

Supplementary Information

Deciphering the Mechanism of Oxygen Atom Transfer by Non-heme Mn^{IV}-Oxo Species: An Ab initio and DFT Exploration

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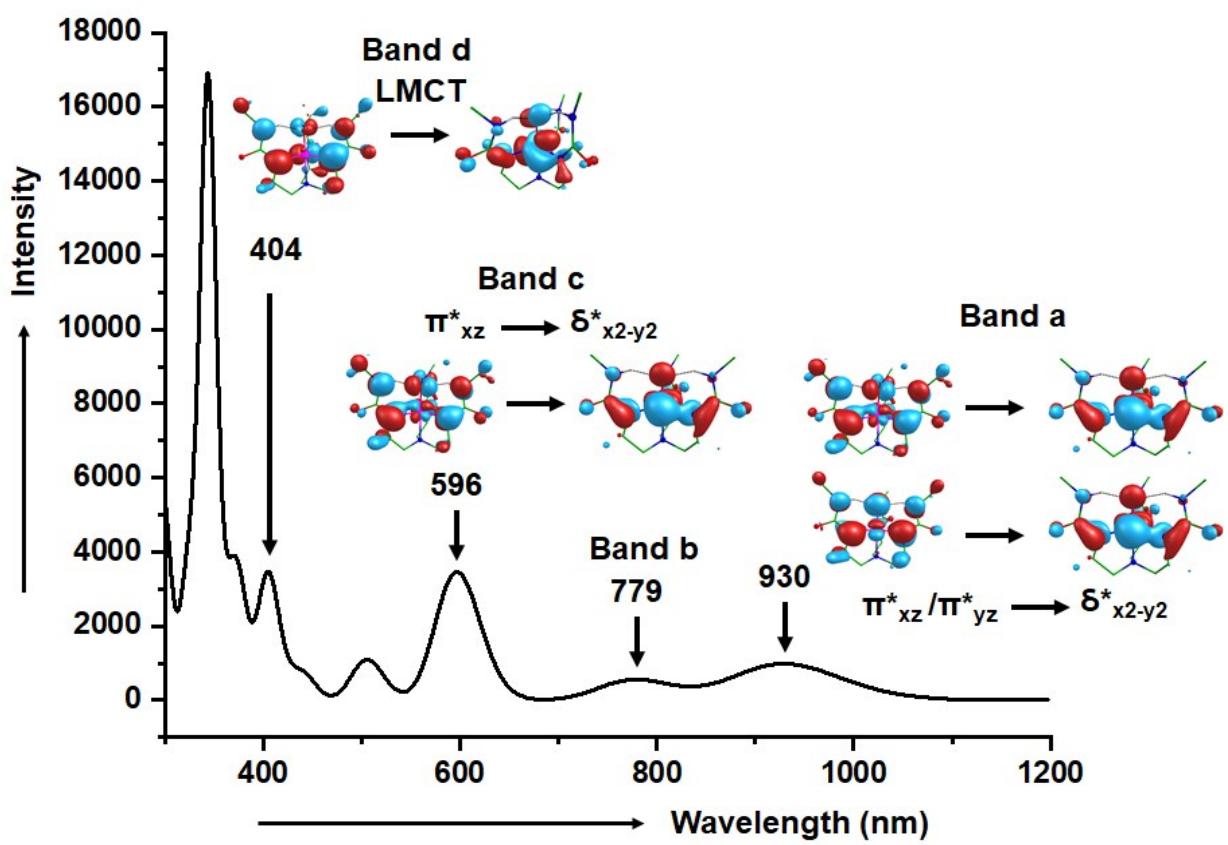


Figure S1: TD-DFT spectrum with the important absorptions for $[\text{Mn}^{\text{IV}}\text{H}_2\text{buea(O)}]^-$ species.

Table S1: Important bond distances (\AA) and angles ($^{\circ}$) involved in the OAT and SAT reactions catalysed by $[\text{Mn}^{\text{IV}}\text{H}_3\text{buea(O)}]^-$ and $[\text{Mn}^{\text{IV}}\text{H}_3\text{buea(S)}]^-$ species.

Spin states		Mn-O(S)	Mn-N1	Mn-N2	Mn-N	Mn-N3	P-O(S)	$\angle \text{N-Mn-O(S)}$	$\angle \text{Mn-O(S)-P}$	O-H1	O-H2	O-H3
Mn^{IV}=O(S)												
Reactant	$S = 5/2$	1.73 (2.33)	2.21 (2.27)	2.05 (2.00)	2.19 (2.00)	2.01 (1.96)	--	174.18 (161.62)	--	1.68 --	1.74 --	1.81 --
	$S = 3/2$	1.68 (2.20)	2.19 (1.93)	1.92 (1.97)	1.95 (2.22)	1.98 (2.00)	--	175.03 (163.38)	--	1.80 --	1.85 --	1.75 --
	$S = 1/2$	1.67 (2.16)	1.93 (1.88)	1.88 (1.97)	2.30 (2.24)	1.94 (1.96)	--	175.93 (163.74)	--	1.76 --	1.88 --	1.87 --
PPh₂Me												
RC	$S = 5/2$	1.73 (2.34)	2.05 (1.96)	2.22 (2.02)	2.19 (2.25)	2.00 (1.96)	4.03 --	173.51 (133.40)	--	1.79 --	1.65 --	1.83 --
	$S = 3/2(\sigma)$	1.67 (2.33)	1.96 (2.27)	1.91 (2.02)	2.25 (2.00)	1.96 (1.96)	3.71 --	176.77 (158.56)	--	1.78 --	2.05 --	1.86 --
	$S = 3/2(\square)$	1.68	1.98	1.91	2.21	1.94	4.55	175.16	--	1.75	1.80	1.93
	$S = 1/2$	1.65 (2.27)	1.93 (1.94)	1.89 (1.92)	2.33 (2.11)	1.96 (2.01)	3.76 --	176.34 (145.28)	--	1.82 --	2.08 --	1.90 --
TS	$S = 5/2$	1.78 (2.46)	2.02 (2.11)	2.23 (2.00)	2.23 (2.33)	2.02 (2.05)	2.33 (2.70)	172.34 (163.87)	155.27 (118.29)	2.09 --	1.74 --	2.10 --
	$S = 3/2(\square)$	1.72 (2.36)	2.04 (2.14)	2.03 (1.98)	2.16 (2.26)	1.99 (2.04)	2.33 (2.26)	174.41 (164.07)	123.49 (119.58)	1.81 --	1.94 --	2.13 --
	$S = 3/2(\sigma)$											
	$S = 1/2$	1.73 (2.32)	2.02 (1.97)	2.04 (2.02)	2.25 (2.14)	1.96 (1.99)	2.16 (2.45)	177.51 (156.31)	158.33 (121.06)	2.05 --	1.90 --	2.33 --
Product	$S = 5/2$	2.25 (2.99)	2.09 (2.11)	2.13 (2.08)	2.38 (2.39)	2.13 (2.11)	1.51 (2.02)	177.01 (161.33)	144.77 (105.02)	2.05 --	2.20 --	3.25 --

	$S = 3/2$	2.09 (2.71)	2.03 (2.14)	2.08 (2.03)	2.13 (2.22)	2.17 (2.06)	1.51 (2.03)	177.68 (160.99)	151.43 (110.66)	2.16 --	2.07 --	3.02 --
	$S = 1/2$	2.10 (2.57)	2.02 (2.04)	2.06 (2.02)	2.13 (2.14)	2.07 (2.06)	1.51 (2.03)	177.69 (163.81)	150.64 (118.24)	1.98 --	2.16 --	3.10 --
PPhMe₂												
RC	$S = 5/2$	1.74	2.01	2.26	2.20	2.01	4.38	173.25	--	1.78	1.67	1.83
	$S = 3/2$	1.68	1.98	1.92	2.23	1.94	4.45	176.59	--	1.74	1.77	2.09
	$S = 1/2$	1.66	1.90	1.88	2.34	1.93	5.03	174.70	--	1.77	1.83	1.84
TS	$S = 5/2$	1.76	2.04	2.11	2.15	2.10	2.53	178.53	123.91	1.82	1.85	1.85
	$S = 3/2$	1.73	2.05	2.04	2.17	1.97	2.37	175.60	117.59	1.79	1.90	2.25
	$S = 1/2$	1.72	2.00	1.92	2.19	1.95	2.06	169.85	121.35	1.81	1.87	2.51
Product	$S = 5/2$	2.30	2.09	2.12	2.42	2.13	1.51	173.97	137.06	2.23	2.17	3.41
	$S = 3/2$	2.11	2.08	2.15	2.14	2.10	1.51	179.11	151.10	1.97	2.23	3.03
	$S = 1/2$	2.14	2.03	2.05	2.12	2.03	1.51	175.76	145.66	1.91	2.31	3.05
PPh₃												
RC	$S = 5/2$	1.73	2.01	2.24	2.20	2.01	4.67	174.07	127.43	1.82	1.70	1.83
	$S = 3/2$	1.68	1.99	1.92	2.23	1.93	4.81	176.48	123.57	1.76	1.79	1.98
	$S = 1/2$	1.65	1.90	1.86	2.37	1.94	4.67	172.04	128.97	1.81	1.83	1.97
TS	$S = 5/2$	1.76	2.00	2.19	2.22	2.07	2.41	175.03	139.81	1.87	1.78	2.46
	$S = 3/2$	1.72	2.04	2.02	2.16	1.99	2.40	174.97	120.61	1.79	1.93	2.12
	$S = 1/2$	1.77	1.96	1.90	2.17	1.95	2.14	173.99	121.95	1.76	1.81	2.09
Product	$S = 5/2$	2.27	2.08	2.11	2.39	2.10	1.51	178.27	148.80	2.15	2.23	2.93
	$S = 3/2$	2.12	2.16	2.05	2.13	2.04	1.51	176.38	153.18	2.19	2.81	2.12
	$S = 1/2$	2.13	2.05	2.03	2.13	2.03	1.50	177.81	154.91	2.14	2.80	2.13
PCy₃												
RC	$S = 5/2$	1.74	2.02	2.25	2.17	2.01	5.26	172.99	--	1.80	1.61	1.81
	$S = 3/2$	1.68	1.98	1.92	2.15	1.97	5.18	174.37	--	1.80	1.80	1.81

	$S = I/2$	1.69	1.94	1.89	2.17	1.93	5.64	175.98	--	1.74	1.73	1.73
TSTS	$S = 5/2$	1.77	2.04	2.15	2.15	2.03	2.83	179.31	114.31	1.79	1.82	1.84
	$S = 3/2$	1.72	2.06	2.04	2.17	1.98	2.53	175.08	121.88	1.83	1.94	2.07
	$S = I/2$	1.75	2.01	1.94	2.17	1.94	2.48	174.97	119.07	1.75	1.83	2.13
<i>Product</i>	$S = 5/2$	2.25	2.15	2.10	2.34	2.14	1.52	163.04	154.23	2.25	3.14	2.41
	$S = 3/2$	2.13	2.04	2.17	2.11	2.00	1.51	165.58	161.83	2.18	3.24	2.58
	$S = I/2$	2.14	2.03	1.96	2.06	2.02	1.51	165.90	148.18	2.60	2.03	2.58
PMe₃												
RC	$S = 5/2$	1.73	2.00	2.23	2.18	2.04	4.39	174.56	--	1.80	1.71	1.76
	$S = 3/2$	1.68	1.98	1.92	2.17	1.95	4.39	174.09	--	1.76	1.81	1.81
	$S = I/2$	1.68	1.96	1.89	2.15	1.92	4.76	175.35	--	1.74	1.77	1.74
TS	$S = 5/2$	1.76	2.04	2.11	2.14	2.09	2.66	179.73	118.90	1.80	1.82	1.83
	$S = 3/2$	1.72	2.05	2.04	2.18	1.99	2.44	177.16	115.40	1.79	1.87	2.19
	$S = I/2$	1.84	1.99	1.95	2.15	1.98	2.10	175.06	112.62	1.74	1.78	2.23
<i>Product</i>	$S = 5/2$	2.31	2.11	2.10	2.39	2.15	1.52	176.08	123.60	2.17	2.11	3.16
	$S = 3/2$	2.14	2.08	2.07	2.08	2.21	1.53	171.52	118.96	2.02	2.06	2.46
	$S = I/2$	2.18	2.06	2.03	2.09	2.09	1.52	172.06	118.38	1.99	2.03	2.42

Table S2: Spin density values of all species involved in oxygen atom transfer (OAT).

Species		PCy ₃			PPh ₃			PPh ₂ Me			PPhMe ₂			PMe ₃		
		Mn	O	P	Mn	O	P	Mn	O	P	Mn	O	P	Mn	O	P
<i>Reactant</i>	S=5/2	3.737	0.146	--	3.737	0.146	--	3.737	0.146	--	3.737	0.146	--	3.737	0.146	--
	S=3/2	2.790	0.243	--	2.790	0.243	--	2.790	0.243	--	2.790	0.243	--	2.790	0.243	--
	S=1/2	0.914	0.076	--	0.914	0.076	--	0.914	0.076	--	0.914	0.076	--	0.914	0.076	--
<i>RC</i>	S=5/2	3.741	0.139	0.000	3.739	0.146	0.000	3.733	0.140	0.000	3.750	0.141	0.000	3.731	0.149	0.000
	S=3/2	2.774	0.243	0.000	2.816	0.236	0.000	2.829* (2.819)	0.217* (0.224)	0.001* (0.000)	2.830	0.229	0.000	2.791	0.239	0.000
	S=1/2	0.904	0.117	0.000	0.892	0.124	0.000	0.922	0.117	0.000	0.899	0.105	0.000	0.899	0.130	0.000
<i>TS</i>	S=5/2	3.800	0.385	0.522	3.800	0.461	0.327	3.862	0.414	0.465	3.783	0.258	0.365	3.776	0.313	0.357
	S=3/2	3.625	-0.290	-0.332	3.544	-0.257	-0.238	3.591# (3.567)	-0.277# (-0.207)	-0.270# (-0.287)	3.616	-0.284	-0.284	3.598	-0.294	-0.271
	S=1/2	0.158	0.367	0.341	0.300	0.365	0.264	--	--	--	1.780	-0.225	-0.420	0.036	0.317	0.500
<i>P</i>	S=5/2	4.807	0.000	0.017	4.807	-0.001	0.016	4.819	0.001	0.015	4.820	0.003	0.012	4.818	0.007	0.009
	S=3/2	2.993	-0.005	0.004	2.978	-0.011	0.003	2.971	-0.009	-0.001	2.988	-0.011	0.003	2.967	-0.008	-0.001
	S=1/2	0.959	-0.001	-0.001	0.995	-0.005	-0.001	1.003	-0.006	0.000	1.013	-0.004	0.000	0.997	-0.005	-0.001

*Values in the bracket are the spin densities of the respective atoms corresponds to ⁴RC_{1(□)}

Values in the bracket are the spin densities of the respective atoms corresponds to ⁴TS_{1(σ)}

Table S3: Electronic configuration of ground state of the [Mn^{IV}H₃buea(O)]⁻ species (⁴R) from CASSCF/NEVPT2 method.

Multiplicity(root)	Energy (cm ⁻¹)	Electronic configuration from CASSCF	Contribution to D(cm ⁻¹)
4(0)	0	$\square_{xy}^1 \square_{yz}^1 \square_{z2}^0 \square_{xz}^1 \square_{x2-y2}^0$ (32%)	
		$\square_{xy}^1 \square_{yz}^0 \square_{z2}^0 \square_{xz}^1 \square_{x2-y2}^1$ (18%)	
		$\square_{xy}^1 \square_{yz}^1 \square_{z2}^1 \square_{xz}^0 \square_{x2-y2}^0$ (17%)	
		$\square_{xy}^1 \square_{yz}^0 \square_{z2}^1 \square_{xz}^0 \square_{x2-y2}^1$ (14%)	
4(1)	7724	$\square_{xy}^1 \square_{yz}^0 \square_{z2}^1 \square_{xz}^1 \square_{x2-y2}^0$ (27%)	-0.412
		$\square_{xy}^1 \square_{yz}^0 \square_{z2}^1 \square_{xz}^0 \square_{x2-y2}^1$ (17%)	
		$\square_{xy}^1 \square_{yz}^1 \square_{z2}^0 \square_{xz}^1 \square_{x2-y2}^0$ (16%)	
		$\square_{xy}^1 \square_{yz}^1 \square_{z2}^1 \square_{xz}^0 \square_{x2-y2}^0$ (13%)	
4(2)	13619	$\square_{xy}^0 \square_{yz}^0 \square_{z2}^1 \square_{xz}^1 \square_{x2-y2}^1$ (40%)	0.919
		$\square_{xy}^1 \square_{yz}^0 \square_{z2}^1 \square_{xz}^1 \square_{x2-y2}^0$ (37%)	
		$\square_{xy}^1 \square_{yz}^0 \square_{z2}^1 \square_{xz}^1 \square_{x2-y2}^0$ (23%)	0.653
		$\square_{xy}^0 \square_{yz}^1 \square_{z2}^1 \square_{xz}^0 \square_{x2-y2}^0$ (21%)	
2(0)		$\square_{xy}^0 \square_{yz}^1 \square_{z2}^0 \square_{xz}^1 \square_{x2-y2}^1$ (17%)	1.801
		$\square_{xy}^1 \square_{yz}^1 \square_{z2}^0 \square_{xz}^1 \square_{x2-y2}^0$ (15%)	
		$\square_{xy}^0 \square_{yz}^2 \square_{z2}^0 \square_{xz}^1 \square_{x2-y2}^0$ (14%)	
		$\square_{xy}^1 \square_{yz}^0 \square_{z2}^0 \square_{xz}^1 \square_{x2-y2}^1$ (11%)	
2(0)	8490	$\square_{xy}^1 \square_{yz}^1 \square_{z2}^1 \square_{xz}^0 \square_{x2-y2}^0$ (21%)	2.458
		$\square_{xy}^1 \square_{yz}^0 \square_{z2}^1 \square_{xz}^0 \square_{x2-y2}^1$ (10%)	

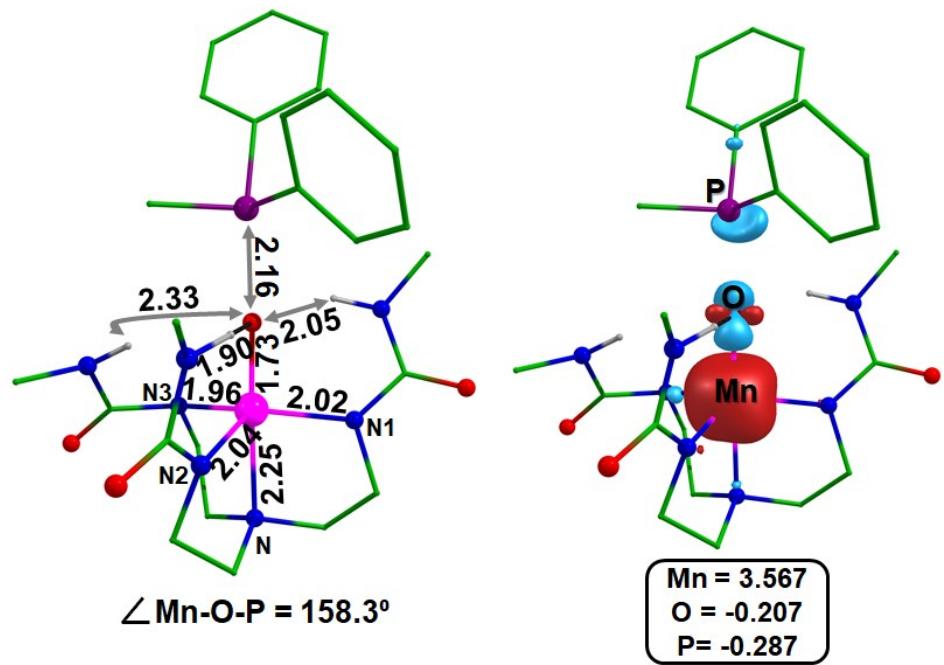


Figure S2. DFT/B3LYP optimised structure and respective spin density of $^4\text{TS}_{1(\sigma)}$.

