

Supporting Information

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

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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, O– CH_2 – 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.

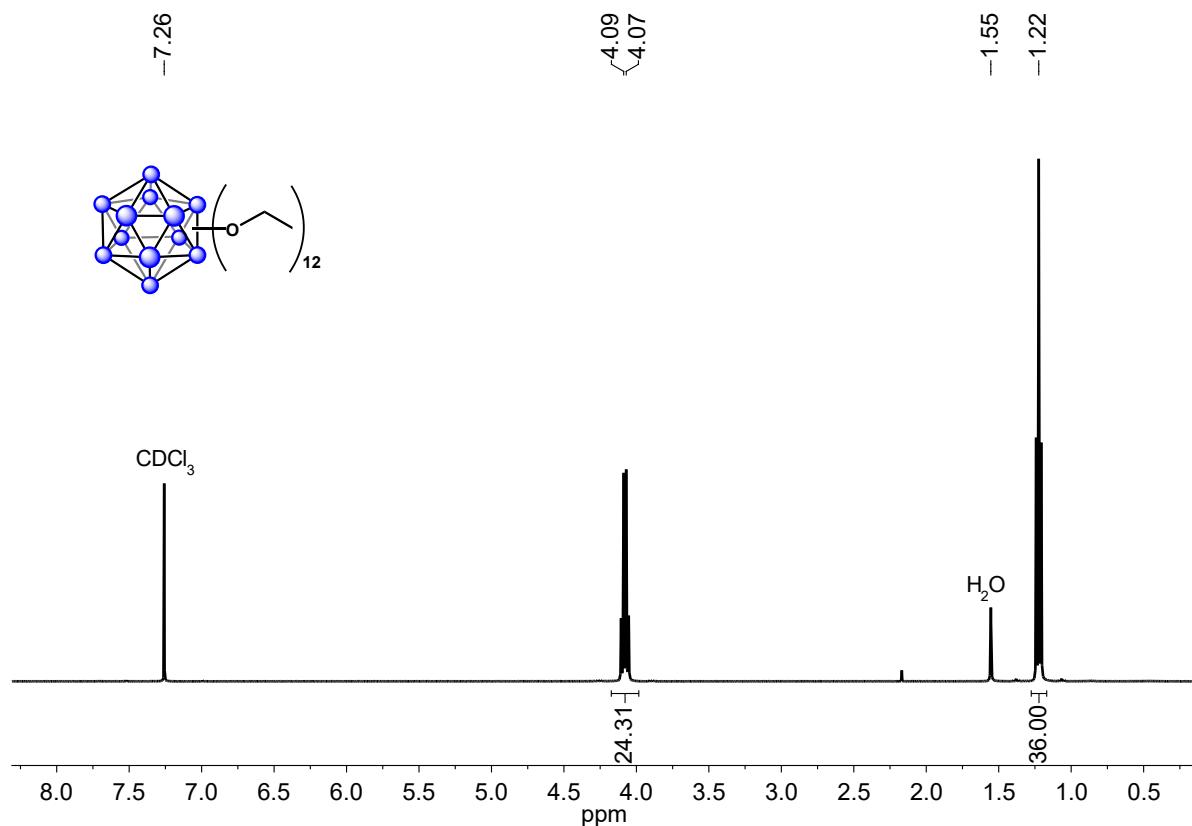


Figure S1. ^1H NMR spectrum of $\text{B}_{12}(\text{O-ethyl})_{12}$ (CDCl_3 , 400 MHz, 25 °C).

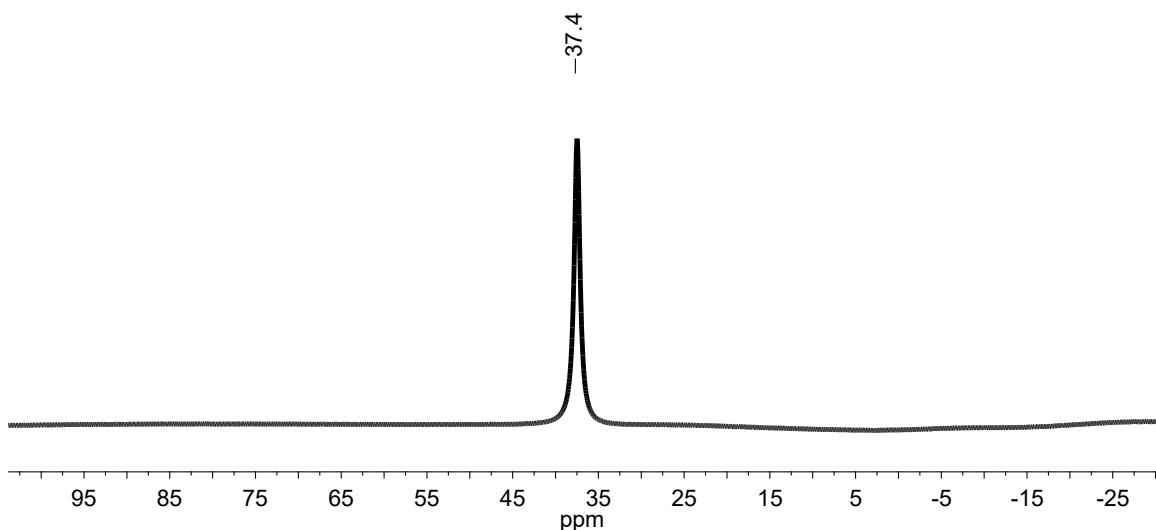


Figure S2. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of $\text{B}_{12}(\text{O-ethyl})_{12}$ (CDCl_3 , 128 MHz, 25 °C).

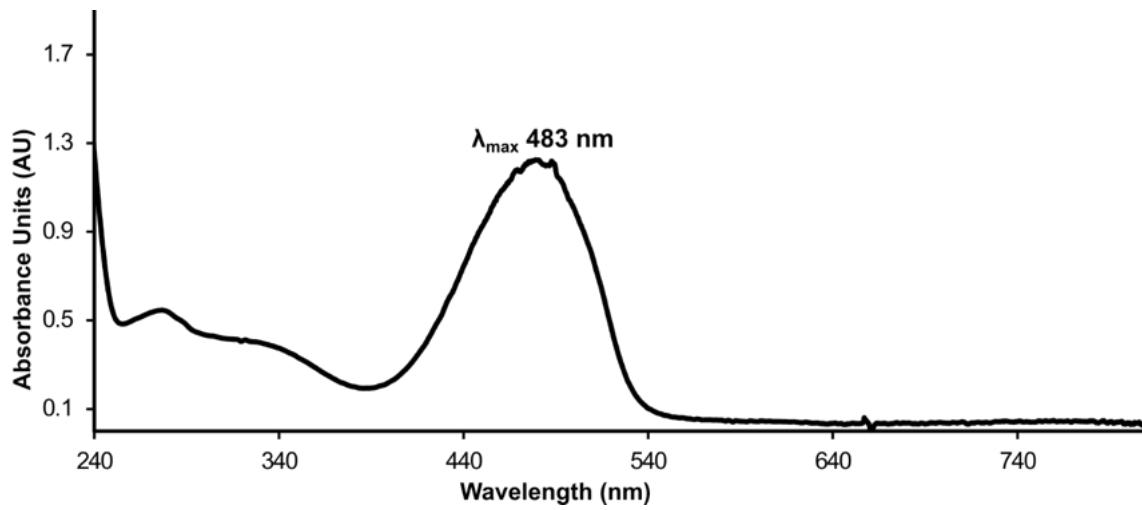


Figure S3. UV-vis spectrum of $\text{B}_{12}(\text{O-ethyl})_{12}$ (DCM, 70 μM , 25 $^{\circ}\text{C}$).

