

Supporting Information

Electronic Structure of Super-Oxidized Radical Cationic Dodecaborate- Based Clusters

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Table of Content

| | |
|---|------------|
| 1. Experimental Section | S2 |
| 1.1 General Considerations | S2 |
| 1.2 Synthetic Procedures and Characterization Data for B ₁₂ (O-ethyl) ₁₂ and [B ₁₂ (O-ethyl) ₁₂][SbCl ₆] | S2 |
| 1.3 Randles-Sevcik Analysis of the [B ₁₂ (O-ethyl) ₁₂] ^{0/+} Redox Couple | S6 |
| 1.4 One-Electron Reduction of [B ₁₂ (O-ethyl) ₁₂][SbCl ₆] to B ₁₂ (O-ethyl) ₁₂ with Ferrocene | S7 |
| 1.5 Electrochemical Characterization of B ₁₂ (OR) ₁₂ Clusters: 0/+ Redox Couple | S9 |
| 2. Computational Details | S10 |
| 2.1 Optimized Structures | S10 |
| 2.2 Electronic Structure Analysis: Frontier Molecular Orbitals | S12 |
| 2.3 Electronic Structure Analysis: Spin Density and Charge Distribution | S17 |
| 2.4 Redox Potential Calculations | S19 |
| 2.5 TD-DFT Calculations for UV-Vis Spectra | S19 |
| 2.6 Electronic Energies, Zero-Point Energies and Free Energies | S71 |
| 2.7 Full Reference for Gaussian 16, Revision C.01 | S72 |
| 3. Reference | S73 |
| 4. Cartesian Coordinates of Optimized Structures | S74 |

1. Experimental Section

1.1 General Considerations

1.1.1 Materials

All manipulations were performed under an inert atmosphere of purified N₂ in a Vacuum Atmospheres NexGen glovebox unless otherwise indicated. All reagents were purchased from Sigma Aldrich, Oakwood Chemicals, TCI, Fisher Scientific, or Alfa Aesar, and used as received unless otherwise noted. Dichloromethane was purified on a JC Meyer Glass Contour Solvent Purification System, and all other solvents were used as received without further purification unless otherwise specified. [TBA][PF₆] was purchased from Sigma Aldrich and recrystallized three times from hot EtOH and dried under vacuum at 80 °C for 12 h prior to use. [TBA]₂[B₁₂(OH)₁₂],¹ B₁₂(OEt)₁₂,¹ B₁₂(OCH₂-3,5-(CF₃)₂-C₆H₃)₁₂,² B₁₂(OCH₂-*p*-(CF₃)-C₆H₄)₁₂,¹ B₁₂(OCH₂C₆F₅)₁₂,³ B₁₂(OCH₂C₆H₅)₁₂,¹ B₁₂(OCH₂-*p*-F-C₆H₄)₁₂, B₁₂(OCH₂-*p*-Br-C₆H₄)₁₂,¹ and B₁₂(OCH₂-*p*-I-C₆H₄)₁₂⁴ were prepared following previously reported procedures, and [TBA]₂[B₁₂(OH)₁₂]¹ was stored under an atmosphere of purified N₂ in a Vacuum Atmospheres NexGen glovebox prior to use. [N(2,4-Br₂C₆H₃)₃][SbCl₆] was prepared according to a reported procedure, and was stored under an inert atmosphere of N₂ at -30 °C prior to use.⁵ CDCl₃ was obtained from Cambridge Isotope Laboratories and degassed and stored over molecular sieves (4 Å beads, 8-12 mesh) for at least 48 h prior to use.

1.1.2 Methods

All NMR spectra were obtained on a Bruker Avance 400 MHz broad band FT NMR spectrometer. ¹H NMR spectra were referenced to residual protio-solvent signals, and ¹¹B{¹H} chemical shifts were referenced to BF₃•Et₂O (15% in CDCl₃, δ 0.0 ppm). UV-vis measurements were conducted using an Ocean Optics Flame-S-UV-VIS-ES miniature spectrometer equipped with a DH-2000 UV-vis NIR light source. All measurements were carried out using quartz cuvettes (1 cm path length) and conducted at 25 °C with solution samples at 0.1 mM concentration. Cyclic voltammetry measurements were performed with a Gamry Instruments Interface 1010E potentiostat using a glassy carbon disc working electrode, platinum wire counter electrode and a Ag/Ag⁺ pseudo-reference electrode wire. Measurements were conducted with [TBA][PF₆] (0.1 M, DCM) supporting electrolyte in dry DCM under an inert atmosphere of purified N₂ and referenced vs. Fc/Fc⁺.

1.2 Synthetic Procedures and Characterization Data for B₁₂(O-ethyl)₁₂ and [B₁₂(O-ethyl)₁₂][SbCl₆]

1.2.1 B₁₂(O-ethyl)₁₂

The B₁₂(O-ethyl)₁₂ cluster was prepared according to the procedure previously reported.¹ ¹H and ¹¹B{¹H} NMR spectra, UV-vis, and CV data are provided below.

^1H NMR (400 MHz, 25 °C, CDCl_3) δ : 4.08 (q, 24H, $\text{O}-\text{CH}_2-\text{CH}_3$, $^3J = 7$ Hz), 1.23 (t, 36H, CH_3 , $^3J = 7$ Hz) ppm. $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, 25 °C, CDCl_3) δ : 37.4 ppm. UV-vis (DCM, 25 °C, 70 μM): λ_{max} 483 nm.

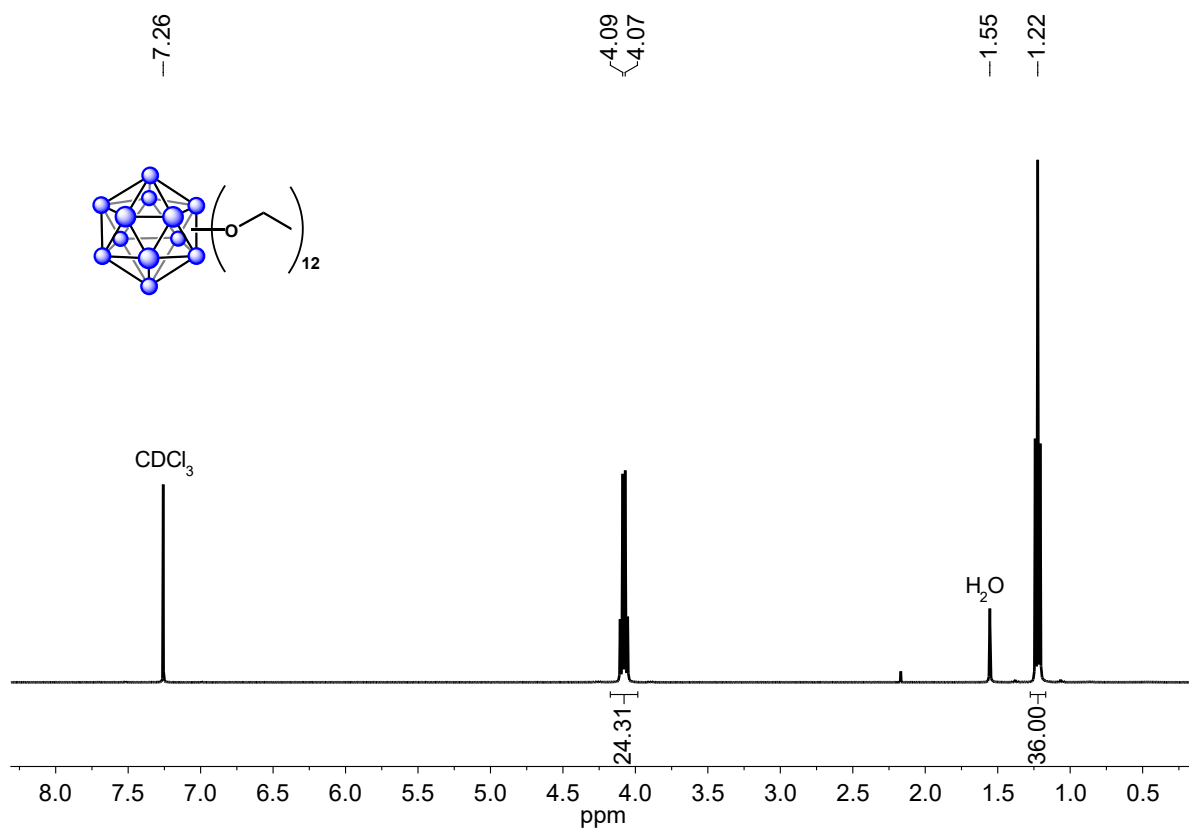


Figure S1. ^1H NMR spectrum of $\text{B}_{12}(\text{O-ethyl})_{12}$ (CDCl_3 , 400 MHz, 25 °C).

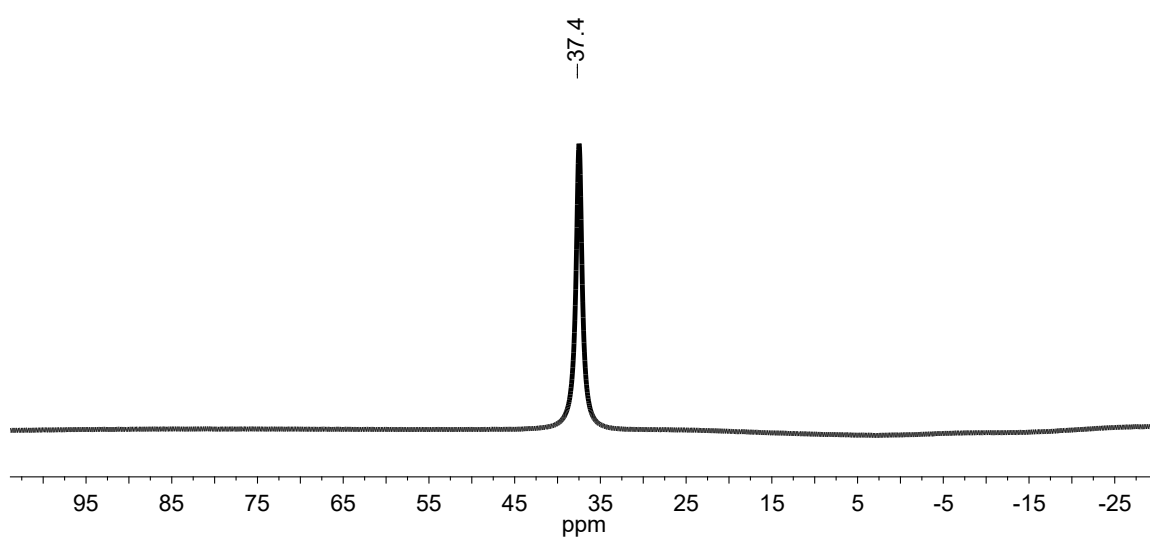


Figure S2. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of $\text{B}_{12}(\text{O-ethyl})_{12}$ (CDCl_3 , 128 MHz, 25 °C).

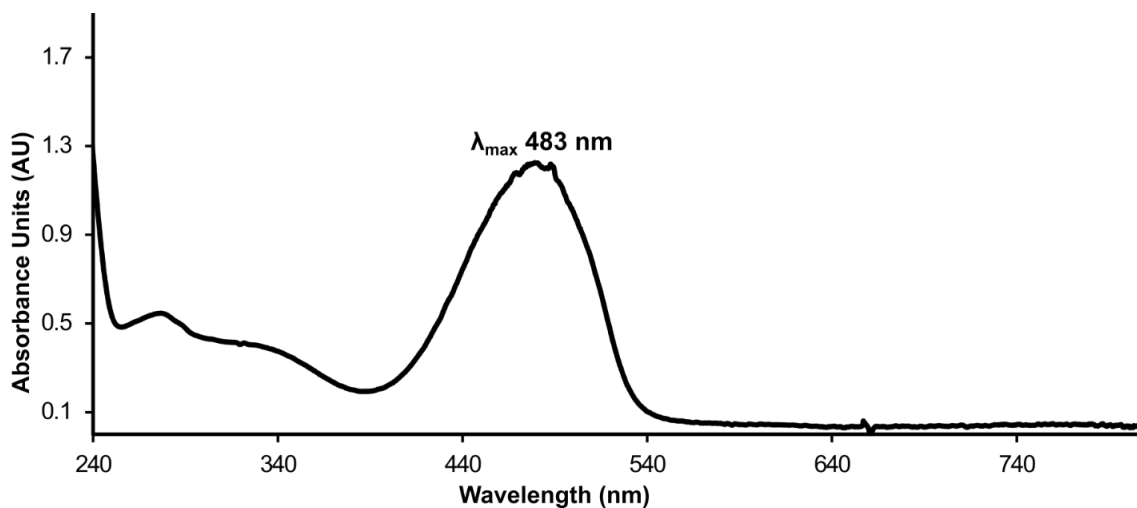


Figure S3. UV-vis spectrum of $B_{12}(O\text{-ethyl})_{12}$ (DCM, $70 \mu\text{M}$, $25 \text{ }^\circ\text{C}$).

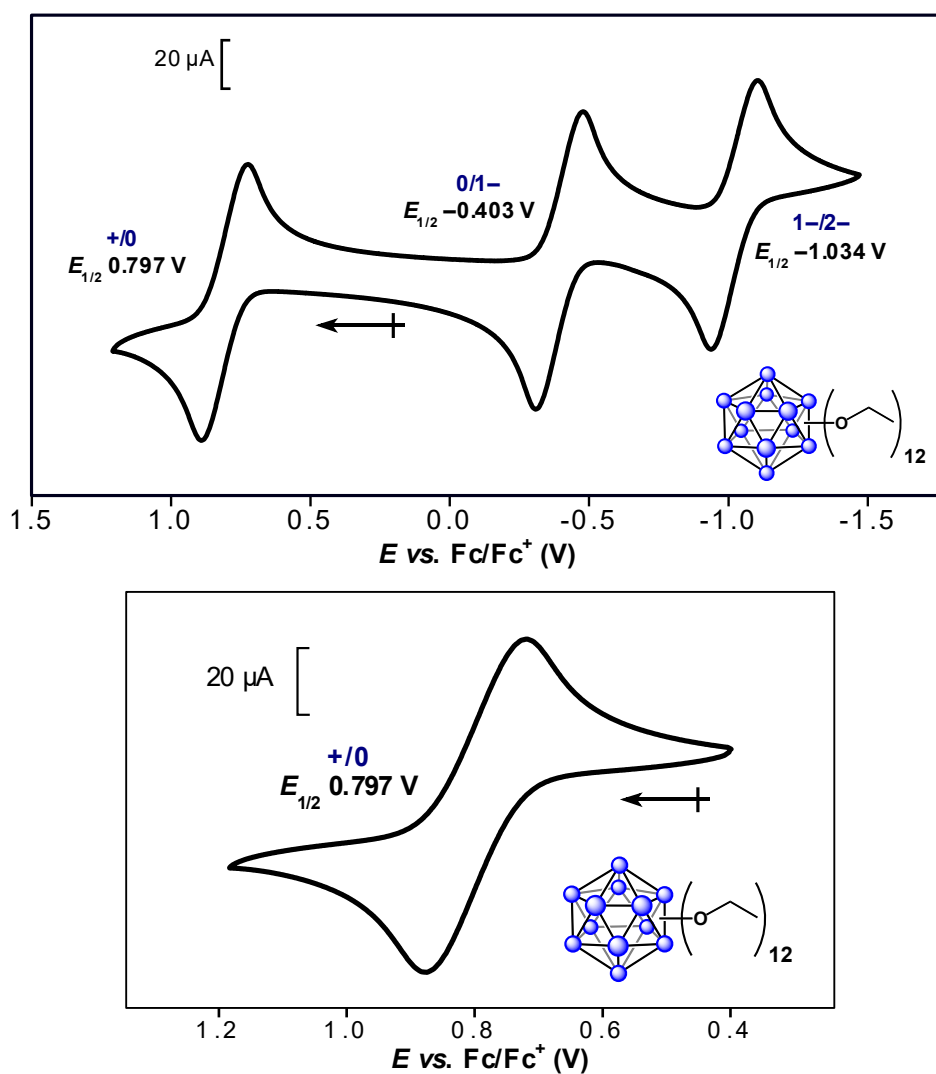
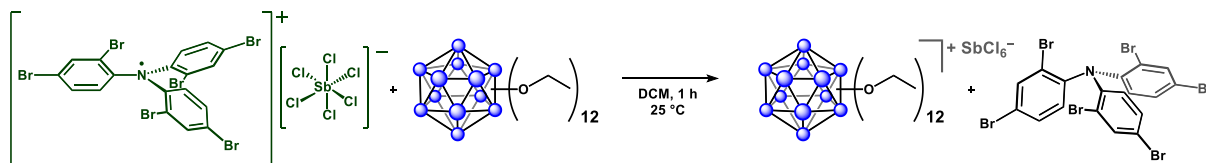


Figure S4. CV of $B_{12}(O\text{-ethyl})_{12}$ measured at a scan rate of 100 mV/s with $0.1 \text{ M [TBA][PF}_6\text{]}$ supporting electrolyte and referenced vs. Fc/Fc^+ (glassy carbon working electrode, platinum counter electrode and Ag/Ag^+ pseudo-reference electrode wire; DCM, 3 mM , $25 \text{ }^\circ\text{C}$).

1.2.2 [B₁₂(O-ethyl)₁₂][SbCl₆]



To a dark yellow solution of B₁₂(O-ethyl)₁₂ (15 mg, 0.022 mmol, 1.0 equiv) in DCM (1 mL) was added a green solution of [N(2,4-Br₂C₆H₃)₃][SbCl₆] (35 mg, 0.033 mmol, 1.5 equiv) in DCM (1 mL) dropwise over 5 min, during which time the color of the reaction mixture darkened to yellow brown. The reaction mixture was allowed to stir at glovebox temperature for 1 h, at which point all volatiles were removed under reduced pressure. The resulting residue was suspended in pentane (2 mL), stirred for 5 min, and then the pentane was decanted and the residue was dried under reduced pressure to afford [B₁₂(O-ethyl)₁₂][SbCl₆] as a yellow-brown solid (17 mg, 0.017 mmol, 78%). ¹H and ¹¹B{¹H} NMR spectra were collected immediately. ¹H NMR (400 MHz, 25 °C, CDCl₃) δ: The O-CH₂-CH₃ resonance is paramagnetically broadened and is therefore not observed due to its proximity to the paramagnetic B₁₂ core, 2.04 (br s, 24H, CH₂) ppm. ¹¹B{¹H} NMR (128 MHz, 25 °C, CDCl₃) δ: A silent NMR spectrum was observed due to paramagnetic broadening of the ¹¹B NMR signal, which suggests the spin density is delocalized throughout the B₁₂ core. UV-vis (DCM, 25 °C, 70 μM): λ_{max} 460, 720 nm.

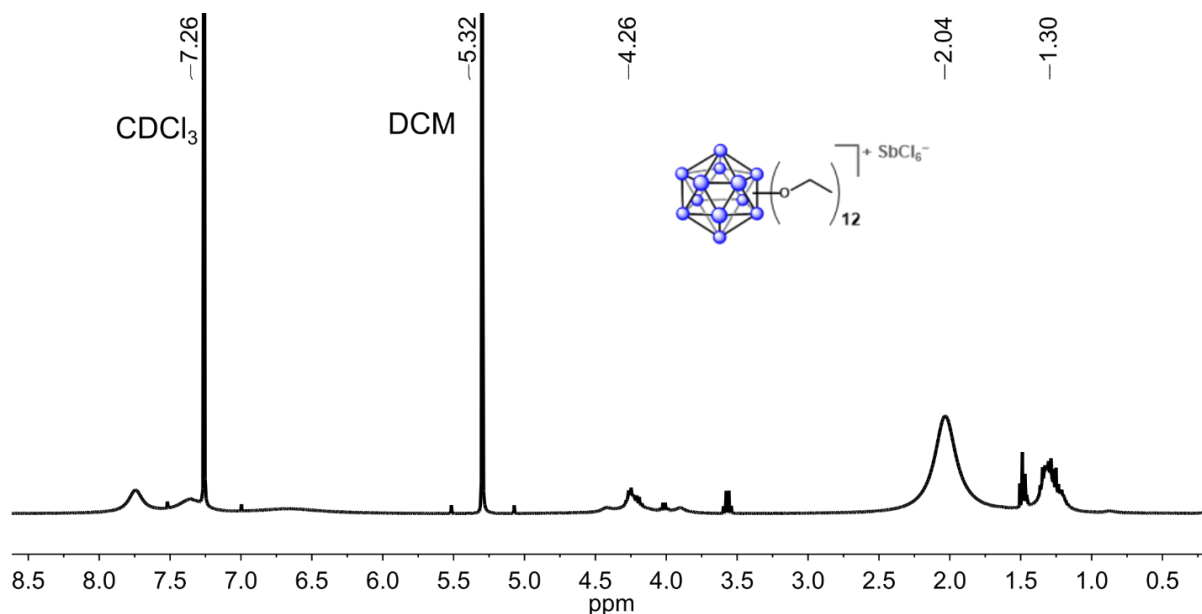


Figure S5. ¹H NMR spectrum of [B₁₂(O-ethyl)₁₂][SbCl₆] (CDCl₃, 400 MHz, 25 °C).

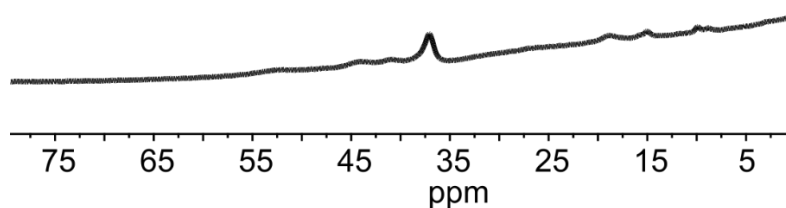


Figure S6. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of $[\text{B}_{12}(\text{O-ethyl})_{12}][\text{SbCl}_6]$ (CDCl_3 , 128 MHz, 25 °C).

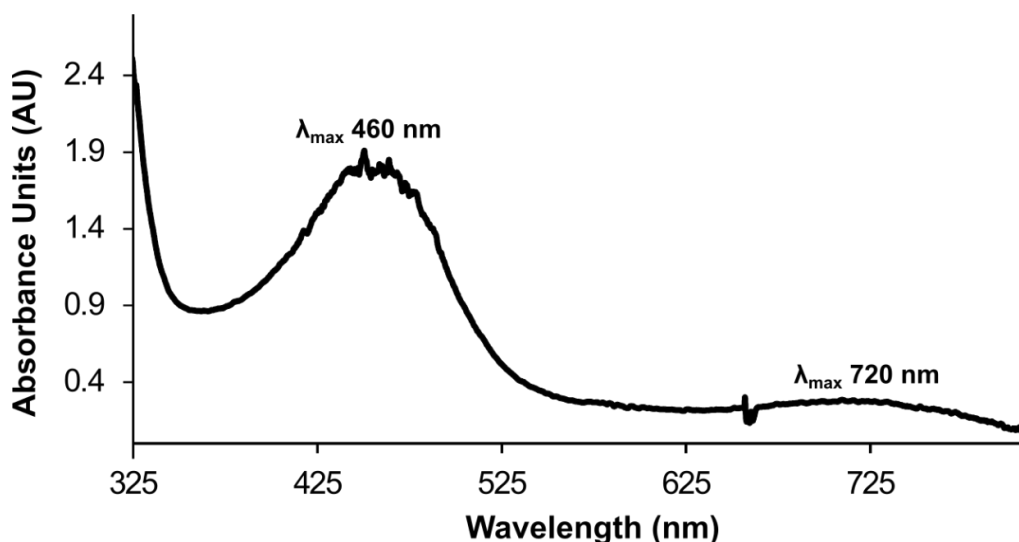


Figure S7. UV-Vis spectrum of $[\text{B}_{12}(\text{O-ethyl})_{12}][\text{SbCl}_6]$ (DCM, 70 μM , 25 °C).

1.3 Randles-Sevcik Analysis of the $[\text{B}_{12}(\text{O-ethyl})_{12}]^{0/+}$ Redox Couple

Electrochemical measurements of $\text{B}_{12}(\text{O-ethyl})_{12}$ (3 mM solution in DCM) were performed under an inert atmosphere of purified N_2 . Scans were collected between 25-300 mV/s with $[\text{TBA}][\text{PF}_6]$ supporting electrolyte (0.1 M solution in DCM) and referenced vs. Fc/Fc^+ (glassy carbon working electrode, Pt wire counter electrode, Ag wire pseudo-reference electrode). The diffusion coefficient (D_0) was calculated according to the Randles-Sevcik equation as described below.⁶ The plot of i_p vs. $v^{1/2}$ is linear, as shown below (right), indicating that the electron transfer for the $[\text{B}_{12}(\text{O-ethyl})_{12}]^{0/+}$ redox event is diffusion controlled.

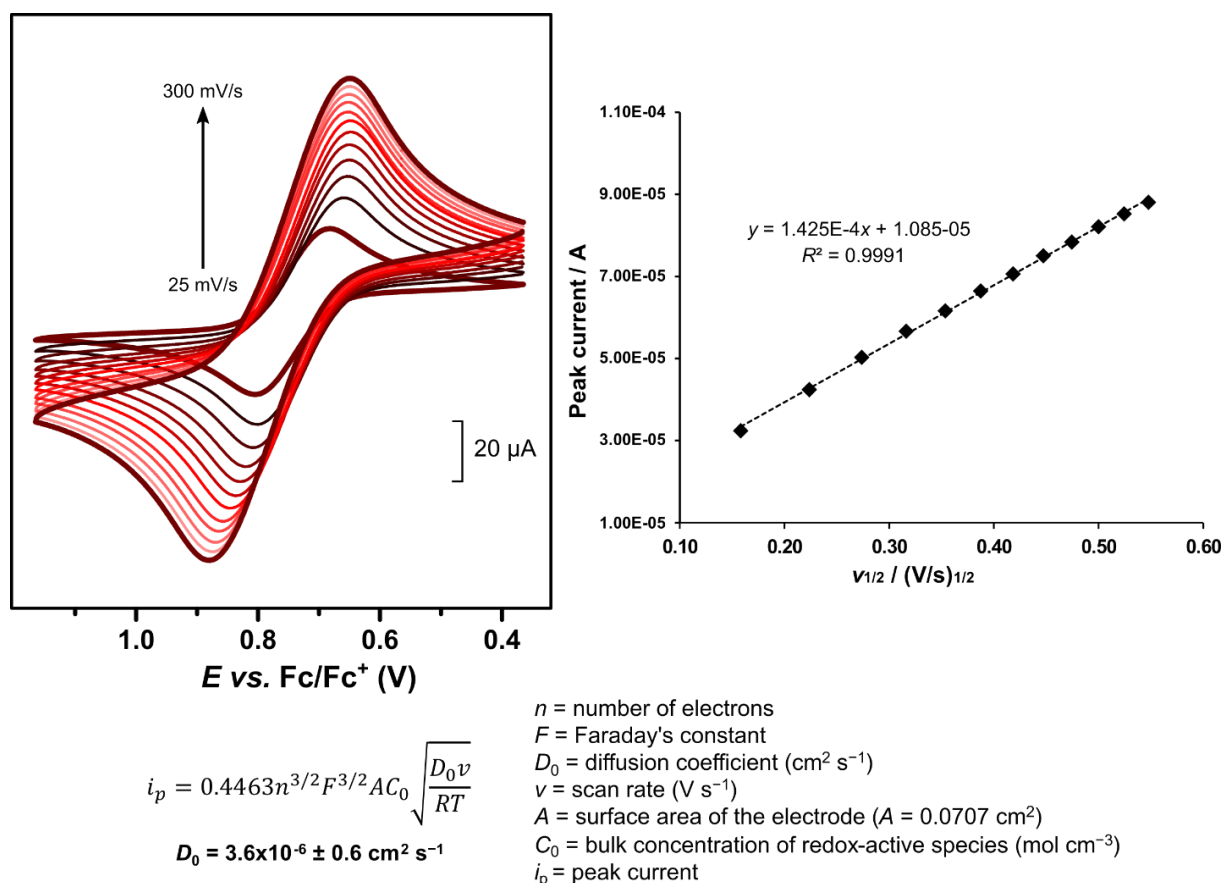
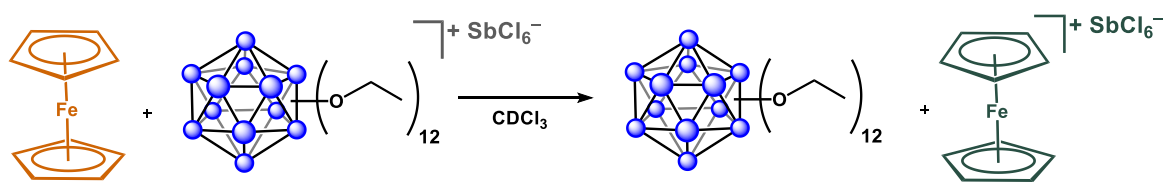


Figure S8. (Left) CV of the $[\text{B}_{12}(\text{O-ethyl})_{12}]^{0/+}$ redox couple recorded at variable scan rates (25-300 mV/s). (Right) Randles-Sevcik plot of the CV data.

1.4 One-Electron Reduction of $[\text{B}_{12}(\text{O-ethyl})_{12}][\text{SbCl}_6]$ to $\text{B}_{12}(\text{O-ethyl})_{12}$ with Ferrocene



The $[\text{B}_{12}(\text{O-ethyl})_{12}][\text{SbCl}_6]$ (0.022 mmol) salt was freshly prepared according to the procedure described in **Section S1.2.2**. The dark yellow brown solids were dissolved in CDCl_3 (0.5 mL) and transferred to an NMR tube. The tube was brought outside of the glovebox and ^1H (**Figure S9**, top) and $^{11}\text{B}\{^1\text{H}\}$ NMR spectra (**Figure S10**, top) were immediately collected to confirm the clean formation of $[\text{B}_{12}(\text{O-ethyl})_{12}][\text{SbCl}_6]$. The NMR sample was then transferred back into the glovebox, and to this solution was added a CDCl_3 solution (0.4 mL) of ferrocene (8 mg, 0.04 mmol, 2 equiv), which resulted in the immediate formation of dark blue-green precipitate. The reaction mixture was filtered through a piece of microfiber glass filter paper and the yellow-orange filtrate was transferred to an NMR tube. The ^1H (**Figure S9**,

bottom) and $^{11}\text{B}\{^1\text{H}\}$ NMR spectra (**Figure S10**, bottom) that were immediately collected display resonances consistent with the *hypercloso*- $\text{B}_{12}(\text{O-ethyl})_{12}$ cluster.

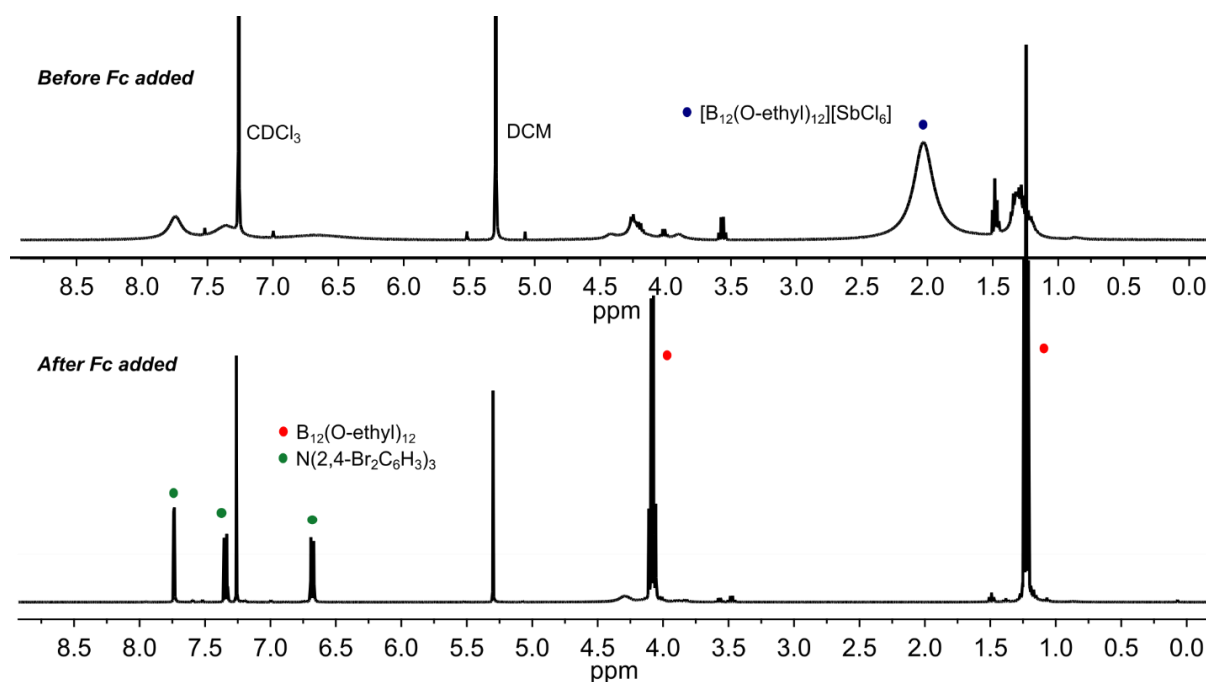


Figure S9. ^1H NMR spectrum of $[\text{B}_{12}(\text{O-ethyl})_{12}][\text{SbCl}_6]$ before (top) and after (bottom) reduction with ferrocene. The spectrum after the reduction of $[\text{B}_{12}(\text{O-ethyl})_{12}][\text{SbCl}_6]$ with ferrocene displays ^1H NMR resonances attributed to *hypercloso*- $\text{B}_{12}(\text{O-ethyl})_{12}$ (•) (CDCl_3 , 400 MHz, 25 °C).

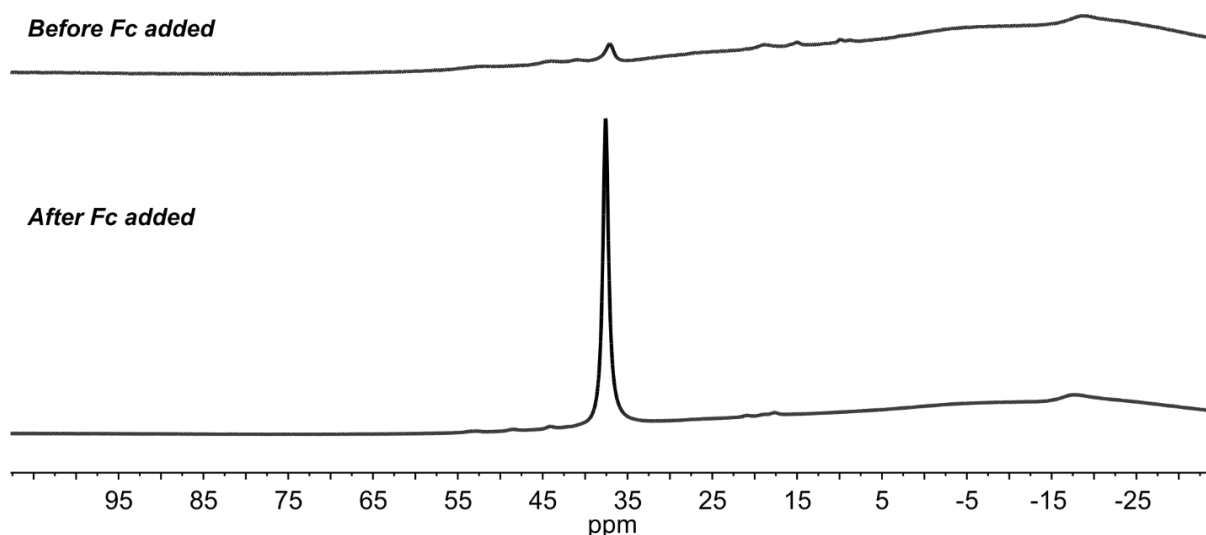


Figure S10. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of $[\text{B}_{12}(\text{O-ethyl})_{12}][\text{SbCl}_6]$ before (top) and after (bottom) reduction with ferrocene. The spectrum after the reduction of $[\text{B}_{12}(\text{O-ethyl})_{12}][\text{SbCl}_6]$ with ferrocene displays the ^{11}B NMR resonance attributed to *hypercloso*- $\text{B}_{12}(\text{O-ethyl})_{12}$ (CDCl_3 , 128 MHz, 25 °C).

1.5 Electrochemical Characterization of $B_{12}(OR)_{12}$ Clusters: $0/+$ Redox Couple

Electrochemical measurements of $B_{12}(OR)_{12}$ clusters (3 mM solution in DCM) were performed under an inert atmosphere of purified N_2 . Scans were collected at 100 mV/s with [TBA][PF₆] supporting electrolyte (0.1 M solution in DCM) and referenced vs. Fc/Fc⁺ (glassy carbon working electrode, Pt wire counter electrode, Ag wire pseudo-reference electrode).

2. Computational Details

2.1 Optimized Structures

All density functional theory (DFT) and time-dependent DFT (TD-DFT) calculations were performed in the Gaussian 16 software package. Geometry optimizations of all boron clusters were performed at the B3LYP-D3/def2-SVP level of theory following our previous study.⁷ X-ray crystal structures were used as initial geometries for all boron clusters. There is no switch between conformers in geometry optimizations. The optimized geometries of the neutral clusters are shown in **Figure S11**. Because two distinct conformers were recognized in the crystal of **6**, both were calculated, and the lower-energy conformer was used in all discussions and subsequent calculations. This conformer is favored by $\Delta E = -3.0$ kcal/mol at the B3LYP-D3/def2-SVP level of theory. The Cartesian coordinates and energies of both conformers are provided.

Overall, the computationally optimized cluster geometries are in good agreement with X-ray crystal structures, which is indicated by the small root-mean-square deviations (RMSDs) of atomic positions (see **Table S1**). Despite displacement of supporting substituents, the overall RMSDs are reasonably small, the largest being 1.850 Å for **6**. By monitoring the RMSD on the B₁₂ cluster core, the influence of side group displacement is alleviated. The resulting RMSD_{cryst-comput,B12} values are notably smaller, ranging from 0.14 Å for **8** to 0.31 Å for **4**.

The electronic structure of the dodecaborate clusters at different oxidation states is among the main focuses of the present study. One underlying reason is the minor influence of redox events on molecular geometries, as reflected by (a) the low RMSD_{0/+} values for the 0/+ redox couples (most all-atom RMSD_{0/+}'s are smaller than 0.25 Å, see **Table S1**) as well as (b) the aligned structures in **Figure S12** (for 0/+ couples) and **Figure S13** (for the [1]^{2-/+} series). It is thereby sufficient to concentrate on their electronic structure in order to rationalize the redox chemistry of these perfunctionalized B₁₂ clusters.

Since cyclic voltammetry and UV-Vis measurements were conducted in dichloromethane (DCM), we anticipate low influence of solvent effects on geometries. Therefore, the gas-phase geometries were used in all subsequent calculations without further specification. The accuracy of our redox potential calculations with respect to CV half-potentials supports the reliability of using these geometries.

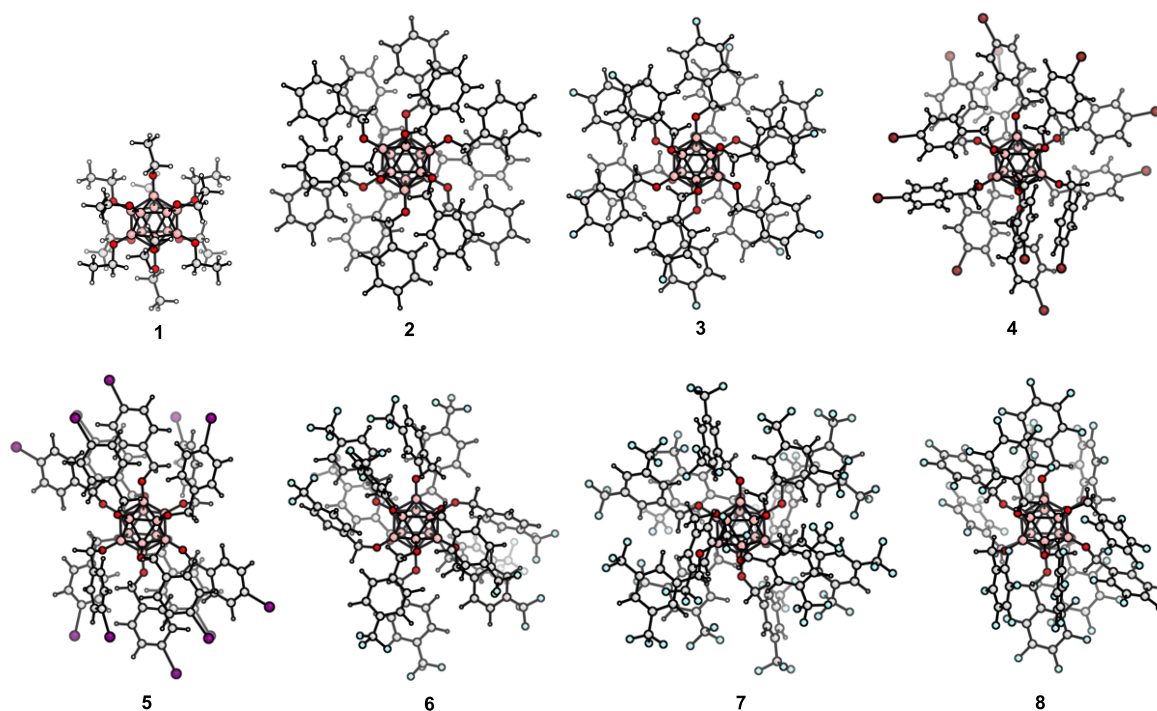


Figure S11. Optimized structures of neutral $B_{12}(OR)_{12}$ boron clusters.

Table S1. Root-mean-square deviations (RMSDs) of atomic positions (unit: Å) between computational geometries and X-ray crystal structures of neutral $B_{12}(OR)_{12}$ clusters for all atoms ($RMSD_{\text{crys-comput}}$) and for the B_{12} core ($RMSD_{\text{crys-comput},B_{12}}$). RMSDs for optimized geometries of all $[B_{12}(OR)_{12}]^{0/+}$ couples are also shown, including $RMSD_{0/+}$ for all atoms and $RMSD_{0/+,B_{12}}$ for the B_{12} cluster core.

| | $RMSD_{\text{crys-comput}}$ | $RMSD_{\text{crys-comput},B_{12}}$ | $RMSD_{0/+}$ | $RMSD_{0/+,B_{12}}$ |
|----------|-----------------------------|------------------------------------|--------------|---------------------|
| 1 | 0.196 | 0.019 | 0.151 | 0.034 |
| 2 | 1.285 | 0.020 | 0.295 | 0.030 |
| 3 | 0.535 | 0.016 | 0.235 | 0.029 |
| 4 | 0.617 | 0.031 | 0.198 | 0.030 |
| 5 | 0.847 | 0.025 | 0.246 | 0.031 |
| 6 | 1.850 | 0.024 | 0.070 | 0.028 |
| 7 | 0.769 | 0.022 | 0.211 | 0.049 |
| 8 | 1.471 | 0.014 | 0.506 | 0.043 |

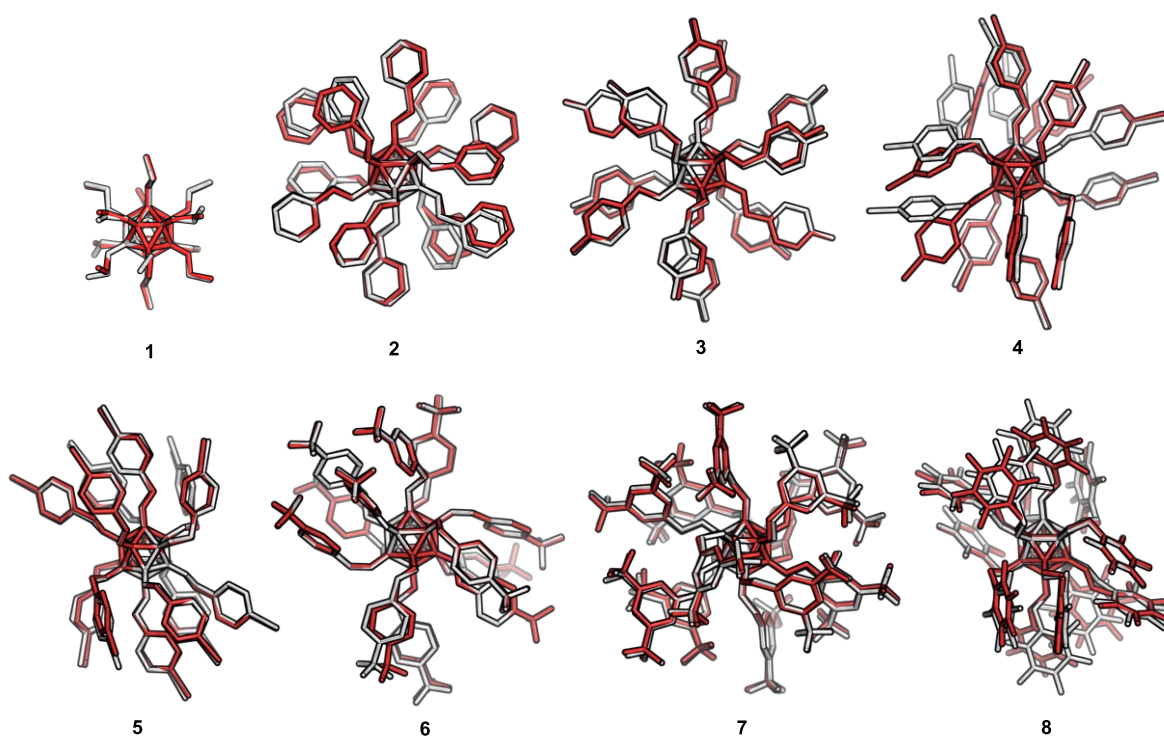


Figure S12. Aligned structures of $[\text{B}_{12}(\text{OR})_{12}]^{0/+}$ couples (white: neutral clusters, red: radical cationic clusters). H atoms are omitted for clarity.

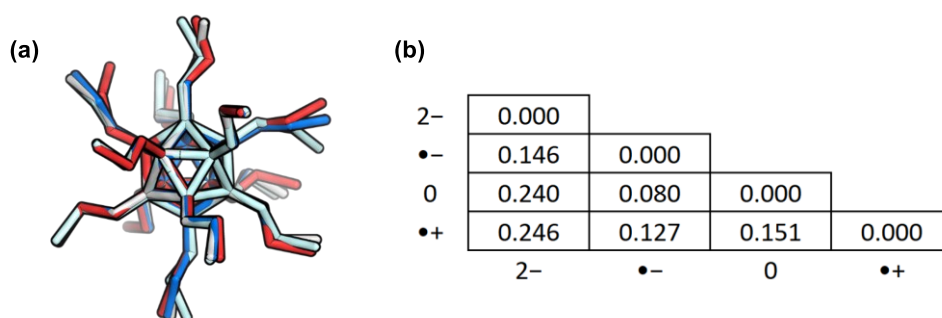


Figure S13. (a) Aligned structures of the $[\mathbf{1}]^{2-/-/0/+}$ redox series (red: $[\mathbf{1}]^{2-}$, blue: $[\mathbf{1}]^{-}$, white: $\mathbf{1}$, pale cyan $[\mathbf{1}]^{+}$). H atoms are omitted for clarity. (b) All-atom RMSDs for the optimized structures of the $[\mathbf{1}]^{2-/-/0/+}$ redox series.

2.2 Electronic Structure Analysis: Frontier Molecular Orbitals

The aforementioned DFT calculations (B3LYP-D3/def2-SVP) yielded frontier molecular orbitals (FMOs) for all boron clusters. The FMO energies of all clusters are reported in **Table S2**. Detailed discussion on $[\mathbf{1}]^{2-/-/0/+}$ (**Figure 2**) and $[\mathbf{2}]^{0/+}$ (**Figure 4**) have been presented in the manuscript, in which we noted that the highest-energy occupied orbitals of $[\mathbf{2}]^{+}$ are mainly distributed in the side groups. **Figure S14** demonstrates the independence of this observation on the theoretical level by FMO diagrams computed using Hartree-Fock theory (HF/def2-SVP).

Despite different FMO energies, the FMO diagrams are highly consistent. **Figure S15-S20** visualize the FMOs of all other clusters, which are in general very similar to the case of $[2]^{0/+}$.

Table S2. HOMO energies, LUMO energies and HOMO-LUMO gaps of all structures studied in this work. All energies are shown in eV, and all calculations are at the B3LYP-D3/def2-SVP level of theory. For radical species, the top, bottom lines specify the orbital energies for α -, β -electrons, respectively.

| | HOMO | LUMO | HOMO – LUMO |
|------------|-------|-------|-------------|
| $[1]^{2-}$ | 1.27 | 5.94 | 4.66 |
| $[1]^{-}$ | -1.79 | 3.20 | 4.99 |
| | -2.40 | -0.53 | 1.87 |
| 1 | -5.70 | -3.67 | 2.03 |
| 2 | -6.05 | -4.16 | 1.89 |
| 3 | -6.32 | -4.52 | 1.80 |
| 4 | -6.42 | -4.65 | 1.77 |
| 5 | -6.28 | -4.45 | 1.83 |
| 6 | -6.75 | -4.99 | 1.76 |
| 7 | -6.98 | -5.36 | 1.62 |
| 8 | -6.91 | -5.00 | 1.91 |
| $[1]^{+}$ | -8.63 | -7.01 | 1.62 |
| | -8.99 | -7.39 | 1.59 |
| $[2]^{+}$ | -8.35 | -6.98 | 1.37 |
| | -8.35 | -7.36 | 0.99 |
| $[3]^{+}$ | -8.60 | -7.23 | 1.37 |
| | -8.59 | -7.69 | 0.90 |
| $[4]^{+}$ | -8.41 | -7.33 | 1.08 |
| | -8.41 | -7.58 | 0.83 |
| $[5]^{+}$ | -8.15 | -7.04 | 1.11 |
| | -8.14 | -7.50 | 0.64 |
| $[6]^{+}$ | -9.31 | -7.74 | 1.57 |
| | -9.30 | -8.09 | 1.21 |
| $[7]^{+}$ | -9.45 | -7.98 | 1.47 |
| | -9.64 | -8.12 | 1.52 |
| $[8]^{+}$ | -9.34 | -7.74 | 1.60 |
| | -9.35 | -8.09 | 1.26 |

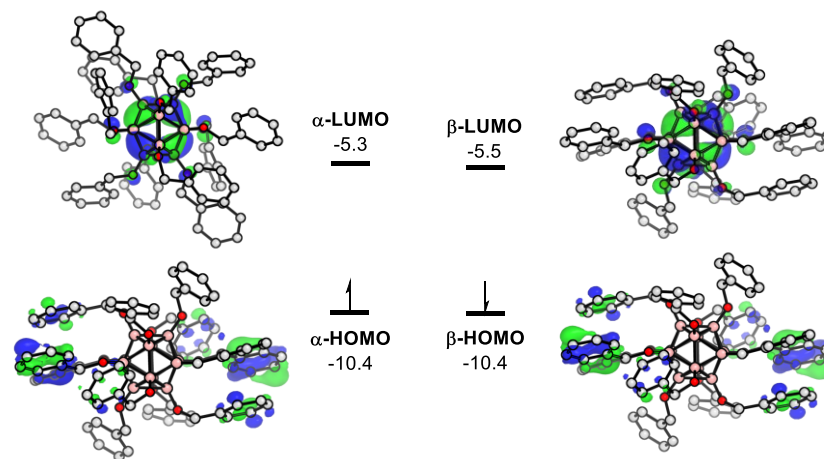


Figure S14. Frontier molecular orbitals of $[2]^{++}$ at the HF//B3LYP-D3/def2-SVP level of theory.

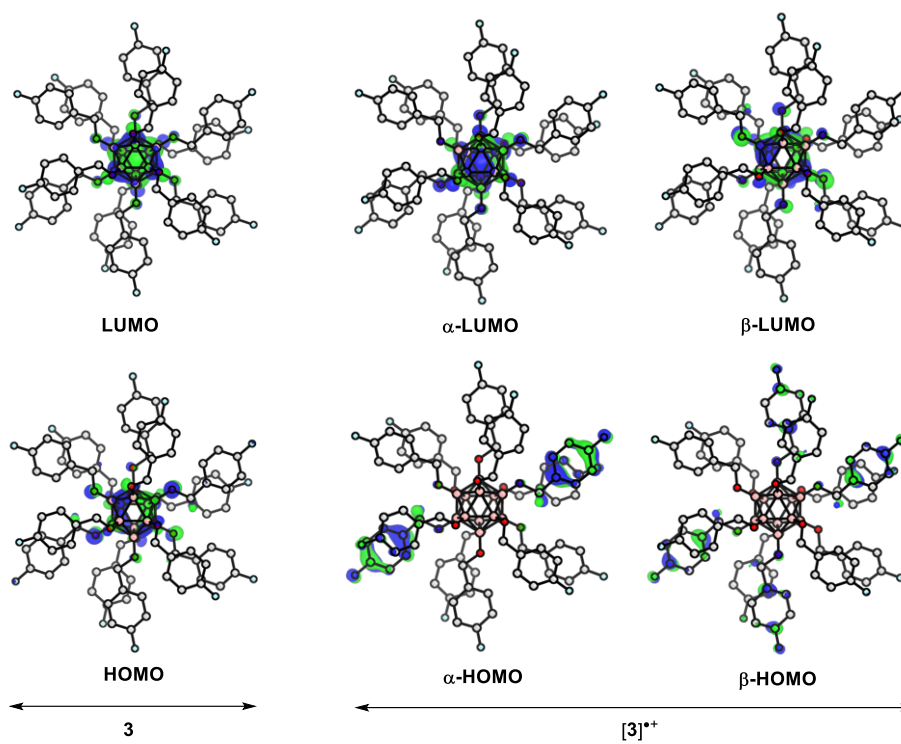


Figure S15. Frontier molecular orbitals of **3** and $[3]^{++}$ at the B3LYP-D3/def2-SVP level of theory.

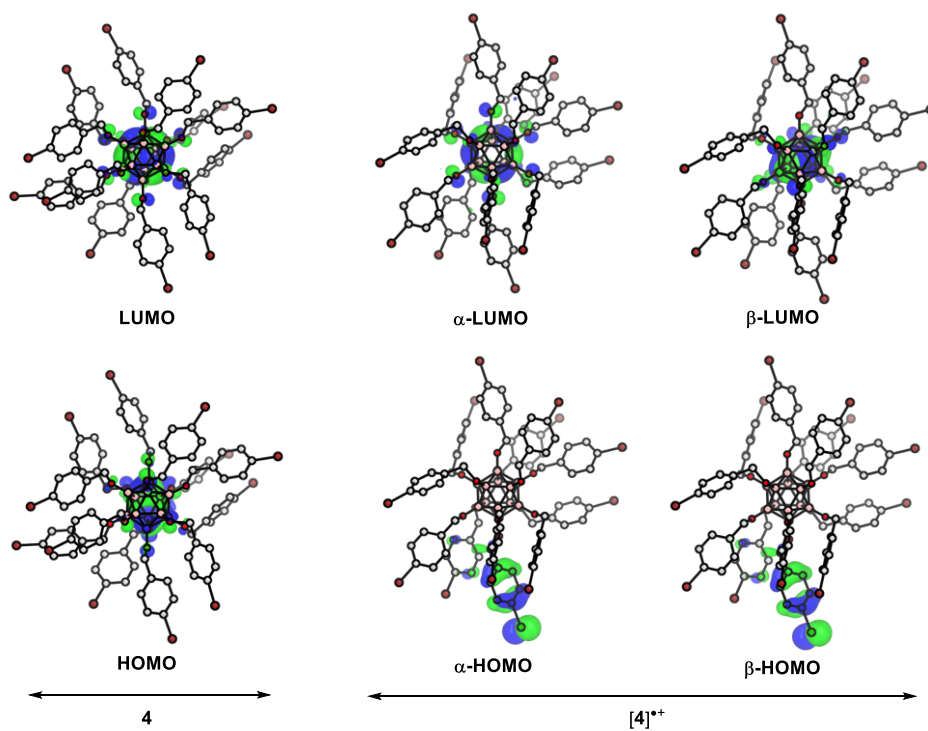


Figure S16. Frontier molecular orbitals of **4** and $[4]^{++}$ at the B3LYP-D3/def2-SVP level of theory.