Table S4: Electronic configuration of ground state of $^4\text{RC}_{1(\sigma)}$ from CASSCF/NEVPT2 method.

Multiplicity(root)	Energy (cm ⁻¹)	Electronic configuration from CASSCF	Contribution to Δ (cm ⁻¹)
4(0)	0	$\square_{xy}^1 \square_{yz}^1 \square_{z2}^1 \square_{x2-y2}^0 \square_{xz}^0$ (38%)	
		$\square_{xy}^1 \square_{yz}^0 \square_{z2}^1 \square_{x2-y2}^1 \square_{xz}^0$ (33%)	
		$\square_{xy}^1 \square_{yz}^0 \square_{z2}^1 \square_{x2-y2}^0 \square_{xz}^1$ (12%)	
4(1)	3580	$\square_{xy}^0 \square_{yz}^1 \square_{z2}^1 \square_{x2-y2}^0 \square_{xz}^1$ (32%)	-8.161
		$\square_{xy}^1 \square_{yz}^0 \square_{z2}^1 \square_{x2-y2}^0 \square_{xz}^1$ (28%)	
		$\square_{xy}^0 \square_{yz}^0 \square_{z2}^1 \square_{x2-y2}^1 \square_{xz}^1$ (27%)	
4(2)	9408	$\square_{xy}^1 \square_{yz}^1 \square_{z2}^0 \square_{x2-y2}^0 \square_{xz}^1$ (40%)	0.716
		$\square_{xy}^1 \square_{yz}^0 \square_{z2}^0 \square_{x2-y2}^1 \square_{xz}^1$ (33%)	
		$\square_{xy}^1 \square_{yz}^1 \square_{z2}^0 \square_{x2-y2}^1 \square_{xz}^0$ (19%)	0.361
	419.3	$\square_{xy}^1 \square_{yz}^0 \square_{z2}^1 \square_{x2-y2}^0 \square_{xz}^1$ (13%)	
		$\square_{xy}^1 \square_{yz}^0 \square_{z2}^2 \square_{x2-y2}^0 \square_{xz}^0$ (10%)	
		$\square_{xy}^1 \square_{yz}^2 \square_{z2}^0 \square_{x2-y2}^0 \square_{xz}^0$ (10%)	
2(3)	2145.8	$\square_{xy}^1 \square_{yz}^0 \square_{z2}^2 \square_{x2-y2}^0 \square_{xz}^0$ (17%)	1.165
		$\square_{xy}^1 \square_{yz}^1 \square_{z2}^1 \square_{x2-y2}^0 \square_{xz}^0$ (11%)	
		$\square_{xy}^0 \square_{yz}^1 \square_{z2}^1 \square_{x2-y2}^0 \square_{xz}^1$ (25%)	0.471
		$\square_{xy}^0 \square_{yz}^0 \square_{z2}^1 \square_{x2-y2}^1 \square_{xz}^1$	

		(22%)	
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Multiplicity (root)	Energy (cm ⁻¹)	Electronic configuration from CASSCF	Contribution to Δ (cm ⁻¹)
4(0)	0	$\square_{xy}^0 \square_{yz}^1 \square_{z2}^0 \square_{xz}^1 \square_{x2-y2}^1$ (27%)	
		$\square_{xy}^0 \square_{yz}^1 \square_{z2}^1 \square_{xz}^0 \square_{x2-y2}^1$ (21%)	
		$\square_{xy}^0 \square_{yz}^0 \square_{z2}^1 \square_{xz}^1 \square_{x2-y2}^1$ (14%)	
		$\square_{xy}^1 \square_{yz}^1 \square_{z2}^0 \square_{xz}^0 \square_{x2-y2}^1$ (12%)	
		$\square_{xy}^1 \square_{yz}^1 \square_{z2}^0 \square_{xz}^1 \square_{x2-y2}^0$ (10%)	
		$\square_{xy}^1 \square_{yz}^0 \square_{z2}^0 \square_{xz}^1 \square_{x2-y2}^1$ (10%)	
4(1)	8352	$\square_{xy}^1 \square_{yz}^1 \square_{z2}^0 \square_{xz}^1 \square_{x2-y2}^0$ (36%)	-0.461
		$\square_{xy}^1 \square_{yz}^1 \square_{z2}^1 \square_{xz}^0 \square_{x2-y2}^0$ (32%)	
		$\square_{xy}^1 \square_{yz}^0 \square_{z2}^1 \square_{xz}^1 \square_{x2-y2}^0$ (14%)	
		$\square_{xy}^1 \square_{yz}^1 \square_{z2}^0 \square_{xz}^0 \square_{x2-y2}^1$ (10%)	

Table S5: Electronic configuration of ground state of ${}^4\text{RC}_1(\square)$ from CASSCF/NEVPT2 method.

4(2)	14123	$\square_{xy}^1 \square_{yz}^0 \square_{z2}^1 \square_{xz}^0 \square_{x2-y2}^1$ (58%)	0.939
		$\square_{xy}^1 \square_{yz}^1 \square_{z2}^0 \square_{xz}^0 \square_{x2-y2}^1$ (17%)	
4(3)	14420	$\square_{xy}^0 \square_{yz}^1 \square_{z2}^0 \square_{xz}^1 \square_{x2-y2}^1$ (36%)	0.567
		$\square_{xy}^1 \square_{yz}^0 \square_{z2}^0 \square_{xz}^1 \square_{x2-y2}^1$ (30%)	
		$\square_{xy}^1 \square_{yz}^1 \square_{z2}^0 \square_{xz}^0 \square_{x2-y2}^1$ (21%)	
2(0)		$\square_{xy}^1 \square_{yz}^1 \square_{z2}^0 \square_{xz}^1 \square_{x2-y2}^0$ (28%)	1.518
2(1)	1299	$\square_{xy}^1 \square_{yz}^1 \square_{z2}^0 \square_{xz}^0 \square_{x2-y2}^1$ (18%)	2.628
		$\square_{xy}^0 \square_{yz}^1 \square_{z2}^0 \square_{xz}^1 \square_{x2-y2}^1$ (14%)	
		$\square_{xy}^0 \square_{yz}^1 \square_{z2}^1 \square_{xz}^0 \square_{x2-y2}^1$ (13%)	

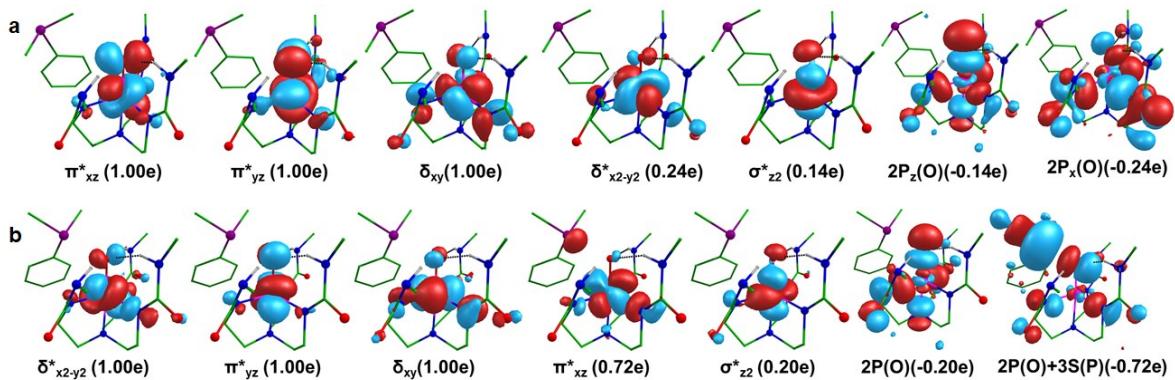


Figure S3. Spin natural orbitals and their occupations in (a) ${}^4\text{RC}_2$ (top panel) (b) ${}^4\text{TS}_2$ (bottom panel). The negative occupation in ϕ signifies a β spin electron.

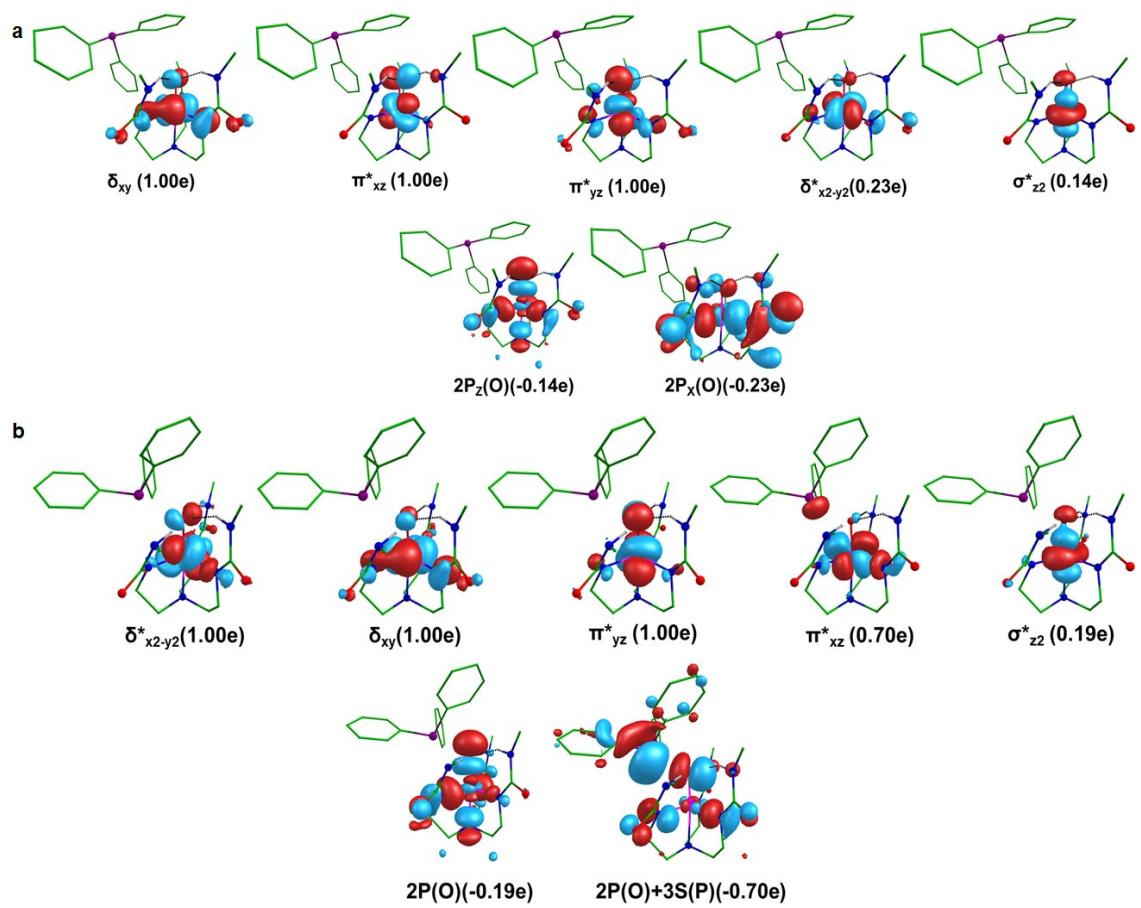


Figure S4. Spin natural orbitals and their occupations in (a) ${}^4\text{RC}_3$ (top panel) (b) ${}^4\text{TS}_3$ (bottom panel). The negative occupation in ϕ signifies a β spin electron.

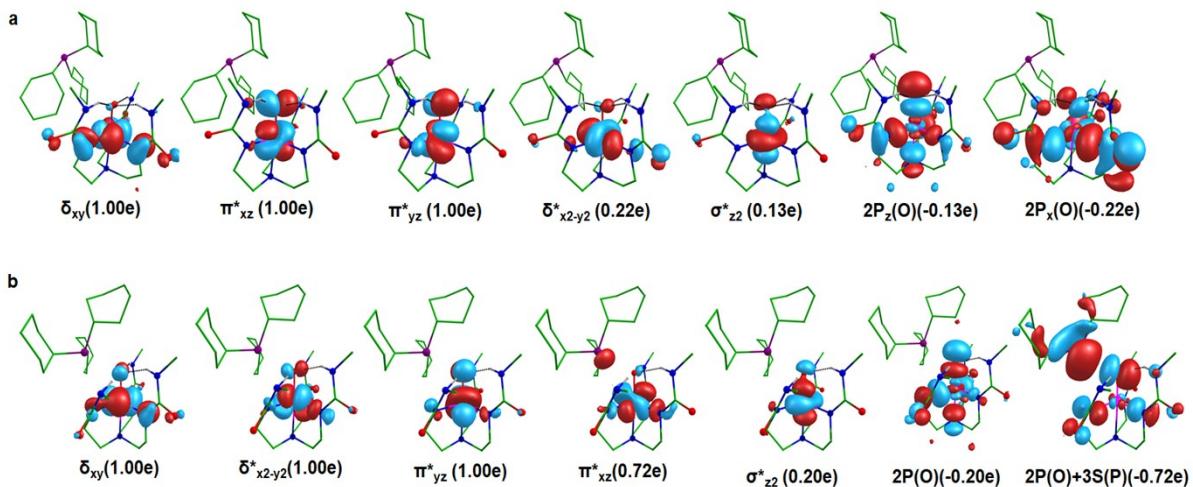


Figure S5. Spin natural orbitals and their occupations in (a) ${}^4\text{RC}_4$ (top panel) (b) ${}^4\text{TS}_4$ (bottom panel). The negative occupation in ϕ signifies a β spin electron.

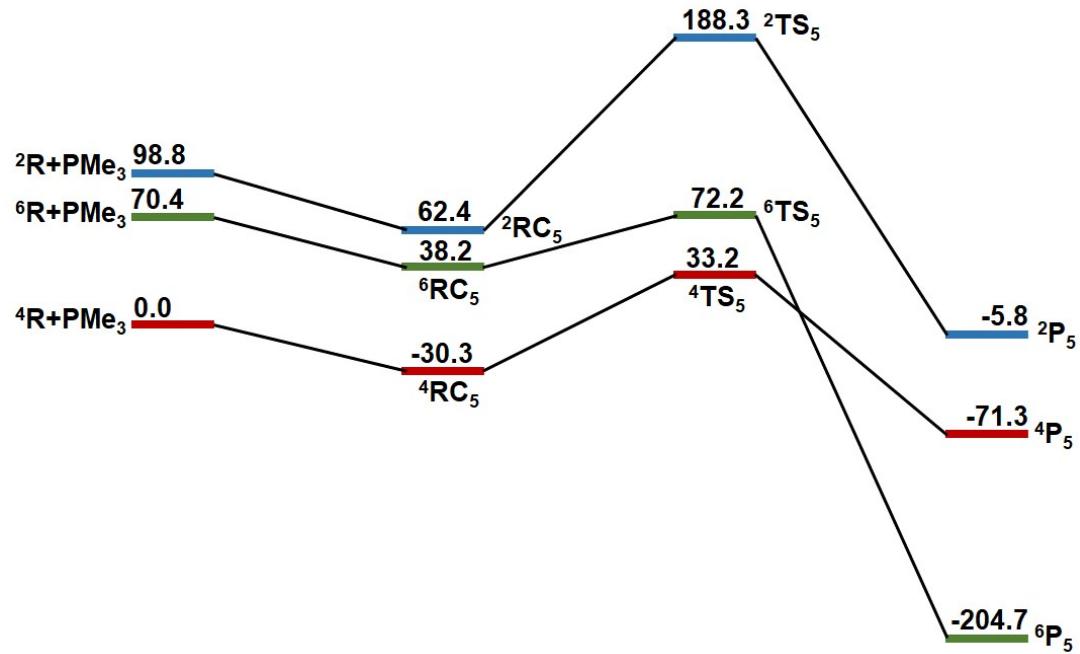


Figure S6. DFT/B3LYP computed energy profile diagram (kJ mol^{-1}) for the oxygen atom transfer reactions for PMe_3 using $[\text{Mn}^{\text{IV}}\text{H}_3\text{buea(O)}]^-$ catalyst

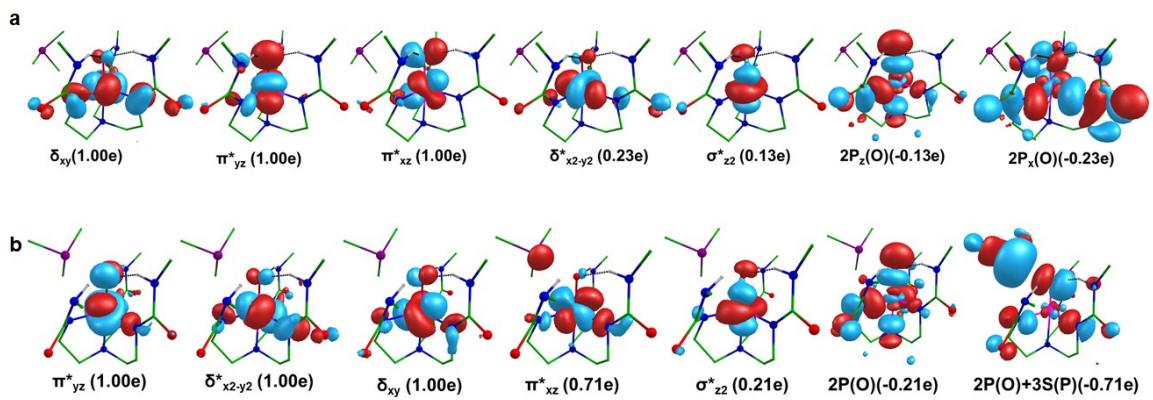


Figure S7. Spin natural orbitals and their occupations in (a) ${}^4\text{RC}_5$ (top panel) (b) ${}^4\text{TS}_5$ (bottom panel). The negative occupation in ϕ signifies a β spin electron.

