

Supporting Information for

Bis(phenothiazine)arene diradicaloids: isolation, characterization and crystal structures

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Experimental Section

All experiments were carried out under a nitrogen atmosphere by using standard Schlenk techniques and a glovebox. Solvents were dried prior to use. $\text{Ag}[\text{Al}(\text{OR}_\text{F})_4]^\text{I}$ ($\text{OR}_\text{F} = \text{OC}(\text{CF}_3)_3$) was synthesized according to literature method. EPR spectra were obtained using Bruker EMX-10/12 variable-temperature apparatus. Magnetic measurements were performed using a Quantum Design MPMS XL-7 SQUID magnetometer in the temperature range 5-350K with field up to 7T. UV-Vis spectra were recorded on the Lambda 750 spectrometer. Element analyses were performed at Shanghai Institute of Organic Chemistry, the Chinese Academy of Sciences. X-ray crystal structures were obtained by using Bruker APEX DUO CCD detectors. All hydrogen atoms were found in different maps and refined using a riding model. CCDC-1046930 ($\mathbf{A} \cdot 2[\text{Al}(\text{OR}_\text{F})_4]^-$), 1046927 ($\mathbf{1}^{2+} \cdot 2[\text{Al}(\text{OR}_\text{F})_4]^-$), 1046928 ($\mathbf{2}^{2+} \cdot 2[\text{Al}(\text{OR}_\text{F})_4]^- \cdot 1.8\text{CH}_2\text{Cl}_2$) and 1046929 ($\mathbf{3}^{2+} \cdot 2[\text{Al}(\text{OR}_\text{F})_4]^- \cdot 1.5\text{CH}_2\text{Cl}_2$) contain the supplementary crystallographic data for this paper.

Table S1 Crystal Data and Structure Refinement

	A •2[Al(OR _F) ₄] ⁻	1 ²⁺ •2[Al(OR _F) ₄] ⁻	2 ²⁺ •2[Al(OR _F) ₄] ⁻ •1.8CH ₂ Cl ₂	3 ²⁺ •2[Al(OR _F) ₄] ⁻ •1.5CH ₂ Cl ₂
formula	C ₆₂ H ₂₄ Al ₂ F ₇₂ N ₂ O ₈	C ₃₁ H ₁₀ AlF ₃₆ NO ₄ S	C _{69.80} H _{27.60} Al ₂ Cl _{3.61} F ₇₂ N ₂ O ₈ S ₂	C _{71.56} H _{27.11} Al ₂ Cl _{3.11} F ₇₂ N ₂ O ₈ S ₂
Mr [g mol ⁻¹]	2346.79	1203.44	2636.02	2639.05
crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic
space group	<i>P</i> 2(1)/c	<i>P</i> 2(1)/c	<i>P</i> 2(1)/n	<i>P</i> 2(1)/c
<i>Z</i>	4	4	2	2
Temp. (K)	123(2)	123(2)	123(2)	123(2)
μ (mm ⁻¹)	0.261	0.311	0.387	0.371
<i>a</i> (Å)	27.656(3)	14.2945(19)	13.604(3)	10.4150(7)
<i>b</i> (Å)	11.298(10)	19.666(3)	20.135(5)	15.3696(11)
<i>c</i> (Å)	25.570(2)	19.9786(19)	16.634(4)	28.611(2)
α	90	90	90	90
β	94.846(2)	134.333(6)	93.113(4)	93.362(1)
γ	90	90	90	90
<i>V</i> [Å ³]	7961.1(12)	4017.3(9)	4549.7(19)	4572.0(6)
<i>R</i> 1 (<i>I</i> > 2σ(<i>I</i>))	0.0503	0.0369	0.1031	0.0536
<i>wR</i> 2 (all data)	0.0995	0.1000	0.2636	0.1479

2²⁺•2[Al(OR_F)₄]⁻•1.8CH₂Cl₂:

Alert level B

Poor Data / Parameter Ratio 7.97 Note

3²⁺•2[Al(OR_F)₄]⁻•1.5CH₂Cl₂:

Alert level B

Poor Data / Parameter Ratio 7.66 Note

Author Response: The low relatively data / parameter ratios are caused by the disorder of the anions. But such a disorder does not influence the structural identification of **2**²⁺•2[Al(OR_F)₄]⁻•1.8CH₂Cl₂ and **3**²⁺•2[Al(OR_F)₄]⁻•1.5CH₂Cl₂, which have also been fully characterized by elemental analysis, UV-Vis, EPR spectroscopy and SQUID measurements, assisted by DFT calculations. We believe the key findings of the structural features of these complexes are unambiguous.

General Procedure for Syntheses of Phenylene Diphenothiazine Dications. A mixture of bis(phenothiazine)arene and $\text{Ag}[\text{Al}(\text{OR}_\text{F})_4]$ ($\text{OR}_\text{F} = \text{OC}(\text{CF}_3)_3$) in CH_2Cl_2 (≈ 30 ml) was stirred at room temperature overnight under anhydrous and anaerobic conditions. The resultant solution was filtered to remove the precipitate. The filtrate was then concentrated and stored at about 5 °C for 1 day to afford crystals.

$\text{A}\cdot\text{2}[\text{Al}(\text{OR}_\text{F})_4]^-$. 1,4-Bis(diphenylamino)benzene (0.122 g, 0.296 mmol) and $\text{Ag}[\text{Al}(\text{OR}_\text{F})_4]$ (0.675 g, 0.628 mmol); dark-brown crystals. Yield: 0.533 g, 76.7%; elemental analysis (%) Calcd $\text{C}_{62}\text{H}_{24}\text{Al}_2\text{F}_{72}\text{N}_2\text{O}_8$: C 31.73, H 1.03, N 1.19; Found: C 31.76, H 1.07, N 1.40.

$\text{1}^{2+}\cdot\text{2}[\text{Al}(\text{OR}_\text{F})_4]^-$. **1** (0.142 g, 0.300 mmol) and $\text{Ag}[\text{Al}(\text{OR}_\text{F})_4]$ (0.660 g, 0.614 mmol); brown crystals. Yield: 0.546 g, 75.6%; elemental analysis (%) Calcd $\text{C}_{62}\text{H}_{20}\text{Al}_2\text{F}_{72}\text{N}_2\text{O}_8\text{S}_2$: C 30.94, H 0.84, N 1.16; Found: C 30.83, H 0.85, N 1.13.

$\text{2}^{2+}\cdot\text{2}[\text{Al}(\text{OR}_\text{F})_4]^-$. **2** (0.109 g, 0.199 mmol) and $\text{Ag}[\text{Al}(\text{OR}_\text{F})_4]$ (0.449 g, 0.418 mmol); purple crystals; Yield: 0.289 g, 58.5%; elemental analysis (%) Calcd $\text{C}_{68}\text{H}_{24}\text{Al}_2\text{F}_{72}\text{N}_2\text{O}_8\text{S}_2$: C, 32.89; H, 0.97; N, 1.13; Found: C 33.04, H 1.01, N 1.10.

$\text{3}^{2+}\cdot\text{2}[\text{Al}(\text{OR}_\text{F})_4]^-$. **3** (0.110 g, 0.192 mmol) and $\text{Ag}[\text{Al}(\text{OR}_\text{F})_4]$ (0.434 g, 0.404 mmol); red-brown crystals; Yield: 0.301 g, 62.5 %; elemental analysis (%) Calcd $\text{C}_{70}\text{H}_{24}\text{Al}_2\text{F}_{72}\text{N}_2\text{O}_8\text{S}_2$: C, 33.54; H, 0.96; N, 1.12; Found: C 33.09, H 1.05, N 0.98.

Computational Details

All the geometry optimizations were carried out at the (U)B3LYP/6-31G(d) level of theory. The obtained stationary points were characterized by frequency calculations. The spin densities were calculated at the optimized geometries. The broken-symmetry approach was applied for open-shell singlet calculations. The diradical character (y) was obtained from the occupation number of the lowest unoccupied natural orbital (LUNO) at both UBH&HLYP/6-31G(d) and LC-UBLYP/6-31G(d) with a range-separating parameter of $\mu = 0.33^{2-4}$. The global ring centers for NICS(0) and NICS(1)_{zz} values were designated at the non-weighted mean centers of and 1 Å above the central bridging benzenoid rings (Figure S3). The NICS values were obtained at the UB3LYP/6-31+G(d) level with gauge independent atomic orbital (GIAO) method based on the optimized geometries. For 2^{2+} , the NICS values were the same for the two central benzenoid rings and only one of them was reported. The spin contamination errors were corrected by the approximate spin-projection method⁵ when evaluating the energy gaps. All calculations were performed with the Gaussian 09 program suite.⁶

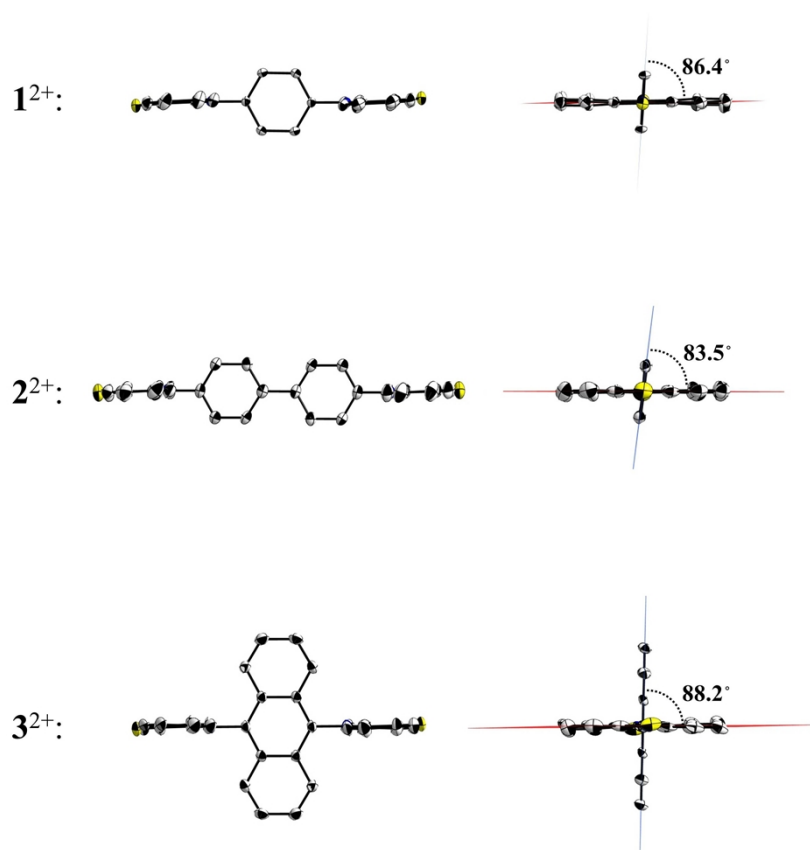


Fig. S1 The angle (θ) between the two planes formed by the bridging aryl moieties and the peripheral phenothiazine units in $1^{2+} - 3^{2+}$.

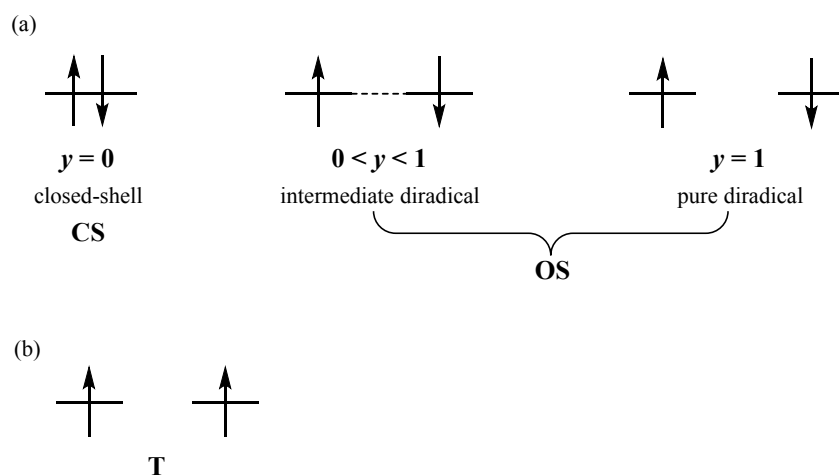


Fig. S2 Schematic illustration of diradical character y and the three electronic configurations of (a) singlet and (b) triplet states.

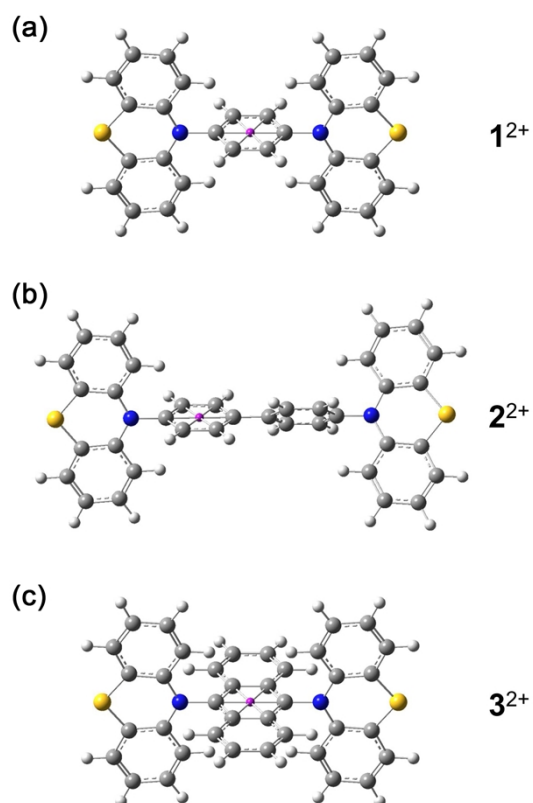


Fig. S3 The designation of the global ring centers (purple dots) for the calculation of NICS values of **1²⁺** – **3²⁺**.

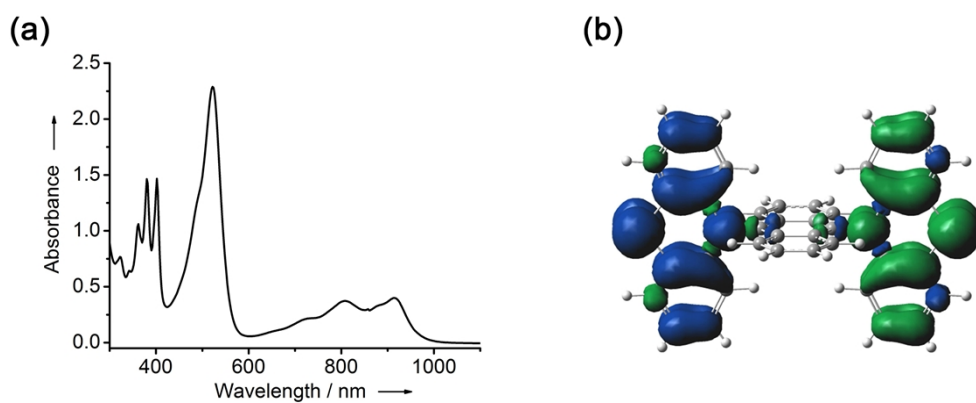
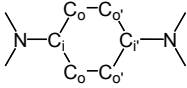
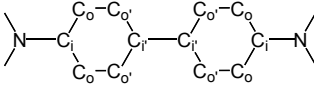


Fig. S4 (a) UV-vis absorption spectrum of 1×10^{-4} M **3²⁺** in CH₂Cl₂ at 25°C, and (b) spin density distribution of **3²⁺**.

Table S2 Selected experimental and calculated bond lengths (Å), relative energy (kcal mol⁻¹), diradical character (y), NICS(0) and NICS(1)_{zz} values for **1**²⁺–**3**²⁺, **A** and **B**.