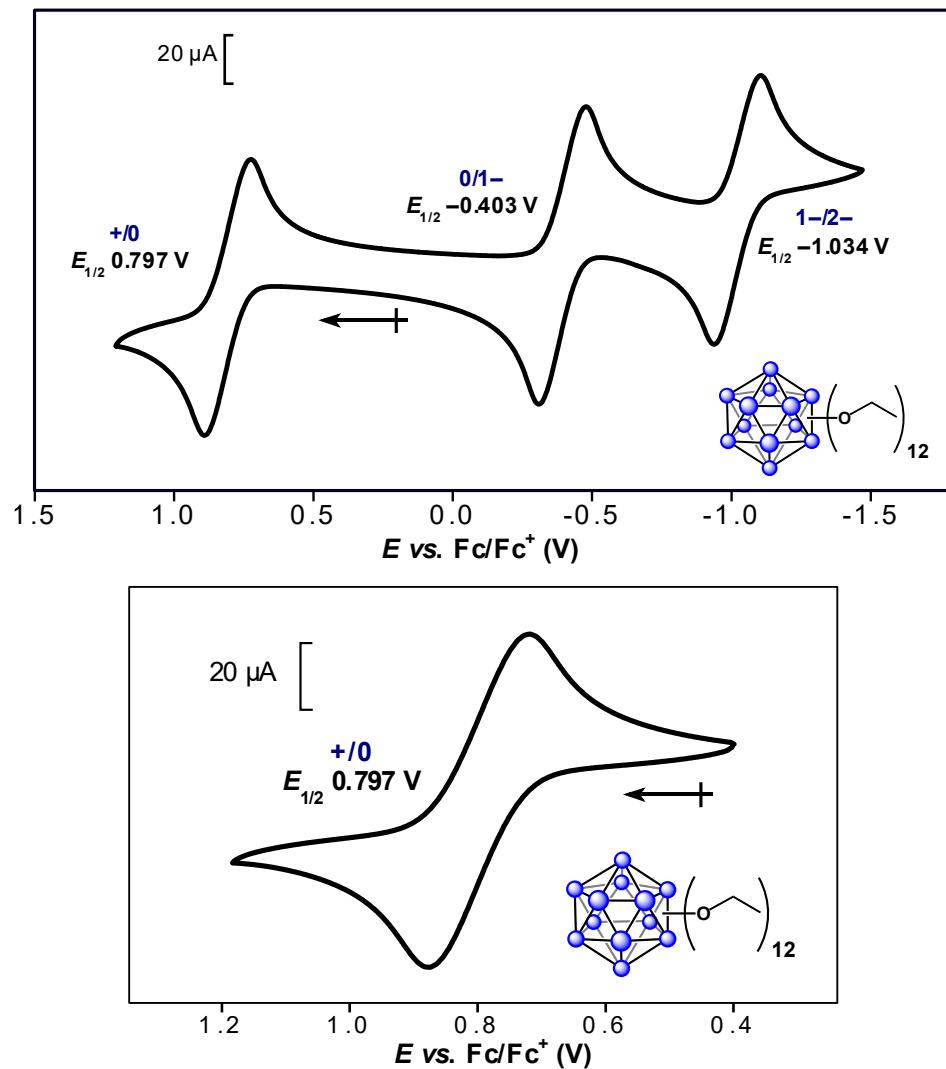
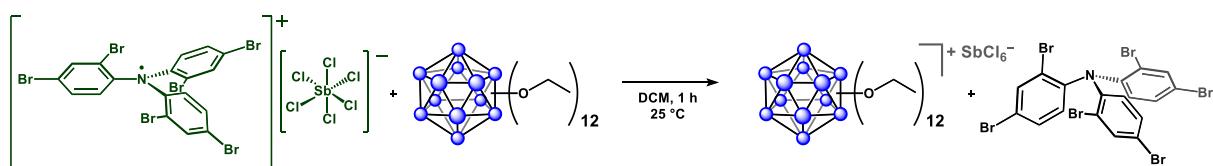


Figure S4. CV of $\text{B}_{12}(\text{O-ethyl})_{12}$ measured at a scan rate of 100 mV/s with 0.1 M [TBA][PF₆] supporting electrolyte and referenced vs. Fc/Fc^+ (glassy carbon working electrode, platinum counter electrode and Ag/Ag⁺ pseudo-reference electrode wire; DCM, 3 mM, 25 $^{\circ}\text{C}$).

1.2.2 $[B_{12}(O\text{-ethyl})_{12}][SbCl_6]$



To a dark yellow solution of $B_{12}(O\text{-ethyl})_{12}$ (15 mg, 0.022 mmol, 1.0 equiv) in DCM (1 mL) was added a green solution of $[N(2,4\text{-Br}_2C_6H_3)_3][SbCl_6]$ (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 $[B_{12}(O\text{-ethyl})_{12}][SbCl_6]$ as a yellow-brown solid (17 mg, 0.017 mmol, 78%). 1H and $^{11}B\{^1H\}$ NMR spectra were collected immediately. 1H NMR (400 MHz, 25 °C, $CDCl_3$) δ: The $O\text{-CH}_2\text{-CH}_3$ resonance is paramagnetically broadened and is therefore not observed due to its proximity to the paramagnetic B_{12} core, 2.04 (br s, 24H, CH_2) ppm. $^{11}B\{^1H\}$ NMR (128 MHz, 25 °C, $CDCl_3$) δ: A silent NMR spectrum was observed due to paramagnetic broadening of the ^{11}B NMR signal, which suggests the spin density is delocalized throughout the B_{12} core. UV-vis (DCM, 25 °C, 70 μM): λ_{max} 460, 720 nm.

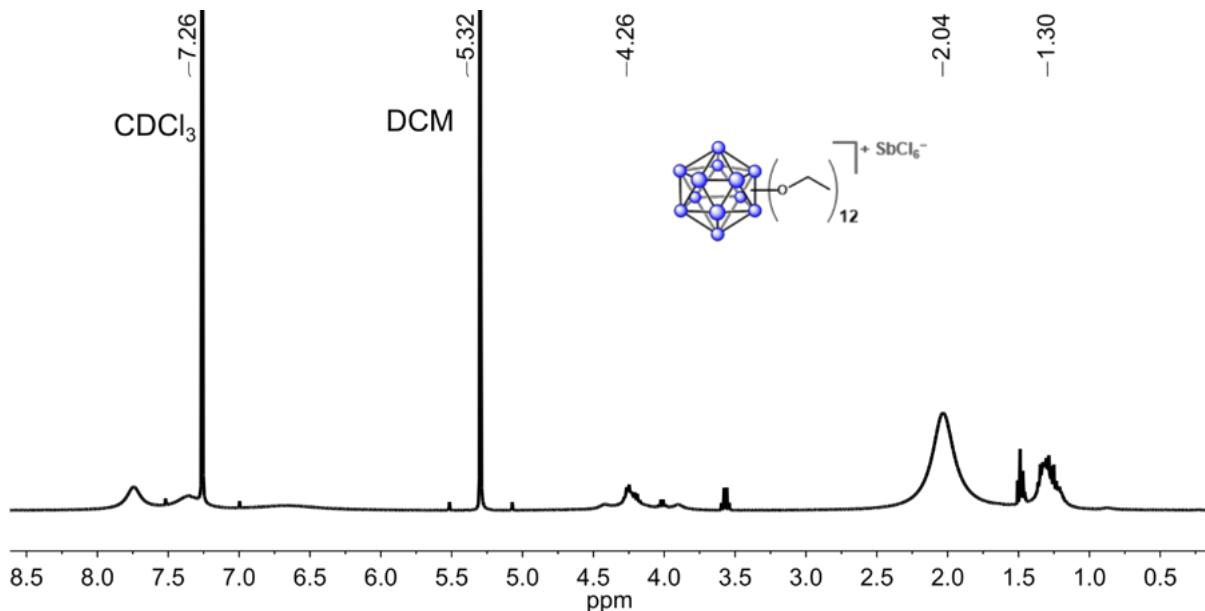


Figure S5. 1H NMR spectrum of $[B_{12}(O\text{-ethyl})_{12}][SbCl_6]$ ($CDCl_3$, 400 MHz, 25 °C).

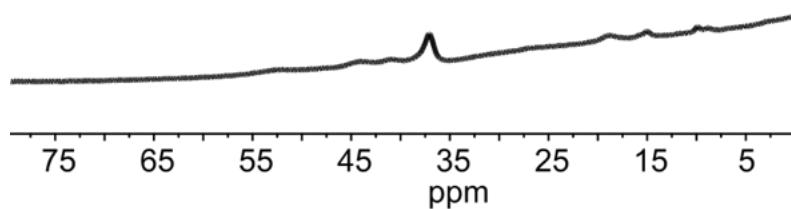


Figure S6. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of $[\text{B}_{12}(\text{O-ethyl})_{12}][\text{SbCl}_6]$ (CDCl_3 , 128 MHz, 25 °C).