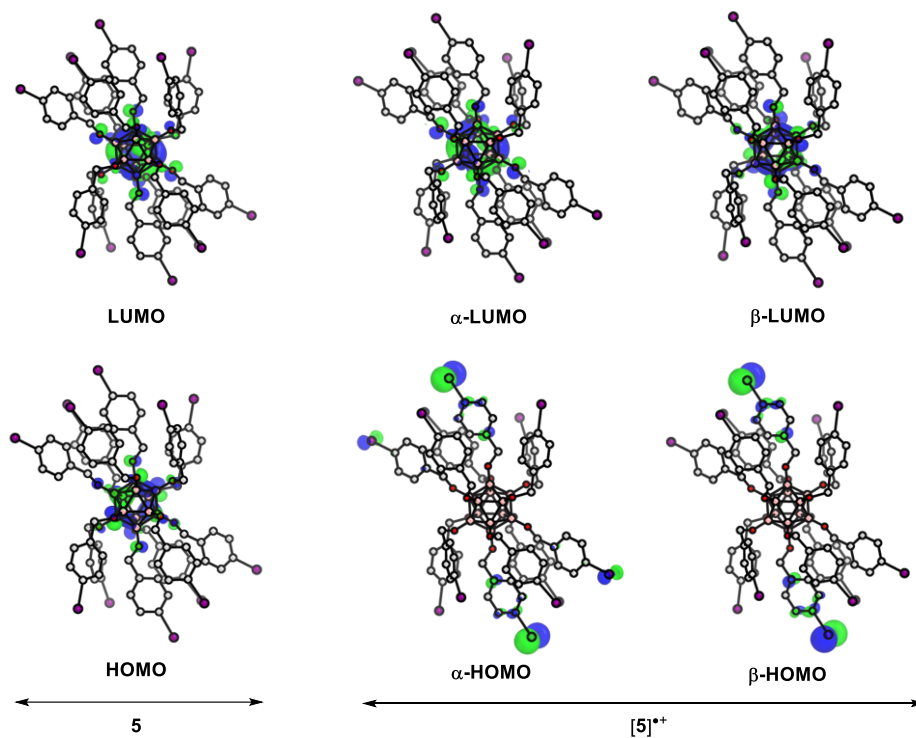


Figure S17. Frontier molecular orbitals of **5** and $[5]^{++}$ at the B3LYP-D3/def2-SVP level of theory.

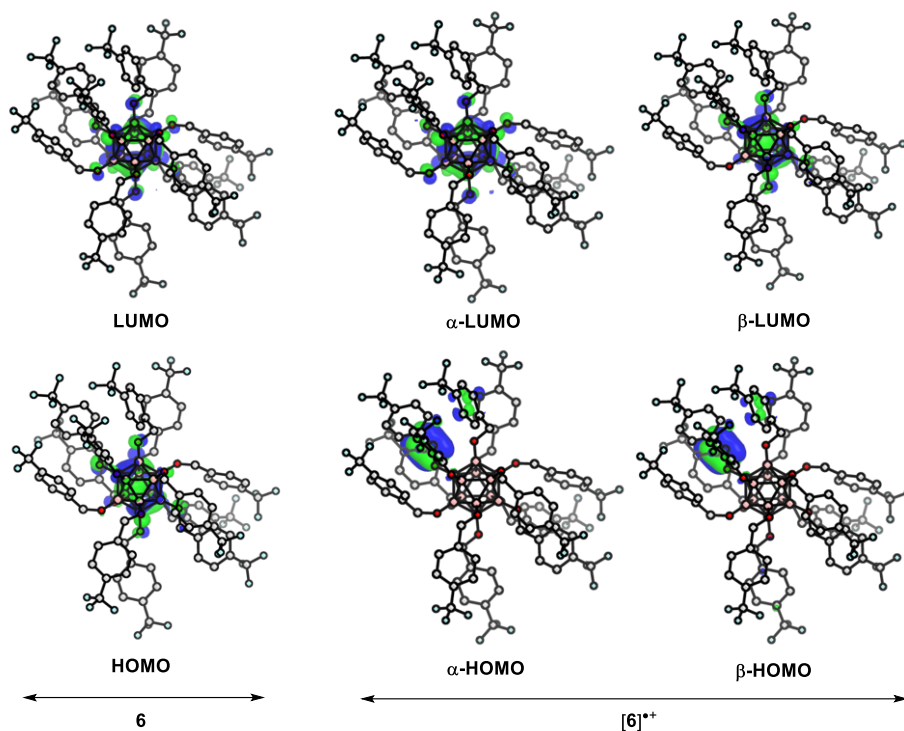


Figure S18. Frontier molecular orbitals of 6 and [6]²⁺ at the B3LYP-D3/def2-SVP level of theory.

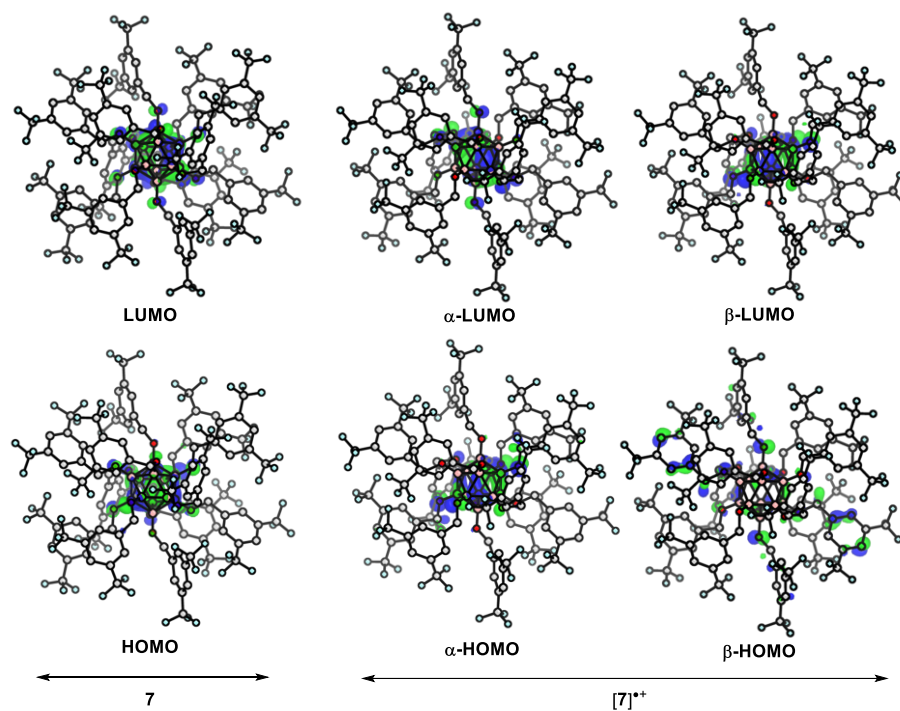


Figure S19. Frontier molecular orbitals of 7 and [7]²⁺ at the B3LYP-D3/def2-SVP level of theory.

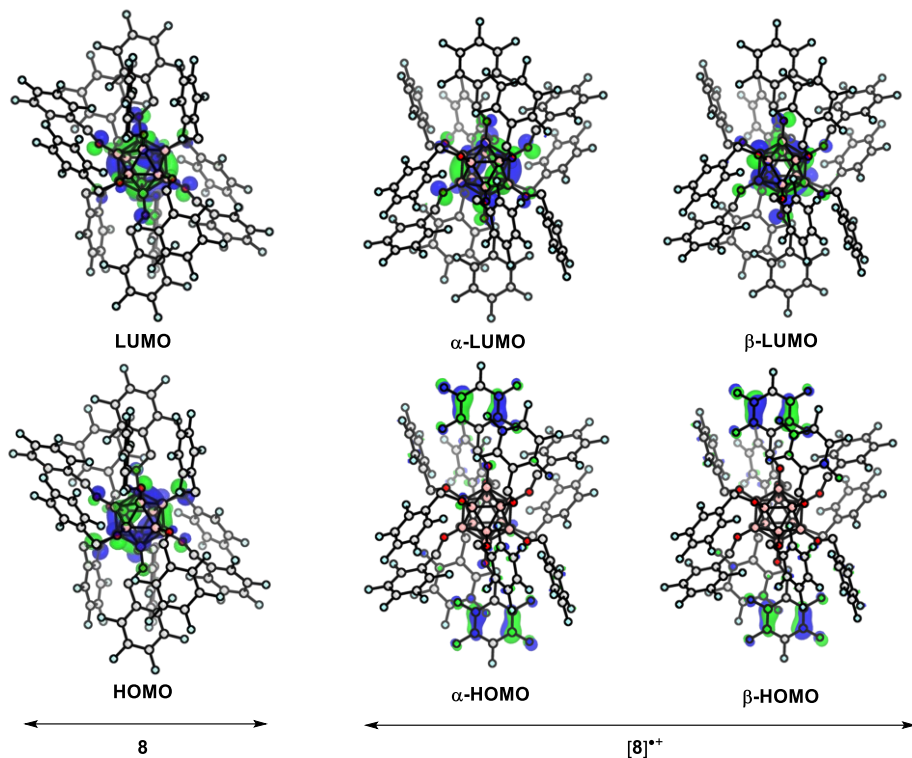


Figure S20. Frontier molecular orbitals of **8** and $[8]^{++}$ at the B3LYP-D3/def2-SVP level of theory.

2.3 Electronic Structure Analysis: Spin Density and Charge Distribution

To characterize the radical cationic nature of the $[B_{12}(OR)_{12}]^{++}$ boron clusters, we studied (a) the spin density isosurfaces of $[1]^{++}$ (**Figure 3**) and $[2]^{++}$ (**Figure S21**), and (b) the Hirshfeld spin density and charge populations of the B_{12} cluster core, the O atoms and the hydrocarbon side groups (**Table S3**). **Figure S22** further describes the average Hirshfeld partial charges for each of the α -C, β -C, $-CH_2-$ and $-CH_3$ in $[1]^{++}$.

Although Hirshfeld population analysis features clear physical meaning, it is necessary to examine the dependence of our conclusions on the population scheme. Thereby, we performed Natural Population Analysis (NPA) at the level of B3LYP-D3/def2-SVP in Gaussian 16 (see **Table S4**). It is known that Hirshfeld atomic charges are generally smaller than natural atomic charges, but for all the noted distribution patterns and redox-dependent tendencies, these two methods are consistent. The spin populations computed by the two methods are also in good agreement, both suggesting that the unpaired electron in $[1]^{+/-/+}$ and $[2]^{++}$ is in the B_{12} core and the O atoms. These results well support our discussions that are based on Hirshfeld population analysis.

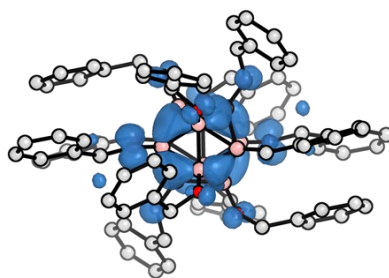


Figure S21. Spin density isosurface (isovalue = 0.002 a.u.) of $[2]^{++}$ at the B3LYP-D3/def2-SVP level of theory. Hydrogen atoms are omitted for clarity.

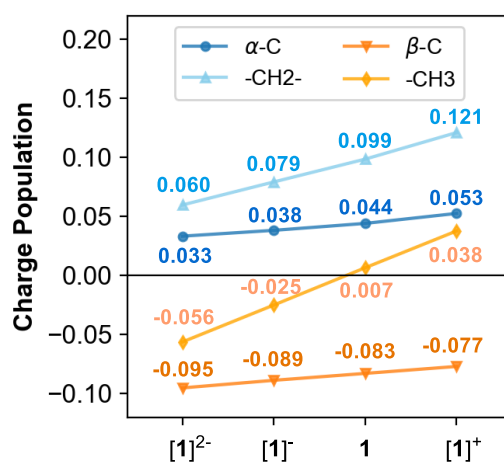


Figure S22. Average Hirshfeld charges on each α -C, β -C, -CH₂- and -CH₃ of $[1]^{2-/-/0/+}$ computed at the B3LYP-D3/def2-SVP level of theory.

Table S3. Hirshfeld spin density and charge population analysis of $[2]^{++}$ through $[8]^{++}$ at the level of B3LYP-D3/def2-SVP.

| | Hirshfeld charge population | | | Hirshfeld spin density | | |
|------------|-----------------------------|-----------|-----------------|------------------------|-----------|-----------------|
| | B ₁₂ core | O linkers | exterior groups | B ₁₂ core | O linkers | exterior groups |
| $[2]^{++}$ | 0.862 | -1.645 | 1.783 | 0.437 | 0.431 | 0.132 |
| $[3]^{++}$ | 0.845 | -1.712 | 1.867 | 0.415 | 0.419 | 0.167 |
| $[4]^{++}$ | 0.840 | -1.690 | 1.850 | 0.458 | 0.431 | 0.110 |
| $[5]^{++}$ | 0.825 | -1.737 | 1.912 | 0.430 | 0.407 | 0.164 |
| $[6]^{++}$ | 0.843 | -1.678 | 1.835 | 0.457 | 0.444 | 0.099 |
| $[7]^{++}$ | 0.850 | -1.660 | 1.810 | 0.471 | 0.437 | 0.092 |
| $[8]^{++}$ | 0.855 | -1.735 | 1.880 | 0.481 | 0.435 | 0.083 |

Table S4. Natural spin density and charge population analysis of $[1]^{2-/-/0/+}$ and $[2]^{0/+}$ at the level of B3LYP-D3/def2-SVP.

| | Hirshfeld charge population | Hirshfeld spin density |
|--|-----------------------------|------------------------|
|--|-----------------------------|------------------------|

| | B ₁₂ core | O linkers | exterior groups | B ₁₂ core | O linkers | exterior groups |
|-------------------|----------------------|-----------|-----------------|----------------------|-----------|-----------------|
| [1] ²⁻ | 3.968 | -9.435 | 3.467 | 0.000 | 0.000 | 0.000 |
| [1] ^{•-} | 4.335 | -9.202 | 3.867 | 0.477 | 0.505 | 0.019 |
| 1 | 4.698 | -8.948 | 4.250 | 0.000 | 0.000 | 0.000 |
| [1] ^{•+} | 5.005 | -8.651 | 4.646 | 0.448 | 0.508 | 0.044 |
| 2 | 4.728 | -8.651 | 3.923 | 0.000 | 0.000 | 0.000 |
| [2] ^{•+} | 4.998 | -8.565 | 4.568 | 0.403 | 0.501 | 0.096 |

2.4 Redox Potential Calculations

Table S5. SMD-DFT calculated and CV measured redox potentials in the [1]^{2-•-/0/+} series. The errors are defined as the difference between SMD-DFT calculations and CV measurements. An MAE of 0.11 V (MSE = -0.11 V) is achieved by these calculations.

| | E_{DFT} (V) vs. Fc/Fc ⁺ | $E_{1/2,\text{CV}}$ (V) vs. Fc/Fc ⁺ | error (V) |
|-------|---|--|-----------|
| 0/•+ | 0.77 | 0.80 | -0.03 |
| •-/0 | -0.47 | -0.40 | -0.07 |
| 2-/•- | -1.27 | -1.03 | -0.24 |

2.5 TD-DFT Calculations for UV-Vis Spectra

We have performed Time-Dependent Density Functional Theory (TD-DFT) calculations to predict the UV-Vis spectra of all neutral and radical cationic boron clusters and reveal the associated excited states (see Methods for computational details). The charge transfer feature of important electronic excitations reported in our previous study motivated us to use the range separated CAM-B3LYP functional. TD-CAM-B3LYP has been successfully applied to the absorption spectra calculations of other clusters and nanoparticles with good accuracy.⁸ For the present study, the necessity of using a long range corrected exchange-correlation functional is supported by the severe underestimation of excitation energies for the diagnostic absorptions of [1]^{•+} and [2]^{•+} by TD-PBE0⁹ (**Figure S23**), whose low share of exact exchange potential is known to cause incorrect descriptions of charge transfer excited states (e.g. underestimated excitation energies). Specifically, the diagnostic modes of excitation of [1]^{•+} at 770 nm, 794 nm and 844 nm (by TD-CAM-B3LYP) are red-shifted to 825 nm, 844 nm and 908 nm (by TD-PBE0, note that the experimental absorption peaks at ca. 710 nm), and the diagnostic excitation of [2]^{•+} at 844 nm (by TD-CAM-B3LYP) is unrealistically shifted to as far as 1510 nm (by TD-PBE0). The main absorption band is also significantly more red-shifted by TD-PBE0 than TD-CAM-B3LYP.

To obtain reasonable results with minimized computational cost, we comparatively tested the predictions by three Ahlrichs basis sets def2-SVP, def2-TZVP and def2-SVPD on [1]^{0/+}. One advantage of Ahlrichs basis sets is the complete definition for (almost) all elements until

Rn. Among the three basis sets, def2-SVP is the split valence double- ζ Ahlrichs basis set with polarization functions on all atoms, def2-SVPD equips def2-SVP with diffuse functions, and def2-TZVP is the valence triple- ζ Ahlrichs basis set with polarization functions on all atoms. Our tests show that def2-SVP yields analogous results as the more extended def2-TZVP and def2-SVPD (**Figure S24**). However, using def2-SVP saves the total CPU time for one order of magnitude compared with def2-TZVP and def2-SVPD (**Table S6**). Taking the extended sizes of the B₁₂ clusters into account, we used the def2-SVP basis set in all TD-DFT calculations.

According to these results, we performed all TD-DFT calculations at the level of TD-CAM-B3LYP/def2-SVP/LR-PCM(DCM). The remaining part of this section presents details of the excitation energies, absorption wavelengths, oscillator strengths and configurations of all excited states whose $\lambda > 300$ nm and $f > 0.01$. We also show the natural transition orbitals (NTOs) for the root 7 of [2]⁺, root 6 of [3]⁺, root 8 of [4]⁺, root 7 of [5]⁺, root 7 of [6]⁺, root 9 of [7]⁺, and root 8 of [8]⁺. These excited states are of primary importance for the diagnostic absorption of these radical cationic clusters. All NTOs are shown with an isovalue of ± 0.01 a.u.

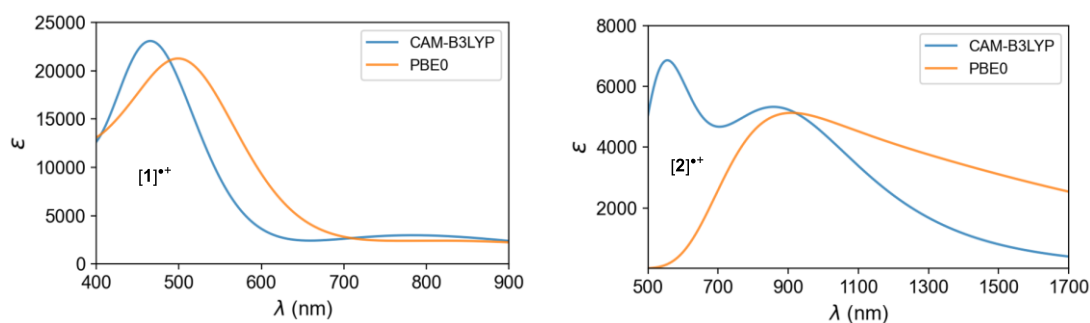


Figure S23, Comparison of TD-CAM-B3LYP and TD-PBE0 calculations for the UV-Vis spectrum of [1]⁺⁺ and [2]⁺⁺. For both methods, the def2-SVP basis set and the LR-PCM(DCM) model are employed.

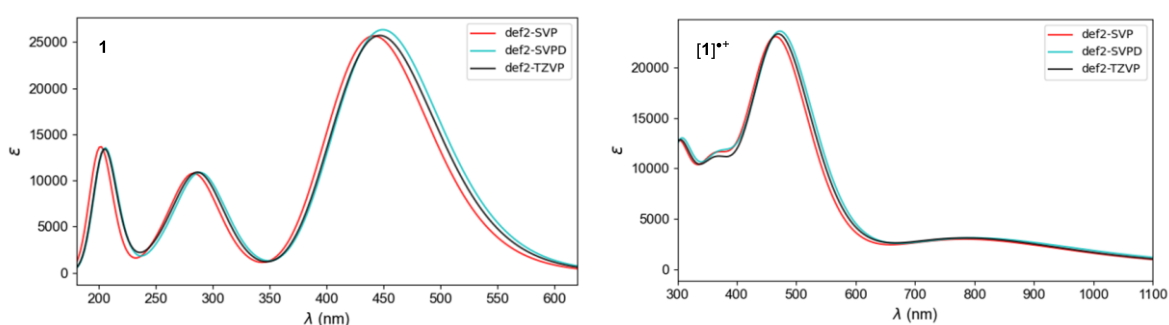


Figure S24. Basis set dependence of the simulated absorption spectra of [1]⁰⁺⁺ in TD-CAM-B3LYP calculations in conjunction with the LR-PCM model.

Table S6. Total job CPU time (hh:mm:ss) for TD-CAM-B3LYP calculations using different Ahlrichs basis sets and the LR-PCM model. All calculations were performed parallelly on 28 shared processors with a total memory of 128 GB.

| | def2-SVP | def2-TZVP | def2-SVPD |
|-------------------------|-----------|------------|------------|
| 1 | 76:07:04 | 698:55:51 | 690:39:07 |
| [1]⁺⁺ | 149:20:36 | 1402:30:08 | 1500:13:29 |

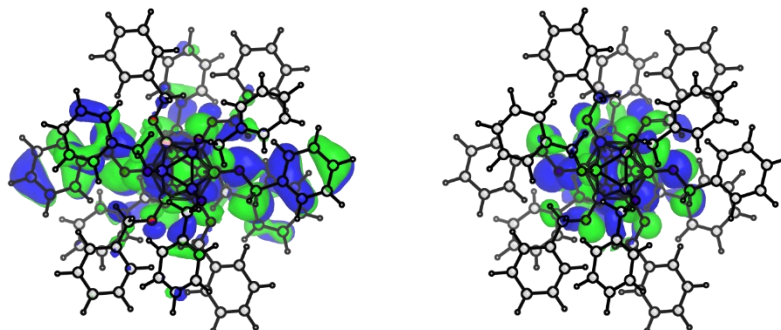


Figure S25. Natural transition orbitals for the root 7 of $[2]^{++}$. The occupied and vacant NTOs are shown on left- and right-hand sides, respectively.

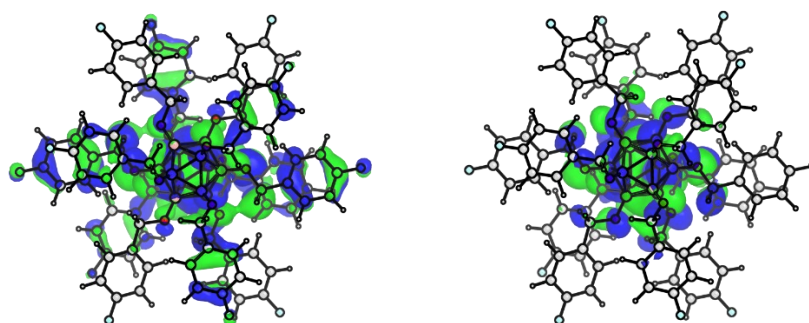


Figure S26. Natural transition orbitals for the root 6 of $[3]^{++}$. The occupied and vacant NTOs are shown on left- and right-hand sides, respectively.

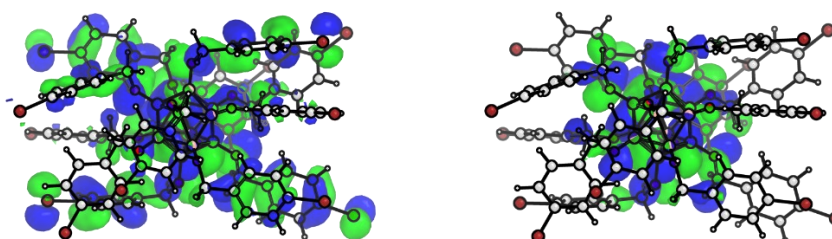


Figure S27. Natural transition orbitals for the root 8 of $[4]^{++}$. The occupied and vacant NTOs are shown on left- and right-hand sides, respectively.

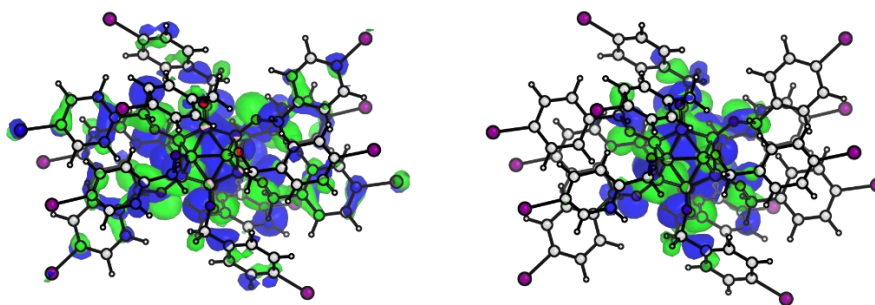


Figure S28. Natural transition orbitals for the root 7 of $[5]^{+}$. The occupied and vacant NTOs are shown on left- and right-hand sides, respectively.

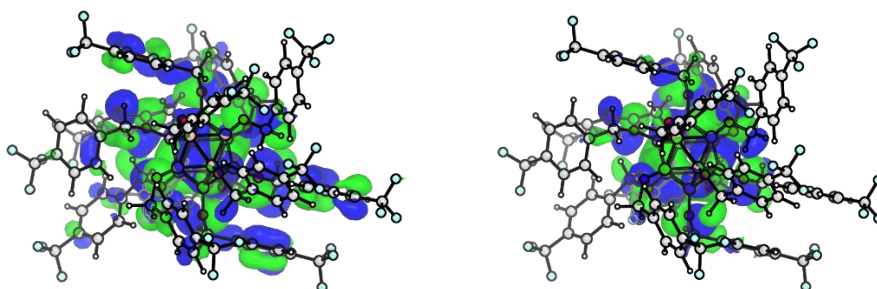


Figure S29. Natural transition orbitals for the root 7 of $[6]^{+}$. The occupied and vacant NTOs are shown on left- and right-hand sides, respectively.

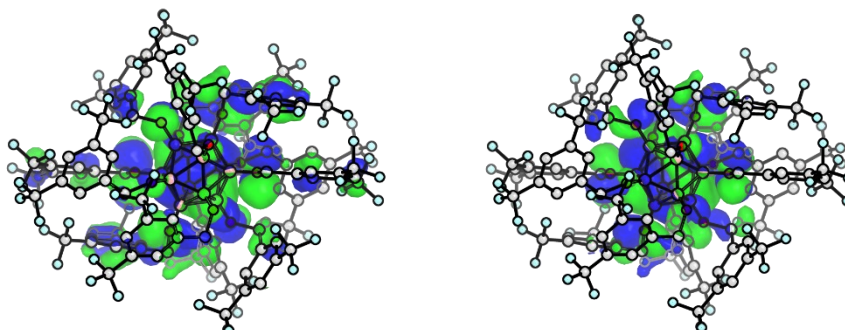


Figure S30. Natural transition orbitals for the root 9 of $[7]^{+}$. The occupied and vacant NTOs are shown on left- and right-hand sides, respectively.

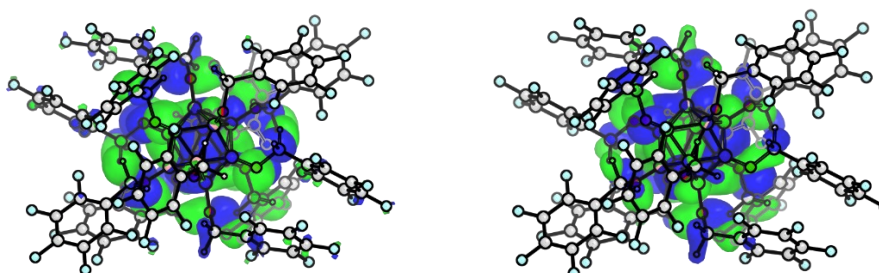


Figure S31. Natural transition orbitals for the root 8 of [8]⁺. The occupied and vacant NTOs are shown on left- and right-hand sides, respectively.

Table S7. Excitation energies, absorption wavelengths, oscillator strengths and configurations of the excited states of **1**. Up to 50 states are computed, and all excited states whose $\lambda > 300$ nm and $f > 0.01$ are presented. Orbital indices: HOMO = 180, LUMO = 181.

| root | E (eV) | λ (nm) | f | configuration (weight) |
|------|--------|----------------|--------|---|
| 4 | 2.77 | 448 | 0.2122 | 177 -> 181 (0.98) |
| 5 | 2.81 | 441 | 0.2138 | 176 -> 181 (0.98) |
| 6 | 2.85 | 436 | 0.2117 | 175 -> 181 (0.98) |
| 7 | 4.05 | 306 | 0.0186 | 167 -> 181 (0.25) 170 -> 181 (0.04) 172 -> 181 (0.06) 173 -> 181 (0.04) 174 -> 181 (0.54) |

Table S8. Excitation energies, absorption wavelengths, oscillator strengths and configurations of the excited states of **2**. Up to 50 states are computed, and all excited states whose $\lambda > 300$ nm and $f > 0.01$ are presented. Orbital indices: HOMO = 372, LUMO = 373.

| root | E (eV) | λ (nm) | f | configuration (weight) |
|------|--------|----------------|--------|--|
| 4 | 2.79 | 444 | 0.1637 | 343 -> 373 (0.13) 344 -> 373 (0.12) 355 -> 373 (0.03) 368 -> 373 (0.67) |
| 5 | 2.80 | 444 | 0.1648 | 343 -> 373 (0.12) 344 -> 373 (0.13) 356 -> 373 (0.03) 367 -> 373 (0.66) |
| 6 | 2.86 | 434 | 0.0673 | 345 -> 373 (0.34) 352 -> 373 (0.06) 364 -> 373 (0.04) 370 -> 373 (0.54) |
| 7 | 2.91 | 427 | 0.0976 | 345 -> 373 (0.21) 352 -> 373 (0.08) 364 -> 373 (0.31) 370 -> 373 (0.38) |
| 10 | 3.01 | 412 | 0.0106 | 343 -> 373 (0.14) 355 -> 373 (0.20) 359 -> 373 (0.04) 360 -> 373 (0.48) |

| | | | | |
|----|------|-----|--------|-------------------|
| | | | | 367 -> 373 (0.07) |
| 11 | 3.01 | 412 | 0.0107 | 344 -> 373 (0.14) |
| | | | | 356 -> 373 (0.19) |
| | | | | 359 -> 373 (0.48) |
| | | | | 360 -> 373 (0.04) |
| | | | | 368 -> 373 (0.06) |
| 15 | 3.07 | 403 | 0.0345 | 345 -> 373 (0.29) |
| | | | | 364 -> 373 (0.60) |
| | | | | 370 -> 373 (0.07) |
| 16 | 3.18 | 389 | 0.0188 | 343 -> 373 (0.05) |
| | | | | 344 -> 373 (0.05) |
| | | | | 355 -> 373 (0.31) |
| | | | | 359 -> 373 (0.11) |
| | | | | 360 -> 373 (0.26) |
| | | | | 367 -> 373 (0.03) |
| | | | | 368 -> 373 (0.14) |
| 17 | 3.19 | 389 | 0.0178 | 343 -> 373 (0.04) |
| | | | | 344 -> 373 (0.05) |
| | | | | 356 -> 373 (0.30) |
| | | | | 359 -> 373 (0.27) |
| | | | | 360 -> 373 (0.10) |
| | | | | 367 -> 373 (0.13) |
| | | | | 368 -> 373 (0.03) |
| 20 | 3.40 | 365 | 0.0315 | 341 -> 373 (0.06) |
| | | | | 343 -> 373 (0.02) |
| | | | | 344 -> 373 (0.36) |
| | | | | 347 -> 373 (0.04) |
| | | | | 355 -> 373 (0.15) |
| | | | | 356 -> 373 (0.21) |
| | | | | 359 -> 373 (0.03) |
| | | | | 360 -> 373 (0.03) |
| | | | | 368 -> 373 (0.06) |
| 21 | 3.40 | 365 | 0.0317 | 342 -> 373 (0.06) |
| | | | | 343 -> 373 (0.36) |
| | | | | 344 -> 373 (0.02) |
| | | | | 348 -> 373 (0.04) |
| | | | | 355 -> 373 (0.21) |
| | | | | 356 -> 373 (0.15) |
| | | | | 359 -> 373 (0.03) |
| | | | | 360 -> 373 (0.03) |
| | | | | 367 -> 373 (0.06) |
| 24 | 3.49 | 355 | 0.0234 | 338 -> 373 (0.04) |
| | | | | 345 -> 373 (0.11) |

| | | | | |
|----|------|-----|--------|-------------------|
| | | | | 351 -> 373 (0.21) |
| | | | | 352 -> 373 (0.63) |
| 29 | 3.79 | 327 | 0.0106 | 342 -> 373 (0.03) |
| | | | | 343 -> 373 (0.04) |
| | | | | 344 -> 373 (0.02) |
| | | | | 347 -> 373 (0.87) |
| 31 | 3.82 | 324 | 0.0327 | 336 -> 373 (0.02) |
| | | | | 341 -> 373 (0.05) |
| | | | | 342 -> 373 (0.70) |
| | | | | 343 -> 373 (0.02) |
| | | | | 347 -> 373 (0.04) |
| | | | | 356 -> 373 (0.06) |
| 32 | 3.82 | 324 | 0.0334 | 335 -> 373 (0.02) |
| | | | | 341 -> 373 (0.71) |
| | | | | 342 -> 373 (0.05) |
| | | | | 344 -> 373 (0.03) |
| | | | | 348 -> 373 (0.03) |
| | | | | 355 -> 373 (0.06) |

Table S9. Excitation energies, absorption wavelengths, oscillator strengths and configurations of the excited states of **3**. Up to 50 states are computed, and all excited states whose $\lambda > 300$ nm and $f > 0.01$ are presented. Orbital indices: HOMO = 420, LUMO = 421.

| root | E (eV) | λ (nm) | f | configuration (weight) |
|------|--------|----------------|--------|------------------------|
| 4 | 2.63 | 471 | 0.0680 | 392 -> 421 (0.17) |
| | | | | 416 -> 421 (0.02) |
| | | | | 417 -> 421 (0.03) |
| | | | | 418 -> 421 (0.74) |
| 5 | 2.63 | 471 | 0.0676 | 391 -> 421 (0.17) |
| | | | | 417 -> 421 (0.75) |
| | | | | 418 -> 421 (0.02) |
| 6 | 2.75 | 451 | 0.1274 | 393 -> 421 (0.02) |
| | | | | 399 -> 421 (0.46) |
| | | | | 411 -> 421 (0.26) |
| | | | | 416 -> 421 (0.22) |
| 7 | 2.80 | 442 | 0.0499 | 399 -> 421 (0.09) |
| | | | | 411 -> 421 (0.14) |
| | | | | 416 -> 421 (0.70) |
| | | | | 418 -> 421 (0.03) |
| 11 | 3.19 | 389 | 0.0581 | 392 -> 421 (0.16) |
| | | | | 409 -> 421 (0.29) |
| | | | | 410 -> 421 (0.46) |
| | | | | 418 -> 421 (0.02) |

| | | | | |
|----|------|-----|--------|--|
| 12 | 3.19 | 389 | 0.0573 | 391 -> 421 (0.15) 409 -> 421 (0.46) 410 -> 421 (0.30) |
| 16 | 3.31 | 375 | 0.0321 | 393 -> 421 (0.03) 399 -> 421 (0.37) 405 -> 421 (0.02) 411 -> 421 (0.56) |
| 17 | 3.34 | 371 | 0.0539 | 392 -> 421 (0.44) 397 -> 421 (0.04) 401 -> 421 (0.05) 402 -> 421 (0.02) 409 -> 421 (0.09) 410 -> 421 (0.13) 417 -> 421 (0.04) 418 -> 421 (0.12) |
| 18 | 3.34 | 371 | 0.0557 | 391 -> 421 (0.45) 396 -> 421 (0.04) 401 -> 421 (0.02) 402 -> 421 (0.04) 409 -> 421 (0.13) 410 -> 421 (0.09) 417 -> 421 (0.12) 418 -> 421 (0.04) |
| 25 | 3.65 | 339 | 0.0167 | 384 -> 421 (0.03) 390 -> 421 (0.85) |
| 26 | 3.66 | 339 | 0.0164 | 383 -> 421 (0.03) 389 -> 421 (0.85) |
| 32 | 4.10 | 302 | 0.0212 | 385 -> 421 (0.07) 393 -> 421 (0.86) 399 -> 421 (0.05) |

Table S10. Excitation energies, absorption wavelengths, oscillator strengths and configurations of the excited states of **4**. Up to 50 states are computed, and all excited states whose $\lambda > 300$ nm and $f > 0.01$ are presented. Orbital indices: HOMO = 576, LUMO = 577.

| root | E (eV) | λ (nm) | f | configuration (weight) |
|------|--------|----------------|--------|---|
| 4 | 2.66 | 466 | 0.2447 | 548 -> 577 (0.19) 549 -> 577 (0.03) 554 -> 577 (0.03) 567 -> 577 (0.13) 569 -> 577 (0.03) 570 -> 577 (0.04) 571 -> 577 (0.03) |

| | | | | |
|----|------|-----|--------|-------------------|
| | | | | 572 -> 577 (0.36) |
| | | | | 574 -> 577 (0.08) |
| 5 | 2.71 | 458 | 0.2059 | 548 -> 577 (0.04) |
| | | | | 549 -> 577 (0.17) |
| | | | | 552 -> 577 (0.04) |
| | | | | 553 -> 577 (0.03) |
| | | | | 554 -> 577 (0.03) |
| | | | | 555 -> 577 (0.02) |
| | | | | 556 -> 577 (0.04) |
| | | | | 563 -> 577 (0.02) |
| | | | | 564 -> 577 (0.02) |
| | | | | 566 -> 577 (0.09) |
| | | | | 567 -> 577 (0.06) |
| | | | | 569 -> 577 (0.11) |
| | | | | 570 -> 577 (0.08) |
| | | | | 572 -> 577 (0.11) |
| | | | | 574 -> 577 (0.02) |
| 6 | 2.76 | 449 | 0.0458 | 547 -> 577 (0.05) |
| | | | | 567 -> 577 (0.17) |
| | | | | 569 -> 577 (0.13) |
| | | | | 570 -> 577 (0.14) |
| | | | | 571 -> 577 (0.06) |
| | | | | 572 -> 577 (0.17) |
| | | | | 573 -> 577 (0.12) |
| | | | | 574 -> 577 (0.07) |
| 7 | 2.79 | 444 | 0.0138 | 562 -> 577 (0.02) |
| | | | | 566 -> 577 (0.05) |
| | | | | 567 -> 577 (0.21) |
| | | | | 571 -> 577 (0.05) |
| | | | | 573 -> 577 (0.05) |
| | | | | 574 -> 577 (0.44) |
| | | | | 575 -> 577 (0.06) |
| 9 | 2.85 | 435 | 0.0247 | 566 -> 577 (0.06) |
| | | | | 568 -> 577 (0.37) |
| | | | | 570 -> 577 (0.20) |
| | | | | 571 -> 577 (0.20) |
| | | | | 572 -> 577 (0.04) |
| 14 | 3.02 | 410 | 0.0284 | 549 -> 577 (0.08) |
| | | | | 554 -> 577 (0.02) |
| | | | | 563 -> 577 (0.22) |
| | | | | 565 -> 577 (0.16) |
| | | | | 566 -> 577 (0.10) |
| | | | | 569 -> 577 (0.06) |

| | | | | |
|----|------|-----|--------|-------------------|
| | | | | 570 -> 577 (0.12) |
| | | | | 571 -> 577 (0.04) |
| | | | | 573 -> 577 (0.06) |
| 15 | 3.06 | 406 | 0.0150 | 548 -> 577 (0.04) |
| | | | | 562 -> 577 (0.29) |
| | | | | 563 -> 577 (0.09) |
| | | | | 565 -> 577 (0.32) |
| | | | | 566 -> 577 (0.06) |
| | | | | 572 -> 577 (0.04) |
| | | | | 574 -> 577 (0.03) |
| | | | | 575 -> 577 (0.03) |
| 16 | 3.15 | 393 | 0.0198 | 549 -> 577 (0.11) |
| | | | | 552 -> 577 (0.02) |
| | | | | 554 -> 577 (0.05) |
| | | | | 556 -> 577 (0.02) |
| | | | | 563 -> 577 (0.38) |
| | | | | 564 -> 577 (0.08) |
| | | | | 565 -> 577 (0.05) |
| | | | | 566 -> 577 (0.06) |
| | | | | 567 -> 577 (0.03) |
| | | | | 569 -> 577 (0.03) |
| | | | | 570 -> 577 (0.02) |
| 17 | 3.22 | 385 | 0.0796 | 547 -> 577 (0.14) |
| | | | | 548 -> 577 (0.37) |
| | | | | 550 -> 577 (0.03) |
| | | | | 557 -> 577 (0.05) |
| | | | | 560 -> 577 (0.02) |
| | | | | 565 -> 577 (0.04) |
| | | | | 567 -> 577 (0.03) |
| | | | | 569 -> 577 (0.10) |
| | | | | 571 -> 577 (0.03) |
| | | | | 572 -> 577 (0.03) |
| 18 | 3.30 | 376 | 0.0647 | 545 -> 577 (0.03) |
| | | | | 547 -> 577 (0.47) |
| | | | | 548 -> 577 (0.08) |
| | | | | 554 -> 577 (0.02) |
| | | | | 559 -> 577 (0.04) |
| | | | | 561 -> 577 (0.04) |
| | | | | 565 -> 577 (0.06) |
| | | | | 570 -> 577 (0.03) |
| | | | | 572 -> 577 (0.05) |
| 19 | 3.41 | 364 | 0.0131 | 547 -> 577 (0.08) |
| | | | | 551 -> 577 (0.03) |

| | | | | |
|----|------|-----|--------|-------------------|
| | | | | 559 -> 577 (0.26) |
| | | | | 560 -> 577 (0.08) |
| | | | | 561 -> 577 (0.45) |
| 21 | 3.49 | 356 | 0.0136 | 532 -> 577 (0.04) |
| | | | | 533 -> 577 (0.02) |
| | | | | 534 -> 577 (0.04) |
| | | | | 549 -> 577 (0.02) |
| | | | | 552 -> 577 (0.03) |
| | | | | 554 -> 577 (0.06) |
| | | | | 556 -> 577 (0.10) |
| | | | | 558 -> 577 (0.28) |
| | | | | 559 -> 577 (0.20) |
| | | | | 560 -> 577 (0.11) |
| 23 | 3.56 | 348 | 0.0161 | 530 -> 577 (0.02) |
| | | | | 531 -> 577 (0.02) |
| | | | | 533 -> 577 (0.03) |
| | | | | 534 -> 577 (0.08) |
| | | | | 553 -> 577 (0.16) |
| | | | | 554 -> 577 (0.13) |
| | | | | 556 -> 577 (0.04) |
| | | | | 557 -> 577 (0.12) |
| | | | | 558 -> 577 (0.25) |

Table S11. Excitation energies, absorption wavelengths, oscillator strengths and configurations of the excited states of **5**. Up to 50 states are computed, and all excited states whose $\lambda > 300$ nm and $f > 0.01$ are presented. Orbital indices: HOMO = 516, LUMO = 517.

| root | E (eV) | λ (nm) | f | configuration (weight) |
|------|--------|----------------|--------|------------------------|
| 4 | 2.76 | 450 | 0.4668 | 486 -> 517 (0.03) |
| | | | | 489 -> 517 (0.06) |
| | | | | 491 -> 517 (0.03) |
| | | | | 495 -> 517 (0.09) |
| | | | | 497 -> 517 (0.17) |
| | | | | 499 -> 517 (0.22) |
| | | | | 508 -> 517 (0.03) |
| | | | | 512 -> 517 (0.14) |
| | | | | 514 -> 517 (0.14) |
| 5 | 2.92 | 425 | 0.1000 | 476 -> 517 (0.19) |
| | | | | 478 -> 517 (0.03) |
| | | | | 504 -> 517 (0.06) |
| | | | | 508 -> 517 (0.25) |
| | | | | 514 -> 517 (0.37) |
| 6 | 2.98 | 416 | 0.0162 | 474 -> 517 (0.06) |

| | | | | |
|----|------|-----|--------|-------------------|
| | | | | 475 -> 517 (0.04) |
| | | | | 476 -> 517 (0.04) |
| | | | | 478 -> 517 (0.04) |
| | | | | 501 -> 517 (0.02) |
| | | | | 504 -> 517 (0.07) |
| | | | | 508 -> 517 (0.02) |
| | | | | 510 -> 517 (0.23) |
| | | | | 512 -> 517 (0.24) |
| | | | | 514 -> 517 (0.16) |
| 7 | 2.99 | 414 | 0.0883 | 475 -> 517 (0.32) |
| | | | | 476 -> 517 (0.05) |
| | | | | 504 -> 517 (0.22) |
| | | | | 507 -> 517 (0.04) |
| | | | | 508 -> 517 (0.03) |
| | | | | 510 -> 517 (0.25) |
| 9 | 3.08 | 403 | 0.0291 | 476 -> 517 (0.05) |
| | | | | 507 -> 517 (0.27) |
| | | | | 508 -> 517 (0.09) |
| | | | | 510 -> 517 (0.30) |
| | | | | 512 -> 517 (0.11) |
| | | | | 514 -> 517 (0.11) |
| 15 | 3.17 | 391 | 0.0594 | 473 -> 517 (0.04) |
| | | | | 476 -> 517 (0.31) |
| | | | | 478 -> 517 (0.04) |
| | | | | 484 -> 517 (0.02) |
| | | | | 489 -> 517 (0.03) |
| | | | | 507 -> 517 (0.17) |
| | | | | 510 -> 517 (0.03) |
| | | | | 512 -> 517 (0.13) |
| | | | | 514 -> 517 (0.07) |
| 17 | 3.21 | 387 | 0.0359 | 470 -> 517 (0.02) |
| | | | | 475 -> 517 (0.11) |
| | | | | 476 -> 517 (0.04) |
| | | | | 478 -> 517 (0.06) |
| | | | | 489 -> 517 (0.02) |
| | | | | 495 -> 517 (0.03) |
| | | | | 497 -> 517 (0.04) |
| | | | | 499 -> 517 (0.05) |
| | | | | 504 -> 517 (0.22) |
| | | | | 508 -> 517 (0.20) |
| | | | | 512 -> 517 (0.08) |
| | | | | 514 -> 517 (0.04) |
| 18 | 3.28 | 378 | 0.0236 | 465 -> 517 (0.02) |

| | | | | |
|----|------|-----|--------|-------------------|
| | | | | 475 -> 517 (0.26) |
| | | | | 486 -> 517 (0.03) |
| | | | | 497 -> 517 (0.03) |
| | | | | 504 -> 517 (0.08) |
| | | | | 507 -> 517 (0.12) |
| | | | | 508 -> 517 (0.08) |
| | | | | 510 -> 517 (0.04) |
| | | | | 512 -> 517 (0.19) |
| 28 | 3.82 | 325 | 0.0144 | 461 -> 517 (0.05) |
| | | | | 462 -> 517 (0.04) |
| | | | | 484 -> 517 (0.08) |
| | | | | 486 -> 517 (0.13) |
| | | | | 487 -> 517 (0.11) |
| | | | | 491 -> 517 (0.38) |
| | | | | 493 -> 517 (0.10) |

Table S12. Excitation energies, absorption wavelengths, oscillator strengths and configurations of the excited states of **6**. Up to 50 states are computed, and all excited states whose $\lambda > 300$ nm and $f > 0.01$ are presented. Orbital indices: HOMO = 564, LUMO = 565.

| root | E (eV) | λ (nm) | f | configuration (weight) |
|------|--------|----------------|--------|------------------------|
| 4 | 2.70 | 459 | 0.2654 | 537 -> 565 (0.14) |
| | | | | 538 -> 565 (0.02) |
| | | | | 547 -> 565 (0.02) |
| | | | | 552 -> 565 (0.03) |
| | | | | 553 -> 565 (0.05) |
| | | | | 555 -> 565 (0.06) |
| | | | | 556 -> 565 (0.04) |
| | | | | 557 -> 565 (0.02) |
| | | | | 558 -> 565 (0.04) |
| | | | | 561 -> 565 (0.49) |
| 5 | 2.88 | 431 | 0.2185 | 535 -> 565 (0.05) |
| | | | | 536 -> 565 (0.35) |
| | | | | 553 -> 565 (0.04) |
| | | | | 554 -> 565 (0.02) |
| | | | | 556 -> 565 (0.03) |
| | | | | 559 -> 565 (0.27) |
| | | | | 560 -> 565 (0.10) |
| | | | | 561 -> 565 (0.04) |
| 6 | 2.98 | 416 | 0.1264 | 535 -> 565 (0.44) |
| | | | | 536 -> 565 (0.08) |
| | | | | 550 -> 565 (0.04) |
| | | | | 552 -> 565 (0.05) |

| | | | | |
|----|------|-----|--------|-------------------|
| | | | | 553 -> 565 (0.08) |
| | | | | 555 -> 565 (0.03) |
| | | | | 556 -> 565 (0.11) |
| | | | | 558 -> 565 (0.07) |
| | | | | 561 -> 565 (0.03) |
| 7 | 3.16 | 392 | 0.0162 | 533 -> 565 (0.05) |
| | | | | 558 -> 565 (0.15) |
| | | | | 559 -> 565 (0.08) |
| | | | | 560 -> 565 (0.55) |
| | | | | 561 -> 565 (0.05) |
| | | | | 562 -> 565 (0.03) |
| 8 | 3.18 | 389 | 0.0113 | 534 -> 565 (0.07) |
| | | | | 553 -> 565 (0.04) |
| | | | | 554 -> 565 (0.04) |
| | | | | 555 -> 565 (0.18) |
| | | | | 558 -> 565 (0.12) |
| | | | | 559 -> 565 (0.14) |
| | | | | 560 -> 565 (0.07) |
| | | | | 561 -> 565 (0.20) |
| 9 | 3.27 | 379 | 0.0251 | 534 -> 565 (0.09) |
| | | | | 535 -> 565 (0.02) |
| | | | | 543 -> 565 (0.02) |
| | | | | 550 -> 565 (0.02) |
| | | | | 553 -> 565 (0.08) |
| | | | | 554 -> 565 (0.05) |
| | | | | 556 -> 565 (0.27) |
| | | | | 557 -> 565 (0.20) |
| | | | | 559 -> 565 (0.08) |
| | | | | 560 -> 565 (0.05) |
| 10 | 3.29 | 377 | 0.0126 | 535 -> 565 (0.03) |
| | | | | 553 -> 565 (0.09) |
| | | | | 554 -> 565 (0.08) |
| | | | | 555 -> 565 (0.03) |
| | | | | 556 -> 565 (0.03) |
| | | | | 557 -> 565 (0.36) |
| | | | | 558 -> 565 (0.18) |
| | | | | 559 -> 565 (0.06) |
| | | | | 560 -> 565 (0.05) |
| 12 | 3.39 | 366 | 0.0210 | 533 -> 565 (0.02) |
| | | | | 534 -> 565 (0.02) |
| | | | | 536 -> 565 (0.09) |
| | | | | 537 -> 565 (0.04) |
| | | | | 541 -> 565 (0.02) |

| | | | | |
|----|------|-----|--------|-------------------|
| | | | | 543 -> 565 (0.03) |
| | | | | 547 -> 565 (0.09) |
| | | | | 549 -> 565 (0.05) |
| | | | | 551 -> 565 (0.04) |
| | | | | 552 -> 565 (0.11) |
| | | | | 555 -> 565 (0.19) |
| | | | | 557 -> 565 (0.02) |
| | | | | 559 -> 565 (0.06) |
| | | | | 561 -> 565 (0.08) |
| 27 | 3.73 | 332 | 0.0108 | 534 -> 565 (0.15) |
| | | | | 537 -> 565 (0.04) |
| | | | | 541 -> 565 (0.06) |
| | | | | 542 -> 565 (0.19) |
| | | | | 543 -> 565 (0.05) |
| | | | | 546 -> 565 (0.24) |
| | | | | 548 -> 565 (0.05) |
| | | | | 550 -> 565 (0.09) |
| | | | | 551 -> 565 (0.02) |
| 28 | 3.73 | 332 | 0.0181 | 534 -> 565 (0.19) |
| | | | | 539 -> 565 (0.38) |
| | | | | 542 -> 565 (0.18) |
| | | | | 543 -> 565 (0.03) |
| | | | | 544 -> 565 (0.06) |
| | | | | 547 -> 565 (0.04) |

Table S13. Excitation energies, absorption wavelengths, oscillator strengths and configurations of the excited states of **7**. Up to 50 states are computed, and all excited states whose $\lambda > 300$ nm and $f > 0.01$ are presented. Orbital indices: HOMO = 756, LUMO = 757.

| root | E (eV) | λ (nm) | f | configuration (weight) |
|------|--------|----------------|--------|------------------------|
| 4 | 2.73 | 454 | 0.2113 | 728 -> 757 (0.15) |
| | | | | 738 -> 757 (0.03) |
| | | | | 740 -> 757 (0.02) |
| | | | | 748 -> 757 (0.25) |
| | | | | 749 -> 757 (0.09) |
| | | | | 752 -> 757 (0.05) |
| | | | | 753 -> 757 (0.31) |
| 5 | 2.78 | 446 | 0.2121 | 727 -> 757 (0.03) |
| | | | | 728 -> 757 (0.08) |
| | | | | 729 -> 757 (0.11) |
| | | | | 735 -> 757 (0.03) |
| | | | | 743 -> 757 (0.14) |
| | | | | 748 -> 757 (0.13) |

| | | | | |
|----|------|-----|--------|-------------------|
| | | | | 749 -> 757 (0.10) |
| | | | | 752 -> 757 (0.28) |
| 6 | 2.87 | 432 | 0.1061 | 727 -> 757 (0.24) |
| | | | | 728 -> 757 (0.04) |
| | | | | 738 -> 757 (0.06) |
| | | | | 743 -> 757 (0.02) |
| | | | | 746 -> 757 (0.09) |
| | | | | 749 -> 757 (0.32) |
| | | | | 752 -> 757 (0.06) |
| | | | | 753 -> 757 (0.13) |
| 7 | 3.03 | 409 | 0.0439 | 726 -> 757 (0.12) |
| | | | | 743 -> 757 (0.02) |
| | | | | 748 -> 757 (0.16) |
| | | | | 749 -> 757 (0.03) |
| | | | | 752 -> 757 (0.23) |
| | | | | 753 -> 757 (0.36) |
| 10 | 3.26 | 381 | 0.0698 | 727 -> 757 (0.03) |
| | | | | 731 -> 757 (0.02) |
| | | | | 738 -> 757 (0.03) |
| | | | | 742 -> 757 (0.08) |
| | | | | 746 -> 757 (0.39) |
| | | | | 748 -> 757 (0.06) |
| | | | | 749 -> 757 (0.06) |
| | | | | 752 -> 757 (0.22) |
| | | | | 753 -> 757 (0.02) |
| 12 | 3.37 | 368 | 0.0401 | 726 -> 757 (0.06) |
| | | | | 727 -> 757 (0.07) |
| | | | | 728 -> 757 (0.04) |
| | | | | 735 -> 757 (0.02) |
| | | | | 742 -> 757 (0.04) |
| | | | | 743 -> 757 (0.41) |
| | | | | 749 -> 757 (0.24) |
| | | | | 753 -> 757 (0.04) |
| 13 | 3.42 | 363 | 0.0130 | 722 -> 757 (0.03) |
| | | | | 726 -> 757 (0.41) |
| | | | | 727 -> 757 (0.03) |
| | | | | 731 -> 757 (0.04) |
| | | | | 735 -> 757 (0.02) |
| | | | | 738 -> 757 (0.08) |
| | | | | 740 -> 757 (0.08) |
| | | | | 743 -> 757 (0.10) |
| | | | | 748 -> 757 (0.06) |
| | | | | 753 -> 757 (0.08) |

| | | | | |
|----|------|-----|--------|---|
| 15 | 3.53 | 352 | 0.0126 | 725 -> 757 (0.09) 727 -> 757 (0.11) 728 -> 757 (0.03) 729 -> 757 (0.04) 731 -> 757 (0.09) 735 -> 757 (0.07) 738 -> 757 (0.03) 746 -> 757 (0.28) 748 -> 757 (0.16) |
| 29 | 3.90 | 318 | 0.0117 | 725 -> 757 (0.11) 726 -> 757 (0.12) 727 -> 757 (0.08) 729 -> 757 (0.02) 735 -> 757 (0.14) 738 -> 757 (0.29) 742 -> 757 (0.16) |
| 30 | 3.93 | 315 | 0.0108 | 725 -> 757 (0.06) 726 -> 757 (0.09) 728 -> 757 (0.02) 729 -> 757 (0.27) 731 -> 757 (0.44) 733 -> 757 (0.05) 735 -> 757 (0.04) |