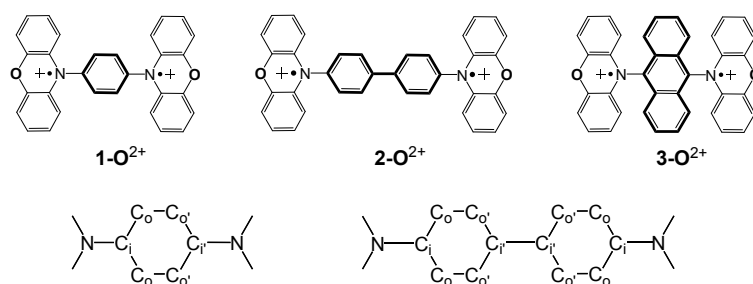
		ΔE_{X-OS}^a	avg. N–Ar	avg. N–C _i and N–C _{i'}	avg C _i –C _o and C _{i'} –C _{o'}	avg C _o –C _{o'}	BLA ^b	y UBH&HLYP (LC-UBLYP)	NICS(0)	NICS(1) _{zz}
A	X-ray		1.440	1.346	1.436	1.344	0.092			
	CS ^c	0	1.429	1.362	1.436	1.365	0.071		–0.47	–9.54
	T	6.0	1.409	1.429	1.405	1.390	0.015			
1 ²⁺	X-ray		1.389	1.456	1.382	1.390	0.008			
	CS	14.8	1.402	1.454	1.396	1.398	0.002			
	OS	0	1.402	1.455	1.397	1.396	0.001	0.993(0.995)	–7.78	–27.85
	T	0.0038	1.402	1.455	1.397	1.396	0.001			
B ⁷	X-ray		1.439	1.339	1.431	1.357	0.074			
	CS	5.2	1.430	1.368	1.432	1.369	0.063		–0.71	–9.21
	OS ^d	0	1.418	1.402	1.414	1.383	0.031	0.813(0.857)		
	T	2.6	1.413	1.418	1.408	1.387	0.021			
2 ²⁺	X-ray		1.397	1.459	1.392	1.390	0.002			
	CS	16.4	1.398	1.455	1.401	1.394	0.002			
	OS	0	1.400	1.456	1.401	1.394	0.007	0.999(0.999)	–7.55	–25.97
	T	0.0013	1.400	1.456	1.401	1.394	0.007			
3 ²⁺	X-ray		1.392	1.454	1.396	1.436	0.040			
	CS	15.4	1.401	1.457	1.409	1.446	0.037			
	OS	0	1.402	1.459	1.408	1.449	0.041	0.995(0.997)	–9.86	–31.62
	T	0.0025	1.402	1.459	1.408	1.449	0.041			

^aEnergy relative to the OS state. X = CS, OS, or T. ^bBLA is defined as the difference between the average of all C_i–C_o and C_{i'}–C_{o'} bond lengths and the average of C_o–C_{o'} bond lengths. ^cAttempted geometry optimization of **A** by using the broken-symmetry method did not converge to open-shell singlet (OS) but to closed-shell singlet (CS) instead. ^dIt is worth mentioning that the most stable electronic states for **B** is OS in the gas phase according to DFT calculations, but experimental characterization shows that **B** should have a CS ground state.⁷ Such a discrepancy between calculation and experimental observation may be ascribed to counterion effects. For example, bis(triarylamine) dicationic species with arylene/vinylene conjugated bridges were reported to be closed-shell singlets in the solid state, but their open-shell singlets have the lowest energy in the gas phase.⁸

Table S3 Singlet–triplet energy gap ΔE_{S-T} (cm⁻¹) for **1**²⁺ – **3**²⁺ calculated at both UB3LYP/6-31G(d) and LC-UBLYP/6-31G(d) ($\mu = 0.33$) in comparison with experimental results.

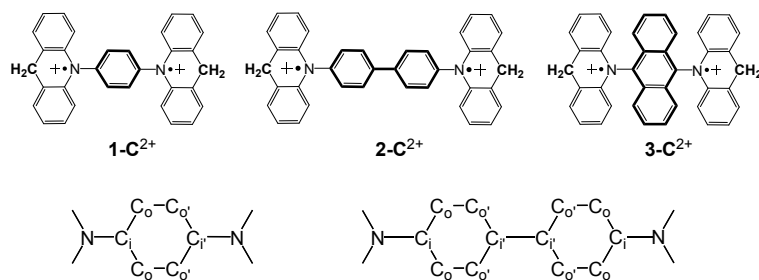
	Exp.	UB3LYP/6-31G(d)	LC-UBLYP/6-31G(d) ($\mu = 0.33$)
1 ²⁺	–6.07	–1.33	–0.90
2 ²⁺	–6.76	–0.44	–0.05
3 ²⁺	–0.75	–0.88	–0.40

Table S4 Selected calculated bond lengths (Å), relative energy (kcal mol⁻¹), dihedral angle θ (deg) and diradical character (y , calculated at UBH&HLYP/6-31G(d)) for oxygen analogues **1-O**²⁺ – **3-O**²⁺.



		ΔE_{X-OS}	avg. N–Ar	avg. N–C _i and N–C _{i'}	avg C _i –C _o and C _{i'} –C _{o'}	avg C _o –C _{o'}	BLA	θ	y
1-O ²⁺	CS	14.8	1.402	1.431	1.403	1.391	0.012	62.1	
	OS	0	1.394	1.450	1.397	1.396	0.001	90.0	0.992
	T	0.0051	1.394	1.450	1.397	1.396	0.001	90.0	
2-O ²⁺	CS	17.6	1.396	1.440	1.404	1.390	0.014	67.0	
	OS	0	1.392	1.452	1.401	1.394	0.007	88.5	0.999
	T	0	1.392	1.452	1.401	1.394	0.007	88.5	
3-O ²⁺	CS	15.8	1.397	1.444	1.411	1.449	0.038	78.0	
	OS	0	1.394	1.454	1.408	1.449	0.041	90.0	0.993
	T	0.0063	1.394	1.454	1.408	1.449	0.041	90.0	

Table S5 Selected calculated bond lengths (Å), relative energy (kcal mol⁻¹), dihedral angle θ (deg) and diradical character (y , calculated at UBH&HLYP/6-31G(d)) for carbon analogues **1-C²⁺** – **3-C²⁺**.



		ΔE_{X-OS}	avg. N-Ar	avg. N-C _i and N-C _{i'}	avg C _i -C _o and C _i -C _{o'}	avg C _o -C _{o'}	BLA	θ	y
1-C²⁺	CS	15.6	1.406	1.436	1.403	1.391	0.012	65.5	
	OS	0	1.400	1.455	1.397	1.396	0.001	90.0	0.992
	T	0.0051	1.400	1.455	1.397	1.396	0.001	90.0	
2-C²⁺	CS	18.1	1.401	1.442	1.404	1.390	0.014	68.8	
	OS	0	1.398	1.455	1.400	1.394	0.006	89.4	0.999
	T	0.0013	1.398	1.455	1.400	1.394	0.006	89.4	
3-C²⁺	CS	15.5	1.404	1.442	1.414	1.448	0.034	77.7	
	OS	0	1.400	1.458	1.407	1.448	0.041	90.0	0.994
	T	0.0064	1.400	1.458	1.407	1.448	0.041	90.0	

Table S6 Triplet–singlet energy gap $\Delta E_{\text{T-CS}}$ (kcal mol⁻¹) for neutral **1** – **3** calculated at UB3LYP/6-31G(d).

		$\Delta E_{\text{T-CS}}^a$
1	CS	0
	T	70.8
2	CS	0
	T	59.9
3	CS	0
	T	37.1

^aAttempted geometry optimization of **1** – **3** by using the broken-symmetry method did not converge to open-shell singlet (OS) but to closed-shell
shell singlet (CS) instead.

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Coordinates for calculated geometries

A-CS

N	0.000000000	0.000000000	2.781753000
N	0.000000000	0.000000000	-2.781753000
C	1.221581000	0.047701000	3.521830000
C	2.292170000	-0.793254000	3.160675000
H	2.178433000	-1.499539000	2.344273000
C	3.466775000	-0.753473000	3.902962000
H	4.287175000	-1.416389000	3.647609000
C	3.580462000	0.118739000	4.992441000
H	4.499475000	0.144544000	5.569657000
C	2.510384000	0.949720000	5.349537000
H	2.605581000	1.628912000	6.190526000
C	1.324241000	0.913376000	4.626899000
H	0.496637000	1.564228000	4.888151000
C	-1.221581000	-0.047701000	3.521830000
C	-1.324241000	-0.913376000	4.626899000
H	-0.496637000	-1.564228000	4.888151000
C	-2.510384000	-0.949720000	5.349537000
H	-2.605581000	-1.628912000	6.190526000
C	-3.580462000	-0.118739000	4.992441000
H	-4.499475000	-0.144544000	5.569657000
C	-3.466775000	0.753473000	3.902962000
H	-4.287175000	1.416389000	3.647609000
C	-2.292170000	0.793254000	3.160675000
H	-2.178433000	1.499539000	2.344273000
C	0.000000000	0.000000000	1.419976000
C	-1.090138000	-0.573673000	0.682351000
H	-1.882884000	-1.080748000	1.220034000
C	-1.090138000	-0.573673000	-0.682351000
H	-1.882884000	-1.080748000	-1.220034000
C	0.000000000	0.000000000	-1.419976000
C	1.090138000	0.573673000	-0.682351000
H	1.882884000	1.080748000	-1.220034000
C	1.090138000	0.573673000	0.682351000
H	1.882884000	1.080748000	1.220034000
C	-1.221581000	-0.047701000	-3.521830000
C	-2.292170000	0.793254000	-3.160675000
H	-2.178433000	1.499539000	-2.344273000
C	-3.466775000	0.753473000	-3.902962000
H	-4.287175000	1.416389000	-3.647609000
C	-3.580462000	-0.118739000	-4.992441000
H	-4.499475000	-0.144544000	-5.569657000
C	-2.510384000	-0.949720000	-5.349537000

H	-2.605581000	-1.628912000	-6.190526000
C	-1.324241000	-0.913376000	-4.626899000
H	-0.496637000	-1.564228000	-4.888151000
C	1.221581000	0.047701000	-3.521830000
C	1.324241000	0.913376000	-4.626899000
H	0.496637000	1.564228000	-4.888151000
C	2.510384000	0.949720000	-5.349537000
H	2.605581000	1.628912000	-6.190526000
C	3.580462000	0.118739000	-4.992441000
H	4.499475000	0.144544000	-5.569657000
C	3.466775000	-0.753473000	-3.902962000
H	4.287175000	-1.416389000	-3.647609000
C	2.292170000	-0.793254000	-3.160675000
H	2.178433000	-1.499539000	-2.344273000

A-T

N	0.000000000	0.000000000	2.825563000
N	0.000000000	0.000000000	-2.825563000
C	-0.369554000	1.165909000	3.525385000
C	0.000000000	2.438714000	3.031927000
H	0.599889000	2.518021000	2.131933000
C	-0.356678000	3.574931000	3.741303000
H	-0.049428000	4.551712000	3.381780000
C	-1.093598000	3.466114000	4.931536000
H	-1.373600000	4.361649000	5.477361000
C	-1.472218000	2.206104000	5.414571000
H	-2.061590000	2.125067000	6.322144000
C	-1.113805000	1.057120000	4.724855000
H	-1.436941000	0.082424000	5.073567000
C	0.369554000	-1.165909000	3.525385000
C	1.113805000	-1.057120000	4.724855000
H	1.436941000	-0.082424000	5.073567000
C	1.472218000	-2.206104000	5.414571000
H	2.061590000	-2.125067000	6.322144000
C	1.093598000	-3.466114000	4.931536000
H	1.373600000	-4.361649000	5.477361000
C	0.356678000	-3.574931000	3.741303000
H	0.049428000	-4.551712000	3.381780000
C	0.000000000	-2.438714000	3.031927000
H	-0.599889000	-2.518021000	2.131933000
C	0.000000000	0.000000000	1.396366000
C	1.072846000	-0.575293000	0.694990000

H	1.916755000	-0.990298000	1.235225000
C	1.072846000	-0.575293000	-0.694990000
H	1.916755000	-0.990298000	-1.235225000
C	0.000000000	0.000000000	-1.396366000
C	-1.072846000	0.575293000	-0.694990000
H	-1.916755000	0.990298000	-1.235225000
C	-1.072846000	0.575293000	0.694990000
H	-1.916755000	0.990298000	1.235225000
C	0.369554000	-1.165909000	-3.525385000
C	0.000000000	-2.438714000	-3.031927000
H	-0.599889000	-2.518021000	-2.131933000
C	0.356678000	-3.574931000	-3.741303000
H	0.049428000	-4.551712000	-3.381780000
C	1.093598000	-3.466114000	-4.931536000
H	1.373600000	-4.361649000	-5.477361000
C	1.472218000	-2.206104000	-5.414571000
H	2.061590000	-2.125067000	-6.322144000
C	1.113805000	-1.057120000	-4.724855000
H	1.436941000	-0.082424000	-5.073567000
C	-0.369554000	1.165909000	-3.525385000
C	-1.113805000	1.057120000	-4.724855000
H	-1.436941000	0.082424000	-5.073567000
C	-1.472218000	2.206104000	-5.414571000
H	-2.061590000	2.125067000	-6.322144000
C	-1.093598000	3.466114000	-4.931536000
H	-1.373600000	4.361649000	-5.477361000
C	-0.356678000	3.574931000	-3.741303000
H	-0.049428000	4.551712000	-3.381780000
C	0.000000000	2.438714000	-3.031927000
H	0.599889000	2.518021000	-2.131933000

1^{2+} -CS

S	-5.983651000	0.000044000	0.000409000
N	-2.839560000	-0.000016000	-0.000064000
C	-3.482869000	-1.245268000	-0.000119000
C	-2.727536000	-2.439371000	-0.000345000
C	-3.348528000	-3.676384000	-0.000402000
C	-4.750695000	-3.780153000	-0.000232000
C	-5.516434000	-2.628403000	-0.000012000
C	-4.903848000	-1.362819000	0.000050000
C	-4.903796000	1.362865000	0.000079000
C	-5.516327000	2.628475000	0.000063000
C	-4.750537000	3.780191000	-0.000122000

C	-3.348374000	3.676362000	-0.000298000
C	-2.727436000	2.439322000	-0.000283000
C	-3.482823000	1.245256000	-0.000097000
C	-1.385615000	-0.000026000	-0.000033000
C	-0.698882000	-0.000003000	1.215941000
C	0.698820000	-0.000003000	1.215971000
H	-1.647616000	-2.391387000	-0.000505000
H	-2.740483000	-4.575158000	-0.000586000
H	-5.230804000	-4.752873000	-0.000285000
H	-6.600854000	-2.690948000	0.000110000
H	-6.600745000	2.691066000	0.000193000
H	-5.230604000	4.752933000	-0.000139000
H	-2.740289000	4.575109000	-0.000451000
H	-1.647517000	2.391286000	-0.000439000
H	-1.245856000	0.000016000	2.153736000
H	1.245757000	0.000015000	2.153788000
S	5.983649000	0.000014000	-0.000409000
N	2.839562000	-0.000015000	0.000064000
C	3.482835000	1.245250000	0.000083000
C	2.727464000	2.439325000	0.000281000
C	3.348417000	3.676356000	0.000299000
C	4.750580000	3.780168000	0.000118000
C	5.516354000	2.628444000	-0.000072000
C	4.903809000	1.362843000	-0.000093000
C	4.903833000	-1.362835000	-0.000036000
C	5.516403000	-2.628425000	0.000021000
C	4.750652000	-3.780163000	0.000236000
C	3.348486000	-3.676378000	0.000401000
C	2.727510000	-2.439360000	0.000348000
C	3.482858000	-1.245269000	0.000133000
C	1.385617000	-0.000023000	0.000033000
C	0.698885000	-0.000040000	-1.215940000
C	-0.698817000	-0.000040000	-1.215972000
H	1.647545000	2.391305000	0.000449000
H	2.740344000	4.575110000	0.000461000
H	5.230658000	4.752903000	0.000139000
H	6.600771000	2.691022000	-0.000199000
H	6.600821000	-2.690982000	-0.000104000
H	5.230749000	-4.752889000	0.000283000
H	2.740431000	-4.575145000	0.000575000
H	1.647591000	-2.391361000	0.000495000
H	1.245858000	-0.000051000	-2.153735000
H	-1.245755000	-0.000051000	-2.153789000

1^{2+} -OS

S	-5.987124000	0.000052000	0.000335000
N	-2.841705000	-0.000019000	-0.000054000
C	-3.487127000	-1.244766000	-0.000085000
C	-2.731691000	-2.439887000	-0.000266000
C	-3.353309000	-3.675513000	-0.000295000
C	-4.755754000	-3.779014000	-0.000142000
C	-5.520300000	-2.628057000	0.000032000
C	-4.905767000	-1.361458000	0.000062000
C	-4.905705000	1.361512000	0.000049000
C	-5.520175000	2.628142000	0.000018000
C	-4.755568000	3.779059000	-0.000149000
C	-3.353127000	3.675487000	-0.000290000
C	-2.731573000	2.439830000	-0.000259000
C	-3.487072000	1.244752000	-0.000093000
C	-1.386869000	-0.000031000	-0.000027000
C	-0.698220000	-0.000026000	1.215593000
C	0.698165000	-0.000026000	1.215619000
H	-1.651704000	-2.392307000	-0.000408000
H	-2.745796000	-4.574713000	-0.000444000
H	-5.235845000	-4.751756000	-0.000169000
H	-6.604804000	-2.689448000	0.000140000
H	-6.604675000	2.689587000	0.000122000
H	-5.235609000	4.751826000	-0.000178000
H	-2.745569000	4.574656000	-0.000426000
H	-1.651587000	2.392189000	-0.000386000
H	-1.244610000	-0.000021000	2.153538000
H	1.244523000	-0.000021000	2.153583000
S	5.987124000	0.000016000	-0.000337000
N	2.841705000	-0.000017000	0.000054000
C	3.487087000	1.244748000	0.000087000
C	2.731606000	2.439838000	0.000269000
C	3.353177000	3.675487000	0.000299000
C	4.755619000	3.779039000	0.000146000
C	5.520209000	2.628111000	-0.000030000
C	4.905721000	1.361489000	-0.000061000
C	4.905750000	-1.361480000	-0.000051000
C	5.520266000	-2.628088000	-0.000021000
C	4.755703000	-3.779034000	0.000146000
C	3.353259000	-3.675513000	0.000287000
C	2.731659000	-2.439879000	0.000258000