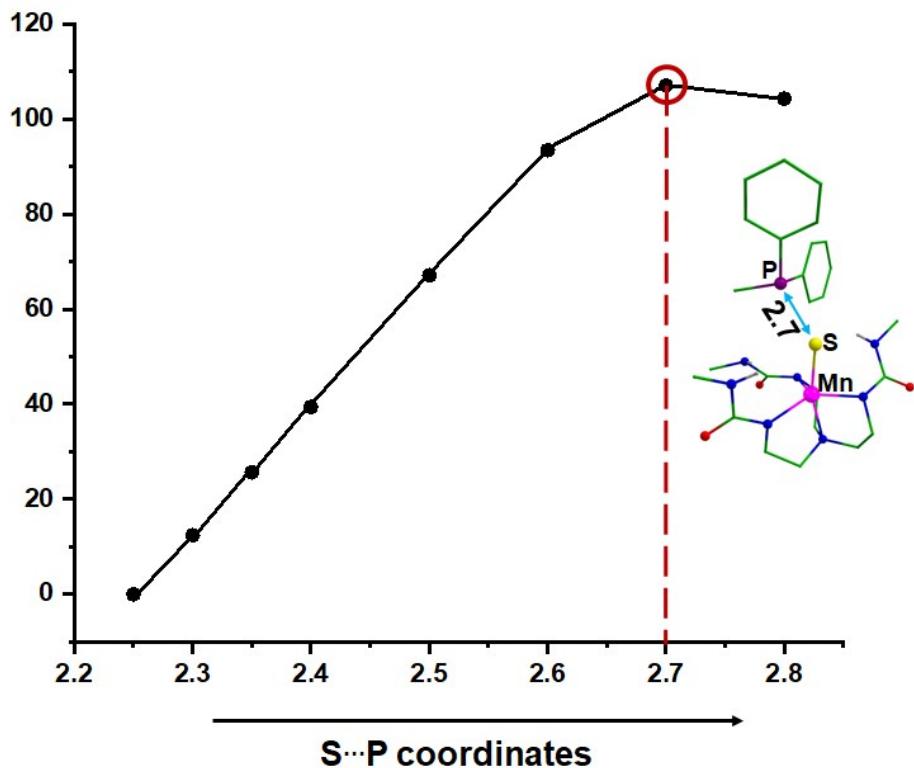


Figure S8. Relaxed potential energy scan graph along the S...P distance for ${}^6\text{TS}_S$.

Here, we can see that when the S...P distance is fixed to 2.7 Å, it gives the highest energy in the potential energy surface. Therefore, we have taken this highest energy structure and have performed the single point calculation on this.

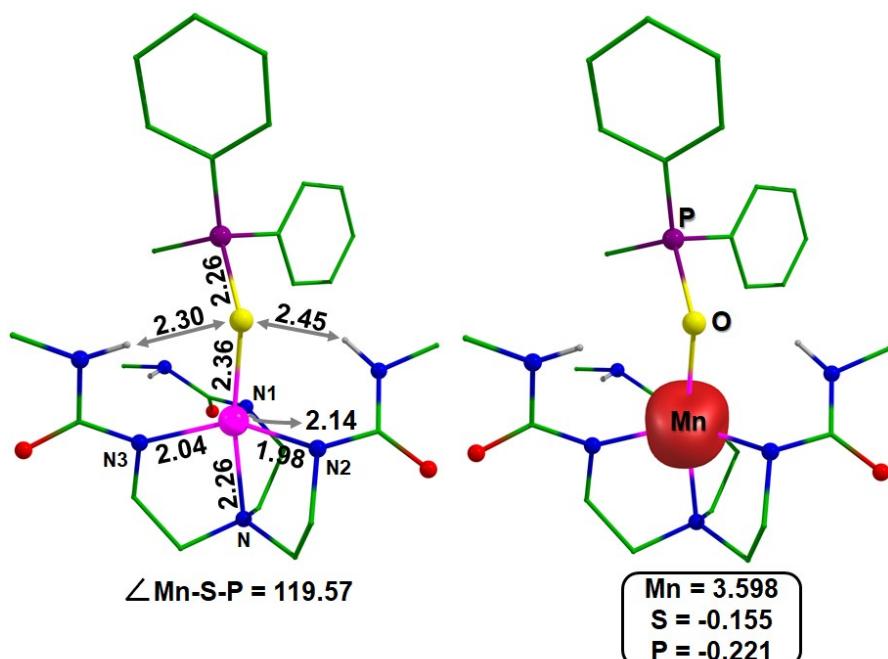


Figure S9. DFT/B3LYP optimised structures and spin density plot of ${}^4\text{TS}_S$ species.

Table S6: Spin density values of all species involved in Sulphur atom transfer (SAT)

Species		PPh ₂ Me		
		Mn	S	P
<i>Reactant</i>	<i>S=5/2</i>	3.937	0.792	--
	<i>S=3/2</i>	3.170	-0.041	--
	<i>S=1/2</i>	1.323	-0.160	--
<i>RC</i>	<i>S=5/2</i>	3.907	0.763	0.000
	<i>S=3/2</i>	4.034	-0.904	0.000
	<i>S=1/2</i>	0.993	0.134	0.000
<i>TS</i>	<i>S=5/2</i>	4.363	0.266	0.216
	<i>S=3/2</i>	3.620	-0.185	-0.214
	<i>S=1/2</i>	1.816	-0.350	-0.276
<i>P</i>	<i>S=5/2</i>	4.818	0.005	0.010
	<i>S=3/2</i>	3.000	-0.024	-0.004
	<i>S=1/2</i>	1.009	-0.009	-0.001

Table S7: EDA values (where, E_{steric} = steric energy, E_{int} = electronic interaction energy, and E_{orb} = orbital interaction energy) (kJ mol⁻¹) of all the species for the OAT reaction.

Species	E_{steric}	E_{int}	E_{orb}
PPh₂Me	184.2	59.1	-125.2
PPhMe₂	168.1	40.8	-127.3
PPh₃	171.4	55.1	-115.5
PCy₃	156.2	58.7	-97.4
PM₃	134.3	38.1	-96.2

Table S8: Computed DFT/B3LYP-D3 bond indices for various TSs involving in the oxygen and sulphur atom transfer reactions from the catalysts $[\text{Mn}^{\text{IV}}\text{H}_3\text{buea(O)}]^-$ and $[\text{Mn}^{\text{IV}}\text{H}_3\text{buea(S)}]^-$ to the various substrates.

Catalyst	Substrate	BF_i	BC_f	BFC_{ave}
$[\text{Mn}^{\text{IV}}\text{H}_3\text{buea(O)}]^-$	PPh₂Me(\square)	27.1	33.8	30.5
	PPh₂Me(σ)	35.0	36.5	35.8
	PPhMe₂	27.9	29.7	28.8
	PPh₃	26.1	25.3	25.7
	PCy₃	22.4	21.0	21.7
	PM₃	23.7	25.7	24.7
$[\text{Mn}^{\text{IV}}\text{H}_3\text{buea(S)}]^-$	PPh₂Me	41.6	34.6	38.1

Reaction Coordinates

⁶ R	⁴ R	⁶ RC ₁
Mn 0.378544000 -0.054401000 -0.244113000	Mn 0.236595000 -0.219811000 -0.229214000	
O 0.013169000 1.617248000 -0.495104000	O 0.036096000 1.238297000 -1.036716000	
N 0.702493000 -2.164632000 0.247258000	N 0.542956000 -2.203580000 0.658365000	
C 1.999848000 -2.455834000 -0.408143000	C 1.879949000 -2.627064000 0.197406000	
H 1.801934000 -2.475838000 -1.484343000	H 1.772034000 -2.925675000 -0.850088000	
H 2.372739000 -3.451216000 -0.112512000	H 2.235424000 -3.500520000 0.768917000	
C 3.024982000 -1.360921000 -0.112240000	C 2.853220000 -1.461588000 0.278386000	
H 3.467469000 -1.513451000 0.888179000	H 3.174921000 -1.295200000 1.319969000	
H 3.866346000 -1.467145000 -0.810148000	H 3.768900000 -1.712317000 -0.268663000	
N 2.386423000 -0.059633000 -0.231148000	N 2.219306000 -0.272188000 -0.281911000	
C 3.289772000 0.985686000 -0.265938000	C 3.163587000 0.717722000 -0.571472000	
O 4.525255000 0.820077000 -0.286828000	O 4.389191000 0.528753000 -0.468347000	
N 2.717519000 2.238157000 -0.249010000	N 2.646106000 1.918824000 -0.968564000	
H 1.696666000 2.263333000 -0.377934000	H 1.634683000 1.933130000 -1.132566000	
C 3.511060000 3.398835000 -0.559063000	C 3.503903000 2.958735000 -1.473803000	
C -0.416299000 -2.961488000 -0.315739000	C -0.536917000 -3.102382000 0.177054000	
H -1.214900000 -2.987078000 0.426643000	H -1.366522000 -3.050121000 0.884730000	
H -0.093786000 -3.997993000 -0.503392000	H -0.179931000 -4.143159000 0.142184000	
C -0.974798000 -2.298369000 -1.575805000	C -1.022665000 -2.591783000 -1.173989000	
H -0.267021000 -2.432510000 -2.412547000	H -0.261986000 -2.799448000 -1.944801000	
H -1.912690000 -2.781666000 -1.871945000	H -1.944527000 -3.098426000 -1.474978000	
N -1.170030000 -0.887356000 -1.305695000	N -1.254013000 -1.160968000 -1.051668000	
C -2.339497000 -0.336097000 -1.814272000	C -2.497643000 -0.706886000 -1.455068000	
O -3.234885000 -0.985791000 -2.382796000	O -3.399149000 -1.448132000 -1.884220000	
N -2.410622000 1.017326000 -1.610299000	N -2.672693000 0.651954000 -1.322276000	
H -1.536016000 1.466797000 -1.280513000	H -1.799533000 1.179724000 -1.265648000	
C -3.515872000 1.787408000 -2.112249000	C -3.833634000 1.276762000 -1.909368000	
C 0.771357000 -2.244372000 1.725195000	C 0.464896000 -1.947974000 2.113504000	
H 1.681100000 -1.723639000 2.028410000	H 1.412444000 -1.506884000 2.427506000	
H 0.846039000 -3.292079000 2.059440000	H 0.316022000 -2.887629000 2.668482000	
C -0.425689000 -1.540533000 2.375768000	C -0.648220000 -0.945970000 2.377357000	
H -1.342737000 -2.147033000 2.345031000	H -1.636000000 -1.398508000 2.200929000	
H -0.229767000 -1.392983000 3.449697000	H -0.634089000 -0.641907000 3.428873000	
N -0.633741000 -0.283187000 1.706389000	N -0.433392000 0.212947000 1.517953000	
C -1.694824000 0.485136000 2.199833000	C -1.147688000 1.337740000 1.925151000	
O -2.481008000 0.107818000 3.079934000	O -1.872082000 1.316986000 2.933376000	
N -1.728661000 1.701715000 1.584318000	N -0.943109000 2.483725000 1.195537000	
H -1.047627000 1.843944000 0.793923000	H -0.504828000 2.325989000 0.285986000	
C -2.824786000 2.606895000 1.809714000	C -1.884817000 3.572199000 1.322041000	
H 3.127795000 4.277387000 -0.024688000	H 3.057756000 3.940532000 -1.276414000	
H 4.541756000 3.212487000 -0.247611000	H 4.472401000 2.896887000 -0.971576000	
H 3.527139000 3.643519000 -1.636328000	H 3.687798000 2.882449000 -2.559306000	
H -3.757302000 2.601649000 -1.416985000	H -3.979249000 2.265860000 -1.461478000	
H -3.313382000 2.238172000 -3.098211000	H -3.761334000 1.399567000 -3.003429000	
H -4.384588000 1.133006000 -2.218446000	H -4.713420000 0.661102000 -1.708740000	
H -2.487364000 3.639606000 1.674443000	H -1.410190000 4.511853000 1.018068000	
H -3.654902000 2.422025000 1.110440000	H -2.790612000 3.428869000 0.709070000	
H -3.205920000 2.471118000 2.825511000	H -2.197435000 3.649820000 2.365334000	
² R	⁶ RC ₁	
Mn 0.191866000 -0.015450000 -0.196734000	Mn -1.793099000 -0.203817000 -0.107222000	
O -0.063740000 -1.637927000 -0.471366000	O -0.639936000 0.496738000 -1.197456000	
N 0.684218000 2.207764000 0.099004000	N -3.399632000 -0.904020000 1.200790000	
C -0.255624000 2.905092000 -0.795618000	C -2.721841000 -0.964755000 2.517305000	
H 0.153868000 2.847559000 -1.808638000	H -1.981633000 -1.763234000 2.446487000	
H -0.352597000 3.969806000 -0.524533000	H -3.435545000 -1.230083000 3.314997000	
C -1.596616000 2.190667000 -0.778608000	C -2.003171000 0.352087000 2.823343000	
H -2.107982000 2.352370000 0.183757000	H -2.690414000 1.091109000 3.265305000	
H -2.254661000 2.604866000 -1.548150000	H -1.251603000 0.168193000 3.603661000	