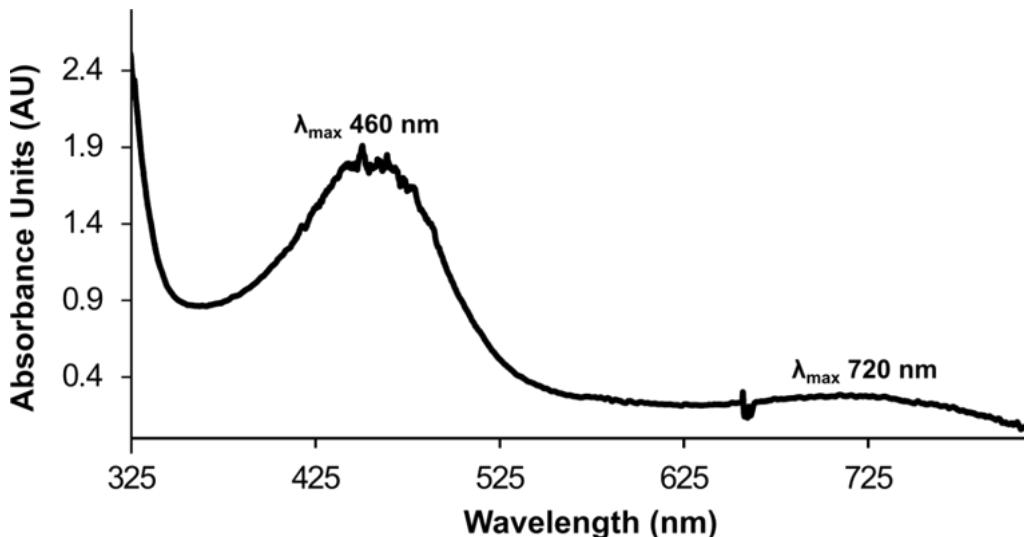


Figure S7. UV-Vis spectrum of $[\text{B}_{12}(\text{O-ethyl})_{12}][\text{SbCl}_6]$ (DCM, 70 μM , 25 °C).

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.

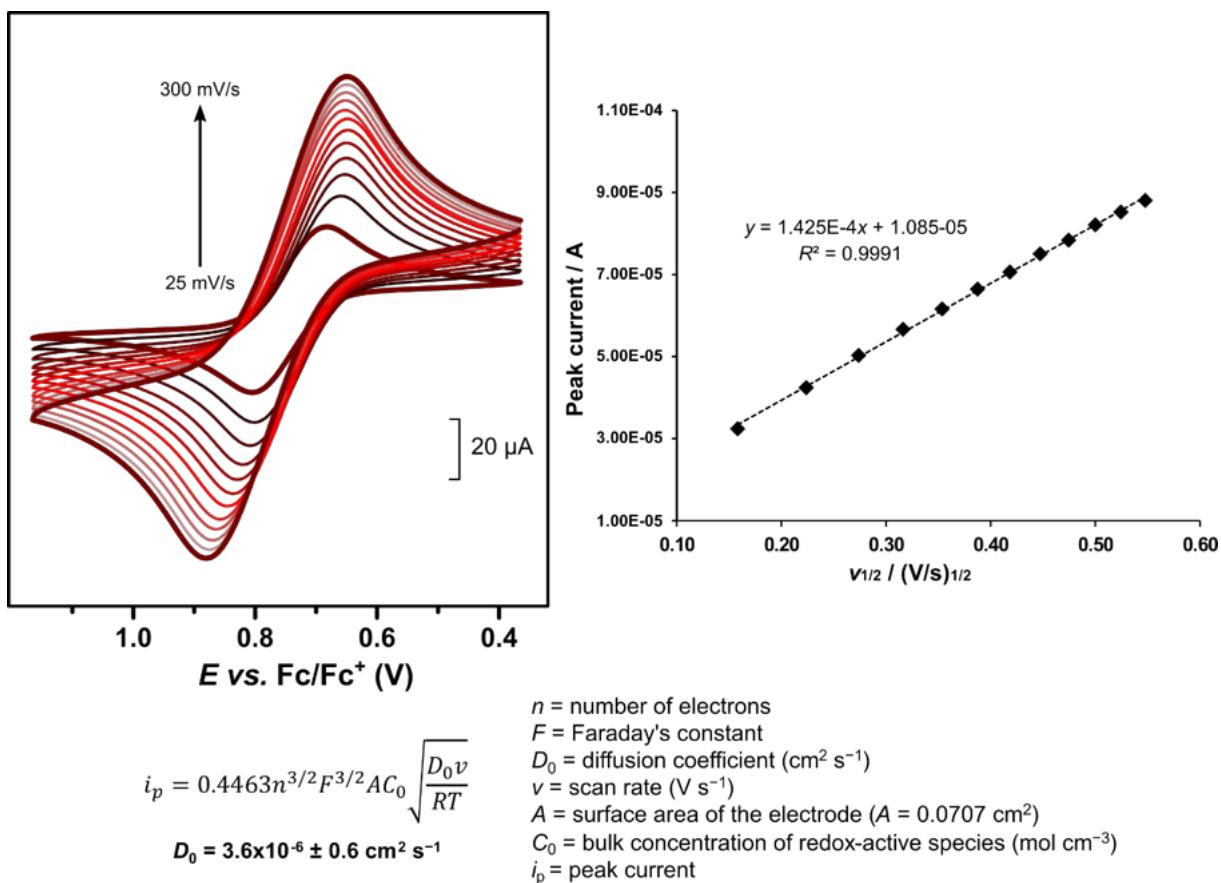
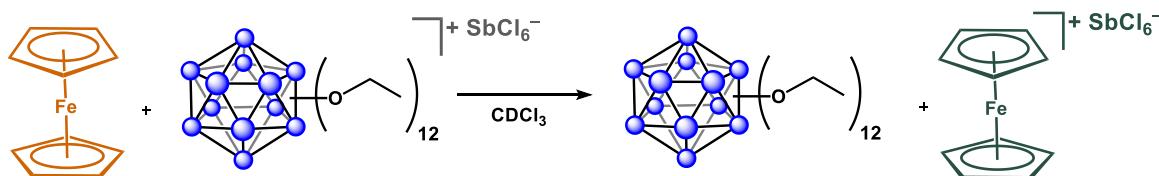


Figure S8. (Left) CV of the $[\text{B}_{12}(\text{O-ethyl})_{12}]^{0/+}$ redox couple recorded at variable scan rates (25-300 mV/s). (Right) Randles-Sevcik plot of the CV data.