C	3.487112000	-1.244770000	0.000092000
C	1.386869000	-0.000027000	0.000028000
C	0.698219000	-0.000025000	-1.215592000
C	-0.698165000	-0.000025000	-1.215619000
H	1.651619000	2.392215000	0.000411000
H	2.745631000	4.574665000	0.000449000
H	5.235674000	4.751799000	0.000174000
H	6.604710000	2.689541000	-0.000138000
H	6.604769000	-2.689494000	-0.000126000
H	5.235780000	-4.751783000	0.000173000
H	2.745734000	-4.574705000	0.000424000
H	1.651672000	-2.392282000	0.000386000
H	1.244610000	-0.000021000	-2.153538000
H	-1.244523000	-0.000021000	-2.153583000

$\mathbf{1}^{2+}\text{-T}$

S	-5.987125000	0.000051000	0.000335000
N	-2.841711000	-0.000018000	-0.000054000
C	-3.487128000	-1.244766000	-0.000085000
C	-2.731691000	-2.439886000	-0.000266000
C	-3.353308000	-3.675513000	-0.000295000
C	-4.755752000	-3.779016000	-0.000142000
C	-5.520301000	-2.628059000	0.000032000
C	-4.905769000	-1.361461000	0.000062000
C	-4.905709000	1.361513000	0.000049000
C	-5.520179000	2.628142000	0.000017000
C	-4.755571000	3.779060000	-0.000149000
C	-3.353131000	3.675488000	-0.000290000
C	-2.731576000	2.439831000	-0.000259000
C	-3.487075000	1.244752000	-0.000093000
C	-1.386884000	-0.000029000	-0.000027000
C	-0.698211000	-0.000024000	1.215590000
C	0.698156000	-0.000024000	1.215617000
H	-1.651704000	-2.392306000	-0.000408000
H	-2.745795000	-4.574713000	-0.000444000
H	-5.235842000	-4.751759000	-0.000169000
H	-6.604804000	-2.689452000	0.000140000
H	-6.604679000	2.689588000	0.000122000
H	-5.235613000	4.751827000	-0.000178000
H	-2.745573000	4.574657000	-0.000426000
H	-1.651590000	2.392190000	-0.000386000

H	-1.244601000	-0.000020000	2.153534000
H	1.244513000	-0.000020000	2.153580000
S	5.987125000	0.000015000	-0.000337000
N	2.841711000	-0.000016000	0.000054000
C	3.487089000	1.244748000	0.000087000
C	2.731608000	2.439839000	0.000269000
C	3.353181000	3.675488000	0.000299000
C	4.755623000	3.779040000	0.000146000
C	5.520213000	2.628111000	-0.000030000
C	4.905725000	1.361491000	-0.000061000
C	4.905752000	-1.361483000	-0.000051000
C	5.520267000	-2.628091000	-0.000021000
C	4.755702000	-3.779036000	0.000146000
C	3.353259000	-3.675513000	0.000287000
C	2.731659000	-2.439878000	0.000258000
C	3.487113000	-1.244770000	0.000092000
C	1.386883000	-0.000025000	0.000028000
C	0.698211000	-0.000023000	-1.215590000
C	-0.698157000	-0.000023000	-1.215616000
H	1.651622000	2.392217000	0.000411000
H	2.745636000	4.574666000	0.000449000
H	5.235678000	4.751800000	0.000174000
H	6.604714000	2.689542000	-0.000138000
H	6.604770000	-2.689498000	-0.000126000
H	5.235778000	-4.751786000	0.000173000
H	2.745733000	-4.574704000	0.000424000
H	1.651672000	-2.392280000	0.000386000
H	1.244600000	-0.000019000	-2.153534000
H	-1.244514000	-0.000020000	-2.153580000

2²⁺-CS

S	0.000000000	0.000000000	-8.146735000
N	0.000000000	0.000000000	-5.003438000
C	1.167116000	0.426444000	-5.645026000
C	2.288683000	0.832417000	-4.885073000
C	3.450912000	1.257836000	-5.503332000
C	3.550149000	1.298204000	-6.905341000
C	2.469620000	0.905367000	-7.674924000
C	1.280508000	0.469853000	-7.065824000
C	-1.280508000	-0.469853000	-7.065824000
C	-2.469620000	-0.905367000	-7.674924000

C	-3.550149000	-1.298204000	-6.905341000
C	-3.450912000	-1.257836000	-5.503332000
C	-2.288683000	-0.832417000	-4.885073000
C	-1.167116000	-0.426444000	-5.645026000
C	0.000000000	0.000000000	-3.548415000
C	0.401206000	-1.144985000	-2.858141000
C	0.399270000	-1.138993000	-1.464472000
H	2.239437000	0.810307000	-3.805398000
H	4.294244000	1.562868000	-4.892319000
H	4.464670000	1.633110000	-7.383118000
H	2.530531000	0.929413000	-8.759141000
H	-2.530531000	-0.929413000	-8.759141000
H	-4.464670000	-1.633110000	-7.383118000
H	-4.294244000	-1.562868000	-4.892319000
H	-2.239437000	-0.810307000	-3.805398000
H	0.720146000	-2.027635000	-3.404072000
H	0.736782000	-2.024535000	-0.934947000
C	0.000000000	0.000000000	-0.743721000
C	-0.399270000	1.138993000	-1.464472000
C	-0.401206000	1.144985000	-2.858141000
H	-0.736782000	2.024535000	-0.934947000
H	-0.720146000	2.027635000	-3.404072000
C	0.000000000	0.000000000	0.743721000
C	0.399327000	1.138973000	1.464473000
C	-0.399327000	-1.138973000	1.464473000
C	0.401265000	1.144965000	2.858142000
H	0.736881000	2.024499000	0.934948000
C	-0.401265000	-1.144965000	2.858142000
H	-0.736881000	-2.024499000	0.934948000
C	0.000000000	0.000000000	3.548416000
H	0.720249000	2.027599000	3.404073000
H	-0.720249000	-2.027599000	3.404073000
N	0.000000000	0.000000000	5.003439000
C	1.167113000	-0.426451000	5.645026000
C	-1.167113000	0.426451000	5.645026000
C	2.288670000	-0.832448000	4.885073000
C	1.280510000	-0.469848000	7.065824000
C	-1.280510000	0.469848000	7.065824000
C	-2.288670000	0.832448000	4.885073000
C	3.450900000	-1.257865000	5.503331000
H	2.239416000	-0.810360000	3.805398000
S	0.000000000	0.000000000	8.146736000
C	2.469623000	-0.905357000	7.674924000
C	-2.469623000	0.905357000	7.674924000

C	-3.450900000	1.257865000	5.503331000
H	-2.239416000	0.810360000	3.805398000
C	3.550146000	-1.298208000	6.905340000
H	4.294224000	-1.562916000	4.892318000
H	2.530539000	-0.929391000	8.759140000
C	-3.550146000	1.298208000	6.905340000
H	-2.530539000	0.929391000	8.759140000
H	-4.294224000	1.562916000	4.892318000
H	4.464669000	-1.633111000	7.383117000
H	-4.464669000	1.633111000	7.383117000

2²⁺-OS

S	0.000000000	0.000000000	-8.149765000
N	0.000000000	0.000000000	-5.004440000
C	1.169431000	0.419703000	-5.648691000
C	2.293106000	0.821556000	-4.888002000
C	3.456919000	1.239011000	-5.506303000
C	3.556870000	1.276000000	-6.908672000
C	2.475380000	0.888819000	-7.677382000
C	1.282204000	0.460708000	-7.066835000
C	-1.282204000	-0.460708000	-7.066835000
C	-2.475380000	-0.888819000	-7.677382000
C	-3.556870000	-1.276000000	-6.908672000
C	-3.456919000	-1.239011000	-5.506303000
C	-2.293106000	-0.821556000	-4.888002000
C	-1.169431000	-0.419703000	-5.648691000
C	0.000000000	0.000000000	-3.548149000
C	0.405386000	-1.143504000	-2.858433000
C	0.403245000	-1.137649000	-1.464668000
H	2.242739000	0.802169000	-3.808276000
H	4.301744000	1.540988000	-4.895774000
H	4.473632000	1.604909000	-7.386405000
H	2.536139000	0.911020000	-8.761653000
H	-2.536139000	-0.911020000	-8.761653000
H	-4.473632000	-1.604909000	-7.386405000
H	-4.301744000	-1.540988000	-4.895774000
H	-2.242739000	-0.802169000	-3.808276000
H	0.727362000	-2.025151000	-3.404212000
H	0.743510000	-2.022051000	-0.935110000
C	0.000000000	0.000000000	-0.743871000
C	-0.403245000	1.137649000	-1.464668000

C	-0.405386000	1.143504000	-2.858433000
H	-0.743510000	2.022051000	-0.935110000
H	-0.727362000	2.025151000	-3.404212000
C	0.000000000	0.000000000	0.743871000
C	0.403264000	1.137642000	1.464668000
C	-0.403264000	-1.137642000	1.464668000
C	0.405406000	1.143497000	2.858433000
H	0.743546000	2.022038000	0.935111000
C	-0.405406000	-1.143497000	2.858433000
H	-0.743546000	-2.022038000	0.935111000
C	0.000000000	0.000000000	3.548148000
H	0.727398000	2.025138000	3.404212000
H	-0.727398000	-2.025138000	3.404212000
N	0.000000000	0.000000000	5.004441000
C	1.169429000	-0.419709000	5.648691000
C	-1.169429000	0.419709000	5.648691000
C	2.293104000	-0.821562000	4.888002000
C	1.282203000	-0.460713000	7.066835000
C	-1.282203000	0.460713000	7.066835000
C	-2.293104000	0.821562000	4.888002000
C	3.456918000	-1.239015000	5.506304000
H	2.242738000	-0.802172000	3.808276000
S	0.000000000	0.000000000	8.149765000
C	2.475379000	-0.888822000	7.677382000
C	-2.475379000	0.888822000	7.677382000
C	-3.456918000	1.239015000	5.506304000
H	-2.242738000	0.802172000	3.808276000
C	3.556869000	-1.276004000	6.908672000
H	4.301742000	-1.540992000	4.895774000
H	2.536140000	-0.911020000	8.761653000
C	-3.556869000	1.276004000	6.908672000
H	-2.536140000	0.911020000	8.761653000
H	-4.301742000	1.540992000	4.895774000
H	4.473632000	-1.604910000	7.386405000
H	-4.473632000	1.604910000	7.386405000

2²⁺-T

S	0.000000000	0.000000000	8.149765000
N	0.000000000	0.000000000	5.004441000
C	-1.169432000	0.419699000	5.648691000
C	-2.293107000	0.821552000	4.888003000

C	-3.456923000	1.239002000	5.506304000
C	-3.556874000	1.275988000	6.908672000
C	-2.475384000	0.888809000	7.677382000
C	-1.282206000	0.460703000	7.066835000
C	1.282206000	-0.460703000	7.066835000
C	2.475384000	-0.888809000	7.677382000
C	3.556874000	-1.275988000	6.908672000
C	3.456923000	-1.239002000	5.506304000
C	2.293107000	-0.821552000	4.888003000
C	1.169432000	-0.419699000	5.648691000
C	0.000000000	0.000000000	3.548148000
C	-0.405392000	-1.143502000	2.858433000
C	-0.403251000	-1.137647000	1.464668000
H	-2.242739000	0.802167000	3.808276000
H	-4.301748000	1.540978000	4.895774000
H	-4.473638000	1.604892000	7.386405000
H	-2.536144000	0.911008000	8.761653000
H	2.536144000	-0.911008000	8.761653000
H	4.473638000	-1.604892000	7.386405000
H	4.301748000	-1.540978000	4.895774000
H	2.242739000	-0.802167000	3.808276000
H	-0.727373000	-2.025147000	3.404212000
H	-0.743522000	-2.022047000	0.935110000
C	0.000000000	0.000000000	0.743871000
C	0.403251000	1.137647000	1.464668000
C	0.405392000	1.143502000	2.858433000
H	0.743522000	2.022047000	0.935110000
H	0.727373000	2.025147000	3.404212000
C	0.000000000	0.000000000	-0.743871000
C	-0.403271000	1.137640000	-1.464668000
C	0.403271000	-1.137640000	-1.464668000
C	-0.405412000	1.143494000	-2.858433000
H	-0.743558000	2.022034000	-0.935110000
C	0.405412000	-1.143494000	-2.858433000
H	0.743558000	-2.022034000	-0.935110000
C	0.000000000	0.000000000	-3.548148000
H	-0.727410000	2.025134000	-3.404212000
H	0.727410000	-2.025134000	-3.404212000
N	0.000000000	0.000000000	-5.004441000
C	-1.169430000	-0.419706000	-5.648691000
C	1.169430000	0.419706000	-5.648691000
C	-2.293105000	-0.821558000	-4.888003000
C	-1.282204000	-0.460708000	-7.066835000
C	1.282204000	0.460708000	-7.066835000

C	2.293105000	0.821558000	-4.888003000
C	-3.456921000	-1.239007000	-5.506304000
H	-2.242738000	-0.802171000	-3.808276000
S	0.000000000	0.000000000	-8.149765000
C	-2.475383000	-0.888812000	-7.677382000
C	2.475383000	0.888812000	-7.677382000
C	3.456921000	1.239007000	-5.506304000
H	2.242738000	0.802171000	-3.808276000
C	-3.556873000	-1.275991000	-6.908672000
H	-4.301746000	-1.540982000	-4.895774000
H	-2.536144000	-0.911008000	-8.761653000
C	3.556873000	1.275991000	-6.908672000
H	2.536144000	0.911008000	-8.761653000
H	4.301746000	1.540982000	-4.895774000
H	-4.473638000	-1.604894000	-7.386405000
H	4.473638000	1.604894000	-7.386405000

3^{2+} -CS

C	-3.672155000	0.000018000	0.711535000
C	-2.492019000	0.000029000	1.406792000
C	-1.236624000	0.000007000	0.723114000
C	-1.236624000	-0.000007000	-0.723114000
C	-2.492019000	-0.000029000	-1.406792000
C	-3.672155000	-0.000018000	-0.711535000
C	0.000000000	0.000000000	1.397612000
C	0.000000000	0.000000000	-1.397612000
C	1.236624000	0.000007000	-0.723114000
C	1.236624000	-0.000007000	0.723114000
C	2.492019000	-0.000029000	1.406792000
H	2.504204000	-0.000054000	2.490935000
C	3.672155000	-0.000018000	0.711535000
C	3.672155000	0.000018000	-0.711535000
C	2.492019000	0.000029000	-1.406792000
H	-4.616714000	0.000035000	1.246335000
H	-2.504204000	0.000054000	2.490935000
H	-2.504204000	-0.000054000	-2.490935000
H	-4.616714000	-0.000035000	-1.246335000
H	4.616714000	-0.000035000	1.246335000
H	4.616714000	0.000035000	-1.246335000
H	2.504204000	0.000054000	-2.490935000
N	0.000000000	0.000000000	2.854733000

C	0.000147000	-1.243169000	3.500253000
C	-0.000147000	1.243169000	3.500253000
C	0.000352000	-2.436250000	2.743058000
C	0.000117000	-1.363176000	4.921254000
C	-0.000117000	1.363176000	4.921254000
C	-0.000352000	2.436250000	2.743058000
C	0.000483000	-3.673813000	3.361555000
H	0.000412000	-2.380677000	1.663485000
S	0.000000000	0.000000000	6.002245000
C	0.000241000	-2.629416000	5.531994000
C	-0.000241000	2.629416000	5.531994000
C	-0.000483000	3.673813000	3.361555000
H	-0.000412000	2.380677000	1.663485000
C	0.000415000	-3.779760000	4.763863000
H	0.000644000	-4.571636000	2.752106000
H	0.000209000	-2.693857000	6.616305000
C	-0.000415000	3.779760000	4.763863000
H	-0.000209000	2.693857000	6.616305000
H	-0.000644000	4.571636000	2.752106000
H	0.000508000	-4.753285000	5.242425000
H	-0.000508000	4.753285000	5.242425000
N	0.000000000	0.000000000	-2.854733000
C	-0.000147000	-1.243169000	-3.500253000
C	0.000147000	1.243169000	-3.500253000
C	-0.000352000	-2.436250000	-2.743058000
C	-0.000117000	-1.363176000	-4.921254000
C	0.000117000	1.363176000	-4.921254000
C	0.000352000	2.436250000	-2.743058000
C	-0.000483000	-3.673813000	-3.361555000
H	-0.000412000	-2.380677000	-1.663485000
S	0.000000000	0.000000000	-6.002245000
C	-0.000241000	-2.629416000	-5.531994000
C	0.000241000	2.629416000	-5.531994000
C	0.000483000	3.673813000	-3.361555000
H	0.000412000	2.380677000	-1.663485000
C	-0.000415000	-3.779760000	-4.763863000
H	-0.000644000	-4.571636000	-2.752106000
H	-0.000209000	-2.693857000	-6.616305000
C	0.000415000	3.779760000	-4.763863000
H	0.000209000	2.693857000	-6.616305000
H	0.000644000	4.571636000	-2.752106000
H	-0.000508000	-4.753285000	-5.242425000
H	0.000508000	4.753285000	-5.242425000