Table S14. Excitation energies, absorption wavelengths, oscillator strengths and configurations of the excited states of **8**. Up to 50 states are computed, and all excited states whose $\lambda > 300$ nm and $f > 0.01$ are presented. Orbital indices: HOMO = 612, LUMO = 613.

| root | E (eV) | λ (nm) | f | configuration (weight) |
|------|--------|----------------|--------|---|
| 4 | 2.81 | 442 | 0.4065 | 585 -> 613 (0.34) 597 -> 613 (0.26) 603 -> 613 (0.30) 605 -> 613 (0.07) |
| 5 | 2.98 | 416 | 0.1267 | 583 -> 613 (0.09) 584 -> 613 (0.39) 589 -> 613 (0.12) 596 -> 613 (0.10) 601 -> 613 (0.08) 602 -> 613 (0.05) 609 -> 613 (0.11) |
| 6 | 2.98 | 416 | 0.1268 | 583 -> 613 (0.39) 584 -> 613 (0.09) 590 -> 613 (0.12) |

| | | | | |
|----|------|-----|--------|-------------------|
| | | | | 595 -> 613 (0.11) |
| | | | | 601 -> 613 (0.05) |
| | | | | 602 -> 613 (0.08) |
| | | | | 608 -> 613 (0.10) |
| 15 | 3.33 | 373 | 0.0194 | 591 -> 613 (0.24) |
| | | | | 597 -> 613 (0.22) |
| | | | | 603 -> 613 (0.48) |
| | | | | 605 -> 613 (0.03) |
| 24 | 3.54 | 351 | 0.0132 | 591 -> 613 (0.65) |
| | | | | 597 -> 613 (0.22) |
| | | | | 603 -> 613 (0.06) |
| | | | | 605 -> 613 (0.03) |

Table S15. Excitation energies, absorption wavelengths, oscillator strengths, $\langle S^2 \rangle$ and configurations of the excited states of $[1]^+$. Up to 50 states are computed, and all excited states whose $\lambda > 300$ nm and $f > 0.01$ are presented. Orbital indices: α -HOMO = 180A, α -LUMO = 181A, β -HOMO = 179B, β -LUMO = 180B.

| root | E (eV) | λ (nm) | f | $\langle S^2 \rangle$ | configuration (weight) |
|------|--------|----------------|--------|-----------------------|------------------------|
| 8 | 1.47 | 844 | 0.0210 | 1.389 | 176A -> 181A (0.01) |
| | | | | | 177A -> 181A (0.20) |
| | | | | | 176B -> 180B (0.07) |
| | | | | | 177B -> 180B (0.65) |
| | | | | | 177B -> 181B (0.05) |
| | | | | | 177A <- 181A (0.01) |
| 9 | 1.56 | 794 | 0.0269 | 0.824 | 176A -> 181A (0.03) |
| | | | | | 177A -> 181A (0.01) |
| | | | | | 175B -> 181B (0.02) |
| | | | | | 176B -> 180B (0.76) |
| | | | | | 177B -> 180B (0.13) |
| | | | | | 177B -> 181B (0.01) |
| 10 | 1.61 | 770 | 0.0224 | 0.807 | 175A -> 181A (0.03) |
| | | | | | 175B -> 180B (0.89) |
| | | | | | 176B -> 180B (0.02) |
| | | | | | 176B -> 181B (0.03) |
| 14 | 2.62 | 473 | 0.1752 | 0.820 | 175A -> 181A (0.01) |
| | | | | | 176A -> 181A (0.33) |
| | | | | | 177A -> 181A (0.23) |
| | | | | | 175B -> 180B (0.01) |
| | | | | | 176B -> 180B (0.01) |
| | | | | | 176B -> 181B (0.14) |
| | | | | | 177B -> 181B (0.20) |
| 15 | 2.65 | 467 | 0.1575 | 0.818 | 175A -> 181A (0.39) |

| | | | | | |
|----|------|-----|--------|-------|---------------------|
| | | | | | 176A -> 181A (0.11) |
| | | | | | 177A -> 181A (0.08) |
| | | | | | 172B -> 180B (0.02) |
| | | | | | 175B -> 181B (0.19) |
| | | | | | 176B -> 181B (0.06) |
| | | | | | 177B -> 180B (0.02) |
| | | | | | 177B -> 181B (0.08) |
| 16 | 2.67 | 464 | 0.2280 | 0.793 | 175A -> 181A (0.17) |
| | | | | | 176A -> 181A (0.13) |
| | | | | | 177A -> 181A (0.26) |
| | | | | | 175B -> 181B (0.15) |
| | | | | | 176B -> 181B (0.13) |
| | | | | | 177B -> 180B (0.03) |
| | | | | | 177B -> 181B (0.07) |
| 19 | 3.34 | 372 | 0.0902 | 0.835 | 175A -> 181A (0.02) |
| | | | | | 176A -> 181A (0.01) |
| | | | | | 168B -> 180B (0.18) |
| | | | | | 169B -> 180B (0.03) |
| | | | | | 170B -> 180B (0.02) |
| | | | | | 171B -> 180B (0.01) |
| | | | | | 172B -> 180B (0.54) |
| | | | | | 173B -> 180B (0.09) |
| 20 | 3.35 | 370 | 0.0346 | 0.839 | 170A -> 181A (0.01) |
| | | | | | 169B -> 180B (0.18) |
| | | | | | 170B -> 180B (0.56) |
| | | | | | 171B -> 180B (0.11) |
| 21 | 3.41 | 364 | 0.0214 | 1.039 | 170A -> 181A (0.02) |
| | | | | | 171A -> 181A (0.03) |
| | | | | | 168B -> 180B (0.06) |
| | | | | | 169B -> 180B (0.32) |
| | | | | | 170B -> 181B (0.02) |
| | | | | | 171B -> 180B (0.43) |
| 22 | 3.44 | 361 | 0.0581 | 0.931 | 171A -> 181A (0.02) |
| | | | | | 175A -> 181A (0.01) |
| | | | | | 168B -> 180B (0.03) |
| | | | | | 169B -> 180B (0.23) |
| | | | | | 170B -> 180B (0.27) |
| | | | | | 171B -> 180B (0.30) |
| | | | | | 171B -> 181B (0.01) |
| | | | | | 172B -> 180B (0.03) |
| 23 | 3.48 | 356 | 0.0334 | 1.138 | 172A -> 181A (0.01) |
| | | | | | 173A -> 181A (0.07) |
| | | | | | 168B -> 180B (0.49) |

| | | | | | |
|----|------|-----|--------|-------|---------------------|
| | | | | | 169B -> 180B (0.06) |
| | | | | | 171B -> 180B (0.01) |
| | | | | | 172B -> 180B (0.21) |
| | | | | | 173B -> 181B (0.03) |
| 35 | 3.91 | 317 | 0.0105 | 1.090 | 168A -> 181A (0.02) |
| | | | | | 169A -> 181A (0.15) |
| | | | | | 170A -> 181A (0.07) |
| | | | | | 172A -> 181A (0.03) |
| | | | | | 161B -> 180B (0.03) |
| | | | | | 162B -> 180B (0.01) |
| | | | | | 163B -> 180B (0.03) |
| | | | | | 164B -> 180B (0.04) |
| | | | | | 165B -> 180B (0.01) |
| | | | | | 167B -> 181B (0.02) |
| | | | | | 168B -> 181B (0.02) |
| | | | | | 169B -> 181B (0.34) |
| | | | | | 170B -> 181B (0.04) |
| | | | | | 171B -> 181B (0.01) |
| | | | | | 172B -> 181B (0.01) |
| 40 | 4.05 | 306 | 0.0115 | 1.006 | 167A -> 181A (0.06) |
| | | | | | 169A -> 181A (0.02) |
| | | | | | 172A -> 181A (0.04) |
| | | | | | 173A -> 181A (0.16) |
| | | | | | 174A -> 181A (0.07) |
| | | | | | 160B -> 180B (0.06) |
| | | | | | 161B -> 180B (0.02) |
| | | | | | 162B -> 180B (0.26) |
| | | | | | 166B -> 181B (0.02) |
| | | | | | 167B -> 181B (0.02) |
| | | | | | 168B -> 181B (0.02) |
| | | | | | 170B -> 181B (0.01) |
| | | | | | 173B -> 181B (0.11) |
| | | | | | 174B -> 181B (0.02) |
| 43 | 4.11 | 302 | 0.0212 | 1.416 | 165A -> 181A (0.02) |
| | | | | | 166A -> 181A (0.06) |
| | | | | | 167A -> 181A (0.05) |
| | | | | | 172A -> 181A (0.05) |
| | | | | | 159B -> 180B (0.07) |
| | | | | | 160B -> 180B (0.02) |
| | | | | | 161B -> 180B (0.33) |
| | | | | | 166B -> 181B (0.08) |
| | | | | | 167B -> 181B (0.06) |
| | | | | | 171B -> 181B (0.03) |

Table S16. Excitation energies, absorption wavelengths, oscillator strengths, $\langle S^2 \rangle$ and configurations of the excited states of $[2]^+$. Up to 50 states are computed, and all excited states whose $\lambda > 300$ nm and $f > 0.01$ are presented. Orbital indices: α -HOMO = 372A, α -LUMO = 373A, β -HOMO = 371B, β -LUMO = 372B.

| root | E (eV) | λ (nm) | f | $\langle S^2 \rangle$ | configuration (weight) |
|---------------------|--------|----------------|--------|-----------------------|------------------------|
| 7 | 1.34 | 924 | 0.1005 | 0.786 | 345B -> 372B (0.47) |
| | | | | | 352B -> 372B (0.01) |
| | | | | | 354B -> 372B (0.06) |
| | | | | | 356B -> 372B (0.05) |
| | | | | | 361B -> 372B (0.01) |
| | | | | | 364B -> 372B (0.08) |
| | | | | | 371B -> 372B (0.28) |
| 12 | 1.65 | 750 | 0.0262 | 1.105 | 344A -> 373A (0.03) |
| | | | | | 345A -> 373A (0.01) |
| | | | | | 343B -> 372B (0.02) |
| | | | | | 344B -> 372B (0.22) |
| | | | | | 345B -> 373B (0.07) |
| | | | | | 356B -> 372B (0.01) |
| | | | | | 361B -> 372B (0.01) |
| | | | | | 363B -> 372B (0.02) |
| | | | | | 367B -> 372B (0.27) |
| | | | | | 368B -> 372B (0.18) |
| 371B -> 372B (0.04) | | | | | |
| 33 | 2.25 | 551 | 0.0142 | 0.976 | 345A -> 373A (0.02) |
| | | | | | 361A -> 373A (0.05) |
| | | | | | 364A -> 373A (0.07) |
| | | | | | 367A -> 373A (0.01) |
| | | | | | 369A -> 373A (0.04) |
| | | | | | 343B -> 372B (0.14) |
| | | | | | 347B -> 372B (0.01) |
| | | | | | 356B -> 372B (0.08) |
| | | | | | 357B -> 372B (0.45) |
| | | | | | 364B -> 372B (0.02) |
| 367B -> 373B (0.01) | | | | | |
| 34 | 2.25 | 551 | 0.0561 | 0.994 | 361A -> 373A (0.04) |
| | | | | | 363A -> 373A (0.02) |
| | | | | | 364A -> 373A (0.08) |
| | | | | | 367A -> 373A (0.22) |
| | | | | | 369A -> 373A (0.16) |
| 343B -> 373B (0.02) | | | | | |

| | | | | | |
|----|------|-----|--------|-------|---------------------|
| | | | | | 344B -> 373B (0.06) |
| | | | | | 356B -> 372B (0.03) |
| | | | | | 363B -> 373B (0.02) |
| | | | | | 367B -> 373B (0.11) |
| | | | | | 368B -> 373B (0.14) |
| 37 | 2.29 | 541 | 0.0120 | 1.128 | 361A -> 373A (0.08) |
| | | | | | 363A -> 373A (0.03) |
| | | | | | 364A -> 373A (0.07) |
| | | | | | 369A -> 373A (0.01) |
| | | | | | 343B -> 372B (0.07) |
| | | | | | 343B -> 373B (0.04) |
| | | | | | 344B -> 372B (0.06) |
| | | | | | 345B -> 372B (0.01) |
| | | | | | 345B -> 373B (0.02) |
| | | | | | 352B -> 372B (0.04) |
| | | | | | 354B -> 373B (0.02) |
| | | | | | 356B -> 372B (0.02) |
| | | | | | 357B -> 372B (0.06) |
| | | | | | 364B -> 372B (0.06) |
| | | | | | 364B -> 373B (0.18) |
| | | | | | 368B -> 373B (0.02) |
| | | | | | 371B -> 373B (0.10) |
| 38 | 2.30 | 539 | 0.0163 | 1.224 | 361A -> 373A (0.29) |
| | | | | | 363A -> 373A (0.04) |
| | | | | | 364A -> 373A (0.13) |
| | | | | | 367A -> 373A (0.03) |
| | | | | | 369A -> 373A (0.12) |
| | | | | | 343B -> 373B (0.04) |
| | | | | | 344B -> 372B (0.02) |
| | | | | | 349B -> 372B (0.03) |
| | | | | | 352B -> 372B (0.01) |
| | | | | | 354B -> 372B (0.03) |
| | | | | | 356B -> 372B (0.04) |
| | | | | | 364B -> 372B (0.01) |
| | | | | | 364B -> 373B (0.06) |
| | | | | | 367B -> 373B (0.03) |
| | | | | | 368B -> 373B (0.04) |
| | | | | | 371B -> 373B (0.02) |
| 40 | 2.31 | 536 | 0.0130 | 1.337 | 356A -> 373A (0.02) |
| | | | | | 357A -> 373A (0.01) |
| | | | | | 361A -> 373A (0.19) |
| | | | | | 363A -> 373A (0.14) |
| | | | | | 367A -> 373A (0.10) |

| | | | | | |
|----|------|-----|--------|-------|---------------------|
| | | | | | 369A -> 373A (0.03) |
| | | | | | 344B -> 372B (0.09) |
| | | | | | 345B -> 372B (0.01) |
| | | | | | 347B -> 372B (0.01) |
| | | | | | 349B -> 372B (0.08) |
| | | | | | 352B -> 372B (0.02) |
| | | | | | 354B -> 372B (0.06) |
| | | | | | 356B -> 372B (0.08) |
| | | | | | 363B -> 372B (0.01) |
| | | | | | 364B -> 372B (0.04) |
| | | | | | 367B -> 372B (0.01) |
| 46 | 2.39 | 518 | 0.0172 | 1.864 | 352A -> 373A (0.02) |
| | | | | | 354A -> 373A (0.02) |
| | | | | | 356A -> 373A (0.02) |
| | | | | | 361A -> 373A (0.17) |
| | | | | | 363A -> 373A (0.53) |
| | | | | | 364A -> 373A (0.02) |
| | | | | | 369A -> 373A (0.02) |
| | | | | | 352B -> 372B (0.03) |
| | | | | | 368B -> 373B (0.11) |

Table S17. Excitation energies, absorption wavelengths, oscillator strengths, $\langle S^2 \rangle$ and configurations of the excited states of $[3]^+$. Up to 50 states are computed, and all excited states whose $\lambda > 300$ nm and $f > 0.01$ are presented. Orbital indices: α -HOMO = 420A, α -LUMO = 421A, β -HOMO = 419B, β -LUMO = 420B.

| root | E (eV) | λ (nm) | f | $\langle S^2 \rangle$ | configuration (weight) |
|------|--------|----------------|--------|-----------------------|------------------------|
| 6 | 1.25 | 991 | 0.0956 | 0.762 | 393B -> 420B (0.21) |
| | | | | | 396B -> 420B (0.06) |
| | | | | | 397B -> 420B (0.02) |
| | | | | | 399B -> 420B (0.29) |
| | | | | | 404B -> 420B (0.01) |
| | | | | | 409B -> 420B (0.04) |
| | | | | | 412B -> 420B (0.19) |
| | | | | | 415B -> 420B (0.01) |
| | | | | | 417B -> 420B (0.13) |
| | | | | | 418B -> 420B (0.01) |
| 8 | 1.44 | 861 | 0.0142 | 1.848 | 393A -> 421A (0.15) |
| | | | | | 396A -> 421A (0.03) |
| | | | | | 409A -> 421A (0.02) |
| | | | | | 391B -> 420B (0.07) |
| | | | | | 391B -> 421B (0.01) |
| | | | | | 392B -> 420B (0.03) |

| | | | | | |
|----|------|-----|--------|-------|---------------------|
| | | | | | 393B -> 421B (0.09) |
| | | | | | 396B -> 420B (0.02) |
| | | | | | 396B -> 421B (0.03) |
| | | | | | 399B -> 421B (0.11) |
| | | | | | 409B -> 420B (0.01) |
| | | | | | 409B -> 421B (0.01) |
| | | | | | 412B -> 420B (0.01) |
| | | | | | 412B -> 421B (0.05) |
| | | | | | 415B -> 420B (0.01) |
| | | | | | 417B -> 420B (0.21) |
| | | | | | 417B -> 421B (0.01) |
| | | | | | 418B -> 420B (0.08) |
| | | | | | 393A <- 421A (0.01) |
| 9 | 1.46 | 847 | 0.0264 | 1.014 | 393A -> 421A (0.03) |
| | | | | | 392B -> 420B (0.12) |
| | | | | | 393B -> 421B (0.02) |
| | | | | | 399B -> 421B (0.02) |
| | | | | | 412B -> 421B (0.01) |
| | | | | | 415B -> 420B (0.19) |
| | | | | | 417B -> 420B (0.01) |
| | | | | | 418B -> 420B (0.53) |
| 13 | 1.61 | 771 | 0.0129 | 0.792 | 391B -> 420B (0.01) |
| | | | | | 415B -> 420B (0.68) |
| | | | | | 417B -> 420B (0.02) |
| | | | | | 418B -> 420B (0.24) |
| 23 | 2.10 | 592 | 0.0165 | 1.521 | 409A -> 421A (0.01) |
| | | | | | 416A -> 421A (0.30) |
| | | | | | 417A -> 421A (0.04) |
| | | | | | 418A -> 421A (0.37) |
| | | | | | 419A -> 421A (0.02) |
| | | | | | 392B -> 421B (0.03) |
| | | | | | 415B -> 421B (0.03) |
| | | | | | 417B -> 421B (0.02) |
| | | | | | 418B -> 421B (0.12) |
| 25 | 2.11 | 587 | 0.0158 | 1.072 | 416A -> 421A (0.29) |
| | | | | | 417A -> 421A (0.05) |
| | | | | | 418A -> 421A (0.02) |
| | | | | | 392B -> 420B (0.02) |
| | | | | | 392B -> 421B (0.07) |
| | | | | | 409B -> 420B (0.01) |
| | | | | | 410B -> 420B (0.02) |
| | | | | | 415B -> 421B (0.09) |
| | | | | | 417B -> 421B (0.01) |

| | | | | | |
|----|------|-----|--------|-------|---------------------|
| | | | | | 418B -> 421B (0.35) |
| 26 | 2.13 | 583 | 0.0101 | 0.790 | 416A -> 421A (0.01) |
| | | | | | 417A -> 421A (0.01) |
| | | | | | 393B -> 420B (0.05) |
| | | | | | 396B -> 420B (0.01) |
| | | | | | 397B -> 420B (0.01) |
| | | | | | 399B -> 420B (0.12) |
| | | | | | 404B -> 420B (0.03) |
| | | | | | 407B -> 420B (0.11) |
| | | | | | 409B -> 420B (0.17) |
| | | | | | 412B -> 420B (0.40) |
| | | | | | 417B -> 421B (0.02) |
| 36 | 2.25 | 552 | 0.0116 | 0.856 | 416A -> 421A (0.02) |
| | | | | | 418A -> 421A (0.02) |
| | | | | | 391B -> 420B (0.09) |
| | | | | | 392B -> 420B (0.26) |
| | | | | | 396B -> 420B (0.06) |
| | | | | | 397B -> 420B (0.02) |
| | | | | | 399B -> 420B (0.01) |
| | | | | | 403B -> 420B (0.04) |
| | | | | | 404B -> 420B (0.13) |
| | | | | | 407B -> 420B (0.05) |
| | | | | | 409B -> 420B (0.15) |
| | | | | | 412B -> 420B (0.01) |
| | | | | | 415B -> 420B (0.01) |
| | | | | | 418B -> 420B (0.05) |
| 42 | 2.37 | 522 | 0.0323 | 0.980 | 393A -> 421A (0.07) |
| | | | | | 396A -> 421A (0.02) |
| | | | | | 409A -> 421A (0.09) |
| | | | | | 410A -> 421A (0.01) |
| | | | | | 412A -> 421A (0.04) |
| | | | | | 390B -> 420B (0.15) |
| | | | | | 391B -> 420B (0.06) |
| | | | | | 393B -> 421B (0.03) |
| | | | | | 396B -> 421B (0.01) |
| | | | | | 397B -> 420B (0.02) |
| | | | | | 399B -> 421B (0.04) |
| | | | | | 403B -> 420B (0.05) |
| | | | | | 409B -> 421B (0.01) |
| | | | | | 410B -> 421B (0.01) |
| | | | | | 412B -> 421B (0.17) |
| | | | | | 415B -> 421B (0.01) |
| | | | | | 417B -> 421B (0.09) |

| | | | | | |
|----|------|-----|--------|-------|--|
| 43 | 2.46 | 504 | 0.0145 | 2.348 | 392A -> 421A (0.09) 404A -> 421A (0.01) 407A -> 421A (0.05) 409A -> 421A (0.15) 410A -> 421A (0.09) 412A -> 421A (0.23) 390B -> 420B (0.03) 391B -> 421B (0.01) 392B -> 420B (0.03) 392B -> 421B (0.05) 407B -> 421B (0.01) 409B -> 421B (0.07) 412B -> 421B (0.02) 415B -> 421B (0.02) 417B -> 421B (0.03) 418B -> 421B (0.05) |
| 47 | 2.59 | 479 | 0.0368 | 1.244 | 392A -> 421A (0.01) 409A -> 421A (0.38) 412A -> 421A (0.02) 418A -> 421A (0.02) 391B -> 421B (0.03) 392B -> 421B (0.07) 407B -> 421B (0.03) 409B -> 421B (0.22) 412B -> 421B (0.09) 417B -> 421B (0.02) 418B -> 421B (0.01) |
| 48 | 2.60 | 477 | 0.0213 | 1.464 | 393A -> 421A (0.03) 409A -> 421A (0.14) 410A -> 421A (0.26) 412A -> 421A (0.17) 390B -> 420B (0.24) 397B -> 420B (0.04) 409B -> 421B (0.02) 410B -> 421B (0.02) |
| 50 | 2.65 | 467 | 0.0224 | 1.422 | 391A -> 421A (0.02) 392A -> 421A (0.01) 410A -> 421A (0.02) 412A -> 421A (0.03) 416A -> 421A (0.01) 390B -> 420B (0.06) 390B -> 421B (0.01) 391B -> 421B (0.07) |

392B -> 421B (0.03)
 397B -> 420B (0.01)
 404B -> 421B (0.01)
 407B -> 421B (0.07)
 409B -> 421B (0.03)
 410B -> 421B (0.52)
 418B -> 421B (0.01)

Table S18. Excitation energies, absorption wavelengths, oscillator strengths, $\langle S^2 \rangle$ and configurations of the excited states of $[4]^{+}$. Up to 50 states are computed, and all excited states whose $\lambda > 300$ nm and $f > 0.01$ are presented. Orbital indices: α -HOMO = 576A, α -LUMO = 577A, β -HOMO = 575B, β -LUMO = 576B.

| root | E (eV) | λ (nm) | f | $\langle S^2 \rangle$ | configuration (weight) |
|---------------------|--------|----------------|--------|-----------------------|------------------------|
| 8 | 1.54 | 807 | 0.0486 | 1.324 | 536A -> 577A (0.07) |
| | | | | | 569A -> 577A (0.01) |
| | | | | | 549B -> 576B (0.31) |
| | | | | | 549B -> 577B (0.09) |
| | | | | | 557B -> 576B (0.01) |
| | | | | | 567B -> 576B (0.02) |
| | | | | | 568B -> 576B (0.06) |
| | | | | | 570B -> 576B (0.18) |
| | | | | | 570B -> 577B (0.02) |
| | | | | | 571B -> 576B (0.04) |
| | | | | | 573B -> 576B (0.05) |
| | | | | | 9 |
| 541A -> 577A (0.04) | | | | | |
| 569A -> 577A (0.01) | | | | | |
| 571A -> 577A (0.02) | | | | | |
| 572A -> 577A (0.01) | | | | | |
| 576A -> 577A (0.02) | | | | | |
| 546B -> 576B (0.09) | | | | | |
| 546B -> 577B (0.03) | | | | | |
| 549B -> 576B (0.03) | | | | | |
| 549B -> 577B (0.15) | | | | | |
| 567B -> 576B (0.02) | | | | | |
| 568B -> 577B (0.01) | | | | | |
| 569B -> 576B (0.03) | | | | | |
| 570B -> 576B (0.11) | | | | | |
| 570B -> 577B (0.06) | | | | | |
| 571B -> 576B (0.05) | | | | | |
| 571B -> 577B (0.02) | | | | | |
| 572B -> 576B (0.03) | | | | | |

| | | | | | |
|----|------|-----|--------|-------|---------------------|
| | | | | | 573B -> 576B (0.04) |
| 14 | 1.78 | 695 | 0.0152 | 0.851 | 535B -> 576B (0.02) |
| | | | | | 549B -> 576B (0.02) |
| | | | | | 568B -> 576B (0.04) |
| | | | | | 569B -> 576B (0.04) |
| | | | | | 570B -> 576B (0.26) |
| | | | | | 571B -> 576B (0.03) |
| | | | | | 572B -> 576B (0.02) |
| | | | | | 573B -> 576B (0.42) |
| | | | | | 574B -> 576B (0.06) |
| 18 | 1.92 | 646 | 0.0155 | 1.968 | 534A -> 577A (0.01) |
| | | | | | 555A -> 577A (0.01) |
| | | | | | 570A -> 577A (0.04) |
| | | | | | 575A -> 577A (0.30) |
| | | | | | 576A -> 577A (0.45) |
| | | | | | 568B -> 576B (0.03) |
| | | | | | 570B -> 577B (0.01) |
| 21 | 1.99 | 623 | 0.0123 | 1.355 | 569A -> 577A (0.03) |
| | | | | | 570A -> 577A (0.03) |
| | | | | | 571A -> 577A (0.21) |
| | | | | | 572A -> 577A (0.05) |
| | | | | | 573A -> 577A (0.05) |
| | | | | | 575A -> 577A (0.01) |
| | | | | | 534B -> 577B (0.02) |
| | | | | | 549B -> 577B (0.02) |
| | | | | | 567B -> 577B (0.01) |
| | | | | | 569B -> 577B (0.02) |
| | | | | | 570B -> 577B (0.07) |
| | | | | | 573B -> 577B (0.02) |
| | | | | | 574B -> 577B (0.36) |
| 22 | 2.00 | 621 | 0.0191 | 1.110 | 570A -> 577A (0.05) |
| | | | | | 571A -> 577A (0.02) |
| | | | | | 572A -> 577A (0.07) |
| | | | | | 574A -> 577A (0.02) |
| | | | | | 576A -> 577A (0.01) |
| | | | | | 535B -> 576B (0.01) |
| | | | | | 546B -> 576B (0.05) |
| | | | | | 546B -> 577B (0.02) |
| | | | | | 563B -> 576B (0.02) |
| | | | | | 564B -> 576B (0.02) |
| | | | | | 566B -> 576B (0.03) |
| | | | | | 567B -> 576B (0.06) |
| | | | | | 568B -> 576B (0.03) |

| | | | | | |
|----|------|-----|--------|-------|---------------------|
| | | | | | 569B -> 576B (0.04) |
| | | | | | 570B -> 576B (0.03) |
| | | | | | 570B -> 577B (0.02) |
| | | | | | 572B -> 576B (0.07) |
| | | | | | 574B -> 577B (0.27) |
| | | | | | 575B -> 577B (0.05) |
| 23 | 2.01 | 617 | 0.0272 | 1.247 | 570A -> 577A (0.06) |
| | | | | | 571A -> 577A (0.12) |
| | | | | | 572A -> 577A (0.08) |
| | | | | | 573A -> 577A (0.06) |
| | | | | | 546B -> 576B (0.05) |
| | | | | | 558B -> 576B (0.01) |
| | | | | | 563B -> 576B (0.03) |
| | | | | | 567B -> 576B (0.15) |
| | | | | | 568B -> 576B (0.02) |
| | | | | | 570B -> 576B (0.04) |
| | | | | | 572B -> 576B (0.07) |
| | | | | | 573B -> 576B (0.03) |
| | | | | | 574B -> 577B (0.14) |
| 25 | 2.03 | 612 | 0.0113 | 1.755 | 563A -> 577A (0.05) |
| | | | | | 567A -> 577A (0.01) |
| | | | | | 569A -> 577A (0.01) |
| | | | | | 570A -> 577A (0.07) |
| | | | | | 572A -> 577A (0.15) |
| | | | | | 573A -> 577A (0.20) |
| | | | | | 574A -> 577A (0.02) |
| | | | | | 575A -> 577A (0.01) |
| | | | | | 571B -> 577B (0.06) |
| | | | | | 575B -> 577B (0.30) |
| 28 | 2.07 | 599 | 0.0193 | 1.648 | 536A -> 577A (0.01) |
| | | | | | 563A -> 577A (0.03) |
| | | | | | 569A -> 577A (0.07) |
| | | | | | 570A -> 577A (0.11) |
| | | | | | 571A -> 577A (0.01) |
| | | | | | 572A -> 577A (0.07) |
| | | | | | 573A -> 577A (0.13) |
| | | | | | 574A -> 577A (0.08) |
| | | | | | 549B -> 576B (0.01) |
| | | | | | 565B -> 576B (0.07) |
| | | | | | 566B -> 576B (0.12) |
| | | | | | 570B -> 576B (0.01) |
| | | | | | 570B -> 577B (0.02) |
| | | | | | 571B -> 577B (0.14) |

| | | | | | |
|----|------|-----|--------|-------|---------------------|
| 31 | 2.11 | 588 | 0.0135 | 1.488 | 573B -> 577B (0.02) |
| | | | | | 569A -> 577A (0.16) |
| | | | | | 535B -> 577B (0.01) |
| | | | | | 549B -> 576B (0.05) |
| | | | | | 563B -> 577B (0.01) |
| | | | | | 564B -> 576B (0.02) |
| | | | | | 565B -> 576B (0.05) |
| | | | | | 566B -> 577B (0.01) |
| | | | | | 567B -> 576B (0.03) |
| | | | | | 569B -> 576B (0.01) |
| | | | | | 569B -> 577B (0.04) |
| | | | | | 570B -> 576B (0.03) |
| | | | | | 570B -> 577B (0.02) |
| | | | | | 572B -> 577B (0.13) |
| | | | | | 573B -> 577B (0.29) |
| | | | | | 575B -> 577B (0.02) |
| 36 | 2.18 | 568 | 0.0171 | 1.651 | 536A -> 577A (0.02) |
| | | | | | 541A -> 577A (0.02) |
| | | | | | 564A -> 577A (0.01) |
| | | | | | 565A -> 577A (0.01) |
| | | | | | 567A -> 577A (0.06) |
| | | | | | 568A -> 577A (0.03) |
| | | | | | 570A -> 577A (0.03) |
| | | | | | 574A -> 577A (0.12) |
| | | | | | 535B -> 577B (0.03) |
| | | | | | 549B -> 576B (0.02) |
| | | | | | 565B -> 576B (0.01) |
| | | | | | 565B -> 577B (0.01) |
| | | | | | 567B -> 577B (0.03) |
| | | | | | 568B -> 576B (0.01) |
| | | | | | 568B -> 577B (0.14) |
| | | | | | 569B -> 577B (0.29) |
| | | | | | 572B -> 577B (0.02) |
| 38 | 2.23 | 557 | 0.0173 | 1.013 | 567A -> 577A (0.01) |
| | | | | | 574A -> 577A (0.04) |
| | | | | | 523B -> 576B (0.01) |
| | | | | | 534B -> 576B (0.01) |
| | | | | | 535B -> 576B (0.13) |
| | | | | | 546B -> 576B (0.06) |
| | | | | | 549B -> 577B (0.02) |
| | | | | | 564B -> 576B (0.28) |
| | | | | | 565B -> 576B (0.03) |
| | | | | | 565B -> 577B (0.01) |

| | | | | | |
|----|------|-----|--------|-------|---------------------|
| | | | | | 566B -> 576B (0.02) |
| | | | | | 566B -> 577B (0.01) |
| | | | | | 567B -> 576B (0.03) |
| | | | | | 567B -> 577B (0.03) |
| | | | | | 568B -> 577B (0.11) |
| | | | | | 573B -> 576B (0.01) |
| 40 | 2.25 | 552 | 0.0103 | 1.199 | 563A -> 577A (0.02) |
| | | | | | 566A -> 577A (0.09) |
| | | | | | 567A -> 577A (0.04) |
| | | | | | 568A -> 577A (0.35) |
| | | | | | 535B -> 576B (0.04) |
| | | | | | 546B -> 576B (0.01) |
| | | | | | 549B -> 577B (0.01) |
| | | | | | 564B -> 576B (0.17) |
| | | | | | 565B -> 577B (0.01) |
| | | | | | 566B -> 577B (0.02) |
| | | | | | 567B -> 576B (0.02) |
| | | | | | 567B -> 577B (0.02) |
| | | | | | 568B -> 577B (0.03) |
| | | | | | 569B -> 577B (0.02) |
| 41 | 2.29 | 541 | 0.0103 | 1.818 | 536A -> 577A (0.02) |
| | | | | | 565A -> 577A (0.02) |
| | | | | | 566A -> 577A (0.07) |
| | | | | | 567A -> 577A (0.07) |
| | | | | | 568A -> 577A (0.02) |
| | | | | | 535B -> 576B (0.09) |
| | | | | | 535B -> 577B (0.02) |
| | | | | | 546B -> 576B (0.01) |
| | | | | | 546B -> 577B (0.04) |
| | | | | | 549B -> 577B (0.01) |
| | | | | | 557B -> 576B (0.01) |
| | | | | | 563B -> 577B (0.02) |
| | | | | | 564B -> 576B (0.05) |
| | | | | | 564B -> 577B (0.02) |
| | | | | | 565B -> 576B (0.01) |
| | | | | | 566B -> 577B (0.06) |
| | | | | | 567B -> 577B (0.03) |
| | | | | | 570B -> 577B (0.10) |
| | | | | | 572B -> 577B (0.05) |
| | | | | | 573B -> 577B (0.05) |
| 43 | 2.33 | 532 | 0.0211 | 1.822 | 536A -> 577A (0.03) |
| | | | | | 564A -> 577A (0.03) |
| | | | | | 566A -> 577A (0.01) |

| | | | | | |
|----|------|-----|--------|-------|---------------------|
| | | | | | 567A -> 577A (0.09) |
| | | | | | 568A -> 577A (0.03) |
| | | | | | 573A -> 577A (0.01) |
| | | | | | 528B -> 577B (0.01) |
| | | | | | 535B -> 576B (0.03) |
| | | | | | 563B -> 577B (0.03) |
| | | | | | 564B -> 577B (0.05) |
| | | | | | 566B -> 577B (0.18) |
| | | | | | 567B -> 577B (0.29) |
| | | | | | 568B -> 577B (0.02) |
| 44 | 2.38 | 520 | 0.0234 | 1.937 | 565A -> 577A (0.50) |
| | | | | | 566A -> 577A (0.01) |
| | | | | | 569A -> 577A (0.02) |
| | | | | | 535B -> 576B (0.04) |
| | | | | | 549B -> 577B (0.02) |
| | | | | | 557B -> 576B (0.01) |
| | | | | | 563B -> 577B (0.01) |
| | | | | | 565B -> 577B (0.02) |
| | | | | | 566B -> 577B (0.11) |
| | | | | | 567B -> 577B (0.06) |
| | | | | | 568B -> 577B (0.03) |
| | | | | | 572B -> 577B (0.01) |
| | | | | | 573B -> 577B (0.02) |
| 50 | 2.50 | 497 | 0.0114 | 1.568 | 523B -> 577B (0.01) |
| | | | | | 535B -> 576B (0.03) |
| | | | | | 535B -> 577B (0.09) |
| | | | | | 549B -> 576B (0.01) |
| | | | | | 549B -> 577B (0.03) |
| | | | | | 553B -> 576B (0.02) |
| | | | | | 554B -> 576B (0.03) |
| | | | | | 557B -> 576B (0.02) |
| | | | | | 559B -> 576B (0.06) |
| | | | | | 560B -> 576B (0.01) |
| | | | | | 561B -> 576B (0.05) |
| | | | | | 562B -> 576B (0.01) |
| | | | | | 564B -> 577B (0.19) |
| | | | | | 565B -> 577B (0.23) |
| | | | | | 567B -> 577B (0.03) |
| | | | | | 573B -> 577B (0.02) |

Table S19. Excitation energies, absorption wavelengths, oscillator strengths, $\langle S^2 \rangle$ and configurations of the excited states of $[5]^+$. Up to 50 states are computed, and all excited states whose $\lambda > 300$ nm and $f >$

0.01 are presented. Orbital indices: α -HOMO = 516A, α -LUMO = 517A, β -HOMO = 515B, β -LUMO = 516B.

| root | E (eV) | λ (nm) | f | $\langle S^2 \rangle$ | configuration (weight) |
|---------------------|--------|----------------|--------|-----------------------|------------------------|
| 7 | 1.31 | 945 | 0.0556 | 0.786 | 477B -> 516B (0.26) |
| | | | | | 479B -> 516B (0.16) |
| | | | | | 481B -> 516B (0.07) |
| | | | | | 483B -> 516B (0.02) |
| | | | | | 489B -> 516B (0.03) |
| | | | | | 491B -> 516B (0.05) |
| | | | | | 493B -> 516B (0.01) |
| | | | | | 495B -> 516B (0.08) |
| | | | | | 498B -> 516B (0.03) |
| | | | | | 505B -> 516B (0.02) |
| | | | | | 511B -> 516B (0.06) |
| | | | | | 513B -> 516B (0.12) |
| | | | | | 514B -> 516B (0.02) |
| 9 | 1.49 | 832 | 0.0189 | 2.628 | 466A -> 517A (0.01) |
| | | | | | 467A -> 517A (0.01) |
| | | | | | 472A -> 517A (0.01) |
| | | | | | 477A -> 517A (0.25) |
| | | | | | 496A -> 517A (0.01) |
| | | | | | 511A -> 517A (0.02) |
| | | | | | 514A -> 517A (0.02) |
| | | | | | 477B -> 517B (0.17) |
| | | | | | 479B -> 517B (0.10) |
| | | | | | 481B -> 517B (0.04) |
| | | | | | 483B -> 517B (0.01) |
| | | | | | 489B -> 517B (0.02) |
| | | | | | 491B -> 517B (0.03) |
| 495B -> 517B (0.05) | | | | | |
| 498B -> 517B (0.02) | | | | | |
| 511B -> 517B (0.02) | | | | | |
| 513B -> 517B (0.04) | | | | | |
| 477A -> 517A (0.01) | | | | | |
| 10 | 1.73 | 718 | 0.0341 | 0.863 | 465B -> 516B (0.01) |
| | | | | | 475B -> 516B (0.03) |
| | | | | | 476B -> 516B (0.21) |
| | | | | | 498B -> 516B (0.01) |
| | | | | | 505B -> 516B (0.02) |
| | | | | | 507B -> 516B (0.09) |
| | | | | | 508B -> 516B (0.13) |
| 511B -> 516B (0.36) | | | | | |
| 514B -> 516B (0.05) | | | | | |

| | | | | | |
|----|------|-----|--------|-------|--|
| 12 | 1.80 | 690 | 0.0256 | 0.781 | 474B -> 516B (0.14) 476B -> 516B (0.01) 505B -> 516B (0.61) 508B -> 516B (0.12) 511B -> 516B (0.02) 514B -> 516B (0.04) |
| 19 | 1.92 | 646 | 0.0109 | 0.790 | 466B -> 516B (0.03) 474B -> 516B (0.03) 500B -> 516B (0.01) 505B -> 516B (0.05) 507B -> 516B (0.69) 511B -> 516B (0.12) 514B -> 516B (0.01) |
| 22 | 2.08 | 597 | 0.0130 | 1.372 | 464A -> 517A (0.03) 475A -> 517A (0.07) 476A -> 517A (0.01) 507A -> 517A (0.02) 509A -> 517A (0.04) 511A -> 517A (0.07) 463B -> 516B (0.04) 465B -> 516B (0.08) 469B -> 516B (0.01) 472B -> 516B (0.04) 475B -> 516B (0.05) 476B -> 516B (0.14) 476B -> 517B (0.02) 505B -> 516B (0.05) 507B -> 516B (0.02) 508B -> 516B (0.10) 511B -> 516B (0.09) 513B -> 516B (0.01) |
| 23 | 2.11 | 589 | 0.0409 | 1.122 | 464A -> 517A (0.01) 475A -> 517A (0.04) 477A -> 517A (0.04) 509A -> 517A (0.01) 514A -> 517A (0.04) 515A -> 517A (0.01) 463B -> 516B (0.07) 466B -> 516B (0.04) 474B -> 516B (0.18) 476B -> 516B (0.04) 476B -> 517B (0.03) 477B -> 517B (0.01) |

| | | | | | |
|----|------|-----|--------|-------|---------------------|
| | | | | | 479B -> 516B (0.01) |
| | | | | | 479B -> 517B (0.01) |
| | | | | | 481B -> 516B (0.02) |
| | | | | | 505B -> 516B (0.06) |
| | | | | | 507B -> 516B (0.09) |
| | | | | | 508B -> 516B (0.04) |
| | | | | | 511B -> 517B (0.04) |
| | | | | | 513B -> 516B (0.03) |
| | | | | | 513B -> 517B (0.01) |
| 24 | 2.19 | 567 | 0.0162 | 1.997 | 476A -> 517A (0.03) |
| | | | | | 509A -> 517A (0.01) |
| | | | | | 511A -> 517A (0.17) |
| | | | | | 514A -> 517A (0.04) |
| | | | | | 515A -> 517A (0.41) |
| | | | | | 463B -> 516B (0.01) |
| | | | | | 465B -> 516B (0.01) |
| | | | | | 472B -> 516B (0.01) |
| | | | | | 475B -> 516B (0.02) |
| | | | | | 476B -> 516B (0.03) |
| | | | | | 476B -> 517B (0.02) |
| | | | | | 511B -> 517B (0.01) |
| | | | | | 513B -> 517B (0.01) |
| | | | | | 514B -> 517B (0.04) |
| 25 | 2.19 | 566 | 0.0300 | 1.681 | 475A -> 517A (0.03) |
| | | | | | 507A -> 517A (0.08) |
| | | | | | 509A -> 517A (0.06) |
| | | | | | 511A -> 517A (0.07) |
| | | | | | 514A -> 517A (0.01) |
| | | | | | 515A -> 517A (0.37) |
| | | | | | 465B -> 516B (0.03) |
| | | | | | 466B -> 516B (0.01) |
| | | | | | 472B -> 516B (0.02) |
| | | | | | 474B -> 516B (0.06) |
| | | | | | 475B -> 516B (0.02) |
| | | | | | 476B -> 516B (0.03) |
| | | | | | 476B -> 517B (0.03) |
| | | | | | 508B -> 516B (0.02) |
| | | | | | 508B -> 517B (0.02) |
| | | | | | 511B -> 517B (0.01) |
| | | | | | 513B -> 517B (0.01) |
| 26 | 2.23 | 556 | 0.0976 | 1.239 | 477A -> 517A (0.02) |
| | | | | | 511A -> 517A (0.02) |
| | | | | | 514A -> 517A (0.10) |

| | | | | | |
|----|------|-----|--------|-------|---------------------|
| | | | | | 515A -> 517A (0.06) |
| | | | | | 462B -> 516B (0.02) |
| | | | | | 463B -> 516B (0.03) |
| | | | | | 465B -> 516B (0.01) |
| | | | | | 466B -> 516B (0.02) |
| | | | | | 474B -> 516B (0.19) |
| | | | | | 474B -> 517B (0.01) |
| | | | | | 475B -> 517B (0.02) |
| | | | | | 476B -> 517B (0.08) |
| | | | | | 477B -> 517B (0.01) |
| | | | | | 479B -> 517B (0.01) |
| | | | | | 505B -> 516B (0.01) |
| | | | | | 505B -> 517B (0.06) |
| | | | | | 507B -> 517B (0.04) |
| | | | | | 508B -> 517B (0.01) |
| | | | | | 511B -> 516B (0.01) |
| | | | | | 511B -> 517B (0.11) |
| | | | | | 513B -> 517B (0.03) |
| | | | | | 514B -> 517B (0.01) |
| 30 | 2.30 | 540 | 0.0130 | 1.402 | 509A -> 517A (0.02) |
| | | | | | 511A -> 517A (0.23) |
| | | | | | 514A -> 517A (0.12) |
| | | | | | 475B -> 517B (0.01) |
| | | | | | 476B -> 517B (0.03) |
| | | | | | 500B -> 517B (0.01) |
| | | | | | 511B -> 517B (0.08) |
| | | | | | 514B -> 517B (0.42) |
| 32 | 2.33 | 532 | 0.0153 | 1.413 | 467A -> 517A (0.01) |
| | | | | | 507A -> 517A (0.50) |
| | | | | | 509A -> 517A (0.07) |
| | | | | | 514A -> 517A (0.10) |
| | | | | | 515A -> 517A (0.02) |
| | | | | | 474B -> 517B (0.01) |
| | | | | | 475B -> 517B (0.01) |
| | | | | | 476B -> 517B (0.02) |
| | | | | | 500B -> 516B (0.01) |
| | | | | | 507B -> 517B (0.01) |
| | | | | | 508B -> 517B (0.06) |
| | | | | | 511B -> 517B (0.05) |
| | | | | | 513B -> 517B (0.02) |
| | | | | | 514B -> 517B (0.03) |
| 34 | 2.34 | 529 | 0.0178 | 2.134 | 463A -> 517A (0.01) |
| | | | | | 472A -> 517A (0.06) |

| | | | | | |
|----|------|-----|--------|-------|---------------------|
| | | | | | 505A -> 517A (0.27) |
| | | | | | 507A -> 517A (0.06) |
| | | | | | 509A -> 517A (0.22) |
| | | | | | 511A -> 517A (0.02) |
| | | | | | 514A -> 517A (0.06) |
| | | | | | 474B -> 517B (0.06) |
| | | | | | 500B -> 516B (0.10) |
| | | | | | 505B -> 517B (0.03) |
| | | | | | 507B -> 517B (0.02) |
| | | | | | 508B -> 517B (0.02) |
| 38 | 2.37 | 524 | 0.0186 | 1.758 | 477A -> 517A (0.01) |
| | | | | | 505A -> 517A (0.10) |
| | | | | | 507A -> 517A (0.21) |
| | | | | | 509A -> 517A (0.10) |
| | | | | | 511A -> 517A (0.13) |
| | | | | | 474B -> 517B (0.03) |
| | | | | | 505B -> 517B (0.05) |
| | | | | | 507B -> 517B (0.03) |
| | | | | | 508B -> 517B (0.05) |
| | | | | | 511B -> 517B (0.03) |
| | | | | | 513B -> 517B (0.07) |
| | | | | | 514B -> 517B (0.09) |
| 48 | 2.50 | 496 | 0.0206 | 1.017 | 462B -> 516B (0.04) |
| | | | | | 474B -> 517B (0.01) |
| | | | | | 476B -> 516B (0.04) |
| | | | | | 477B -> 516B (0.06) |
| | | | | | 479B -> 516B (0.07) |
| | | | | | 488B -> 516B (0.08) |
| | | | | | 489B -> 516B (0.02) |
| | | | | | 491B -> 516B (0.06) |
| | | | | | 493B -> 516B (0.17) |
| | | | | | 495B -> 516B (0.11) |
| | | | | | 498B -> 516B (0.01) |
| | | | | | 502B -> 516B (0.04) |
| | | | | | 505B -> 517B (0.04) |
| | | | | | 507B -> 517B (0.03) |
| | | | | | 508B -> 517B (0.03) |
| | | | | | 513B -> 517B (0.09) |
| | | | | | 514B -> 517B (0.01) |

Table S20. Excitation energies, absorption wavelengths, oscillator strengths, $\langle S^2 \rangle$ and configurations of the excited states of $[6]^{+}$. Up to 50 states are computed, and all excited states whose $\lambda > 300$ nm and $f >$

0.01 are presented. Orbital indices: α -HOMO = 564A, α -LUMO = 565A, β -HOMO = 563B, β -LUMO = 564B.