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

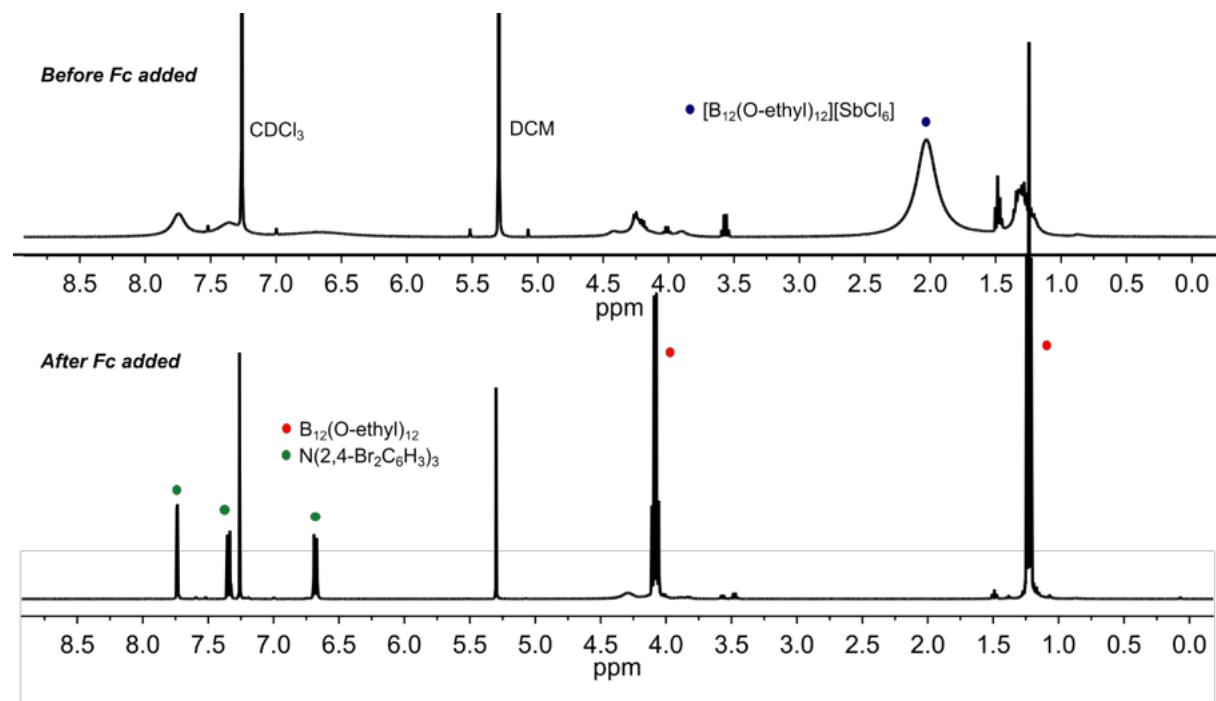


Figure S9. ^1H NMR spectrum of $[\text{B}_{12}(\text{O-ethyl})_{12}][\text{SbCl}_6]$ before (top) and after (bottom) reduction with ferrocene. The spectrum after the reduction of $[\text{B}_{12}(\text{O-ethyl})_{12}][\text{SbCl}_6]$ with ferrocene displays ^1H NMR resonances attributed to *hypercloso*-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

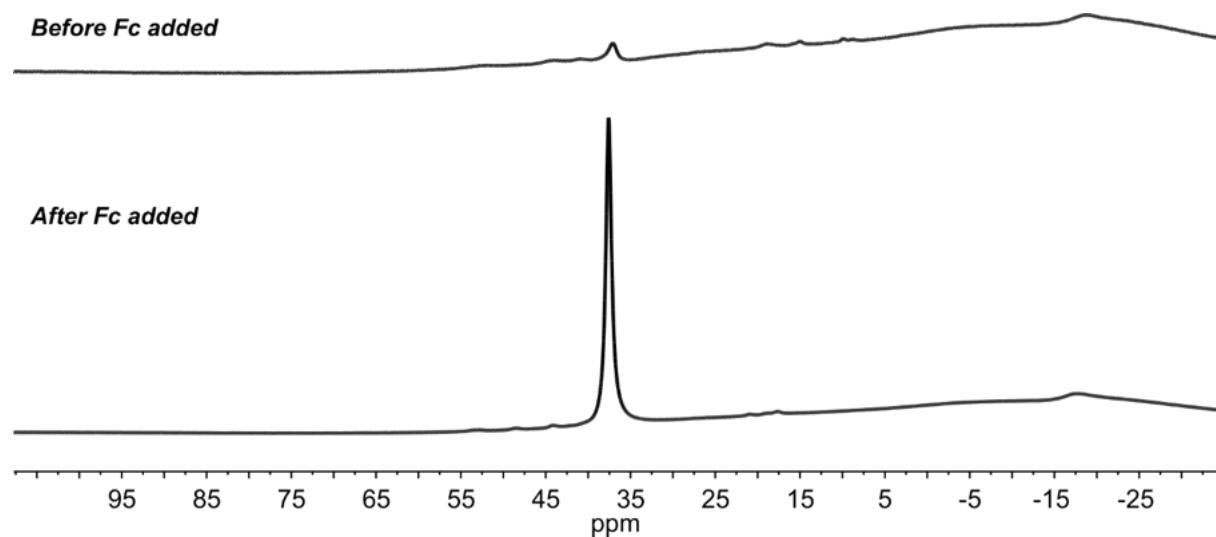


Figure S10. $^{11}\text{B}\{\text{H}\}$ NMR spectrum of $[\text{B}_{12}(\text{O-ethyl})_{12}][\text{SbCl}_6]$ before (top) and after (bottom) reduction with ferrocene. The spectrum after the reduction of $[\text{B}_{12}(\text{O-ethyl})_{12}][\text{SbCl}_6]$ with ferrocene displays the ^{11}B NMR resonance 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/ $\bullet+$ Redox Couple

Electrochemical measurements of $B_{12}(OR)_{12}$ clusters (3 mM solution in DCM) were performed under an inert atmosphere of purified N₂. 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_{crys-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-/•-/0/+} 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.

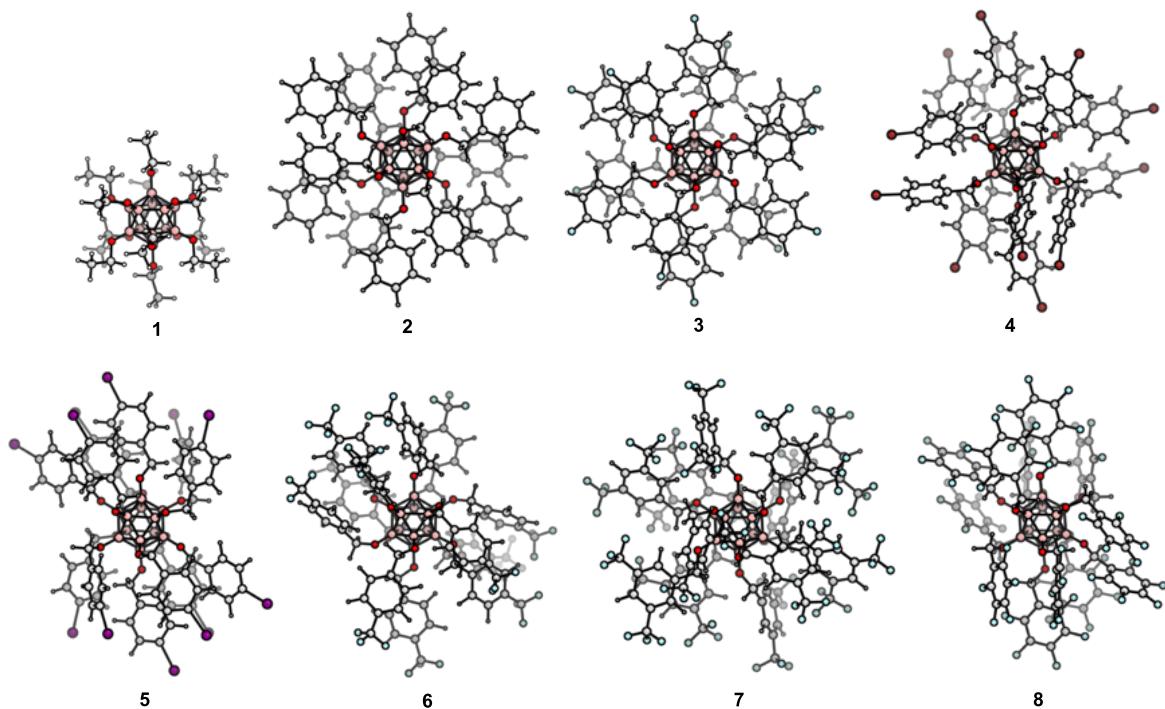


Figure S11. Optimized structures of neutral $\text{B}_{12}(\text{OR})_{12}$ boron clusters.

Table S1. Root-mean-square deviations (RMSDs) of atomic positions (unit: Å) between computational geometries and X-ray crystal structures of neutral $\text{B}_{12}(\text{OR})_{12}$ clusters for all atoms ($\text{RMSD}_{\text{crys-comput}}$) and for the B_{12} core ($\text{RMSD}_{\text{crys-comput,B12}}$). RMSDs for optimized geometries of all $[\text{B}_{12}(\text{OR})_{12}]^{0/+}$ couples are also shown, including $\text{RMSD}_{0/+}$ for all atoms and $\text{RMSD}_{0/+,\text{B12}}$ for the B_{12} cluster core.