3²⁺-OS

C	-3.672552000	0.000016000	0.711494000
C	-2.492817000	0.000025000	1.407512000
C	-1.236962000	0.000006000	0.724256000
C	-1.236962000	-0.000006000	-0.724256000
C	-2.492817000	-0.000025000	-1.407512000
C	-3.672552000	-0.000016000	-0.711494000
C	0.000000000	0.000000000	1.396041000
C	0.000000000	0.000000000	-1.396041000
C	1.236962000	0.000006000	-0.724256000
C	1.236962000	-0.000006000	0.724256000
C	2.492817000	-0.000025000	1.407512000
H	2.506916000	-0.000048000	2.491570000
C	3.672552000	-0.000016000	0.711494000
C	3.672552000	0.000016000	-0.711494000
C	2.492817000	0.000025000	-1.407512000
H	-4.617273000	0.000034000	1.245991000
H	-2.506916000	0.000048000	2.491570000
H	-2.506916000	-0.000048000	-2.491570000
H	-4.617273000	-0.000034000	-1.245991000
H	4.617273000	-0.000034000	1.245991000
H	4.617273000	0.000034000	-1.245991000
H	2.506916000	0.000048000	-2.491570000
N	0.000000000	0.000000000	2.854642000
C	-0.000101000	-1.242689000	3.503154000
C	0.000101000	1.242689000	3.503154000
C	-0.000134000	-2.436796000	2.745726000
C	-0.000188000	-1.361377000	4.921587000
C	0.000188000	1.361377000	4.921587000
C	0.000134000	2.436796000	2.745726000
C	-0.000294000	-3.672903000	3.364634000
H	-0.000032000	-2.381506000	1.666081000
S	0.000000000	0.000000000	6.004648000
C	-0.000371000	-2.628878000	5.534202000
C	0.000371000	2.628878000	5.534202000
C	0.000294000	3.672903000	3.364634000
H	0.000032000	2.381506000	1.666081000
C	-0.000433000	-3.778342000	4.767360000
H	-0.000308000	-4.571202000	2.755801000
H	-0.000451000	-2.692149000	6.618595000
C	0.000433000	3.778342000	4.767360000

H	0.000451000	2.692149000	6.618595000
H	0.000308000	4.571202000	2.755801000
H	-0.000580000	-4.751864000	5.245983000
H	0.000580000	4.751864000	5.245983000
N	0.000000000	0.000000000	-2.854642000
C	0.000101000	-1.242689000	-3.503154000
C	-0.000101000	1.242689000	-3.503154000
C	0.000134000	-2.436796000	-2.745726000
C	0.000188000	-1.361377000	-4.921587000
C	-0.000188000	1.361377000	-4.921587000
C	-0.000134000	2.436796000	-2.745726000
C	0.000294000	-3.672903000	-3.364634000
H	0.000032000	-2.381506000	-1.666081000
S	0.000000000	0.000000000	-6.004648000
C	0.000371000	-2.628878000	-5.534202000
C	-0.000371000	2.628878000	-5.534202000
C	-0.000294000	3.672903000	-3.364634000
H	-0.000032000	2.381506000	-1.666081000
C	0.000433000	-3.778342000	-4.767360000
H	0.000308000	-4.571202000	-2.755801000
H	0.000451000	-2.692149000	-6.618595000
C	-0.000433000	3.778342000	-4.767360000
H	-0.000451000	2.692149000	-6.618595000
H	-0.000308000	4.571202000	-2.755801000
H	0.000580000	-4.751864000	-5.245983000
H	-0.000580000	4.751864000	-5.245983000

3^{2+} -T

C	-3.672552000	0.000016000	0.711494000
C	-2.492817000	0.000025000	1.407512000
C	-1.236962000	0.000006000	0.724256000
C	-1.236962000	-0.000006000	-0.724256000
C	-2.492817000	-0.000025000	-1.407512000
C	-3.672552000	-0.000016000	-0.711494000
C	0.000000000	0.000000000	1.396041000
C	0.000000000	0.000000000	-1.396041000
C	1.236962000	0.000006000	-0.724256000
C	1.236962000	-0.000006000	0.724256000
C	2.492817000	-0.000025000	1.407512000
H	2.506916000	-0.000048000	2.491570000
C	3.672552000	-0.000016000	0.711494000

C	3.672552000	0.000016000	-0.711494000
C	2.492817000	0.000025000	-1.407512000
H	-4.617273000	0.000034000	1.245991000
H	-2.506916000	0.000048000	2.491570000
H	-2.506916000	-0.000048000	-2.491570000
H	-4.617273000	-0.000034000	-1.245991000
H	4.617273000	-0.000034000	1.245991000
H	4.617273000	0.000034000	-1.245991000
H	2.506916000	0.000048000	-2.491570000
N	0.000000000	0.000000000	2.854642000
C	-0.000101000	-1.242689000	3.503154000
C	0.000101000	1.242689000	3.503154000
C	-0.000134000	-2.436796000	2.745726000
C	-0.000188000	-1.361377000	4.921587000
C	0.000188000	1.361377000	4.921587000
C	0.000134000	2.436796000	2.745726000
C	-0.000294000	-3.672903000	3.364634000
H	-0.000032000	-2.381506000	1.666081000
S	0.000000000	0.000000000	6.004648000
C	-0.000371000	-2.628878000	5.534202000
C	0.000371000	2.628878000	5.534202000
C	0.000294000	3.672903000	3.364634000
H	0.000032000	2.381506000	1.666081000
C	-0.000433000	-3.778342000	4.767360000
H	-0.000308000	-4.571202000	2.755801000
H	-0.000451000	-2.692149000	6.618595000
C	0.000433000	3.778342000	4.767360000
H	0.000451000	2.692149000	6.618595000
H	0.000308000	4.571202000	2.755801000
H	-0.000580000	-4.751864000	5.245983000
H	0.000580000	4.751864000	5.245983000
N	0.000000000	0.000000000	-2.854642000
C	0.000101000	-1.242689000	-3.503154000
C	-0.000101000	1.242689000	-3.503154000
C	0.000134000	-2.436796000	-2.745726000
C	0.000188000	-1.361377000	-4.921587000
C	-0.000188000	1.361377000	-4.921587000
C	-0.000134000	2.436796000	-2.745726000
C	0.000294000	-3.672903000	-3.364634000
H	0.000032000	-2.381506000	-1.666081000
S	0.000000000	0.000000000	-6.004648000
C	0.000371000	-2.628878000	-5.534202000
C	-0.000371000	2.628878000	-5.534202000
C	-0.000294000	3.672903000	-3.364634000

H	-0.000032000	2.381506000	-1.666081000
C	0.000433000	-3.778342000	-4.767360000
H	0.000308000	-4.571202000	-2.755801000
H	0.000451000	-2.692149000	-6.618595000
C	-0.000433000	3.778342000	-4.767360000
H	-0.000451000	2.692149000	-6.618595000
H	-0.000308000	4.571202000	-2.755801000
H	0.000580000	-4.751864000	-5.245983000
H	-0.000580000	4.751864000	-5.245983000

1-O²⁺-CS

O	-5.624261000	-0.000200000	-0.000364000
N	-2.826117000	0.000016000	0.000141000
C	-3.529727000	-1.066880000	0.577056000
C	-2.904378000	-2.211716000	1.110798000
C	-3.667595000	-3.226146000	1.665176000
C	-5.074067000	-3.143787000	1.692221000
C	-5.715315000	-2.047694000	1.136954000
C	-4.950371000	-1.025712000	0.575900000
C	-4.950330000	1.025538000	-0.576169000
C	-5.715208000	2.047496000	-1.137353000
C	-5.073901000	3.143772000	-1.692195000
C	-3.667448000	3.226331000	-1.664610000
C	-2.904298000	2.211913000	-1.110125000
C	-3.529696000	1.066904000	-0.576805000
C	-1.394782000	0.000033000	0.000087000
C	-0.695252000	-0.007696000	1.216720000
C	0.695405000	0.007949000	1.216635000
H	-1.827207000	-2.307622000	1.080311000
H	-3.172061000	-4.101074000	2.072573000
H	-5.657745000	-3.946202000	2.130785000
H	-6.796188000	-1.959728000	1.114460000
H	-6.796077000	1.959379000	-1.115282000
H	-5.657527000	3.946181000	-2.130835000
H	-3.171892000	4.101412000	-2.071652000
H	-1.827147000	2.307939000	-1.079209000
H	-1.234855000	-0.009073000	2.158155000
H	1.235125000	0.009489000	2.158002000
O	5.624263000	-0.000193000	0.000346000
N	2.826121000	0.000013000	-0.000138000
C	3.529698000	1.066908000	0.576794000

C	2.904296000	2.211910000	1.110121000
C	3.667444000	3.226335000	1.664596000
C	5.073898000	3.143786000	1.692165000
C	5.715209000	2.047513000	1.137322000
C	4.950332000	1.025548000	0.576147000
C	4.950372000	-1.025718000	-0.575896000
C	5.715313000	-2.047705000	-1.136945000
C	5.074061000	-3.143805000	-1.692196000
C	3.667588000	-3.226162000	-1.665144000
C	2.904374000	-2.211727000	-1.110771000
C	3.529728000	-1.066889000	-0.577040000
C	1.394787000	0.000030000	-0.000083000
C	0.695258000	-0.007819000	-1.216716000
C	-0.695399000	0.007828000	-1.216632000
H	1.827143000	2.307923000	1.079221000
H	3.171886000	4.101411000	2.071645000
H	5.657523000	3.946201000	2.130799000
H	6.796078000	1.959402000	1.115243000
H	6.796186000	-1.959738000	-1.114461000
H	5.657735000	-3.946223000	-2.130756000
H	3.172052000	-4.101093000	-2.072531000
H	1.827202000	-2.307627000	-1.080282000
H	1.234862000	-0.009297000	-2.158150000
H	-1.235118000	0.009268000	-2.158000000

1-O²⁺-OS

O	-5.623493000	0.000017000	-0.000066000
N	-2.834649000	-0.000009000	-0.000069000
C	-3.528271000	-1.209653000	-0.000080000
C	-2.887404000	-2.464130000	-0.000094000
C	-3.643839000	-3.623760000	-0.000106000
C	-5.052801000	-3.571524000	-0.000100000
C	-5.705842000	-2.349031000	-0.000087000
C	-4.948255000	-1.177744000	-0.000079000
C	-4.948233000	1.177766000	-0.000078000
C	-5.705797000	2.349067000	-0.000086000
C	-5.052733000	3.571547000	-0.000099000
C	-3.643769000	3.623756000	-0.000103000
C	-2.887357000	2.464112000	-0.000092000
C	-3.528249000	1.209648000	-0.000079000
C	-1.384214000	-0.000018000	-0.000035000

C	-0.698162000	-0.000021000	1.217145000
C	0.698101000	-0.000021000	1.217181000
H	-1.806054000	-2.517534000	-0.000100000
H	-3.142941000	-4.586177000	-0.000120000
H	-5.629454000	-4.490418000	-0.000107000
H	-6.787720000	-2.271138000	-0.000083000
H	-6.787677000	2.271195000	-0.000083000
H	-5.629368000	4.490453000	-0.000105000
H	-3.142853000	4.586163000	-0.000117000
H	-1.806005000	2.517493000	-0.000097000
H	-1.244787000	-0.000021000	2.154878000
H	1.244678000	-0.000021000	2.154941000
O	5.623493000	0.000014000	0.000066000
N	2.834649000	-0.000009000	0.000069000
C	3.528250000	1.209647000	0.000080000
C	2.887361000	2.464112000	0.000095000
C	3.643774000	3.623755000	0.000107000
C	5.052738000	3.571545000	0.000101000
C	5.705800000	2.349063000	0.000088000
C	4.948234000	1.177763000	0.000079000
C	4.948253000	-1.177747000	0.000078000
C	5.705838000	-2.349035000	0.000086000
C	5.052796000	-3.571527000	0.000098000
C	3.643833000	-3.623760000	0.000103000
C	2.887401000	-2.464130000	0.000092000
C	3.528269000	-1.209654000	0.000079000
C	1.384214000	-0.000018000	0.000035000
C	0.698163000	-0.000014000	-1.217145000
C	-0.698100000	-0.000014000	-1.217181000
H	1.806009000	2.517496000	0.000101000
H	3.142859000	4.586163000	0.000121000
H	5.629374000	4.490449000	0.000108000
H	6.787681000	2.271189000	0.000084000
H	6.787717000	-2.271143000	0.000082000
H	5.629448000	-4.490422000	0.000104000
H	3.142934000	-4.586176000	0.000116000
H	1.806050000	-2.517532000	0.000097000
H	1.244787000	-0.000009000	-2.154877000
H	-1.244678000	-0.000008000	-2.154941000

1-O²⁺-T

O	5.623493000	0.000017000	0.000066000
N	2.834649000	-0.000009000	0.000069000
C	3.528271000	-1.209653000	0.000080000
C	2.887404000	-2.464130000	0.000094000
C	3.643839000	-3.623760000	0.000106000
C	5.052801000	-3.571524000	0.000100000
C	5.705842000	-2.349031000	0.000087000
C	4.948255000	-1.177744000	0.000079000
C	4.948233000	1.177766000	0.000078000
C	5.705797000	2.349067000	0.000086000
C	5.052733000	3.571547000	0.000099000
C	3.643769000	3.623756000	0.000103000
C	2.887357000	2.464112000	0.000092000
C	3.528249000	1.209648000	0.000079000
C	1.384214000	-0.000018000	0.000035000
C	0.698162000	-0.000021000	-1.217145000
C	-0.698101000	-0.000021000	-1.217181000
H	1.806054000	-2.517534000	0.000100000
H	3.142941000	-4.586177000	0.000120000
H	5.629454000	-4.490418000	0.000107000
H	6.787720000	-2.271138000	0.000083000
H	6.787677000	2.271195000	0.000083000
H	5.629368000	4.490453000	0.000105000
H	3.142853000	4.586163000	0.000117000
H	1.806005000	2.517493000	0.000097000
H	1.244787000	-0.000021000	-2.154878000
H	-1.244678000	-0.000021000	-2.154941000
O	-5.623493000	0.000014000	-0.000066000
N	-2.834649000	-0.000009000	-0.000069000
C	-3.528250000	1.209647000	-0.000080000
C	-2.887361000	2.464112000	-0.000095000
C	-3.643774000	3.623755000	-0.000107000
C	-5.052738000	3.571545000	-0.000101000
C	-5.705800000	2.349063000	-0.000088000
C	-4.948234000	1.177763000	-0.000079000
C	-4.948253000	-1.177747000	-0.000078000
C	-5.705838000	-2.349035000	-0.000086000
C	-5.052796000	-3.571527000	-0.000098000
C	-3.643833000	-3.623760000	-0.000103000
C	-2.887401000	-2.464130000	-0.000092000
C	-3.528269000	-1.209654000	-0.000079000
C	-1.384214000	-0.000018000	-0.000035000
C	-0.698163000	-0.000014000	1.217145000

C	0.698100000	-0.000014000	1.217181000
H	-1.806009000	2.517496000	-0.000101000
H	-3.142859000	4.586163000	-0.000121000
H	-5.629374000	4.490449000	-0.000108000
H	-6.787681000	2.271189000	-0.000084000
H	-6.787717000	-2.271143000	-0.000082000
H	-5.629448000	-4.490422000	-0.000104000
H	-3.142934000	-4.586176000	-0.000116000
H	-1.806050000	-2.517532000	-0.000097000
H	-1.244787000	-0.000009000	2.154877000
H	1.244678000	-0.000008000	2.154941000

2-O²⁺-CS

N	0.000000000	0.000000000	-4.991021000
C	1.154184000	0.361435000	-5.689104000
C	2.371149000	0.684612000	-5.055725000
C	3.475456000	1.036479000	-5.814811000
C	3.408732000	1.066813000	-7.221297000
C	2.231157000	0.723451000	-7.869365000
C	1.118896000	0.366731000	-7.110274000
C	-1.118896000	-0.366731000	-7.110274000
C	-2.231157000	-0.723451000	-7.869365000
C	-3.408732000	-1.066813000	-7.221297000
C	-3.475456000	-1.036479000	-5.814811000
C	-2.371149000	-0.684612000	-5.055725000
C	-1.154184000	-0.361435000	-5.689104000
C	0.000000000	0.000000000	-3.551434000
C	-0.126587000	-1.207779000	-2.854509000
C	-0.122706000	-1.201364000	-1.464109000
H	2.443152000	0.650070000	-3.976634000
H	4.406341000	1.282744000	-5.314949000
H	4.282114000	1.344932000	-7.801582000
H	2.147603000	0.715351000	-8.950721000
H	-2.147603000	-0.715351000	-8.950721000
H	-4.282114000	-1.344932000	-7.801582000
H	-4.406341000	-1.282744000	-5.314949000
H	-2.443152000	-0.650070000	-3.976634000
H	-0.198645000	-2.144911000	-3.397557000
H	-0.177471000	-2.148746000	-0.937508000
C	0.000000000	0.000000000	-0.739496000
C	0.122706000	1.201364000	-1.464109000