N	-1.369384000	0.766383000	-1.011780000	N	-1.394392000	0.857172000	1.605428000
C	-2.471227000	0.139974000	-1.609575000	C	-0.535363000	1.918495000	1.826688000
O	-3.487855000	0.762380000	-1.964789000	O	-0.288076000	2.382070000	2.955678000
N	-2.372133000	-1.208986000	-1.792314000	N	0.030154000	2.423951000	0.681925000
H	-1.515510000	-1.665867000	-1.474259000	H	-0.035295000	1.806892000	-0.142307000
C	-3.438820000	-1.940130000	-2.426285000	C	1.066584000	3.418660000	0.780369000
C	2.099180000	2.390293000	-0.292072000	C	-3.790896000	-2.241126000	0.690848000
H	2.721615000	2.252610000	0.595750000	H	-4.476055000	-2.076285000	-0.144825000
H	2.271053000	3.409298000	-0.674877000	H	-4.326886000	-2.807734000	1.470480000
C	2.462642000	1.305089000	-1.298618000	C	-2.570899000	-2.993427000	0.167496000
H	1.936945000	1.489931000	-2.248900000	H	-1.955091000	-3.349594000	1.012027000
H	3.537244000	1.303566000	-1.503240000	H	-2.898623000	-3.900752000	-0.354497000
N	2.058512000	0.027927000	-0.735510000	N	-1.836339000	-2.107574000	-0.720652000
C	3.057684000	-0.917511000	-0.599580000	C	-1.008503000	-2.767377000	-1.606042000
O	4.241887000	-0.726006000	-0.932223000	O	-0.838251000	-4.003504000	-1.599432000
N	2.654522000	-2.108339000	-0.030977000	N	-0.399094000	-1.951878000	-2.532548000
H	1.646978000	-2.267817000	-0.061390000	H	-0.386148000	-0.955014000	-2.285313000
C	3.536692000	-3.249528000	-0.096842000	C	0.613016000	-2.488672000	-3.411220000
C	0.450825000	2.473290000	1.535367000	C	-4.524279000	0.059435000	1.200500000
H	-0.606168000	2.705238000	1.683443000	H	-4.257005000	0.881572000	1.864241000
H	1.044765000	3.335540000	1.877955000	H	-5.438863000	-0.414348000	1.590371000
C	0.762318000	1.186375000	2.295442000	C	-4.766091000	0.656043000	-0.192732000
H	1.834528000	0.960534000	2.231019000	H	-5.182625000	-0.112131000	-0.865066000
H	0.478704000	1.281064000	3.346862000	H	-5.488010000	1.479514000	-0.141487000
N	0.012870000	0.108359000	1.670917000	N	-3.500026000	1.073096000	-0.731580000
C	-1.071606000	-0.387460000	2.393427000	C	-3.459029000	2.328916000	-1.366605000
O	-1.450971000	0.105253000	3.469079000	O	-4.389119000	3.146199000	-1.367405000
N	-1.673556000	-1.481161000	1.830149000	N	-2.253963000	2.503576000	-1.969592000
H	-1.284783000	-1.808107000	0.946517000	H	-1.532426000	1.750138000	-1.799305000
C	-2.947894000	-1.969468000	2.291963000	C	-1.905990000	3.768856000	-2.563047000
H	-3.338408000	-3.003376000	-2.184292000	P	3.247595000	-0.561928000	-1.245339000
H	-4.410069000	-1.580724000	-2.071163000	C	7.286580000	0.887747000	0.627387000
H	-3.437548000	-1.837334000	-3.523121000	C	6.675053000	1.638313000	-0.377146000
H	3.229680000	-3.993188000	0.646845000	C	5.451257000	1.232478000	-0.914991000
H	3.550767000	-3.738093000	-1.086261000	C	4.808111000	0.067167000	-0.463138000
H	4.557157000	-2.925837000	0.120019000	C	5.443533000	-0.680622000	0.546384000
H	-3.728419000	-1.841650000	1.527996000	C	6.662273000	-0.275144000	1.087450000
H	-2.903560000	-3.035213000	2.558258000	H	8.235674000	1.206020000	1.050825000
H	-3.225500000	-1.402246000	3.182718000	H	7.146221000	2.548760000	-0.740015000
PPh₂Me							
P	-0.033181000	1.404611000	-0.692544000	H	4.991070000	1.839017000	-1.689854000
C	1.426248000	0.332577000	-0.312171000	H	4.962842000	-1.578689000	0.925381000
C	2.458550000	0.708639000	0.560007000	H	7.123865000	-0.865164000	1.875552000
C	1.543968000	-0.892851000	-0.992997000	C	0.773826000	-1.811180000	2.492194000
C	3.570147000	-0.116859000	0.750179000	C	0.853587000	-2.645702000	1.378034000
H	2.405872000	1.646539000	1.103413000	C	1.602648000	-2.254551000	0.265457000
C	2.647002000	-1.719734000	-0.796335000	C	2.282637000	-1.029371000	0.258762000
H	0.755531000	-1.207205000	-1.672176000	C	2.173389000	-0.189446000	1.380511000
C	3.667712000	-1.333323000	0.076625000	C	1.422044000	-0.571680000	2.488134000
H	4.357461000	0.192837000	1.431899000	H	0.191018000	-2.112112000	3.359519000
H	2.711874000	-2.666150000	-1.325758000	H	0.323441000	-3.592604000	1.348683000
H	4.530444000	-1.975342000	0.228120000	H	1.629737000	-2.906077000	-0.602267000
C	-1.424689000	0.282221000	-0.196533000	H	2.676285000	0.772892000	1.385529000
C	-1.344667000	-0.608841000	0.886056000	H	1.304107000	0.118313000	3.318258000
C	-2.622971000	0.356020000	-0.920580000	C	2.416940000	1.021548000	-1.732768000
C	-2.437478000	-1.399860000	1.236703000	H	1.339282000	0.816902000	-1.786368000
H	-0.417722000	-0.691040000	1.446477000	H	2.577239000	1.815350000	-0.997318000
C	-3.720995000	-0.431753000	-0.566677000	H	2.777343000	1.358346000	-2.710154000
H	-2.694750000	1.031585000	-1.769135000	H	1.193351000	3.909421000	-0.190296000
C	-3.629406000	-1.311186000	0.512032000	H	0.789664000	4.164706000	1.530177000
H	-2.360620000	-2.086798000	2.074976000	H	2.043502000	3.004594000	1.083214000
				H	0.336367000	-3.508324000	-3.689682000
				H	0.678807000	-1.873930000	-4.316650000

H	-4.642645000	-0.362769000	-1.137543000	H	1.617659000	-2.524628000	-2.960103000
H	-4.479867000	-1.929192000	0.785412000	H	-1.165170000	3.612458000	-3.353172000
C	-0.046363000	2.560525000	0.772637000	H	-2.800603000	4.238659000	-2.981125000
H	0.757113000	3.296704000	0.680066000	H	-1.478320000	4.459740000	-1.820766000
H	-0.998627000	3.097203000	0.763489000				
H	0.051300000	2.031012000	1.725244000				
⁴RC_{1(σ)}				⁴RC_{1(□)}			
Mn	1.812034000	0.436163000	-0.087226000	Mn	-1.424290091	-0.055104814	-0.112860807
O	0.484088000	0.151959000	-1.064561000	O	-0.729525872	0.324659238	1.372750873
N	3.520636000	0.863485000	1.317313000	N	-2.165903430	-0.602962020	-2.119679268
C	3.444031000	-0.235101000	2.299236000	C	-1.989397946	-2.066204319	-2.206459045
H	2.622410000	0.000118000	2.983479000	H	-0.927169870	-2.247534312	-2.390329089
H	4.372661000	-0.304624000	2.889273000	H	-2.566248244	-2.482699094	-3.048845195
C	3.129270000	-1.541759000	1.584210000	C	-2.368130103	-2.714163340	-0.884506013
H	3.998842000	-1.886348000	1.003466000	H	-3.463609031	-2.734918200	-0.762389896
H	2.930869000	-2.326922000	2.321344000	H	-2.049837396	-3.761069088	-0.886794176
N	1.962331000	-1.343593000	0.728536000	N	-1.735679151	-1.981054937	0.209050943
C	1.313178000	-2.541495000	0.432095000	C	-1.508295921	-2.780802101	1.326645247
O	1.676910000	-3.642390000	0.885172000	O	-1.630303027	-4.022068303	1.317163978
N	0.229010000	-2.442815000	-0.389212000	N	-1.116159175	-2.117480007	2.454937926
H	-0.047938000	-1.503457000	-0.673248000	H	-0.887246093	-1.125971179	2.329881171
C	-0.562529000	-3.605964000	-0.693541000	C	-0.662482819	-2.856178109	3.606427091
C	3.287056000	2.204714000	1.903784000	C	-1.366138274	0.130923214	-3.136210242
H	3.801869000	2.938286000	1.278450000	H	-1.892537342	1.052415013	-3.393396206
H	3.712591000	2.263033000	2.917865000	H	-1.264808239	-0.473214109	-4.049686064
C	1.796564000	2.518281000	1.871785000	C	-0.0266626082	0.501442011	-2.506975100
H	1.272392000	1.906620000	2.626109000	H	0.597842230	-0.394924981	-2.390302101
H	1.615493000	3.567458000	2.124915000	H	0.512122925	1.218449137	-3.133384436
N	1.299944000	2.225261000	0.533760000	N	-0.295218991	1.080729170	-1.199071195
C	0.527857000	3.223340000	-0.049461000	C	-0.028824814	2.425818361	-1.034375889
O	0.297789000	4.320551000	0.486423000	O	0.370851120	3.172510214	-1.950032980
N	0.055906000	2.904336000	-1.299808000	N	-0.212880070	2.877926235	0.244922281
H	0.091945000	1.908959000	-1.527829000	H	-0.330419862	2.154778007	0.953620266
C	-0.927196000	3.747935000	-1.940142000	C	0.181770268	4.213835259	0.619092930
C	4.745782000	0.824898000	0.481582000	C	-3.579969287	-0.166440003	-2.092397006
H	5.096160000	-0.204439000	0.399981000	H	-4.154876446	-0.915696249	-1.544762054
H	5.543919000	1.433378000	0.933547000	H	-3.985554544	-0.093437885	-3.113456149
C	4.348863000	1.280965000	-0.921344000	C	-3.670385041	1.154639886	-1.344060999
H	4.027179000	2.328381000	-0.910653000	H	-3.195777079	1.964534024	-1.918790884
H	5.193904000	1.170656000	-1.607267000	H	-4.717707252	1.439702907	-1.208858858
N	3.228621000	0.466466000	-1.374462000	N	-3.030992342	0.983998215	-0.043439102
C	3.589162000	-0.739508000	-1.981888000	C	-3.437113126	1.920545107	0.907057960
O	4.766151000	-1.116535000	-2.088064000	O	-4.291922241	2.781905436	0.647787038
N	2.534726000	-1.447070000	-2.504921000	N	-2.898509114	1.785845154	2.162669098
H	1.617471000	-1.109882000	-2.223739000	H	-2.058809067	1.205838843	2.204579407
C	2.678524000	-2.874464000	-2.723494000	C	-3.038166398	2.870993484	3.106247168
P	-3.120566000	0.810636000	-0.466995000	H	-0.615045783	-2.183165192	4.468024492
C	-7.703031000	-0.101692000	-0.157942000	H	-1.355393859	-3.673326208	3.825541398
C	-7.051890000	-0.270406000	-1.379407000	H	0.334523102	-3.309265490	3.470782029
C	-5.677171000	-0.039171000	-1.485204000	H	-0.372573063	4.521070278	1.511811245
C	-4.921528000	0.370587000	-0.374187000	H	1.260083215	4.298225271	0.828816987
C	-5.598975000	0.543419000	0.848878000	H	-0.051520168	4.899038303	-0.198902911
C	-6.966857000	0.305340000	0.959227000	H	-2.889963430	2.494784973	4.124105318
H	-8.770893000	-0.286059000	-0.074326000	H	-2.319002346	3.689245447	2.932911456
H	-7.611491000	-0.590656000	-2.255077000	H	-4.042301395	3.291154399	3.021350203
H	-5.194365000	-0.188467000	-2.446057000	P	3.620871513	-1.024301942	1.381486002
H	-5.037914000	0.852014000	1.727660000	C	2.711283028	-1.925474393	0.043991034
H	-7.461171000	0.436649000	1.918641000	C	1.665619259	-2.806776237	0.362212831
C	-1.219877000	-1.929321000	2.783868000	C	3.122481267	-1.846067113	-1.299538142
C	-0.714981000	-0.655537000	2.527468000	C	1.051259819	-3.587547105	-0.617923978
C	-1.324101000	0.166425000	1.577466000	H	1.293593894	-2.875719037	1.378218332
C	-2.442515000	-0.284035000	0.860700000	C	2.508829338	-2.622300286	-2.283019351

C	-2.949682000	-1.565882000	1.134105000	H	3.915336427	-1.158018154	-1.579598322
C	-2.346527000	-2.380176000	2.091195000	C	1.475539849	-3.501967502	-1.944762903
H	-0.727100000	-2.577011000	3.503163000	H	0.228575996	-4.232235281	-0.324330090
H	0.172673000	-0.307600000	3.045350000	H	2.836848322	-2.537051419	-3.316391391
H	-0.892718000	1.137887000	1.356501000	H	0.998464863	-4.107393372	-2.711705311
H	-3.818645000	-1.927388000	0.590790000	C	3.991735334	0.588028109	0.554139069
H	-2.741264000	-3.374713000	2.283075000	C	3.011940374	1.331022072	-0.128118045
C	-2.585249000	-0.130072000	-1.974187000	C	5.297621486	1.096790229	0.626278099
H	-1.491039000	-0.109091000	-1.983018000	C	3.331890993	2.552464235	-0.725478195
H	-2.929684000	-1.170095000	-1.962989000	H	1.996283071	0.951867102	-0.198755270
H	-2.946529000	0.363213000	-2.882519000	C	5.620287314	2.322167355	0.036709026
H	-1.325474000	-3.326600000	-1.426327000	H	6.064326293	0.527112929	1.146848280
H	0.059588000	-4.405803000	-1.112669000	C	4.637555420	3.047232263	-0.638659788
H	-1.067530000	-4.010181000	0.193926000	H	2.560284416	3.101136374	-1.257783940
H	-0.716111000	4.789141000	-1.687130000	H	6.636207617	2.704979998	0.101740147
H	-0.867613000	3.623395000	-3.027457000	H	4.886695244	3.998721532	-1.102596891
H	-1.955261000	3.521435000	-1.618866000	C	2.218826976	-0.522346100	2.493496956
H	1.893666000	-3.218077000	-3.404566000	H	1.890670405	-1.379542863	3.089004456
H	3.653170000	-3.065037000	-3.176878000	H	2.595834015	0.235955902	3.187416079
H	2.606775000	-3.450884000	-1.790360000	H	1.354824993	-0.124549803	1.949662026
²RC₁				⁶TS₁			
Mn	1.785041000	0.402129000	-0.125445000	Mn	1.690467000	0.587056000	-0.264019000
O	0.515234000	0.156531000	-1.147959000	O	0.039711000	-0.066037000	-0.128773000
N	3.521440000	0.883195000	1.347497000	N	3.835797000	1.186087000	-0.247164000
C	3.551692000	-0.286184000	2.241645000	C	4.504237000	0.492019000	0.882304000
H	2.756736000	-0.156068000	2.982913000	H	4.229587000	1.015457000	1.800954000
H	4.511929000	-0.356029000	2.779391000	H	5.597611000	0.554555000	0.769626000
C	3.262388000	-1.541564000	1.435011000	C	4.040256000	-0.957403000	1.002250000
H	4.098223000	-1.764679000	0.754595000	H	4.378254000	-1.548229000	0.133685000
H	3.161746000	-2.404956000	2.099080000	H	4.489690000	-1.432594000	1.884774000
N	2.026683000	-1.331825000	0.681313000	N	2.599992000	-0.966788000	1.046433000
C	1.358359000	-2.527533000	0.399412000	C	2.039601000	-2.099785000	1.607289000
O	1.746904000	-3.632592000	0.820032000	O	2.672181000	-3.097228000	1.992050000
N	0.242097000	-2.436746000	-0.377755000	N	0.672602000	-1.991603000	1.705562000
H	-0.049492000	-1.513918000	-0.686755000	H	0.248225000	-1.213838000	1.171289000
C	-0.526475000	-3.616964000	-0.681247000	C	-0.120872000	-3.119927000	2.121655000
C	3.167891000	2.143989000	2.033734000	C	3.819247000	2.657458000	-0.046677000
H	3.592311000	2.973884000	1.462541000	H	3.584279000	3.111608000	-1.013415000
H	3.597361000	2.172900000	3.048170000	H	4.814167000	3.010748000	0.271608000
C	1.652538000	2.294209000	2.025407000	C	2.719903000	3.039868000	0.939547000
H	1.202862000	1.545441000	2.697837000	H	2.982906000	2.695430000	1.953930000
H	1.353387000	3.283271000	2.384126000	H	2.637071000	4.130597000	1.001719000
N	1.191803000	2.095466000	0.661075000	N	1.473418000	2.454652000	0.469243000
C	0.470488000	3.142343000	0.108897000	C	0.374670000	3.270768000	0.621087000
O	0.221417000	4.200981000	0.711595000	O	0.373584000	4.350465000	1.239326000
N	0.061426000	2.938513000	-1.190780000	N	-0.761946000	2.823437000	-0.030280000
H	0.100038000	1.972672000	-1.509255000	H	-0.738078000	1.860335000	-0.349581000
C	-0.906827000	3.832433000	-1.785505000	C	-2.051192000	3.390165000	0.292135000
C	4.731463000	1.015809000	0.505010000	C	4.421417000	0.796635000	-1.562045000
H	5.193182000	0.0360666000	0.374838000	H	4.853230000	-0.201103000	-1.474127000
H	5.465832000	1.687557000	0.975891000	H	5.221051000	1.499967000	-1.841757000
C	4.271658000	1.486706000	-0.874418000	C	3.298425000	0.701862000	-2.598433000
H	3.844538000	2.493804000	-0.815286000	H	2.885334000	1.698985000	-2.801666000
H	5.113745000	1.493221000	-1.573649000	H	3.705168000	0.297266000	-3.533152000
N	3.231087000	0.580444000	-1.336445000	N	2.238487000	-0.140945000	-2.064696000
C	3.691200000	-0.570695000	-1.972578000	C	2.440100000	-1.490917000	-2.226731000
O	4.894177000	-0.859462000	-2.069505000	O	3.453619000	-2.003487000	-2.738989000
N	2.699139000	-1.350892000	-2.526019000	N	1.379903000	-2.261664000	-1.773083000
H	1.754252000	-1.074046000	-2.278338000	H	0.735573000	-1.734208000	-1.190176000
C	2.934227000	-2.769421000	-2.723630000	C	1.603468000	-3.653186000	-1.430569000
P	-3.126245000	0.784986000	-0.468262000	P	-2.224451000	-0.220891000	-0.655167000
C	-7.730669000	-0.024290000	-0.213567000	C	-6.553661000	0.543548000	-2.306081000