	$\text{RMSD}_{\text{crys-comput}}$	$\text{RMSD}_{\text{crys-comput,B12}}$	$\text{RMSD}_{0/+}$	$\text{RMSD}_{0/+,\text{B12}}$
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

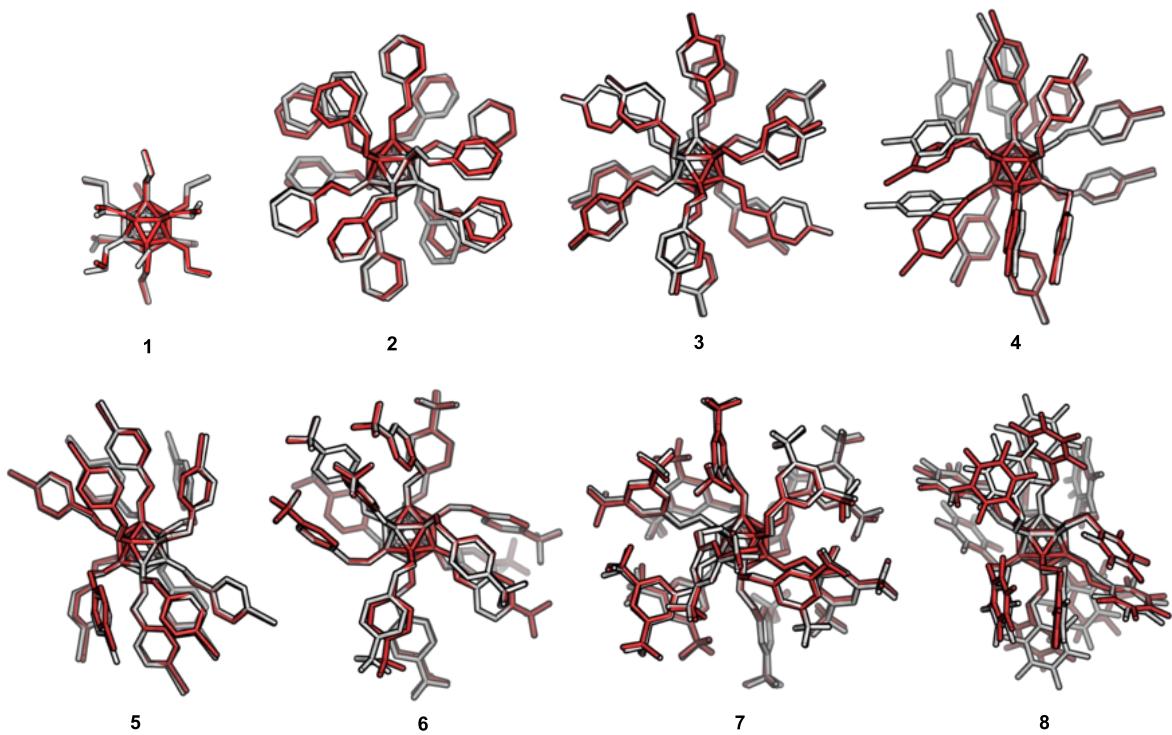


Figure S12. Aligned structures of $[B_{12}(OR)_{12}]^{0/+}$ couples (white: neutral clusters, red: radical cationic clusters). H atoms are omitted for clarity.

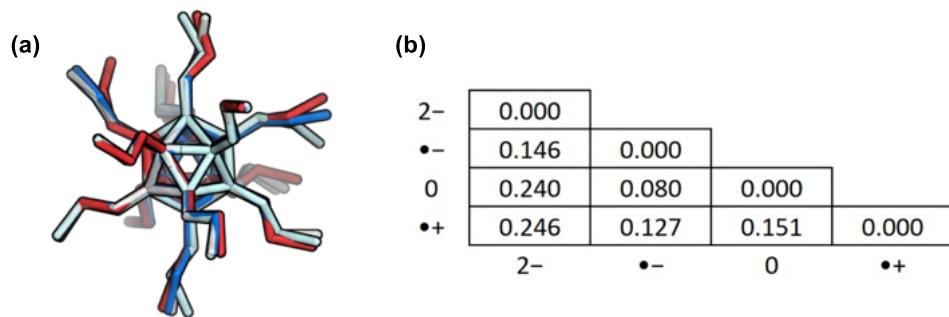


Figure S13. (a) Aligned structures of the $[1]^{2-/•-/0/+}$ redox series (red: $[1]^{2-}$, blue: $[1]^{•-}$, white: **1**, pale cyan $[1]^{0/+}$). H atoms are omitted for clarity. (b) All-atom RMSDs for the optimized structures of the $[1]^{2-/•-/0/+}$ redox series.

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 $[1]^{2-/•-/0/+}$ (**Figure 2**) and $[2]^{0/+}$ (**Figure 4**) have been presented in the manuscript, in which we noted that the highest-energy occupied orbitals of $[2]^{0/+}$ 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 - $, \beta$ -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

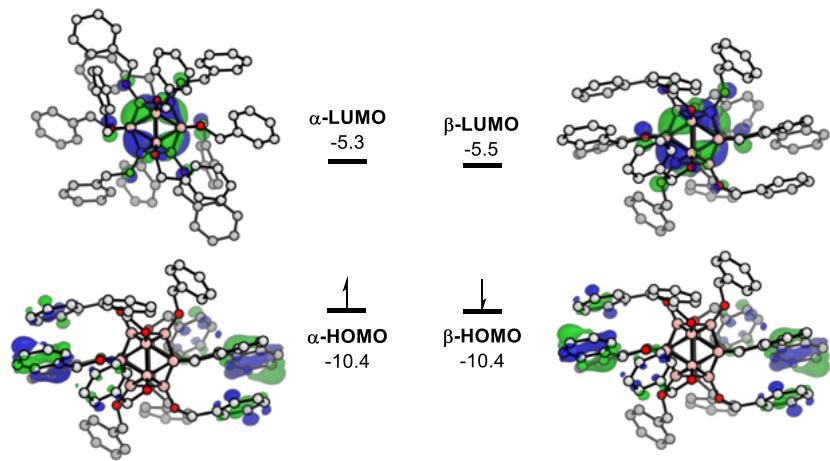


Figure S14. Frontier molecular orbitals of $[2]^{+}$ at the HF//B3LYP-D3/def2-SVP level of theory.

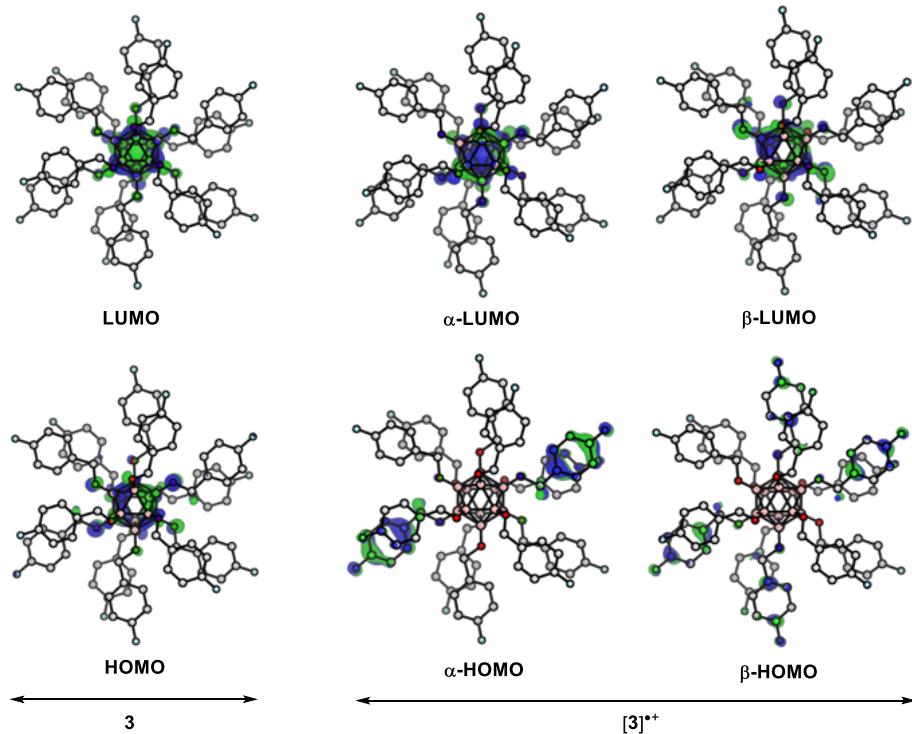


Figure S15. Frontier molecular orbitals of **3** and $[3]^{+}$ at the B3LYP-D3/def2-SVP level of theory.