C	0.126587000	1.207779000	-2.854509000
H	0.177471000	2.148746000	-0.937508000
H	0.198645000	2.144911000	-3.397557000
C	0.000000000	0.000000000	0.742544000
C	0.789623000	0.913512000	1.465768000
C	-0.789623000	-0.913512000	1.465768000
C	0.799779000	0.914019000	2.857042000
H	1.421991000	1.620704000	0.938402000
C	-0.799779000	-0.914019000	2.857042000
H	-1.421991000	-1.620704000	0.938402000
C	0.000000000	0.000000000	3.551828000
H	1.415590000	1.623740000	3.400645000
H	-1.415590000	-1.623740000	3.400645000
N	0.000000000	0.000000000	4.993117000
C	1.132317000	-0.424052000	5.689882000
C	-1.132317000	0.424052000	5.689882000
C	2.292212000	-0.909912000	5.053862000
C	1.107172000	-0.401519000	7.111109000
C	-1.107172000	0.401519000	7.111109000
C	-2.292212000	0.909912000	5.053862000
C	3.379581000	-1.313327000	5.811702000
H	2.328262000	-0.972929000	3.974085000
C	2.203645000	-0.806689000	7.868810000
C	-2.203645000	0.806689000	7.868810000
C	-3.379581000	1.313327000	5.811702000
H	-2.328262000	0.972929000	3.974085000
C	3.343845000	-1.256449000	7.218686000
H	4.266855000	-1.685992000	5.310786000
H	2.133301000	-0.765350000	8.950347000
C	-3.343845000	1.256449000	7.218686000
H	-2.133301000	0.765350000	8.950347000
H	-4.266855000	1.685992000	5.310786000
H	4.203720000	-1.575941000	7.797838000
H	-4.203720000	1.575941000	7.797838000
O	0.000000000	0.000000000	7.787140000
O	0.000000000	0.000000000	-7.786345000

2-O²⁺-OS

N	0.000000000	0.000000000	4.996947000
C	-1.123612000	0.440769000	5.690677000
C	-2.291272000	0.896087000	5.045069000
C	-3.371980000	1.320202000	5.798452000

C	-3.324945000	1.304247000	7.207299000
C	-2.187787000	0.859498000	7.864061000
C	-1.096029000	0.430816000	7.109914000
C	1.096029000	-0.430816000	7.109914000
C	2.187787000	-0.859498000	7.864061000
C	3.324945000	-1.304247000	7.207299000
C	3.371980000	-1.320202000	5.798452000
C	2.291272000	-0.896087000	5.045069000
C	1.123612000	-0.440769000	5.690677000
C	0.000000000	0.000000000	3.545439000
C	-0.413590000	-1.141959000	2.857309000
C	-0.410385000	-1.135584000	1.463687000
H	-2.334986000	0.910818000	3.963374000
H	-4.267403000	1.669303000	5.294998000
H	-4.181410000	1.640441000	7.782147000
H	-2.117989000	0.833011000	8.946098000
H	2.117989000	-0.833011000	8.946098000
H	4.181410000	-1.640441000	7.782147000
H	4.267403000	-1.669303000	5.294998000
H	2.334986000	-0.910818000	3.963374000
H	-0.741978000	-2.021248000	3.402955000
H	-0.756041000	-2.017514000	0.933566000
C	0.000000000	0.000000000	0.743968000
C	0.410385000	1.135584000	1.463687000
C	0.413590000	1.141959000	2.857309000
H	0.756041000	2.017514000	0.933566000
H	0.741978000	2.021248000	3.402955000
C	0.000000000	0.000000000	-0.743968000
C	-0.410385000	1.135584000	-1.463687000
C	0.410385000	-1.135584000	-1.463687000
C	-0.413590000	1.141959000	-2.857309000
H	-0.756040000	2.017514000	-0.933566000
C	0.413590000	-1.141959000	-2.857309000
H	0.756040000	-2.017514000	-0.933566000
C	0.000000000	0.000000000	-3.545439000
H	-0.741977000	2.021248000	-3.402955000
H	0.741977000	-2.021248000	-3.402955000
N	0.000000000	0.000000000	-4.996947000
C	-1.123612000	-0.440768000	-5.690677000
C	1.123612000	0.440768000	-5.690677000
C	-2.291272000	-0.896087000	-5.045069000
C	-1.096029000	-0.430816000	-7.109914000
C	1.096029000	0.430816000	-7.109914000
C	2.291272000	0.896087000	-5.045069000

C	-3.371980000	-1.320202000	-5.798452000
H	-2.334986000	-0.910818000	-3.963374000
C	-2.187787000	-0.859498000	-7.864061000
C	2.187787000	0.859498000	-7.864061000
C	3.371980000	1.320202000	-5.798452000
H	2.334986000	0.910818000	-3.963374000
C	-3.324945000	-1.304247000	-7.207299000
H	-4.267403000	-1.669303000	-5.294998000
H	-2.117989000	-0.833011000	-8.946098000
C	3.324945000	1.304247000	-7.207299000
H	2.117989000	0.833011000	-8.946098000
H	4.267403000	1.669303000	-5.294998000
H	-4.181410000	-1.640441000	-7.782147000
H	4.181410000	1.640441000	-7.782147000
O	0.000000000	0.000000000	-7.788004000
O	0.000000000	0.000000000	7.788004000

2-O²⁺-T

N	0.000000000	0.000000000	4.996947000
C	-1.123618000	0.440753000	5.690677000
C	-2.291283000	0.896058000	5.045068000
C	-3.371997000	1.320159000	5.798452000
C	-3.324963000	1.304203000	7.207298000
C	-2.187799000	0.859468000	7.864061000
C	-1.096035000	0.430801000	7.109914000
C	1.096035000	-0.430801000	7.109914000
C	2.187799000	-0.859468000	7.864061000
C	3.324963000	-1.304203000	7.207298000
C	3.371997000	-1.320159000	5.798452000
C	2.291283000	-0.896058000	5.045068000
C	1.123618000	-0.440753000	5.690677000
C	0.000000000	0.000000000	3.545438000
C	-0.413602000	-1.141954000	2.857309000
C	-0.410397000	-1.135580000	1.463686000
H	-2.334996000	0.910792000	3.963374000
H	-4.267423000	1.669250000	5.294997000
H	-4.181432000	1.640385000	7.782146000
H	-2.118001000	0.832982000	8.946097000
H	2.118001000	-0.832982000	8.946097000
H	4.181432000	-1.640385000	7.782146000
H	4.267423000	-1.669250000	5.294997000
H	2.334996000	-0.910792000	3.963374000

H	-0.741999000	-2.021240000	3.402954000
H	-0.756062000	-2.017506000	0.933565000
C	0.000000000	0.000000000	0.743968000
C	0.410397000	1.135580000	1.463686000
C	0.413602000	1.141954000	2.857309000
H	0.756062000	2.017506000	0.933565000
H	0.741999000	2.021240000	3.402954000
C	0.000000000	0.000000000	-0.743968000
C	-0.410397000	1.135580000	-1.463686000
C	0.410397000	-1.135580000	-1.463686000
C	-0.413602000	1.141954000	-2.857309000
H	-0.756062000	2.017506000	-0.933565000
C	0.413602000	-1.141954000	-2.857309000
H	0.756062000	-2.017506000	-0.933565000
C	0.000000000	0.000000000	-3.545438000
H	-0.741998000	2.021240000	-3.402954000
H	0.741998000	-2.021240000	-3.402954000
N	0.000000000	0.000000000	-4.996947000
C	-1.123618000	-0.440753000	-5.690677000
C	1.123618000	0.440753000	-5.690677000
C	-2.291283000	-0.896058000	-5.045068000
C	-1.096035000	-0.430801000	-7.109914000
C	1.096035000	0.430801000	-7.109914000
C	2.291283000	0.896058000	-5.045068000
C	-3.371997000	-1.320159000	-5.798452000
H	-2.334996000	-0.910792000	-3.963374000
C	-2.187799000	-0.859468000	-7.864061000
C	2.187799000	0.859468000	-7.864061000
C	3.371997000	1.320159000	-5.798452000
H	2.334996000	0.910792000	-3.963374000
C	-3.324963000	-1.304203000	-7.207298000
H	-4.267423000	-1.669250000	-5.294997000
H	-2.118001000	-0.832982000	-8.946097000
C	3.324963000	1.304203000	-7.207298000
H	2.118001000	0.832982000	-8.946097000
H	4.267423000	1.669250000	-5.294997000
H	-4.181432000	-1.640385000	-7.782146000
H	4.181432000	1.640385000	-7.782146000
O	0.000000000	0.000000000	-7.788004000
O	0.000000000	0.000000000	7.788004000

3-O²⁺-CS

C	-3.676684000	0.018618000	-0.710223000
C	-2.495489000	0.026386000	-1.406334000
C	-1.240363000	0.001289000	-0.724612000
C	-1.240363000	-0.001289000	0.724612000
C	-2.495489000	-0.026386000	1.406334000
C	-3.676684000	-0.018618000	0.710223000
C	0.000000000	0.000000000	-1.397437000
C	0.000000000	0.000000000	1.397437000
C	1.240363000	0.001289000	0.724612000
C	1.240363000	-0.001289000	-0.724612000
C	2.495489000	-0.026386000	-1.406334000
H	2.513296000	-0.051348000	-2.489648000
C	3.676684000	-0.018618000	-0.710223000
C	3.676684000	0.018618000	0.710223000
C	2.495489000	0.026386000	1.406334000
H	-4.620679000	0.038094000	-1.245527000
H	-2.513296000	0.051348000	-2.489648000
H	-2.513296000	-0.051348000	2.489648000
H	-4.620679000	-0.038094000	1.245527000
H	4.620679000	-0.038094000	-1.245527000
H	4.620679000	0.038094000	1.245527000
H	2.513296000	0.051348000	2.489648000
N	0.000000000	0.000000000	-2.841535000
C	0.258057000	1.181391000	-3.540875000
C	-0.258057000	-1.181391000	-3.540875000
C	0.487255000	2.415756000	-2.903842000
C	0.260918000	1.148452000	-4.961963000
C	-0.260918000	-1.148452000	-4.961963000
C	-0.487255000	-2.415756000	-2.903842000
C	0.737382000	3.549216000	-3.660245000
H	0.465903000	2.473816000	-1.823165000
C	0.512120000	2.291163000	-5.719556000
C	-0.512120000	-2.291163000	-5.719556000
C	-0.737382000	-3.549216000	-3.660245000
H	-0.465903000	-2.473816000	-1.823165000
C	0.756667000	3.491139000	-5.068359000
H	0.913167000	4.495333000	-3.159287000
H	0.505137000	2.211498000	-6.801275000
C	-0.756667000	-3.491139000	-5.068359000
H	-0.505137000	-2.211498000	-6.801275000
H	-0.913167000	-4.495333000	-3.159287000
H	0.952523000	4.387940000	-5.646433000
H	-0.952523000	-4.387940000	-5.646433000

N	0.000000000	0.000000000	2.841535000
C	-0.258057000	1.181391000	3.540875000
C	0.258057000	-1.181391000	3.540875000
C	-0.487255000	2.415756000	2.903842000
C	-0.260918000	1.148452000	4.961963000
C	0.260918000	-1.148452000	4.961963000
C	0.487255000	-2.415756000	2.903842000
C	-0.737382000	3.549216000	3.660245000
H	-0.465903000	2.473816000	1.823165000
C	-0.512120000	2.291163000	5.719556000
C	0.512120000	-2.291163000	5.719556000
C	0.737382000	-3.549216000	3.660245000
H	0.465903000	-2.473816000	1.823165000
C	-0.756667000	3.491139000	5.068359000
H	-0.913167000	4.495333000	3.159287000
H	-0.505137000	2.211498000	6.801275000
C	0.756667000	-3.491139000	5.068359000
H	0.505137000	-2.211498000	6.801275000
H	0.913167000	-4.495333000	3.159287000
H	-0.952523000	4.387940000	5.646433000
H	0.952523000	-4.387940000	5.646433000
O	0.000000000	0.000000000	-5.637921000
O	0.000000000	0.000000000	5.637921000

3-O²⁺-OS

C	-3.673704000	0.000000000	0.711520000
C	-2.494223000	0.000000000	1.407964000
C	-1.238758000	0.000000000	0.724283000
C	-1.238758000	0.000000000	-0.724283000
C	-2.494223000	0.000000000	-1.407964000
C	-3.673704000	0.000000000	-0.711520000
C	0.000000000	0.000000000	1.392704000
C	0.000000000	0.000000000	-1.392704000
C	1.238758000	0.000000000	-0.724283000
C	1.238758000	0.000000000	0.724283000
C	2.494223000	0.000000000	1.407964000
H	2.509571000	0.000000000	2.492030000
C	3.673704000	0.000000000	0.711520000
C	3.673704000	0.000000000	-0.711520000
C	2.494223000	0.000000000	-1.407964000
H	-4.618484000	0.000001000	1.245841000

H	-2.509571000	0.000000000	2.492030000
H	-2.509571000	0.000000000	-2.492030000
H	-4.618484000	-0.000001000	-1.245841000
H	4.618484000	-0.000001000	1.245841000
H	4.618484000	0.000001000	-1.245841000
H	2.509571000	0.000000000	-2.492030000
N	0.000000000	0.000000000	2.846472000
C	-0.000002000	-1.207309000	3.543128000
C	0.000002000	1.207309000	3.543128000
C	-0.000005000	-2.461100000	2.900212000
C	-0.000001000	-1.177407000	4.962943000
C	0.000001000	1.177407000	4.962943000
C	0.000005000	2.461100000	2.900212000
C	-0.000006000	-3.621545000	3.654139000
H	-0.000006000	-2.507280000	1.818535000
C	-0.000003000	-2.349946000	5.718719000
C	0.000003000	2.349946000	5.718719000
C	0.000006000	3.621545000	3.654139000
H	0.000006000	2.507280000	1.818535000
C	-0.000005000	-3.571301000	5.063394000
H	-0.000008000	-4.583251000	3.151864000
H	-0.000002000	-2.273958000	6.800716000
C	0.000005000	3.571301000	5.063394000
H	0.000002000	2.273958000	6.800716000
H	0.000008000	4.583251000	3.151864000
H	-0.000007000	-4.491053000	5.638735000
H	0.000007000	4.491053000	5.638735000
N	0.000000000	0.000000000	-2.846472000
C	0.000002000	-1.207309000	-3.543128000
C	-0.000002000	1.207309000	-3.543128000
C	0.000005000	-2.461100000	-2.900212000
C	0.000001000	-1.177407000	-4.962943000
C	-0.000001000	1.177407000	-4.962943000
C	-0.000005000	2.461100000	-2.900212000
C	0.000006000	-3.621545000	-3.654139000
H	0.000006000	-2.507280000	-1.818535000
C	0.000003000	-2.349946000	-5.718719000
C	-0.000003000	2.349946000	-5.718719000
C	-0.000006000	3.621545000	-3.654139000
H	-0.000006000	2.507280000	-1.818535000
C	0.000005000	-3.571301000	-5.063394000
H	0.000008000	-4.583251000	-3.151864000
H	0.000002000	-2.273958000	-6.800716000
C	-0.000005000	3.571301000	-5.063394000

H	-0.000002000	2.273958000	-6.800716000
H	-0.000008000	4.583251000	-3.151864000
H	0.000007000	-4.491053000	-5.638735000
H	-0.000007000	4.491053000	-5.638735000
O	0.000000000	0.000000000	5.640159000
O	0.000000000	0.000000000	-5.640159000

3-O²⁺-T

C	-3.673696000	0.000000000	0.711521000
C	-2.494209000	0.000000000	1.407954000
C	-1.238752000	0.000000000	0.724267000
C	-1.238752000	0.000000000	-0.724267000
C	-2.494209000	0.000000000	-1.407954000
C	-3.673696000	0.000000000	-0.711521000
C	0.000000000	0.000000000	1.392725000
C	0.000000000	0.000000000	-1.392725000
C	1.238752000	0.000000000	-0.724267000
C	1.238752000	0.000000000	0.724267000
C	2.494209000	0.000000000	1.407954000
H	2.509533000	0.000000000	2.492021000
C	3.673696000	0.000000000	0.711521000
C	3.673696000	0.000000000	-0.711521000
C	2.494209000	0.000000000	-1.407954000
H	-4.618474000	0.000001000	1.245846000
H	-2.509533000	0.000000000	2.492021000
H	-2.509533000	0.000000000	-2.492021000
H	-4.618474000	-0.000001000	-1.245846000
H	4.618474000	-0.000001000	1.245846000
H	4.618474000	0.000001000	-1.245846000
H	2.509533000	0.000000000	-2.492021000
N	0.000000000	0.000000000	2.846490000
C	-0.000002000	-1.207311000	3.543143000
C	0.000002000	1.207311000	3.543143000
C	-0.000004000	-2.461101000	2.900228000
C	-0.000001000	-1.177409000	4.962959000
C	0.000001000	1.177409000	4.962959000
C	0.000004000	2.461101000	2.900228000
C	-0.000005000	-3.621546000	3.654155000
H	-0.000005000	-2.507281000	1.818551000
C	-0.000002000	-2.349947000	5.718735000
C	0.000002000	2.349947000	5.718735000
C	0.000005000	3.621546000	3.654155000