| root | E (eV) | λ (nm) | f | $\langle S^2 \rangle$ | configuration (weight) |
|---------------------|--------|----------------|--------|-----------------------|------------------------|
| 7 | 1.34 | 927 | 0.0695 | 0.830 | 537A -> 565A (0.01) |
| | | | | | 535B -> 564B (0.02) |
| | | | | | 537B -> 564B (0.32) |
| | | | | | 551B -> 564B (0.03) |
| | | | | | 553B -> 564B (0.17) |
| | | | | | 556B -> 564B (0.04) |
| | | | | | 557B -> 564B (0.03) |
| | | | | | 558B -> 564B (0.03) |
| | | | | | 561B -> 564B (0.03) |
| | | | | | 562B -> 564B (0.15) |
| | | | | | 563B -> 564B (0.05) |
| 10 | 1.70 | 730 | 0.0349 | 1.043 | 536A -> 565A (0.04) |
| | | | | | 537A -> 565A (0.04) |
| | | | | | 536B -> 564B (0.45) |
| | | | | | 536B -> 565B (0.01) |
| | | | | | 550B -> 564B (0.04) |
| | | | | | 554B -> 564B (0.02) |
| | | | | | 556B -> 564B (0.01) |
| | | | | | 557B -> 564B (0.02) |
| | | | | | 559B -> 564B (0.02) |
| | | | | | 560B -> 564B (0.17) |
| | | | | | 561B -> 564B (0.06) |
| 11 | 1.92 | 645 | 0.0376 | 0.819 | 535B -> 564B (0.30) |
| | | | | | 537B -> 564B (0.03) |
| | | | | | 544B -> 564B (0.01) |
| | | | | | 548B -> 564B (0.02) |
| | | | | | 550B -> 564B (0.05) |
| | | | | | 552B -> 564B (0.02) |
| | | | | | 553B -> 564B (0.11) |
| | | | | | 555B -> 564B (0.02) |
| | | | | | 556B -> 564B (0.03) |
| | | | | | 557B -> 564B (0.04) |
| | | | | | 558B -> 564B (0.01) |
| 560B -> 564B (0.03) | | | | | |
| 561B -> 564B (0.02) | | | | | |
| 562B -> 564B (0.15) | | | | | |
| 563B -> 564B (0.06) | | | | | |
| 12 | 2.04 | 607 | 0.0104 | 1.345 | 536A -> 565A (0.05) |
| | | | | | 537A -> 565A (0.03) |
| | | | | | 560A -> 565A (0.01) |

| | | | | | |
|----|------|-----|--------|-------|---------------------|
| | | | | | 561A -> 565A (0.01) |
| | | | | | 535B -> 564B (0.03) |
| | | | | | 535B -> 565B (0.02) |
| | | | | | 536B -> 565B (0.09) |
| | | | | | 556B -> 564B (0.02) |
| | | | | | 560B -> 565B (0.03) |
| | | | | | 561B -> 564B (0.28) |
| | | | | | 561B -> 565B (0.01) |
| | | | | | 562B -> 564B (0.23) |
| | | | | | 562B -> 565B (0.01) |
| | | | | | 563B -> 564B (0.04) |
| 17 | 2.25 | 550 | 0.0512 | 1.259 | 535A -> 565A (0.01) |
| | | | | | 537A -> 565A (0.02) |
| | | | | | 551A -> 565A (0.01) |
| | | | | | 562A -> 565A (0.05) |
| | | | | | 563A -> 565A (0.07) |
| | | | | | 534B -> 564B (0.01) |
| | | | | | 535B -> 565B (0.03) |
| | | | | | 536B -> 565B (0.09) |
| | | | | | 537B -> 565B (0.05) |
| | | | | | 544B -> 564B (0.02) |
| | | | | | 550B -> 564B (0.01) |
| | | | | | 550B -> 565B (0.02) |
| | | | | | 552B -> 564B (0.02) |
| | | | | | 553B -> 565B (0.04) |
| | | | | | 556B -> 565B (0.03) |
| | | | | | 557B -> 564B (0.27) |
| | | | | | 558B -> 565B (0.01) |
| | | | | | 559B -> 564B (0.01) |
| | | | | | 561B -> 565B (0.02) |
| | | | | | 562B -> 565B (0.01) |
| 23 | 2.37 | 524 | 0.0101 | 1.059 | 536A -> 565A (0.01) |
| | | | | | 560A -> 565A (0.02) |
| | | | | | 561A -> 565A (0.03) |
| | | | | | 562A -> 565A (0.10) |
| | | | | | 563A -> 565A (0.12) |
| | | | | | 564A -> 565A (0.01) |
| | | | | | 535B -> 564B (0.05) |
| | | | | | 535B -> 565B (0.02) |
| | | | | | 536B -> 564B (0.03) |
| | | | | | 536B -> 565B (0.01) |
| | | | | | 537B -> 564B (0.08) |
| | | | | | 540B -> 564B (0.02) |

| | | | | | |
|----|------|-----|--------|-------|---------------------|
| | | | | | 542B -> 564B (0.06) |
| | | | | | 547B -> 564B (0.02) |
| | | | | | 548B -> 564B (0.02) |
| | | | | | 549B -> 564B (0.01) |
| | | | | | 550B -> 565B (0.02) |
| | | | | | 551B -> 564B (0.01) |
| | | | | | 552B -> 564B (0.03) |
| | | | | | 553B -> 564B (0.02) |
| | | | | | 555B -> 564B (0.12) |
| | | | | | 557B -> 564B (0.01) |
| | | | | | 558B -> 564B (0.01) |
| | | | | | 560B -> 564B (0.05) |
| | | | | | 560B -> 565B (0.01) |
| 27 | 2.42 | 512 | 0.0300 | 1.692 | 536A -> 565A (0.03) |
| | | | | | 551A -> 565A (0.02) |
| | | | | | 558A -> 565A (0.05) |
| | | | | | 560A -> 565A (0.06) |
| | | | | | 561A -> 565A (0.34) |
| | | | | | 562A -> 565A (0.07) |
| | | | | | 535B -> 565B (0.01) |
| | | | | | 536B -> 564B (0.01) |
| | | | | | 542B -> 564B (0.02) |
| | | | | | 544B -> 564B (0.02) |
| | | | | | 551B -> 564B (0.06) |
| | | | | | 552B -> 564B (0.03) |
| | | | | | 553B -> 564B (0.02) |
| | | | | | 562B -> 565B (0.08) |
| | | | | | 563B -> 565B (0.02) |
| 30 | 2.47 | 503 | 0.0217 | 1.500 | 535A -> 565A (0.01) |
| | | | | | 537A -> 565A (0.01) |
| | | | | | 548A -> 565A (0.01) |
| | | | | | 549A -> 565A (0.01) |
| | | | | | 550A -> 565A (0.01) |
| | | | | | 551A -> 565A (0.03) |
| | | | | | 558A -> 565A (0.02) |
| | | | | | 559A -> 565A (0.17) |
| | | | | | 560A -> 565A (0.02) |
| | | | | | 561A -> 565A (0.13) |
| | | | | | 563A -> 565A (0.05) |
| | | | | | 534B -> 565B (0.01) |
| | | | | | 536B -> 565B (0.01) |
| | | | | | 542B -> 564B (0.01) |
| | | | | | 543B -> 564B (0.03) |

| | | | | | |
|----|------|-----|--------|-------|---------------------|
| | | | | | 544B -> 564B (0.01) |
| | | | | | 546B -> 564B (0.01) |
| | | | | | 552B -> 564B (0.04) |
| | | | | | 554B -> 564B (0.15) |
| | | | | | 556B -> 564B (0.03) |
| | | | | | 562B -> 565B (0.06) |
| | | | | | 563B -> 565B (0.02) |
| 32 | 2.50 | 497 | 0.0245 | 1.326 | 551A -> 565A (0.02) |
| | | | | | 558A -> 565A (0.02) |
| | | | | | 559A -> 565A (0.08) |
| | | | | | 560A -> 565A (0.22) |
| | | | | | 561A -> 565A (0.01) |
| | | | | | 563A -> 565A (0.01) |
| | | | | | 535B -> 564B (0.03) |
| | | | | | 538B -> 564B (0.03) |
| | | | | | 541B -> 564B (0.05) |
| | | | | | 543B -> 564B (0.11) |
| | | | | | 544B -> 564B (0.10) |
| | | | | | 546B -> 564B (0.05) |
| | | | | | 550B -> 564B (0.03) |
| | | | | | 562B -> 565B (0.05) |
| | | | | | 563B -> 565B (0.02) |
| 33 | 2.52 | 492 | 0.0301 | 1.311 | 536A -> 565A (0.03) |
| | | | | | 537A -> 565A (0.02) |
| | | | | | 551A -> 565A (0.14) |
| | | | | | 552A -> 565A (0.02) |
| | | | | | 557A -> 565A (0.06) |
| | | | | | 559A -> 565A (0.24) |
| | | | | | 561A -> 565A (0.06) |
| | | | | | 562A -> 565A (0.01) |
| | | | | | 563A -> 565A (0.02) |
| | | | | | 535B -> 564B (0.02) |
| | | | | | 535B -> 565B (0.01) |
| | | | | | 537B -> 564B (0.02) |
| | | | | | 538B -> 564B (0.02) |
| | | | | | 539B -> 564B (0.02) |
| | | | | | 541B -> 564B (0.01) |
| | | | | | 543B -> 564B (0.01) |
| | | | | | 544B -> 564B (0.02) |
| | | | | | 545B -> 564B (0.01) |
| | | | | | 546B -> 564B (0.03) |
| | | | | | 550B -> 564B (0.05) |
| | | | | | 553B -> 565B (0.02) |

| | | | | | |
|----|------|-----|--------|-------|---------------------|
| | | | | | 560B -> 565B (0.02) |
| 34 | 2.52 | 492 | 0.0464 | 1.054 | 551A -> 565A (0.01) |
| | | | | | 557A -> 565A (0.04) |
| | | | | | 560A -> 565A (0.10) |
| | | | | | 562A -> 565A (0.03) |
| | | | | | 535B -> 564B (0.03) |
| | | | | | 536B -> 564B (0.01) |
| | | | | | 538B -> 564B (0.05) |
| | | | | | 543B -> 564B (0.03) |
| | | | | | 544B -> 564B (0.01) |
| | | | | | 545B -> 564B (0.01) |
| | | | | | 546B -> 564B (0.03) |
| | | | | | 548B -> 564B (0.02) |
| | | | | | 549B -> 564B (0.01) |
| | | | | | 550B -> 564B (0.06) |
| | | | | | 551B -> 564B (0.06) |
| | | | | | 553B -> 564B (0.03) |
| | | | | | 553B -> 565B (0.01) |
| | | | | | 554B -> 564B (0.02) |
| | | | | | 556B -> 564B (0.02) |
| | | | | | 559B -> 565B (0.02) |
| | | | | | 560B -> 565B (0.04) |
| | | | | | 562B -> 565B (0.14) |
| | | | | | 563B -> 565B (0.06) |
| 39 | 2.57 | 482 | 0.0144 | 1.805 | 545A -> 565A (0.02) |
| | | | | | 551A -> 565A (0.03) |
| | | | | | 553A -> 565A (0.09) |
| | | | | | 554A -> 565A (0.07) |
| | | | | | 555A -> 565A (0.07) |
| | | | | | 556A -> 565A (0.04) |
| | | | | | 558A -> 565A (0.28) |
| | | | | | 559A -> 565A (0.15) |
| | | | | | 560A -> 565A (0.01) |
| | | | | | 561A -> 565A (0.04) |
| | | | | | 536B -> 564B (0.01) |
| | | | | | 539B -> 564B (0.02) |
| | | | | | 544B -> 564B (0.01) |
| 42 | 2.61 | 475 | 0.0111 | 1.335 | 535A -> 565A (0.02) |
| | | | | | 548A -> 565A (0.02) |
| | | | | | 549A -> 565A (0.01) |
| | | | | | 550A -> 565A (0.05) |
| | | | | | 551A -> 565A (0.03) |
| | | | | | 554A -> 565A (0.02) |

| | | | | | |
|----|------|-----|--------|-------|---------------------|
| | | | | | 556A -> 565A (0.03) |
| | | | | | 557A -> 565A (0.03) |
| | | | | | 558A -> 565A (0.06) |
| | | | | | 561A -> 565A (0.02) |
| | | | | | 534B -> 565B (0.01) |
| | | | | | 538B -> 564B (0.02) |
| | | | | | 542B -> 564B (0.03) |
| | | | | | 545B -> 564B (0.04) |
| | | | | | 547B -> 564B (0.01) |
| | | | | | 551B -> 564B (0.02) |
| | | | | | 553B -> 565B (0.03) |
| | | | | | 555B -> 565B (0.01) |
| | | | | | 556B -> 565B (0.01) |
| | | | | | 560B -> 565B (0.05) |
| | | | | | 561B -> 565B (0.31) |
| | | | | | 563B -> 565B (0.03) |
| 45 | 2.66 | 465 | 0.0163 | 1.737 | 535A -> 565A (0.01) |
| | | | | | 548A -> 565A (0.08) |
| | | | | | 549A -> 565A (0.02) |
| | | | | | 550A -> 565A (0.11) |
| | | | | | 552A -> 565A (0.02) |
| | | | | | 554A -> 565A (0.05) |
| | | | | | 555A -> 565A (0.02) |
| | | | | | 556A -> 565A (0.04) |
| | | | | | 557A -> 565A (0.08) |
| | | | | | 558A -> 565A (0.06) |
| | | | | | 540B -> 564B (0.02) |
| | | | | | 556B -> 565B (0.02) |
| | | | | | 557B -> 565B (0.02) |
| | | | | | 558B -> 565B (0.06) |
| | | | | | 559B -> 565B (0.23) |
| | | | | | 561B -> 565B (0.02) |
| | | | | | 563B -> 565B (0.02) |
| 48 | 2.69 | 461 | 0.0137 | 1.558 | 541A -> 565A (0.01) |
| | | | | | 548A -> 565A (0.05) |
| | | | | | 549A -> 565A (0.01) |
| | | | | | 550A -> 565A (0.08) |
| | | | | | 551A -> 565A (0.04) |
| | | | | | 552A -> 565A (0.04) |
| | | | | | 555A -> 565A (0.03) |
| | | | | | 560A -> 565A (0.02) |
| | | | | | 534B -> 565B (0.02) |
| | | | | | 535B -> 565B (0.05) |

536B -> 565B (0.02)
 550B -> 565B (0.02)
 552B -> 565B (0.05)
 553B -> 565B (0.02)
 554B -> 565B (0.01)
 557B -> 565B (0.18)
 559B -> 565B (0.08)
 560B -> 565B (0.07)
 562B -> 565B (0.04)
 563B -> 565B (0.01)

Table S21. Excitation energies, absorption wavelengths, oscillator strengths, $\langle S^2 \rangle$ and configurations of the excited states of [7]⁺. Up to 50 states are computed, and all excited states whose $\lambda > 300$ nm and $f > 0.01$ are presented. Orbital indices: α -HOMO = 756A, α -LUMO = 757A, β -HOMO = 755B, β -LUMO = 756B.

| root | E (eV) | λ (nm) | f | $\langle S^2 \rangle$ | configuration (weight) |
|------|--------|----------------|--------|-----------------------|------------------------|
| 9 | 1.58 | 785 | 0.1278 | 0.823 | 729B -> 756B (0.24) |
| | | | | | 740B -> 756B (0.09) |
| | | | | | 742B -> 756B (0.02) |
| | | | | | 743B -> 756B (0.03) |
| | | | | | 748B -> 756B (0.29) |
| | | | | | 749B -> 756B (0.10) |
| | | | | | 754B -> 756B (0.15) |
| | | | | | 754B -> 756B (0.15) |
| 12 | 2.08 | 597 | 0.0126 | 0.857 | 729A -> 757A (0.02) |
| | | | | | 740A -> 757A (0.01) |
| | | | | | 727B -> 756B (0.14) |
| | | | | | 728B -> 756B (0.20) |
| | | | | | 738B -> 756B (0.04) |
| | | | | | 740B -> 756B (0.01) |
| | | | | | 749B -> 756B (0.26) |
| | | | | | 749B -> 757B (0.02) |
| | | | | | 752B -> 756B (0.13) |
| | | | | | 754B -> 756B (0.06) |
| 13 | 2.20 | 563 | 0.0132 | 2.118 | 727A -> 757A (0.03) |
| | | | | | 729A -> 757A (0.02) |
| | | | | | 740A -> 757A (0.01) |
| | | | | | 743A -> 757A (0.01) |
| | | | | | 748A -> 757A (0.02) |
| | | | | | 750A -> 757A (0.02) |
| | | | | | 754A -> 757A (0.02) |
| | | | | | 726B -> 757B (0.03) |
| | | | | | 727B -> 757B (0.23) |
| | | | | | 727B -> 757B (0.23) |

| | | | | | |
|----|------|-----|--------|-------|---------------------|
| | | | | | 729B -> 757B (0.03) |
| | | | | | 738B -> 757B (0.05) |
| | | | | | 746B -> 757B (0.06) |
| | | | | | 748B -> 757B (0.01) |
| | | | | | 749B -> 756B (0.03) |
| | | | | | 749B -> 757B (0.15) |
| | | | | | 752B -> 757B (0.04) |
| | | | | | 754B -> 756B (0.10) |
| | | | | | 754B -> 757B (0.04) |
| 15 | 2.27 | 545 | 0.0508 | 1.325 | 728A -> 757A (0.06) |
| | | | | | 729A -> 757A (0.04) |
| | | | | | 740A -> 757A (0.03) |
| | | | | | 743A -> 757A (0.03) |
| | | | | | 748A -> 757A (0.03) |
| | | | | | 750A -> 757A (0.05) |
| | | | | | 752A -> 757A (0.04) |
| | | | | | 754A -> 757A (0.02) |
| | | | | | 726B -> 757B (0.03) |
| | | | | | 727B -> 756B (0.01) |
| | | | | | 727B -> 757B (0.09) |
| | | | | | 748B -> 756B (0.04) |
| | | | | | 754B -> 756B (0.14) |
| | | | | | 754B -> 757B (0.33) |
| 17 | 2.40 | 517 | 0.0963 | 0.999 | 727A -> 757A (0.01) |
| | | | | | 729A -> 757A (0.02) |
| | | | | | 752A -> 757A (0.49) |
| | | | | | 754A -> 757A (0.04) |
| | | | | | 728B -> 757B (0.04) |
| | | | | | 749B -> 757B (0.04) |
| | | | | | 752B -> 756B (0.06) |
| | | | | | 752B -> 757B (0.15) |
| | | | | | 754B -> 756B (0.02) |
| 19 | 2.43 | 511 | 0.0300 | 2.200 | 726A -> 757A (0.02) |
| | | | | | 728A -> 757A (0.01) |
| | | | | | 750A -> 757A (0.10) |
| | | | | | 754A -> 757A (0.48) |
| | | | | | 726B -> 757B (0.01) |
| | | | | | 748B -> 757B (0.01) |
| | | | | | 752B -> 757B (0.22) |
| | | | | | 754B -> 757B (0.05) |
| 20 | 2.45 | 506 | 0.0267 | 1.165 | 727A -> 757A (0.05) |
| | | | | | 728A -> 757A (0.04) |
| | | | | | 738A -> 757A (0.02) |

| | | | | | |
|----|------|-----|--------|-------|---------------------|
| | | | | | 746A -> 757A (0.02) |
| | | | | | 750A -> 757A (0.32) |
| | | | | | 752A -> 757A (0.02) |
| | | | | | 754A -> 757A (0.30) |
| | | | | | 727B -> 757B (0.01) |
| | | | | | 748B -> 757B (0.01) |
| | | | | | 749B -> 757B (0.04) |
| | | | | | 752B -> 757B (0.04) |
| | | | | | 754B -> 757B (0.07) |
| 26 | 2.54 | 488 | 0.0566 | 0.776 | 729A -> 757A (0.02) |
| | | | | | 740A -> 757A (0.02) |
| | | | | | 750A -> 757A (0.10) |
| | | | | | 752A -> 757A (0.04) |
| | | | | | 754A -> 757A (0.02) |
| | | | | | 726B -> 756B (0.05) |
| | | | | | 727B -> 756B (0.06) |
| | | | | | 728B -> 757B (0.01) |
| | | | | | 729B -> 756B (0.02) |
| | | | | | 736B -> 756B (0.03) |
| | | | | | 738B -> 756B (0.04) |
| | | | | | 740B -> 757B (0.02) |
| | | | | | 743B -> 756B (0.08) |
| | | | | | 746B -> 756B (0.16) |
| | | | | | 748B -> 756B (0.06) |
| | | | | | 748B -> 757B (0.04) |
| | | | | | 749B -> 757B (0.08) |
| | | | | | 752B -> 757B (0.04) |
| | | | | | 754B -> 756B (0.01) |
| | | | | | 754B -> 757B (0.02) |
| 32 | 2.66 | 467 | 0.0403 | 1.056 | 740A -> 757A (0.01) |
| | | | | | 742A -> 757A (0.02) |
| | | | | | 743A -> 757A (0.14) |
| | | | | | 746A -> 757A (0.02) |
| | | | | | 748A -> 757A (0.20) |
| | | | | | 752A -> 757A (0.02) |
| | | | | | 726B -> 757B (0.02) |
| | | | | | 727B -> 756B (0.01) |
| | | | | | 729B -> 756B (0.02) |
| | | | | | 738B -> 757B (0.04) |
| | | | | | 743B -> 756B (0.01) |
| | | | | | 743B -> 757B (0.09) |
| | | | | | 746B -> 756B (0.01) |
| | | | | | 746B -> 757B (0.16) |

| | | | | | |
|----|------|-----|--------|-------|---------------------|
| | | | | | 748B -> 757B (0.01) |
| | | | | | 749B -> 756B (0.02) |
| | | | | | 749B -> 757B (0.07) |
| | | | | | 752B -> 757B (0.03) |
| 33 | 2.67 | 464 | 0.0537 | 1.419 | 729A -> 757A (0.01) |
| | | | | | 740A -> 757A (0.03) |
| | | | | | 748A -> 757A (0.02) |
| | | | | | 722B -> 757B (0.01) |
| | | | | | 726B -> 756B (0.01) |
| | | | | | 726B -> 757B (0.01) |
| | | | | | 727B -> 756B (0.13) |
| | | | | | 727B -> 757B (0.03) |
| | | | | | 729B -> 756B (0.02) |
| | | | | | 736B -> 756B (0.03) |
| | | | | | 736B -> 757B (0.01) |
| | | | | | 738B -> 757B (0.02) |
| | | | | | 743B -> 757B (0.07) |
| | | | | | 746B -> 757B (0.05) |
| | | | | | 748B -> 757B (0.30) |
| | | | | | 749B -> 756B (0.02) |
| | | | | | 749B -> 757B (0.03) |
| | | | | | 752B -> 757B (0.02) |
| | | | | | 754B -> 757B (0.08) |
| 38 | 2.77 | 448 | 0.0149 | 1.189 | 738A -> 757A (0.05) |
| | | | | | 746A -> 757A (0.07) |
| | | | | | 748A -> 757A (0.02) |
| | | | | | 750A -> 757A (0.02) |
| | | | | | 726B -> 756B (0.04) |
| | | | | | 729B -> 756B (0.20) |
| | | | | | 731B -> 756B (0.01) |
| | | | | | 734B -> 756B (0.01) |
| | | | | | 738B -> 756B (0.18) |
| | | | | | 738B -> 757B (0.02) |
| | | | | | 742B -> 756B (0.05) |
| | | | | | 743B -> 756B (0.04) |
| | | | | | 746B -> 757B (0.01) |
| | | | | | 748B -> 756B (0.06) |
| | | | | | 749B -> 756B (0.07) |
| | | | | | 754B -> 756B (0.01) |
| 39 | 2.79 | 445 | 0.0151 | 1.584 | 726A -> 757A (0.02) |
| | | | | | 728A -> 757A (0.01) |
| | | | | | 738A -> 757A (0.10) |
| | | | | | 742A -> 757A (0.01) |

| | | | | | |
|----|------|-----|--------|-------|---------------------|
| | | | | | 746A -> 757A (0.24) |
| | | | | | 750A -> 757A (0.02) |
| | | | | | 726B -> 756B (0.04) |
| | | | | | 726B -> 757B (0.02) |
| | | | | | 727B -> 756B (0.05) |
| | | | | | 727B -> 757B (0.10) |
| | | | | | 729B -> 756B (0.03) |
| | | | | | 731B -> 756B (0.01) |
| | | | | | 736B -> 756B (0.06) |
| | | | | | 736B -> 757B (0.02) |
| | | | | | 738B -> 756B (0.04) |
| | | | | | 742B -> 756B (0.05) |
| | | | | | 748B -> 756B (0.01) |
| | | | | | 754B -> 757B (0.05) |
| 41 | 2.84 | 437 | 0.0910 | 0.852 | 728A -> 757A (0.01) |
| | | | | | 738A -> 757A (0.10) |
| | | | | | 740A -> 757A (0.20) |
| | | | | | 743A -> 757A (0.02) |
| | | | | | 750A -> 757A (0.02) |
| | | | | | 726B -> 756B (0.03) |
| | | | | | 726B -> 757B (0.01) |
| | | | | | 727B -> 756B (0.01) |
| | | | | | 728B -> 756B (0.03) |
| | | | | | 728B -> 757B (0.02) |
| | | | | | 736B -> 756B (0.06) |
| | | | | | 738B -> 757B (0.18) |
| | | | | | 740B -> 757B (0.11) |
| | | | | | 742B -> 756B (0.01) |
| | | | | | 743B -> 756B (0.01) |
| | | | | | 746B -> 756B (0.05) |
| | | | | | 748B -> 757B (0.02) |
| | | | | | 749B -> 756B (0.01) |
| | | | | | 749B -> 757B (0.03) |
| 42 | 2.87 | 432 | 0.0124 | 1.381 | 728A -> 757A (0.02) |
| | | | | | 729A -> 757A (0.01) |
| | | | | | 738A -> 757A (0.04) |
| | | | | | 740A -> 757A (0.08) |
| | | | | | 748A -> 757A (0.01) |
| | | | | | 752A -> 757A (0.01) |
| | | | | | 724B -> 756B (0.02) |
| | | | | | 726B -> 756B (0.03) |
| | | | | | 728B -> 756B (0.24) |
| | | | | | 728B -> 757B (0.04) |

| | | | | | |
|----|------|-----|--------|-------|---------------------|
| | | | | | 738B -> 756B (0.05) |
| | | | | | 740B -> 756B (0.06) |
| | | | | | 742B -> 756B (0.04) |
| | | | | | 743B -> 756B (0.02) |
| | | | | | 746B -> 756B (0.08) |
| | | | | | 746B -> 757B (0.03) |
| | | | | | 749B -> 756B (0.06) |
| | | | | | 749B -> 757B (0.01) |
| | | | | | 752B -> 756B (0.03) |
| | | | | | 752B -> 757B (0.01) |
| 44 | 2.89 | 429 | 0.0116 | 0.804 | 740A -> 757A (0.03) |
| | | | | | 724B -> 756B (0.02) |
| | | | | | 726B -> 756B (0.01) |
| | | | | | 727B -> 756B (0.06) |
| | | | | | 728B -> 756B (0.03) |
| | | | | | 731B -> 756B (0.02) |
| | | | | | 736B -> 756B (0.06) |
| | | | | | 738B -> 756B (0.03) |
| | | | | | 738B -> 757B (0.02) |
| | | | | | 740B -> 756B (0.03) |
| | | | | | 742B -> 756B (0.15) |
| | | | | | 743B -> 756B (0.22) |
| | | | | | 746B -> 756B (0.22) |
| | | | | | 748B -> 756B (0.02) |
| | | | | | 749B -> 756B (0.01) |
| 48 | 2.92 | 424 | 0.0192 | 1.927 | 727A -> 757A (0.02) |
| | | | | | 729A -> 757A (0.11) |
| | | | | | 734A -> 757A (0.03) |
| | | | | | 736A -> 757A (0.04) |
| | | | | | 738A -> 757A (0.02) |
| | | | | | 740A -> 757A (0.05) |
| | | | | | 743A -> 757A (0.11) |
| | | | | | 746A -> 757A (0.08) |
| | | | | | 748A -> 757A (0.09) |
| | | | | | 752A -> 757A (0.01) |
| | | | | | 727B -> 757B (0.05) |
| | | | | | 736B -> 756B (0.05) |
| | | | | | 738B -> 757B (0.09) |
| | | | | | 740B -> 757B (0.05) |
| | | | | | 742B -> 756B (0.01) |
| | | | | | 743B -> 756B (0.04) |
| | | | | | 746B -> 756B (0.02) |
| | | | | | 746B -> 757B (0.02) |

748B -> 757B (0.02)
 749B -> 756B (0.01)
 749B -> 757B (0.03)

Table S22. Excitation energies, absorption wavelengths, oscillator strengths, $\langle S^2 \rangle$ and configurations of the excited states of $[\mathbf{8}]^+$. Up to 50 states are computed, and all excited states whose $\lambda > 300$ nm and $f > 0.01$ are presented. Orbital indices: α -HOMO = 612A, α -LUMO = 613A, β -HOMO = 611B, β -LUMO = 612B.

| root | E (eV) | λ (nm) | f | $\langle S^2 \rangle$ | configuration (weight) |
|---------------------|--------|----------------|--------|-----------------------|------------------------|
| 8 | 1.40 | 883 | 0.0406 | 1.110 | 585A -> 613A (0.04) |
| | | | | | 585B -> 612B (0.62) |
| | | | | | 585B -> 613B (0.05) |
| | | | | | 592B -> 612B (0.06) |
| | | | | | 593B -> 612B (0.02) |
| | | | | | 596B -> 612B (0.03) |
| | | | | | 597B -> 612B (0.07) |
| | | | | | 604B -> 612B (0.03) |
| | | | | | 605B -> 612B (0.02) |
| | | | | | 9 |
| 585A -> 613A (0.31) | | | | | |
| 591A -> 613A (0.01) | | | | | |
| 582B -> 613B (0.01) | | | | | |
| 583B -> 613B (0.01) | | | | | |
| 585B -> 612B (0.08) | | | | | |
| 585B -> 613B (0.40) | | | | | |
| 592B -> 613B (0.03) | | | | | |
| 593B -> 613B (0.01) | | | | | |
| 596B -> 613B (0.02) | | | | | |
| 597B -> 613B (0.04) | | | | | |
| 604B -> 613B (0.02) | | | | | |
| 585A <- 613A (0.02) | | | | | |
| 585B <- 613B (0.02) | | | | | |
| 11 | 2.09 | 593 | 0.0405 | 0.829 | 584A -> 613A (0.03) |
| | | | | | 585A -> 613A (0.03) |
| | | | | | 583B -> 612B (0.39) |
| | | | | | 584B -> 612B (0.04) |
| | | | | | 585B -> 613B (0.01) |
| | | | | | 588B -> 612B (0.17) |
| | | | | | 593B -> 612B (0.02) |
| | | | | | 596B -> 612B (0.01) |
| | | | | | 600B -> 612B (0.01) |
| | | | | | 604B -> 612B (0.06) |

| | | | | | |
|----|------|-----|--------|-------|---------------------|
| | | | | | 605B -> 612B (0.10) |
| | | | | | 608B -> 612B (0.04) |
| 20 | 2.27 | 546 | 0.0146 | 0.820 | 585A -> 613A (0.03) |
| | | | | | 583B -> 612B (0.10) |
| | | | | | 584B -> 612B (0.02) |
| | | | | | 585B -> 612B (0.03) |
| | | | | | 585B -> 613B (0.02) |
| | | | | | 589B -> 612B (0.02) |
| | | | | | 605B -> 612B (0.63) |
| | | | | | 608B -> 612B (0.08) |
| 21 | 2.31 | 537 | 0.0333 | 1.095 | 585A -> 613A (0.10) |
| | | | | | 591A -> 613A (0.01) |
| | | | | | 582B -> 612B (0.19) |
| | | | | | 582B -> 613B (0.01) |
| | | | | | 583B -> 612B (0.04) |
| | | | | | 583B -> 613B (0.03) |
| | | | | | 584B -> 612B (0.07) |
| | | | | | 584B -> 613B (0.04) |
| | | | | | 585B -> 613B (0.09) |
| | | | | | 588B -> 612B (0.08) |
| | | | | | 588B -> 613B (0.02) |
| | | | | | 593B -> 613B (0.01) |
| | | | | | 596B -> 613B (0.01) |
| | | | | | 597B -> 613B (0.01) |
| | | | | | 602B -> 612B (0.10) |
| | | | | | 603B -> 612B (0.02) |
| | | | | | 604B -> 613B (0.02) |
| | | | | | 605B -> 612B (0.02) |
| | | | | | 605B -> 613B (0.01) |
| | | | | | 610B -> 612B (0.02) |
| 22 | 2.35 | 529 | 0.0138 | 0.904 | 585A -> 613A (0.02) |
| | | | | | 582B -> 612B (0.03) |
| | | | | | 583B -> 612B (0.02) |
| | | | | | 583B -> 613B (0.03) |
| | | | | | 584B -> 612B (0.02) |
| | | | | | 585B -> 613B (0.03) |
| | | | | | 588B -> 612B (0.02) |
| | | | | | 596B -> 612B (0.02) |
| | | | | | 600B -> 612B (0.04) |
| | | | | | 602B -> 612B (0.52) |
| | | | | | 603B -> 612B (0.09) |
| | | | | | 605B -> 612B (0.01) |
| | | | | | 608B -> 612B (0.01) |

| | | | | | |
|----|------|-----|--------|-------|---------------------|
| | | | | | 610B -> 612B (0.05) |
| 42 | 2.57 | 482 | 0.0129 | 1.627 | 588A -> 613A (0.01) |
| | | | | | 593A -> 613A (0.02) |
| | | | | | 606A -> 613A (0.71) |
| | | | | | 582B -> 612B (0.03) |
| | | | | | 589B -> 612B (0.02) |
| | | | | | 604B -> 613B (0.02) |
| | | | | | 608B -> 613B (0.02) |
| | | | | | 610B -> 613B (0.11) |
| 46 | 2.60 | 476 | 0.0241 | 1.011 | 606A -> 613A (0.03) |
| | | | | | 582B -> 613B (0.01) |
| | | | | | 583B -> 612B (0.03) |
| | | | | | 583B -> 613B (0.01) |
| | | | | | 584B -> 612B (0.02) |
| | | | | | 584B -> 613B (0.01) |
| | | | | | 585B -> 612B (0.07) |
| | | | | | 588B -> 612B (0.10) |
| | | | | | 589B -> 612B (0.16) |
| | | | | | 592B -> 612B (0.13) |
| | | | | | 593B -> 612B (0.06) |
| | | | | | 596B -> 612B (0.06) |
| | | | | | 604B -> 612B (0.01) |
| | | | | | 604B -> 613B (0.09) |
| | | | | | 605B -> 613B (0.01) |
| | | | | | 608B -> 613B (0.06) |
| 47 | 2.61 | 474 | 0.0188 | 1.702 | 584A -> 613A (0.05) |
| | | | | | 593A -> 613A (0.02) |
| | | | | | 604A -> 613A (0.02) |
| | | | | | 606A -> 613A (0.01) |
| | | | | | 582B -> 613B (0.05) |
| | | | | | 583B -> 612B (0.05) |
| | | | | | 588B -> 612B (0.12) |
| | | | | | 592B -> 612B (0.01) |
| | | | | | 593B -> 612B (0.01) |
| | | | | | 602B -> 613B (0.03) |
| | | | | | 604B -> 613B (0.40) |
| | | | | | 608B -> 613B (0.02) |
| | | | | | 610B -> 613B (0.07) |
| 49 | 2.64 | 470 | 0.0176 | 1.494 | 588A -> 613A (0.01) |
| | | | | | 589A -> 613A (0.02) |
| | | | | | 591A -> 613A (0.02) |
| | | | | | 593A -> 613A (0.03) |
| | | | | | 600A -> 613A (0.05) |

603A -> 613A (0.29)
 604A -> 613A (0.02)
 610A -> 613A (0.03)
 583B -> 612B (0.03)
 584B -> 613B (0.02)
 588B -> 612B (0.05)
 600B -> 613B (0.01)
 604B -> 613B (0.04)
 605B -> 613B (0.01)
 608B -> 613B (0.24)
 610B -> 613B (0.02)

2.6 Electronic Energies, Zero-Point Energies and Free Energies

This section contains a summary of the electronic energies (E), zero-point energies (ZPE) and free energies (G) of all computed boron clusters at the levels of (a) B3LYP-D3/def2-SVP (**Level I**) and (b) SMD-M06-2X/def2-TZVP//B3LYP-D3/def2-SVP (**Level II**) (**Table S23**). All reported ZPE and G (298 K, 1 mol/L) have included quasi-harmonic corrections. Note that the ZPE computed at **Level II** is identical to **Level I**.

We predicted the redox potential of Fc/Fc⁺ using energetics at both **Level II** and the SMD-M06/def2-TZVP//B3LYP-D3/def2-SVP (**Level III**) level of theory. The computed E, ZPE and G at all of the three levels (**Level I** through **III**) are tabulated in **Table S24**.

Table S23. Electronic energies, zero-point energies and free energies of all boron clusters at two levels of theory (see text for explanations). Results for the higher-energy conformation of **6** are presented in the second line of the corresponding entry.

| | Oxidation States | Level I | | | Level II | |
|----------|------------------|--------------|------------|--------------|--------------|--------------|
| | | E (a.u.) | ZPE (a.u.) | G (a.u.) | E (a.u.) | G (a.u.) |
| 1 | 2- | -2150.944231 | 0.906828 | -2150.128602 | -2152.404257 | -2151.588627 |
| | •- | -2150.955849 | 0.907704 | -2150.143124 | -2152.265304 | -2151.452579 |
| | 0 | -2150.855481 | 0.909662 | -2150.039725 | -2152.102944 | -2151.287188 |
| | •+ | -2150.615840 | 0.907938 | -2149.803309 | -2151.888836 | -2151.076306 |
| 2 | 0 | -4450.378687 | 1.552840 | -4448.957058 | -4452.959564 | -4451.537934 |
| | •+ | -4450.132969 | 1.551681 | -4448.713299 | -4452.728780 | -4451.309109 |
| 3 | 0 | -5640.289868 | 1.455944 | -5638.977686 | -5643.986668 | -5642.674486 |
| | •+ | -5640.032103 | 1.453380 | -5638.724843 | -5643.751674 | -5642.444415 |
| 4 | 0 | -35329.65626 | 1.430690 | -35328.38490 | -35336.14549 | -35334.87414 |
| | •+ | -35329.40572 | 1.429303 | -35328.13638 | -35335.91033 | -35334.64100 |
| 5 | 0 | -8016.734111 | 1.429070 | -8015.466426 | -8017.330241 | -8016.062556 |
| | •+ | -8016.480413 | 1.426333 | -8015.218309 | -8017.107592 | -8015.845488 |

| | | | | | | |
|----------|----|--------------|----------|--------------|--------------|--------------|
| 6 | 0 | -8491.951502 | 1.614683 | -8490.520668 | -8498.078042 | -8496.647208 |
| | | -8491.946769 | 1.614171 | -8490.517571 | | |
| | •+ | -8491.678218 | 1.612449 | -8490.251471 | -8497.839462 | -8496.412715 |
| 7 | 0 | -12533.53366 | 1.672728 | -12532.09686 | -12543.16600 | -12541.72920 |
| | •+ | -12533.25648 | 1.671333 | -12531.81918 | -12542.91722 | -12541.47992 |
| 8 | 0 | -10399.60183 | 1.070718 | -10398.71263 | -10407.68634 | -10406.79714 |
| | •+ | -10399.31341 | 1.066391 | -10398.43479 | -10407.43101 | -10406.55239 |

Table S24. Electronic energies, zero-point energies and free energies of the Fc/Fc⁺ reference electrode at three levels of theory (see text for explanations).

| | Level I | | | Level II | | Level III | |
|-----------------|--------------|------------|--------------|--------------|--------------|--------------|--------------|
| | E (a.u.) | ZPE (a.u.) | G (a.u.) | E (a.u.) | G (a.u.) | E (a.u.) | G (a.u.) |
| Fc | -1650.444598 | 0.169288 | -1650.306575 | -1650.714870 | -1650.576847 | -1650.613783 | -1650.475761 |
| Fc ⁺ | -1650.184627 | 0.169780 | -1650.047416 | -1650.518999 | -1650.381788 | -1650.430434 | -1650.293223 |

2.7 Full Reference for Gaussian 16, Revision C.01

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3. Reference

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4. Cartesian Coordinates of Optimized Structures

1

| | | | |
|---|-------------|-------------|-------------|
| O | -2.32250900 | 0.09489200 | -2.03502700 |
| O | -2.70013600 | 1.06230400 | 1.10091800 |
| O | -0.90686100 | 2.75198800 | -1.14790500 |
| O | -0.77246800 | -0.55884500 | 2.97928400 |
| O | 2.74293400 | -1.07271500 | -1.08233000 |
| O | 2.25307900 | 2.15826700 | -0.39461400 |
| O | 0.82435100 | 0.57248700 | -2.95226000 |
| O | 0.19222400 | 2.44630600 | 1.96267600 |
| O | -2.20724900 | -2.12921500 | 0.40744700 |
| O | -0.14228100 | -2.42519500 | -1.93678300 |
| O | 2.38901600 | -0.07598300 | 2.05475200 |
| O | 0.95040300 | -2.73593700 | 1.18357400 |
| H | -4.42121500 | 0.06889400 | -3.64177500 |
| H | -5.12615300 | 1.79959700 | 1.84499200 |
| H | -4.85025800 | -1.64676400 | -3.38343000 |
| H | -5.69509500 | 2.28830000 | 0.22263400 |
| H | -4.94114000 | -0.48586000 | -2.02954700 |
| H | -5.28406400 | 0.58220200 | 0.55251300 |
| H | -2.36015700 | -1.39928300 | -3.45571600 |
| H | -3.29779400 | 2.94465800 | 0.50994900 |
| H | -2.87470000 | -1.89798800 | -1.83393100 |
| H | -3.43891500 | 1.69119100 | -0.73711100 |
| H | -1.87305500 | 5.11396000 | -1.83264000 |
| H | -1.53488900 | -1.37073800 | 5.37607900 |
| H | -0.46714400 | 6.07003800 | -1.28174100 |
| H | 0.08438700 | -1.87760700 | 5.93721900 |
| H | -0.29012000 | 4.90364500 | -2.62205200 |
| H | -0.24392400 | -0.15994300 | 5.57635600 |
| H | -0.89962800 | 4.20290200 | 0.32344200 |
| H | -0.19758100 | -2.46759600 | 3.52370100 |
| H | 0.65128200 | 3.94978000 | -0.48336000 |
| H | 1.05472000 | -1.23563200 | 3.69419300 |
| H | 5.11042500 | -1.92547200 | -1.88952400 |
| H | 4.31062700 | 3.79643100 | -0.69372500 |
| H | 5.37463500 | -3.07787100 | -0.54940800 |
| H | 4.71476500 | 3.30021500 | -2.36190800 |
| H | 4.03711200 | -3.33595100 | -1.70437300 |
| H | 3.15169600 | 4.09120900 | -2.01512400 |
| H | 4.25797700 | -1.01156100 | 0.31768700 |
| H | 4.02330300 | 1.30004800 | -1.02225000 |

| | | | |
|---|-------------|-------------|-------------|
| H | 3.16504300 | -2.39135300 | 0.46600200 |
| H | 2.84569300 | 1.60297400 | -2.30526900 |
| H | 0.21806400 | 0.20403100 | -5.53688000 |
| H | -0.96574000 | 4.67833300 | 2.88654400 |
| H | -0.04013200 | 1.93547400 | -5.88837000 |
| H | -1.14849700 | 4.08273400 | 4.56003100 |
| H | 1.56743100 | 1.35464500 | -5.36803600 |
| H | 0.47894300 | 4.27723000 | 3.84771600 |
| H | -0.98516600 | 1.33245700 | -3.62466800 |
| H | -1.64814400 | 2.24433700 | 2.90040500 |
| H | 0.32697100 | 2.50674400 | -3.48102600 |
| H | -0.24345100 | 1.84947000 | 3.89342700 |
| H | -4.22186400 | -3.80709600 | 0.74446100 |
| H | -5.10112100 | -2.82468400 | 1.95120200 |
| H | -4.88551100 | -2.21753500 | 0.28579500 |
| H | -2.63616300 | -2.65389000 | 2.35477900 |
| H | -3.27925400 | -1.08174200 | 1.84625900 |
| H | -0.43323900 | -4.27766400 | -3.79674100 |
| H | 1.17223400 | -4.05670800 | -4.55037600 |
| H | 1.04272800 | -4.64246300 | -2.86864700 |
| H | 0.24380700 | -1.83561500 | -3.87913500 |
| H | 1.67596300 | -2.20064300 | -2.91136300 |
| H | 4.98756500 | 0.38268800 | 2.50519000 |
| H | 4.71901500 | 1.64769400 | 3.73653200 |
| H | 4.15387100 | -0.02240500 | 4.02655700 |
| H | 3.06030700 | 1.87574100 | 1.84568000 |
| H | 2.24768700 | 1.51064500 | 3.37257500 |
| H | 0.27833800 | -4.90490500 | 2.60645400 |
| H | 0.50902400 | -6.05612300 | 1.26134400 |
| H | 1.89189400 | -5.10843200 | 1.87937700 |
| H | -0.57589000 | -3.92806200 | 0.43998200 |
| H | 1.00868900 | -4.16942600 | -0.30323600 |
| C | -4.36832700 | -0.76754700 | -2.92741600 |
| C | -5.00191900 | 1.62577100 | 0.76467800 |
| C | -2.92904500 | -1.07860800 | -2.56444700 |
| C | -3.57087800 | 1.88803300 | 0.33586100 |
| C | -0.78651600 | 5.08435300 | -1.65546200 |
| C | -0.45389600 | -1.19435800 | 5.26145400 |
| C | -0.43503400 | 3.99898700 | -0.65708700 |
| C | -0.02354100 | -1.42005400 | 3.82548300 |
| C | 4.60578000 | -2.57036700 | -1.15318200 |
| C | 3.89860200 | 3.38101200 | -1.62671500 |
| C | 3.68610600 | -1.75497800 | -0.26559200 |

| | | | |
|---|-------------|-------------|-------------|
| C | 3.26999600 | 2.02381900 | -1.38075300 |
| C | 0.48270600 | 1.22713800 | -5.22648100 |
| C | -0.55976200 | 3.97947900 | 3.63484600 |
| C | 0.09651700 | 1.46918500 | -3.78069200 |
| C | -0.61494300 | 2.55211300 | 3.12689900 |
| C | -4.40300700 | -2.78083200 | 1.10037100 |
| C | -3.10467600 | -2.11413000 | 1.51215900 |
| C | 0.60423300 | -3.95777600 | -3.61183500 |
| C | 0.64393800 | -2.52570100 | -3.11564900 |
| C | 4.27831400 | 0.75804700 | 3.25962400 |
| C | 2.94712600 | 1.10270100 | 2.62184000 |
| C | 0.81340000 | -5.07504300 | 1.65884700 |
| C | 0.50227700 | -3.97861000 | 0.65932600 |
| B | -1.26929800 | 0.05837000 | -1.13213300 |
| B | -1.47977300 | 0.60344300 | 0.62479800 |
| B | -0.50155700 | 1.53255000 | -0.62370400 |
| B | -0.42415200 | -0.31188100 | 1.65804200 |
| B | 1.53901800 | -0.58447700 | -0.59632100 |
| B | 1.26413200 | 1.20268000 | -0.20689800 |
| B | 0.48077100 | 0.32979200 | -1.62747200 |
| B | 0.13204500 | 1.35687500 | 1.10162600 |
| B | -1.20714500 | -1.18429400 | 0.23530400 |
| B | -0.07334700 | -1.33980900 | -1.07301500 |
| B | 1.32819500 | -0.04216900 | 1.16008600 |
| B | 0.55652700 | -1.51305900 | 0.65327800 |

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|---|-------------|-------------|-------------|
| B | 1.47116300 | 0.83569700 | 0.38015800 |
| B | 0.92257300 | 0.57455700 | -1.35417500 |
| B | 1.46034400 | -0.85725700 | -0.37486200 |
| B | 0.95584800 | -0.50942300 | 1.35739400 |
| B | -0.03998400 | 1.08582600 | 1.35469200 |
| B | 0.01290400 | 1.69265800 | -0.37839100 |
| O | 2.61843400 | 1.59873600 | 0.57241800 |
| C | 3.76806900 | 1.08442100 | 1.21139800 |
| H | 4.03386500 | 0.10912600 | 0.77578800 |
| H | 3.55419800 | 0.90500900 | 2.28036400 |
| C | 4.92487500 | 2.03841100 | 1.07648300 |
| C | 4.73275300 | 3.37453500 | 0.71185100 |
| H | 3.72146800 | 3.73842900 | 0.53605800 |
| C | 5.82617800 | 4.23506700 | 0.58413600 |
| H | 5.65999300 | 5.27683700 | 0.29914900 |
| C | 7.12159800 | 3.77251100 | 0.83074100 |

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|---|------------|-------------|-------------|
| H | 7.97598300 | 4.44597000 | 0.72875800 |
| C | 7.31751100 | 2.44030500 | 1.21161400 |
| H | 8.32667900 | 2.06839600 | 1.40519100 |
| C | 6.22496700 | 1.57995400 | 1.32949200 |
| H | 6.38296400 | 0.53289000 | 1.60432500 |
| O | 1.56936200 | 1.03016300 | -2.48588600 |
| C | 2.34289200 | 0.22277200 | -3.35575000 |
| H | 2.17117500 | 0.61821000 | -4.37268800 |
| H | 1.97400900 | -0.81343100 | -3.34593100 |
| C | 3.82435000 | 0.25766900 | -3.06214300 |
| C | 4.39731300 | 1.27611900 | -2.29361400 |
| H | 3.75574400 | 2.02723700 | -1.83424100 |
| C | 5.78089800 | 1.31824200 | -2.09822300 |
| H | 6.21467700 | 2.11631900 | -1.49463800 |
| C | 6.60166500 | 0.34216200 | -2.66835700 |
| H | 7.68214200 | 0.37386100 | -2.50923300 |
| C | 6.03287600 | -0.68296400 | -3.42984400 |
| H | 6.66415000 | -1.46501000 | -3.85752200 |
| C | 4.65197700 | -0.72431800 | -3.62339000 |
| H | 4.21094600 | -1.53599100 | -4.20921500 |
| O | 2.69620200 | -1.46816100 | -0.56231000 |
| C | 2.83114500 | -2.72176500 | -1.19809500 |
| H | 2.56069900 | -2.63277300 | -2.26555300 |
| H | 2.12805800 | -3.44381900 | -0.75483700 |
| C | 4.24100200 | -3.23441700 | -1.07007100 |
| C | 5.29460200 | -2.39299800 | -0.70019800 |
| H | 5.09469900 | -1.33800600 | -0.51846400 |
| C | 6.59119200 | -2.89884500 | -0.57621900 |
| H | 7.40436300 | -2.22845400 | -0.28738900 |
| C | 6.85040500 | -4.24792800 | -0.83193900 |
| H | 7.86441900 | -4.64274500 | -0.73287200 |
| C | 5.80217000 | -5.09047400 | -1.21887100 |
| H | 5.99429900 | -6.14724900 | -1.42022500 |
| C | 4.50623100 | -4.58534900 | -1.33307000 |
| H | 3.68442000 | -5.25118100 | -1.61262200 |
| O | 1.67196200 | -0.84004500 | 2.49095200 |
| C | 1.36071200 | -1.91479700 | 3.35980500 |
| H | 0.27888000 | -2.11380700 | 3.35081600 |
| H | 1.61829300 | -1.56936300 | 4.37680300 |
| C | 2.13227300 | -3.17972800 | 3.06476200 |
| C | 1.69517300 | -4.38878400 | 3.62273200 |
| H | 0.77036400 | -4.41442500 | 4.20631800 |
| C | 2.42288800 | -5.56310800 | 3.42894200 |

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| H | 2.06096300 | -6.50182900 | 3.85415600 |
| C | 3.59725800 | -5.54082900 | 2.67090600 |
| H | 4.16636400 | -6.45989600 | 2.51213500 |
| C | 4.03285100 | -4.34054500 | 2.10419300 |
| H | 4.94305500 | -4.31513100 | 1.50390300 |
| C | 3.30281600 | -3.16443400 | 2.29936700 |
| H | 3.63273700 | -2.23217000 | 1.84242300 |
| O | -0.11435300 | 1.87485400 | 2.48560800 |
| C | 0.96905900 | 2.14219800 | 3.35844500 |
| H | 1.68107700 | 1.30373400 | 3.35341800 |
| H | 0.53726300 | 2.19465200 | 4.37373700 |
| C | 1.68200900 | 3.44126500 | 3.06405200 |
| C | 1.08659300 | 4.44831300 | 2.29751000 |
| H | 0.11378900 | 4.27034500 | 1.84051700 |
| C | 1.74385100 | 5.66638900 | 2.10099200 |
| H | 1.26955500 | 6.44242600 | 1.49910400 |
| C | 3.00143500 | 5.88638900 | 2.66814300 |
| H | 3.51573700 | 6.83702100 | 2.50820800 |
| C | 3.60452200 | 4.87978400 | 3.42795200 |
| H | 4.59858000 | 5.03352500 | 3.85365600 |
| C | 2.94791000 | 3.66433900 | 3.62262200 |
| H | 3.43009200 | 2.87543700 | 4.20713500 |
| O | -0.07320800 | 3.06832800 | -0.56821600 |
| C | 0.94860800 | 3.80744800 | -1.20377100 |
| H | 1.00313700 | 3.53129300 | -2.27211700 |
| H | 1.92462900 | 3.55239200 | -0.76304900 |
| C | 0.69778600 | 5.28603500 | -1.07182400 |
| C | 1.74250400 | 6.18426900 | -1.32928500 |
| H | 2.72811800 | 5.79892700 | -1.60664000 |
| C | 1.54164400 | 7.56037500 | -1.21245300 |
| H | 2.36646100 | 8.24963500 | -1.40947000 |
| C | 0.29017100 | 8.05505700 | -0.82844800 |
| H | 0.13251700 | 9.13155100 | -0.72731900 |
| C | -0.75577600 | 7.16295000 | -0.57776400 |
| H | -1.74088600 | 7.53858900 | -0.29043700 |
| C | -0.55516200 | 5.78591500 | -0.70422200 |
| H | -1.37414600 | 5.09065500 | -0.52553400 |
| B | -0.92258800 | -0.57444600 | 1.35418300 |
| B | -1.47112200 | -0.83580600 | -0.38017600 |
| B | -1.46034900 | 0.85723100 | 0.37477600 |
| B | -0.95591900 | 0.50936200 | -1.35738700 |
| B | 0.04001000 | -1.08579000 | -1.35475200 |
| B | -0.01291900 | -1.69268400 | 0.37845500 |

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| O | -2.61831900 | -1.59896700 | -0.57235600 |
| C | -3.76793600 | -1.08515200 | -1.21176300 |
| H | -4.03380000 | -0.10958300 | -0.77681000 |
| H | -3.55396400 | -0.90639300 | -2.28081900 |
| C | -4.92473100 | -2.03909300 | -1.07619000 |
| C | -4.73254800 | -3.37489700 | -0.71040400 |
| H | -3.72125800 | -3.73857600 | -0.53421100 |
| C | -5.82593300 | -4.23536000 | -0.58191200 |
| H | -5.65968700 | -5.27685900 | -0.29597500 |
| C | -7.12137400 | -3.77307100 | -0.82891900 |
| H | -7.97573300 | -4.44646600 | -0.72630200 |
| C | -7.31735700 | -2.44120600 | -1.21094600 |
| H | -8.32654800 | -2.06950000 | -1.40479800 |
| C | -6.22485400 | -1.58089600 | -1.32953200 |
| H | -6.38291000 | -0.53405600 | -1.60518600 |
| O | -1.56955800 | -1.02966500 | 2.48591900 |
| C | -2.34222000 | -0.22120700 | 3.35552800 |
| H | -2.17037000 | -0.61576700 | 4.37279000 |
| H | -1.97246000 | 0.81467200 | 3.34466300 |
| C | -3.82384300 | -0.25480200 | 3.06261700 |
| C | -4.39843800 | -1.27313700 | 2.29516600 |
| H | -3.75807800 | -2.02556200 | 1.83628500 |
| C | -5.78217400 | -1.31359500 | 2.10038700 |
| H | -6.21727100 | -2.11169300 | 1.49778000 |
| C | -6.60140200 | -0.33586900 | 2.66989900 |
| H | -7.68198500 | -0.36627400 | 2.51123200 |
| C | -6.03094100 | 0.68918100 | 3.43025600 |
| H | -6.66098400 | 1.47248200 | 3.85745600 |
| C | -4.64994000 | 0.72877500 | 3.62333800 |
| H | -4.20758000 | 1.54041400 | 4.20821900 |
| O | 0.07332400 | -3.06829200 | 0.56869200 |
| C | -0.94845200 | -3.80744100 | 1.20433000 |
| H | -1.00370200 | -3.53014700 | 2.27234700 |
| H | -1.92440600 | -3.55357500 | 0.76282500 |
| C | -0.69624800 | -5.28597700 | 1.07451500 |
| C | -1.74072800 | -6.18480200 | 1.33082200 |
| H | -2.72735900 | -5.79997200 | 1.60525200 |
| C | -1.53825400 | -7.56090800 | 1.21667000 |
| H | -2.36287400 | -8.25065400 | 1.41280800 |
| C | -0.28537700 | -8.05499000 | 0.83651500 |
| H | -0.12643200 | -9.13149400 | 0.73751000 |
| C | 0.76033900 | -7.16226900 | 0.58698600 |
| H | 1.74652000 | -7.53742000 | 0.30270000 |

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| C | 0.55811100 | -5.78523300 | 0.71082700 |
| H | 1.37691000 | -5.08948500 | 0.53316200 |
| O | 0.11454000 | -1.87473800 | -2.48571000 |
| C | -0.96844800 | -2.14188900 | -3.35914200 |
| H | -1.68117900 | -1.30404400 | -3.35338700 |
| H | -0.53629600 | -2.19275700 | -4.37437000 |
| C | -1.68026100 | -3.44199500 | -3.06666600 |
| C | -1.08432500 | -4.44916600 | -2.30069700 |
| H | -0.11215900 | -4.27054000 | -1.84261500 |
| C | -1.74026900 | -5.66822100 | -2.10615600 |
| H | -1.26560600 | -6.44433500 | -1.50467200 |
| C | -2.99701700 | -5.88911100 | -2.67479200 |
| H | -3.51028800 | -6.84055200 | -2.51644000 |
| C | -3.60062200 | -4.88241000 | -3.43404100 |
| H | -4.59406200 | -5.03689300 | -3.86090900 |
| C | -2.94535800 | -3.66595800 | -3.62668000 |
| H | -3.42794100 | -2.87701500 | -4.21079800 |
| O | -2.69636600 | 1.46793800 | 0.56175300 |
| C | -2.83214200 | 2.72181500 | 1.19672600 |
| H | -2.56197400 | 2.63409800 | 2.26435300 |
| H | -2.12924600 | 3.44377800 | 0.75295200 |
| C | -4.24211600 | 3.23381300 | 1.06717600 |
| C | -5.29505100 | 2.39187500 | 0.69657400 |
| H | -5.09473300 | 1.33673600 | 0.51615600 |
| C | -6.59155700 | 2.89738100 | 0.57022700 |
| H | -7.40418400 | 2.22656800 | 0.28085200 |
| C | -6.85136000 | 4.24665900 | 0.82425100 |
| H | -7.86528800 | 4.64122800 | 0.72330200 |
| C | -5.80380900 | 5.08974800 | 1.21189300 |
| H | -5.99639300 | 6.14669200 | 1.41192200 |
| C | -4.50796400 | 4.58494800 | 1.32854100 |
| H | -3.68666200 | 5.25121400 | 1.60857300 |
| O | -1.67243100 | 0.83997400 | -2.49070000 |
| C | -1.36273300 | 1.91547000 | -3.35913900 |
| H | -0.28115300 | 2.11589000 | -3.35050800 |
| H | -1.62030900 | 1.57018100 | -4.37618800 |
| C | -2.13601400 | 3.17915700 | -3.06312700 |
| C | -1.70223100 | 4.38879100 | -3.62244100 |
| H | -0.77865400 | 4.41588800 | -4.20790800 |
| C | -2.43170300 | 5.56185800 | -3.42765500 |
| H | -2.07235900 | 6.50106500 | -3.85398600 |
| C | -3.60441400 | 5.53779100 | -2.66710100 |
| H | -4.17481300 | 6.45591200 | -2.50750200 |

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| C | -4.03664000 | 4.33696400 | -2.09896300 |
| H | -4.94547800 | 4.31013400 | -1.49663700 |
| C | -3.30496200 | 3.16206100 | -2.29533300 |
| H | -3.63228600 | 2.22939300 | -1.83735900 |

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|---|-------------|-------------|-------------|
| B | 1.09438300 | 0.06809800 | 1.35025800 |
| O | 1.85375600 | 0.24800100 | 2.48179200 |
| C | 2.36569100 | -0.81741200 | 3.28066100 |
| H | 1.80075000 | -1.74090200 | 3.10227000 |
| H | 2.20024800 | -0.51360400 | 4.32830200 |
| C | 3.83731600 | -1.04002700 | 3.03289800 |
| C | 4.72876800 | 0.04284700 | 3.00004700 |
| H | 4.34768100 | 1.05685900 | 3.13876100 |
| C | 6.09042200 | -0.15639800 | 2.77858500 |
| H | 6.79406600 | 0.67511400 | 2.73358700 |
| C | 6.55618500 | -1.45415300 | 2.58274200 |
| C | 5.69887500 | -2.54934000 | 2.61224500 |
| H | 6.09441100 | -3.55180900 | 2.44229800 |
| C | 4.33777800 | -2.33257400 | 2.84036300 |
| H | 3.65522700 | -3.18328800 | 2.84281200 |
| F | 7.86239500 | -1.65008000 | 2.34842300 |
| B | 0.74616600 | 1.52161800 | 0.38444200 |
| O | 1.30200200 | 2.78132900 | 0.63716100 |
| C | 2.69641200 | 2.99852600 | 0.58984300 |
| H | 3.10587200 | 2.56810800 | -0.33463300 |
| H | 3.19009100 | 2.47418700 | 1.42783800 |
| C | 3.02864400 | 4.46705800 | 0.61492700 |
| C | 4.35751800 | 4.86399700 | 0.82365200 |
| H | 5.11995900 | 4.10903700 | 1.03542800 |
| C | 4.72936900 | 6.20537700 | 0.74708500 |
| H | 5.76263000 | 6.52473600 | 0.88956200 |
| C | 3.75122500 | 7.15789700 | 0.46939900 |
| C | 2.42178200 | 6.79672400 | 0.27415300 |
| H | 1.68154400 | 7.57082400 | 0.06231100 |
| C | 2.07003300 | 5.44639200 | 0.34043400 |
| H | 1.04046800 | 5.14371900 | 0.16962900 |
| F | 4.09876000 | 8.45085600 | 0.39233500 |
| B | -0.49109000 | -0.97679000 | 1.35307200 |
| B | -0.60299500 | 0.91849700 | 1.34789000 |
| B | 0.60356000 | -0.91851700 | -1.34553600 |
| B | -1.09387400 | -0.06821100 | -1.34780800 |
| B | 0.49155600 | 0.97677100 | -1.35070500 |