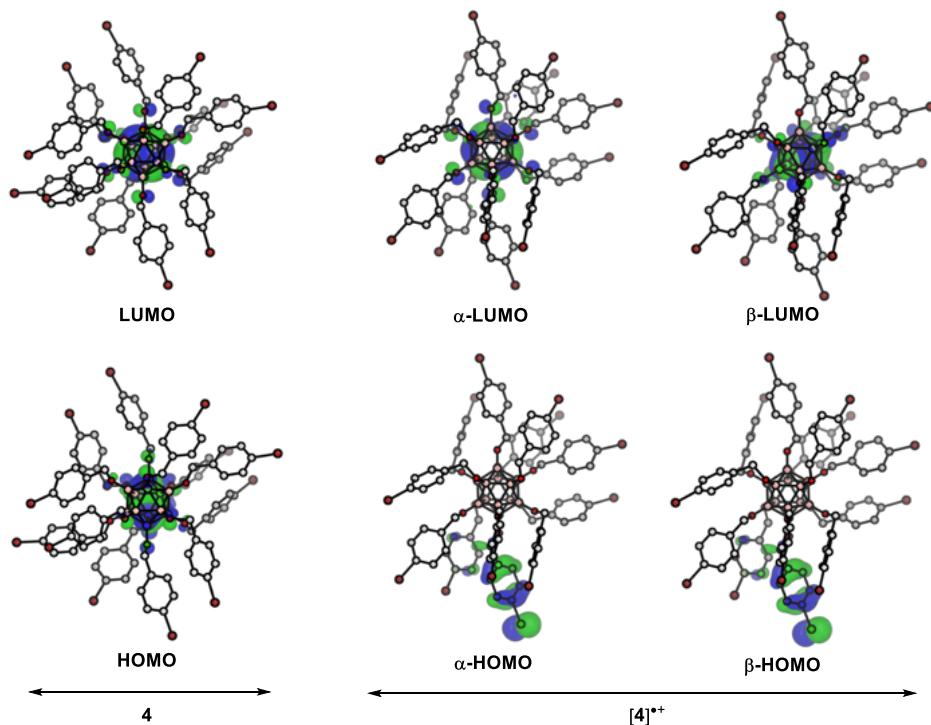


Figure S16. Frontier molecular orbitals of **4** and $[4]^{•+}$ at the B3LYP-D3/def2-SVP level of theory.

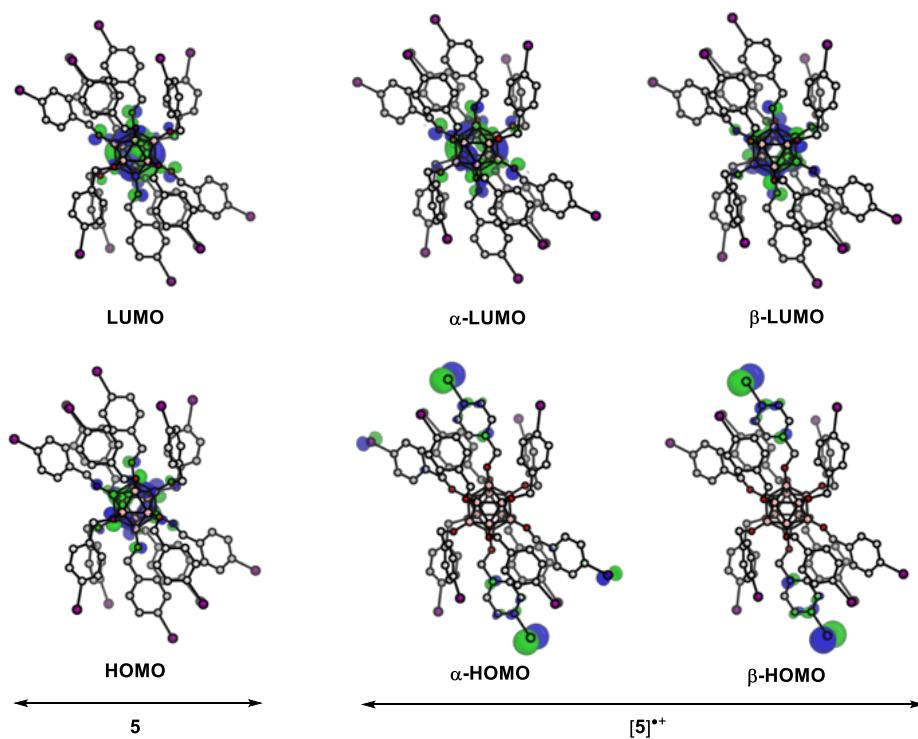


Figure S17. Frontier molecular orbitals of **5** and $[5]^{•+}$ at the B3LYP-D3/def2-SVP level of theory.

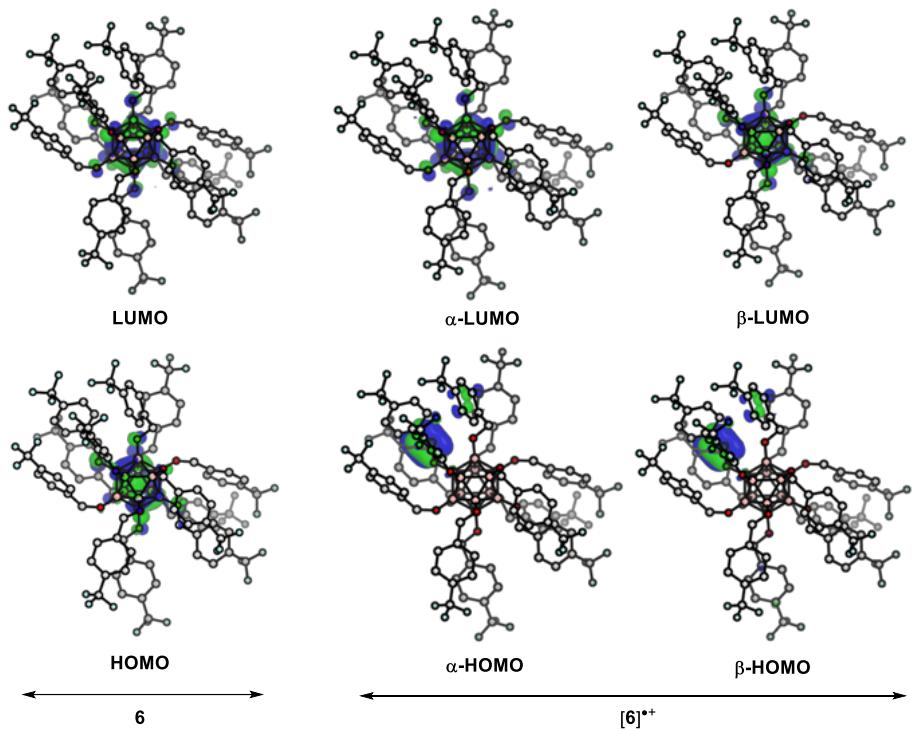


Figure S18. Frontier molecular orbitals of **6** and $[6]^{•+}$ at the B3LYP-D3/def2-SVP level of theory.