C	-7.075201000	-0.184122000	-1.433843000	C	-5.695084000	-0.329563000	-2.976356000
C	-5.694761000	0.017310000	-1.526221000	C	-4.428369000	-0.608566000	-2.459328000
C	-4.937936000	0.387812000	-0.402438000	C	-3.987698000	-0.031671000	-1.252915000
C	-5.619735000	0.552959000	0.819335000	C	-4.862382000	0.863055000	-0.602420000
C	-6.993309000	0.344089000	0.916208000	C	-6.127714000	1.140490000	-1.115351000
H	-8.803071000	-0.185295000	-0.140628000	H	-7.539938000	0.760908000	-2.707699000
H	-7.635997000	-0.473914000	-2.319283000	H	-6.012132000	-0.798505000	-3.905028000
H	-5.208955000	-0.124330000	-2.486680000	H	-3.777856000	-1.287800000	-3.004371000
H	-5.057994000	0.832476000	1.707409000	H	-4.548634000	1.334749000	0.325065000
H	-7.491268000	0.468633000	1.874602000	H	-6.785767000	1.823749000	-0.583685000
C	-1.321765000	-2.125306000	2.690645000	C	-3.020547000	-0.789434000	3.912442000
C	-0.766994000	-0.866358000	2.466725000	C	-2.038423000	0.100099000	3.474320000
C	-1.348287000	0.006196000	1.544300000	C	-1.804147000	0.278722000	2.109073000
C	-2.484645000	-0.380343000	0.818560000	C	-2.557571000	-0.428648000	1.158944000
C	-3.038932000	-1.650291000	1.055344000	C	-3.552397000	-1.312374000	1.612575000
C	-2.466239000	-2.513119000	1.988431000	C	-3.780232000	-1.496800000	2.976677000
H	-0.853189000	-2.810888000	3.390866000	H	-3.193375000	-0.933167000	4.976077000
H	0.141653000	-0.572247000	2.981147000	H	-1.440149000	0.651974000	4.193847000
H	-0.880055000	0.966183000	1.349405000	H	-1.013173000	0.938164000	1.772321000
H	-3.922732000	-1.962790000	0.505492000	H	-4.155112000	-1.857856000	0.891627000
H	-2.899478000	-3.496417000	2.154025000	H	-4.548091000	-2.191517000	3.308293000
C	-2.604230000	-0.108044000	-2.009167000	C	-1.895303000	-1.969352000	-1.172934000
H	-1.510086000	-0.103029000	-2.020639000	H	-1.201469000	-2.401294000	-0.452569000
H	-2.965429000	-1.142061000	-2.038439000	H	-2.809050000	-2.570389000	-1.194059000
H	-2.957000000	0.425115000	-2.898187000	H	-1.408957000	-1.996227000	-2.151239000
H	-1.416518000	-3.316689000	-1.240938000	H	-1.106603000	-2.770261000	2.439208000
H	0.048345000	-4.334759000	-1.281668000	H	-0.251294000	-3.865872000	1.320905000
H	-0.847350000	-4.132213000	0.231465000	H	0.383935000	-3.626100000	2.949441000
H	-0.691921000	4.852297000	-1.459737000	H	-1.949856000	4.472994000	0.389298000
H	-0.830850000	3.780572000	-2.877466000	H	-2.760757000	3.159901000	-0.509090000
H	-1.941496000	3.594054000	-1.494635000	H	-2.471220000	3.006577000	1.237971000
H	2.255950000	-3.152581000	-3.493331000	H	0.643982000	-4.183670000	-1.416796000
H	3.964061000	-2.906856000	-3.057779000	H	2.242265000	-4.099201000	-2.195477000
H	2.781395000	-3.350884000	-1.802858000	H	2.089337000	-3.789460000	-0.453505000
⁴TS_{1(g)}				⁴TS_{1(̄)}			
Mn	1.630860000	0.462213000	-0.275977000	Mn	1.308943000	-0.587820000	0.036527000
O	-0.024458000	0.004797000	-0.041931000	O	-0.273121000	0.039434000	-0.238682000
N	3.774781000	1.115705000	-0.502347000	N	3.208422000	-1.480821000	0.542916000
C	4.508615000	0.470551000	0.613658000	C	4.109104000	-1.102060000	-0.576950000
H	4.363956000	1.083441000	1.506472000	H	3.856986000	-1.737513000	-1.427841000
H	5.586183000	0.436212000	0.389069000	H	5.158417000	-1.287124000	-0.298012000
C	3.933489000	-0.911382000	0.885503000	C	3.870875000	0.353256000	-0.971701000
H	4.149724000	-1.586614000	0.041744000	H	4.244284000	1.035033000	-0.190122000
H	4.415333000	-1.347105000	1.766923000	H	4.458548000	0.580805000	-1.870413000
N	2.499565000	-0.772812000	1.103125000	N	2.447913000	0.532274000	-1.213434000
C	1.968138000	-1.726073000	1.941287000	C	2.138610000	1.706487000	-1.858121000
O	2.644442000	-2.563854000	2.568694000	O	2.992559000	2.552323000	-2.191002000
N	0.585657000	-1.723749000	2.043946000	N	0.797895000	1.883800000	-2.152253000
H	0.121609000	-0.936464000	1.604051000	H	0.147956000	1.250715000	-1.697495000
C	-0.056313000	-2.356837000	3.173958000	C	0.301025000	3.152961000	-2.627617000
C	3.767408000	2.592255000	-0.388822000	C	2.947651000	-2.937619000	0.630317000
H	3.497600000	2.998212000	-1.368178000	H	2.419048000	-3.103031000	1.573883000
H	4.771076000	2.962283000	-0.121752000	H	3.896719000	-3.496615000	0.668566000
C	2.695088000	3.017432000	0.611048000	C	2.062859000	-3.404742000	-0.515836000
H	2.971564000	2.682931000	1.623170000	H	2.653739000	-3.504093000	-1.441849000
H	2.615646000	4.108877000	0.647100000	H	1.699569000	-4.417233000	-0.296705000
N	1.440065000	2.422383000	0.178940000	N	0.964574000	-2.461550000	-0.684769000
C	0.373270000	3.295829000	0.153109000	C	0.007195000	-2.936592000	-1.564029000
O	0.385634000	4.449058000	0.618377000	O	-0.021873000	-4.111786000	-1.976672000
N	-0.747340000	2.812808000	-0.503044000	N	-0.922226000	-2.007305000	-1.976855000
H	-0.754474000	1.813617000	-0.674323000	H	-0.927784000	-1.133717000	-1.451445000
C	-2.023558000	3.467779000	-0.321114000	C	-2.107148000	-2.416772000	-2.688522000

C	4.231278000	0.632475000	-1.834680000	C	3.654202000	-0.927557000	1.851325000
H	4.731890000	-0.329418000	-1.712053000	H	4.208785000	-0.005905000	1.669782000
H	4.945022000	1.343172000	-2.277202000	H	4.318341000	-1.643509000	2.360124000
C	2.994837000	0.391280000	-2.701145000	C	2.410024000	-0.559002000	2.659552000
H	2.497475000	1.342284000	-2.930286000	H	1.856569000	-1.463660000	2.945247000
H	3.280579000	-0.090144000	-3.642661000	H	2.701384000	-0.026194000	3.570117000
N	2.065999000	-0.450804000	-1.951549000	N	1.558713000	0.268102000	1.814318000
C	2.350664000	-1.804620000	-1.993590000	C	1.789701000	1.632374000	1.938111000
O	3.290853000	-2.293476000	-2.641677000	O	2.626966000	2.124950000	2.711244000
N	1.464756000	-2.587877000	-1.276077000	N	0.969192000	2.427754000	1.157254000
H	0.882446000	-2.062721000	-0.636569000	H	0.458100000	1.926621000	0.440015000
C	1.889408000	-3.890930000	-0.791715000	C	1.400676000	3.771491000	0.808894000
P	-2.081428000	-0.416590000	-0.548700000	P	-1.789096000	0.501018000	1.470877000
C	-6.249209000	-0.059284000	-2.688636000	C	-3.223477000	3.724536000	-1.568223000
C	-5.359297000	-1.069787000	-3.057198000	C	-3.325216000	2.368858000	-1.888967000
C	-4.145821000	-1.221687000	-2.383034000	C	-2.941839000	1.395587000	-0.966730000
C	-3.791851000	-0.373486000	-1.317120000	C	-2.457030000	1.755706000	0.303334000
C	-4.695936000	0.651631000	-0.972237000	C	-2.344196000	3.124099000	0.606038000
C	-5.908863000	0.802496000	-1.641301000	C	-2.727280000	4.097817000	-0.317769000
H	-7.194236000	0.058644000	-3.212414000	H	-3.513408000	4.482145000	-2.291352000
H	-5.610754000	-1.746123000	-3.870980000	H	-3.695615000	2.066360000	-2.865098000
H	-3.469152000	-2.014375000	-2.691293000	H	-3.017024000	0.346150000	-1.232128000
H	-4.448796000	1.328585000	-0.158582000	H	-1.927879000	3.435485000	1.559266000
H	-6.592840000	1.593919000	-1.343897000	H	-2.627262000	5.149695000	-0.062360000
C	-3.250312000	0.141797000	3.942014000	H	-0.425674000	3.010868000	-3.437599000
C	-2.227294000	0.908295000	3.383050000	H	-0.194515000	3.736222000	-1.837771000
C	-1.879849000	0.751093000	2.039318000	H	1.151403000	3.724705000	-3.004373000
C	-2.558442000	-0.174336000	1.229410000	H	-2.461950000	-1.595563000	-3.322812000
C	-3.596116000	-0.930351000	1.802173000	H	-1.859950000	-3.273612000	-3.318934000
C	-3.936576000	-0.779565000	3.146707000	H	-2.930046000	-2.715464000	-2.019018000
H	-3.512176000	0.259504000	4.990494000	H	0.525727000	4.369040000	0.530696000
H	-1.687363000	1.628388000	3.991558000	H	1.879360000	4.218873000	1.681656000
H	-1.064702000	1.326913000	1.618520000	H	2.109691000	3.777023000	-0.030206000
H	-4.145835000	-1.638849000	1.188728000	C	-2.792453000	-1.008908000	1.120495000
H	-4.735622000	-1.381096000	3.573044000	C	-2.115431000	-2.215169000	0.887089000
C	-1.754686000	-2.236250000	-0.596752000	C	-4.197872000	-1.010010000	1.099837000
H	-1.068312000	-2.473643000	0.218101000	C	-2.823587000	-3.394079000	0.639806000
H	-2.674290000	-2.816252000	-0.476357000	H	-1.031146000	-2.227881000	0.856123000
H	-1.264011000	-2.511563000	-1.533877000	C	-4.907186000	-2.187170000	0.860960000
H	-1.120564000	-2.489787000	2.955363000	H	-4.739467000	-0.080085000	1.254015000
H	0.408767000	-3.329870000	3.347546000	C	-4.218961000	-3.382623000	0.629595000
H	0.027419000	-1.773253000	4.104931000	H	-2.275309000	-4.304029000	0.413975000
H	-1.890278000	4.547261000	-0.417545000	H	-5.994380000	-2.171134000	0.842805000
H	-2.7211103000	3.116733000	-1.088162000	H	-4.770498000	-4.297533000	0.427537000
H	-2.475099000	3.273808000	0.666599000	C	-2.626432000	1.071832000	3.058460000
H	1.020391000	-4.551021000	-0.691146000	H	-2.470670000	0.299160000	3.817311000
H	2.578093000	-4.318165000	-1.522252000	H	-2.138716000	1.985429000	3.409972000
H	2.390164000	-3.826494000	0.184018000	H	-3.700984000	1.258422000	2.952678000
⁶P₁				⁴P₁			
Mn	1.392815000	-0.342213000	0.322988000	Mn	-1.381164000	-0.016195000	0.590147000
O	-0.824883000	-0.346176000	-0.069532000	O	0.603017000	0.365914000	0.075416000
N	3.713528000	-0.403318000	0.841010000	N	-3.376085000	-0.454841000	1.179871000
C	4.293555000	-1.032437000	-0.359883000	C	-4.093044000	0.844287000	1.086256000
H	4.171192000	-2.114899000	-0.257654000	H	-3.827930000	1.426974000	1.974044000
H	5.376569000	-0.822895000	-0.433221000	H	-5.184224000	0.681991000	1.092743000
C	3.574118000	-0.600816000	-1.649357000	C	-3.636394000	1.622533000	-0.150902000
H	3.726607000	0.480363000	-1.795991000	H	-3.951689000	1.083244000	-1.058053000
H	4.037288000	-1.111610000	-2.501229000	H	-4.130717000	2.600609000	-0.167751000
N	2.146038000	-0.904694000	-1.584267000	N	-2.184528000	1.761759000	-0.118906000
C	1.655331000	-1.641122000	-2.615825000	C	-1.728005000	3.027086000	-0.330318000

O	2.276281000	-2.074536000	-3.601654000	O	-2.408089000	4.040788000	-0.570463000
N	0.257580000	-1.875414000	-2.524244000	N	-0.317305000	3.138162000	-0.286509000
H	-0.100697000	-1.772653000	-1.582478000	H	0.111907000	2.375460000	0.221785000
C	-0.278945000	-3.009324000	-3.254576000	C	0.242498000	4.449765000	-0.020946000
C	3.784068000	-1.234327000	2.057412000	C	-3.315900000	-0.983522000	2.574082000
H	3.636853000	-0.570925000	2.915268000	H	-3.214181000	-2.069746000	2.504146000
H	4.780056000	-1.704012000	2.160427000	H	-4.254267000	-0.757043000	3.106752000
C	2.666982000	-2.287994000	2.094689000	C	-2.077247000	-0.452196000	3.292268000
H	2.828625000	-3.012296000	1.278659000	H	-2.193266000	0.630658000	3.474398000
H	2.728072000	-2.845358000	3.036673000	H	-1.971664000	-0.932709000	4.272230000
N	1.367596000	-1.644389000	1.958384000	N	-0.930665000	-0.727358000	2.438499000
C	0.462952000	-1.943438000	2.928394000	C	0.120371000	-1.341524000	3.043717000
O	0.602390000	-2.757787000	3.861005000	O	0.261398000	-1.549124000	4.265072000
N	-0.729201000	-1.197884000	2.836755000	N	1.085857000	-1.810737000	2.140820000
H	-0.888461000	-0.775199000	1.931665000	H	0.999100000	-1.428441000	1.212254000
C	-1.902570000	-1.675449000	3.531933000	C	2.413975000	-2.136936000	2.602033000
C	4.119391000	1.001678000	1.057545000	C	-3.937516000	-1.478337000	0.244761000
H	4.518981000	1.402455000	0.121782000	H	-4.439546000	-0.966293000	-0.578793000
H	4.920662000	1.067056000	1.813489000	H	-4.689729000	-2.085726000	0.772046000
C	2.897303000	1.866238000	1.432755000	C	-2.799858000	-2.309125000	-0.370004000
H	2.478688000	1.514946000	2.385340000	H	-2.259927000	-2.846653000	0.420753000
H	3.218347000	2.908047000	1.556054000	H	-3.230494000	-3.040728000	-1.065895000
N	1.883867000	1.724668000	0.390250000	N	-1.886065000	-1.381574000	-1.024779000
C	2.078070000	2.546945000	-0.676351000	C	-2.285905000	-1.024818000	-2.273644000
O	2.792654000	3.564112000	-0.716750000	O	-3.129755000	-1.600078000	-2.987084000
N	1.343559000	2.154228000	-1.830084000	N	-1.621748000	0.135700000	-2.758899000
H	1.375054000	1.138416000	-1.942078000	H	-1.535328000	0.817044000	-2.002544000
C	1.679563000	2.856656000	-3.060556000	C	-2.175528000	0.723355000	-3.969740000
P	-1.975591000	0.434189000	-0.665378000	P	1.747445000	0.328559000	-0.905888000
C	-2.753902000	4.205849000	1.860415000	C	2.792430000	-4.064561000	-1.809156000
C	-1.457669000	3.745074000	1.620401000	C	1.466071000	-3.644214000	-1.690265000
C	-1.244834000	2.593892000	0.861322000	C	1.166374000	-2.307736000	-1.423323000
C	-2.349290000	1.901434000	0.331824000	C	2.217263000	-1.383010000	-1.277437000
C	-3.651578000	2.361038000	0.581575000	C	3.550420000	-1.807609000	-1.390791000
C	-3.851254000	3.512567000	1.343125000	C	3.835290000	-3.146271000	-1.659293000
H	-2.911616000	5.101186000	2.456434000	H	3.016543000	-5.109136000	-2.010360000
H	-0.600761000	4.275450000	2.025317000	H	0.653180000	-4.356846000	-1.795952000
H	-0.223808000	2.239006000	0.698171000	H	0.122039000	-1.993611000	-1.305949000
H	-4.509003000	1.815248000	0.198849000	H	4.363797000	-1.101282000	-1.251015000
H	-4.861213000	3.862397000	1.539739000	H	4.868319000	-3.474204000	-1.739109000
C	-5.650499000	-2.364536000	-0.627691000	C	5.299425000	2.342572000	1.245286000
C	-4.503220000	-2.664259000	0.109518000	C	4.203295000	1.849579000	1.957101000
C	-3.405929000	-1.803195000	0.078069000	C	3.140938000	1.250123000	1.280615000
C	-3.452308000	-0.629577000	-0.691143000	C	3.171896000	1.138383000	-0.119708000
C	-4.605147000	-0.340522000	-1.438321000	C	4.273093000	1.641732000	-0.829101000
C	-5.700865000	-1.203082000	-1.403210000	C	5.334032000	2.239443000	-0.147595000
H	-6.503592000	-3.037228000	-0.603645000	H	6.125089000	2.810946000	1.774334000
H	-4.457937000	-3.568785000	0.708866000	H	4.171829000	1.931482000	3.039552000
H	-2.505804000	-2.033191000	0.639316000	H	2.281201000	0.866699000	1.822476000
H	-4.651012000	0.555536000	-2.051524000	H	4.304879000	1.574276000	-1.913218000
H	-6.589539000	-0.973569000	-1.984663000	H	6.182690000	2.629795000	-0.702595000
C	-1.656476000	0.983195000	-2.351193000	C	1.411167000	1.158546000	-2.468356000
H	-1.262685000	0.129443000	-2.914629000	H	1.062258000	2.172024000	-2.245051000
H	-2.550025000	1.396618000	-2.827018000	H	2.287381000	1.170767000	-3.122763000
H	-0.868976000	1.743682000	-2.288414000	H	0.584583000	0.609642000	-2.938586000
H	-1.372275000	-2.936670000	-3.295795000	H	1.320563000	4.434342000	-0.220679000
H	0.122804000	-2.987152000	-4.268976000	H	-0.237136000	5.174085000	-0.681698000
H	-0.014570000	-3.986204000	-2.815899000	H	0.089168000	4.798565000	1.014444000
H	-2.638318000	-0.867300000	3.619920000	H	2.903432000	-2.803111000	1.882272000
H	-2.400639000	-2.535371000	3.044645000	H	3.070692000	-1.259695000	2.747815000
H	-1.604486000	-2.002326000	4.529767000	H	2.325948000	-2.643929000	3.564931000
H	1.014744000	2.511680000	-3.860533000	H	-1.538430000	1.557444000	-4.285437000