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| O | -1.13537800 | 1.49118500 | 2.47843300 |
| O | -0.71876800 | -1.71942400 | 2.48700100 |
| O | 1.13623200 | -1.49099500 | -2.47599000 |
| O | -1.85311700 | -0.24855600 | -2.47930800 |
| O | 0.71893500 | 1.71941000 | -2.48462700 |
| C | -0.46591800 | 2.46766700 | 3.27454400 |
| C | -1.89882600 | -1.62535800 | 3.28324200 |
| C | 0.46803900 | -2.46859200 | -3.27173000 |
| C | -2.36741900 | 0.81642400 | -3.27725600 |
| C | 1.89901500 | 1.62585200 | -3.28087800 |
| H | 0.61585800 | 2.43934400 | 3.09343700 |
| H | -2.41305100 | -0.67319100 | 3.10215400 |
| H | -0.61356600 | -2.44308300 | -3.08926200 |
| H | -1.80538600 | 1.74135100 | -3.09717400 |
| H | 2.41517000 | 0.67513800 | -3.09772400 |
| H | -0.64368400 | 2.17371200 | 4.32298000 |
| H | -1.55509000 | -1.63309200 | 4.33157300 |
| H | 0.64377600 | -2.17370300 | -4.32025200 |
| H | -2.20034400 | 0.51444500 | -4.32515300 |
| H | 1.55513700 | 1.63060400 | -4.32918500 |
| C | -1.00907800 | 3.85327600 | 3.02636400 |
| C | -2.83019300 | -2.78632600 | 3.03536900 |
| C | 1.01501000 | -3.85296100 | -3.02484200 |
| C | -3.83986300 | 1.03410000 | -3.02992000 |
| C | 2.82799800 | 2.78928200 | -3.03559600 |
| C | -2.39264400 | 4.08482700 | 3.00065900 |
| C | -2.34066700 | -4.10073200 | 3.00141000 |
| C | 2.39919000 | -4.08078500 | -2.99957500 |
| C | -4.72819000 | -0.05147800 | -3.00184100 |
| C | 2.33596600 | 4.10284700 | -3.00599800 |
| H | -3.08009100 | 3.24893700 | 3.14690000 |
| H | -1.27239400 | -4.27972700 | 3.14060900 |
| H | 3.08435000 | -3.24289900 | -3.14513300 |
| H | -4.34413500 | -1.06381300 | -3.14467800 |
| H | 1.26745100 | 4.27942500 | -3.14649100 |
| C | -2.90127600 | 5.36305700 | 2.77654400 |
| C | -3.19572300 | -5.17830200 | 2.77673200 |
| C | 2.91130000 | -5.35790100 | -2.77694400 |
| C | -6.09053600 | 0.14295300 | -2.78041500 |
| C | 3.18887400 | 5.18274000 | -2.78430000 |
| H | -3.97333400 | 5.55724000 | 2.73685600 |
| H | -2.82917800 | -6.20396000 | 2.72990400 |
| H | 3.98389500 | -5.54927100 | -2.73785000 |

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| H | -6.79190700 | -0.69069600 | -2.73953300 |
| H | 2.82039000 | 6.20786900 | -2.74120300 |
| C | -2.01060200 | 6.41383100 | 2.57134700 |
| C | -4.55177000 | -4.92992400 | 2.57929700 |
| C | 2.02350500 | -6.41130600 | -2.57279400 |
| C | -6.56017700 | 1.43858300 | -2.57966000 |
| C | 4.54526000 | 4.93756500 | -2.58529200 |
| C | -0.63347500 | 6.21813600 | 2.59430800 |
| C | -5.06928100 | -3.63901700 | 2.61139400 |
| C | 0.64583500 | -6.21929300 | -2.59524800 |
| C | -5.70603100 | 2.53635700 | -2.60440000 |
| C | 5.06521200 | 3.64751800 | -2.61283400 |
| H | 0.03661100 | 7.06074000 | 2.41745700 |
| H | -6.13470200 | -3.47797200 | 2.44050000 |
| H | -0.02191200 | -7.06397900 | -2.41942800 |
| H | -6.10465300 | 3.53701400 | -2.43098900 |
| H | 6.13086900 | 3.48909000 | -2.44094600 |
| C | -0.14026900 | 4.93159000 | 2.82489200 |
| C | -4.19929800 | -2.57066400 | 2.84248900 |
| C | 0.14912200 | -4.93383100 | -2.82436400 |
| C | -4.34419300 | 2.32444300 | -2.83267100 |
| C | 4.19738600 | 2.57679200 | -2.84105200 |
| H | 0.93762700 | 4.76511000 | 2.82194200 |
| H | -4.59317700 | -1.55357300 | 2.84638400 |
| H | -0.92923000 | -4.77029600 | -2.82138000 |
| H | -3.66413800 | 3.17714600 | -2.83181600 |
| H | 4.59318500 | 1.56043400 | -2.84171600 |
| F | -2.49442000 | 7.64233100 | 2.33451800 |
| F | -5.37595100 | -5.96107500 | 2.34068100 |
| F | 2.51071400 | -7.63879700 | -2.33765900 |
| F | -7.86711500 | 1.62972600 | -2.34557000 |
| F | 5.36735800 | 5.97107000 | -2.34974300 |
| B | -1.68980700 | -0.11315600 | 0.38884200 |
| B | 0.94397000 | -1.40575400 | 0.39212300 |
| B | 1.69032300 | 0.11307600 | -0.38639800 |
| B | -0.74572900 | -1.52165200 | -0.38215200 |
| B | -0.94348700 | 1.40565800 | -0.38975300 |
| O | 3.05865400 | 0.26073400 | -0.64251500 |
| O | 1.75580000 | -2.51643200 | 0.65104300 |
| O | -1.30181800 | -2.78118500 | -0.63524100 |
| O | -3.05812100 | -0.26072000 | 0.64508100 |
| O | -1.75552300 | 2.51618200 | -0.64884900 |
| C | 3.94504200 | -0.83735200 | -0.59596900 |

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| C | 1.24936100 | -3.83345300 | 0.60006200 |
| C | -2.69636200 | -2.99796500 | -0.58881500 |
| C | -3.94347300 | 0.83829700 | 0.60068200 |
| C | -1.25002800 | 3.83353300 | -0.59763900 |
| H | 3.77702800 | -1.40918700 | 0.32729500 |
| H | 0.67365400 | -3.97236500 | -0.32561500 |
| H | -3.10585100 | -2.56996000 | 0.33676800 |
| H | -3.77508200 | 1.41149100 | -0.32163000 |
| H | -0.67480700 | 3.97287600 | 0.32828800 |
| H | 3.73957500 | -1.52579300 | -1.43554900 |
| H | 0.54761100 | -4.00197100 | 1.43680200 |
| H | -3.18967600 | -2.47116200 | -1.42543500 |
| H | -3.73695300 | 1.52506300 | 1.44138900 |
| H | -0.54810000 | 4.00253800 | -1.43412000 |
| C | 5.38252400 | -0.38905100 | -0.61957700 |
| C | 2.35697400 | -4.85342800 | 0.62529900 |
| C | -3.02890400 | -4.46631200 | -0.61819200 |
| C | -5.38150800 | 0.39187000 | 0.62388200 |
| C | -2.35843200 | 4.85267300 | -0.62361200 |
| C | 6.39236600 | -1.34139300 | -0.82053000 |
| C | 2.03816700 | -6.20413900 | 0.82785000 |
| C | -4.35783600 | -4.86227700 | -0.82827100 |
| C | -6.38984900 | 1.34509200 | 0.82828200 |
| C | -2.04086100 | 6.20336100 | -0.82809700 |
| H | 6.12156400 | -2.38091200 | -1.02591700 |
| H | 1.00281500 | -6.48983300 | 1.03408500 |
| H | -5.12007300 | -4.10646100 | -1.03769700 |
| H | -6.11736300 | 2.38355500 | 1.03679600 |
| H | -1.00584400 | 6.48966800 | -1.03514000 |
| C | 7.73935900 | -0.99042300 | -0.74428300 |
| C | 3.01618600 | -7.19464000 | 0.75199400 |
| C | -4.73001500 | -6.20379800 | -0.75590800 |
| C | -7.73739700 | 0.99630300 | 0.75192000 |
| C | -3.01968200 | 7.19315300 | -0.75310800 |
| H | 8.53371900 | -1.72546000 | -0.88065700 |
| H | 2.77756100 | -8.25010600 | 0.88956900 |
| H | -5.76334500 | -6.52243600 | -0.89950500 |
| H | -8.53062600 | 1.73204200 | 0.89109100 |
| H | -2.78198300 | 8.24861700 | -0.89229300 |
| C | 8.07299300 | 0.33513900 | -0.47447500 |
| C | 4.33055000 | -6.82029900 | 0.48091700 |
| C | -3.75208300 | -7.15744200 | -0.48134500 |
| C | -8.07309300 | -0.32791600 | 0.47816100 |

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| C | -4.33365400 | 6.81809200 | -0.48113700 |
| C | 7.09389200 | 1.30569700 | -0.28671000 |
| C | 4.68062000 | -5.48704700 | 0.29176000 |
| C | -2.42257600 | -6.79718300 | -0.28469600 |
| C | -7.09551100 | -1.29933500 | 0.28704500 |
| C | -4.68252300 | 5.48480500 | -0.28989600 |
| H | 7.39229800 | 2.33560400 | -0.08108300 |
| H | 5.72150000 | -5.23005600 | 0.08543100 |
| H | -1.68251900 | -7.57212600 | -0.07534600 |
| H | -7.39559900 | -2.32815900 | 0.07847200 |
| H | -5.72308600 | 5.22717900 | -0.08276100 |
| C | 5.74917200 | 0.93290800 | -0.35284200 |
| C | 3.68487400 | -4.50945400 | 0.35760000 |
| C | -2.07053600 | -5.44670700 | -0.34653800 |
| C | -5.75021200 | -0.92874400 | 0.35349600 |
| C | -3.68595700 | 4.50799100 | -0.35479400 |
| H | 4.97104800 | 1.67321700 | -0.18817000 |
| H | 3.93638300 | -3.46543800 | 0.19206800 |
| H | -1.04092900 | -5.14481800 | -0.17441900 |
| H | -4.97320800 | -1.66965700 | 0.18622000 |
| H | -3.93655800 | 3.46405200 | -0.18751600 |
| F | 9.36594500 | 0.68291800 | -0.39767900 |
| F | 5.27869800 | -7.76564000 | 0.40435100 |
| F | -4.09986500 | -8.45060200 | -0.40878100 |
| F | -9.36655900 | -0.67352300 | 0.40078800 |
| F | -5.28261600 | 7.76272800 | -0.40575000 |

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| B | 0.05531200 | -0.81034900 | 1.38782000 |
| O | 0.17269200 | -1.63076900 | 2.51076500 |
| C | -0.92485300 | -2.27442800 | 3.15787900 |
| H | -1.86234300 | -1.74247100 | 2.94956800 |
| H | -0.72444000 | -2.21103300 | 4.24073000 |
| C | -1.04081300 | -3.71974400 | 2.73849400 |
| C | 0.03950800 | -4.59434900 | 2.91539200 |
| H | 0.95329700 | -4.23722700 | 3.39585800 |
| C | -0.01829100 | -5.91168500 | 2.46298400 |
| H | 0.83677500 | -6.57742300 | 2.57981300 |
| C | -1.17966500 | -6.35851700 | 1.82747800 |
| C | -2.28302700 | -5.51718900 | 1.66769900 |
| H | -3.18470100 | -5.87327500 | 1.16762100 |
| C | -2.20337500 | -4.20108300 | 2.12662700 |
| H | -3.05076400 | -3.53339200 | 1.96648100 |

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| Br | -1.24025700 | -8.13353000 | 1.13524500 |
| B | 1.55691900 | 0.05453800 | 0.90309700 |
| O | 2.76579400 | -0.01369200 | 1.59140400 |
| C | 2.88932200 | 0.27533300 | 2.96740400 |
| H | 2.25482100 | -0.42367200 | 3.54316800 |
| H | 2.51753100 | 1.28859400 | 3.18293700 |
| C | 4.32565000 | 0.16456900 | 3.40894000 |
| C | 5.34130500 | -0.25095400 | 2.54365300 |
| H | 5.09782700 | -0.50125000 | 1.51330000 |
| C | 6.66889800 | -0.31792800 | 2.97224600 |
| H | 7.45678700 | -0.62154400 | 2.28286000 |
| C | 6.98281700 | 0.03669100 | 4.28356100 |
| C | 5.98328700 | 0.45120000 | 5.16911500 |
| H | 6.23921700 | 0.72884800 | 6.19257500 |
| C | 4.66318800 | 0.51050000 | 4.72467400 |
| H | 3.88298500 | 0.84490400 | 5.41485000 |
| Br | 8.79300800 | -0.02340200 | 4.87108500 |
| B | 1.08914400 | -1.27757800 | -0.10785300 |
| O | 1.74696300 | -2.47536600 | -0.22424400 |
| C | 2.56080000 | -3.04590200 | 0.77902500 |
| H | 2.15696400 | -2.79552300 | 1.77231200 |
| H | 3.57408400 | -2.61212300 | 0.72561800 |
| C | 2.62087500 | -4.54234000 | 0.60651700 |
| C | 3.53319000 | -5.29243700 | 1.35964700 |
| H | 4.22865900 | -4.78554800 | 2.03496000 |
| C | 3.56588800 | -6.68487400 | 1.26778500 |
| H | 4.27474300 | -7.26415300 | 1.86098800 |
| C | 2.68076400 | -7.33371300 | 0.40120300 |
| C | 1.77289100 | -6.60393800 | -0.36748700 |
| H | 1.07590400 | -7.12026900 | -1.02760700 |
| C | 1.74520600 | -5.21318900 | -0.25321500 |
| H | 1.02067800 | -4.63521500 | -0.82439300 |
| Br | 2.69942100 | -9.23359900 | 0.28570300 |
| B | -0.75102300 | -1.33657300 | -0.22588800 |
| O | -1.45955400 | -2.49622600 | -0.13506800 |
| C | -1.79424900 | -3.42094400 | -1.14503000 |
| H | -1.35701100 | -4.39360500 | -0.86049900 |
| H | -1.35192600 | -3.12147100 | -2.10823700 |
| C | -3.29681300 | -3.56215300 | -1.24249600 |
| C | -4.14317600 | -2.67084400 | -0.57568400 |
| H | -3.71236700 | -1.86975300 | 0.01823900 |
| C | -5.53034300 | -2.80103000 | -0.64747400 |
| H | -6.17619000 | -2.09426300 | -0.12884800 |

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| C | -6.07558500 | -3.83733900 | -1.40324900 |
| C | -5.25116800 | -4.73999200 | -2.08312700 |
| H | -5.69056000 | -5.54932800 | -2.66795000 |
| C | -3.86512400 | -4.59807700 | -1.99620200 |
| H | -3.22115800 | -5.31403000 | -2.51518700 |
| Br | -7.96711300 | -4.00999400 | -1.52223900 |
| B | -1.35258500 | 0.04951800 | 0.84504000 |
| O | -2.56155300 | -0.03198200 | 1.51741600 |
| C | -3.71028400 | 0.68285500 | 1.08904300 |
| H | -3.73631700 | 0.72104900 | -0.00782200 |
| H | -3.64210600 | 1.71832800 | 1.45639800 |
| C | -4.97755100 | 0.03515800 | 1.57472000 |
| C | -4.97919800 | -1.04811300 | 2.45788900 |
| H | -4.03153700 | -1.42377100 | 2.84103200 |
| C | -6.17432100 | -1.66811500 | 2.83224100 |
| H | -6.16535800 | -2.52511400 | 3.50698200 |
| C | -7.38209900 | -1.19467100 | 2.31645500 |
| C | -7.40608100 | -0.09712700 | 1.45005800 |
| H | -8.35326500 | 0.26477000 | 1.04854500 |
| C | -6.20393800 | 0.50912200 | 1.08827500 |
| H | -6.22191200 | 1.35872500 | 0.40203800 |
| Br | -9.01066600 | -2.06852800 | 2.77165900 |
| B | 0.10441300 | 1.01024400 | 1.45565400 |
| O | 0.12601600 | 1.73485300 | 2.65808500 |
| C | -0.72928600 | 1.48855900 | 3.75640600 |
| H | -0.18493900 | 1.82708000 | 4.65584500 |
| H | -0.91732400 | 0.41099600 | 3.87993300 |
| C | -2.04665200 | 2.22496600 | 3.64681700 |
| C | -3.22352400 | 1.66318000 | 4.15656500 |
| H | -3.19251200 | 0.68630100 | 4.64551200 |
| C | -4.45502000 | 2.30036100 | 3.99499300 |
| H | -5.37295100 | 1.83284000 | 4.35202800 |
| C | -4.50117000 | 3.51700200 | 3.30966200 |
| C | -3.33532100 | 4.12137400 | 2.83381000 |
| H | -3.38163300 | 5.07250400 | 2.30419100 |
| C | -2.11429500 | 3.46859800 | 3.00789000 |
| H | -1.20982200 | 3.90941300 | 2.59063900 |
| Br | -6.18857400 | 4.33001700 | 2.94856400 |
| B | 0.19340200 | 1.11323100 | -1.51095600 |
| O | 0.11730500 | 1.93131700 | -2.63834900 |
| C | 1.20281500 | 2.73491700 | -3.09000100 |
| H | 2.13689700 | 2.45174900 | -2.58946900 |
| H | 1.32365500 | 2.53762500 | -4.17003900 |

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| C | 0.91932600 | 4.20194000 | -2.87165500 |
| C | -0.25057000 | 4.77829700 | -3.38722500 |
| H | -0.95442600 | 4.15697600 | -3.94627800 |
| C | -0.53574700 | 6.12886400 | -3.19177700 |
| H | -1.45631800 | 6.56647000 | -3.57947900 |
| C | 0.37135800 | 6.92028000 | -2.48145700 |
| C | 1.54762300 | 6.37313500 | -1.96637700 |
| H | 2.24849200 | 6.99966200 | -1.41273700 |
| C | 1.80962200 | 5.01356700 | -2.15936800 |
| H | 2.72085600 | 4.57955700 | -1.74405400 |
| Br | -0.01953100 | 8.76079500 | -2.19277400 |
| B | -1.30624100 | 0.24293900 | -1.04313100 |
| O | -2.51999700 | 0.31784000 | -1.71575700 |
| C | -2.83771400 | -0.31867500 | -2.93889400 |
| H | -2.38158500 | 0.25739200 | -3.76654600 |
| H | -2.41053900 | -1.32972300 | -2.98496800 |
| C | -4.33770900 | -0.38516700 | -3.08715500 |
| C | -5.15253700 | 0.62589900 | -2.56195500 |
| H | -4.69204400 | 1.47654600 | -2.05894200 |
| C | -6.54198900 | 0.55076500 | -2.65586200 |
| H | -7.17160700 | 1.33555400 | -2.23426900 |
| C | -7.12565600 | -0.54582900 | -3.29468600 |
| C | -6.33324200 | -1.55653800 | -3.84213400 |
| H | -6.79843700 | -2.41953800 | -4.31863200 |
| C | -4.94462000 | -1.46934800 | -3.73024400 |
| H | -4.32913900 | -2.28442500 | -4.11815500 |
| Br | -9.02290600 | -0.66166200 | -3.40054200 |
| B | -0.84491500 | 1.56791500 | -0.02503500 |
| O | -1.50569900 | 2.76059100 | 0.11542600 |
| C | -2.36962600 | 3.34501400 | -0.84115100 |
| H | -1.92537900 | 3.24361800 | -1.84402300 |
| H | -3.33382700 | 2.81260100 | -0.85432300 |
| C | -2.57155200 | 4.78995100 | -0.47733000 |
| C | -3.82909700 | 5.39368300 | -0.56459700 |
| H | -4.69349600 | 4.80860300 | -0.88919700 |
| C | -4.00649600 | 6.73593600 | -0.21630300 |
| H | -4.99078700 | 7.20121200 | -0.27957500 |
| C | -2.90882200 | 7.47043800 | 0.23551200 |
| C | -1.64444600 | 6.88206100 | 0.34016200 |
| H | -0.79487900 | 7.47120300 | 0.68501600 |
| C | -1.48324200 | 5.54773900 | -0.02460600 |
| H | -0.49979900 | 5.08014000 | 0.04051300 |
| Br | -3.12740900 | 9.30278000 | 0.70399800 |

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| B | 0.99714200 | 1.63418500 | 0.09566700 |
| O | 1.71136000 | 2.80236700 | 0.03532500 |
| C | 2.22225800 | 3.52088900 | 1.14505800 |
| H | 2.05775200 | 4.59075200 | 0.92522900 |
| H | 1.66430300 | 3.27711300 | 2.06008700 |
| C | 3.70219100 | 3.26304700 | 1.32682000 |
| C | 4.48886900 | 2.82350900 | 0.25595700 |
| H | 4.01774300 | 2.61116600 | -0.70211100 |
| C | 5.86282000 | 2.63084200 | 0.40328400 |
| H | 6.46428900 | 2.28666400 | -0.43727600 |
| C | 6.45577600 | 2.87845900 | 1.64215500 |
| C | 5.69050700 | 3.30229900 | 2.73048200 |
| H | 6.16000500 | 3.46448600 | 3.70099200 |
| C | 4.31690800 | 3.49120800 | 2.56426500 |
| H | 3.71705400 | 3.81409100 | 3.41992700 |
| Br | 8.33003700 | 2.61323700 | 1.84888900 |
| B | 1.59983100 | 0.24627300 | -0.97252700 |
| O | 2.78925400 | 0.32658900 | -1.67516800 |
| C | 3.94171200 | -0.38751100 | -1.26717400 |
| H | 4.03992200 | -0.32918500 | -0.17399800 |
| H | 3.81829300 | -1.44944400 | -1.53376100 |
| C | 5.18847300 | 0.15462700 | -1.90618100 |
| C | 5.16946900 | 1.23587700 | -2.79078500 |
| H | 4.21580200 | 1.69443700 | -3.04960500 |
| C | 6.35394500 | 1.72972400 | -3.34356700 |
| H | 6.33447900 | 2.57874400 | -4.02826600 |
| C | 7.56891500 | 1.12800500 | -3.00873700 |
| C | 7.60818400 | 0.03682400 | -2.13510300 |
| H | 8.56014200 | -0.43252900 | -1.88510600 |
| C | 6.41711800 | -0.44017600 | -1.59067100 |
| H | 6.44706300 | -1.29956300 | -0.91568800 |
| Br | 9.18997900 | 1.80053900 | -3.74829800 |
| B | 0.13589800 | -0.71031800 | -1.58943100 |
| O | 0.10602200 | -1.42657800 | -2.79758600 |
| C | 0.92816600 | -1.13215200 | -3.90953200 |
| H | 0.37064700 | -1.45890400 | -4.80524800 |
| H | 1.08785400 | -0.04695800 | -4.00570600 |
| C | 2.26325100 | -1.84165200 | -3.85268600 |
| C | 3.40043700 | -1.26879600 | -4.43347900 |
| H | 3.32623200 | -0.29926600 | -4.93218500 |
| C | 4.64762700 | -1.88729100 | -4.33892500 |
| H | 5.53539500 | -1.41227800 | -4.75711400 |
| C | 4.75500100 | -3.09340300 | -3.64311500 |

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| C | 3.62946000 | -3.70235600 | -3.08205100 |
| H | 3.72057300 | -4.64213300 | -2.53568100 |
| C | 2.38925900 | -3.07268600 | -3.19947200 |
| H | 1.51348700 | -3.51982600 | -2.73325500 |
| Br | 6.47225500 | -3.88617400 | -3.40342200 |

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| I | -7.96151700 | -1.43645400 | 3.86238500 |
| I | -9.84075000 | 1.28203800 | 1.08281400 |
| I | -6.57082600 | 4.11764500 | -4.16018300 |
| I | -8.72382800 | -1.85447100 | -2.25878500 |
| I | 5.05070000 | -6.88111000 | -1.89122200 |
| I | -7.98887600 | -6.22081800 | -0.78033600 |
| O | -1.06131800 | -1.03720400 | 2.76519800 |
| O | -2.77771800 | 1.04735100 | 0.91815400 |
| O | -0.60110100 | 2.99349300 | -0.66521500 |
| O | -2.10587600 | 0.58147300 | -2.21558500 |
| O | -0.09398200 | -2.04091700 | -2.38321400 |
| O | -2.36862800 | -1.99895800 | -0.13906800 |
| C | -1.64497000 | -0.24841500 | 3.80122400 |
| H | -1.43720900 | 0.81563600 | 3.63606100 |
| H | -1.14679400 | -0.54684200 | 4.73928800 |
| C | -3.13139800 | -0.49223000 | 3.91346900 |
| C | -4.05531300 | 0.50835300 | 3.59552500 |
| H | -3.70148000 | 1.49047100 | 3.28580800 |
| C | -5.42999500 | 0.25842100 | 3.61125800 |
| H | -6.13166000 | 1.04327000 | 3.32791900 |
| C | -5.88241300 | -1.01753400 | 3.94913400 |
| C | -4.98095000 | -2.03187100 | 4.29456200 |
| H | -5.34205100 | -3.02654800 | 4.55910600 |
| C | -3.61340900 | -1.75795500 | 4.27927100 |
| H | -2.90614400 | -2.55131100 | 4.53583500 |
| C | -3.52020100 | 2.04845900 | 0.22484800 |
| H | -3.30732900 | 1.97571900 | -0.84966500 |
| H | -3.18924200 | 3.03710800 | 0.56607200 |
| C | -4.99162600 | 1.86476100 | 0.46703900 |
| C | -5.59861900 | 0.62440100 | 0.23139000 |
| H | -4.99742200 | -0.21174600 | -0.12562300 |
| C | -6.96730000 | 0.44576300 | 0.42573800 |
| H | -7.42799200 | -0.52149800 | 0.23037400 |
| C | -7.74599000 | 1.52941700 | 0.84374300 |
| C | -7.16481800 | 2.77747000 | 1.08118100 |
| H | -7.77121800 | 3.62412900 | 1.40602900 |

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|---|-------------|-------------|-------------|
| C | -5.78753000 | 2.93295800 | 0.89436900 |
| H | -5.33456100 | 3.90798600 | 1.07930700 |
| C | -0.55991800 | 3.62910600 | -1.93743600 |
| H | 0.06355100 | 3.05832300 | -2.63800600 |
| H | -0.08433400 | 4.61146800 | -1.77304400 |
| C | -1.94303200 | 3.82612700 | -2.51223700 |
| C | -2.28520200 | 3.30479200 | -3.76348600 |
| H | -1.53204400 | 2.77112200 | -4.34838100 |
| C | -3.58458600 | 3.42779400 | -4.26444600 |
| H | -3.84105400 | 3.00517100 | -5.23702500 |
| C | -4.55785200 | 4.06037400 | -3.48615600 |
| C | -4.23247100 | 4.61471900 | -2.24393300 |
| H | -4.99061400 | 5.11412400 | -1.63896200 |
| C | -2.92353700 | 4.50455000 | -1.77616000 |
| H | -2.66978300 | 4.91923000 | -0.80058600 |
| C | -2.57535600 | -0.27043300 | -3.25943800 |
| H | -1.94270100 | -1.16220900 | -3.33976800 |
| H | -2.48294900 | 0.30910900 | -4.19247700 |
| C | -4.01762500 | -0.64802800 | -3.03663500 |
| C | -5.02325900 | 0.32702100 | -3.10499200 |
| H | -4.75622600 | 1.36377500 | -3.30821600 |
| C | -6.36219700 | -0.00391300 | -2.90064600 |
| H | -7.12732200 | 0.77179000 | -2.94468700 |
| C | -6.69709400 | -1.33315200 | -2.62359900 |
| C | -5.71458000 | -2.32148600 | -2.54958500 |
| H | -5.97900800 | -3.35272800 | -2.32156400 |
| C | -4.37773700 | -1.96897800 | -2.75139700 |
| H | -3.60624200 | -2.73643000 | -2.67151300 |
| C | -0.36464500 | -3.42227100 | -2.24630100 |
| H | -0.95584300 | -3.72037800 | -3.13192700 |
| H | -0.97994800 | -3.62050100 | -1.35767200 |
| C | 0.89673500 | -4.25188400 | -2.19187800 |
| C | 2.02677500 | -3.88475900 | -2.93110200 |
| H | 1.99288800 | -2.98422600 | -3.54462200 |
| C | 3.20334900 | -4.63493200 | -2.87290700 |
| H | 4.08119200 | -4.32187200 | -3.43993500 |
| C | 3.24355900 | -5.77744300 | -2.06875600 |
| C | 2.11603400 | -6.18335300 | -1.34869500 |
| H | 2.14932100 | -7.07713200 | -0.72406400 |
| C | 0.95373100 | -5.41172800 | -1.41140300 |
| H | 0.08446100 | -5.70746000 | -0.81853500 |
| C | -3.23686600 | -2.26433800 | 0.96077600 |
| H | -3.64680500 | -1.32014000 | 1.34340600 |

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|---|-------------|-------------|-------------|
| H | -2.64587300 | -2.70299100 | 1.78022800 |
| C | -4.34007400 | -3.19775500 | 0.55007000 |
| C | -5.66274600 | -2.92277100 | 0.91052900 |
| H | -5.89055100 | -2.01878300 | 1.47343200 |
| C | -6.70423200 | -3.78318800 | 0.55641200 |
| H | -7.72863900 | -3.54044500 | 0.83933900 |
| C | -6.41250500 | -4.93537000 | -0.17568700 |
| C | -5.09446700 | -5.23754300 | -0.54004600 |
| H | -4.87290700 | -6.14067600 | -1.11077900 |
| C | -4.06718300 | -4.36754900 | -0.17163400 |
| H | -3.03900900 | -4.59428400 | -0.46247900 |
| B | -0.65548700 | -0.52172600 | 1.52374200 |
| B | -1.51842900 | 0.65760900 | 0.53283400 |
| B | -0.39336500 | 1.63162200 | -0.43938700 |
| B | -1.14300800 | 0.27621900 | -1.28730000 |
| B | -1.31190800 | -1.12988400 | -0.02463800 |
| B | -0.08036900 | -1.15096900 | -1.29091300 |
| I | 7.96154000 | 1.43625600 | -3.86212700 |
| I | 9.84076300 | -1.28243900 | -1.08273000 |
| I | 6.57085600 | -4.11773600 | 4.16013700 |
| I | 8.72381000 | 1.85435400 | 2.25863800 |
| I | -5.05057200 | 6.88131800 | 1.89079100 |
| I | 7.98876600 | 6.22100200 | 0.78043800 |
| O | 1.06130700 | 1.03730300 | -2.76513800 |
| O | 2.77769200 | -1.04728000 | -0.91809400 |
| O | 0.60109900 | -2.99339800 | 0.66525600 |
| O | 2.10584100 | -0.58136100 | 2.21565600 |
| O | 0.09395600 | 2.04102600 | 2.38325200 |
| O | 2.36860700 | 1.99904900 | 0.13912000 |
| C | 1.64493800 | 0.24851400 | -3.80117500 |
| H | 1.43712800 | -0.81553300 | -3.63604700 |
| H | 1.14679100 | 0.54699000 | -4.73923900 |
| C | 3.13137900 | 0.49226600 | -3.91338000 |
| C | 4.05523700 | -0.50838100 | -3.59547500 |
| H | 3.70134800 | -1.49050200 | -3.28582900 |
| C | 5.42993100 | -0.25851500 | -3.61115700 |
| H | 6.13155200 | -1.04341700 | -3.32785400 |
| C | 5.88241800 | 1.01743900 | -3.94894000 |
| C | 4.98101300 | 2.03184300 | -4.29432700 |
| H | 5.34216900 | 3.02651900 | -4.55880100 |
| C | 3.61345800 | 1.75799200 | -4.27909100 |
| H | 2.90623700 | 2.55139700 | -4.53562200 |
| C | 3.52015500 | -2.04839300 | -0.22476900 |

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|---|-------------|-------------|-------------|
| H | 3.30730900 | -1.97560600 | 0.84974800 |
| H | 3.18914000 | -3.03704000 | -0.56594400 |
| C | 4.99158600 | -1.86478600 | -0.46700300 |
| C | 5.59866200 | -0.62445400 | -0.23141500 |
| H | 4.99752200 | 0.21174800 | 0.12556300 |
| C | 6.96735900 | -0.44592200 | -0.42575500 |
| H | 7.42812000 | 0.52131200 | -0.23041400 |
| C | 7.74597800 | -1.52964700 | -0.84370400 |
| C | 7.16471800 | -2.77766700 | -1.08110400 |
| H | 7.77106300 | -3.62438400 | -1.40590700 |
| C | 5.78741900 | -2.93305200 | -0.89429300 |
| H | 5.33438500 | -3.90806000 | -1.07918100 |
| C | 0.55992400 | -3.62903500 | 1.93746300 |
| H | -0.06354000 | -3.05827400 | 2.63805500 |
| H | 0.08434600 | -4.61139600 | 1.77304800 |
| C | 1.94305100 | -3.82606000 | 2.51223100 |
| C | 2.28523900 | -3.30478300 | 3.76349900 |
| H | 1.53208400 | -2.77115800 | 4.34843900 |
| C | 3.58462800 | -3.42782200 | 4.26444100 |
| H | 3.84110500 | -3.00526600 | 5.23704700 |
| C | 4.55788200 | -4.06037500 | 3.48611100 |
| C | 4.23248900 | -4.61463000 | 2.24385100 |
| H | 4.99062200 | -5.11401100 | 1.63884600 |
| C | 2.92355200 | -4.50442400 | 1.77609500 |
| H | 2.66978500 | -4.91905400 | 0.80050200 |
| C | 2.57530700 | 0.27058600 | 3.25948100 |
| H | 1.94267200 | 1.16238300 | 3.33973400 |
| H | 2.48285600 | -0.30889400 | 4.19255500 |
| C | 4.01759100 | 0.64813200 | 3.03669800 |
| C | 5.02320900 | -0.32691800 | 3.10524900 |
| H | 4.75615500 | -1.36363500 | 3.30863200 |
| C | 6.36215600 | 0.00396200 | 2.90088100 |
| H | 7.12726700 | -0.77174700 | 2.94505900 |
| C | 6.69707700 | 1.33314500 | 2.62359600 |
| C | 5.71458100 | 2.32148200 | 2.54939900 |
| H | 5.97902700 | 3.35267800 | 2.32118500 |
| C | 4.37773000 | 1.96903200 | 2.75125800 |
| H | 3.60624600 | 2.73648000 | 2.67121500 |
| C | 0.36466600 | 3.42236800 | 2.24631400 |
| H | 0.95584400 | 3.72048600 | 3.13195100 |
| H | 0.98000400 | 3.62055100 | 1.35770000 |
| C | -0.89668400 | 4.25201700 | 2.19180700 |
| C | -2.02676800 | 3.88496000 | 2.93099800 |

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|---|-------------|-------------|-------------|
| H | -1.99293500 | 2.98445600 | 3.54456300 |
| C | -3.20331700 | 4.63516500 | 2.87270800 |
| H | -4.08119800 | 4.32215500 | 3.43970600 |
| C | -3.24346000 | 5.77763100 | 2.06849000 |
| C | -2.11588800 | 6.18347500 | 1.34846600 |
| H | -2.14912300 | 7.07721700 | 0.72377900 |
| C | -0.95360900 | 5.41182200 | 1.41127200 |
| H | -0.08430300 | 5.70749900 | 0.81842800 |
| C | 3.23683500 | 2.26444900 | -0.96072500 |
| H | 3.64679100 | 1.32026100 | -1.34335900 |
| H | 2.64583500 | 2.70309800 | -1.78017600 |
| C | 4.34002500 | 3.19788300 | -0.55001000 |
| C | 5.66270600 | 2.92291700 | -0.91045200 |
| H | 5.89052900 | 2.01893100 | -1.47335200 |
| C | 6.70417500 | 3.78334600 | -0.55631800 |
| H | 7.72859000 | 3.54061700 | -0.83923000 |
| C | 6.41242300 | 4.93552700 | 0.17577400 |
| C | 5.09437600 | 5.23768400 | 0.54011100 |
| H | 4.87279400 | 6.14081600 | 1.11083700 |
| C | 4.06711000 | 4.36767300 | 0.17169000 |
| H | 3.03892900 | 4.59439500 | 0.46252100 |
| B | 0.65546600 | 0.52181800 | -1.52368900 |
| B | 1.51840400 | -0.65752700 | -0.53278200 |
| B | 0.39334700 | -1.63152900 | 0.43943900 |
| B | 1.14298600 | -0.27612200 | 1.28735400 |
| B | 1.31188600 | 1.12997500 | 0.02468900 |
| B | 0.08034500 | 1.15106700 | 1.29095900 |

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Lower-energy conformer:

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|---|-------------|-------------|-------------|
| F | -8.33124000 | -4.08625800 | -4.49998700 |
| F | -7.41337600 | -5.57428300 | -3.23026700 |
| F | -8.99892200 | -4.31408900 | -2.45211200 |
| F | 4.69803800 | -2.01950800 | -7.39897400 |
| F | 5.12299400 | 0.10871400 | -7.38432700 |
| F | 5.47884900 | -1.07960200 | -5.61167500 |
| F | 9.66049400 | 0.21874000 | -1.77979700 |
| F | 8.95129600 | 0.49251400 | 0.24422800 |
| F | 9.43154500 | -1.49332400 | -0.46808300 |
| F | 7.92549300 | 3.66684300 | -2.55316500 |
| F | 7.60762000 | 5.16746600 | -1.02256800 |
| F | 7.66890000 | 3.07620200 | -0.48186300 |
| F | 7.34922200 | 3.06098000 | 5.78428000 |

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|---|-------------|-------------|-------------|
| F | 8.85566800 | 1.94283000 | 4.69547400 |
| F | 7.46376000 | 0.91401200 | 5.99886000 |
| F | -2.56221600 | 7.90170500 | -1.83024600 |
| F | -2.41997400 | 9.00335300 | 0.02143900 |
| F | -4.12702800 | 7.71938400 | -0.33809500 |
| F | -9.26863600 | -1.08738000 | 0.45410200 |
| F | -9.28850400 | -1.79223000 | 2.50114000 |
| F | -9.86925900 | 0.24763100 | 2.04697700 |
| F | -4.85966300 | 2.04502900 | 6.88913900 |
| F | -5.42174400 | -0.01590800 | 6.50675900 |
| F | -5.58642300 | 1.46468100 | 4.93635700 |
| F | -7.33774700 | 7.11124800 | -2.07908900 |
| F | -8.30727100 | 5.37310500 | -1.21447000 |
| F | -7.19066500 | -5.69142500 | -0.28648900 |
| F | -7.83875100 | -4.08659300 | 1.01116500 |
| F | -7.37404000 | -6.02634600 | 1.84974400 |
| F | 2.86186700 | -7.91368400 | 1.01855700 |
| F | 4.55756500 | -6.91147800 | 0.10638800 |
| F | 3.48277900 | -8.43469900 | -0.98755100 |
| F | 7.69689000 | -1.51489300 | 4.41688000 |
| F | 8.28605700 | -3.44610000 | 3.62215000 |
| F | 8.28300100 | -1.70242200 | 2.34101500 |
| B | 0.14765200 | -1.16517100 | -1.47441600 |
| B | -0.51308000 | -1.52612000 | 0.21683900 |
| B | -1.44798500 | -0.56732000 | -1.05105100 |
| B | -0.19329600 | 0.53215200 | -1.92969800 |
| B | 1.43896200 | 0.13647400 | -1.19647600 |
| B | 1.21408500 | -1.11252200 | 0.01475600 |
| B | 1.37907500 | 0.69725500 | 0.51382400 |
| B | 0.44545100 | 1.65504200 | -0.74560700 |
| B | -1.27604200 | 1.23067100 | -0.54641300 |
| B | -1.48991000 | -0.00811500 | 0.66839700 |
| B | 0.13615100 | -0.40037000 | 1.39780100 |
| B | -0.22019100 | 1.29136400 | 0.94056500 |
| O | -0.44462900 | 0.99554900 | -3.20757400 |
| O | 2.56661300 | 0.30742200 | -1.99463700 |
| O | 0.82786500 | 2.97385400 | -0.98569100 |
| O | 2.46013700 | 1.16445300 | 1.21491400 |
| O | -0.47954200 | 2.25227800 | 1.92824200 |
| O | -2.61661200 | -0.18963200 | 1.46847500 |
| O | 0.37158200 | -0.84858700 | 2.68600300 |
| O | -2.32218900 | 2.08218100 | -0.82184100 |
| O | -2.53798400 | -1.02979300 | -1.74747000 |

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|---|-------------|-------------|-------------|
| O | -0.92827000 | -2.82850200 | 0.48053100 |
| O | 0.38060200 | -2.12503300 | -2.46963900 |
| O | 2.24223900 | -1.99158400 | 0.26498900 |
| C | -0.59728400 | 0.15122000 | -4.34432700 |
| H | -1.25411000 | 0.69682900 | -5.04151900 |
| H | -1.09668300 | -0.78645700 | -4.06669800 |
| C | 0.73342400 | -0.12820600 | -5.00433400 |
| C | 1.09102700 | -1.42343900 | -5.39257600 |
| H | 0.39888400 | -2.24843400 | -5.21891700 |
| C | 2.33360700 | -1.67611800 | -5.97623000 |
| H | 2.61015600 | -2.69054100 | -6.26715000 |
| C | 3.23800000 | -0.62751400 | -6.16477200 |
| C | 2.88239300 | 0.67679900 | -5.80135000 |
| H | 3.58634700 | 1.49478300 | -5.96308600 |
| C | 1.63573100 | 0.92000200 | -5.23232200 |
| H | 1.35943300 | 1.93563000 | -4.94652400 |
| C | 4.63474900 | -0.90663000 | -6.65230500 |
| C | 3.32194700 | -0.81233500 | -2.46923000 |
| H | 3.24509300 | -0.81423200 | -3.56378700 |
| H | 2.89369100 | -1.74652100 | -2.09441000 |
| C | 4.77041300 | -0.71106500 | -2.06585300 |
| C | 5.31914600 | -1.60246700 | -1.13531700 |
| H | 4.68701500 | -2.37247200 | -0.69340000 |
| C | 6.65693900 | -1.49929000 | -0.75260100 |
| H | 7.07309100 | -2.18395300 | -0.01418100 |
| C | 7.45874800 | -0.49366100 | -1.30122300 |
| C | 6.92266100 | 0.40140000 | -2.23475200 |
| H | 7.55433700 | 1.17918700 | -2.66316500 |
| C | 5.58682800 | 0.28702500 | -2.61311300 |
| H | 5.16804700 | 0.97933200 | -3.34346600 |
| C | 8.88089900 | -0.32538700 | -0.83207800 |
| C | 1.48666600 | 3.41014300 | -2.15356200 |
| H | 1.05072500 | 4.39096500 | -2.41863200 |
| H | 1.29482600 | 2.72579100 | -2.99085600 |
| C | 2.97732600 | 3.56968900 | -1.95808600 |
| C | 3.82809400 | 3.58889200 | -3.07020100 |
| H | 3.41124200 | 3.47298900 | -4.07379900 |
| C | 5.20637500 | 3.72673200 | -2.91199800 |
| H | 5.86431800 | 3.72012400 | -3.78185100 |
| C | 5.75250000 | 3.83473400 | -1.62937600 |
| C | 4.91020300 | 3.84204000 | -0.51342800 |
| H | 5.33267100 | 3.91540700 | 0.49017300 |
| C | 3.53193400 | 3.71581700 | -0.68130800 |

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|---|-------------|-------------|-------------|
| H | 2.87978900 | 3.68287500 | 0.19001800 |
| C | 7.24082100 | 3.93926300 | -1.42456900 |
| C | 3.79194400 | 0.81873500 | 0.86306500 |
| H | 4.05061000 | 1.26964700 | -0.10508200 |
| H | 3.85861700 | -0.27078100 | 0.72595300 |
| C | 4.75322100 | 1.24061100 | 1.93433600 |
| C | 6.12583500 | 1.12121400 | 1.68841500 |
| H | 6.47647000 | 0.81618300 | 0.70483300 |
| C | 7.05428600 | 1.36200400 | 2.69868400 |
| H | 8.11699600 | 1.23179500 | 2.49934700 |
| C | 6.61210000 | 1.74617700 | 3.96755400 |
| C | 5.24401700 | 1.91765200 | 4.20934300 |
| H | 4.90344700 | 2.23810300 | 5.19603400 |
| C | 4.31928200 | 1.66396900 | 3.19656600 |
| H | 3.25173400 | 1.77592600 | 3.38463900 |
| C | 7.58063500 | 1.91871600 | 5.10685300 |
| C | 0.19155200 | 3.49309200 | 1.98680200 |
| H | 1.20046300 | 3.42548200 | 1.55658800 |
| H | 0.31047800 | 3.74410200 | 3.05697600 |
| C | -0.59159500 | 4.59733600 | 1.31448300 |
| C | 0.06447900 | 5.59437300 | 0.58051200 |
| H | 1.14883100 | 5.55214400 | 0.45957200 |
| C | -0.65629800 | 6.63110200 | -0.00867500 |
| H | -0.13737600 | 7.40557700 | -0.57729700 |
| C | -2.04981000 | 6.67752900 | 0.12632400 |
| C | -2.71526200 | 5.68111600 | 0.84486400 |
| H | -3.80154600 | 5.71000300 | 0.93170800 |
| C | -1.98551100 | 4.64829200 | 1.43519400 |
| H | -2.50021700 | 3.86178900 | 1.98832100 |
| C | -2.79981500 | 7.82339900 | -0.49994800 |
| C | -3.42830000 | 0.89344900 | 1.89992900 |
| H | -3.29308900 | 1.76683500 | 1.24799600 |
| H | -3.10982000 | 1.19068100 | 2.91017100 |
| C | -4.87702600 | 0.48026900 | 1.91429300 |
| C | -5.88484600 | 1.43163700 | 1.70912900 |
| H | -5.61932700 | 2.47954800 | 1.55217400 |
| C | -7.22714800 | 1.05310600 | 1.69154200 |
| H | -8.00736600 | 1.79676900 | 1.52114100 |
| C | -7.57239600 | -0.28906200 | 1.88281100 |
| C | -6.57504800 | -1.24057300 | 2.11775600 |
| H | -6.84750300 | -2.28466400 | 2.26139700 |
| C | -5.23624400 | -0.85572000 | 2.13116700 |
| H | -4.45895200 | -1.60307800 | 2.27763600 |

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|---|-------------|-------------|-------------|
| C | -9.00341600 | -0.73028500 | 1.73497000 |
| C | 0.47717600 | -0.00437800 | 3.82662900 |
| H | 0.97300600 | 0.93997600 | 3.56565000 |
| H | 1.12080900 | -0.54186500 | 4.54283700 |
| C | -0.87271900 | 0.26604200 | 4.45166900 |
| C | -1.79228200 | -0.77702700 | 4.62338700 |
| H | -1.51386200 | -1.78913600 | 4.32931500 |
| C | -3.06146800 | -0.53370500 | 5.14340800 |
| H | -3.78198100 | -1.34591100 | 5.24667800 |
| C | -3.41710900 | 0.76386300 | 5.52585000 |
| C | -2.49143100 | 1.80562900 | 5.40591200 |
| H | -2.76581200 | 2.81499800 | 5.71667600 |
| C | -1.23089900 | 1.55498500 | 4.86279800 |
| H | -0.52497100 | 2.37743900 | 4.73778200 |
| C | -4.82379000 | 1.06132200 | 5.97488000 |
| C | -2.24794000 | 3.19791400 | -1.68645000 |
| H | -1.87512000 | 2.87176400 | -2.67315600 |
| H | -1.52177100 | 3.92786100 | -1.29336500 |
| C | -3.60569100 | 3.83668700 | -1.81324500 |
| C | -3.73061000 | 5.05844200 | -2.48794700 |
| H | -2.84545800 | 5.54241800 | -2.90568500 |
| C | -4.96625100 | 5.69041200 | -2.58979800 |
| H | -5.04506800 | 6.65887500 | -3.08516600 |
| C | -6.10152000 | 5.10164300 | -2.01921500 |
| C | -5.98833500 | 3.88059600 | -1.35092500 |
| H | -6.86941400 | 3.42185900 | -0.89955300 |
| C | -4.74526900 | 3.25307400 | -1.25008200 |
| H | -4.65617900 | 2.30949700 | -0.71612900 |
| C | -7.44169800 | 5.77368600 | -2.16251200 |
| C | -3.85402500 | -0.55575000 | -1.49016500 |
| H | -3.96961000 | 0.42353300 | -1.98755300 |
| H | -3.99298900 | -0.38912500 | -0.41487600 |
| C | -4.89764400 | -1.51981800 | -1.98281500 |
| C | -4.62548200 | -2.45787600 | -2.98636100 |
| H | -3.62802900 | -2.49865400 | -3.42594500 |
| C | -5.61188400 | -3.35425500 | -3.39552700 |
| H | -5.39207400 | -4.09802100 | -4.16406300 |
| C | -6.88092200 | -3.31990600 | -2.80321000 |
| C | -7.16628500 | -2.37470300 | -1.81483900 |
| H | -8.14299300 | -2.35830200 | -1.33284700 |
| C | -6.17558600 | -1.47963000 | -1.41177500 |
| H | -6.39614400 | -0.76324100 | -0.61928300 |
| C | -7.91570600 | -4.32381300 | -3.23974000 |

| | | | |
|---|-------------|-------------|-------------|
| C | -1.55030000 | -3.21385500 | 1.68474600 |
| H | -1.60418900 | -2.36791900 | 2.38124000 |
| H | -0.92711400 | -3.99448000 | 2.15954300 |
| C | -2.94367700 | -3.75224400 | 1.46260800 |
| C | -3.70807700 | -4.16246000 | 2.56668900 |
| H | -3.28195100 | -4.10985600 | 3.57271200 |
| C | -5.00903700 | -4.63138800 | 2.39704900 |
| H | -5.59848300 | -4.94539100 | 3.26016500 |
| C | -5.56016500 | -4.70357400 | 1.11069300 |
| C | -4.80127500 | -4.31319300 | 0.00711800 |
| H | -5.22682500 | -4.37676200 | -0.99243600 |
| C | -3.50315200 | -3.83345100 | 0.18532000 |
| H | -2.92608500 | -3.49852500 | -0.67406300 |
| C | -6.98943100 | -5.13844400 | 0.91900200 |
| C | -0.21217600 | -3.40815400 | -2.46006400 |
| H | -0.39080200 | -3.68646800 | -3.51461000 |
| H | -1.18598500 | -3.40110500 | -1.95264600 |
| C | 0.69679800 | -4.43858000 | -1.82947200 |
| C | 0.20482000 | -5.37860000 | -0.91745600 |
| H | -0.84786200 | -5.35247000 | -0.63116500 |
| C | 1.05214700 | -6.33699000 | -0.35735200 |
| H | 0.66401000 | -7.06450000 | 0.35687000 |
| C | 2.40782800 | -6.35218500 | -0.69835900 |
| C | 2.91153800 | -5.41205100 | -1.60714200 |
| H | 3.97084200 | -5.42032700 | -1.87020500 |
| C | 2.05755900 | -4.46594800 | -2.16766900 |
| H | 2.44733500 | -3.73219000 | -2.87443400 |
| C | 3.32292400 | -7.40767600 | -0.13587100 |
| C | 2.24689100 | -3.00650400 | 1.27587800 |
| H | 2.07691700 | -3.97640100 | 0.78944000 |
| H | 1.44118100 | -2.82223800 | 1.99709900 |
| C | 3.59460900 | -2.95490500 | 1.94935200 |
| C | 3.87583300 | -1.91640100 | 2.84732200 |
| H | 3.08250100 | -1.22217700 | 3.12952300 |
| C | 5.16526900 | -1.72871100 | 3.34145200 |
| H | 5.38521500 | -0.90091400 | 4.01487600 |
| C | 6.18913900 | -2.59228900 | 2.94205000 |
| C | 5.90960400 | -3.66845200 | 2.09259300 |
| H | 6.70547100 | -4.35786700 | 1.80461500 |
| C | 4.61701400 | -3.84509200 | 1.59744500 |
| H | 4.40994800 | -4.67167100 | 0.91754600 |
| C | 7.61442300 | -2.31664200 | 3.34529600 |
| F | -8.00743800 | 5.49954000 | -3.35396500 |

Higher-energy conformer:

| | | | |
|---|--------------|-------------|-------------|
| F | 1.65749700 | 8.10377600 | 1.20055700 |
| F | 1.71724800 | 9.05982200 | -0.73470900 |
| F | 3.44787700 | 7.97192400 | -0.01755400 |
| F | 5.75382300 | 1.69269500 | -6.53151200 |
| F | 6.40848300 | -0.21839400 | -5.73807500 |
| F | 6.17814200 | 1.48374000 | -4.42103600 |
| F | 8.10800800 | -4.53420600 | -1.73052400 |
| F | 7.59947000 | -5.74134900 | -0.00468600 |
| F | 7.99015200 | -3.62773200 | 0.23371000 |
| F | -6.48814500 | -7.68174000 | -2.36004300 |
| F | -7.67876500 | -5.97796100 | -1.73620800 |
| F | -7.05243800 | -6.16906500 | -3.79797800 |
| F | -10.06323400 | -0.86342900 | 1.14953200 |
| F | -9.70834400 | 1.24848300 | 1.49608600 |
| F | -9.44715500 | 0.41270600 | -0.48393500 |
| F | -9.03048100 | 3.19370100 | -3.60131700 |
| F | -7.72148900 | 4.81225600 | -3.00108900 |
| F | -7.66901600 | 4.08418000 | -5.03661800 |
| O | 0.67372300 | 2.02619800 | -2.28598300 |
| O | 0.11671400 | -1.20550900 | -2.87041200 |
| O | 1.12700600 | -2.89415800 | -0.27127500 |
| O | -2.05843600 | -2.21118400 | -0.70661800 |
| O | -2.83765500 | 0.20656100 | 1.28441200 |
| O | -2.30202400 | 0.79516400 | -1.94321900 |
| B | 0.30473800 | 1.13278900 | -1.27314800 |
| B | 0.12625600 | -0.63160000 | -1.61244500 |
| B | -1.12227300 | -1.26077300 | -0.35758900 |
| B | -1.59352700 | 0.05437100 | 0.68658200 |
| B | -1.29919900 | 0.46814400 | -1.05874600 |
| B | 0.63788700 | -1.59161700 | -0.24351200 |
| C | -0.07247500 | 3.18761800 | -2.59000200 |
| H | -1.13224900 | 3.06753800 | -2.32401500 |
| H | -0.01968800 | 3.32564100 | -3.68549100 |
| C | 0.49677900 | 4.41470400 | -1.91549300 |
| C | 1.88289800 | 4.58676000 | -1.81808400 |
| H | 2.54383200 | 3.81105200 | -2.20681200 |
| C | 2.41912700 | 5.72571300 | -1.21556900 |
| H | 3.49884100 | 5.84982900 | -1.13082100 |
| C | 1.56563100 | 6.70711000 | -0.70498700 |
| C | 0.17710400 | 6.54166300 | -0.79106900 |
| H | -0.48990400 | 7.30506600 | -0.38509800 |
| C | -0.35038600 | 5.39986500 | -1.39087400 |