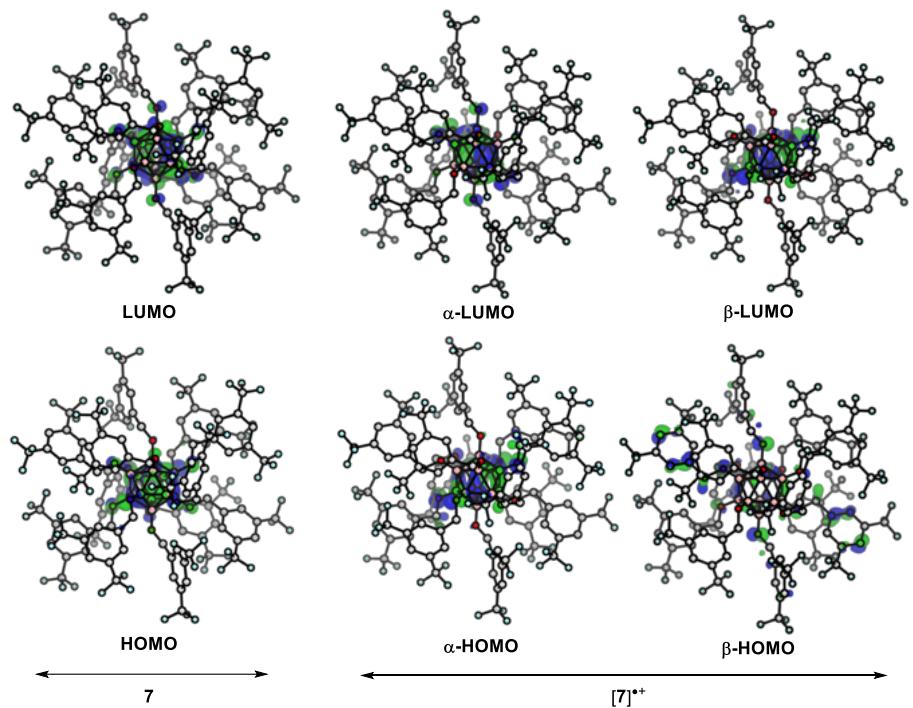


Figure S19. Frontier molecular orbitals of **7** and $[7]^{•+}$ at the B3LYP-D3/def2-SVP level of theory.

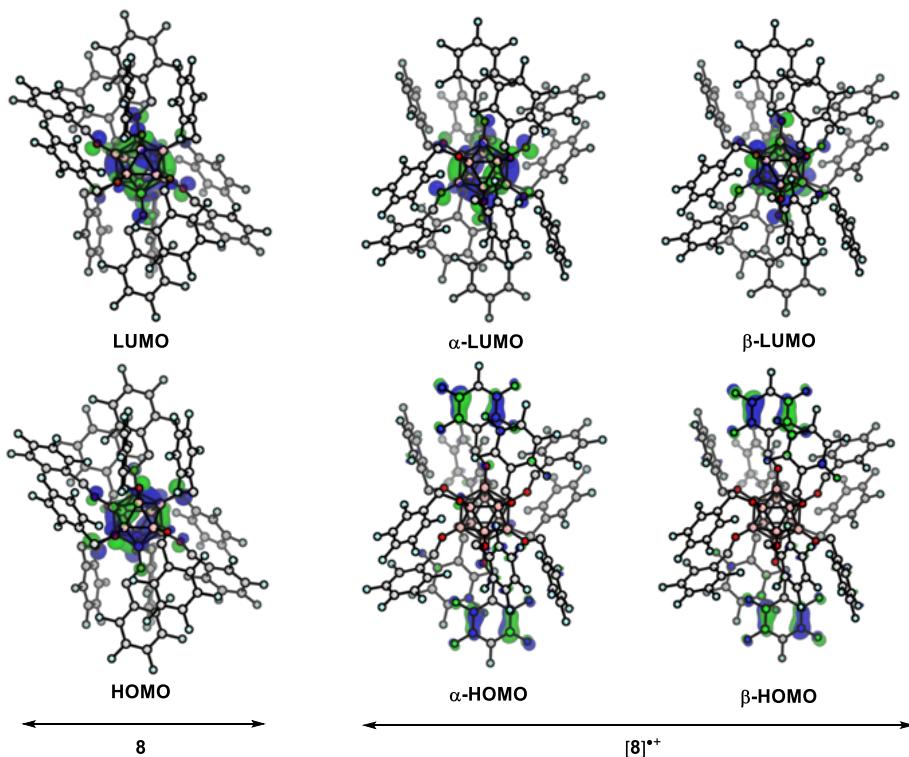


Figure S20. Frontier molecular orbitals of **8** and $[8]^{•+}$ at the B3LYP-D3/def2-SVP level of theory.

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, -CH₂- and -CH₃ 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.

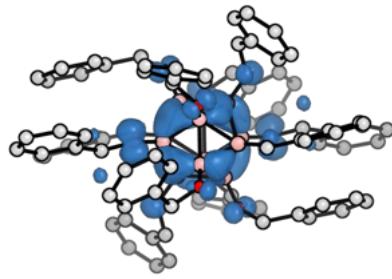


Figure S21. Spin density isosurface (iso value = 0.002 a.u.) of $[2]^{•+}$ at the B3LYP-D3/def2-SVP level of theory. Hydrogen atoms are omitted for clarity.

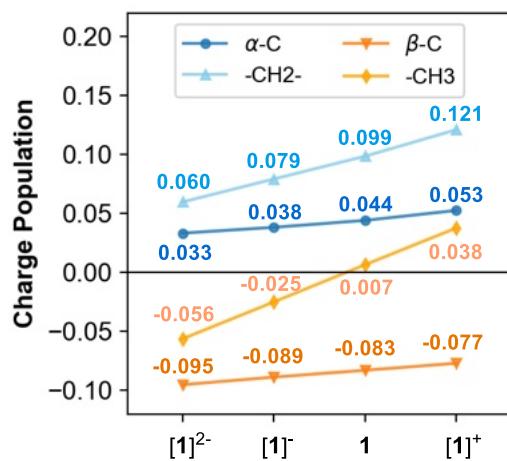


Figure S22. Average Hirshfeld charges on each $\alpha\text{-C}$, $\beta\text{-C}$, $-\text{CH}_2-$ and $-\text{CH}_3$ of $[1]^{2-/-0/+}$ computed at the B3LYP-D3/def2-SVP level of theory.

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,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-SVPPD 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 B_{12} 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.

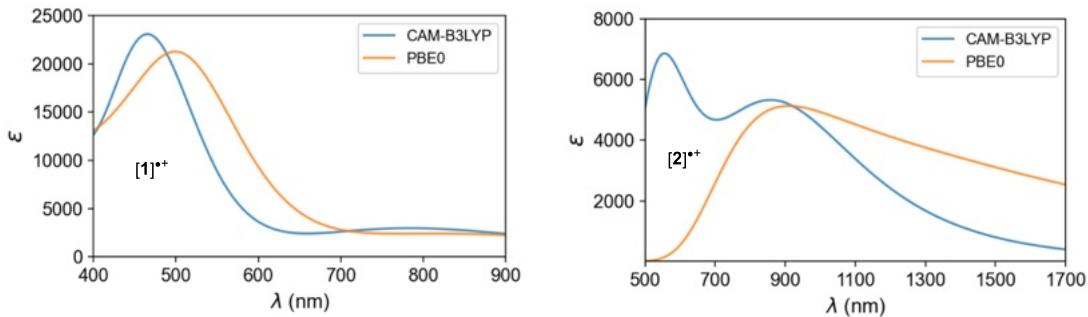


Figure S23. Comparison of TD-CAM-B3LYP and TD-PBE0 calculations for the UV-Vis spectrum of $[1]^{*+}$ and $[2]^{*+}$. For both methods, the def2-SVP basis set and the LR-PCM(DCM) model are employed.

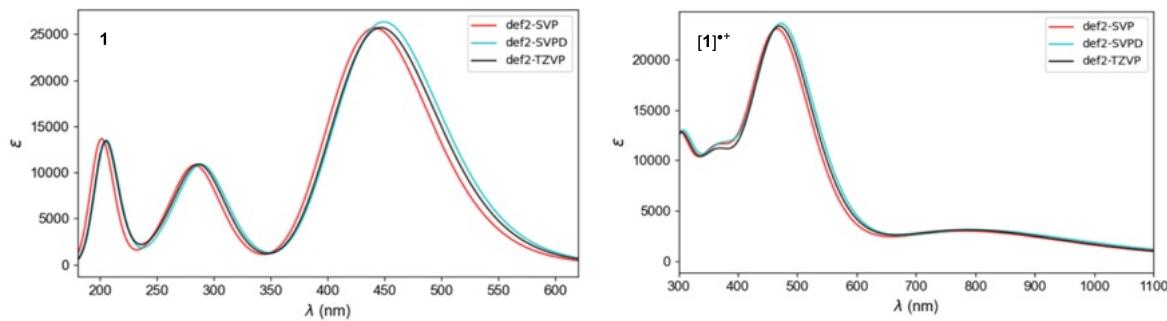


Figure S24. Basis set dependence of the simulated absorption spectra of $[1]^{0/+}$ in TD-CAM-B3LYP calculations in conjunction with the LR-PCM model.