H	0.000005000	2.507281000	1.818551000
C	-0.000005000	-3.571303000	5.063410000
H	-0.000007000	-4.583252000	3.151880000
H	-0.000002000	-2.273959000	6.800732000
C	0.000005000	3.571303000	5.063410000
H	0.000002000	2.273959000	6.800732000
H	0.000007000	4.583252000	3.151880000
H	-0.000006000	-4.491055000	5.638751000
H	0.000006000	4.491055000	5.638751000
N	0.000000000	0.000000000	-2.846490000
C	0.000002000	-1.207311000	-3.543143000
C	-0.000002000	1.207311000	-3.543143000
C	0.000004000	-2.461101000	-2.900228000
C	0.000001000	-1.177409000	-4.962959000
C	-0.000001000	1.177409000	-4.962959000
C	-0.000004000	2.461101000	-2.900228000
C	0.000005000	-3.621546000	-3.654155000
H	0.000005000	-2.507281000	-1.818551000
C	0.000002000	-2.349947000	-5.718735000
C	-0.000002000	2.349947000	-5.718735000
C	-0.000005000	3.621546000	-3.654155000
H	-0.000005000	2.507281000	-1.818551000
C	0.000005000	-3.571303000	-5.063410000
H	0.000007000	-4.583252000	-3.151880000
H	0.000002000	-2.273959000	-6.800732000
C	-0.000005000	3.571303000	-5.063410000
H	-0.000002000	2.273959000	-6.800732000
H	-0.000007000	4.583252000	-3.151880000
H	0.000006000	-4.491055000	-5.638751000
H	-0.000006000	4.491055000	-5.638751000
O	0.000000000	0.000000000	5.640173000
O	0.000000000	0.000000000	-5.640173000

1-C²⁺-CS

N	0.000000000	0.000000000	2.829710000
C	-0.514682000	1.120747000	3.504804000
C	-0.940265000	2.266397000	2.785106000
C	-1.471929000	3.351920000	3.455131000
C	-1.571813000	3.340546000	4.856414000
C	-1.103236000	2.241514000	5.571894000
C	-0.562823000	1.130491000	4.925746000

C	0.562823000	-1.130491000	4.925746000
C	1.103236000	-2.241514000	5.571894000
C	1.571813000	-3.340546000	4.856414000
C	1.471929000	-3.351920000	3.455131000
C	0.940265000	-2.266397000	2.785106000
C	0.514682000	-1.120747000	3.504804000
C	0.000000000	0.000000000	1.393438000
C	-1.216861000	0.010126000	0.695661000
C	-1.216861000	-0.010126000	-0.695661000
H	-0.840699000	2.308013000	1.709356000
H	-1.797648000	4.221320000	2.893564000
H	-1.988682000	4.193885000	5.381544000
H	-1.145468000	2.246362000	6.657554000
H	1.145468000	-2.246362000	6.657554000
H	1.988682000	-4.193885000	5.381544000
H	1.797648000	-4.221320000	2.893564000
H	0.840699000	-2.308013000	1.709356000
H	-2.156852000	0.016780000	1.237742000
H	-2.156852000	-0.016780000	-1.237742000
N	0.000000000	0.000000000	-2.829710000
C	-0.514682000	-1.120747000	-3.504804000
C	-0.940265000	-2.266397000	-2.785106000
C	-1.471929000	-3.351920000	-3.455131000
C	-1.571813000	-3.340546000	-4.856414000
C	-1.103236000	-2.241514000	-5.571894000
C	-0.562823000	-1.130491000	-4.925746000
C	0.562823000	1.130491000	-4.925746000
C	1.103236000	2.241514000	-5.571894000
C	1.571813000	3.340546000	-4.856414000
C	1.471929000	3.351920000	-3.455131000
C	0.940265000	2.266397000	-2.785106000
C	0.514682000	1.120747000	-3.504804000
C	0.000000000	0.000000000	-1.393438000
C	1.216861000	0.010126000	-0.695661000
C	1.216861000	-0.010126000	0.695661000
H	-0.840699000	-2.308013000	-1.709356000
H	-1.797648000	-4.221320000	-2.893564000
H	-1.988682000	-4.193885000	-5.381544000
H	-1.145468000	-2.246362000	-6.657554000
H	1.145468000	2.246362000	-6.657554000
H	1.988682000	4.193885000	-5.381544000
H	1.797648000	4.221320000	-2.893564000
H	0.840699000	2.308013000	-1.709356000
H	2.156852000	0.016780000	-1.237742000

H	2.156852000	-0.016780000	1.237742000
C	0.000000000	0.000000000	5.731622000
H	0.775986000	0.394028000	6.406658000
H	-0.775986000	-0.394028000	6.406658000
C	0.000000000	0.000000000	-5.731622000
H	0.775986000	-0.394028000	-6.406658000
H	-0.775986000	0.394028000	-6.406658000

1-C²⁺-OS

N	2.839174000	0.000000000	0.000000000
C	3.505033000	1.231081000	0.000000000
C	2.769794000	2.443010000	0.000000000
C	3.433961000	3.654416000	0.000000000
C	4.839051000	3.692019000	0.000000000
C	5.565315000	2.503309000	0.000000000
C	4.926236000	1.264153000	0.000000000
C	4.926236000	-1.264153000	0.000000000
C	5.565315000	-2.503309000	0.000000000
C	4.839051000	-3.692019000	0.000000000
C	3.433961000	-3.654416000	0.000000000
C	2.769794000	-2.443010000	0.000000000
C	3.505033000	-1.231081000	0.000000000
C	1.384597000	0.000000000	0.000000000
C	0.698127000	0.000000000	1.216391000
C	-0.698127000	0.000000000	1.216391000
H	1.688226000	2.424829000	0.000000000
H	2.866199000	4.579020000	0.000000000
H	5.358431000	4.644954000	0.000000000
H	6.651289000	2.534006000	0.000000000
H	6.651289000	-2.534006000	0.000000000
H	5.358431000	-4.644954000	0.000000000
H	2.866199000	-4.579020000	0.000000000
H	1.688226000	-2.424829000	0.000000000
H	1.244461000	0.000000000	2.154248000
H	-1.244461000	0.000000000	2.154248000
N	-2.839174000	0.000000000	0.000000000
C	-3.505033000	-1.231081000	0.000000000
C	-2.769794000	-2.443010000	0.000000000
C	-3.433961000	-3.654416000	0.000000000
C	-4.839051000	-3.692019000	0.000000000
C	-5.565315000	-2.503309000	0.000000000
C	-4.926236000	-1.264153000	0.000000000

C	-4.926236000	1.264153000	0.000000000
C	-5.565315000	2.503309000	0.000000000
C	-4.839051000	3.692019000	0.000000000
C	-3.433961000	3.654416000	0.000000000
C	-2.769794000	2.443010000	0.000000000
C	-3.505033000	1.231081000	0.000000000
C	-1.384597000	0.000000000	0.000000000
C	-0.698127000	0.000000000	-1.216391000
C	0.698127000	0.000000000	-1.216391000
H	-1.688226000	-2.424829000	0.000000000
H	-2.866199000	-4.579020000	0.000000000
H	-5.358431000	-4.644954000	0.000000000
H	-6.651289000	-2.534006000	0.000000000
H	-6.651289000	2.534006000	0.000000000
H	-5.358431000	4.644954000	0.000000000
H	-2.866199000	4.579020000	0.000000000
H	-1.688226000	2.424829000	0.000000000
H	-1.244461000	0.000000000	-2.154248000
H	1.244461000	0.000000000	-2.154248000
C	5.732652000	0.000000000	0.000000000
H	6.407028000	0.000000000	-0.870377000
H	6.407028000	0.000000000	0.870377000
C	-5.732652000	0.000000000	0.000000000
H	-6.407028000	0.000000000	-0.870377000
H	-6.407028000	0.000000000	0.870377000

1-C²⁺-T

N	2.839184000	0.000000000	0.000000000
C	3.505037000	1.231080000	0.000000000
C	2.769795000	2.443008000	0.000000000
C	3.433960000	3.654417000	0.000000000
C	4.839049000	3.692021000	0.000000000
C	5.565316000	2.503311000	0.000000000
C	4.926242000	1.264154000	0.000000000
C	4.926242000	-1.264154000	0.000000000
C	5.565316000	-2.503311000	0.000000000
C	4.839049000	-3.692021000	0.000000000
C	3.433960000	-3.654417000	0.000000000
C	2.769795000	-2.443008000	0.000000000
C	3.505037000	-1.231080000	0.000000000
C	1.384624000	0.000000000	0.000000000
C	0.698112000	0.000000000	1.216386000

C	-0.698112000	0.000000000	1.216386000
H	1.688227000	2.424825000	0.000000000
H	2.866196000	4.579019000	0.000000000
H	5.358427000	4.644957000	0.000000000
H	6.651290000	2.534012000	0.000000000
H	6.651290000	-2.534012000	0.000000000
H	5.358427000	-4.644957000	0.000000000
H	2.866196000	-4.579019000	0.000000000
H	1.688227000	-2.424825000	0.000000000
H	1.244446000	0.000000000	2.154240000
H	-1.244446000	0.000000000	2.154240000
N	-2.839184000	0.000000000	0.000000000
C	-3.505037000	-1.231080000	0.000000000
C	-2.769795000	-2.443008000	0.000000000
C	-3.433960000	-3.654417000	0.000000000
C	-4.839049000	-3.692021000	0.000000000
C	-5.565316000	-2.503311000	0.000000000
C	-4.926242000	-1.264154000	0.000000000
C	-4.926242000	1.264154000	0.000000000
C	-5.565316000	2.503311000	0.000000000
C	-4.839049000	3.692021000	0.000000000
C	-3.433960000	3.654417000	0.000000000
C	-2.769795000	2.443008000	0.000000000
C	-3.505037000	1.231080000	0.000000000
C	-1.384624000	0.000000000	0.000000000
C	-0.698112000	0.000000000	-1.216386000
C	0.698112000	0.000000000	-1.216386000
H	-1.688227000	-2.424825000	0.000000000
H	-2.866196000	-4.579019000	0.000000000
H	-5.358427000	-4.644957000	0.000000000
H	-6.651290000	-2.534012000	0.000000000
H	-6.651290000	2.534012000	0.000000000
H	-5.358427000	4.644957000	0.000000000
H	-2.866196000	4.579019000	0.000000000
H	-1.688227000	2.424825000	0.000000000
H	-1.244446000	0.000000000	-2.154240000
H	1.244446000	0.000000000	-2.154240000
C	5.732659000	0.000000000	0.000000000
H	6.407034000	0.000000000	-0.870377000
H	6.407034000	0.000000000	0.870377000
C	-5.732659000	0.000000000	0.000000000
H	-6.407034000	0.000000000	-0.870377000
H	-6.407034000	0.000000000	0.870377000

2-C²⁺-CS

N	0.000000000	0.000000000	-4.994197000
C	1.181109000	0.343131000	-5.666070000
C	2.370361000	0.609529000	-4.940361000
C	3.525398000	0.972267000	-5.607611000
C	3.536985000	1.059617000	-7.008880000
C	2.384098000	0.753150000	-7.729018000
C	1.203426000	0.384848000	-7.087224000
C	-1.203426000	-0.384848000	-7.087224000
C	-2.384098000	-0.753150000	-7.729018000
C	-3.536985000	-1.059617000	-7.008880000
C	-3.525398000	-0.972267000	-5.607611000
C	-2.370361000	-0.609529000	-4.940361000
C	-1.181109000	-0.343131000	-5.666070000
C	0.000000000	0.000000000	-3.553062000
C	-0.112152000	-1.209017000	-2.854585000
C	-0.103749000	-1.203419000	-1.464914000
H	2.384110000	0.517951000	-3.863115000
H	4.428767000	1.175808000	-5.042006000
H	4.444717000	1.343421000	-7.531615000
H	2.400232000	0.789968000	-8.814834000
H	-2.400232000	-0.789968000	-8.814834000
H	-4.444717000	-1.343421000	-7.531615000
H	-4.428767000	-1.175808000	-5.042006000
H	-2.384110000	-0.517951000	-3.863115000
H	-0.174748000	-2.146106000	-3.398724000
H	-0.140733000	-2.152233000	-0.939533000
C	0.000000000	0.000000000	-0.738812000
C	0.103749000	1.203419000	-1.464914000
C	0.112152000	1.209017000	-2.854585000
H	0.140733000	2.152233000	-0.939533000
H	0.174748000	2.146106000	-3.398724000
C	0.000000000	0.000000000	0.741646000
C	0.751144000	0.945720000	1.466005000
C	-0.751144000	-0.945720000	1.466005000
C	0.764104000	0.943890000	2.856609000
H	1.353373000	1.679222000	0.939470000
C	-0.764104000	-0.943890000	2.856609000
H	-1.353373000	-1.679222000	0.939470000
C	0.000000000	0.000000000	3.552866000
H	1.353154000	1.675108000	3.401166000
H	-1.353154000	-1.675108000	3.401166000

N	0.000000000	0.000000000	4.995574000
C	1.159896000	-0.408652000	5.666394000
C	-1.159896000	0.408652000	5.666394000
C	2.283678000	-0.877008000	4.938864000
C	1.201606000	-0.391151000	7.087685000
C	-1.201606000	0.391151000	7.087685000
C	-2.283678000	0.877008000	4.938864000
C	3.433297000	-1.257369000	5.605489000
H	2.243669000	-0.949810000	3.860715000
C	2.375443000	-0.781941000	7.728731000
C	-2.375443000	0.781941000	7.728731000
C	-3.433297000	1.257369000	5.605489000
H	-2.243669000	0.949810000	3.860715000
C	3.491477000	-1.201344000	7.007416000
H	4.287923000	-1.612488000	5.039014000
H	2.409772000	-0.764831000	8.814614000
C	-3.491477000	1.201344000	7.007416000
H	-2.409772000	0.764831000	8.814614000
H	-4.287923000	1.612488000	5.039014000
H	4.394311000	-1.501500000	7.529491000
H	-4.394311000	1.501500000	7.529491000
C	0.000000000	0.000000000	7.895418000
C	0.000000000	0.000000000	-7.895086000
H	0.270302000	-0.827500000	-8.569611000
H	-0.270302000	0.827500000	-8.569611000
H	0.264521000	0.829312000	8.570067000
H	-0.264521000	-0.829312000	8.570067000

2-C²⁺-OS

N	0.000000000	0.000000000	-5.001498000
C	-0.426632000	1.152426000	-5.667661000
C	-0.845515000	2.287820000	-4.929133000
C	-1.266565000	3.425028000	-5.591585000
C	-1.281367000	3.462376000	-6.995926000
C	-0.869527000	2.348587000	-7.724848000
C	-0.439087000	1.185492000	-7.088358000
C	0.439087000	-1.185492000	-7.088358000
C	0.869527000	-2.348587000	-7.724848000
C	1.281367000	-3.462376000	-6.995926000
C	1.266565000	-3.425028000	-5.591585000
C	0.845515000	-2.287820000	-4.929133000
C	0.426632000	-1.152426000	-5.667661000

C	0.000000000	0.000000000	-3.546016000
C	1.142652000	0.410156000	-2.857976000
C	1.136184000	0.407452000	-1.464285000
H	-0.836059000	2.266244000	-3.847643000
H	-1.586041000	4.290902000	-5.021016000
H	-1.612501000	4.356814000	-7.513871000
H	-0.881081000	2.379257000	-8.810873000
H	0.881081000	-2.379257000	-8.810873000
H	1.612501000	-4.356814000	-7.513871000
H	1.586041000	-4.290902000	-5.021016000
H	0.836059000	-2.266244000	-3.847643000
H	2.022823000	0.735683000	-3.403825000
H	2.019319000	0.750893000	-0.934681000
C	0.000000000	0.000000000	-0.743871000
C	-1.136184000	-0.407452000	-1.464285000
C	-1.142652000	-0.410156000	-2.857976000
H	-2.019319000	-0.750893000	-0.934681000
H	-2.022823000	-0.735683000	-3.403825000
C	0.000000000	0.000000000	0.743871000
C	-1.136184000	0.407452000	1.464285000
C	1.136184000	-0.407452000	1.464285000
C	-1.142652000	0.410156000	2.857976000
H	-2.019319000	0.750893000	0.934681000
C	1.142652000	-0.410156000	2.857976000
H	2.019319000	-0.750893000	0.934681000
C	0.000000000	0.000000000	3.546016000
H	-2.022823000	0.735683000	3.403825000
H	2.022823000	-0.735683000	3.403825000
N	0.000000000	0.000000000	5.001498000
C	0.426632000	1.152426000	5.667661000
C	-0.426632000	-1.152426000	5.667661000
C	0.845515000	2.287820000	4.929133000
C	0.439087000	1.185492000	7.088358000
C	-0.439087000	-1.185492000	7.088358000
C	-0.845515000	-2.287820000	4.929133000
C	1.266565000	3.425028000	5.591585000
H	0.836059000	2.266244000	3.847643000
C	0.869527000	2.348587000	7.724848000
C	-0.869527000	-2.348587000	7.724848000
C	-1.266565000	-3.425028000	5.591585000
H	-0.836059000	-2.266244000	3.847643000
C	1.281367000	3.462376000	6.995926000
H	1.586041000	4.290902000	5.021016000
H	0.881081000	2.379257000	8.810873000