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|---|-------------|-------------|-------------|
| H | -1.43282100 | 5.26373400 | -1.43790300 |
| C | 2.10767800 | 7.95956500 | -0.06840000 |
| C | 0.14860900 | -0.46867400 | -4.08775500 |
| H | -0.45098500 | 0.44800200 | -4.00181600 |
| H | -0.32522500 | -1.11481400 | -4.84504500 |
| C | 1.56475400 | -0.14037500 | -4.50631100 |
| C | 1.88110400 | 1.11037500 | -5.04975700 |
| H | 1.09753300 | 1.86048000 | -5.17202400 |
| C | 3.19217100 | 1.41865900 | -5.41407900 |
| H | 3.43199000 | 2.39925000 | -5.82843000 |
| C | 4.20754200 | 0.47479800 | -5.22500000 |
| C | 3.89975800 | -0.78571900 | -4.70426300 |
| H | 4.69104800 | -1.52137700 | -4.55851900 |
| C | 2.58570800 | -1.08737200 | -4.35513000 |
| H | 2.35582100 | -2.06356600 | -3.93108600 |
| C | 5.64145700 | 0.85386200 | -5.48783700 |
| C | 1.74183300 | -3.51419900 | -1.37557200 |
| H | 1.55869500 | -2.94765200 | -2.29806600 |
| H | 1.26257200 | -4.50314100 | -1.50099600 |
| C | 3.22257600 | -3.72573400 | -1.16975800 |
| C | 4.03068600 | -4.09229600 | -2.25490700 |
| H | 3.59444500 | -4.18434600 | -3.25351700 |
| C | 5.39032000 | -4.34838400 | -2.07578400 |
| H | 6.01576800 | -4.62409100 | -2.92572800 |
| C | 5.95533800 | -4.24123900 | -0.80027700 |
| C | 5.15752000 | -3.87059500 | 0.28576800 |
| H | 5.59792100 | -3.78086500 | 1.27682700 |
| C | 3.80140300 | -3.60853800 | 0.09839000 |
| H | 3.18664500 | -3.29172400 | 0.93923200 |
| C | 7.41544700 | -4.54183400 | -0.57579700 |
| C | -1.77412500 | -3.39794400 | -1.41824600 |
| H | -1.09939300 | -4.03659000 | -0.82634700 |
| H | -1.24737900 | -3.14647500 | -2.35564700 |
| C | -3.05131900 | -4.14031200 | -1.71070100 |
| C | -2.98646100 | -5.43571100 | -2.24008900 |
| H | -2.01605900 | -5.90050100 | -2.42493500 |
| C | -4.14843100 | -6.16056700 | -2.48956800 |
| H | -4.08477400 | -7.18117200 | -2.86842300 |
| C | -5.39816600 | -5.59177000 | -2.21621100 |
| C | -5.47313700 | -4.29836500 | -1.69333200 |
| H | -6.44525800 | -3.85542200 | -1.47051500 |
| C | -4.30398800 | -3.57799800 | -1.44326600 |
| H | -4.36256000 | -2.57673700 | -1.02247400 |

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|---|-------------|-------------|-------------|
| C | -6.65729100 | -6.35890100 | -2.52411700 |
| C | -3.61962300 | -0.91179300 | 1.68626200 |
| H | -3.41579000 | -1.11506000 | 2.74819700 |
| H | -3.33179700 | -1.81067700 | 1.12566300 |
| C | -5.08413500 | -0.62625300 | 1.48849400 |
| C | -5.58726000 | 0.67392500 | 1.61894100 |
| H | -4.90416500 | 1.49447200 | 1.83178400 |
| C | -6.94831200 | 0.92233100 | 1.45390300 |
| H | -7.34153000 | 1.92971600 | 1.56740200 |
| C | -7.81835400 | -0.12391400 | 1.13527500 |
| C | -7.32811300 | -1.42841500 | 1.01341600 |
| H | -8.00969600 | -2.24740900 | 0.77736600 |
| C | -5.96740000 | -1.67384700 | 1.19445000 |
| H | -5.58787100 | -2.69385500 | 1.10219600 |
| C | -9.26387300 | 0.16962900 | 0.83727500 |
| C | -3.58110800 | 0.17697400 | -1.88121900 |
| H | -3.82886000 | -0.08699100 | -0.84677100 |
| H | -3.53315700 | -0.76652000 | -2.45373200 |
| C | -4.66202500 | 1.06759200 | -2.42849600 |
| C | -5.98196700 | 0.85820600 | -2.00810000 |
| H | -6.20575200 | 0.06953500 | -1.28735000 |
| C | -7.01408200 | 1.67275800 | -2.47007300 |
| H | -8.03057600 | 1.52324800 | -2.10832800 |
| C | -6.72694500 | 2.71072500 | -3.36113500 |
| C | -5.41488500 | 2.91308900 | -3.80600700 |
| H | -5.19966900 | 3.72146700 | -4.50718700 |
| C | -4.38722500 | 2.09264800 | -3.34141700 |
| H | -3.36015400 | 2.25776200 | -3.66964900 |
| C | -7.79724500 | 3.69354800 | -3.75478000 |
| F | -1.65708300 | -8.10370100 | -1.20068800 |
| F | -1.71628800 | -9.06002900 | 0.73445300 |
| F | -3.44728500 | -7.97241500 | 0.01774100 |
| F | -5.75399600 | -1.69240900 | 6.53170800 |
| F | -6.40885400 | 0.21812900 | 5.73710800 |
| F | -6.17790400 | -1.48467600 | 4.42103200 |
| F | -8.10795700 | 4.53548800 | 1.73041500 |
| F | -7.59933500 | 5.74128200 | 0.00364800 |
| F | -7.99038500 | 3.62755200 | -0.23315400 |
| F | 6.48792400 | 7.68160000 | 2.36124700 |
| F | 7.67853400 | 5.97808600 | 1.73666800 |
| F | 7.05237600 | 6.16838900 | 3.79856000 |
| F | 10.06323300 | 0.86320200 | -1.15035900 |
| F | 9.70816400 | -1.24886900 | -1.49575300 |

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|---|-------------|-------------|-------------|
| F | 9.44729200 | -0.41202300 | 0.48386600 |
| F | 9.03062300 | -3.19363100 | 3.60039700 |
| F | 7.72114900 | -4.81226600 | 3.00141300 |
| F | 7.66963500 | -4.08330300 | 5.03664500 |
| O | -0.67381700 | -2.02622400 | 2.28595300 |
| O | -0.11684100 | 1.20549200 | 2.87041000 |
| O | -1.12712800 | 2.89412600 | 0.27126100 |
| O | 2.05834100 | 2.21119600 | 0.70659500 |
| O | 2.83760700 | -0.20659600 | -1.28437600 |
| O | 2.30195900 | -0.79518100 | 1.94320000 |
| B | -0.30481700 | -1.13280200 | 1.27313900 |
| B | -0.12631800 | 0.63159900 | 1.61243200 |
| B | 1.12219100 | 1.26076800 | 0.35757800 |
| B | 1.59345700 | -0.05439300 | -0.68659100 |
| B | 1.29911800 | -0.46817200 | 1.05873900 |
| B | -0.63795500 | 1.59160800 | 0.24351000 |
| C | 0.07244900 | -3.18758000 | 2.59005500 |
| H | 1.13223200 | -3.06742000 | 2.32413800 |
| H | 0.01959500 | -3.32558000 | 3.68554400 |
| C | -0.49665300 | -4.41473500 | 1.91554500 |
| C | -1.88274700 | -4.58692700 | 1.81805500 |
| H | -2.54378400 | -3.81126900 | 2.20671100 |
| C | -2.41882800 | -5.72594900 | 1.21553400 |
| H | -3.49852500 | -5.85016600 | 1.13071700 |
| C | -1.56520600 | -6.70727900 | 0.70503800 |
| C | -0.17669800 | -6.54170300 | 0.79121700 |
| H | 0.49041000 | -7.30505600 | 0.38531700 |
| C | 0.35064100 | -5.39983500 | 1.39101700 |
| H | 1.43306100 | -5.26359400 | 1.43810700 |
| C | -2.10708300 | -7.95976600 | 0.06837300 |
| C | -0.14872700 | 0.46863900 | 4.08774300 |
| H | 0.45086800 | -0.44803500 | 4.00178700 |
| H | 0.32510800 | 1.11476600 | 4.84504400 |
| C | -1.56487100 | 0.14032100 | 4.50629200 |
| C | -1.88120500 | -1.11044400 | 5.04972000 |
| H | -1.09761800 | -1.86053100 | 5.17200100 |
| C | -3.19227500 | -1.41876900 | 5.41398400 |
| H | -3.43208200 | -2.39937900 | 5.82830100 |
| C | -4.20766900 | -0.47493700 | 5.22486600 |
| C | -3.89989900 | 0.78559800 | 4.70417500 |
| H | -4.69120700 | 1.52122900 | 4.55839600 |
| C | -2.58584100 | 1.08729500 | 4.35510200 |
| H | -2.35596900 | 2.06349700 | 3.93107300 |

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|---|-------------|-------------|-------------|
| C | -5.64157100 | -0.85411000 | 5.48760800 |
| C | -1.74194400 | 3.51417700 | 1.37556400 |
| H | -1.55886800 | 2.94759500 | 2.29804500 |
| H | -1.26262500 | 4.50308400 | 1.50102400 |
| C | -3.22267300 | 3.72580500 | 1.16972900 |
| C | -4.03080700 | 4.09225600 | 2.25489300 |
| H | -3.59460400 | 4.18415100 | 3.25353400 |
| C | -5.39042600 | 4.34844200 | 2.07575400 |
| H | -6.01588600 | 4.62408200 | 2.92570800 |
| C | -5.95539400 | 4.24151000 | 0.80021400 |
| C | -5.15754900 | 3.87096600 | -0.28585500 |
| H | -5.59791300 | 3.78140100 | -1.27694900 |
| C | -3.80145900 | 3.60880700 | -0.09846100 |
| H | -3.18668800 | 3.29206700 | -0.93932100 |
| C | -7.41547800 | 4.54216900 | 0.57565400 |
| C | 1.77399200 | 3.39793400 | 1.41824500 |
| H | 1.09933000 | 4.03662000 | 0.82630800 |
| H | 1.24715300 | 3.14644200 | 2.35558600 |
| C | 3.05117000 | 4.14026800 | 1.71085600 |
| C | 2.98628200 | 5.43561800 | 2.24035900 |
| H | 2.01586800 | 5.90039900 | 2.42516900 |
| C | 4.14824000 | 6.16043200 | 2.49001700 |
| H | 4.08456700 | 7.18100000 | 2.86896800 |
| C | 5.39799000 | 5.59164800 | 2.21671100 |
| C | 5.47299000 | 4.29829700 | 1.69370200 |
| H | 6.44512500 | 3.85536500 | 1.47091800 |
| C | 4.30385500 | 3.57796800 | 1.44346800 |
| H | 4.36244900 | 2.57675000 | 1.02257900 |
| C | 6.65711400 | 6.35870400 | 2.52480500 |
| C | 3.61956700 | 0.91175200 | -1.68625300 |
| H | 3.41571700 | 1.11500200 | -2.74818800 |
| H | 3.33175900 | 1.81064700 | -1.12566300 |
| C | 5.08408200 | 0.62620700 | -1.48851200 |
| C | 5.58722900 | -0.67393800 | -1.61918800 |
| H | 4.90414600 | -1.49445700 | -1.83218100 |
| C | 6.94829100 | -0.92235000 | -1.45421800 |
| H | 7.34154300 | -1.92969400 | -1.56796400 |
| C | 7.81831100 | 0.12385400 | -1.13540000 |
| C | 7.32804400 | 1.42832400 | -1.01329200 |
| H | 8.00961200 | 2.24729300 | -0.77710100 |
| C | 5.96732900 | 1.67376500 | -1.19427800 |
| H | 5.58778400 | 2.69374900 | -1.10184300 |
| C | 9.26384900 | -0.16964600 | -0.83745100 |

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|---|------------|-------------|------------|
| C | 3.58097900 | -0.17684900 | 1.88129400 |
| H | 3.82871700 | 0.08727000 | 0.84688300 |
| H | 3.53292600 | 0.76656800 | 2.45392700 |
| C | 4.66198000 | -1.06741300 | 2.42848100 |
| C | 5.98188400 | -0.85793900 | 2.00802200 |
| H | 6.20558400 | -0.06925200 | 1.28726300 |
| C | 7.01407600 | -1.67243700 | 2.46993300 |
| H | 8.03054300 | -1.52286100 | 2.10814000 |
| C | 6.72704500 | -2.71044600 | 3.36097000 |
| C | 5.41501300 | -2.91290300 | 3.80590300 |
| H | 5.19987700 | -3.72132200 | 4.50706200 |
| C | 4.38728500 | -2.09251100 | 3.34139400 |
| H | 3.36023900 | -2.25769300 | 3.66967100 |
| C | 7.79738800 | -3.69323700 | 3.75458300 |

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| F | 4.81432000 | 0.09816000 | -5.84577500 |
| F | 5.74857200 | -0.15585400 | -3.90948000 |
| F | 6.24222700 | -1.50496900 | -5.53010500 |
| F | 4.96801800 | -5.31078000 | -2.61808800 |
| F | 3.33555200 | -6.11180500 | -3.79259800 |
| F | 2.95866800 | -5.37496100 | -1.79629900 |
| F | 0.70393100 | -4.24627300 | 4.85362100 |
| F | 2.82242200 | -4.20960400 | 4.44317300 |
| F | 1.93333500 | -5.97121200 | 5.33542300 |
| F | 1.52751100 | -9.13389300 | -0.03352600 |
| F | 1.88659800 | -9.56325400 | 2.06306700 |
| F | -0.13746800 | -9.32787400 | 1.33232400 |
| F | -5.76567700 | -6.42890700 | -2.94631400 |
| F | -6.74791700 | -6.42627800 | -1.01830000 |
| F | -7.84512400 | -5.83175100 | -2.78847000 |
| F | -8.82539700 | -1.32095700 | -0.65272000 |
| F | -8.24029900 | -0.56282700 | -2.59013200 |
| F | -7.25723300 | 0.17087000 | -0.80648300 |
| F | -8.24752500 | 3.24716700 | 2.96202400 |
| F | -8.92779900 | 1.85165400 | 1.45643700 |
| F | -9.26501600 | 3.97730300 | 1.19108900 |
| F | -6.11410700 | 6.34921400 | -1.56518600 |
| F | -4.12292000 | 6.28265200 | -0.71238800 |
| F | -4.57524400 | 5.12197200 | -2.47784400 |
| F | 2.50798800 | 6.02595500 | 0.36976100 |
| F | 2.31788300 | 7.06253400 | -1.51928900 |
| F | 4.20820600 | 7.09140300 | -0.45347000 |

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| F | 7.43195300 | 3.54839500 | -1.25252800 |
| F | 7.11167700 | 2.82477300 | -3.26663000 |
| F | 6.65502000 | 1.54650600 | -1.58507500 |
| F | -3.13567700 | -3.78663900 | -4.43860400 |
| F | -5.08447400 | -2.91305400 | -4.79629700 |
| F | -3.84732000 | -3.52771300 | -6.46896300 |
| F | -0.73037800 | 1.68831900 | -7.62719200 |
| F | 0.59124000 | 0.19361600 | -6.78929700 |
| F | -0.75517000 | -0.33622400 | -8.40492800 |
| O | -0.36709900 | -3.07202200 | 0.34413800 |
| O | -2.77427000 | -1.16904900 | -0.80271500 |
| O | -2.49809900 | 1.74234600 | 0.58904900 |
| O | -1.35691300 | 1.40997600 | -2.41638800 |
| O | 1.80776100 | 0.87522800 | -2.41117700 |
| O | -0.17677600 | -1.75344900 | -2.55754200 |
| C | 0.36776800 | -1.48995300 | -3.84807100 |
| H | 0.34494700 | -0.41835400 | -4.07313200 |
| H | -0.29324800 | -2.00338800 | -4.56193700 |
| C | 1.77690100 | -2.02263300 | -3.95375800 |
| C | 2.80249400 | -1.24974000 | -4.50343800 |
| H | 2.58481700 | -0.25840200 | -4.89910000 |
| C | 4.11392200 | -1.73431400 | -4.52535500 |
| C | 4.41964900 | -2.99623000 | -4.00832700 |
| H | 5.44944000 | -3.35303700 | -3.99179900 |
| C | 3.38963700 | -3.77366400 | -3.47580500 |
| C | 2.07888600 | -3.29333200 | -3.45637000 |
| H | 1.28473100 | -3.89974700 | -3.02274300 |
| C | 5.23226400 | -0.83050900 | -4.97553300 |
| C | 3.67275900 | -5.14815300 | -2.92150300 |
| C | 0.37884700 | -4.10086200 | -0.28092100 |
| H | 1.26908600 | -3.68833600 | -0.77379400 |
| H | -0.24550100 | -4.58788300 | -1.04856800 |
| C | 0.79134900 | -5.10746200 | 0.76409300 |
| C | 1.12620500 | -4.65662800 | 2.04288600 |
| H | 1.09322900 | -3.58904600 | 2.25519000 |
| C | 1.45790400 | -5.56207500 | 3.05086300 |
| C | 1.48932600 | -6.93148300 | 2.78933400 |
| H | 1.74755500 | -7.64143700 | 3.57397900 |
| C | 1.17341300 | -7.38015700 | 1.50473500 |
| C | 0.82276800 | -6.47784600 | 0.49804500 |
| H | 0.55621900 | -6.85005400 | -0.49235200 |
| C | 1.73868800 | -5.01577100 | 4.42467400 |
| C | 1.11882100 | -8.85995300 | 1.21602300 |

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| C | -2.98177200 | -2.52322700 | -1.16396600 |
| H | -2.61475800 | -3.18842800 | -0.36904100 |
| H | -2.39507200 | -2.75440300 | -2.06962800 |
| C | -4.44305600 | -2.77750500 | -1.41204800 |
| C | -5.39564200 | -1.76339600 | -1.29124600 |
| H | -5.08550400 | -0.76176800 | -1.00585300 |
| C | -6.74711800 | -2.03213800 | -1.50971200 |
| C | -7.16802700 | -3.32099700 | -1.83809600 |
| H | -8.22572300 | -3.54035300 | -1.98381100 |
| C | -6.21536900 | -4.33464500 | -1.95274600 |
| C | -4.86082400 | -4.06632900 | -1.75387500 |
| H | -4.13007900 | -4.86974800 | -1.85238400 |
| C | -7.77160000 | -0.93123800 | -1.38319900 |
| C | -6.64820400 | -5.75860700 | -2.19031700 |
| C | -3.77396000 | 1.26592900 | 0.96757600 |
| H | -3.77789500 | 1.03902500 | 2.04244000 |
| H | -4.00277300 | 0.31911600 | 0.45421400 |
| C | -4.81141100 | 2.30758600 | 0.65224100 |
| C | -4.50915400 | 3.39514400 | -0.16798900 |
| H | -3.50739700 | 3.49120600 | -0.58312800 |
| C | -5.47490400 | 4.36946500 | -0.43245900 |
| C | -6.74962300 | 4.27400500 | 0.12401400 |
| H | -7.49814000 | 5.04116500 | -0.06798900 |
| C | -7.04867400 | 3.18090500 | 0.94205800 |
| C | -6.09352300 | 2.19749400 | 1.19827000 |
| H | -6.34523700 | 1.34707700 | 1.83434800 |
| C | -5.08225100 | 5.53899600 | -1.29756800 |
| C | -8.38508300 | 3.06616000 | 1.62906800 |
| C | 1.77906300 | 2.10889500 | -3.11196300 |
| H | 0.79801400 | 2.59461300 | -3.04460100 |
| H | 1.96038000 | 1.87986900 | -4.17649100 |
| C | 2.86348500 | 3.01892200 | -2.58957100 |
| C | 2.56928400 | 4.28205600 | -2.07737600 |
| H | 1.54459100 | 4.64818000 | -2.09590700 |
| C | 3.57540900 | 5.05806600 | -1.49261900 |
| C | 4.89652000 | 4.60633100 | -1.45735500 |
| H | 5.67539100 | 5.20710900 | -0.99022200 |
| C | 5.19358300 | 3.35235300 | -2.00050800 |
| C | 4.18382500 | 2.55850500 | -2.54598200 |
| H | 4.42606500 | 1.56930700 | -2.93436500 |
| C | 6.60695000 | 2.82550100 | -2.02438400 |
| C | 3.16738700 | 6.32593100 | -0.78945900 |
| C | -2.71496900 | 1.30851700 | -2.84889700 |

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|---|-------------|-------------|-------------|
| H | -3.07077800 | 2.32870500 | -3.05066300 |
| H | -3.34757300 | 0.85618800 | -2.07650200 |
| C | -2.70035300 | 0.47104900 | -4.10341700 |
| C | -3.36407200 | -0.75313900 | -4.17257300 |
| H | -4.01054500 | -1.07005000 | -3.35604600 |
| C | -3.18718400 | -1.59118700 | -5.27885800 |
| C | -2.34376500 | -1.21610200 | -6.32470600 |
| H | -2.18817300 | -1.87881500 | -7.17555400 |
| C | -1.68865500 | 0.01789000 | -6.25769800 |
| C | -1.87690500 | 0.86442900 | -5.16609500 |
| H | -1.35234300 | 1.82005100 | -5.12269300 |
| C | -3.82683300 | -2.95633500 | -5.25950400 |
| C | -0.65683900 | 0.39552400 | -7.28924400 |
| B | -0.19845800 | -1.70940200 | 0.12654100 |
| B | -1.54614500 | -0.68153500 | -0.39055900 |
| B | -1.43054300 | 0.90260200 | 0.32086100 |
| B | -0.78086800 | 0.76734100 | -1.34771600 |
| B | -0.02443100 | -0.95456500 | -1.44967800 |
| B | 0.95992200 | 0.55276400 | -1.34277900 |
| F | -4.81411000 | -0.09867000 | 5.84565500 |
| F | -5.74852400 | 0.15564100 | 3.90947200 |
| F | -6.24205200 | 1.50449800 | 5.53034900 |
| F | -4.96812000 | 5.31047600 | 2.61825200 |
| F | -3.33590200 | 6.11159300 | 3.79303700 |
| F | -2.95867700 | 5.37497000 | 1.79671800 |
| F | -0.70436900 | 4.24632000 | -4.85343400 |
| F | -2.82284700 | 4.21001600 | -4.44288900 |
| F | -1.93350100 | 5.97147500 | -5.33516700 |
| F | -1.52729400 | 9.13394300 | 0.03391800 |
| F | -1.88661900 | 9.56338400 | -2.06261600 |
| F | 0.13753000 | 9.32793800 | -1.33212200 |
| F | 5.76582000 | 6.42924800 | 2.94542800 |
| F | 6.74822300 | 6.42624400 | 1.01749700 |
| F | 7.84525200 | 5.83196700 | 2.78785800 |
| F | 8.82601800 | 1.32118000 | 0.65354000 |
| F | 8.23938600 | 0.56213400 | 2.59013700 |
| F | 7.25750000 | -0.17047800 | 0.80541100 |
| F | 8.24700000 | -3.24833600 | -2.96235700 |
| F | 8.92767400 | -1.85253600 | -1.45721400 |
| F | 9.26470700 | -3.97815900 | -1.19141700 |
| F | 6.11389600 | -6.34925700 | 1.56566600 |
| F | 4.12256200 | -6.28258000 | 0.71321700 |
| F | 4.57536800 | -5.12164100 | 2.47838000 |

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| F | -2.50781100 | -6.02589900 | -0.36979600 |
| F | -2.31792300 | -7.06253800 | 1.51924000 |
| F | -4.20815800 | -7.09127800 | 0.45326600 |
| F | -7.43173500 | -3.54794200 | 1.25198600 |
| F | -7.11166500 | -2.82459200 | 3.26622300 |
| F | -6.65466000 | -1.54615900 | 1.58489700 |
| F | 3.13525300 | 3.78688700 | 4.43840500 |
| F | 5.08417000 | 2.91354100 | 4.79602600 |
| F | 3.84703700 | 3.52814100 | 6.46873400 |
| F | 0.73068700 | -1.68815700 | 7.62736900 |
| F | -0.59112100 | -0.19365100 | 6.78942400 |
| F | 0.75528000 | 0.33643600 | 8.40498100 |
| O | 0.36713800 | 3.07203900 | -0.34405300 |
| O | 2.77433200 | 1.16909000 | 0.80278800 |
| O | 2.49814000 | -1.74237700 | -0.58895800 |
| O | 1.35698400 | -1.40991300 | 2.41650600 |
| O | -1.80763600 | -0.87521800 | 2.41131200 |
| O | 0.17684300 | 1.75346200 | 2.55763400 |
| C | -0.36766700 | 1.48990800 | 3.84816900 |
| H | -0.34478500 | 0.41830300 | 4.07319000 |
| H | 0.29333300 | 2.00335700 | 4.56204300 |
| C | -1.77683100 | 2.02250500 | 3.95388900 |
| C | -2.80237800 | 1.24951900 | 4.50352500 |
| H | -2.58464200 | 0.25816800 | 4.89912300 |
| C | -4.11383400 | 1.73401400 | 4.52546300 |
| C | -4.41963400 | 2.99594500 | 4.00850900 |
| H | -5.44944800 | 3.35268800 | 3.99199300 |
| C | -3.38966500 | 3.77347000 | 3.47603000 |
| C | -2.07888900 | 3.29321300 | 3.45657400 |
| H | -1.28477200 | 3.89969500 | 3.02297500 |
| C | -5.23213100 | 0.83012900 | 4.97558900 |
| C | -3.67287700 | 5.14797700 | 2.92181400 |
| C | -0.37878500 | 4.10087900 | 0.28103800 |
| H | -1.26901100 | 3.68836400 | 0.77394300 |
| H | 0.24560000 | 4.58787700 | 1.04866900 |
| C | -0.79131700 | 5.10752300 | -0.76392800 |
| C | -1.12627300 | 4.65674800 | -2.04271500 |
| H | -1.09334900 | 3.58917400 | -2.25506000 |
| C | -1.45803400 | 5.56224400 | -3.05063100 |
| C | -1.48940800 | 6.93164000 | -2.78904700 |
| H | -1.74768300 | 7.64163200 | -3.57364300 |
| C | -1.17340300 | 7.38025400 | -1.50445000 |
| C | -0.82270800 | 6.47789700 | -0.49782000 |

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| H | -0.55611000 | 6.85006000 | 0.49258100 |
| C | -1.73897500 | 5.01599600 | -4.42443200 |
| C | -1.11875600 | 8.86003700 | -1.21568800 |
| C | 2.98183700 | 2.52328100 | 1.16398700 |
| H | 2.61473000 | 3.18845400 | 0.36908300 |
| H | 2.39522700 | 2.75446500 | 2.06970600 |
| C | 4.44314400 | 2.77758600 | 1.41189900 |
| C | 5.39572000 | 1.76347600 | 1.29108800 |
| H | 5.08555800 | 0.76182000 | 1.00581300 |
| C | 6.74722300 | 2.03224500 | 1.50939300 |
| C | 7.16815900 | 3.32113600 | 1.83759100 |
| H | 8.22587100 | 3.54051000 | 1.98315100 |
| C | 6.21550200 | 4.33479200 | 1.95225600 |
| C | 4.86094000 | 4.06644800 | 1.75356700 |
| H | 4.13020200 | 4.86987200 | 1.85207300 |
| C | 7.77163100 | 0.93125900 | 1.38304900 |
| C | 6.64837700 | 5.75877600 | 2.18962000 |
| C | 3.77403100 | -1.26603900 | -0.96749400 |
| H | 3.77796900 | -1.03914900 | -2.04236200 |
| H | 4.00291100 | -0.31923500 | -0.45414600 |
| C | 4.81139900 | -2.30778400 | -0.65216500 |
| C | 4.50911400 | -3.39519700 | 0.16825100 |
| H | 3.50740800 | -3.49106600 | 0.58355600 |
| C | 5.47476700 | -4.36961600 | 0.43271200 |
| C | 6.74941100 | -4.27441500 | -0.12397800 |
| H | 7.49784400 | -5.04166300 | 0.06800400 |
| C | 7.04849400 | -3.18146100 | -0.94220600 |
| C | 6.09345000 | -2.19793700 | -1.19838600 |
| H | 6.34519500 | -1.34763200 | -1.83460200 |
| C | 5.08210200 | -5.53894800 | 1.29808800 |
| C | 8.38480200 | -3.06702300 | -1.62946300 |
| C | -1.77895600 | -2.10893200 | 3.11201400 |
| H | -0.79790500 | -2.59464600 | 3.04463900 |
| H | -1.96029700 | -1.87997900 | 4.17655300 |
| C | -2.86337300 | -3.01891000 | 2.58954100 |
| C | -2.56920800 | -4.28205900 | 2.07736200 |
| H | -1.54453400 | -4.64824000 | 2.09595600 |
| C | -3.57533600 | -5.05799700 | 1.49251400 |
| C | -4.89641300 | -4.60616700 | 1.45712900 |
| H | -5.67527900 | -5.20688900 | 0.98991400 |
| C | -5.19344500 | -3.35218500 | 2.00028800 |
| C | -4.18368100 | -2.55841500 | 2.54586100 |
| H | -4.42588500 | -1.56920500 | 2.93423500 |

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| C | -6.60677300 | -2.82521900 | 2.02404400 |
| C | -3.16732900 | -6.32587000 | 0.78935800 |
| C | 2.71505200 | -1.30839100 | 2.84896900 |
| H | 3.07092800 | -2.32855100 | 3.05075600 |
| H | 3.34760100 | -0.85604200 | 2.07654200 |
| C | 2.70040900 | -0.47087500 | 4.10345400 |
| C | 3.36400000 | 0.75338900 | 4.17251600 |
| H | 4.01039800 | 1.07032900 | 3.35594100 |
| C | 3.18705600 | 1.59148300 | 5.27875900 |
| C | 2.34371800 | 1.21636100 | 6.32465900 |
| H | 2.18808400 | 1.87910200 | 7.17547800 |
| C | 1.68873700 | -0.01770400 | 6.25774100 |
| C | 1.87703600 | -0.86428100 | 5.16617700 |
| H | 1.35257100 | -1.81996000 | 5.12284300 |
| C | 3.82654800 | 2.95670200 | 5.25930300 |
| C | 0.65699400 | -0.39539000 | 7.28934300 |
| B | 0.19851600 | 1.70941400 | -0.12644800 |
| B | 1.54621400 | 0.68154900 | 0.39064600 |
| B | 1.43061300 | -0.90259800 | -0.32076500 |
| B | 0.78093900 | -0.76732400 | 1.34780900 |
| B | 0.02448700 | 0.95458100 | 1.44976600 |
| B | -0.95984400 | -0.55275900 | 1.34287400 |

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| O | -0.56489000 | 3.00045000 | -0.65258200 |
| O | -2.46579700 | 0.59106300 | -1.80508800 |
| B | -0.37838800 | 1.63523700 | -0.41704800 |
| B | -1.35339700 | 0.29710400 | -1.05180000 |
| F | -1.94703900 | 2.33877800 | -4.17807400 |
| F | -4.55274200 | 2.69802000 | -4.77293000 |
| F | -6.12872900 | 4.20890400 | -3.16275600 |
| F | -5.05412400 | 5.49917000 | -1.00733100 |
| F | -2.39247200 | 5.28040200 | -0.50675700 |
| F | -4.02940400 | -1.02355000 | -5.14447500 |
| F | -6.44739600 | -0.34473500 | -6.11383800 |
| F | -8.17546400 | 1.11089400 | -4.58759100 |
| F | -7.44241900 | 1.87883600 | -2.06945300 |
| F | -5.06772800 | 1.17870500 | -1.08117700 |
| C | -2.67250900 | 3.15184200 | -3.40727900 |
| C | -2.09080500 | 3.81298200 | -2.32576200 |
| C | -2.91688900 | 4.62679000 | -1.54465600 |
| C | -4.28227100 | 4.75751700 | -1.79479300 |
| C | -4.83472700 | 4.09434200 | -2.89464300 |

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| C | -4.02385500 | 3.31124300 | -3.71628100 |
| C | -4.85777500 | -0.32800600 | -4.36444600 |
| C | -6.10565000 | 0.01968200 | -4.88391800 |
| C | -6.99242800 | 0.76174000 | -4.10351900 |
| C | -6.61627100 | 1.15666300 | -2.81851800 |
| C | -5.37223200 | 0.77763700 | -2.31935300 |
| C | -4.45523700 | 0.04495300 | -3.07792400 |
| C | -0.64787600 | 3.61469700 | -1.92921700 |
| H | -0.12943100 | 3.02472600 | -2.69325200 |
| H | -0.15434000 | 4.59342200 | -1.83596500 |
| C | -3.13113500 | -0.42638600 | -2.54121000 |
| H | -3.29620200 | -1.29034500 | -1.88315800 |
| H | -2.49798900 | -0.75691200 | -3.37341400 |
| O | -0.56455500 | -2.06454500 | -2.27243000 |
| O | -2.46609600 | -1.85857500 | 0.39016200 |
| B | -0.37826700 | -1.17848100 | -1.20755000 |
| B | -1.35352200 | -1.05927200 | 0.26851800 |
| F | -1.93970000 | -4.79069300 | 0.06244900 |
| F | -4.54493700 | -5.48778900 | 0.05226100 |
| F | -6.12467800 | -4.84862200 | -2.05858100 |
| F | -5.05441800 | -3.62469400 | -4.25433800 |
| F | -2.39319000 | -3.07917600 | -4.31862000 |
| F | -4.02164300 | -3.94887600 | 3.45648100 |
| F | -6.43682800 | -5.13339200 | 3.35549700 |
| F | -8.16903400 | -4.54162100 | 1.33460700 |
| F | -7.44328000 | -2.74123500 | -0.58839700 |
| F | -5.07146500 | -1.52879100 | -0.47815500 |
| C | -2.66721600 | -4.52958800 | -1.02570200 |
| C | -2.08781500 | -3.92198000 | -2.13933900 |
| C | -2.91563800 | -3.65245600 | -3.23332200 |
| C | -4.28073800 | -3.93572000 | -3.21968900 |
| C | -4.83095500 | -4.55799200 | -2.09508600 |
| C | -4.01821600 | -4.87807700 | -1.00748600 |
| C | -4.85229600 | -3.62165500 | 2.46585400 |
| C | -6.09865000 | -4.24845500 | 2.42554800 |
| C | -6.98748800 | -3.94480300 | 1.39418600 |
| C | -6.61494800 | -3.02745000 | 0.41011000 |
| C | -5.37249600 | -2.40231600 | 0.48783100 |
| C | -4.45348100 | -2.69170000 | 1.50022400 |
| C | -0.64553900 | -3.47746100 | -2.16700900 |
| H | -0.12604600 | -3.84400600 | -1.27460900 |
| H | -0.15227600 | -3.88487100 | -3.06193600 |
| C | -3.13116500 | -1.98782100 | 1.63943100 |

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|---|-------------|-------------|-------------|
| H | -3.29858000 | -0.98592800 | 2.05769900 |
| H | -2.49660600 | -2.54108400 | 2.34218200 |
| O | -0.56537100 | -0.93497500 | 2.92444100 |
| O | -2.46618800 | 1.26752500 | 1.41420000 |
| B | -0.37867600 | -0.45640200 | 1.62444500 |
| B | -1.35368800 | 0.76233600 | 0.78283900 |
| F | -1.94735200 | 2.44894200 | 4.11560500 |
| F | -4.55361800 | 2.78424600 | 4.72201000 |
| F | -6.13044700 | 0.63416600 | 5.22141400 |
| F | -5.05575700 | -1.87766200 | 5.26193300 |
| F | -2.39345300 | -2.20144300 | 4.82560800 |
| F | -4.02217000 | 4.96872900 | 1.69012400 |
| F | -6.43995200 | 5.47385600 | 2.76046500 |
| F | -8.17384200 | 3.42805800 | 3.25370200 |
| F | -7.44673200 | 0.86232200 | 2.65774700 |
| F | -5.07260800 | 0.35118900 | 1.55914200 |
| C | -2.67327000 | 1.37472500 | 4.43280900 |
| C | -2.09171500 | 0.10748200 | 4.46440200 |
| C | -2.91803900 | -0.97590400 | 4.77780600 |
| C | -4.28370200 | -0.82479600 | 5.01442200 |
| C | -4.83614700 | 0.45928200 | 4.98974000 |
| C | -4.02489500 | 1.56250100 | 4.72404800 |
| C | -4.85344600 | 3.94729900 | 1.90013600 |
| C | -6.10117700 | 4.22597100 | 2.45994700 |
| C | -6.99085700 | 3.18108500 | 2.71021500 |
| C | -6.61768800 | 1.87016700 | 2.40868200 |
| C | -5.37371100 | 1.62468800 | 1.83179700 |
| C | -4.45386500 | 2.64603100 | 1.57858100 |
| C | -0.64867900 | -0.13693800 | 4.09506400 |
| H | -0.13004700 | 0.81970000 | 3.96687700 |
| H | -0.15577200 | -0.70756100 | 4.89607200 |
| C | -3.12968400 | 2.41545700 | 0.90261700 |
| H | -3.29443300 | 2.27973100 | -0.17495400 |
| H | -2.49503900 | 3.30007600 | 1.03430500 |
| O | 0.56490300 | -3.00032900 | 0.65256900 |
| O | 2.46579200 | -0.59093100 | 1.80510900 |
| B | 0.37839500 | -1.63511500 | 0.41705200 |
| B | 1.35339600 | -0.29698000 | 1.05181200 |
| F | 1.94715200 | -2.33876800 | 4.17805300 |
| F | 4.55288600 | -2.69800100 | 4.77278700 |
| F | 6.12882000 | -4.20881900 | 3.16250200 |
| F | 5.05415200 | -5.49898200 | 1.00704600 |
| F | 2.39248200 | -5.28021200 | 0.50657800 |

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|---|------------|-------------|-------------|
| F | 4.02934600 | 1.02367100 | 5.14451700 |
| F | 6.44733200 | 0.34485800 | 6.11390200 |
| F | 8.17543100 | -1.11073500 | 4.58765300 |
| F | 7.44242500 | -1.87863500 | 2.06949000 |
| F | 5.06774000 | -1.17851500 | 1.08119900 |
| C | 2.67260100 | -3.15179500 | 3.40719800 |
| C | 2.09086200 | -3.81289800 | 2.32567700 |
| C | 2.91692700 | -4.62665600 | 1.54449800 |
| C | 4.28232000 | -4.75738200 | 1.79457900 |
| C | 4.83480800 | -4.09425600 | 2.89444100 |
| C | 4.02396000 | -3.31119500 | 3.71614100 |
| C | 4.85773400 | 0.32814600 | 4.36448900 |
| C | 6.10560400 | -0.01954300 | 4.88397100 |
| C | 6.99239700 | -0.76158200 | 4.10357200 |
| C | 6.61626100 | -1.15648400 | 2.81855900 |
| C | 5.37222500 | -0.77746300 | 2.31938600 |
| C | 4.45521400 | -0.04479700 | 3.07795700 |
| C | 0.64791900 | -3.61460500 | 1.92918700 |
| H | 0.12949600 | -3.02465400 | 2.69325300 |
| H | 0.15438200 | -4.59332900 | 1.83592200 |
| C | 3.13111000 | 0.42652700 | 2.54123700 |
| H | 3.29616400 | 1.29049600 | 1.88319400 |
| H | 2.49795300 | 0.75703600 | 3.37344000 |
| O | 0.56456800 | 2.06466900 | 2.27243500 |
| O | 2.46611800 | 1.85867500 | -0.39014300 |
| B | 0.37827100 | 1.17860500 | 1.20755600 |
| B | 1.35352900 | 1.05938900 | -0.26850800 |
| F | 1.93938200 | 4.79114500 | -0.06241900 |
| F | 4.54461600 | 5.48825500 | -0.05249700 |
| F | 6.12463600 | 4.84887500 | 2.05806800 |
| F | 5.05468700 | 3.62465500 | 4.25381100 |
| F | 2.39348000 | 3.07904400 | 4.31836000 |
| F | 4.02164900 | 3.94918800 | -3.45622400 |
| F | 6.43687300 | 5.13362700 | -3.35520100 |
| F | 8.16917200 | 4.54151900 | -1.33449000 |
| F | 7.44347900 | 2.74087500 | 0.58829300 |
| F | 5.07161800 | 1.52851200 | 0.47800900 |
| C | 2.66705300 | 4.52988100 | 1.02559000 |
| C | 2.08780700 | 3.92212200 | 2.13922700 |
| C | 2.91577600 | 3.65247900 | 3.23307000 |
| C | 4.28086700 | 3.93577900 | 3.21929700 |
| C | 4.83092700 | 4.55819800 | 2.09469700 |
| C | 4.01804400 | 4.87839500 | 1.00723800 |

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|---|------------|-------------|-------------|
| C | 4.85234600 | 3.62181100 | -2.46568400 |
| C | 6.09871800 | 4.24857100 | -2.42535600 |
| C | 6.98760300 | 3.94474800 | -1.39408500 |
| C | 6.61509000 | 3.02726800 | -0.41011700 |
| C | 5.37261500 | 2.40218300 | -0.48785600 |
| C | 4.45355500 | 2.69173600 | -1.50016100 |
| C | 0.64553700 | 3.47758800 | 2.16702200 |
| H | 0.12595900 | 3.84415000 | 1.27467900 |
| H | 0.15235500 | 3.88497300 | 3.06200300 |
| C | 3.13121400 | 1.98790900 | -1.63939900 |
| H | 3.29859800 | 0.98602100 | -2.05768800 |
| H | 2.49668500 | 2.54121500 | -2.34214200 |
| O | 0.56537200 | 0.93508300 | -2.92443500 |
| O | 2.46619500 | -1.26739700 | -1.41418700 |
| B | 0.37867800 | 0.45652100 | -1.62443700 |
| B | 1.35369200 | -0.76221200 | -0.78282900 |
| F | 1.94653100 | -2.44919100 | -4.11558300 |
| F | 4.55273300 | -2.78520500 | -4.72188200 |
| F | 6.13017500 | -0.63556100 | -5.22118100 |
| F | 5.05618900 | 1.87656900 | -5.26170800 |
| F | 2.39395000 | 2.20108500 | -4.82548400 |
| F | 4.02228600 | -4.96861300 | -1.68990600 |
| F | 6.44012800 | -5.47373500 | -2.76010900 |
| F | 8.17398000 | -3.42791700 | -3.25339800 |
| F | 7.44675800 | -0.86215900 | -2.65765700 |
| F | 5.07254500 | -0.35102400 | -1.55925200 |
| C | 2.67276700 | -1.37516700 | -4.43271500 |
| C | 2.09156400 | -0.10776200 | -4.46431300 |
| C | 2.91819800 | 0.97540200 | -4.77767200 |
| C | 4.28383100 | 0.82391800 | -5.01422900 |
| C | 4.83592100 | -0.46031500 | -4.98953900 |
| C | 4.02435200 | -1.56331300 | -4.72389900 |
| C | 4.85352500 | -3.94716600 | -1.89997700 |
| C | 6.10129300 | -4.22583700 | -2.45970700 |
| C | 6.99095400 | -3.18094000 | -2.71000200 |
| C | 6.61772600 | -1.87001200 | -2.40858700 |
| C | 5.37370800 | -1.62453400 | -1.83178700 |
| C | 4.45388900 | -2.64588900 | -1.57852700 |
| C | 0.64857100 | 0.13702900 | -4.09505500 |
| H | 0.12970800 | -0.81948700 | -3.96688900 |
| H | 0.15583600 | 0.70776000 | -4.89609300 |
| C | 3.12969600 | -2.41531600 | -0.90258500 |
| H | 3.29444200 | -2.27955600 | 0.17498100 |

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|------------------|-------------|-------------|-------------|
| H | 2.49505900 | -3.29994500 | -1.03425100 |
| [1] ⁺ | | | |
| O | 1.35491200 | -2.76802100 | -0.02311400 |
| O | 2.85547800 | -0.14186300 | -1.24529000 |
| O | 2.31606600 | -0.54521200 | 1.95892700 |
| O | 0.76398700 | 1.88475500 | -2.39941200 |
| O | -2.89036400 | 0.17953900 | 1.16808900 |
| O | -0.17768800 | 1.41882300 | 2.74264200 |
| O | -0.79430900 | -1.83741600 | 2.33696700 |
| O | 1.90911300 | 2.38932200 | 0.61323000 |
| O | 0.11846800 | -1.36900000 | -2.81406100 |
| O | -1.94147100 | -2.34281100 | -0.67622000 |
| O | -1.38620700 | 2.81465100 | -0.02763300 |
| O | -2.34809400 | 0.59688100 | -2.02246900 |
| H | 2.25480000 | -5.24102600 | 0.35335300 |
| H | 5.44629300 | 0.19069800 | -1.75942000 |
| H | 1.33233500 | -5.98452000 | -0.98134400 |
| H | 5.93726200 | -1.46600200 | -1.31564900 |
| H | 2.58443700 | -4.76544600 | -1.33467100 |
| H | 4.84391100 | -1.19983200 | -2.69933600 |
| H | -0.06630800 | -4.25540000 | 0.16345700 |
| H | 4.16977000 | -0.63785700 | 0.26585000 |
| H | 0.28304100 | -3.74740800 | -1.50090000 |
| H | 3.55965500 | -2.00599900 | -0.66776400 |
| H | 4.84451600 | -0.07583700 | 2.74200200 |
| H | 1.31867700 | 3.16726600 | -4.66064900 |
| H | 4.40116600 | 0.51187300 | 4.36581400 |
| H | -0.19212300 | 4.11611100 | -4.71650400 |
| H | 4.02896600 | -1.16804700 | 3.89200800 |
| H | 0.97325700 | 4.37147100 | -3.39087000 |
| H | 2.76810700 | 1.36029100 | 2.63118800 |
| H | -0.66497400 | 1.80216900 | -3.88989400 |
| H | 1.96966200 | 0.31095600 | 3.80949300 |
| H | -0.98261800 | 2.98225400 | -2.60424600 |
| H | -5.34937200 | 0.28345600 | 2.15854600 |
| H | -0.56072200 | 2.83262700 | 4.96055900 |
| H | -6.05038500 | 1.25859000 | 0.83813400 |
| H | -1.73048600 | 1.70836500 | 5.70426000 |
| H | -5.43292000 | -0.38142400 | 0.50491700 |
| H | -0.04966100 | 1.18605200 | 5.41785200 |
| H | -3.72923300 | 2.05734200 | 1.34072100 |
| H | -2.13511900 | 1.85307900 | 3.24007500 |

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|---|-------------|-------------|-------------|
| H | -3.79021900 | 1.35618400 | -0.28522700 |
| H | -1.59396500 | 0.21984700 | 3.66848000 |
| H | -0.98791200 | -4.33248600 | 3.30172900 |
| H | 4.43592000 | 3.15410400 | 1.08883400 |
| H | 0.16819500 | -4.08320100 | 4.63724700 |
| H | 4.51356000 | 4.31348300 | -0.26433300 |
| H | -1.35047500 | -3.14697000 | 4.58387300 |
| H | 3.35413000 | 4.57240700 | 1.06732600 |
| H | 0.96246700 | -2.91849000 | 2.54482100 |
| H | 3.26137400 | 2.22775700 | -0.94874800 |
| H | 0.62294500 | -1.75407500 | 3.83901700 |
| H | 2.21067000 | 3.64869500 | -0.99836900 |
| H | 1.54221000 | -3.37876000 | -3.90710200 |
| H | 2.90478500 | -2.36025300 | -4.44299600 |
| H | 2.56876200 | -2.55119500 | -2.70360800 |
| H | 0.72421000 | -1.16388700 | -4.74655400 |
| H | 1.75215900 | -0.31760200 | -3.55778000 |
| H | -3.70510400 | -4.22906100 | -1.27834900 |
| H | -4.74116400 | -3.99484800 | 0.15618000 |
| H | -4.58130600 | -2.69131500 | -1.05092300 |
| H | -2.33604100 | -3.73036900 | 0.79913700 |
| H | -3.18430000 | -2.18444000 | 0.97935700 |
| H | -2.69515700 | 4.72902800 | 1.31959000 |
| H | -1.43940000 | 5.97614600 | 1.09687400 |
| H | -2.28838700 | 5.30073000 | -0.32032700 |
| H | -0.38773900 | 3.72590300 | 1.54257100 |
| H | 0.02845200 | 4.32075100 | -0.07627600 |
| H | -4.35699500 | 1.07768100 | -3.68673500 |
| H | -4.60780100 | -0.61783100 | -4.18486900 |
| H | -4.89034700 | -0.13481100 | -2.49118800 |
| H | -2.15732600 | -0.16325800 | -3.93228000 |
| H | -2.68583000 | -1.33150800 | -2.70872600 |
| C | 1.79155000 | -5.04946100 | -0.62627800 |
| C | 5.10266600 | -0.85251600 | -1.68781100 |
| C | 0.74487900 | -3.96231700 | -0.52438200 |
| C | 3.91745300 | -0.96818100 | -0.75539600 |
| C | 4.07884900 | -0.12941800 | 3.53138900 |
| C | 0.52086900 | 3.61175300 | -4.04672300 |
| C | 2.73309000 | 0.32867600 | 3.01412200 |
| C | -0.18808500 | 2.55034400 | -3.23428900 |
| C | -5.26051000 | 0.53488200 | 1.09080900 |
| C | -0.88073600 | 1.78081000 | 5.00855600 |
| C | -3.89922600 | 1.12062900 | 0.78306800 |

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|---|-------------|-------------|-------------|
| C | -1.28382100 | 1.27683600 | 3.64014400 |
| C | -0.54537500 | -3.57725000 | 3.96927500 |
| C | 3.83411000 | 3.80739200 | 0.43830100 |
| C | 0.15866700 | -2.50085400 | 3.17246900 |
| C | 2.80006600 | 3.00681500 | -0.32254000 |
| C | 2.10328100 | -2.45647600 | -3.69436300 |
| C | 1.19225600 | -1.24384800 | -3.75303000 |
| C | -4.03934500 | -3.49551400 | -0.52914100 |
| C | -2.86423700 | -2.93629200 | 0.24434800 |
| C | -1.87089200 | 5.05864700 | 0.66868500 |
| C | -0.80960500 | 3.98619300 | 0.55828200 |
| C | -4.24793500 | 0.02924200 | -3.37045400 |
| C | -2.80451300 | -0.29265600 | -3.04819400 |
| B | 0.75035900 | -1.54084000 | -0.01739500 |
| B | 1.59430400 | -0.09755300 | -0.71483300 |
| B | 1.27425400 | -0.29042200 | 1.11157500 |
| B | 0.42799600 | 1.05373000 | -1.36416400 |
| B | -1.62641400 | 0.14138700 | 0.64875300 |
| B | -0.10006600 | 0.81140800 | 1.51866000 |
| B | -0.45985500 | -1.00743500 | 1.29905900 |
| B | 1.04832300 | 1.37146600 | 0.30363100 |
| B | 0.06615700 | -0.76500900 | -1.58944000 |
| B | -1.08130600 | -1.32499000 | -0.36814400 |
| B | -0.78446000 | 1.58662100 | -0.04385900 |
| B | -1.30572200 | 0.34084900 | -1.17624100 |

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|---|-------------|-------------|-------------|
| B | 1.30571800 | -1.10645100 | 0.26205100 |
| B | 0.82695200 | -0.55519300 | -1.43508800 |
| B | -0.26098100 | -1.66931300 | -0.47182900 |
| B | -0.13974000 | -1.17382700 | 1.29515500 |
| B | 1.03828900 | 0.35890300 | 1.35251800 |
| B | 1.59655400 | 0.62122900 | -0.35854200 |
| O | 2.43861700 | -1.85186800 | 0.46137600 |
| C | 2.48710800 | -3.25778600 | 0.62796800 |
| H | 2.02106600 | -3.74157700 | -0.24658200 |
| H | 1.88422700 | -3.53695300 | 1.51108100 |
| C | 3.91105100 | -3.72457800 | 0.77052400 |
| C | 4.99009500 | -2.83837300 | 0.70824800 |
| H | 4.80801200 | -1.76806600 | 0.62929700 |
| C | 6.30067600 | -3.32051000 | 0.76768700 |
| H | 7.13218100 | -2.61407900 | 0.72269700 |
| C | 6.54390800 | -4.68927300 | 0.90047900 |

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|---|-------------|-------------|-------------|
| H | 7.56846800 | -5.06529500 | 0.94624200 |
| C | 5.46536800 | -5.57742300 | 0.98749800 |
| H | 5.64609700 | -6.64878300 | 1.10163700 |
| C | 4.15799900 | -5.09637500 | 0.92206600 |
| H | 3.31857800 | -5.79591500 | 0.96886000 |
| O | 1.44162500 | -0.88201000 | -2.61311400 |
| C | 1.15352100 | -2.03270300 | -3.41270600 |
| H | 1.35268600 | -1.72296300 | -4.45145400 |
| H | 0.08847000 | -2.29150800 | -3.33619400 |
| C | 2.02314700 | -3.20783900 | -3.04197300 |
| C | 3.39288900 | -3.03009500 | -2.79441500 |
| H | 3.82401600 | -2.02927800 | -2.84707400 |
| C | 4.19979700 | -4.12079500 | -2.47158300 |
| H | 5.25898500 | -3.97137800 | -2.25465500 |
| C | 3.64785000 | -5.40392600 | -2.40169400 |
| H | 4.28029200 | -6.25380900 | -2.13891700 |
| C | 2.28673600 | -5.58872600 | -2.65182400 |
| H | 1.84307000 | -6.58471000 | -2.58996900 |
| C | 1.47737800 | -4.49335900 | -2.96823300 |
| H | 0.41172700 | -4.64535600 | -3.14776000 |
| O | -0.42402400 | -3.01282500 | -0.75710400 |
| C | -1.64360600 | -3.53869000 | -1.25574300 |
| H | -1.77486200 | -3.22623800 | -2.30793700 |
| H | -2.48720500 | -3.10979300 | -0.69404500 |
| C | -1.67924700 | -5.04046800 | -1.14982300 |
| C | -0.61692000 | -5.77653500 | -0.61635400 |
| H | 0.28148500 | -5.25416200 | -0.29198900 |
| C | -0.70949900 | -7.16682200 | -0.49940800 |
| H | 0.12530400 | -7.73093500 | -0.07663200 |
| C | -1.86350200 | -7.83407600 | -0.91725400 |
| H | -1.93568900 | -8.91984000 | -0.82400100 |
| C | -2.92668100 | -7.10231300 | -1.45809800 |
| H | -3.83212100 | -7.61594600 | -1.78913600 |
| C | -2.83390700 | -5.71483700 | -1.57262200 |
| H | -3.67186800 | -5.14610400 | -1.98644500 |
| O | -0.13060800 | -2.06431200 | 2.31927200 |
| C | -1.08322800 | -2.17270300 | 3.37856500 |
| H | -1.51827000 | -1.18557500 | 3.59030100 |
| H | -0.50624100 | -2.48862700 | 4.26326000 |
| C | -2.16540400 | -3.18450700 | 3.08687900 |
| C | -3.40193000 | -3.07203900 | 3.73669000 |
| H | -3.59675200 | -2.22144700 | 4.39615200 |
| C | -4.38611800 | -4.04536900 | 3.55455800 |