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

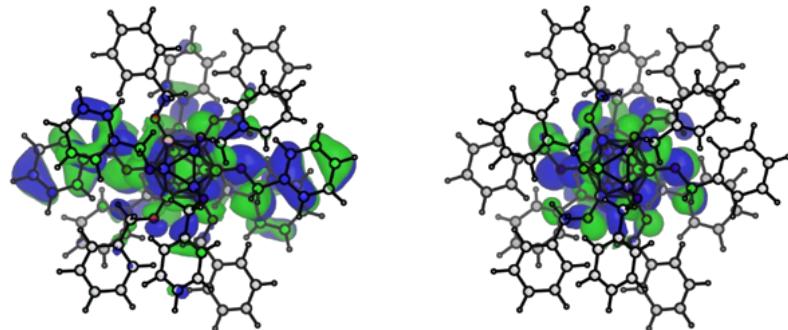


Figure S25. Natural transition orbitals for the root 7 of $[2]^{•+}$. The occupied and vacant NTOs are shown on left- and right-hand sides, respectively.

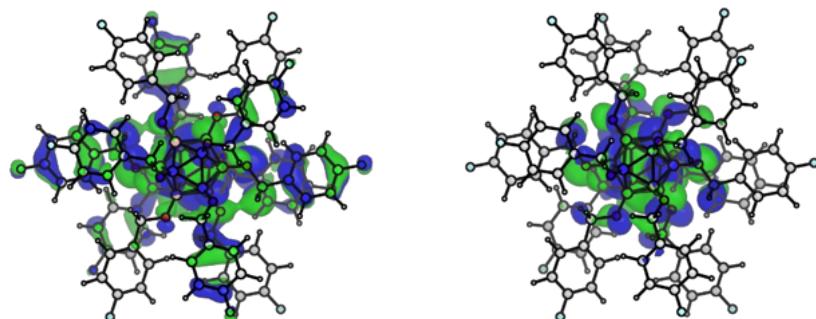


Figure S26. Natural transition orbitals for the root 6 of $[3]^{•+}$. The occupied and vacant NTOs are shown on left- and right-hand sides, respectively.

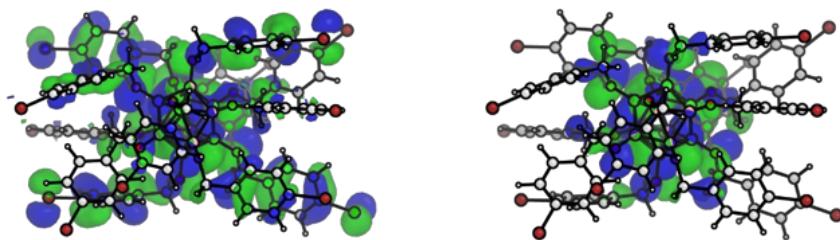


Figure S27. Natural transition orbitals for the root 8 of $[4]^{•+}$. The occupied and vacant NTOs are shown on left- and right-hand sides, respectively.

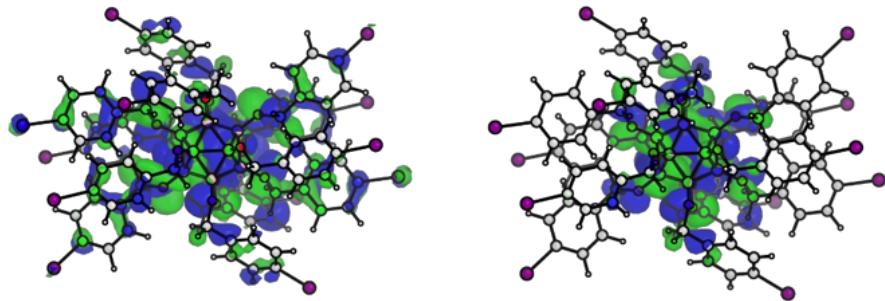


Figure S28. Natural transition orbitals for the root 7 of $[5]^{+}$. The occupied and vacant NTOs are shown on left- and right-hand sides, respectively.

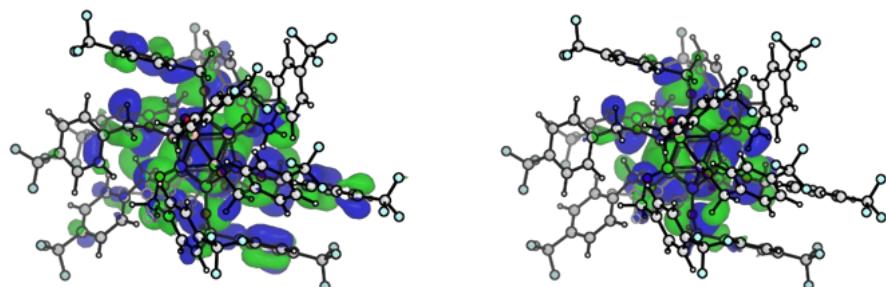


Figure S29. Natural transition orbitals for the root 7 of $[6]^{+}$. The occupied and vacant NTOs are shown on left- and right-hand sides, respectively.

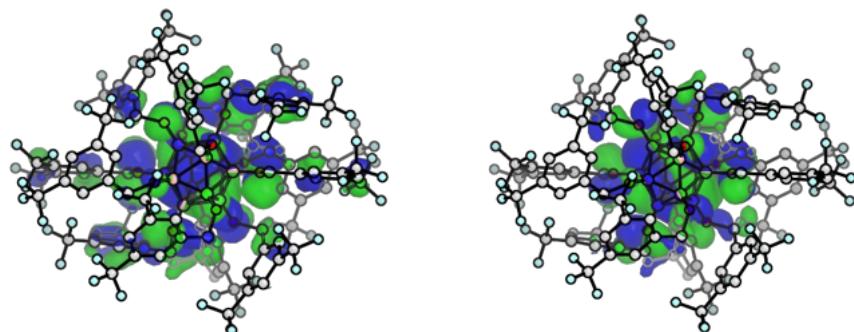


Figure S30. Natural transition orbitals for the root 9 of $[7]^{+}$. The occupied and vacant NTOs are shown on left- and right-hand sides, respectively.

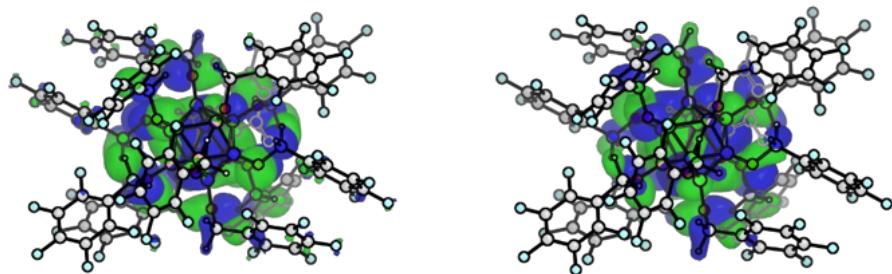


Figure S31. Natural transition orbitals for the root 8 of $[8]^{+}$. The occupied and vacant NTOs are shown on left- and right-hand sides, respectively.

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	1.57	789	0.0125	1.794	536A -> 577A (0.07) 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)

					573B -> 577B (0.02)
31	2.11	588	0.0135	1.488	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)
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)

					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 $[8]^{*+}$. 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	1.47	841	0.0273	2.333	584A -> 613A (0.01) 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

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

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

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

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

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

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

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

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

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	-0.724444000	-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

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

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

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

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	3.464448600	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

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

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

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

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

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:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

[2]⁺

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

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

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

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

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

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

[3]⁺

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

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

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

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

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

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

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

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

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

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

[5]⁺

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

[1]²⁻

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

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

Fc⁺

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