C	-1.281367000	-3.462376000	6.995926000
H	-0.881081000	-2.379257000	8.810873000
H	-1.586041000	-4.290902000	5.021016000
H	1.612501000	4.356814000	7.513871000
H	-1.612501000	-4.356814000	7.513871000
C	0.000000000	0.000000000	-7.896441000
C	0.000000000	0.000000000	7.896441000
H	-0.816588000	-0.302343000	-8.570105000
H	0.816588000	0.302343000	-8.570105000
H	0.816588000	-0.302343000	8.570105000
H	-0.816588000	0.302343000	8.570105000

2-C²⁺-T

N	0.000000000	0.000000000	-5.001499000
C	-0.426624000	1.152429000	-5.667661000
C	-0.845501000	2.287825000	-4.929133000
C	-1.266541000	3.425037000	-5.591585000
C	-1.281339000	3.462387000	-6.995925000
C	-0.869506000	2.348594000	-7.724848000
C	-0.439076000	1.185496000	-7.088359000
C	0.439076000	-1.185496000	-7.088359000
C	0.869506000	-2.348594000	-7.724848000
C	1.281339000	-3.462387000	-6.995925000
C	1.266541000	-3.425037000	-5.591585000
C	0.845501000	-2.287825000	-4.929133000
C	0.426624000	-1.152429000	-5.667661000
C	0.000000000	0.000000000	-3.546016000
C	1.142647000	0.410171000	-2.857976000
C	1.136179000	0.407467000	-1.464285000
H	-0.836049000	2.266247000	-3.847643000
H	-1.586013000	4.290912000	-5.021015000
H	-1.612465000	4.356827000	-7.513870000
H	-0.881059000	2.379266000	-8.810874000
H	0.881059000	-2.379266000	-8.810874000
H	1.612465000	-4.356827000	-7.513870000
H	1.586013000	-4.290912000	-5.021015000
H	0.836049000	-2.266247000	-3.847643000
H	2.022814000	0.735708000	-3.403825000
H	2.019309000	0.750918000	-0.934681000
C	0.000000000	0.000000000	-0.743871000
C	-1.136179000	-0.407467000	-1.464285000
C	-1.142647000	-0.410171000	-2.857976000

H	-2.019309000	-0.750918000	-0.934681000
H	-2.022814000	-0.735708000	-3.403825000
C	0.000000000	0.000000000	0.743871000
C	-1.136179000	0.407467000	1.464285000
C	1.136179000	-0.407467000	1.464285000
C	-1.142647000	0.410171000	2.857976000
H	-2.019309000	0.750918000	0.934681000
C	1.142647000	-0.410171000	2.857976000
H	2.019309000	-0.750918000	0.934681000
C	0.000000000	0.000000000	3.546016000
H	-2.022814000	0.735708000	3.403825000
H	2.022814000	-0.735708000	3.403825000
N	0.000000000	0.000000000	5.001499000
C	0.426624000	1.152429000	5.667661000
C	-0.426624000	-1.152429000	5.667661000
C	0.845501000	2.287825000	4.929133000
C	0.439076000	1.185496000	7.088359000
C	-0.439076000	-1.185496000	7.088359000
C	-0.845501000	-2.287825000	4.929133000
C	1.266541000	3.425037000	5.591585000
H	0.836049000	2.266247000	3.847643000
C	0.869506000	2.348594000	7.724848000
C	-0.869506000	-2.348594000	7.724848000
C	-1.266541000	-3.425037000	5.591585000
H	-0.836049000	-2.266247000	3.847643000
C	1.281339000	3.462387000	6.995925000
H	1.586013000	4.290912000	5.021015000
H	0.881059000	2.379266000	8.810874000
C	-1.281339000	-3.462387000	6.995925000
H	-0.881059000	-2.379266000	8.810874000
H	-1.586013000	-4.290912000	5.021015000
H	1.612465000	4.356827000	7.513870000
H	-1.612465000	-4.356827000	7.513870000
C	0.000000000	0.000000000	-7.896442000
C	0.000000000	0.000000000	7.896442000
H	-0.816591000	-0.302336000	-8.570106000
H	0.816591000	0.302336000	-8.570106000
H	0.816591000	-0.302336000	8.570106000
H	-0.816591000	0.302336000	8.570106000

3-C²⁺-CS

C	-3.677233000	0.017220000	0.709055000
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C	-2.493745000	0.022489000	1.405370000
C	-1.240515000	-0.003926000	0.723992000
C	-1.240515000	0.003926000	-0.723992000
C	-2.493745000	-0.022489000	-1.405370000
C	-3.677233000	-0.017220000	-0.709055000
C	0.000000000	0.000000000	1.402688000
C	0.000000000	0.000000000	-1.402688000
C	1.240515000	-0.003926000	-0.723992000
C	1.240515000	0.003926000	0.723992000
C	2.493745000	-0.022489000	1.405370000
H	2.510773000	-0.040757000	2.488683000
C	3.677233000	-0.017220000	0.709055000
C	3.677233000	0.017220000	-0.709055000
C	2.493745000	0.022489000	-1.405370000
H	-4.620516000	0.035207000	1.245629000
H	-2.510773000	0.040757000	2.488683000
H	-2.510773000	-0.040757000	-2.488683000
H	-4.620516000	-0.035207000	-1.245629000
H	4.620516000	-0.035207000	1.245629000
H	4.620516000	0.035207000	-1.245629000
H	2.510773000	0.040757000	-2.488683000
N	0.000000000	0.000000000	2.844491000
C	-0.268430000	-1.201794000	3.519722000
C	0.268430000	1.201794000	3.519722000
C	-0.462004000	-2.401190000	2.791975000
C	-0.302460000	-1.227150000	4.939728000
C	0.302460000	1.227150000	4.939728000
C	0.462004000	2.401190000	2.791975000
C	-0.744202000	-3.579789000	3.456432000
H	-0.383975000	-2.400123000	1.712912000
C	-0.582584000	-2.433762000	5.580972000
C	0.582584000	2.433762000	5.580972000
C	0.744202000	3.579789000	3.456432000
H	0.383975000	2.400123000	1.712912000
C	-0.816476000	-3.601711000	4.859439000
H	-0.894745000	-4.492958000	2.889976000
H	-0.609569000	-2.455545000	6.666975000
C	0.816476000	3.601711000	4.859439000
H	0.609569000	2.455545000	6.666975000
H	0.894745000	4.492958000	2.889976000
H	-1.032940000	-4.528572000	5.380769000
H	1.032940000	4.528572000	5.380769000
N	0.000000000	0.000000000	-2.844491000
C	0.268430000	-1.201794000	-3.519722000

C	-0.268430000	1.201794000	-3.519722000
C	0.462004000	-2.401190000	-2.791975000
C	0.302460000	-1.227150000	-4.939728000
C	-0.302460000	1.227150000	-4.939728000
C	-0.462004000	2.401190000	-2.791975000
C	0.744202000	-3.579789000	-3.456432000
H	0.383975000	-2.400123000	-1.712912000
C	0.582584000	-2.433762000	-5.580972000
C	-0.582584000	2.433762000	-5.580972000
C	-0.744202000	3.579789000	-3.456432000
H	-0.383975000	2.400123000	-1.712912000
C	0.816476000	-3.601711000	-4.859439000
H	0.894745000	-4.492958000	-2.889976000
H	0.609569000	-2.455545000	-6.666975000
C	-0.816476000	3.601711000	-4.859439000
H	-0.609569000	2.455545000	-6.666975000
H	-0.894745000	4.492958000	-2.889976000
H	1.032940000	-4.528572000	-5.380769000
H	-1.032940000	4.528572000	-5.380769000
C	0.000000000	0.000000000	5.748184000
C	0.000000000	0.000000000	-5.748184000
H	-0.843324000	0.213847000	6.423398000
H	0.843324000	0.213847000	-6.423398000
H	0.843324000	-0.213847000	6.423398000
H	-0.843324000	-0.213847000	-6.423398000

3-C²⁺-OS

C	-3.672964000	0.000000000	-0.711507000
C	-2.493526000	0.000000000	-1.407830000
C	-1.237818000	0.000000000	-0.724177000
C	-1.237818000	0.000000000	0.724177000
C	-2.493526000	0.000000000	1.407830000
C	-3.672964000	0.000000000	0.711507000
C	0.000000000	0.000000000	-1.393536000
C	0.000000000	0.000000000	1.393536000
C	1.237818000	0.000000000	0.724177000
C	1.237818000	0.000000000	-0.724177000
C	2.493526000	0.000000000	-1.407830000
H	2.508262000	-0.000001000	-2.491904000
C	3.672964000	0.000000000	-0.711507000
C	3.672964000	0.000000000	0.711507000
C	2.493526000	0.000000000	1.407830000

H	-4.617689000	0.000000000	-1.245944000
H	-2.508262000	0.000001000	-2.491904000
H	-2.508262000	-0.000001000	2.491904000
H	-4.617689000	0.000000000	1.245944000
H	4.617689000	0.000000000	-1.245944000
H	4.617689000	0.000000000	1.245944000
H	2.508262000	0.000001000	2.491904000
N	0.000000000	0.000000000	-2.851845000
C	-0.000004000	1.229058000	-3.521455000
C	0.000004000	-1.229058000	-3.521455000
C	-0.000008000	2.440105000	-2.785261000
C	-0.000004000	1.263729000	-4.942556000
C	0.000004000	-1.263729000	-4.942556000
C	0.000008000	-2.440105000	-2.785261000
C	-0.000013000	3.652301000	-3.447521000
H	-0.000009000	2.415136000	-1.703830000
C	-0.000008000	2.503687000	-5.580342000
C	0.000008000	-2.503687000	-5.580342000
C	0.000013000	-3.652301000	-3.447521000
H	0.000009000	-2.415136000	-1.703830000
C	-0.000012000	3.691536000	-4.852474000
H	-0.000016000	4.576140000	-2.878496000
H	-0.000008000	2.535730000	-6.666335000
C	0.000012000	-3.691536000	-4.852474000
H	0.000008000	-2.535730000	-6.666335000
H	0.000016000	-4.576140000	-2.878496000
H	-0.000016000	4.645019000	-5.370935000
H	0.000016000	-4.645019000	-5.370935000
N	0.000000000	0.000000000	2.851845000
C	0.000004000	1.229058000	3.521455000
C	-0.000004000	-1.229058000	3.521455000
C	0.000008000	2.440105000	2.785261000
C	0.000004000	1.263729000	4.942556000
C	-0.000004000	-1.263729000	4.942556000
C	-0.000008000	-2.440105000	2.785261000
C	0.000013000	3.652301000	3.447521000
H	0.000009000	2.415136000	1.703830000
C	0.000008000	2.503687000	5.580342000
C	-0.000008000	-2.503687000	5.580342000
C	-0.000013000	-3.652301000	3.447521000
H	-0.000009000	-2.415136000	1.703830000
C	0.000012000	3.691536000	4.852474000
H	0.000016000	4.576140000	2.878496000
H	0.000008000	2.535730000	6.666335000

C	-0.000012000	-3.691536000	4.852474000
H	-0.000008000	-2.535730000	6.666335000
H	-0.000016000	-4.576140000	2.878496000
H	0.000016000	4.645019000	5.370935000
H	-0.000016000	-4.645019000	5.370935000
C	0.000000000	0.000000000	-5.750468000
C	0.000000000	0.000000000	5.750468000
H	-0.870161000	-0.000003000	-6.425024000
H	0.870161000	0.000003000	-6.425024000
H	0.870161000	-0.000003000	6.425024000
H	-0.870161000	0.000003000	6.425024000

3-C²⁺-T

C	-3.672955000	0.000000000	-0.711508000
C	-2.493513000	0.000000000	-1.407821000
C	-1.237810000	0.000000000	-0.724161000
C	-1.237810000	0.000000000	0.724161000
C	-2.493513000	0.000000000	1.407821000
C	-3.672955000	0.000000000	0.711508000
C	0.000000000	0.000000000	-1.393557000
C	0.000000000	0.000000000	1.393557000
C	1.237810000	0.000000000	0.724161000
C	1.237810000	0.000000000	-0.724161000
C	2.493513000	0.000000000	-1.407821000
H	2.508223000	-0.000001000	-2.491896000
C	3.672955000	0.000000000	-0.711508000
C	3.672955000	0.000000000	0.711508000
C	2.493513000	0.000000000	1.407821000
H	-4.617678000	0.000000000	-1.245949000
H	-2.508223000	0.000001000	-2.491896000
H	-2.508223000	-0.000001000	2.491896000
H	-4.617678000	0.000000000	1.245949000
H	4.617678000	0.000000000	-1.245949000
H	4.617678000	0.000000000	1.245949000
H	2.508223000	0.000001000	2.491896000
N	0.000000000	0.000000000	-2.851861000
C	-0.000003000	1.229060000	-3.521468000
C	0.000003000	-1.229060000	-3.521468000
C	-0.000006000	2.440105000	-2.785273000
C	-0.000003000	1.263730000	-4.942570000
C	0.000003000	-1.263730000	-4.942570000
C	0.000006000	-2.440105000	-2.785273000

C	-0.000009000	3.652302000	-3.447533000
H	-0.000006000	2.415135000	-1.703842000
C	-0.000006000	2.503688000	-5.580355000
C	0.000006000	-2.503688000	-5.580355000
C	0.000009000	-3.652302000	-3.447533000
H	0.000006000	-2.415135000	-1.703842000
C	-0.000009000	3.691538000	-4.852486000
H	-0.000011000	4.576141000	-2.878507000
H	-0.000006000	2.535732000	-6.666347000
C	0.000009000	-3.691538000	-4.852486000
H	0.000006000	-2.535732000	-6.666347000
H	0.000011000	-4.576141000	-2.878507000
H	-0.000011000	4.645021000	-5.370947000
H	0.000011000	-4.645021000	-5.370947000
N	0.000000000	0.000000000	2.851861000
C	0.000003000	1.229060000	3.521468000
C	-0.000003000	-1.229060000	3.521468000
C	0.000006000	2.440105000	2.785273000
C	0.000003000	1.263730000	4.942570000
C	-0.000003000	-1.263730000	4.942570000
C	-0.000006000	-2.440105000	2.785273000
C	0.000009000	3.652302000	3.447533000
H	0.000006000	2.415135000	1.703842000
C	0.000006000	2.503688000	5.580355000
C	-0.000006000	-2.503688000	5.580355000
C	-0.000009000	-3.652302000	3.447533000
H	-0.000006000	-2.415135000	1.703842000
C	0.000009000	3.691538000	4.852486000
H	0.000011000	4.576141000	2.878507000
H	0.000006000	2.535732000	6.666347000
C	-0.000009000	-3.691538000	4.852486000
H	-0.000006000	-2.535732000	6.666347000
H	-0.000011000	-4.576141000	2.878507000
H	0.000011000	4.645021000	5.370947000
H	-0.000011000	-4.645021000	5.370947000
C	0.000000000	0.000000000	-5.750481000
C	0.000000000	0.000000000	5.750481000
H	-0.870161000	-0.000002000	-6.425037000
H	0.870161000	0.000002000	-6.425037000
H	0.870161000	-0.000002000	6.425037000
H	-0.870161000	0.000002000	6.425037000

1-CS

S	0.420737000	3.437442000	4.634018000
N	0.360715000	2.029448000	1.951628000
C	1.666901000	2.246958000	2.469276000
C	2.811113000	1.762910000	1.816298000
C	4.083467000	1.977310000	2.347587000
C	4.247519000	2.704437000	3.524153000
C	3.119394000	3.201644000	4.176966000
C	1.841108000	2.954565000	3.674789000
C	-0.714288000	3.771007000	3.302797000
C	-1.701252000	4.742086000	3.476465000
C	-2.697163000	4.922249000	2.516439000
C	-2.680263000	4.135014000	1.367595000
C	-1.671995000	3.191383000	1.167177000
C	-0.670030000	2.992379000	2.129689000
C	0.183151000	1.013533000	0.951017000
C	0.448938000	1.258865000	-0.401961000
C	-0.266191000	-0.249657000	1.347229000
H	2.709024000	1.205742000	0.892976000
H	4.947831000	1.579063000	1.823457000
H	5.237183000	2.883869000	3.933438000
H	3.221279000	3.769555000	5.097533000
H	-1.694884000	5.341229000	4.382756000
H	-3.473267000	5.666191000	2.669275000
H	-3.447352000	4.256457000	0.607796000
H	-1.673325000	2.599550000	0.259938000
H	0.798579000	2.240400000	-0.708280000
H	-0.469551000	-0.430128000	2.398189000
C	0.266191000	0.249657000	-1.347229000
C	-0.183151000	-1.013533000	-0.951017000
N	-0.360715000	-2.029448000	-1.951628000
C	-1.666901000	-2.246958000	-2.469276000
C	-2.811113000	-1.762910000	-1.816298000
C	-4.083467000	-1.977310000	-2.347587000
C	-4.247519000	-2.704437000	-3.524153000
C	-3.119394000	-3.201644000	-4.176966000
C	-1.841108000	-2.954565000	-3.674789000
S	-0.420737000	-3.437442000	-4.634018000
C	0.714288000	-3.771007000	-3.302797000
C	1.701252000	-4.742086000	-3.476465000
C	2.697163000	-4.922249000	-2.516439000
C	2.680263000	-4.135014000	-1.367595000
C	1.671995000	-3.191383000	-1.167177000
C	0.670030000	-2.992379000	-2.129689000