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| H | -5.34823200 | -3.94527400 | 4.06104400 |
| C | -4.14538700 | -5.13534800 | 2.71331600 |
| H | -4.91701500 | -5.89431400 | 2.56719600 |
| C | -2.92143900 | -5.24250600 | 2.04807500 |
| H | -2.72792300 | -6.08367800 | 1.38075800 |
| C | -1.93398000 | -4.27171600 | 2.23701600 |
| H | -0.97972900 | -4.35721600 | 1.71841600 |
| O | 1.73980500 | 0.62001700 | 2.48654900 |
| C | 2.40910700 | -0.32598700 | 3.31594100 |
| H | 1.99364900 | -1.33015300 | 3.14823500 |
| H | 2.17268900 | -0.03700700 | 4.35387500 |
| C | 3.90561000 | -0.33552500 | 3.12205500 |
| C | 4.56402500 | 0.64322000 | 2.37292600 |
| H | 3.98824800 | 1.41657000 | 1.86643300 |
| C | 5.95760800 | 0.61994000 | 2.25756600 |
| H | 6.46069400 | 1.38412900 | 1.66482000 |
| C | 6.69893600 | -0.37696200 | 2.89358300 |
| H | 7.78729400 | -0.39190900 | 2.80198500 |
| C | 6.04248000 | -1.36103200 | 3.63979800 |
| H | 6.61377800 | -2.15498800 | 4.12536400 |
| C | 4.65303500 | -1.34190200 | 3.74985000 |
| H | 4.14416700 | -2.12145800 | 4.32395300 |
| O | 2.84706900 | 1.16011800 | -0.52856900 |
| C | 3.87161300 | 0.52256500 | -1.28533200 |
| H | 3.60772100 | 0.58743500 | -2.35449900 |
| H | 3.91061700 | -0.54378200 | -1.02118100 |
| C | 5.20207800 | 1.17624200 | -1.04091600 |
| C | 6.37402200 | 0.42014000 | -1.17130200 |
| H | 6.30803900 | -0.64683000 | -1.40136600 |
| C | 7.62437000 | 1.01574500 | -0.99141900 |
| H | 8.53205600 | 0.41659500 | -1.09324000 |
| C | 7.71228100 | 2.37297800 | -0.66693600 |
| H | 8.68882400 | 2.83928600 | -0.51850000 |
| C | 6.54373800 | 3.12940100 | -0.53156400 |
| H | 6.60406600 | 4.19176100 | -0.28393200 |
| C | 5.29428600 | 2.53560600 | -0.72312000 |
| H | 4.38574900 | 3.13024000 | -0.63301300 |
| B | -0.82680700 | 0.55663100 | 1.43571500 |
| B | -1.30558600 | 1.10783700 | -0.26138300 |
| B | 0.26108300 | 1.67072200 | 0.47248500 |
| B | 0.13989400 | 1.17529000 | -1.29450600 |
| B | -1.03809300 | -0.35750500 | -1.35185100 |
| B | -1.59634900 | -0.61985600 | 0.35919800 |

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| O | -2.43866800 | 1.85292300 | -0.46071400 |
| C | -2.48809500 | 3.25868100 | -0.62826000 |
| H | -2.02296500 | 3.74342400 | 0.24625700 |
| H | -1.88491000 | 3.53774000 | -1.51119900 |
| C | -3.91242100 | 3.72404500 | -0.77203400 |
| C | -4.99057700 | 2.83665500 | -0.71072000 |
| H | -4.80744600 | 1.76657000 | -0.63132700 |
| C | -6.30163700 | 3.31731900 | -0.77166000 |
| H | -7.13238200 | 2.60994600 | -0.72746200 |
| C | -6.54624500 | 4.68577600 | -0.90497300 |
| H | -7.57117700 | 5.06063400 | -0.95197200 |
| C | -5.46859900 | 5.57511800 | -0.99088300 |
| H | -5.65039200 | 6.64626000 | -1.10535800 |
| C | -4.16075000 | 5.09555300 | -0.92395500 |
| H | -3.32207600 | 5.79604300 | -0.96988100 |
| O | -1.44153700 | 0.88346900 | 2.61370700 |
| C | -1.15348100 | 2.03418900 | 3.41326000 |
| H | -1.35334300 | 1.72469300 | 4.45194200 |
| H | -0.08827600 | 2.29253800 | 3.33731200 |
| C | -2.02244200 | 3.20962100 | 3.04187900 |
| C | -3.39192500 | 3.03223900 | 2.79265000 |
| H | -3.82331000 | 2.03149900 | 2.84443200 |
| C | -4.19821300 | 4.12318900 | 2.46911900 |
| H | -5.25715100 | 3.97402500 | 2.25077200 |
| C | -3.64590700 | 5.40622800 | 2.40029200 |
| H | -4.27784800 | 6.25632900 | 2.13700400 |
| C | -2.28506000 | 5.59067500 | 2.65216400 |
| H | -1.84111000 | 6.58658000 | 2.59114700 |
| C | -1.47630500 | 4.49504700 | 2.96917800 |
| H | -0.41081400 | 4.64675400 | 3.14991600 |
| O | -2.84676200 | -1.15898200 | 0.52918200 |
| C | -3.87165700 | -0.52188200 | 1.28590000 |
| H | -3.60770600 | -0.58663300 | 2.35507500 |
| H | -3.91123500 | 0.54441700 | 1.02169300 |
| C | -5.20168000 | -1.17639700 | 1.04131300 |
| C | -6.37413100 | -0.42072400 | 1.16953700 |
| H | -6.30893000 | 0.64663800 | 1.39794900 |
| C | -7.62401100 | -1.01731500 | 0.98960600 |
| H | -8.53209800 | -0.41848400 | 1.08971900 |
| C | -7.71092500 | -2.37511200 | 0.66725300 |
| H | -8.68709800 | -2.84220300 | 0.51883900 |
| C | -6.54185700 | -3.13110700 | 0.53394200 |
| H | -6.60137700 | -4.19390500 | 0.28799900 |

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| C | -5.29289400 | -2.53630000 | 0.72547100 |
| H | -4.38396000 | -3.13055900 | 0.63688100 |
| O | -1.73963400 | -0.61859000 | -2.48585700 |
| C | -2.40960400 | 0.32716900 | -3.31491700 |
| H | -1.99609300 | 1.33187400 | -3.14569500 |
| H | -2.17171500 | 0.03976400 | -4.35295700 |
| C | -3.90629600 | 0.33381100 | -3.12238500 |
| C | -4.56336300 | -0.64543600 | -2.37272500 |
| H | -3.98650200 | -1.41727000 | -1.86518200 |
| C | -5.95703500 | -0.62455500 | -2.25813100 |
| H | -6.45903800 | -1.38912400 | -1.66490900 |
| C | -6.69980000 | 0.37045700 | -2.89541900 |
| H | -7.78823100 | 0.38354800 | -2.80442700 |
| C | -6.04469900 | 1.35500700 | -3.64221700 |
| H | -6.61716100 | 2.14744100 | -4.12890500 |
| C | -4.65517400 | 1.33825100 | -3.75154800 |
| H | -4.14739900 | 2.11819700 | -4.32609500 |
| O | 0.42400900 | 3.01423900 | 0.75772900 |
| C | 1.64342200 | 3.54017500 | 1.25664400 |
| H | 1.77458900 | 3.22758900 | 2.30879700 |
| H | 2.48715200 | 3.11145000 | 0.69498200 |
| C | 1.67885400 | 5.04197400 | 1.15094100 |
| C | 0.61695900 | 5.77781400 | 0.61630400 |
| H | -0.28100800 | 5.25523400 | 0.29105700 |
| C | 0.70939100 | 7.16811700 | 0.49941000 |
| H | -0.12504500 | 7.73203900 | 0.07566400 |
| C | 1.86278000 | 7.83561700 | 0.91853900 |
| H | 1.93484900 | 8.92139400 | 0.82533500 |
| C | 2.92548100 | 7.10409300 | 1.46064600 |
| H | 3.83042000 | 7.61793000 | 1.79273900 |
| C | 2.83286500 | 5.71659900 | 1.57509000 |
| H | 3.67044800 | 5.14806100 | 1.98995000 |
| O | 0.13059600 | 2.06580000 | -2.31860000 |
| C | 1.08289500 | 2.17437500 | -3.37816200 |
| H | 1.51723900 | 1.18712200 | -3.59078000 |
| H | 0.50573900 | 2.49137700 | -4.26236200 |
| C | 2.16584700 | 3.18521000 | -3.08601100 |
| C | 3.40263000 | 3.07167600 | -3.73514200 |
| H | 3.59704200 | 2.22098200 | -4.39459600 |
| C | 4.38760700 | 4.04409000 | -3.55236000 |
| H | 5.34991600 | 3.94316500 | -4.05831300 |
| C | 4.14739100 | 5.13423400 | -2.71118800 |
| H | 4.91965200 | 5.89245500 | -2.56453900 |

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|---|------------|------------|-------------|
| C | 2.92312600 | 5.24251300 | -2.04670400 |
| H | 2.72995700 | 6.08386700 | -1.37949400 |
| C | 1.93491000 | 4.27262900 | -2.23626800 |
| H | 0.98042300 | 4.35899700 | -1.71824300 |

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| B | 0.57915900 | -1.02939500 | -1.28435700 |
| O | 0.84715200 | -1.83910000 | -2.33906000 |
| C | 1.96639800 | -1.74998800 | -3.24080400 |
| H | 2.44589400 | -0.76745500 | -3.14866800 |
| H | 1.53642100 | -1.83465000 | -4.25107700 |
| C | 2.94060300 | -2.86497400 | -2.97115600 |
| C | 2.51855500 | -4.20314500 | -3.02743700 |
| H | 1.48528500 | -4.43414100 | -3.29784100 |
| C | 3.39788600 | -5.24308600 | -2.73607400 |
| H | 3.08584300 | -6.28733100 | -2.76372400 |
| C | 4.71032700 | -4.93325200 | -2.38252400 |
| C | 5.16362400 | -3.61811500 | -2.33484100 |
| H | 6.19822600 | -3.41127200 | -2.05829900 |
| C | 4.26990400 | -2.58720400 | -2.63144200 |
| H | 4.61490200 | -1.55422500 | -2.58086300 |
| F | 5.55101500 | -5.92595300 | -2.07606700 |
| B | -0.91695600 | -1.43124900 | -0.35226700 |
| O | -1.70541100 | -2.53183000 | -0.63424700 |
| C | -1.18003400 | -3.84909000 | -0.70053100 |
| H | -0.55365400 | -4.01885200 | 0.18727300 |
| H | -0.51712200 | -3.93321400 | -1.57905900 |
| C | -2.26822200 | -4.88426000 | -0.74131800 |
| C | -1.95410000 | -6.18359900 | -1.16755600 |
| H | -0.94768700 | -6.40620100 | -1.53340600 |
| C | -2.90319400 | -7.20348600 | -1.12354400 |
| H | -2.67044100 | -8.22025200 | -1.44312000 |
| C | -4.18437400 | -6.90898500 | -0.65967000 |
| C | -4.52831900 | -5.62551800 | -0.24319600 |
| H | -5.54063500 | -5.43482800 | 0.11736700 |
| C | -3.56063600 | -4.62092700 | -0.27582900 |
| H | -3.80851600 | -3.62237400 | 0.07651200 |
| F | -5.10116200 | -7.87729100 | -0.61493100 |
| B | 0.65626500 | 0.85687900 | -1.37984400 |
| B | -1.04323500 | 0.03662300 | -1.40680500 |
| B | 1.04313600 | -0.03606900 | 1.40827000 |
| B | -0.57929700 | 1.02993500 | 1.28572800 |
| B | -0.65631800 | -0.85633300 | 1.38121800 |

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|---|-------------|-------------|-------------|
| O | -1.72853100 | 0.14721100 | -2.56423800 |
| O | 1.22872400 | 1.37534900 | -2.50611100 |
| O | 1.72802600 | -0.14653700 | 2.56594100 |
| O | -0.84753700 | 1.83965600 | 2.34030900 |
| O | -1.22885700 | -1.37510700 | 2.50727400 |
| C | -2.33409500 | -0.90893800 | -3.33146300 |
| C | 0.64876300 | 2.38814500 | -3.34634300 |
| C | 2.33433500 | 0.90960400 | 3.33258000 |
| C | -1.96684700 | 1.74978100 | 3.24187300 |
| C | -0.64859400 | -2.38778100 | 3.34742000 |
| H | -1.81337300 | -1.85446700 | -3.13227000 |
| H | -0.43996500 | 2.40942900 | -3.21507100 |
| H | 1.81379000 | 1.85519300 | 3.13325900 |
| H | -2.44514700 | 0.76663400 | 3.15004500 |
| H | 0.44022000 | -2.40816400 | 3.21671400 |
| H | -2.16418800 | -0.62901200 | -4.38227800 |
| H | 0.87187000 | 2.07134900 | -4.37702800 |
| H | 2.16478600 | 0.63011700 | 4.38356700 |
| H | -1.53735000 | 1.83550500 | 4.25226200 |
| H | -0.87251800 | -2.07170400 | 4.37814800 |
| C | -3.80590500 | -1.03355500 | -3.04480100 |
| C | 1.25113800 | 3.74029700 | -3.06568300 |
| C | 3.80600800 | 1.03406300 | 3.04520700 |
| C | -2.94232800 | 2.86334300 | 2.97106000 |
| C | -1.24969200 | -3.74022600 | 3.06550800 |
| C | -4.65977400 | 0.06823200 | -3.21362200 |
| C | 2.63305500 | 3.94547700 | -3.20689000 |
| C | 4.66024800 | -0.06727600 | 3.21514300 |
| C | -2.52227300 | 4.20211700 | 3.02785000 |
| C | -2.63151200 | -3.94669900 | 3.20577400 |
| H | -4.25040100 | 1.02477100 | -3.54773200 |
| H | 3.27236700 | 3.12220000 | -3.53557300 |
| H | 4.25128900 | -1.02351600 | 3.55062400 |
| H | -1.48968400 | 4.43459900 | 3.29958200 |
| H | -3.27172800 | -3.12421400 | 3.53467300 |
| C | -6.02510600 | -0.04368400 | -2.96309100 |
| C | 3.20152000 | 5.18857800 | -2.93776200 |
| C | 6.02550500 | 0.04485100 | 2.96427200 |
| C | -3.40272700 | 5.24078200 | 2.73535000 |
| C | -3.19874100 | -5.19007900 | 2.93532700 |
| H | -6.70455200 | 0.80071400 | -3.08291000 |
| H | 4.27288500 | 5.36667000 | -3.03777400 |
| H | 6.70530100 | -0.79913400 | 3.08513800 |

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| H | -3.09222400 | 6.28547300 | 2.76342000 |
| H | -4.27000400 | -5.36918600 | 3.03462000 |
| C | -6.53324900 | -1.27054300 | -2.53638400 |
| C | 2.37461700 | 6.22999300 | -2.51810000 |
| C | 6.53318100 | 1.27142900 | 2.53613500 |
| C | -4.71424300 | 4.92904400 | 2.38002800 |
| C | -2.37069700 | -6.23043900 | 2.51529800 |
| C | -5.71450300 | -2.38310900 | -2.37123600 |
| C | 0.99990900 | 6.06299400 | -2.38586500 |
| C | 5.71406100 | 2.38355000 | 2.36994900 |
| C | -5.16558200 | 3.61324900 | 2.33174200 |
| C | -0.99606900 | -6.06212500 | 2.38387800 |
| H | -6.14592700 | -3.32906300 | -2.04110400 |
| H | 0.38162900 | 6.90180600 | -2.06320000 |
| H | 6.14519300 | 3.32931000 | 2.03888900 |
| H | -6.19951600 | 3.40492100 | 2.05381600 |
| H | -0.37689000 | -6.90014200 | 2.06087700 |
| C | -4.34823200 | -2.25593800 | -2.63055700 |
| C | 0.44463800 | 4.81194400 | -2.66486500 |
| C | 4.34786200 | 2.25617000 | 2.62956200 |
| C | -4.27076700 | 2.58362900 | 2.62953500 |
| C | -0.44204500 | -4.81081800 | 2.66418100 |
| H | -3.69941500 | -3.12211500 | -2.50140200 |
| H | -0.63018400 | 4.66835500 | -2.55513100 |
| H | 3.69870700 | 3.12202500 | 2.49983500 |
| H | -4.61417100 | 1.55013100 | 2.57842100 |
| H | 0.63271000 | -4.66618100 | 2.55513200 |
| F | -7.83927000 | -1.37421100 | -2.27357400 |
| F | 2.92158300 | 7.41441300 | -2.22603300 |
| F | 7.83911200 | 1.37523300 | 2.27297700 |
| F | -5.55594400 | 5.92052600 | 2.07241100 |
| F | -2.91645200 | -7.41515100 | 2.22211900 |
| B | -0.72940400 | 1.52675000 | -0.45816400 |
| B | 1.72142600 | -0.08965600 | -0.29672600 |
| B | 0.72946900 | -1.52617400 | 0.45958500 |
| B | 0.91698100 | 1.43172900 | 0.35369900 |
| B | -1.72145700 | 0.09018700 | 0.29812300 |
| O | 1.29184500 | -2.74640000 | 0.79839200 |
| O | 3.08335400 | -0.24326800 | -0.46724100 |
| O | 1.70567100 | 2.53213100 | 0.63576300 |
| O | -1.29176500 | 2.74703400 | -0.79680100 |
| O | -3.08338300 | 0.24388100 | 0.46849700 |
| C | 2.68860500 | -2.99174600 | 0.68824800 |

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| C | 3.96060500 | 0.85486700 | -0.66616500 |
| C | 1.18043800 | 3.84943200 | 0.70234000 |
| C | -2.68844800 | 2.99245300 | -0.68587100 |
| C | -3.96092100 | -0.85420900 | 0.66628600 |
| H | 3.05771800 | -2.57662000 | -0.25950700 |
| H | 3.79489100 | 1.58661800 | 0.13733000 |
| H | 0.55391100 | 4.01926400 | -0.18534000 |
| H | -3.05699700 | 2.57726400 | 0.26208900 |
| H | -3.79456500 | -1.58586300 | -0.13715800 |
| H | 3.21346700 | -2.45509600 | 1.49804500 |
| H | 3.71420100 | 1.35793300 | -1.61722900 |
| H | 0.51774500 | 3.93355000 | 1.58102300 |
| H | -3.21379900 | 2.45584700 | -1.49538400 |
| H | -3.71545600 | -1.35746100 | 1.61752000 |
| C | 3.00997400 | -4.46068600 | 0.72972200 |
| C | 5.40031800 | 0.41988500 | -0.64181600 |
| C | 2.26871800 | 4.88450200 | 0.74283700 |
| C | -3.00996900 | 4.46138500 | -0.72707800 |
| C | -5.40058700 | -0.41912200 | 0.64066200 |
| C | 4.31361700 | -4.85978600 | 1.05863000 |
| C | 6.39180800 | 1.33909000 | -1.01690900 |
| C | 1.95504800 | 6.18359100 | 1.17013100 |
| C | -4.31396600 | 4.86038900 | -1.05469600 |
| C | -6.39251600 | -1.33887700 | 1.01325800 |
| H | 5.04872900 | -4.11004700 | 1.36399600 |
| H | 6.10373600 | 2.33148100 | -1.37564200 |
| H | 0.94904100 | 6.40596800 | 1.53722500 |
| H | -5.04934500 | 4.11060000 | -1.35929600 |
| H | -6.10484500 | -2.33169800 | 1.37111600 |
| C | 4.69700700 | -6.19809600 | 0.98777400 |
| C | 7.74377800 | 1.01306500 | -0.93072000 |
| C | 2.90403400 | 7.20355800 | 1.12550300 |
| C | -4.69737900 | 6.19867600 | -0.98351600 |
| C | -7.74437500 | -1.01293300 | 0.92546500 |
| H | 5.71185100 | -6.51886900 | 1.22641800 |
| H | 8.52561000 | 1.72118800 | -1.20874600 |
| H | 2.67159000 | 8.22015400 | 1.44584400 |
| H | -5.71248500 | 6.51936200 | -1.22115600 |
| H | -8.52652400 | -1.72154700 | 1.20132200 |
| C | 3.75447100 | -7.14675100 | 0.59595100 |
| C | 8.10097900 | -0.25309700 | -0.46895200 |
| C | 4.18465600 | 6.90938400 | 0.65990400 |
| C | -3.75448700 | 7.14742100 | -0.59276800 |

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| C | -8.10106200 | 0.25365200 | 0.46445900 |
| C | 2.44767200 | -6.78335800 | 0.28045100 |
| C | 7.13864900 | -1.18900100 | -0.10139100 |
| C | 4.52818100 | 5.62615300 | 0.24234700 |
| C | -2.44733700 | 6.78413000 | -0.27859200 |
| C | -7.13831800 | 1.19014200 | 0.09947100 |
| H | 1.73567100 | -7.55461400 | -0.01929600 |
| H | 7.45716600 | -2.17022800 | 0.25528900 |
| H | 5.54003900 | 5.43572700 | -0.11963300 |
| H | -1.73506600 | 7.55545300 | 0.02033500 |
| H | -7.45643000 | 2.17172200 | -0.25661300 |
| C | 2.08670600 | -5.43620600 | 0.33986200 |
| C | 5.78858100 | -0.84153200 | -0.18267700 |
| C | 3.56060600 | 4.62148000 | 0.27568700 |
| C | -2.08637000 | 5.43699100 | -0.33821100 |
| C | -5.78830600 | 0.84280600 | 0.18250400 |
| H | 1.07707300 | -5.13963800 | 0.06805800 |
| H | 5.02636300 | -1.55539500 | 0.11954800 |
| H | 3.80807500 | 3.62320300 | -0.07774200 |
| H | -1.07645500 | 5.14049300 | -0.06744700 |
| H | -5.02574200 | 1.55709000 | -0.11784200 |
| F | 4.11036700 | -8.43215500 | 0.52418100 |
| F | 9.39379800 | -0.57453200 | -0.37920100 |
| F | 5.10130800 | 7.87778800 | 0.61447800 |
| F | -4.11037200 | 8.43281800 | -0.52076800 |
| F | -9.39381100 | 0.57494500 | 0.37294200 |

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| B | -0.19066400 | 1.56216100 | 1.20012700 |
| O | -0.53401600 | 2.39809100 | 2.25502400 |
| C | -0.00806600 | 3.71625200 | 2.45930400 |
| H | 0.85744100 | 3.89309500 | 1.80812200 |
| H | 0.32963000 | 3.76085300 | 3.50737700 |
| C | -1.08964500 | 4.73532100 | 2.20795900 |
| C | -2.20712500 | 4.78942800 | 3.05530100 |
| H | -2.24729800 | 4.14881400 | 3.94005900 |
| C | -3.28560800 | 5.62654800 | 2.77106000 |
| H | -4.15888800 | 5.65224500 | 3.42402200 |
| C | -3.24096300 | 6.43187000 | 1.62706300 |
| C | -2.12118500 | 6.42382900 | 0.79176700 |
| H | -2.08899300 | 7.07137100 | -0.08569500 |
| C | -1.05456300 | 5.57070900 | 1.08572100 |
| H | -0.18860300 | 5.54404800 | 0.42462700 |

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| Br | -4.72819300 | 7.52892200 | 1.19146000 |
| B | -1.22631300 | 0.05898900 | 0.97653200 |
| O | -2.31956000 | -0.26234200 | 1.74993300 |
| C | -2.37582900 | -0.11651800 | 3.16038700 |
| H | -2.07674700 | 0.91043100 | 3.43107700 |
| H | -1.63754100 | -0.79559200 | 3.61858300 |
| C | -3.75591900 | -0.43261500 | 3.66994400 |
| C | -4.82788300 | -0.67963200 | 2.80747600 |
| H | -4.66828200 | -0.66407200 | 1.73205500 |
| C | -6.09255500 | -0.99659700 | 3.30389400 |
| H | -6.91617600 | -1.20748800 | 2.62219700 |
| C | -6.28625300 | -1.07871400 | 4.68358300 |
| C | -5.22856200 | -0.83044700 | 5.56543800 |
| H | -5.38793800 | -0.89705800 | 6.64248600 |
| C | -3.97289300 | -0.50615200 | 5.05284100 |
| H | -3.14684000 | -0.32241900 | 5.74601200 |
| Br | -7.99082200 | -1.55892600 | 5.36525100 |
| B | -1.39017200 | 1.35439300 | -0.23086900 |
| O | -2.50342500 | 2.08085200 | -0.43153200 |
| C | -3.44065700 | 2.50282600 | 0.58511200 |
| H | -2.97651100 | 3.33641300 | 1.12508400 |
| H | -3.59033800 | 1.67328400 | 1.28810200 |
| C | -4.73437900 | 2.91469400 | -0.04509300 |
| C | -5.84604700 | 2.06325600 | -0.01223500 |
| H | -5.77731900 | 1.10554700 | 0.50786900 |
| C | -7.04755200 | 2.42656700 | -0.62046900 |
| H | -7.90776800 | 1.75781100 | -0.59937300 |
| C | -7.13563200 | 3.66196800 | -1.26846100 |
| C | -6.04165000 | 4.53478400 | -1.30040600 |
| H | -6.12832700 | 5.50402500 | -1.79257800 |
| C | -4.84784100 | 4.15427300 | -0.68840900 |
| H | -3.99412400 | 4.83412200 | -0.70380600 |
| Br | -8.75375700 | 4.15445500 | -2.12621200 |
| B | 0.28589400 | 2.10790200 | -0.51585200 |
| O | 0.44759600 | 3.44477100 | -0.71852000 |
| C | 0.70362800 | 4.08403100 | -1.96979100 |
| H | 0.17477500 | 5.05078500 | -1.92641000 |
| H | 0.27810500 | 3.49776700 | -2.79468200 |
| C | 2.18481600 | 4.30115800 | -2.17323900 |
| C | 3.02732800 | 4.55460800 | -1.08424300 |
| H | 2.61573500 | 4.58419200 | -0.07543800 |
| C | 4.39798600 | 4.73819800 | -1.26493000 |
| H | 5.04743400 | 4.92454200 | -0.41133000 |

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| C | 4.93229400 | 4.66248200 | -2.55310400 |
| C | 4.10639100 | 4.44552200 | -3.65989000 |
| H | 4.53345400 | 4.39636800 | -4.66233700 |
| C | 2.73552700 | 4.26534300 | -3.46049200 |
| H | 2.09009800 | 4.08667000 | -4.32492000 |
| Br | 6.81527600 | 4.79200600 | -2.78630500 |
| B | 1.43981600 | 1.24124700 | 0.64346200 |
| O | 2.51720100 | 1.84783300 | 1.23136100 |
| C | 3.85264900 | 1.60679300 | 0.80161500 |
| H | 3.88297200 | 1.55416900 | -0.29508400 |
| H | 4.16327000 | 0.62463800 | 1.19437100 |
| C | 4.79871900 | 2.66673700 | 1.28002500 |
| C | 4.38581000 | 3.75703400 | 2.04910100 |
| H | 3.33832600 | 3.84196600 | 2.33886600 |
| C | 5.29994400 | 4.73732300 | 2.44395100 |
| H | 4.97495000 | 5.59188200 | 3.03904000 |
| C | 6.64061100 | 4.61963500 | 2.06541200 |
| C | 7.07286100 | 3.52589000 | 1.30680700 |
| H | 8.12129500 | 3.43781900 | 1.02053000 |
| C | 6.14884700 | 2.55694900 | 0.92135600 |
| H | 6.48743500 | 1.69958200 | 0.33436000 |
| Br | 7.88612200 | 5.95714200 | 2.58220200 |
| B | 0.47048600 | -0.07541200 | 1.53160800 |
| O | 0.76335300 | -0.56514700 | 2.78937900 |
| C | 1.48006700 | 0.12876400 | 3.80915100 |
| H | 1.11014800 | -0.27865400 | 4.76445300 |
| H | 1.23719600 | 1.20158800 | 3.78296300 |
| C | 2.97148400 | -0.07593200 | 3.68439500 |
| C | 3.85740800 | 0.95627900 | 4.01431500 |
| H | 3.47149800 | 1.91328200 | 4.37237500 |
| C | 5.23361500 | 0.80428500 | 3.84209400 |
| H | 5.91288000 | 1.62774800 | 4.06286400 |
| C | 5.72342500 | -0.39669400 | 3.32194600 |
| C | 4.86305000 | -1.46049300 | 3.03706100 |
| H | 5.25713100 | -2.39959300 | 2.65163700 |
| C | 3.49075400 | -1.29282000 | 3.22220800 |
| H | 2.81645200 | -2.10839700 | 2.96135800 |
| Br | 7.57727700 | -0.56532000 | 2.92997000 |
| B | 0.37230800 | -0.71094400 | -1.39821500 |
| O | 0.73061600 | -1.58817100 | -2.41665600 |
| C | 0.11067400 | -2.86572100 | -2.61439000 |
| H | -0.82314400 | -2.93272000 | -2.04356100 |
| H | -0.13980500 | -2.92393900 | -3.68702800 |

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| C | 1.03637200 | -3.99638500 | -2.24001800 |
| C | 2.31090600 | -4.08905800 | -2.81763600 |
| H | 2.63116000 | -3.33624300 | -3.54011800 |
| C | 3.18069400 | -5.12577300 | -2.48476200 |
| H | 4.17711800 | -5.18027900 | -2.92454200 |
| C | 2.76256800 | -6.10255600 | -1.57513000 |
| C | 1.49069000 | -6.04253600 | -1.00133200 |
| H | 1.17047000 | -6.81271000 | -0.29815900 |
| C | 0.63970000 | -4.98363400 | -1.33028800 |
| H | -0.35034900 | -4.93194200 | -0.87375200 |
| Br | 3.94640300 | -7.50958000 | -1.10400000 |
| B | 1.39566200 | 0.79443700 | -1.18491100 |
| O | 2.47117600 | 1.16623400 | -1.95156400 |
| C | 2.75610400 | 0.79490200 | -3.30158800 |
| H | 2.06230200 | 0.01544200 | -3.64335100 |
| H | 2.61382600 | 1.69602000 | -3.91861000 |
| C | 4.18264200 | 0.31115600 | -3.35913600 |
| C | 4.50376700 | -0.94421400 | -3.88421100 |
| H | 3.72439000 | -1.55232200 | -4.34926400 |
| C | 5.80395600 | -1.44921200 | -3.79595700 |
| H | 6.04428500 | -2.43896300 | -4.18610500 |
| C | 6.79192300 | -0.68097100 | -3.17519800 |
| C | 6.50251200 | 0.59784400 | -2.68485400 |
| H | 7.28560000 | 1.20653900 | -2.23084600 |
| C | 5.19980800 | 1.08440100 | -2.78008700 |
| H | 4.96899000 | 2.07155900 | -2.38051300 |
| Br | 8.54043600 | -1.39374300 | -2.96030100 |
| B | 1.55419100 | -0.49380800 | 0.03040000 |
| O | 2.64610600 | -1.23586000 | 0.26131800 |
| C | 3.66143200 | -1.62369700 | -0.67032300 |
| H | 3.16472700 | -1.93468500 | -1.60071700 |
| H | 4.28725700 | -0.75175700 | -0.89919000 |
| C | 4.47719200 | -2.73502300 | -0.08821500 |
| C | 5.87125600 | -2.72609500 | -0.19371100 |
| H | 6.37827100 | -1.89674200 | -0.68976100 |
| C | 6.63279300 | -3.76868500 | 0.33985500 |
| H | 7.71966300 | -3.75719500 | 0.25442500 |
| C | 5.98561400 | -4.81778800 | 0.99658500 |
| C | 4.59060300 | -4.83683300 | 1.11941800 |
| H | 4.10008200 | -5.66844400 | 1.62508700 |
| C | 3.84449600 | -3.79990100 | 0.56658100 |
| H | 2.75572700 | -3.81521500 | 0.64067400 |
| Br | 7.00143000 | -6.24991400 | 1.71802200 |

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| B | -0.12015200 | -1.25592100 | 0.31507200 |
| O | -0.26211200 | -2.59388900 | 0.50256100 |
| C | -0.48177900 | -3.26224700 | 1.74490900 |
| H | 0.06109400 | -4.21867700 | 1.66490300 |
| H | -0.04433300 | -2.68735000 | 2.57200800 |
| C | -1.95291800 | -3.51414600 | 1.98015900 |
| C | -2.81946200 | -3.74703200 | 0.90515600 |
| H | -2.44159200 | -3.69650700 | -0.11532000 |
| C | -4.16884500 | -4.02783600 | 1.11800300 |
| H | -4.83441900 | -4.20602600 | 0.27423500 |
| C | -4.65704700 | -4.07821200 | 2.42589400 |
| C | -3.81226200 | -3.84620300 | 3.51378900 |
| H | -4.20816200 | -3.86588900 | 4.52950700 |
| C | -2.46462900 | -3.56280700 | 3.28261800 |
| H | -1.80725000 | -3.37555000 | 4.13612100 |
| Br | -6.49839200 | -4.44579400 | 2.71992700 |
| B | -1.26459200 | -0.39230900 | -0.85218000 |
| O | -2.32057300 | -1.01959100 | -1.45569600 |
| C | -3.66802900 | -0.84345500 | -1.04361200 |
| H | -3.70694600 | -0.79932200 | 0.05306400 |
| H | -4.02108600 | 0.12698400 | -1.43083700 |
| C | -4.55753300 | -1.94847500 | -1.53460500 |
| C | -4.07225700 | -3.04816900 | -2.24649700 |
| H | -3.01199400 | -3.10242400 | -2.49069500 |
| C | -4.93089600 | -4.07163200 | -2.65336700 |
| H | -4.54722100 | -4.93130900 | -3.20448700 |
| C | -6.29236600 | -3.98939100 | -2.34653300 |
| C | -6.79777800 | -2.88898500 | -1.64620900 |
| H | -7.86232900 | -2.82569500 | -1.41919500 |
| C | -5.92652600 | -1.87748800 | -1.24663400 |
| H | -6.32601400 | -1.01330700 | -0.71078700 |
| Br | -7.46546100 | -5.38193700 | -2.88576600 |
| B | -0.31023000 | 0.92683600 | -1.73383400 |
| O | -0.59525600 | 1.40777300 | -2.99565700 |
| C | -1.19149200 | 0.65228400 | -4.04677300 |
| H | -0.84107000 | 1.11609200 | -4.98349100 |
| H | -0.82040100 | -0.38354800 | -4.02650600 |
| C | -2.70061200 | 0.66521400 | -3.99210300 |
| C | -3.42385100 | -0.45287700 | -4.42494100 |
| H | -2.89375500 | -1.34306200 | -4.77219100 |
| C | -4.81771900 | -0.46676200 | -4.38838500 |
| H | -5.37166800 | -1.35273300 | -4.69944800 |
| C | -5.49540300 | 0.65331300 | -3.90136500 |

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|----|-------------|------------|-------------|
| C | -4.79502800 | 1.78637100 | -3.47814000 |
| H | -5.33198300 | 2.65471400 | -3.10014500 |
| C | -3.39995700 | 1.78679900 | -3.52904100 |
| H | -2.85249000 | 2.66011500 | -3.17332400 |
| Br | -7.39265700 | 0.61873600 | -3.78007400 |

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| I | -7.88488100 | 1.35885100 | -3.98272200 |
| I | -9.72732400 | -1.30103900 | -1.11708700 |
| I | -5.69729300 | -4.29266700 | 5.11119300 |
| I | -8.69934100 | 1.62839900 | 2.53135500 |
| I | 4.92336400 | 6.71917800 | 2.64536800 |
| I | -8.23389000 | 5.86591000 | 0.87177100 |
| O | -1.00228300 | 1.05209900 | -2.78539500 |
| O | -2.68294700 | -1.18612900 | -1.03086000 |
| O | -0.48453600 | -3.03495700 | 0.55169500 |
| O | -2.16577100 | -0.73429400 | 2.07678800 |
| O | -0.31877500 | 1.93878300 | 2.42922800 |
| O | -2.44940000 | 1.88588500 | 0.05966600 |
| C | -1.55135300 | 0.29327800 | -3.87493400 |
| H | -1.32000100 | -0.77036800 | -3.74493200 |
| H | -1.03649700 | 0.65025100 | -4.78131400 |
| C | -3.03850200 | 0.50992100 | -3.99765700 |
| C | -3.94435700 | -0.50849700 | -3.68199400 |
| H | -3.57490200 | -1.48895000 | -3.38468300 |
| C | -5.32232900 | -0.27934400 | -3.69878800 |
| H | -6.01112800 | -1.07789000 | -3.42345200 |
| C | -5.79901100 | 0.98881500 | -4.03627100 |
| C | -4.91294900 | 2.01813000 | -4.37992800 |
| H | -5.29027600 | 3.00459600 | -4.65246500 |
| C | -3.54072600 | 1.76765200 | -4.36435200 |
| H | -2.84864300 | 2.57251800 | -4.62740200 |
| C | -3.41750100 | -2.24847300 | -0.40611600 |
| H | -3.17256700 | -2.27366100 | 0.66275700 |
| H | -3.09596600 | -3.19802700 | -0.85546900 |
| C | -4.89015900 | -2.02734100 | -0.59698800 |
| C | -5.49975700 | -0.87228900 | -0.08572900 |
| H | -4.90627500 | -0.13622500 | 0.45890000 |
| C | -6.86683300 | -0.65487500 | -0.24826100 |
| H | -7.33104200 | 0.24147900 | 0.15990000 |
| C | -7.64169000 | -1.60965800 | -0.91653100 |
| C | -7.05478300 | -2.77095200 | -1.42807600 |
| H | -7.65653800 | -3.51893300 | -1.94628600 |

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| C | -5.67990300 | -2.96735600 | -1.26801900 |
| H | -5.22406200 | -3.87278300 | -1.67004900 |
| C | -0.24099200 | -3.76460800 | 1.75422000 |
| H | 0.54020900 | -3.27824400 | 2.35166400 |
| H | 0.12488000 | -4.75462300 | 1.43766900 |
| C | -1.50498200 | -3.91340800 | 2.56236900 |
| C | -1.57466700 | -3.45921200 | 3.88283000 |
| H | -0.69775500 | -2.99345400 | 4.33926700 |
| C | -2.75411600 | -3.58465400 | 4.62398700 |
| H | -2.79421900 | -3.23457600 | 5.65673500 |
| C | -3.88297200 | -4.14935600 | 4.02317900 |
| C | -3.83238700 | -4.61187000 | 2.70212300 |
| H | -4.71282900 | -5.05675700 | 2.23626100 |
| C | -2.64136000 | -4.50099200 | 1.98686800 |
| H | -2.59829800 | -4.86419200 | 0.95829200 |
| C | -2.57424500 | -0.10779600 | 3.30828000 |
| H | -1.91236000 | 0.74038200 | 3.52141700 |
| H | -2.45716700 | -0.87141300 | 4.08845800 |
| C | -4.00822900 | 0.31853900 | 3.18658000 |
| C | -5.04041200 | -0.59728400 | 3.43283700 |
| H | -4.80073700 | -1.61125400 | 3.75435600 |
| C | -6.37575500 | -0.23420600 | 3.26195700 |
| H | -7.16702300 | -0.96084100 | 3.45024500 |
| C | -6.67999300 | 1.06543400 | 2.83976000 |
| C | -5.66610600 | 1.99492500 | 2.59164700 |
| H | -5.90681300 | 3.00366200 | 2.26089500 |
| C | -4.33439200 | 1.61317200 | 2.76099000 |
| H | -3.54278300 | 2.33294700 | 2.54764800 |
| C | -0.54864900 | 3.34420200 | 2.36292900 |
| H | -1.17520700 | 3.58874300 | 3.23677300 |
| H | -1.11368300 | 3.60159700 | 1.45728600 |
| C | 0.74212300 | 4.12612900 | 2.42088300 |
| C | 1.74112900 | 3.78973100 | 3.34384800 |
| H | 1.58974200 | 2.94869100 | 4.02252500 |
| C | 2.93186100 | 4.51523200 | 3.41340000 |
| H | 3.69985400 | 4.23877900 | 4.13732800 |
| C | 3.12320800 | 5.60282400 | 2.55340200 |
| C | 2.13317600 | 5.96257700 | 1.63333900 |
| H | 2.27836300 | 6.81539400 | 0.96850500 |
| C | 0.95340600 | 5.21745800 | 1.57138500 |
| H | 0.18740700 | 5.49235700 | 0.84348800 |
| C | -3.40331400 | 2.07750800 | -0.99599600 |
| H | -3.78244500 | 1.10109900 | -1.32578900 |

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| H | -2.86952200 | 2.51727900 | -1.85199500 |
| C | -4.51978500 | 2.97198200 | -0.54732900 |
| C | -5.84107600 | 2.64344400 | -0.86573000 |
| H | -6.05188800 | 1.72782100 | -1.41655100 |
| C | -6.90142700 | 3.46718500 | -0.48407400 |
| H | -7.92397800 | 3.18672300 | -0.73746100 |
| C | -6.63347500 | 4.63539700 | 0.23407700 |
| C | -5.31520300 | 4.98849600 | 0.55345100 |
| H | -5.11021000 | 5.90439300 | 1.10972500 |
| C | -4.26675500 | 4.15723400 | 0.15633500 |
| H | -3.23961300 | 4.43033200 | 0.40921300 |
| B | -0.61730600 | 0.51515200 | -1.56244700 |
| B | -1.47733000 | -0.72250200 | -0.59016900 |
| B | -0.29900900 | -1.68475100 | 0.35984700 |
| B | -1.17637300 | -0.38179700 | 1.23193200 |
| B | -1.37637800 | 1.06586000 | -0.04300500 |
| B | -0.16813100 | 1.11057800 | 1.32570400 |
| I | 7.88486600 | -1.35888300 | 3.98276500 |
| I | 9.72733100 | 1.30127200 | 1.11734000 |
| I | 5.69730000 | 4.29251700 | -5.11133400 |
| I | 8.69931900 | -1.62848900 | -2.53104600 |
| I | -4.92345400 | -6.71909700 | -2.64547200 |
| I | 8.23399400 | -5.86581300 | -0.87176400 |
| O | 1.00227600 | -1.05215000 | 2.78529400 |
| O | 2.68297200 | 1.18607500 | 1.03073500 |
| O | 0.48455400 | 3.03492300 | -0.55180600 |
| O | 2.16575400 | 0.73429500 | -2.07691300 |
| O | 0.31878600 | -1.93880600 | -2.42932800 |
| O | 2.44942100 | -1.88589300 | -0.05975800 |
| C | 1.55132700 | -0.29335500 | 3.87486100 |
| H | 1.31996500 | 0.77029400 | 3.74489200 |
| H | 1.03646700 | -0.65036300 | 4.78122500 |
| C | 3.03847700 | -0.50999100 | 3.99759600 |
| C | 3.94433300 | 0.50844300 | 3.68198600 |
| H | 3.57488100 | 1.48890600 | 3.38470300 |
| C | 5.32230700 | 0.27929800 | 3.69880500 |
| H | 6.01110900 | 1.07785800 | 3.42351600 |
| C | 5.79898900 | -0.98886800 | 4.03626100 |
| C | 4.91292600 | -2.01819800 | 4.37986900 |
| H | 5.29025400 | -3.00467000 | 4.65238600 |
| C | 3.54070100 | -1.76773100 | 4.36426500 |
| H | 2.84861700 | -2.57260800 | 4.62727700 |
| C | 3.41751100 | 2.24843000 | 0.40600100 |

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| H | 3.17263600 | 2.27357400 | -0.66288900 |
| H | 3.09591300 | 3.19798900 | 0.85529800 |
| C | 4.89016700 | 2.02737000 | 0.59695800 |
| C | 5.49982700 | 0.87229900 | 0.08581600 |
| H | 4.90639300 | 0.13617000 | -0.45877900 |
| C | 6.86690200 | 0.65493800 | 0.24843300 |
| H | 7.33115900 | -0.24143600 | -0.15962900 |
| C | 7.64169600 | 1.60980000 | 0.91666400 |
| C | 7.05472800 | 2.77111700 | 1.42808900 |
| H | 7.65643500 | 3.51915400 | 1.94627200 |
| C | 5.67984800 | 2.96746500 | 1.26795100 |
| H | 5.22395600 | 3.87290500 | 1.66989200 |
| C | 0.24100700 | 3.76456000 | -1.75434200 |
| H | -0.54019500 | 3.27818900 | -2.35178000 |
| H | -0.12486100 | 4.75458200 | -1.43780400 |
| C | 1.50499400 | 3.91334600 | -2.56249600 |
| C | 1.57466400 | 3.45914800 | -3.88295800 |
| H | 0.69774600 | 2.99339100 | -4.33938600 |
| C | 2.75411300 | 3.58456500 | -4.62411900 |
| H | 2.79420800 | 3.23447100 | -5.65686200 |
| C | 3.88297900 | 4.14925200 | -4.02331700 |
| C | 3.83240500 | 4.61178200 | -2.70226700 |
| H | 4.71285600 | 5.05665800 | -2.23641100 |
| C | 2.64138000 | 4.50092300 | -1.98700600 |
| H | 2.59832800 | 4.86412600 | -0.95843100 |
| C | 2.57429400 | 0.10777100 | -3.30837000 |
| H | 1.91241800 | -0.74040700 | -3.52153200 |
| H | 2.45725900 | 0.87137700 | -4.08856400 |
| C | 4.00826900 | -0.31857000 | -3.18658600 |
| C | 5.04047400 | 0.59727700 | -3.43266500 |
| H | 4.80082500 | 1.61127900 | -3.75409400 |
| C | 6.37580100 | 0.23418300 | -3.26169800 |
| H | 7.16708600 | 0.96083900 | -3.44983100 |
| C | 6.68000000 | -1.06549900 | -2.83960000 |
| C | 5.66609300 | -1.99501700 | -2.59167800 |
| H | 5.90676900 | -3.00378500 | -2.26100400 |
| C | 4.33439300 | -1.61324700 | -2.76110400 |
| H | 3.54276500 | -2.33304300 | -2.54790600 |
| C | 0.54862900 | -3.34422900 | -2.36303100 |
| H | 1.17518600 | -3.58878500 | -3.23687100 |
| H | 1.11365300 | -3.60163600 | -1.45738600 |
| C | -0.74215900 | -4.12613100 | -2.42098600 |
| C | -1.74114900 | -3.78973300 | -3.34396900 |

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|---|-------------|-------------|-------------|
| H | -1.58973900 | -2.94870900 | -4.02266000 |
| C | -2.93189300 | -4.51521300 | -3.41352200 |
| H | -3.69987200 | -4.23875700 | -4.13746400 |
| C | -3.12327200 | -5.60278500 | -2.55350600 |
| C | -2.13325700 | -5.96254100 | -1.63342600 |
| H | -2.27846800 | -6.81534400 | -0.96858000 |
| C | -0.95347400 | -5.21744100 | -1.57147200 |
| H | -0.18748900 | -5.49234100 | -0.84356000 |
| C | 3.40328400 | -2.07755600 | 0.99594100 |
| H | 3.78239200 | -1.10116000 | 1.32579800 |
| H | 2.86945500 | -2.51737300 | 1.85189500 |
| C | 4.51978800 | -2.97199800 | 0.54729400 |
| C | 5.84106200 | -2.64343300 | 0.86573300 |
| H | 6.05183800 | -1.72780900 | 1.41656700 |
| C | 6.90144100 | -3.46714100 | 0.48408700 |
| H | 7.92398000 | -3.18665500 | 0.73749900 |
| C | 6.63353400 | -4.63534900 | -0.23408700 |
| C | 5.31527700 | -4.98848000 | -0.55349100 |
| H | 5.11032000 | -5.90437400 | -1.10978300 |
| C | 4.26680100 | -4.15724800 | -0.15638900 |
| H | 3.23967200 | -4.43036800 | -0.40929500 |
| B | 0.61731100 | -0.51518300 | 1.56235200 |
| B | 1.47733500 | 0.72247000 | 0.59007200 |
| B | 0.29901300 | 1.68471900 | -0.35995100 |
| B | 1.17639000 | 0.38176200 | -1.23203600 |
| B | 1.37639000 | -1.06587900 | 0.04289700 |
| B | 0.16814400 | -1.11060400 | -1.32579800 |

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|---|-------------|-------------|-------------|
| F | -8.34395500 | -3.96411700 | -4.44112700 |
| F | -7.39995100 | -5.45840900 | -3.19642300 |
| F | -8.98434900 | -4.21582800 | -2.38654300 |
| F | 4.70085400 | -1.80281400 | -7.43976700 |
| F | 5.17122400 | 0.30949000 | -7.26982500 |
| F | 5.46231500 | -1.00667300 | -5.57554100 |
| F | 9.65441000 | 0.45171400 | -1.84757000 |
| F | 8.97800300 | 0.54171100 | 0.20581500 |
| F | 9.51767300 | -1.36298900 | -0.66683300 |
| F | 7.98677700 | 3.78884100 | -2.48278100 |
| F | 7.66609800 | 5.21189300 | -0.87859500 |
| F | 7.72433100 | 3.09492100 | -0.44485400 |
| F | 7.30704500 | 3.08254300 | 5.84875300 |
| F | 8.87984200 | 2.10118100 | 4.72111300 |

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|---|-------------|-------------|-------------|
| F | 7.54407100 | 0.93679200 | 5.96838600 |
| F | -3.28235700 | 7.65411000 | -1.53655300 |
| F | -3.53472600 | 8.50987700 | 0.43230600 |
| F | -4.84004100 | 6.91043600 | -0.21740300 |
| F | -9.22089200 | -1.08719100 | 0.55621400 |
| F | -9.21199700 | -1.81863300 | 2.59505400 |
| F | -9.80808800 | 0.22425100 | 2.17449600 |
| F | -4.82390400 | 1.80908000 | 6.97279800 |
| F | -5.39118800 | -0.21959900 | 6.44985300 |
| F | -5.51824900 | 1.36031900 | 4.97372800 |
| F | -7.59011400 | 6.63420200 | -2.77712100 |
| F | -8.41711400 | 5.10618200 | -1.47610700 |
| F | -7.18854400 | -5.64660300 | -0.28916900 |
| F | -7.81104400 | -4.04354500 | 1.02434800 |
| F | -7.36851900 | -5.99729400 | 1.84505000 |
| F | 3.18773200 | -7.71691200 | 0.88596800 |
| F | 4.79450100 | -6.71726700 | -0.17779900 |
| F | 3.66972300 | -8.29177800 | -1.14438000 |
| F | 7.80829900 | -1.42983300 | 4.31656400 |
| F | 8.41873900 | -3.34457400 | 3.49772000 |
| F | 8.36123100 | -1.59193400 | 2.22858300 |
| B | 0.17280200 | -1.13554000 | -1.45734900 |
| B | -0.49092500 | -1.51540100 | 0.23809700 |
| B | -1.44222900 | -0.51212800 | -0.98270200 |
| B | -0.18026000 | 0.61194800 | -1.89416700 |
| B | 1.45146600 | 0.15060100 | -1.23037800 |
| B | 1.24359600 | -1.11760000 | 0.03300100 |
| B | 1.46215000 | 0.70425100 | 0.50944200 |
| B | 0.50604700 | 1.71046400 | -0.70281700 |
| B | -1.21707600 | 1.29901700 | -0.49611600 |
| B | -1.41802900 | 0.03683800 | 0.76243100 |
| B | 0.20741300 | -0.41730600 | 1.42789400 |
| B | -0.15476900 | 1.32346200 | 0.99187300 |
| O | -0.47638100 | 1.06465300 | -3.15257400 |
| O | 2.57039100 | 0.31292700 | -2.00847500 |
| O | 0.89481400 | 3.01569500 | -0.92888700 |
| O | 2.54599500 | 1.15675800 | 1.15993700 |
| O | -0.29811700 | 2.23045100 | 2.02305500 |
| O | -2.54460400 | -0.14897400 | 1.52673700 |
| O | 0.48405600 | -0.86489500 | 2.69416600 |
| O | -2.26026300 | 2.14922900 | -0.72121100 |
| O | -2.53332900 | -0.95732000 | -1.63375500 |
| O | -0.91749100 | -2.80332900 | 0.48062600 |

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| O | 0.31097300 | -2.05023900 | -2.48126700 |
| O | 2.27157600 | -1.98795500 | 0.23577700 |
| C | -0.59916300 | 0.26542700 | -4.33433900 |
| H | -1.24436900 | 0.84432800 | -5.01294800 |
| H | -1.10623600 | -0.67945900 | -4.09683600 |
| C | 0.74010400 | 0.00505100 | -4.98074600 |
| C | 1.10283900 | -1.28418000 | -5.38615600 |
| H | 0.41019400 | -2.11342900 | -5.23549900 |
| C | 2.34724600 | -1.52315100 | -5.97138500 |
| H | 2.62593100 | -2.53057400 | -6.28430400 |
| C | 3.24886200 | -0.46815200 | -6.13940500 |
| C | 2.88629100 | 0.83008300 | -5.76327000 |
| H | 3.58476200 | 1.65326300 | -5.92117000 |
| C | 1.63549700 | 1.06166900 | -5.19659900 |
| H | 1.34900500 | 2.07629700 | -4.91601400 |
| C | 4.65058800 | -0.74299800 | -6.62431700 |
| C | 3.35421400 | -0.79799000 | -2.48681700 |
| H | 3.24958700 | -0.79710800 | -3.57855200 |
| H | 2.94982400 | -1.73480800 | -2.09379900 |
| C | 4.80340800 | -0.65650800 | -2.10696100 |
| C | 5.38791900 | -1.54952200 | -1.20005700 |
| H | 4.78679100 | -2.34777300 | -0.76481600 |
| C | 6.72825800 | -1.41705200 | -0.83714600 |
| H | 7.17642200 | -2.10467800 | -0.12061000 |
| C | 7.49402900 | -0.38120300 | -1.38079700 |
| C | 6.92183100 | 0.51237900 | -2.29315800 |
| H | 7.52905700 | 1.30976600 | -2.72075900 |
| C | 5.58342100 | 0.36951000 | -2.65417300 |
| H | 5.13825400 | 1.05951300 | -3.37062800 |
| C | 8.92293200 | -0.19182100 | -0.92944100 |
| C | 1.55431900 | 3.48268400 | -2.09337300 |
| H | 1.10635900 | 4.46294700 | -2.33359300 |
| H | 1.36223800 | 2.81197300 | -2.94134000 |
| C | 3.04307500 | 3.64157000 | -1.88960400 |
| C | 3.89504900 | 3.66041800 | -3.00030100 |
| H | 3.48169400 | 3.54686900 | -4.00543300 |
| C | 5.27281900 | 3.80289500 | -2.83808700 |
| H | 5.93275400 | 3.80186800 | -3.70634700 |
| C | 5.81469100 | 3.91256000 | -1.55461700 |
| C | 4.97029800 | 3.92322300 | -0.44009600 |
| H | 5.39021900 | 4.00815200 | 0.56358400 |
| C | 3.59254500 | 3.79471900 | -0.61087300 |
| H | 2.94008100 | 3.77711400 | 0.26112900 |

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| C | 7.30549300 | 4.00937100 | -1.34412000 |
| C | 3.89908600 | 0.83079600 | 0.83635900 |
| H | 4.15111400 | 1.29718400 | -0.12649400 |
| H | 3.97204000 | -0.25776200 | 0.69829400 |
| C | 4.83171500 | 1.26962100 | 1.92336500 |
| C | 6.20798500 | 1.16906700 | 1.69219900 |
| H | 6.57655400 | 0.86659600 | 0.71469200 |
| C | 7.11973500 | 1.42877400 | 2.71279700 |
| H | 8.18723000 | 1.31817300 | 2.52629000 |
| C | 6.65545500 | 1.80751300 | 3.97512500 |
| C | 5.28251800 | 1.95775300 | 4.20122000 |
| H | 4.92703800 | 2.27649300 | 5.18289400 |
| C | 4.37365000 | 1.68708200 | 3.17820500 |
| H | 3.30274400 | 1.78564300 | 3.35703000 |
| C | 7.61062500 | 1.98779800 | 5.12853500 |
| C | 0.20168000 | 3.56352700 | 2.02975900 |
| H | 1.17122000 | 3.61623600 | 1.51756400 |
| H | 0.36422700 | 3.81923600 | 3.08981400 |
| C | -0.77565600 | 4.53631600 | 1.41572300 |
| C | -0.33640300 | 5.54455300 | 0.54905500 |
| H | 0.72273800 | 5.61694800 | 0.29403600 |
| C | -1.24449400 | 6.45280700 | 0.00221900 |
| H | -0.89776300 | 7.23799500 | -0.67199100 |
| C | -2.60571800 | 6.34904000 | 0.30942500 |
| C | -3.05332800 | 5.34381800 | 1.17127800 |
| H | -4.11620700 | 5.26308300 | 1.40079600 |
| C | -2.13932000 | 4.44866900 | 1.72495000 |
| H | -2.48491000 | 3.66875500 | 2.40410300 |
| C | -3.57557000 | 7.35894800 | -0.25478200 |
| C | -3.38464900 | 0.91288200 | 1.97570200 |
| H | -3.25231700 | 1.79883700 | 1.34255800 |
| H | -3.06305600 | 1.18041400 | 2.99368200 |
| C | -4.82518000 | 0.47912900 | 1.98099500 |
| C | -5.83784200 | 1.42965300 | 1.79629000 |
| H | -5.58054600 | 2.48177200 | 1.65469700 |
| C | -7.17850800 | 1.04499000 | 1.79037100 |
| H | -7.96466000 | 1.78675900 | 1.64100800 |
| C | -7.51407300 | -0.30060200 | 1.97093900 |
| C | -6.51062600 | -1.25041500 | 2.18410000 |
| H | -6.77886300 | -2.29613400 | 2.32234600 |
| C | -5.17294400 | -0.86097200 | 2.18754700 |
| H | -4.39373600 | -1.60839100 | 2.32433300 |
| C | -8.94843800 | -0.74688500 | 1.83901400 |