H	1.539771000	3.930094000	-2.915393000	H	-2.199288000	-0.030535000	-4.759575000
H	2.721204000	2.704304000	-3.379690000	H	-3.202994000	1.097072000	-3.844765000
²P₁				⁶RC₂			
Mn	-1.419135000	-0.314137000	-0.381575000	Mn	-0.568779000	-0.534363000	-0.016486000
O	0.646082000	-0.127579000	-0.030393000	O	-0.670600000	0.380016000	1.458300000
N	-3.495523000	-0.498334000	-0.821475000	N	-0.698575000	-1.709849000	-1.876880000
C	-4.115561000	-1.101669000	0.387877000	C	0.610078000	-2.407916000	-1.884844000
H	-3.939014000	-2.179859000	0.348254000	H	1.371341000	-1.647862000	-2.084667000
H	-5.205643000	-0.932107000	0.384859000	H	0.648915000	-3.156252000	-2.694653000
C	-3.443979000	-0.561121000	1.652802000	C	0.899587000	-3.038586000	-0.524723000
H	-3.659741000	0.513181000	1.749821000	H	0.331905000	-3.978223000	-0.407105000
H	-3.857238000	-1.066047000	2.532885000	H	1.953387000	-3.337693000	-0.498749000
N	-2.006008000	-0.778042000	1.541687000	N	0.585590000	-2.082725000	0.527639000
C	-1.471572000	-1.603922000	2.483264000	C	1.239849000	-2.328657000	1.715867000
O	-2.048098000	-2.095288000	3.469993000	O	2.096219000	-3.228055000	1.860131000
N	-0.093059000	-1.870019000	2.289028000	N	0.886143000	-1.495476000	2.752412000
H	0.185723000	-1.749030000	1.323356000	H	0.294226000	-0.692197000	2.492830000
C	0.455851000	-3.048184000	2.935144000	C	1.695487000	-1.441673000	3.943401000
C	-3.595456000	-1.389384000	-2.006202000	C	-0.852649000	-0.770043000	-3.020087000
H	-3.435899000	-0.766891000	-2.891629000	H	-1.918303000	-0.668156000	-3.234930000
H	-4.603175000	-1.835365000	-2.071516000	H	-0.364830000	-1.179886000	-3.917819000
C	-2.487095000	-2.439359000	-1.973007000	C	-0.312370000	0.609927000	-2.638812000
H	-2.663143000	-3.140921000	-1.141411000	H	0.787934000	0.577910000	-2.592001000
H	-2.504402000	-3.028501000	-2.897286000	H	-0.598221000	1.349396000	-3.394523000
N	-1.220132000	-1.736944000	-1.808128000	N	-0.846287000	0.962636000	-1.335007000
C	-0.249648000	-2.108757000	-2.696527000	C	-1.521129000	2.166702000	-1.243669000
O	-0.300972000	-3.066244000	-3.492182000	O	-1.783218000	2.907121000	-2.206821000
N	0.867458000	-1.266204000	-2.706533000	N	-1.878777000	2.475677000	0.049713000
H	0.940449000	-0.635958000	-1.920078000	H	-1.422389000	1.898052000	0.768906000
C	2.077018000	-1.674952000	-3.377969000	C	-2.377299000	3.787131000	0.371961000
C	-4.039163000	0.863277000	-1.109818000	C	-1.842435000	-2.643910000	-1.757132000
H	-4.488955000	1.262972000	-0.197591000	H	-1.562720000	-3.407757000	-1.030509000
H	-4.828321000	0.802858000	-1.875599000	H	-2.039473000	-3.143952000	-2.718891000
C	-2.883793000	1.797285000	-1.490375000	C	-3.099148000	-1.937588000	-1.239401000
H	-2.435367000	1.470061000	-2.438693000	H	-3.553885000	-1.284624000	-1.999995000
H	-3.258849000	2.820386000	-1.615432000	H	-3.881863000	-2.670506000	-0.993439000
N	-1.894408000	1.696807000	-0.422863000	N	-2.738989000	-1.146900000	-0.094724000
C	-2.108107000	2.567212000	0.602913000	C	-3.813075000	-0.591666000	0.619788000
O	-2.809041000	3.596303000	0.573911000	O	-5.001894000	-0.708806000	0.299468000
N	-1.420085000	2.213340000	1.787158000	N	-3.349158000	0.077883000	1.710343000
H	-1.393373000	1.195285000	1.890981000	H	-2.302470000	0.205454000	1.777709000
C	-1.822396000	2.910579000	2.997315000	C	-4.253109000	0.850265000	2.522583000
P	1.809051000	0.566615000	0.632724000	H	1.090518000	-1.102818000	4.792155000
C	2.798524000	4.321158000	-1.841952000	H	2.087801000	-2.438958000	4.155857000
C	1.483705000	3.886343000	-1.659723000	H	2.560290000	-0.758991000	3.855527000
C	1.215653000	2.736245000	-0.916480000	H	-3.009132000	3.738870000	1.266791000
C	2.283035000	2.021015000	-0.341737000	H	-1.574552000	4.520160000	0.562399000
C	3.603305000	2.453285000	-0.534398000	H	-2.969799000	4.158574000	-0.467193000
C	3.858638000	3.602646000	-1.283133000	H	-3.820234000	0.992195000	3.516911000
H	2.999798000	5.215759000	-2.425947000	H	-4.446007000	1.839912000	2.081401000
H	0.657272000	4.437900000	-2.098617000	H	-5.212479000	0.331089000	2.602805000
H	0.186258000	2.387557000	-0.793514000	P	2.883842000	2.844726000	0.746291000
H	4.432588000	1.887136000	-0.120578000	C	3.259622000	1.255906000	-0.125899000
H	4.882977000	3.931731000	-1.436782000	C	3.285076000	0.017466000	0.533881000
C	5.252866000	-2.510781000	0.797946000	C	3.631273000	1.284196000	-1.484699000
C	4.076638000	-2.779370000	0.095678000	C	3.685939000	-1.147686000	-0.124435000
C	3.055248000	-1.829355000	0.048119000	H	2.956584000	-0.063452000	1.563579000
C	3.206457000	-0.598347000	0.706125000	C	4.009665000	0.120286000	-2.152990000
C	4.386001000	-0.342266000	1.423944000	H	3.624742000	2.226028000	-2.028815000
C	5.407026000	-1.291611000	1.463466000	C	4.048868000	-1.100404000	-1.470416000
H	6.046696000	-3.252041000	0.833944000	H	3.662165000	-2.085976000	0.421586000
H	3.948147000	-3.728502000	-0.416064000	H	4.281241000	0.167408000	-3.205278000

H	2.136627000	-2.032895000	-0.493231000	H	4.349097000	-2.008258000	-1.988044000
H	4.509066000	0.594096000	1.961842000	C	1.872942000	2.266457000	2.189383000
H	6.316924000	-1.085038000	2.020293000	H	2.508887000	1.767614000	2.927917000
C	1.515370000	1.112787000	2.323433000	H	1.451920000	3.154426000	2.674943000
H	1.119414000	0.252313000	2.874096000	H	1.050494000	1.597604000	1.897333000
H	2.432328000	1.489279000	2.785868000	C	1.512740000	3.477524000	-0.337335000
H	0.750012000	1.894826000	2.282700000	H	1.042540000	4.344003000	0.139422000
H	1.547029000	-3.040109000	2.832119000	H	1.900590000	3.803705000	-1.306343000
H	0.191618000	-3.024761000	3.993903000	H	0.760455000	2.704003000	-0.494968000
H	0.075082000	-3.997280000	2.523188000				
H	2.691917000	-0.796064000	-3.604210000				
H	2.701358000	-2.380253000	-2.799546000				
H	1.804229000	-2.173803000	-4.310055000				
H	-1.148925000	2.629288000	3.815227000				
H	-1.758361000	3.988263000	2.832605000				
H	-2.855353000	2.688450000	3.307389000				
⁴RC₂				²RC₂			
Mn	-0.688307000	-0.525200000	-0.063871000	Mn	-1.155352000	-0.008986000	-0.057390000
O	-0.634808000	0.054295000	1.513532000	O	-1.129874000	0.743542000	1.427620000
N	-0.638644000	-1.241294000	-2.173630000	N	-1.061290000	-0.908447000	-2.215309000
C	0.418546000	-2.272027000	-2.209489000	C	-0.570848000	-2.285631000	-2.030635000
H	1.375134000	-1.745643000	-2.254828000	H	0.519968000	-2.253099000	-1.985150000
H	0.323175000	-2.902205000	-3.109372000	H	-0.861606000	-2.931615000	-2.875416000
C	0.383740000	-3.095916000	-0.930983000	C	-1.090798000	-2.811395000	-0.703084000
H	-0.488568000	-3.769789000	-0.932632000	H	-2.178390000	-2.969929000	-0.757051000
H	1.270221000	-3.735412000	-0.879551000	H	-0.629684000	-3.770987000	-0.456898000
N	0.332195000	-2.197731000	0.219924000	N	-0.786844000	-1.827367000	0.332382000
C	1.053477000	-2.664945000	1.315633000	C	-0.269396000	-2.362776000	1.510808000
O	1.871314000	-3.604364000	1.250711000	O	-0.002103000	-3.573567000	1.640085000
N	0.825988000	-1.996463000	2.488513000	N	-0.017032000	-1.478304000	2.523423000
H	0.253370000	-1.148424000	2.400880000	H	-0.358543000	-0.520865000	2.401632000
C	1.723331000	-2.167761000	3.605749000	C	0.427607000	-1.958919000	3.808914000
C	-0.337472000	-0.076919000	-3.048274000	C	-0.114335000	-0.061860000	-2.969115000
H	-1.274628000	0.354882000	-3.402168000	H	-0.666024000	0.777579000	-3.401038000
H	0.252936000	-0.395986000	-3.919413000	H	0.350232000	-0.628063000	-3.792490000
C	0.362019000	0.975757000	-2.192595000	C	0.901127000	0.486522000	-1.975824000
H	1.370607000	0.645022000	-1.921716000	H	1.506191000	-0.327676000	-1.567891000
H	0.444202000	1.917979000	-2.744409000	H	1.570504000	1.204809000	-2.454168000
N	-0.404074000	1.168508000	-0.968052000	N	0.161006000	1.129519000	-0.898627000
C	-1.422416000	2.110282000	-1.030410000	C	0.297371000	2.500499000	-0.809280000
O	-1.789720000	2.664735000	-2.078096000	O	1.044965000	3.167206000	-1.555266000
N	-1.956529000	2.413896000	0.202111000	N	-0.437364000	3.110829000	0.182677000
H	-1.650673000	1.796139000	0.950132000	H	-0.818489000	2.475079000	0.884120000
C	-3.283226000	2.994812000	0.293806000	C	-0.108916000	4.462948000	0.569459000
C	-2.003084000	-1.768589000	-2.394338000	C	-2.444048000	-0.831576000	-2.721822000
H	-2.059089000	-2.763261000	-1.946211000	H	-2.982345000	-1.726238000	-2.396596000
H	-2.216209000	-1.859406000	-3.470703000	H	-2.464834000	-0.800547000	-3.823103000
C	-2.998125000	-0.859813000	-1.688356000	C	-3.107514000	0.384612000	-2.087513000
H	-3.041320000	0.126939000	-2.172643000	H	-2.637784000	1.305024000	-2.461577000
H	-4.004278000	-1.284367000	-1.743276000	H	-4.174268000	0.420376000	-2.322387000
N	-2.586130000	-0.742650000	-0.290733000	N	-2.910411000	0.292979000	-0.646103000
C	-3.623676000	-0.409784000	0.577416000	C	-4.069563000	0.373370000	0.129541000
O	-4.795623000	-0.276729000	0.181731000	O	-5.207615000	0.459912000	-0.358440000
N	-3.293308000	-0.288038000	1.902060000	N	-3.865716000	0.335582000	1.486013000
H	-2.292327000	-0.198115000	2.093990000	H	-2.907869000	0.529262000	1.789165000
C	-4.250119000	0.270620000	2.828121000	C	-4.966833000	0.622881000	2.374891000
H	1.229346000	-1.835186000	4.524309000	H	0.853322000	-1.123643000	4.374445000
H	1.990888000	-3.222701000	3.701371000	H	-0.381881000	-2.405355000	4.407014000
H	2.662593000	-1.598764000	3.497425000	H	1.194151000	-2.727192000	3.672989000
H	-4.078825000	2.240099000	0.224525000	H	-0.948883000	4.900231000	1.119487000
H	-3.386690000	3.529192000	1.244678000	H	0.790527000	4.525559000	1.205370000
H	-3.405160000	3.705220000	-0.526041000	H	0.083383000	5.057164000	-0.326229000

H	-4.004680000	-0.048827000	3.846574000	H	-4.724080000	0.263564000	3.380366000
H	-4.275666000	1.372722000	2.809456000	H	-5.205694000	1.697166000	2.438547000
H	-5.249399000	-0.086173000	2.570295000	H	-5.863647000	0.111113000	2.017948000
P	2.992822000	2.624188000	1.365373000	P	3.873745000	1.232341000	1.378117000
C	3.345799000	1.251670000	0.171505000	C	3.636031000	-0.225870000	0.263484000
C	3.070963000	-0.098620000	0.435933000	C	2.807409000	-1.293409000	0.650635000
C	3.985022000	1.568482000	-1.042969000	C	4.345036000	-0.351063000	-0.945309000
C	3.428138000	-1.102151000	-0.470287000	C	2.682967000	-2.440572000	-0.136367000
H	2.545249000	-0.385927000	1.338265000	H	2.212640000	-1.226962000	1.554212000
C	4.320845000	0.575321000	-1.961497000	C	4.216765000	-1.491176000	-1.739807000
H	4.218973000	2.606092000	-1.274354000	H	4.992467000	0.453618000	-1.283816000
C	4.050977000	-0.767031000	-1.672983000	C	3.387676000	-2.542250000	-1.337904000
H	3.2001138000	-2.134416000	-0.220925000	H	2.014909000	-3.230409000	0.195790000
H	4.800866000	0.846498000	-2.898998000	H	4.762339000	-1.555637000	-2.678504000
H	4.324652000	-1.544504000	-2.382123000	H	3.287334000	-3.429175000	-1.958644000
C	1.920448000	1.785325000	2.623516000	C	2.171450000	1.421263000	2.096956000
H	2.510594000	1.087355000	3.226352000	H	2.011452000	0.692329000	2.896132000
H	1.533885000	2.554972000	3.300742000	H	2.098361000	2.418995000	2.543554000
H	1.072996000	1.253846000	2.172568000	H	1.374839000	1.300409000	1.358842000
C	1.678177000	3.533205000	0.414106000	C	3.876667000	2.640990000	0.164909000
H	1.303382000	4.368080000	1.015671000	H	3.887323000	3.575828000	0.736693000
H	2.102411000	3.947343000	-0.505744000	H	4.795453000	2.622487000	-0.429895000
H	0.851257000	2.865310000	0.158043000	H	3.009720000	2.656510000	-0.503266000
⁶TS₂				⁴TS₂			
Mn	-0.778251000	-0.290010000	-0.123675000	Mn	0.405224000	0.452885000	-0.275583000
O	0.026021000	0.322452000	1.321358000	O	0.097415000	-0.046694000	1.355362000
N	-1.722353000	-1.007652000	-1.914907000	N	0.627815000	1.063395000	-2.349801000
C	-3.164316000	-1.101561000	-1.564101000	C	2.004141000	1.616112000	-2.446109000
H	-3.263592000	-1.924397000	-0.854799000	H	1.985102000	2.622252000	-2.024116000
H	-3.761029000	-1.339862000	-2.459494000	H	2.309785000	1.683678000	-3.501832000
C	-3.650521000	0.182783000	-0.888821000	C	2.969428000	0.768505000	-1.623018000
H	-3.799964000	0.990494000	-1.622628000	H	3.107740000	-0.221818000	-2.086115000
H	-4.651767000	-0.000441000	-0.467509000	H	3.957488000	1.245061000	-1.622529000
N	-2.691784000	0.564956000	0.126912000	N	2.438279000	0.658578000	-0.273472000
C	-3.055160000	1.686915000	0.838807000	C	3.359814000	0.266519000	0.660784000
O	-4.050253000	2.389260000	0.587026000	O	4.560824000	0.044260000	0.403771000
N	-2.209637000	1.953917000	1.899989000	N	2.874265000	0.155439000	1.957789000
H	-1.352699000	1.388455000	1.938619000	H	1.860684000	0.116870000	2.039747000
C	-2.253049000	3.236125000	2.554786000	C	3.660588000	-0.517408000	2.964047000
C	-1.093841000	-2.328401000	-2.159491000	C	-0.431834000	2.074730000	-2.569014000
H	-0.068276000	-2.129328000	-2.482023000	H	-1.379234000	1.529715000	-2.621571000
H	-1.613821000	-2.859001000	-2.974356000	H	-0.277581000	2.594448000	-3.528928000
C	-1.059351000	-3.159266000	-0.878972000	C	-0.493234000	3.049939000	-1.401842000
H	-2.028337000	-3.652245000	-0.704085000	H	0.337418000	3.771952000	-1.449352000
H	-0.345044000	-3.985714000	-1.017524000	H	-1.404262000	3.657428000	-1.491849000
N	-0.685831000	-2.294722000	0.229693000	N	-0.480674000	2.292317000	-0.157080000
C	-0.588954000	-2.971164000	1.417818000	C	-0.802253000	3.074969000	0.925694000
O	-0.818576000	-4.188629000	1.544612000	O	-1.050887000	4.291903000	0.855776000
N	-0.164035000	-2.197015000	2.493304000	N	-0.893318000	2.394832000	2.137753000
H	-0.176020000	-1.184568000	2.318319000	H	-0.442856000	1.476052000	2.127560000
C	-0.394979000	-2.672018000	3.837940000	C	-0.846605000	3.160802000	3.364394000
C	-1.460177000	-0.054630000	-3.021423000	C	0.433698000	-0.138633000	-3.208761000
H	-2.197613000	0.746030000	-2.952451000	H	1.401504000	-0.613232000	-3.375094000
H	-1.584798000	-0.557046000	-3.993832000	H	0.011614000	0.154008000	-4.182334000
C	-0.069205000	0.564961000	-2.870142000	C	-0.432562000	-1.131982000	-2.435768000
H	0.707294000	-0.188436000	-3.067539000	H	-1.449102000	-0.744911000	-2.306416000
H	0.070145000	1.373777000	-3.595896000	H	-0.489980000	-2.081368000	-2.978487000
N	0.052189000	1.049200000	-1.510181000	N	0.161867000	-1.316751000	-1.116305000
C	0.544159000	2.327393000	-1.373943000	C	1.174122000	-2.267762000	-1.071952000
O	0.894788000	3.080021000	-2.299212000	O	1.577610000	-2.891483000	-2.067573000
N	0.637224000	2.705864000	-0.049082000	N	1.666844000	-2.511614000	0.192246000
H	0.319127000	2.021857000	0.646758000	H	1.361586000	-1.852657000	0.899076000