H	1.673325000	-2.599550000	-0.259938000
H	3.447352000	-4.256457000	-0.607796000
H	3.473267000	-5.666191000	-2.669275000
H	1.694884000	-5.341229000	-4.382756000
H	-3.221279000	-3.769555000	-5.097533000
H	-5.237183000	-2.883869000	-3.933438000
H	-4.947831000	-1.579063000	-1.823457000
H	-2.709024000	-1.205742000	-0.892976000
C	-0.448938000	-1.258865000	0.401961000
H	-0.798579000	-2.240400000	0.708280000
H	0.469551000	0.430128000	-2.398189000

1-T

S	0.581532000	3.834623000	4.413060000
N	0.425513000	2.155231000	1.796973000
C	1.694381000	2.282833000	2.380998000
C	2.802888000	1.606991000	1.827620000
C	4.061269000	1.698828000	2.403594000
C	4.262291000	2.470786000	3.562640000
C	3.188334000	3.141740000	4.125086000
C	1.908236000	3.060818000	3.552630000
C	-0.673095000	3.882554000	3.178735000
C	-1.775559000	4.722590000	3.406214000
C	-2.850392000	4.737408000	2.531960000
C	-2.831958000	3.896373000	1.404126000
C	-1.751945000	3.059086000	1.166977000
C	-0.644912000	3.027868000	2.041888000
C	0.209860000	1.061090000	0.881760000
C	0.466345000	1.236221000	-0.508813000
C	-0.248202000	-0.158179000	1.371858000
H	2.660364000	1.016351000	0.931382000
H	4.893629000	1.171944000	1.946760000
H	5.247589000	2.547035000	4.012228000
H	3.323893000	3.741568000	5.021234000
H	-1.772548000	5.363848000	4.283736000
H	-3.693262000	5.396338000	2.716677000
H	-3.663259000	3.900651000	0.705532000
H	-1.744884000	2.421430000	0.291851000
H	0.823378000	2.189961000	-0.882242000
H	-0.435534000	-0.264347000	2.437420000
C	0.248202000	0.158179000	-1.371858000
C	-0.209860000	-1.061090000	-0.881760000

N	-0.425513000	-2.155231000	-1.796973000
C	-1.694381000	-2.282833000	-2.380998000
C	-2.802888000	-1.606991000	-1.827620000
C	-4.061269000	-1.698828000	-2.403594000
C	-4.262291000	-2.470786000	-3.562640000
C	-3.188334000	-3.141740000	-4.125086000
C	-1.908236000	-3.060818000	-3.552630000
S	-0.581532000	-3.834623000	-4.413060000
C	0.673095000	-3.882554000	-3.178735000
C	1.775559000	-4.722590000	-3.406214000
C	2.850392000	-4.737408000	-2.531960000
C	2.831958000	-3.896373000	-1.404126000
C	1.751945000	-3.059086000	-1.166977000
C	0.644912000	-3.027868000	-2.041888000
H	1.744884000	-2.421430000	-0.291851000
H	3.663259000	-3.900651000	-0.705532000
H	3.693262000	-5.396338000	-2.716677000
H	1.772548000	-5.363848000	-4.283736000
H	-3.323893000	-3.741568000	-5.021234000
H	-5.247589000	-2.547035000	-4.012228000
H	-4.893629000	-1.171944000	-1.946760000
H	-2.660364000	-1.016351000	-0.931382000
C	-0.466345000	-1.236221000	0.508813000
H	-0.823378000	-2.189961000	0.882242000
H	0.435534000	0.264347000	-2.437420000

2-CS

S	-7.858404000	-0.391085000	0.989306000
N	-5.003582000	-0.035889000	0.028178000
C	-5.690426000	-1.129285000	-0.565772000
C	-5.051489000	-2.012694000	-1.449884000
C	-5.741615000	-3.085688000	-2.014960000
C	-7.091317000	-3.287175000	-1.736325000
C	-7.741258000	-2.411681000	-0.866266000
C	-7.046981000	-1.361708000	-0.263977000
C	-7.031669000	1.162183000	0.716751000
C	-7.710949000	2.351754000	0.982961000
C	-7.047484000	3.577408000	0.923939000
C	-5.700173000	3.601501000	0.571141000
C	-5.025242000	2.420023000	0.262378000
C	-5.677473000	1.178790000	0.329160000
C	-3.566546000	-0.026730000	-0.004729000

C	-2.860991000	-0.428107000	1.132552000
C	-1.467833000	-0.426765000	1.133468000
H	-4.004992000	-1.869920000	-1.689482000
H	-5.213606000	-3.757414000	-2.686150000
H	-7.634650000	-4.113780000	-2.184303000
H	-8.792385000	-2.550443000	-0.628929000
H	-8.760891000	2.306582000	1.258731000
H	-7.578915000	4.496302000	1.152912000
H	-5.162929000	4.544575000	0.521140000
H	-3.980727000	2.462959000	-0.021148000
H	-3.415440000	-0.748430000	2.009355000
H	-0.935764000	-0.766667000	2.017300000
C	-0.742438000	-0.026298000	-0.000906000
C	-1.463529000	0.375304000	-1.138382000
C	-2.856635000	0.377243000	-1.142166000
H	-0.927959000	0.715221000	-2.020143000
H	-3.401051000	0.700996000	-2.024652000
C	0.742438000	-0.026299000	0.000910000
C	1.467832000	-0.426776000	-1.133461000
C	1.463530000	0.375315000	1.138381000
C	2.860991000	-0.428119000	-1.132545000
H	0.935763000	-0.766686000	-2.017290000
C	2.856635000	0.377253000	1.142165000
H	0.927960000	0.715242000	2.020138000
C	3.566546000	-0.026734000	0.004733000
H	3.415439000	-0.748451000	-2.009345000
H	3.401051000	0.701016000	2.024647000
N	5.003582000	-0.035891000	-0.028176000
C	5.690431000	-1.129284000	0.565774000
C	5.677468000	1.178790000	-0.329161000
C	5.051501000	-2.012697000	1.449888000
C	7.046987000	-1.361702000	0.263976000
C	7.031663000	1.162188000	-0.716754000
C	5.025231000	2.420020000	-0.262377000
C	5.741633000	-3.085688000	2.014962000
H	4.005004000	-1.869928000	1.689488000
S	7.858403000	-0.391076000	-0.989310000
C	7.741270000	-2.411671000	0.866264000
C	7.710937000	2.351762000	-0.982967000
C	5.700156000	3.601500000	-0.571142000
H	3.980717000	2.462950000	0.021153000
C	7.091336000	-3.287168000	1.736325000
H	5.213629000	-3.757416000	2.686153000
H	8.792397000	-2.550429000	0.628923000

C	7.047466000	3.577413000	-0.923944000
H	8.760878000	2.306595000	-1.258739000
H	5.162908000	4.544572000	-0.521140000
H	7.634673000	-4.113770000	2.184301000
H	7.578892000	4.496309000	-1.152918000

2-T

S	-8.088313000	-0.126950000	0.398166000
N	-5.018371000	0.026564000	-0.138160000
C	-5.636580000	1.202564000	0.276894000
C	-4.883425000	2.378490000	0.537242000
C	-5.484405000	3.546137000	0.947774000
C	-6.904130000	3.606566000	1.141305000
C	-7.662320000	2.482325000	0.922879000
C	-7.075046000	1.270931000	0.485233000
C	-7.097883000	-1.306472000	-0.387467000
C	-7.707459000	-2.525488000	-0.771038000
C	-6.967487000	-3.568030000	-1.272463000
C	-5.544105000	-3.431489000	-1.383623000
C	-4.921961000	-2.263591000	-1.006075000
C	-5.656062000	-1.152931000	-0.511575000
C	-3.572003000	0.010143000	-0.123013000
C	-2.860638000	0.371637000	-1.269603000
C	-1.465739000	0.357740000	-1.245673000
H	-3.810011000	2.358211000	0.396530000
H	-4.875042000	4.426554000	1.125282000
H	-7.375238000	4.533230000	1.453149000
H	-8.738933000	2.507825000	1.075193000
H	-8.786245000	-2.617439000	-0.667485000
H	-7.455323000	-4.485934000	-1.584571000
H	-4.948816000	-4.253769000	-1.767525000
H	-3.846237000	-2.184191000	-1.100606000
H	-3.398469000	0.670560000	-2.163815000
H	-0.917857000	0.667505000	-2.130662000
C	-0.761699000	-0.013160000	-0.089075000
C	-1.504034000	-0.374674000	1.053621000
C	-2.896804000	-0.362846000	1.038312000
H	-0.985349000	-0.693681000	1.952412000
H	-3.463773000	-0.649158000	1.918880000
C	0.721489000	-0.017615000	-0.068578000
C	1.429916000	0.386299000	1.077156000
C	1.462527000	-0.424907000	-1.191479000

C	2.822497000	0.386101000	1.099002000
H	0.884558000	0.731841000	1.950639000
C	2.855153000	-0.427891000	-1.172358000
H	0.942594000	-0.769677000	-2.080598000
C	3.547094000	-0.023181000	-0.027461000
H	3.355683000	0.712482000	1.987413000
H	3.420255000	-0.753135000	-2.040544000
N	4.984475000	-0.034897000	-0.041139000
C	5.664236000	1.178098000	-0.335393000
C	5.661338000	-1.127295000	0.565715000
C	5.012118000	2.420118000	-0.283060000
C	7.024399000	1.159434000	-0.701644000
C	7.022215000	-1.361889000	0.285705000
C	5.007970000	-2.007998000	1.442070000
C	5.692848000	3.600116000	-0.584669000
H	3.963196000	2.464682000	-0.016593000
S	7.854041000	-0.395183000	-0.957142000
C	7.708810000	2.347625000	-0.960699000
C	7.706051000	-2.411008000	0.901316000
C	5.688221000	-3.080132000	2.020539000
H	3.958033000	-1.863473000	1.664941000
C	7.045594000	3.574020000	-0.915876000
H	5.155528000	4.543699000	-0.546209000
H	8.762917000	2.300721000	-1.219825000
C	7.041904000	-3.283674000	1.763426000
H	8.760601000	-2.551303000	0.680614000
H	5.149198000	-3.749652000	2.685177000
H	7.581359000	4.491798000	-1.139183000
H	7.577411000	-4.109657000	2.221880000

3-CS

C	0.711868000	0.000001000	3.717098000
C	1.405784000	0.000000000	2.536580000
C	0.722715000	-0.000003000	1.278147000
C	-0.722715000	0.000003000	1.278147000
C	-1.405784000	0.000000000	2.536580000
C	-0.711868000	-0.000001000	3.717098000
C	1.415418000	-0.000008000	0.050294000
C	-1.415418000	0.000008000	0.050294000
C	-0.722668000	0.000004000	-1.177874000
C	0.722668000	-0.000004000	-1.177874000
C	1.407731000	-0.000007000	-2.433362000

H	2.491891000	-0.000014000	-2.432497000
C	0.711554000	-0.000004000	-3.612559000
C	-0.711554000	0.000004000	-3.612559000
C	-1.407731000	0.000007000	-2.433362000
H	1.248889000	0.000000000	4.661447000
H	2.489953000	-0.000001000	2.536127000
H	-2.489953000	0.000001000	2.536127000
H	-1.248889000	0.000000000	4.661447000
H	1.248112000	-0.000007000	-4.557285000
H	-1.248112000	0.000007000	-4.557285000
H	-2.491891000	0.000014000	-2.432497000
N	2.854000000	-0.000012000	0.019524000
C	3.541394000	-1.241858000	0.098833000
C	3.541394000	1.241830000	0.098876000
C	2.921692000	-2.388599000	0.620188000
C	4.870171000	-1.357109000	-0.353942000
C	4.870171000	1.357097000	-0.353894000
C	2.921692000	2.388551000	0.620274000
C	3.604327000	-3.602791000	0.692966000
H	1.896663000	-2.333869000	0.964449000
S	5.645085000	0.000010000	-1.208155000
C	5.561298000	-2.564111000	-0.236497000
C	5.561298000	2.564095000	-0.236403000
C	3.604327000	3.602740000	0.693098000
H	1.896662000	2.333808000	0.964533000
C	4.930448000	-3.697002000	0.276851000
H	3.090878000	-4.473462000	1.091232000
H	6.592515000	-2.613507000	-0.575090000
C	4.930448000	3.696966000	0.276988000
H	6.592516000	2.613504000	-0.574992000
H	3.090878000	4.473396000	1.091397000
H	5.469588000	-4.637106000	0.345168000
H	5.469589000	4.637068000	0.345341000
N	-2.854000000	0.000012000	0.019524000
C	-3.541394000	-1.241830000	0.098876000
C	-3.541394000	1.241858000	0.098833000
C	-2.921692000	-2.388551000	0.620274000
C	-4.870171000	-1.357097000	-0.353894000
C	-4.870171000	1.357109000	-0.353942000
C	-2.921692000	2.388599000	0.620188000
C	-3.604327000	-3.602740000	0.693098000
H	-1.896662000	-2.333808000	0.964533000
S	-5.645085000	-0.000010000	-1.208155000
C	-5.561298000	-2.564095000	-0.236403000

C	-5.561298000	2.564111000	-0.236497000
C	-3.604327000	3.602791000	0.692966000
H	-1.896663000	2.333869000	0.964449000
C	-4.930448000	-3.696966000	0.276988000
H	-3.090878000	-4.473396000	1.091397000
H	-6.592516000	-2.613504000	-0.574992000
C	-4.930448000	3.697002000	0.276851000
H	-6.592515000	2.613507000	-0.575090000
H	-3.090878000	4.473462000	1.091232000
H	-5.469589000	-4.637068000	0.345341000
H	-5.469588000	4.637106000	0.345168000

3-T

C	-0.000012000	0.691681000	3.769780000
C	-0.000016000	1.393369000	2.546845000
C	0.000000000	0.719943000	1.318632000
C	0.000000000	-0.719943000	1.318632000
C	0.000016000	-1.393369000	2.546845000
C	0.000012000	-0.691681000	3.769780000
C	0.000015000	1.423646000	0.058478000
C	-0.000015000	-1.423646000	0.058478000
C	-0.000004000	-0.719232000	-1.200257000
C	0.000004000	0.719232000	-1.200257000
C	0.000021000	1.394377000	-2.426151000
H	0.000045000	2.479028000	-2.429818000
C	0.000010000	0.691509000	-3.648400000
C	-0.000010000	-0.691509000	-3.648400000
C	-0.000021000	-1.394377000	-2.426151000
H	-0.000022000	1.246283000	4.703537000
H	-0.000022000	2.477896000	2.550622000
H	0.000022000	-2.477896000	2.550622000
H	0.000022000	-1.246283000	4.703537000
H	0.000019000	1.246190000	-4.582157000
H	-0.000019000	-1.246190000	-4.582157000
H	-0.000045000	-2.479028000	-2.429818000
N	-0.000003000	2.855262000	0.027348000
C	1.242053000	3.543609000	0.100404000
C	-1.242120000	3.543524000	0.100174000
C	2.388452000	2.920857000	0.618760000
C	1.358324000	4.870827000	-0.355745000
C	-1.358441000	4.870704000	-0.356046000
C	-2.388551000	2.920676000	0.618359000

C	3.605341000	3.599368000	0.684038000
H	2.329585000	1.897715000	0.968330000
S	0.000000000	5.648494000	-1.206037000
C	2.568386000	5.558008000	-0.245430000
C	-2.568606000	5.557763000	-0.246012000
C	-3.605525000	3.599052000	0.683350000
H	-2.329634000	1.897562000	0.968006000
C	3.701519000	4.924276000	0.264063000
H	4.476286000	3.084485000	1.079840000
H	2.620038000	6.588340000	-0.586463000
C	-3.701767000	4.923932000	0.263281000
H	-2.620291000	6.588074000	-0.587099000
H	-4.476496000	3.084105000	1.079013000
H	4.643620000	5.460614000	0.326810000
H	-4.643948000	5.460157000	0.325799000
N	0.000003000	-2.855262000	0.027348000
C	1.242120000	-3.543524000	0.100174000
C	-1.242053000	-3.543609000	0.100404000
C	2.388551000	-2.920676000	0.618359000
C	1.358441000	-4.870704000	-0.356046000
C	-1.358324000	-4.870827000	-0.355745000
C	-2.388452000	-2.920857000	0.618760000
C	3.605525000	-3.599052000	0.683350000
H	2.329634000	-1.897562000	0.968006000
S	0.000000000	-5.648494000	-1.206037000
C	2.568606000	-5.557763000	-0.246012000
C	-2.568386000	-5.558008000	-0.245430000
C	-3.605341000	-3.599368000	0.684038000
H	-2.329585000	-1.897715000	0.968330000
C	3.701767000	-4.923932000	0.263281000
H	4.476496000	-3.084105000	1.079013000
H	2.620291000	-6.588074000	-0.587099000
C	-3.701519000	-4.924276000	0.264063000
H	-2.620038000	-6.588340000	-0.586463000
H	-4.476286000	-3.084485000	1.079840000
H	4.643948000	-5.460157000	0.325799000
H	-4.643620000	-5.460614000	0.326810000