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| C | 0.55236700 | -0.07738700 | 3.88740000 |
| H | 1.05426800 | 0.87674500 | 3.67937000 |
| H | 1.18082500 | -0.65559100 | 4.58257000 |
| C | -0.81015000 | 0.16408000 | 4.49229300 |
| C | -1.70826700 | -0.89819400 | 4.66144300 |
| H | -1.40443300 | -1.90853700 | 4.38554500 |
| C | -2.98591200 | -0.67916100 | 5.17337000 |
| H | -3.68947600 | -1.50553900 | 5.27941100 |
| C | -3.36801800 | 0.61070300 | 5.55435500 |
| C | -2.46107400 | 1.67042900 | 5.44403700 |
| H | -2.75320200 | 2.67176600 | 5.76513300 |
| C | -1.19404900 | 1.44620400 | 4.90359900 |
| H | -0.50050900 | 2.28101300 | 4.79164900 |
| C | -4.78254600 | 0.88587200 | 6.00288100 |
| C | -2.25460200 | 3.23061900 | -1.64234900 |
| H | -1.80231600 | 2.89981100 | -2.59111100 |
| H | -1.61358600 | 4.03046600 | -1.23659500 |
| C | -3.65225600 | 3.74162400 | -1.86371400 |
| C | -3.85129900 | 4.81562000 | -2.74132300 |
| H | -2.99821900 | 5.27088300 | -3.25033100 |
| C | -5.12724400 | 5.33262700 | -2.94899900 |
| H | -5.27147000 | 6.18651900 | -3.61205200 |
| C | -6.22310200 | 4.77758200 | -2.27970300 |
| C | -6.03431300 | 3.70390600 | -1.40722200 |
| H | -6.88727900 | 3.27372200 | -0.88004700 |
| C | -4.75401100 | 3.18852800 | -1.20323500 |
| H | -4.61064200 | 2.35706100 | -0.51750100 |
| C | -7.61029100 | 5.31617000 | -2.52965100 |
| C | -3.85694100 | -0.42383000 | -1.49147000 |
| H | -3.90062900 | 0.51009000 | -2.07765600 |
| H | -4.03281900 | -0.16385900 | -0.44019200 |
| C | -4.89534000 | -1.40463200 | -1.95517800 |
| C | -4.63630400 | -2.32354600 | -2.98055000 |
| H | -3.65239300 | -2.34698800 | -3.45235100 |
| C | -5.62265300 | -3.22304000 | -3.38013500 |
| H | -5.41619800 | -3.95070500 | -4.16731900 |
| C | -6.87855400 | -3.20761700 | -2.75854500 |
| C | -7.14986300 | -2.28337000 | -1.74834500 |
| H | -8.11686000 | -2.28287900 | -1.24713200 |
| C | -6.15707100 | -1.38660800 | -1.35054100 |
| H | -6.36712500 | -0.68391200 | -0.54346800 |
| C | -7.91630600 | -4.21498500 | -3.19134500 |
| C | -1.52759100 | -3.22879800 | 1.68560400 |

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|---|-------------|-------------|-------------|
| H | -1.56424300 | -2.40319400 | 2.40699600 |
| H | -0.89337300 | -4.02295400 | 2.11883800 |
| C | -2.92379200 | -3.75623400 | 1.45949300 |
| C | -3.67821600 | -4.18787600 | 2.56179300 |
| H | -3.24357100 | -4.16294400 | 3.56512400 |
| C | -4.98245900 | -4.64865500 | 2.39218700 |
| H | -5.56487400 | -4.98250100 | 3.25253200 |
| C | -5.54481300 | -4.68870100 | 1.10978800 |
| C | -4.79409400 | -4.27950000 | 0.00771500 |
| H | -5.22775300 | -4.32277900 | -0.98950700 |
| C | -3.49249000 | -3.80901800 | 0.18487100 |
| H | -2.92332200 | -3.46352200 | -0.67559500 |
| C | -6.98116000 | -5.10974000 | 0.92064400 |
| C | -0.21173900 | -3.37634700 | -2.47657100 |
| H | -0.40143400 | -3.62955600 | -3.53245500 |
| H | -1.16842200 | -3.41511400 | -1.94079000 |
| C | 0.76506100 | -4.36418400 | -1.88610600 |
| C | 0.34879400 | -5.30328300 | -0.93588900 |
| H | -0.68762600 | -5.30477800 | -0.59456800 |
| C | 1.25091800 | -6.23582700 | -0.41914400 |
| H | 0.92254100 | -6.96906600 | 0.31881500 |
| C | 2.58458100 | -6.22031700 | -0.83841200 |
| C | 3.01161400 | -5.28145900 | -1.78640800 |
| H | 4.05260600 | -5.27203700 | -2.11401700 |
| C | 2.10232900 | -4.36541600 | -2.30960900 |
| H | 2.43029900 | -3.64483800 | -3.06040300 |
| C | 3.55829300 | -7.24768700 | -0.31379100 |
| C | 2.33997000 | -3.00409400 | 1.25795000 |
| H | 2.18656000 | -3.97059400 | 0.76086000 |
| H | 1.54074200 | -2.84257300 | 1.99081800 |
| C | 3.69935800 | -2.91970300 | 1.89784500 |
| C | 3.96987600 | -1.89934400 | 2.81962700 |
| H | 3.16546200 | -1.23531500 | 3.14076500 |
| C | 5.26328300 | -1.69553800 | 3.29786100 |
| H | 5.47585200 | -0.88478300 | 3.99405400 |
| C | 6.29913800 | -2.52306200 | 2.85677200 |
| C | 6.03082800 | -3.58319100 | 1.98386700 |
| H | 6.83658200 | -4.24834900 | 1.66775700 |
| C | 4.73548600 | -3.77629600 | 1.50389100 |
| H | 4.53846900 | -4.59014400 | 0.80625300 |
| C | 7.72768000 | -2.22649900 | 3.24310000 |
| F | -8.17957500 | 4.71932100 | -3.59196100 |

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|---|-------------|-------------|-------------|
| F | 4.48393600 | 0.20588600 | -6.08228600 |
| F | 5.48408200 | 0.04304200 | -4.16863700 |
| F | 5.99951600 | -1.31706000 | -5.77483800 |
| F | 4.99101000 | -5.11213700 | -2.75022100 |
| F | 3.41279600 | -6.02464500 | -3.91849900 |
| F | 2.99142800 | -5.30163600 | -1.92486700 |
| F | 0.86017000 | -4.41319600 | 4.81001600 |
| F | 2.93610100 | -4.13239900 | 4.29840600 |
| F | 2.29343100 | -6.00084600 | 5.19186900 |
| F | 1.54039500 | -9.18064200 | -0.12174400 |
| F | 1.87183800 | -9.62376700 | 1.97712500 |
| F | -0.13709800 | -9.29181000 | 1.23900900 |
| F | -5.90275100 | -6.28764200 | -3.13166400 |
| F | -6.77779700 | -6.38070400 | -1.15447900 |
| F | -7.96619900 | -5.68823200 | -2.83054000 |
| F | -8.40832600 | -0.97192100 | -0.12971300 |
| F | -8.64177400 | -0.78011100 | -2.26931200 |
| F | -7.11978800 | 0.37263400 | -1.23595300 |
| F | -8.42185800 | 2.69978700 | 3.03267400 |
| F | -9.02155600 | 1.47417800 | 1.35370200 |
| F | -9.35389700 | 3.61634800 | 1.30032900 |
| F | -6.21192400 | 6.03419200 | -1.40691600 |
| F | -4.19225500 | 5.96072700 | -0.62294000 |
| F | -4.71884000 | 4.77424600 | -2.35034300 |
| F | 2.41587400 | 5.97184400 | 0.49909400 |
| F | 2.21927300 | 7.13637400 | -1.31507200 |
| F | 4.13561000 | 7.02536800 | -0.30052300 |
| F | 7.16392400 | 3.37000600 | -1.29118900 |
| F | 6.82295200 | 2.74042600 | -3.33395800 |
| F | 6.26352000 | 1.43383400 | -1.70451500 |
| F | -2.91855100 | -3.72799600 | -4.51121500 |
| F | -4.93206600 | -3.03681300 | -4.90758600 |
| F | -3.59197900 | -3.47313000 | -6.55792500 |
| F | -1.03035300 | 2.06164900 | -7.46385600 |
| F | 0.46246900 | 0.77878000 | -6.56329200 |
| F | -0.71342800 | 0.06248400 | -8.24242200 |
| O | -0.22925800 | -3.10199000 | 0.28135600 |
| O | -2.78023200 | -1.25026600 | -0.62879700 |
| O | -2.50713200 | 1.57448300 | 0.94282000 |
| O | -1.67035700 | 1.44483900 | -2.16131800 |
| O | 1.43889000 | 1.02101100 | -2.57749000 |
| O | -0.33687000 | -1.68111700 | -2.58618700 |

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|---|-------------|-------------|-------------|
| C | 0.19454600 | -1.52481500 | -3.90805400 |
| H | 0.12104500 | -0.47548800 | -4.21208300 |
| H | -0.46929500 | -2.12139900 | -4.54751000 |
| C | 1.61902000 | -2.00388300 | -4.02994100 |
| C | 2.58991200 | -1.19035500 | -4.62008900 |
| H | 2.31576900 | -0.21273500 | -5.01570600 |
| C | 3.91660000 | -1.62525800 | -4.70085300 |
| C | 4.29261800 | -2.86943100 | -4.18909300 |
| H | 5.33570300 | -3.18575900 | -4.21581300 |
| C | 3.31764300 | -3.68630600 | -3.61224100 |
| C | 1.98833700 | -3.26424100 | -3.55077300 |
| H | 1.23534000 | -3.91114700 | -3.10253100 |
| C | 4.97660600 | -0.67980800 | -5.20931400 |
| C | 3.68930000 | -5.04075400 | -3.05540600 |
| C | 0.54813900 | -4.10901400 | -0.35766000 |
| H | 1.43087800 | -3.66279400 | -0.83360000 |
| H | -0.06638400 | -4.58185400 | -1.14035700 |
| C | 0.95574400 | -5.12940900 | 0.67292600 |
| C | 1.34491000 | -4.68939100 | 1.93938000 |
| H | 1.37456800 | -3.62177500 | 2.14774800 |
| C | 1.65912400 | -5.60261600 | 2.94438200 |
| C | 1.62846000 | -6.97321600 | 2.68676100 |
| H | 1.87552400 | -7.69183500 | 3.46760900 |
| C | 1.26397400 | -7.41268400 | 1.41155300 |
| C | 0.92201700 | -6.50010500 | 0.41043300 |
| H | 0.61179000 | -6.86571500 | -0.56969000 |
| C | 1.95231900 | -5.06000300 | 4.31750500 |
| C | 1.14103200 | -8.89209800 | 1.12619200 |
| C | -3.00522600 | -2.56833900 | -1.10798800 |
| H | -2.63961400 | -3.29675100 | -0.36971200 |
| H | -2.42042700 | -2.72653200 | -2.02952300 |
| C | -4.47088100 | -2.77362400 | -1.37311500 |
| C | -5.39463600 | -1.73520400 | -1.23170300 |
| H | -5.06449900 | -0.75239100 | -0.90773100 |
| C | -6.74821700 | -1.94885900 | -1.49142800 |
| C | -7.20201000 | -3.21167800 | -1.87632600 |
| H | -8.26053500 | -3.38901800 | -2.06761200 |
| C | -6.27969000 | -4.25203300 | -2.00177500 |
| C | -4.92034800 | -4.03497000 | -1.77066000 |
| H | -4.21351900 | -4.85732400 | -1.89136900 |
| C | -7.73903100 | -0.82681600 | -1.28099900 |
| C | -6.74173100 | -5.65881500 | -2.29556100 |
| C | -3.79277900 | 1.05067800 | 1.24672900 |

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|---|-------------|-------------|-------------|
| H | -3.83081600 | 0.82475000 | 2.32005300 |
| H | -3.95406800 | 0.10026300 | 0.71944000 |
| C | -4.84943600 | 2.05750200 | 0.88818200 |
| C | -4.56123800 | 3.13711500 | 0.05254000 |
| H | -3.55259100 | 3.26725500 | -0.33596400 |
| C | -5.55382200 | 4.06715900 | -0.26516400 |
| C | -6.84318000 | 3.93038700 | 0.24745900 |
| H | -7.61564100 | 4.66019600 | 0.00924400 |
| C | -7.12794900 | 2.84497600 | 1.07967600 |
| C | -6.14299600 | 1.91025400 | 1.39784100 |
| H | -6.38320800 | 1.06789300 | 2.04877600 |
| C | -5.18270500 | 5.22192500 | -1.16021400 |
| C | -8.49838700 | 2.66339800 | 1.68716300 |
| C | 1.44749700 | 2.31655600 | -3.18547400 |
| H | 0.48624200 | 2.82221000 | -3.03966600 |
| H | 1.57683300 | 2.13986900 | -4.26417500 |
| C | 2.58001300 | 3.14349900 | -2.63300700 |
| C | 2.34800200 | 4.38955700 | -2.05046500 |
| H | 1.34117200 | 4.80271400 | -2.03225700 |
| C | 3.39704600 | 5.08847400 | -1.44499000 |
| C | 4.69595600 | 4.57499300 | -1.45152400 |
| H | 5.50668200 | 5.11483900 | -0.96381100 |
| C | 4.92844400 | 3.33854200 | -2.06089400 |
| C | 3.87894200 | 2.62466800 | -2.64038800 |
| H | 4.07557300 | 1.65356000 | -3.09423800 |
| C | 6.31044900 | 2.73222500 | -2.10034200 |
| C | 3.05793500 | 6.32848600 | -0.65703100 |
| C | -2.99555200 | 1.25120000 | -2.68900300 |
| H | -3.40993200 | 2.25617400 | -2.84445200 |
| H | -3.61678000 | 0.70788500 | -1.96840800 |
| C | -2.85637400 | 0.49348700 | -3.98249800 |
| C | -3.41569100 | -0.77492600 | -4.13492600 |
| H | -4.05002500 | -1.19164800 | -3.35395600 |
| C | -3.15651000 | -1.52621400 | -5.28481900 |
| C | -2.33785000 | -1.01850400 | -6.29471000 |
| H | -2.11754600 | -1.61326100 | -7.18113300 |
| C | -1.78526400 | 0.25700500 | -6.14086700 |
| C | -2.05321500 | 1.01709900 | -5.00255700 |
| H | -1.61160800 | 2.00871500 | -4.89978700 |
| C | -3.66653800 | -2.94560700 | -5.33588500 |
| C | -0.77951100 | 0.79397900 | -7.12958600 |
| B | -0.11889800 | -1.74241500 | 0.12054100 |
| B | -1.54156600 | -0.74157300 | -0.30910800 |

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|---|-------------|-------------|-------------|
| B | -1.43641800 | 0.81679200 | 0.56033200 |
| B | -0.98954300 | 0.77736900 | -1.21155700 |
| B | -0.10541000 | -0.94600200 | -1.46651300 |
| B | 0.82045300 | 0.66691600 | -1.39791500 |
| F | -4.48430500 | -0.20653200 | 6.08006100 |
| F | -5.48524000 | -0.04157000 | 4.16698300 |
| F | -5.99980000 | 1.31694100 | 5.77480100 |
| F | -4.99222500 | 5.11199700 | 2.74837500 |
| F | -3.41617200 | 6.02539200 | 3.91884300 |
| F | -2.99181800 | 5.30344000 | 1.92543800 |
| F | -0.85851400 | 4.41571100 | -4.81013800 |
| F | -2.93439700 | 4.13410300 | -4.29880900 |
| F | -2.29227000 | 6.00293500 | -5.19186600 |
| F | -1.54098900 | 9.18264000 | 0.12119900 |
| F | -1.86801700 | 9.62596500 | -1.97831800 |
| F | 0.13925500 | 9.29270400 | -1.23623200 |
| F | 5.91029800 | 6.28195500 | 3.13629300 |
| F | 6.78151400 | 6.37685500 | 1.15752200 |
| F | 7.97262200 | 5.68113400 | 2.83035100 |
| F | 8.40463200 | 0.96276400 | 0.12842700 |
| F | 8.64145600 | 0.77326000 | 2.26788300 |
| F | 7.11597900 | -0.37845800 | 1.23844300 |
| F | 8.41551900 | -2.70595900 | -3.04122400 |
| F | 9.01977900 | -1.47670700 | -1.36652500 |
| F | 9.35137800 | -3.61890100 | -1.30901300 |
| F | 6.21255000 | -6.03212800 | 1.40670400 |
| F | 4.19261300 | -5.95974700 | 0.62330700 |
| F | 4.71945900 | -4.77179800 | 2.34960200 |
| F | -2.41492500 | -5.97153500 | -0.49657200 |
| F | -2.21837700 | -7.13553900 | 1.31794300 |
| F | -4.13463000 | -7.02505600 | 0.30317300 |
| F | -7.16443800 | -3.37146300 | 1.29581800 |
| F | -6.82180900 | -2.73968900 | 3.33765500 |
| F | -6.26442300 | -1.43452900 | 1.70638600 |
| F | 2.91916400 | 3.72918000 | 4.51200200 |
| F | 4.93214100 | 3.03746900 | 4.91016800 |
| F | 3.59076600 | 3.47431500 | 6.55932100 |
| F | 1.02887900 | -2.06031400 | 7.46429500 |
| F | -0.46379400 | -0.77769100 | 6.56315300 |
| F | 0.71147500 | -0.06111800 | 8.24259500 |
| O | 0.22908800 | 3.10344000 | -0.28117100 |
| O | 2.77999900 | 1.25117700 | 0.62881800 |
| O | 2.50665500 | -1.57313000 | -0.94268300 |

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|---|-------------|-------------|-------------|
| O | 1.66991400 | -1.44312200 | 2.16167300 |
| O | -1.43916800 | -1.01941700 | 2.57767800 |
| O | 0.33640600 | 1.68274600 | 2.58621700 |
| C | -0.19510400 | 1.52655900 | 3.90806000 |
| H | -0.12138000 | 0.47728900 | 4.21224000 |
| H | 0.46854100 | 2.12338800 | 4.54748200 |
| C | -1.61971800 | 2.00525500 | 4.02973600 |
| C | -2.59049300 | 1.19139200 | 4.61962200 |
| H | -2.31617500 | 0.21380700 | 5.01517800 |
| C | -3.91730700 | 1.62592000 | 4.70019900 |
| C | -4.29357200 | 2.87003500 | 4.18848900 |
| H | -5.33674100 | 3.18610800 | 4.21511300 |
| C | -3.31873800 | 3.68722900 | 3.61183900 |
| C | -1.98930400 | 3.26553500 | 3.55057400 |
| H | -1.23642900 | 3.91268400 | 3.10247500 |
| C | -4.97723100 | 0.68012300 | 5.20818300 |
| C | -3.69079600 | 5.04159700 | 3.05505200 |
| C | -0.54822300 | 4.11053300 | 0.35784000 |
| H | -1.43115100 | 3.66440000 | 0.83353700 |
| H | 0.06620400 | 4.58312600 | 1.14076400 |
| C | -0.95538300 | 5.13111700 | -0.67274700 |
| C | -1.34443400 | 4.69122100 | -1.93929700 |
| H | -1.37442700 | 3.62361400 | -2.14767000 |
| C | -1.65807400 | 5.60452800 | -2.94438200 |
| C | -1.62700600 | 6.97514100 | -2.68676500 |
| H | -1.87360400 | 7.69383800 | -3.46768400 |
| C | -1.26268500 | 7.41448300 | -1.41148600 |
| C | -0.92124600 | 6.50179100 | -0.41026600 |
| H | -0.61107200 | 6.86730200 | 0.56991300 |
| C | -1.95092400 | 5.06204700 | -4.31763700 |
| C | -1.13936500 | 8.89383100 | -1.12594800 |
| C | 3.00622700 | 2.56883400 | 1.10837900 |
| H | 2.64146300 | 3.29781100 | 0.37024700 |
| H | 2.42157700 | 2.72749800 | 2.02992400 |
| C | 4.47216700 | 2.77217200 | 1.37355700 |
| C | 5.39440800 | 1.73244700 | 1.23181000 |
| H | 5.06282400 | 0.75026000 | 0.90743600 |
| C | 6.74826000 | 1.94385100 | 1.49186400 |
| C | 7.20393600 | 3.20581500 | 1.87735000 |
| H | 8.26268100 | 3.38145300 | 2.06895700 |
| C | 6.28318200 | 4.24753200 | 2.00299800 |
| C | 4.92351500 | 4.03267100 | 1.77162800 |
| H | 4.21791800 | 4.85605100 | 1.89263000 |

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| C | 7.73710800 | 0.82014500 | 1.28107100 |
| C | 6.74710000 | 5.65350000 | 2.29771700 |
| C | 3.79219100 | -1.04936700 | -1.24712000 |
| H | 3.82965600 | -0.82302400 | -2.32037800 |
| H | 3.95391400 | -0.09918500 | -0.71955600 |
| C | 4.84880100 | -2.05657700 | -0.88960100 |
| C | 4.56121100 | -3.13551600 | -0.05288700 |
| H | 3.55311000 | -3.26473100 | 0.33735500 |
| C | 5.55362000 | -4.06615800 | 0.26359800 |
| C | 6.84213900 | -3.93079500 | -0.25151300 |
| H | 7.61439200 | -4.66118600 | -0.01440900 |
| C | 7.12627200 | -2.84608500 | -1.08485000 |
| C | 6.14159300 | -1.91058200 | -1.40151700 |
| H | 6.38137400 | -1.06872400 | -2.05325800 |
| C | 5.18306100 | -5.22027700 | 1.15971600 |
| C | 8.49535200 | -2.66647900 | -1.69590400 |
| C | -1.44716200 | -2.31474100 | 3.18612300 |
| H | -0.48580400 | -2.82013500 | 3.04011200 |
| H | -1.57616500 | -2.13776200 | 4.26480800 |
| C | -2.57960900 | -3.14218300 | 2.63431200 |
| C | -2.34735900 | -4.38825800 | 2.05192200 |
| H | -1.34035900 | -4.80100200 | 2.03333800 |
| C | -3.39640800 | -5.08776200 | 1.44716400 |
| C | -4.69553800 | -4.57484400 | 1.45425900 |
| H | -5.50630700 | -5.11519900 | 0.96718000 |
| C | -4.92824500 | -3.33834500 | 2.06346000 |
| C | -3.87874000 | -2.62388200 | 2.64222600 |
| H | -4.07554500 | -1.65275300 | 3.09596200 |
| C | -6.31047500 | -2.73255200 | 2.10353500 |
| C | -3.05708400 | -6.32795000 | 0.65958000 |
| C | 2.99499900 | -1.24951500 | 2.68965100 |
| H | 3.40939900 | -2.25449500 | 2.84501500 |
| H | 3.61633500 | -0.70606200 | 1.96926400 |
| C | 2.85562200 | -0.49201400 | 3.98325500 |
| C | 3.41516800 | 0.77624500 | 4.13607100 |
| H | 4.04983200 | 1.19295300 | 3.35536000 |
| C | 3.15583900 | 1.52740200 | 5.28601800 |
| C | 2.33681300 | 1.01969900 | 6.29560900 |
| H | 2.11637400 | 1.61435900 | 7.18206100 |
| C | 1.78403700 | -0.25569000 | 6.14141400 |
| C | 2.05211600 | -1.01564300 | 5.00303500 |
| H | 1.61034800 | -2.00715500 | 4.90000900 |
| C | 3.66622200 | 2.94665800 | 5.33739600 |

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|---|-------------|-------------|-------------|
| C | 0.77801800 | -0.79270000 | 7.12984300 |
| B | 0.11861700 | 1.74389800 | -0.12040300 |
| B | 1.54117500 | 0.74293500 | 0.30922000 |
| B | 1.43596900 | -0.81539300 | -0.56020300 |
| B | 0.98916200 | -0.77587600 | 1.21171600 |
| B | 0.10502200 | 0.94751500 | 1.46661300 |
| B | -0.82082700 | -0.66544500 | 1.39804200 |

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|---|-------------|-------------|-------------|
| O | -1.33131900 | 2.74292000 | 0.61724100 |
| O | -2.51773600 | 0.79350700 | -1.59441500 |
| B | -0.73762700 | 1.54601500 | 0.31432300 |
| B | -1.38507800 | 0.43466700 | -0.95988100 |
| F | -3.00128600 | 4.63660600 | -2.35365500 |
| F | -5.44446100 | 5.77003500 | -2.07298300 |
| F | -6.42129300 | 6.29803800 | 0.41383000 |
| F | -4.92178600 | 5.74428900 | 2.61646400 |
| F | -2.45535400 | 4.67266900 | 2.34024700 |
| F | -2.12896500 | 2.27464800 | -5.12169700 |
| F | -3.66775600 | 4.31252600 | -6.00709900 |
| F | -6.03709500 | 4.86266000 | -4.78119200 |
| F | -6.86417400 | 3.35946700 | -2.66808000 |
| F | -5.36686000 | 1.27354400 | -1.82233100 |
| C | -3.45797000 | 4.90432100 | -1.12430800 |
| C | -2.66585900 | 4.60862900 | -0.01329100 |
| C | -3.17857100 | 4.92525700 | 1.24903000 |
| C | -4.44847400 | 5.48004400 | 1.40920200 |
| C | -5.22157800 | 5.76186300 | 0.27754200 |
| C | -4.72068700 | 5.48403700 | -0.99723000 |
| C | -3.30556500 | 2.50751700 | -4.52681000 |
| C | -4.08499000 | 3.56599200 | -4.99520900 |
| C | -5.30088100 | 3.84807300 | -4.36894100 |
| C | -5.72578000 | 3.07384300 | -3.28411400 |
| C | -4.93757600 | 2.00980200 | -2.85312600 |
| C | -3.71304200 | 1.70854200 | -3.45747100 |
| C | -1.32995300 | 3.93566000 | -0.16660600 |
| H | -1.13422200 | 3.70902900 | -1.22031900 |
| H | -0.52098900 | 4.58122500 | 0.20664600 |
| C | -2.86795600 | 0.57282700 | -2.96739100 |
| H | -3.43278700 | -0.36858400 | -3.00081400 |
| H | -1.97156300 | 0.46134900 | -3.58191100 |
| O | -0.10801600 | -0.93109300 | -2.98146100 |
| O | -1.90236500 | -2.35597500 | -0.63867200 |

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|---|-------------|-------------|-------------|
| B | -0.04971400 | -0.57010900 | -1.65254500 |
| B | -1.05358800 | -1.36008800 | -0.30655700 |
| F | -0.45181700 | -4.71769900 | -2.24316800 |
| F | -2.77166300 | -6.04819000 | -2.55066500 |
| F | -4.73259300 | -5.02751900 | -4.14741000 |
| F | -4.37131400 | -2.62952100 | -5.38327000 |
| F | -2.00186700 | -1.34159800 | -5.16676100 |
| F | -3.60541200 | -5.67915400 | 0.49054700 |
| F | -5.78109900 | -6.68471800 | -0.76973600 |
| F | -7.30629500 | -5.07288800 | -2.34204100 |
| F | -6.63785400 | -2.45050300 | -2.67303000 |
| F | -4.50071800 | -1.43284900 | -1.36881900 |
| C | -1.38353800 | -4.19959400 | -3.04595800 |
| C | -1.15185000 | -2.98912700 | -3.70146500 |
| C | -2.17899800 | -2.49088800 | -4.50857500 |
| C | -3.40105900 | -3.14866400 | -4.64492800 |
| C | -3.58838200 | -4.37544600 | -4.00181300 |
| C | -2.58048300 | -4.90095300 | -3.19240500 |
| C | -4.34917600 | -4.87530100 | -0.26524400 |
| C | -5.47062200 | -5.40619300 | -0.90782900 |
| C | -6.25757700 | -4.57846000 | -1.71173300 |
| C | -5.91270300 | -3.23282500 | -1.88446000 |
| C | -4.80386500 | -2.72917000 | -1.21489300 |
| C | -3.99062900 | -3.53372900 | -0.41340700 |
| C | 0.13722200 | -2.22105200 | -3.54378400 |
| H | 0.84912400 | -2.78830500 | -2.93357700 |
| H | 0.58421800 | -2.03461300 | -4.53017600 |
| C | -2.80654800 | -2.96231900 | 0.29910300 |
| H | -3.13029900 | -2.19955000 | 1.01956600 |
| H | -2.26814500 | -3.75040200 | 0.83719800 |
| O | -0.31613300 | -2.21588700 | 2.18299400 |
| O | -2.74726000 | -0.00082100 | 1.49503500 |
| B | -0.25801400 | -1.17185900 | 1.27782500 |
| B | -1.52807400 | 0.03672600 | 0.85985900 |
| F | -2.34205800 | -0.06088800 | 4.62397400 |
| F | -4.96917500 | -0.43183700 | 5.10045200 |
| F | -6.17146400 | -2.76284800 | 4.39271200 |
| F | -4.70056100 | -4.78678600 | 3.29369700 |
| F | -2.02272000 | -4.48705800 | 2.99924900 |
| F | -4.48438500 | 2.91266900 | 3.07847900 |
| F | -6.76318100 | 2.84558900 | 4.52608800 |
| F | -8.45238700 | 0.72102200 | 4.31358300 |
| F | -7.83990300 | -1.35003100 | 2.65276200 |

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|---|-------------|-------------|-------------|
| F | -5.54697300 | -1.30566300 | 1.22624300 |
| C | -2.88665700 | -1.24569100 | 4.33856400 |
| C | -2.10342900 | -2.27681600 | 3.81996300 |
| C | -2.74094900 | -3.48054400 | 3.50505800 |
| C | -4.11464300 | -3.65530800 | 3.65925300 |
| C | -4.86932400 | -2.61598600 | 4.21415900 |
| C | -4.25124000 | -1.41553400 | 4.56848900 |
| C | -5.29514300 | 1.85712800 | 2.96160000 |
| C | -6.47388300 | 1.84451900 | 3.70955900 |
| C | -7.34065500 | 0.75439300 | 3.60203700 |
| C | -7.02601700 | -0.30986800 | 2.74990100 |
| C | -5.84304700 | -0.26461200 | 2.01739300 |
| C | -4.96558400 | 0.82149800 | 2.08299200 |
| C | -0.62931400 | -2.11107000 | 3.57399300 |
| H | -0.29265900 | -1.15011800 | 3.97752000 |
| H | -0.07312200 | -2.91650500 | 4.07085500 |
| C | -3.78769800 | 0.93479200 | 1.16519200 |
| H | -4.10673400 | 0.73885700 | 0.13294400 |
| H | -3.38087700 | 1.95121900 | 1.20547400 |
| O | 1.33117200 | -2.74331600 | -0.61757600 |
| O | 2.51772700 | -0.79381700 | 1.59407200 |
| B | 0.73758300 | -1.54636600 | -0.31462400 |
| B | 1.38503300 | -0.43503300 | 0.95956000 |
| F | 3.00114100 | -4.63699400 | 2.35377200 |
| F | 5.44445100 | -5.77022800 | 2.07359600 |
| F | 6.42193100 | -6.29794500 | -0.41302600 |
| F | 4.92299200 | -5.74394000 | -2.61597600 |
| F | 2.45661900 | -4.67210500 | -2.34031500 |
| F | 2.12901300 | -2.27511100 | 5.12134400 |
| F | 3.66814600 | -4.31267300 | 6.00692800 |
| F | 6.03756700 | -4.86253200 | 4.78105700 |
| F | 6.86437600 | -3.35940400 | 2.66779300 |
| F | 5.36684600 | -1.27364600 | 1.82202400 |
| C | 3.45820700 | -4.90441600 | 1.12450400 |
| C | 2.66639400 | -4.60853800 | 0.01332900 |
| C | 3.17948300 | -4.92492500 | -1.24890600 |
| C | 4.44939200 | -5.47977800 | -1.40881100 |
| C | 5.22220000 | -5.76174700 | -0.27698600 |
| C | 4.72096600 | -5.48409800 | 0.99768500 |
| C | 3.30568100 | -2.50781000 | 4.52652400 |
| C | 4.08526400 | -3.56614100 | 4.99499000 |
| C | 5.30120000 | -3.84808000 | 4.36874200 |
| C | 5.72596400 | -3.07387800 | 3.28384300 |

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|---|-------------|-------------|-------------|
| C | 4.93763500 | -2.00993800 | 2.85282900 |
| C | 3.71305700 | -1.70882000 | 3.45715800 |
| C | 1.33030000 | -3.93587800 | 0.16650900 |
| H | 1.13456100 | -3.70908800 | 1.22018900 |
| H | 0.52151400 | -4.58179000 | -0.20653400 |
| C | 2.86783400 | -0.57319800 | 2.96708900 |
| H | 3.43249900 | 0.36831000 | 3.00064400 |
| H | 1.97137400 | -0.46191800 | 3.58155100 |
| O | 0.10796800 | 0.93069400 | 2.98115400 |
| O | 1.90212700 | 2.35574200 | 0.63842300 |
| B | 0.04964400 | 0.56971400 | 1.65224800 |
| B | 1.05351700 | 1.35974600 | 0.30623500 |
| F | 0.45219000 | 4.71734900 | 2.24325800 |
| F | 2.77197300 | 6.04774100 | 2.55166100 |
| F | 4.73237800 | 5.02680800 | 4.14889400 |
| F | 4.37060200 | 2.62871000 | 5.38441600 |
| F | 2.00121100 | 1.34085600 | 5.16694700 |
| F | 3.60498400 | 5.67903400 | -0.49080000 |
| F | 5.78015700 | 6.68502900 | 0.77002000 |
| F | 7.30505800 | 5.07359300 | 2.34301900 |
| F | 6.63685000 | 2.45116700 | 2.67413600 |
| F | 4.50028700 | 1.43304500 | 1.36932800 |
| C | 1.38363900 | 4.19912300 | 3.04628600 |
| C | 1.15170100 | 2.98859600 | 3.70159000 |
| C | 2.17858200 | 2.49022700 | 4.50896300 |
| C | 3.40061400 | 3.14795600 | 4.64579700 |
| C | 3.58818400 | 4.37480300 | 4.00287500 |
| C | 2.58055900 | 4.90043200 | 3.19320400 |
| C | 4.34861000 | 4.87536700 | 0.26533100 |
| C | 5.46979600 | 5.40648100 | 0.90818700 |
| C | 6.25660600 | 4.57894900 | 1.71243700 |
| C | 5.91186500 | 3.23328400 | 1.88520500 |
| C | 4.80331400 | 2.72938400 | 1.21534200 |
| C | 3.99020900 | 3.53376000 | 0.41352900 |
| C | -0.13737600 | 2.22061900 | 3.54350000 |
| H | -0.84910500 | 2.78793600 | 2.93314900 |
| H | -0.58464600 | 2.03414000 | 4.52976300 |
| C | 2.80640900 | 2.96211200 | -0.29924200 |
| H | 3.13044400 | 2.19931300 | -1.01954200 |
| H | 2.26801700 | 3.75006800 | -0.83754500 |
| O | 0.31606100 | 2.21545500 | -2.18337700 |
| O | 2.74721300 | 0.00053300 | -1.49532800 |
| B | 0.25798600 | 1.17149500 | -1.27815100 |

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|---|------------|-------------|-------------|
| B | 1.52803700 | -0.03704900 | -0.86015500 |
| F | 2.34208300 | 0.06015700 | -4.62393600 |
| F | 4.96905000 | 0.43133700 | -5.10117000 |
| F | 6.17115400 | 2.76276700 | -4.39456800 |
| F | 4.70032800 | 4.78668100 | -3.29540000 |
| F | 2.02261900 | 4.48662200 | -3.00002900 |
| F | 4.48649700 | -2.91280200 | -3.07952300 |
| F | 6.76581600 | -2.84364500 | -4.52615900 |
| F | 8.45328900 | -0.71780000 | -4.31255400 |
| F | 7.83851000 | 1.35241700 | -2.65150700 |
| F | 5.54512100 | 1.30596500 | -1.22593000 |
| C | 2.88661400 | 1.24509100 | -4.33892300 |
| C | 2.10338400 | 2.27624800 | -3.82038200 |
| C | 2.74084400 | 3.48009500 | -3.50582000 |
| C | 4.11446600 | 3.65502300 | -3.66048200 |
| C | 4.86911000 | 2.61571100 | -4.21545500 |
| C | 4.25111200 | 1.41506100 | -4.56925900 |
| C | 5.29637700 | -1.85664800 | -2.96206600 |
| C | 6.47541300 | -1.84296300 | -3.70955000 |
| C | 7.34130100 | -0.75219500 | -3.60145700 |
| C | 7.02547400 | 0.31164200 | -2.74923600 |
| C | 5.84226100 | 0.26530500 | -2.01719600 |
| C | 4.96558900 | -0.82139900 | -2.08346000 |
| C | 0.62928600 | 2.11048400 | -3.57435200 |
| H | 0.29266500 | 1.14947300 | -3.97775600 |
| H | 0.07307000 | 2.91582800 | -4.07132700 |
| C | 3.78726000 | -0.93577900 | -1.16634900 |
| H | 4.10585500 | -0.74146100 | -0.13364100 |
| H | 3.38022200 | -1.95205000 | -1.20833300 |

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|---|-------------|-------------|-------------|
| O | -1.72371800 | -1.47986400 | -2.10936300 |
| O | -2.78775500 | -0.99963000 | 0.96502600 |
| O | -2.44541700 | 1.48614500 | -1.25933700 |
| O | -0.33716200 | -0.92583400 | 2.97772800 |
| O | 2.82365000 | 0.99352600 | -0.95542400 |
| O | 0.27585400 | 3.11687200 | -0.39260700 |
| O | 0.36009000 | 0.98109000 | -2.94567600 |
| O | -1.57720100 | 1.95553400 | 1.90408300 |
| O | -0.28549600 | -3.06411900 | 0.39644600 |
| O | 1.59726400 | -1.90301600 | -1.87469300 |
| O | 1.74816300 | 1.53304300 | 2.13899000 |
| O | 2.46633800 | -1.43629000 | 1.29221900 |

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|---|-------------|-------------|-------------|
| H | -3.17006900 | -2.89748300 | -3.79498800 |
| H | -5.13260500 | -2.04541800 | 1.55703400 |
| H | -2.30443500 | -4.44522800 | -3.55308200 |
| H | -5.82029000 | -1.95092500 | -0.09278500 |
| H | -3.21110500 | -3.69823600 | -2.20433100 |
| H | -4.40900400 | -2.99887700 | 0.23741300 |
| H | -0.67031300 | -2.55303300 | -3.52637300 |
| H | -4.43898300 | 0.08283500 | 0.35986700 |
| H | -0.75278100 | -3.30360800 | -1.92183500 |
| H | -3.67680500 | -0.89723500 | -0.90747500 |
| H | -4.60286000 | 2.69548100 | -2.15367600 |
| H | -0.49067300 | -1.94731800 | 5.39925800 |
| H | -4.26450200 | 4.29013700 | -1.41473400 |
| H | 1.09899900 | -1.35517900 | 5.96938700 |
| H | -3.18268500 | 3.63301300 | -2.67781800 |
| H | -0.19695600 | -0.19767600 | 5.54616600 |
| H | -3.57874500 | 2.47970000 | 0.15682100 |
| H | 1.27395200 | -2.07275300 | 3.58468000 |
| H | -2.14580100 | 3.35087500 | -0.40361300 |
| H | 1.51332900 | -0.32667900 | 3.69704400 |
| H | 5.26452300 | 1.64590800 | -1.69955800 |
| H | 0.69648400 | 5.69821000 | -0.74161500 |
| H | 6.09001700 | 1.06506000 | -0.22152000 |
| H | 1.50114500 | 5.55454800 | -2.33333500 |
| H | 5.24449300 | -0.08864600 | -1.29594300 |
| H | -0.21070900 | 5.07251700 | -2.14062800 |
| H | 3.90821800 | 2.12322700 | 0.39127800 |
| H | 2.21534000 | 3.67190900 | -0.84664700 |
| H | 3.85402500 | 0.38996700 | 0.74208200 |
| H | 1.27598800 | 3.04219100 | -2.20753600 |
| H | 0.18859600 | 0.25239400 | -5.51014700 |
| H | -4.00904900 | 2.73531800 | 2.69185900 |
| H | -1.09185500 | 1.42939400 | -5.92738200 |
| H | -3.79236500 | 2.23724000 | 4.39593500 |
| H | 0.51164500 | 1.99764300 | -5.37340200 |
| H | -2.74661000 | 3.50320300 | 3.68428200 |
| H | -1.50535700 | 0.41486100 | -3.65024400 |
| H | -2.77783300 | 0.53675000 | 2.82378100 |
| H | -1.23392800 | 2.15720800 | -3.54130200 |
| H | -1.55262300 | 1.27612000 | 3.85862800 |
| H | -0.72351400 | -5.63971600 | 0.73918700 |
| H | -2.03454600 | -5.46425000 | 1.94496200 |
| H | -2.25899300 | -4.86481300 | 0.27500800 |

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|---|-------------|-------------|-------------|
| H | -0.28001400 | -3.72965500 | 2.35156500 |
| H | -1.78583100 | -2.95476200 | 1.82526700 |
| H | 2.84198900 | -3.46112200 | -3.58725800 |
| H | 3.77670700 | -2.16895300 | -4.39995800 |
| H | 4.07099100 | -2.54838100 | -2.67774600 |
| H | 1.49480900 | -1.32761000 | -3.85863900 |
| H | 2.68991500 | -0.45929300 | -2.88597000 |
| H | 3.27770800 | 3.66264300 | 2.62850800 |
| H | 2.20126300 | 4.35705900 | 3.87692100 |
| H | 2.96626900 | 2.75959100 | 4.13095900 |
| H | 0.86088500 | 3.39802100 | 1.96276100 |
| H | 0.53108100 | 2.54162800 | 3.47506800 |
| H | 3.29749600 | -3.55894600 | 2.68413700 |
| H | 4.34129700 | -4.20623700 | 1.38424800 |
| H | 4.68497700 | -2.60529000 | 2.10527600 |
| H | 2.17913000 | -3.30292100 | 0.43893800 |
| H | 3.57374400 | -2.40173300 | -0.16418800 |
| C | -2.57460000 | -3.48699100 | -3.07885300 |
| C | -4.88368600 | -2.03516600 | 0.48330200 |
| C | -1.33191000 | -2.72199100 | -2.65431200 |
| C | -3.94185200 | -0.88690800 | 0.15968200 |
| C | -3.80222600 | 3.36835900 | -1.80562600 |
| C | 0.26817400 | -1.15821300 | 5.27147600 |
| C | -2.96119600 | 2.68960400 | -0.73712000 |
| C | 0.76406300 | -1.12357800 | 3.83538600 |
| C | 5.20673500 | 0.92579600 | -0.86705200 |
| C | 0.77640600 | 5.08024500 | -1.65083800 |
| C | 3.92173600 | 1.12049700 | -0.07871800 |
| C | 1.20636300 | 3.66540600 | -1.30186700 |
| C | -0.25865400 | 1.22132000 | -5.23558000 |
| C | -3.26240200 | 2.55052700 | 3.48096000 |
| C | -0.74406200 | 1.19876600 | -3.79571100 |
| C | -2.26723600 | 1.48934500 | 3.04113000 |
| C | -1.52998600 | -4.97732700 | 1.09382400 |
| C | -0.97491700 | -3.62097400 | 1.49605400 |
| C | 3.29305000 | -2.46428100 | -3.45388200 |
| C | 2.23683100 | -1.45019600 | -3.04618800 |
| C | 2.50748900 | 3.42205100 | 3.37895700 |
| C | 1.31718500 | 2.74294800 | 2.72279800 |
| C | 3.88084200 | -3.28954200 | 1.78884800 |
| C | 2.99257100 | -2.62664000 | 0.74936200 |
| B | -0.92151000 | -0.80715300 | -1.16287400 |
| B | -1.53397400 | -0.51801500 | 0.52906500 |

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|---|-------------|-------------|-------------|
| B | -1.34571000 | 0.83209600 | -0.66441400 |
| B | -0.16382800 | -0.50645100 | 1.64074600 |
| B | 1.55753200 | 0.57137000 | -0.49875300 |
| B | 0.17464700 | 1.72064000 | -0.21258200 |
| B | 0.18600400 | 0.55763200 | -1.60862200 |
| B | -0.85218900 | 1.07542200 | 1.06894000 |
| B | -0.15263800 | -1.66873500 | 0.24342000 |
| B | 0.87486000 | -1.02361800 | -1.03828300 |
| B | 0.94693700 | 0.85952100 | 1.19175500 |
| B | 1.36540100 | -0.78084900 | 0.69561400 |

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|---|-------------|-------------|-------------|
| O | -0.05920300 | 0.87179800 | -2.99092600 |
| O | -0.60469200 | -2.27408600 | -1.98549500 |
| O | -2.78631800 | 0.27188400 | -1.42178200 |
| O | 0.95958900 | -2.84155200 | 0.78435900 |
| O | 0.55145800 | 2.40352400 | 2.05965100 |
| O | -2.47069800 | 1.11525400 | 1.70534700 |
| O | -1.01967400 | 2.95264700 | -0.63712600 |
| O | -2.24195200 | -1.98835300 | 0.93899900 |
| O | 2.37630600 | -1.01871700 | -1.67550500 |
| O | 2.22958000 | 2.06877800 | -0.81830400 |
| O | -0.00394200 | -0.66307500 | 3.11370200 |
| O | 2.73810600 | -0.09349900 | 1.54463400 |
| H | 0.18663700 | -0.54893800 | -5.26892300 |
| H | -1.50848400 | -4.30603400 | -3.39275600 |
| H | 1.97984600 | -0.54791100 | -5.27523000 |
| H | -2.43536100 | -3.33072700 | -4.57587800 |
| H | 1.08021200 | -1.35756800 | -3.95362300 |
| H | -0.65253100 | -3.18930500 | -4.48483700 |
| H | 1.06673000 | 1.66694900 | -4.49389400 |
| H | -2.65211200 | -2.33413400 | -2.30111400 |
| H | 2.00307200 | 0.85396600 | -3.21231200 |
| H | -1.75665900 | -1.22821300 | -3.35209600 |
| H | -5.15185100 | 0.53975300 | -2.51471400 |
| H | 1.89043200 | -5.19534500 | 1.47562200 |
| H | -6.10852800 | 0.24929900 | -1.02678400 |
| H | 2.40178900 | -4.73853800 | 3.13156900 |
| H | -5.05195400 | 1.68909100 | -1.15865600 |
| H | 0.66966700 | -4.70783000 | 2.67564400 |
| H | -4.13193400 | -1.25086800 | -1.02686400 |
| H | 2.87900200 | -2.86720200 | 1.56483600 |
| H | -3.94889700 | -0.05142600 | 0.26318500 |

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|---|-------------|-------------|-------------|
| H | 1.60816200 | -2.37360700 | 2.69619100 |
| H | 2.61916000 | 4.12297100 | 2.21319700 |
| H | -4.48678400 | 2.12140300 | 3.06239000 |
| H | 3.65784500 | 3.05137800 | 3.20777900 |
| H | -4.02205200 | 3.84133100 | 2.86994600 |
| H | 3.17853900 | 2.56844600 | 1.54655400 |
| H | -4.46665700 | 2.85556100 | 1.44084000 |
| H | 1.24053600 | 2.90130300 | 3.91031700 |
| H | -1.97112700 | 2.44900000 | 3.21071600 |
| H | 1.83937000 | 1.34197200 | 3.29097800 |
| H | -1.97420100 | 3.12198700 | 1.57462600 |
| H | -0.88077000 | 4.88740600 | -2.46800000 |
| H | -4.01034300 | -3.68704900 | -0.12302700 |
| H | -2.63969700 | 4.91292200 | -2.80806300 |
| H | -3.34373100 | -5.13654900 | 0.69260500 |
| H | -2.02511300 | 5.31757200 | -1.17438500 |
| H | -4.01743900 | -3.78220400 | 1.65406600 |
| H | -1.79670900 | 2.54556400 | -2.51372600 |
| H | -1.49440700 | -3.60838700 | -0.11640600 |
| H | -2.98860200 | 2.97555700 | -1.27875500 |
| H | -1.48203300 | -3.78176000 | 1.64195900 |
| H | 4.65093800 | -2.01978900 | -2.54124500 |
| H | 4.03183000 | -3.67075600 | -2.85883300 |
| H | 3.40442300 | -2.27290900 | -3.78621100 |
| H | 3.02513300 | -2.76770100 | -0.76857300 |
| H | 1.76405700 | -2.97177700 | -1.98972300 |
| H | 3.81021900 | 3.60608600 | -2.26003700 |
| H | 3.05832100 | 5.16035500 | -1.77918600 |
| H | 3.87451900 | 4.13299900 | -0.55992700 |
| H | 1.29427200 | 3.41105900 | -2.08895000 |
| H | 1.36722800 | 3.90311000 | -0.39471000 |
| H | -0.93051500 | 0.08977100 | 5.48676300 |
| H | -1.88189900 | -1.40100100 | 5.78133700 |
| H | -0.09942800 | -1.47910900 | 5.61481200 |
| H | -2.05874000 | -0.66830400 | 3.37055400 |
| H | -1.27650700 | -2.25122800 | 3.51104600 |
| H | 5.04411100 | -0.71253900 | 2.64338200 |
| H | 6.07262600 | -0.09396100 | 1.31312100 |
| H | 5.04760700 | 1.02655900 | 2.26305500 |
| H | 4.05095600 | -1.19767200 | 0.38109300 |
| H | 3.99247300 | 0.53498100 | 0.02133700 |
| C | 1.08416800 | -0.49161600 | -4.62962100 |
| C | -1.57033600 | -3.32300500 | -3.88946800 |

| | | | |
|---|-------------|-------------|-------------|
| C | 1.07647700 | 0.79417800 | -3.80633100 |
| C | -1.69894700 | -2.21247200 | -2.85545500 |
| C | -5.14295300 | 0.62061700 | -1.41426300 |
| C | 1.69272600 | -4.50879300 | 2.31642200 |
| C | -3.97616100 | -0.16813400 | -0.83137900 |
| C | 1.82547400 | -3.06038600 | 1.86145100 |
| C | 2.84027600 | 3.07106800 | 2.46340000 |
| C | -3.95097400 | 2.83703200 | 2.41531800 |
| C | 1.58981300 | 2.37399000 | 2.99675400 |
| C | -2.49840600 | 2.41240200 | 2.23518200 |
| C | -1.87597500 | 4.66300500 | -2.05007100 |
| C | -3.43718300 | -4.03745700 | 0.75105800 |
| C | -1.96435100 | 3.19751400 | -1.64015000 |
| C | -2.06845300 | -3.36850100 | 0.79481900 |
| C | 3.75059600 | -2.60474100 | -2.79433600 |
| C | 2.66755700 | -2.38583700 | -1.74556900 |
| C | 3.24378100 | 4.11828900 | -1.46415200 |
| C | 1.93779500 | 3.38595000 | -1.18691000 |
| C | -1.01234000 | -0.98241800 | 5.24401700 |
| C | -1.14848400 | -1.17169100 | 3.73852600 |
| C | 5.09784900 | 0.01947600 | 1.81983400 |
| C | 3.94563800 | -0.19660600 | 0.84654600 |
| B | 0.00042600 | 0.47580900 | -1.60954000 |
| B | -0.37959300 | -1.19751200 | -1.05371500 |
| B | -1.53012600 | 0.14414300 | -0.73741600 |
| B | 0.53352200 | -1.50700900 | 0.45917700 |
| B | 0.32956400 | 1.31038600 | 1.16015400 |
| B | -1.32275900 | 0.65358000 | 0.97129400 |
| B | -0.57368100 | 1.61649700 | -0.35425500 |
| B | -1.20331100 | -1.07965200 | 0.53818300 |
| B | 1.27501900 | -0.55430000 | -0.87503300 |
| B | 1.16017200 | 1.18404000 | -0.43678300 |
| B | -0.04445400 | -0.35241100 | 1.71010600 |
| B | 1.48749300 | -0.02877600 | 0.83657600 |

Fc

| | | | |
|---|-------------|-------------|-------------|
| H | 1.86340500 | -1.65112700 | 1.35390900 |
| H | 1.86340500 | -1.65112700 | -1.35390900 |
| C | 0.98275400 | -1.67155800 | 0.71426000 |
| C | 0.98275400 | -1.67155800 | -0.71426000 |
| C | -0.37593500 | -1.67043300 | 1.15576000 |
| C | -0.37593500 | -1.67043300 | -1.15576000 |
| H | -0.71212200 | -1.64879400 | 2.19095100 |

| | | | |
|----|-------------|-------------|-------------|
| H | -0.71212200 | -1.64879400 | -2.19095100 |
| C | -1.21557600 | -1.66981100 | 0.00000000 |
| H | -2.30397500 | -1.64718400 | 0.00000000 |
| C | 1.21518600 | 1.67109500 | 0.00000000 |
| H | 0.71182600 | 1.64965500 | -2.19093000 |
| H | 0.71182600 | 1.64965500 | 2.19093000 |
| C | 0.37554600 | 1.67083000 | -1.15576000 |
| C | 0.37554600 | 1.67083000 | 1.15576000 |
| C | -0.98314400 | 1.67051400 | -0.71426100 |
| C | -0.98314400 | 1.67051400 | 0.71426100 |
| H | -1.86374500 | 1.64894600 | -1.35394300 |
| H | -1.86374500 | 1.64894600 | 1.35394300 |
| H | 2.30361400 | 1.64993300 | 0.00000000 |
| Fe | 0.00051300 | -0.00000200 | 0.00000000 |

Fe⁺

| | | | |
|----|-------------|-------------|-------------|
| H | 1.66882100 | 1.86384800 | 1.35502200 |
| H | 1.66882100 | 1.86384800 | -1.35502200 |
| C | 1.69447900 | 0.98293300 | 0.71507600 |
| C | 1.69447900 | 0.98293300 | -0.71507600 |
| C | 1.69264700 | -0.37723100 | 1.15703800 |
| C | 1.69264700 | -0.37723100 | -1.15703800 |
| H | 1.66542900 | -0.71360400 | 2.19256800 |
| H | 1.66542900 | -0.71360400 | -2.19256800 |
| C | 1.69160200 | -1.21788600 | 0.00000000 |
| H | 1.66301800 | -2.30662000 | 0.00000000 |
| C | -1.69324000 | 1.21732100 | 0.00000000 |
| H | -1.66638300 | 0.71315400 | -2.19254300 |
| H | -1.66638300 | 0.71315400 | 2.19254300 |
| C | -1.69315400 | 0.37668700 | -1.15703100 |
| C | -1.69315400 | 0.37668700 | 1.15703100 |
| C | -1.69315400 | -0.98349200 | -0.71508700 |
| C | -1.69315400 | -0.98349200 | 0.71508700 |
| H | -1.66633700 | -1.86434900 | -1.35506200 |
| H | -1.66633700 | -1.86434900 | 1.35506200 |
| H | -1.66609600 | 2.30609500 | 0.00000000 |
| Fe | 0.00000100 | 0.00073300 | 0.00000000 |