C	0.912984000	4.068869000	0.319675000	C	2.984447000	-3.101876000	0.353199000	
P	2.501359000	0.825392000	1.452710000	P	-1.535829000	-1.732037000	1.698270000	
C	3.051560000	-1.599661000	-2.478452000	C	-4.284635000	-0.297867000	-1.781383000	
C	3.371870000	-0.239966000	-2.432446000	C	-4.074622000	-1.665052000	-1.578961000	
C	3.209381000	0.477689000	-1.248616000	C	-3.281193000	-2.106201000	-0.519878000	
C	2.748289000	-0.151756000	-0.078090000	C	-2.688297000	-1.193173000	0.371266000	
C	2.395835000	-1.510437000	-0.147555000	C	-2.902724000	0.179347000	0.151597000	
C	2.551742000	-2.226830000	-1.334873000	C	-3.690398000	0.619916000	-0.913884000	
H	3.171509000	-2.159281000	-3.402939000	H	-4.896196000	0.045543000	-2.611954000	
H	3.724385000	0.270222000	-3.324788000	H	-4.521820000	-2.391222000	-2.253455000	
H	3.411967000	1.544610000	-1.251602000	H	-3.115936000	-3.172453000	-0.401371000	
H	1.955136000	-2.004625000	0.709281000	H	-2.434440000	0.914701000	0.793517000	
H	2.263671000	-3.274288000	-1.362920000	H	-3.825140000	1.687902000	-1.062774000	
C	4.197025000	1.643021000	1.557960000	C	-2.226560000	-3.432928000	2.098321000	
H	4.279130000	2.148518000	2.526394000	H	-1.792812000	-3.755488000	3.050698000	
H	5.022856000	0.928437000	1.459041000	H	-3.320187000	-3.449393000	2.182310000	
H	4.293904000	2.404626000	0.779249000	H	-1.911159000	-4.152891000	1.338047000	
H	-1.924166000	3.141912000	3.596446000	H	3.434663000	-1.594824000	3.043258000	
H	-1.616319000	3.993768000	2.065879000	H	4.713627000	-0.417044000	2.694410000	
H	-3.281254000	3.604660000	2.531659000	H	3.496894000	-0.064794000	3.950114000	
H	-0.261277000	-3.755963000	3.854098000	H	-1.493809000	4.034635000	3.262990000	
H	0.323838000	-2.210608000	4.526248000	H	-1.204298000	2.542094000	4.195444000	
H	-1.409929000	-2.453085000	4.210054000	H	0.163727000	3.523570000	3.615139000	
H	1.395354000	4.091863000	1.301657000	H	3.044956000	-3.605924000	1.324701000	
H	1.572872000	4.514753000	-0.428910000	H	3.126422000	-3.840531000	-0.437667000	
H	-0.002431000	4.679773000	0.366693000	H	3.788487000	-2.356470000	0.293129000	
C	2.728591000	-0.426591000	2.792178000	C	-2.190908000	-0.809995000	3.165050000	
H	2.729715000	0.092352000	3.756383000	H	-1.586128000	-1.059623000	4.043108000	
H	1.901158000	-1.138144000	2.782266000	H	-2.099087000	0.262953000	2.987023000	
H	3.674609000	-0.969199000	2.681657000	H	-3.238559000	-1.054820000	3.371821000	
²T_{S2}								
Mn	0.368703000	0.375975000	-0.352121000	⁶P₂	Mn	-0.846085000	0.405019000	-0.396751000
O	-0.120162000	0.156685000	1.279621000	O	0.832939000	-0.881613000	-1.292668000	
N	0.613511000	0.633088000	-2.511760000	N	-2.571705000	1.925082000	0.357644000	
C	2.030051000	1.020561000	-2.705912000	C	-3.782469000	1.109071000	0.169437000	
H	2.115657000	2.088439000	-2.497160000	H	-4.065444000	1.182367000	-0.885458000	
H	2.346713000	0.841408000	-3.745579000	H	-4.625733000	1.498753000	0.769767000	
C	2.889122000	0.262884000	-1.702179000	C	-3.552505000	-0.377681000	0.488482000	
H	2.943669000	-0.803511000	-1.971648000	H	-3.310052000	-0.475811000	1.558912000	
H	3.915004000	0.644331000	-1.715048000	H	-4.487924000	-0.923584000	0.320240000	
N	2.286010000	0.441008000	-0.386390000	N	-2.477367000	-0.943268000	-0.324952000	
C	3.161359000	0.330569000	0.667073000	C	-2.751793000	-2.136132000	-0.915526000	
O	4.384336000	0.129762000	0.529718000	O	-3.816675000	-2.776249000	-0.870613000	
N	2.606716000	0.465386000	1.930634000	N	-1.643827000	-2.686429000	-1.611501000	
H	1.592703000	0.389971000	1.985035000	H	-0.937203000	-2.000514000	-1.850621000	
C	3.381689000	0.075626000	3.086145000	C	-1.922844000	-3.662414000	-2.647007000	
C	-0.348905000	1.688114000	-2.882282000	C	-2.472133000	3.089439000	-0.541322000	
H	-1.343912000	1.234092000	-2.837613000	H	-1.770889000	3.802339000	-0.099549000	
H	-0.174419000	2.041670000	-3.912695000	H	-3.448816000	3.596708000	-0.649483000	
C	-0.287746000	2.822095000	-1.876012000	C	-1.879187000	2.686723000	-1.902849000	
H	0.607629000	3.443703000	-2.033309000	H	-2.567064000	2.001367000	-2.417510000	
H	-1.138641000	3.496247000	-2.034337000	H	-1.774033000	3.591180000	-2.516107000	
N	-0.314826000	2.245633000	-0.536424000	N	-0.603326000	2.008521000	-1.720479000	
C	-0.557778000	3.214809000	0.418458000	C	0.464202000	2.843468000	-1.605731000	
O	-0.715285000	4.418233000	0.145663000	O	0.459865000	4.086909000	-1.683902000	
N	-0.688317000	2.772356000	1.727380000	N	1.662168000	2.155314000	-1.327825000	
H	-0.327918000	1.839152000	1.901572000	H	1.641140000	1.178663000	-1.589834000	
C	-0.623071000	3.737887000	2.801852000	C	2.929900000	2.835984000	-1.441202000	
C	0.275338000	-0.663312000	-3.159381000	C	-2.232182000	2.235810000	1.761101000	
H	1.191348000	-1.233087000	-3.319657000	H	-2.772046000	1.551126000	2.421352000	
H	-0.203482000	-0.491013000	-4.135379000	H	-2.543853000	3.261324000	2.022488000	
C	-0.594820000	-1.461944000	-2.186264000	C	-0.725912000	2.008982000	2.008053000	

H	-1.572338000	-0.986310000	-2.051365000	H	-0.140917000	2.673380000	1.358450000
H	-0.753753000	-2.476305000	-2.568265000	H	-0.491432000	2.245442000	3.053351000
N	0.097842000	-1.472544000	-0.901760000	N	-0.404419000	0.622206000	1.675795000
C	1.100286000	-2.435685000	-0.816248000	C	-0.680680000	-0.255021000	2.678000000
O	1.425264000	-3.180738000	-1.755621000	O	-0.868739000	0.013402000	3.877786000
N	1.692461000	-2.534503000	0.423830000	N	-0.730572000	-1.606947000	2.241181000
H	1.420484000	-1.817101000	1.082545000	H	-1.190390000	-1.670245000	1.331290000
C	3.026296000	-3.090811000	0.564257000	C	-1.249912000	-2.572536000	3.197797000
P	-1.320286000	-1.417712000	1.834295000	P	1.927687000	-1.791818000	-0.776563000
C	-4.521700000	-0.411873000	-1.413016000	C	5.023054000	0.714043000	1.546901000
C	-4.253734000	-1.743258000	-1.085659000	C	3.652478000	0.876823000	1.758404000
C	-3.331760000	-2.050930000	-0.084157000	C	2.729480000	0.100017000	1.057635000
C	-2.653067000	-1.038162000	0.616562000	C	3.188060000	-0.857848000	0.133922000
C	-2.937277000	0.299062000	0.278225000	C	4.567533000	-1.017568000	-0.075881000
C	-3.858264000	0.605974000	-0.724577000	C	5.481739000	-0.235054000	0.629858000
H	-5.233865000	-0.172292000	-2.198790000	H	5.735095000	1.329028000	2.091326000
H	-4.755101000	-2.547627000	-1.618807000	H	3.288604000	1.618884000	2.462664000
H	-3.124954000	-3.094201000	0.130004000	H	1.660388000	0.256140000	1.229977000
H	-2.411701000	1.107308000	0.773169000	H	4.938516000	-1.743819000	-0.793677000
H	-4.043985000	1.648206000	-0.970946000	H	6.547555000	-0.360458000	0.458767000
C	-1.928556000	-3.116503000	2.446984000	C	1.307787000	-3.101330000	0.293406000
H	-1.386427000	-3.341364000	3.372153000	H	0.471709000	-3.593473000	-0.216587000
H	-3.007252000	-3.161678000	2.647562000	H	2.093026000	-3.820321000	0.546244000
H	-1.662378000	-3.889130000	1.719943000	H	0.902227000	-2.634829000	1.202459000
H	3.385450000	-1.013528000	3.265188000	H	-1.005148000	-4.206916000	-2.903757000
H	4.418027000	0.385355000	2.939243000	H	-2.661373000	-4.368005000	-2.262660000
H	2.982264000	0.566165000	3.980905000	H	-2.332766000	-3.226304000	-3.574195000
H	-1.236560000	4.603298000	2.542694000	H	3.674858000	2.351044000	-0.799300000
H	-1.009664000	3.284386000	3.721380000	H	3.328875000	2.869920000	-2.470855000
H	0.398398000	4.101998000	2.998784000	H	2.787916000	3.867772000	-1.113599000
H	3.121767000	-3.599842000	1.531147000	H	-1.136818000	-3.580879000	2.783933000
H	3.170035000	-3.821464000	-0.233366000	H	-0.683156000	-2.498065000	4.128162000
H	3.803598000	-2.318698000	0.493409000	H	-2.309700000	-2.413349000	3.447053000
C	-1.865319000	-0.444692000	3.317730000	C	2.768370000	-2.628816000	-2.158576000
H	-1.161460000	-0.604589000	4.141382000	H	2.007991000	-3.168391000	-2.730662000
H	-1.872553000	0.618880000	3.075132000	H	3.238939000	-1.891395000	-2.814013000
H	-2.865534000	-0.743535000	3.648112000	H	3.521036000	-3.343999000	-1.814622000
⁴P₂				²P₂			
Mn	0.963604000	0.018823000	-0.475120000	Mn	0.868722000	-0.542928000	-0.482319000
O	-0.732254000	0.888923000	0.420642000	O	-0.500631000	1.103228000	-0.445572000
N	2.665646000	-0.888932000	-1.395558000	N	2.128025000	-2.245000000	-0.619367000
C	3.608717000	-1.232775000	-0.294054000	C	2.690093000	-2.463538000	0.743818000
H	4.146637000	-0.320377000	-0.025588000	H	3.548056000	-1.801219000	0.873910000
H	4.344387000	-1.974722000	-0.646909000	H	3.041450000	-3.503321000	0.849215000
C	2.852326000	-1.715322000	0.949240000	C	1.645836000	-2.073833000	1.796291000
H	2.351074000	-2.669387000	0.720800000	H	0.775775000	-2.736326000	1.712782000
H	3.571092000	-1.907387000	1.754890000	H	2.079886000	-2.187542000	2.795906000
N	1.875226000	-0.705437000	1.333677000	N	1.225529000	-0.699599000	1.535337000
C	2.017124000	-0.203599000	2.584317000	C	1.952379000	0.234916000	2.217961000
O	2.817406000	-0.563429000	3.466814000	O	2.770516000	0.015345000	3.127045000
N	1.090168000	0.839721000	2.874320000	N	1.680711000	1.574012000	1.825705000
H	0.766702000	1.286690000	2.023981000	H	1.324000000	1.604456000	0.877471000
C	1.454682000	1.761428000	3.935944000	C	2.751756000	2.545831000	2.031013000
C	3.219672000	0.144001000	-2.310630000	C	3.163259000	-1.865224000	-1.608099000
H	2.618176000	0.115302000	-3.224005000	H	2.696524000	-1.936888000	-2.596388000
H	4.262518000	-0.102733000	-2.572911000	H	4.016452000	-2.565398000	-1.576308000
C	3.092647000	1.542071000	-1.710357000	C	3.608376000	-0.422593000	-1.389319000
H	3.767195000	1.640363000	-0.842462000	H	4.199753000	-0.338427000	-0.463580000
H	3.430857000	2.284352000	-2.444154000	H	4.292328000	-0.133051000	-2.199304000
N	1.702601000	1.757580000	-1.341195000	N	2.422586000	0.429156000	-1.351556000
C	1.278673000	3.041471000	-1.481451000	C	2.739158000	1.750961000	-1.484674000
O	1.983902000	4.020800000	-1.791597000	O	3.893514000	2.221795000	-1.492856000

N	-0.107193000	3.207964000	-1.287820000	N	1.635086000	2.599009000	-1.646752000
H	-0.526137000	2.424766000	-0.803034000	H	0.744536000	2.166446000	-1.435852000
C	-0.582047000	4.511200000	-0.879736000	C	1.775985000	4.004773000	-1.349762000
C	2.216593000	-2.097882000	-2.151934000	C	1.307539000	-3.410148000	-1.068941000
H	2.345210000	-2.975185000	-1.513473000	H	1.056909000	-4.011343000	-0.190808000
H	2.844634000	-2.236250000	-3.046104000	H	1.890691000	-4.045147000	-1.754531000
C	0.717801000	-1.984030000	-2.463271000	C	-0.012327000	-2.913547000	-1.675753000
H	0.538537000	-1.146915000	-3.151367000	H	0.186543000	-2.427903000	-2.643436000
H	0.374139000	-2.910083000	-2.940940000	H	-0.688150000	-3.759746000	-1.852074000
N	0.039587000	-1.724559000	-1.198107000	N	-0.572957000	-1.951145000	-0.739830000
C	-0.247786000	-2.857313000	-0.495815000	C	-1.538022000	-2.428459000	0.086108000
O	-0.299484000	-4.016835000	-0.946191000	O	-2.242097000	-3.442867000	-0.085938000
N	-0.510996000	-2.617922000	0.875042000	N	-1.738352000	-1.615067000	1.222514000
H	0.121613000	-1.898961000	1.239624000	H	-0.869937000	-1.182763000	1.542426000
C	-0.569155000	-3.798855000	1.723120000	C	-2.606396000	-2.139972000	2.257300000
P	-2.064781000	0.770592000	1.121969000	P	-1.657357000	1.746329000	0.280418000
C	-5.279863000	-0.804598000	-1.776376000	C	-5.680684000	-0.021002000	-1.092632000
C	-3.928231000	-1.094685000	-1.969446000	C	-4.472802000	-0.604848000	-1.478779000
C	-2.963069000	-0.595435000	-1.092591000	C	-3.260331000	-0.036781000	-1.085303000
C	-3.363433000	0.199055000	-0.004867000	C	-3.258443000	1.112879000	-0.282771000
C	-4.724601000	0.485716000	0.189917000	C	-4.474648000	1.695740000	0.106761000
C	-5.679317000	-0.013414000	-0.695357000	C	-5.683095000	1.132977000	-0.303021000
H	-6.025081000	-1.194565000	-2.465147000	H	-6.623354000	-0.467916000	-1.398311000
H	-3.614347000	-1.716608000	-2.802830000	H	-4.464164000	-1.517442000	-2.066573000
H	-1.906705000	-0.839595000	-1.239081000	H	-2.315223000	-0.502250000	-1.356293000
H	-5.048096000	1.098671000	1.027580000	H	-4.486180000	2.581985000	0.737889000
H	-6.731014000	0.214922000	-0.543916000	H	-6.623397000	1.586167000	-0.000105000
C	-2.050725000	-0.326342000	2.551569000	C	-1.601929000	1.622736000	2.083412000
H	-1.161019000	-0.084732000	3.146286000	H	-0.569047000	1.818535000	2.400217000
H	-2.967218000	-0.219842000	3.140263000	H	-2.293575000	2.337342000	2.540682000
H	-1.952934000	-1.347267000	2.172367000	H	-1.875443000	0.610808000	2.377162000
H	0.579223000	2.353388000	4.232365000	H	2.333955000	3.559885000	2.062391000
H	1.800128000	1.179353000	4.791882000	H	3.231252000	2.326832000	2.986000000
H	2.263495000	2.458557000	3.661361000	H	3.506156000	2.508676000	1.232699000
H	-1.646811000	4.624891000	-1.123773000	H	1.063862000	4.598393000	-1.937337000
H	-0.456877000	4.716293000	0.200654000	H	1.625556000	4.253390000	-0.282692000
H	-0.011903000	5.266270000	-1.424207000	H	2.792754000	4.302959000	-1.612474000
H	-0.830032000	-3.494018000	2.742975000	H	-2.788833000	-1.365814000	3.012411000
H	-1.333448000	-4.482259000	1.346312000	H	-3.560430000	-2.429070000	1.810763000
H	0.378259000	-4.357584000	1.758399000	H	-2.201857000	-3.029255000	2.766022000
C	-2.559039000	2.408602000	1.738375000	C	-1.671664000	3.535526000	-0.061597000
H	-1.802696000	2.740494000	2.455847000	H	-0.753964000	3.978934000	0.335401000
H	-2.582664000	3.119276000	0.908226000	H	-1.694378000	3.695281000	-1.142661000
H	-3.532901000	2.395078000	2.235119000	H	-2.535241000	4.031069000	0.391200000
⁴RC₃				⁴RC₃			
Mn	1.755685000	0.200456000	-0.386084000	Mn	1.897267000	0.031036000	-0.169677000
O	0.579173000	-0.053509000	0.859114000	O	0.799757000	-0.041988000	1.093883000
N	3.380199000	0.375494000	-1.853533000	N	3.275697000	0.221294000	-1.908600000
C	3.202614000	1.763467000	-2.341779000	C	3.648051000	1.649599000	-1.979793000
H	2.281907000	1.765679000	-2.934098000	H	2.831724000	2.169428000	-2.490365000
H	4.032124000	2.056097000	-3.007321000	H	4.566371000	1.785095000	-2.574760000
C	3.052499000	2.739609000	-1.174061000	C	3.781218000	2.223616000	-0.577502000
H	4.040252000	3.007386000	-0.763793000	H	4.697105000	1.841404000	-0.097408000
H	2.643663000	3.685313000	-1.556749000	H	3.884502000	3.311636000	-0.629382000
N	2.189403000	2.147952000	-0.160705000	N	2.601370000	1.855832000	0.201117000
C	1.824036000	3.048985000	0.823058000	C	2.186531000	2.869338000	1.073783000
O	2.137763000	4.253117000	0.787242000	O	2.624873000	4.031770000	1.024600000
N	1.079606000	2.513161000	1.851410000	N	1.239366000	2.490152000	1.986203000
H	0.736007000	1.556300000	1.692165000	H	0.873131000	1.540002000	1.872524000
C	0.331594000	3.402661000	2.707039000	C	0.461287000	3.490333000	2.676580000
C	3.157674000	-0.639498000	-2.915763000	C	2.546181000	-0.237993000	-3.118462000
H	3.680867000	-1.551753000	-2.623265000	H	2.730127000	-1.304743000	-3.258294000

H	3.583051000	-0.294894000	-3.871609000	H	2.907911000	0.294245000	-4.010917000
C	1.666987000	-0.969598000	-3.024605000	C	1.053798000	-0.048568000	-2.862784000
H	1.133414000	-0.124273000	-3.490113000	H	0.800092000	1.020093000	-2.851187000
H	1.521168000	-1.844100000	-3.667314000	H	0.466268000	-0.536164000	-3.645996000
N	1.155093000	-1.214499000	-1.687432000	N	0.735027000	-0.623220000	-1.564857000
C	0.476753000	-2.402440000	-1.503434000	C	0.141881000	-1.876261000	-1.573823000
O	0.322104000	-3.269137000	-2.389654000	O	-0.071199000	-2.528189000	-2.615397000
N	-0.024894000	-2.553767000	-0.235822000	N	-0.227962000	-2.321263000	-0.338319000
H	-0.010422000	-1.710576000	0.354543000	H	-0.099977000	-1.677236000	0.439551000
C	-0.798644000	-3.714119000	0.123415000	C	-0.817635000	-3.619508000	-0.136227000
C	4.661869000	0.183499000	-1.136315000	C	4.396395000	-0.672219000	-1.547247000
H	4.811782000	1.059650000	-0.504352000	H	5.023209000	-0.146559000	-0.822978000
H	5.501969000	0.123709000	-1.846776000	H	5.009387000	-0.909212000	-2.431423000
C	4.623862000	-1.051010000	-0.229666000	C	3.838231000	-1.925191000	-0.888901000
H	4.692987000	-1.990735000	-0.799215000	H	3.294907000	-2.543027000	-1.620071000
H	5.498465000	-1.065157000	0.437234000	H	4.656138000	-2.544323000	-0.509489000
N	3.395096000	-1.038735000	0.516121000	N	2.968243000	-1.519458000	0.211935000
C	3.301890000	-2.000977000	1.535154000	C	2.779885000	-2.526126000	1.161638000
O	4.177001000	-2.840013000	1.780041000	O	3.357145000	-3.622532000	1.071344000
N	2.119538000	-1.862393000	2.197020000	N	1.982759000	-2.209528000	2.229746000
H	1.450302000	-1.131952000	1.836308000	H	1.426806000	-1.356515000	2.140150000
C	1.737229000	-2.783004000	3.235833000	C	1.626897000	-3.216076000	3.197802000
H	0.156623000	2.932628000	3.681262000	H	0.148817000	3.116482000	3.657822000
H	0.906578000	4.319620000	2.852907000	H	1.075569000	4.382299000	2.813832000
H	-0.645585000	3.686208000	2.280746000	H	-0.441454000	3.780246000	2.115034000
H	-0.613548000	-3.978825000	1.170591000	H	-0.425112000	-4.070172000	0.781579000
H	-1.880272000	-3.559510000	-0.004646000	H	-1.914985000	-3.575591000	-0.068903000
H	-0.501993000	-4.546424000	-0.518463000	H	-0.561223000	-4.256222000	-0.985397000
H	1.713837000	-2.289537000	4.217419000	H	1.631769000	-2.796639000	4.211395000
H	0.734360000	-3.175977000	3.037080000	H	0.629758000	-3.647844000	3.017016000
H	2.459502000	-3.601335000	3.269284000	H	2.360710000	-4.022214000	3.142431000
P	-4.035595000	0.644042000	0.592633000	P	-3.875965000	0.999181000	0.621368000
C	-2.870929000	-0.080489000	1.833630000	C	-2.746007000	0.166019000	1.830517000
C	-2.803252000	-1.467995000	2.040024000	C	-2.605059000	-1.227856000	1.903838000
C	-2.138371000	0.754141000	2.694271000	C	-2.061049000	0.953025000	2.773716000
C	-2.025414000	-2.002196000	3.067781000	C	-1.795373000	-1.814498000	2.878294000
H	-3.349634000	-2.138205000	1.383707000	H	-3.113012000	-1.861655000	1.185250000
C	-1.355444000	0.219978000	3.715443000	C	-1.243659000	0.367772000	3.737587000
H	-2.154316000	1.829448000	2.546967000	H	-2.140246000	2.035999000	2.732956000
C	-1.299227000	-1.160358000	3.911041000	C	-1.107776000	-1.020717000	3.794832000
H	-1.981750000	-3.079999000	3.201699000	H	-1.689562000	-2.895437000	2.905317000
H	-0.777422000	0.883555000	4.351857000	H	-0.700089000	0.996340000	4.437208000
H	-0.686529000	-1.576013000	4.705617000	H	-0.462712000	-1.478199000	4.538734000
C	-3.044210000	2.012640000	-0.155413000	C	-2.721589000	2.165292000	-0.232492000
C	-1.644765000	1.995190000	-0.298176000	C	-1.329258000	1.986759000	-0.294645000
C	-3.764994000	3.111583000	-0.653469000	C	-3.289942000	3.283694000	-0.867196000
C	-0.994952000	3.049487000	-0.944072000	C	-0.530471000	2.904203000	-0.981349000
H	-1.043916000	1.181003000	0.107231000	H	-0.849323000	1.144851000	0.195652000
C	-3.111650000	4.163379000	-1.298102000	C	-2.491374000	4.193650000	-1.560981000
H	-4.845833000	3.141567000	-0.532012000	H	-4.364916000	3.443157000	-0.812098000
C	-1.723778000	4.130820000	-1.445146000	C	-1.108023000	4.005077000	-1.616448000
H	0.085008000	3.014326000	-1.038476000	H	0.543767000	2.750424000	-1.000009000
H	-3.683788000	5.007756000	-1.675403000	H	-2.946157000	5.054272000	-2.045707000
H	-1.206664000	4.951602000	-1.935832000	H	-0.480082000	4.720773000	-2.141040000
C	-3.993435000	-0.637654000	-0.745309000	C	-4.086370000	-0.339143000	-0.640964000
C	-5.217219000	-1.151777000	-1.200609000	C	-5.350497000	-0.935556000	-0.769145000
C	-2.802459000	-1.119515000	-1.317126000	C	-3.026857000	-0.826520000	-1.425002000
C	-5.254981000	-2.125607000	-2.202398000	C	-5.550044000	-2.002086000	-1.649723000
H	-6.144180000	-0.788157000	-0.762965000	H	-6.179516000	-0.565747000	-0.169792000
C	-2.835103000	-2.100750000	-2.309680000	C	-3.218668000	-1.898498000	-2.297886000
H	-1.843301000	-0.749954000	-0.971611000	H	-2.040504000	-0.384205000	-1.338104000
C	-4.064236000	-2.600957000	-2.752709000	C	-4.483007000	-2.485861000	-2.408817000

H	-6.210951000	-2.515311000	-2.544405000	H	-6.534329000	-2.456183000	-1.736894000
H	-1.903690000	-2.492766000	-2.708695000	H	-2.366355000	-2.281609000	-2.851212000
H	-4.088549000	-3.367554000	-3.523390000	H	-4.632970000	-3.324220000	-3.084833000
²RC₃				⁶TS₃			
Mn	1.766794000	-0.063891000	-0.249394000	Mn	1.967551000	0.137806000	-0.068357000
O	0.666854000	-0.000798000	0.976980000	O	0.311307000	0.423782000	0.455612000
N	3.103297000	-0.274955000	-2.196573000	N	4.081264000	-0.324211000	-0.567366000
C	3.570576000	1.093559000	-2.463560000	C	4.609280000	-1.162170000	0.539737000
H	2.790917000	1.604921000	-3.036179000	H	4.817990000	-0.501177000	1.384326000
H	4.493433000	1.097373000	-3.067936000	H	5.555095000	-1.637647000	0.237284000
C	3.754208000	1.825875000	-1.145255000	C	3.583485000	-2.204089000	0.988662000
H	4.617217000	1.412279000	-0.600931000	H	3.399975000	-2.937366000	0.184920000
H	3.952676000	2.886351000	-1.318615000	H	3.966407000	-2.777947000	1.842787000
N	2.540910000	1.666586000	-0.345340000	N	2.352337000	-1.520519000	1.307104000
C	2.156756000	2.828999000	0.344522000	C	1.518800000	-2.193022000	2.194544000
O	2.676409000	3.933644000	0.113478000	O	1.768231000	-3.303231000	2.694228000
N	1.174476000	2.681670000	1.285308000	N	0.377752000	-1.485958000	2.461836000
H	0.746580000	1.760279000	1.370779000	H	0.212448000	-0.653763000	1.873606000
C	0.482791000	3.834426000	1.810688000	C	-0.662464000	-2.033046000	3.296171000
C	2.222813000	-0.801550000	-3.258521000	C	4.753570000	0.998475000	-0.641939000
H	2.262391000	-1.893216000	-3.248889000	H	4.526189000	1.415540000	-1.627286000
H	2.549845000	-0.454636000	-4.252054000	H	5.846420000	0.877903000	-0.558792000
C	0.793711000	-0.394513000	-2.909583000	C	4.187575000	1.939639000	0.412602000
H	0.680436000	0.694344000	-2.968921000	H	4.510006000	1.615946000	1.417986000
H	0.081443000	-0.857018000	-3.599211000	H	4.591515000	2.947415000	0.267972000
N	0.531007000	-0.812149000	-1.544492000	N	2.738098000	1.948518000	0.289534000
C	-0.008062000	-2.078146000	-1.409135000	C	2.156478000	3.182690000	0.510854000
O	-0.271899000	-2.820663000	-2.379625000	O	2.796543000	4.233905000	0.702926000
N	-0.270866000	-2.458623000	-0.118980000	N	0.781397000	3.177559000	0.496674000
H	-0.153103000	-1.750514000	0.600192000	H	0.336585000	2.285694000	0.284940000
C	-0.912783000	-3.711891000	0.185072000	C	0.031443000	4.407438000	0.486572000
C	4.163802000	-1.217229000	-1.798349000	C	4.113700000	-1.040686000	-1.873870000
H	4.964454000	-0.653506000	-1.311919000	H	4.140750000	-2.115585000	-1.693567000
H	4.590217000	-1.732974000	-2.674057000	H	5.016225000	-0.760165000	-2.437167000
C	3.572313000	-2.188760000	-0.782368000	C	2.813462000	-0.750593000	-2.630392000
H	2.812394000	-2.819971000	-1.264434000	H	2.771431000	0.309374000	-2.916352000
H	4.344577000	-2.838661000	-0.363649000	H	2.784348000	-1.360665000	-3.541789000
N	2.953151000	-1.399742000	0.274983000	N	1.689318000	-1.034506000	-1.746052000
C	3.328718000	-1.725705000	1.579861000	C	1.364325000	-2.371274000	-1.679336000
O	4.195713000	-2.574907000	1.840702000	O	2.007030000	-3.284182000	-2.233936000
N	2.676916000	-1.030205000	2.568827000	N	0.224810000	-2.637911000	-0.940773000
H	1.814838000	-0.557454000	2.289089000	H	-0.097208000	-1.856618000	-0.378483000
C	2.844828000	-1.426476000	3.946112000	C	0.021581000	-3.963075000	-0.381156000
H	0.214849000	3.668330000	2.860334000	P	-1.943316000	-0.169819000	-0.158475000
H	1.144801000	4.699442000	1.743319000	C	-3.295403000	0.969556000	4.153476000
H	-0.438266000	4.055643000	1.249930000	C	-2.253106000	1.660309000	3.529929000
H	-0.531333000	-4.108363000	1.132739000	C	-1.886785000	1.359546000	2.218737000
H	-2.007469000	-3.622016000	0.257196000	C	-2.567796000	0.363410000	1.489562000
H	-0.692707000	-4.420965000	-0.615850000	C	-3.609952000	-0.329816000	2.134872000
H	2.601470000	-0.583615000	4.601923000	C	-3.970196000	-0.029282000	3.448918000
H	2.209272000	-2.281190000	4.232311000	H	-3.573199000	1.201700000	5.178400000
H	3.883236000	-1.721681000	4.110774000	H	-1.709063000	2.431820000	4.068305000
P	-3.904258000	0.938088000	0.777521000	H	-1.040263000	1.866808000	1.774046000
C	-2.623418000	0.328184000	1.971918000	H	-4.142804000	-1.116162000	1.610310000
C	-2.385016000	-1.033540000	2.210257000	H	-4.777228000	-0.582354000	3.923189000
C	-1.905682000	1.270900000	2.729584000	C	-5.641819000	-2.147753000	-2.266784000
C	-1.446002000	-1.438955000	3.161268000	C	-4.367160000	-2.711444000	-2.319474000
H	-2.915703000	-1.784235000	1.634202000	C	-3.300161000	-2.095381000	-1.657889000
C	-0.962505000	0.865901000	3.671202000	C	-3.489360000	-0.904061000	-0.939477000
H	-2.060238000	2.332853000	2.556074000	C	-4.779042000	-0.344643000	-0.902519000
C	-0.728352000	-0.493222000	3.891516000	C	-5.845988000	-0.960739000	-1.555236000
H	-1.261152000	-2.499328000	3.312773000	H	-6.473935000	-2.627011000	-2.776793000

H	-0.396548000	1.612281000	4.222233000	H	-4.199840000	-3.632217000	-2.872522000
H	0.017059000	-0.810755000	4.614550000	H	-2.303071000	-2.529354000	-1.706052000
C	-2.883964000	2.029681000	-0.312938000	H	-4.948698000	0.574423000	-0.349445000
C	-1.513010000	1.825781000	-0.543384000	H	-6.837256000	-0.515191000	-1.513179000
C	-3.522668000	3.112210000	-0.941888000	H	-1.361994000	-2.668530000	2.731564000
C	-0.801824000	2.684955000	-1.382826000	H	-0.209214000	-2.651813000	4.075166000
H	-0.981762000	1.012945000	-0.057873000	H	-1.236473000	-1.218987000	3.746138000
C	-2.812185000	3.965443000	-1.787917000	H	-0.119185000	4.812513000	-0.526101000
H	-4.580485000	3.290614000	-0.760308000	H	-0.959394000	4.239145000	0.922874000
C	-1.448088000	3.754038000	-2.006401000	H	0.567195000	5.155427000	1.076228000
H	0.260865000	2.517633000	-1.526358000	H	-1.038819000	-4.092668000	-0.136653000
H	-3.318793000	4.801077000	-2.264827000	H	0.308016000	-4.703616000	-1.130239000
H	-0.887766000	4.427144000	-2.650240000	H	0.612214000	-4.137483000	0.528551000
C	-4.162007000	-0.560563000	-0.278867000	C	-1.839784000	1.378528000	-1.150639000
C	-5.400801000	-1.216015000	-0.191617000	C	-0.856493000	1.439082000	-2.152219000
C	-3.175196000	-1.095107000	-1.124816000	C	-2.703232000	2.469038000	-0.976577000
C	-5.646066000	-2.381656000	-0.921829000	C	-0.755907000	2.564666000	-2.969753000
H	-6.175087000	-0.810657000	0.456022000	H	-0.150303000	0.617810000	-2.254371000
C	-3.413874000	-2.262593000	-1.851944000	C	-2.598217000	3.595452000	-1.794798000
H	-2.207268000	-0.613594000	-1.207960000	H	-3.444852000	2.448716000	-0.183218000
C	-4.651192000	-2.905749000	-1.749119000	C	-1.626165000	3.644060000	-2.795428000
H	-6.609913000	-2.878771000	-0.841502000	H	0.016402000	2.606032000	-3.733249000
H	-2.611160000	-2.672577000	-2.457680000	H	-3.265818000	4.439656000	-1.640994000
H	-4.835962000	-3.817816000	-2.311532000	H	-1.537356000	4.524654000	-3.426536000
⁴TS₃				²TS₃			
Mn	1.788883000	0.129747000	-0.309284000	Mn	1.768040000	0.166285000	-0.275737000
O	0.392199000	0.293521000	0.674349000	O	0.261748000	0.226526000	0.660046000
N	3.446157000	-0.000549000	-1.689043000	N	3.483192000	0.113833000	-1.607859000
C	4.581224000	-0.469678000	-0.853083000	C	4.583946000	-0.387644000	-0.758146000
H	4.923239000	0.382189000	-0.261893000	H	4.924741000	0.439440000	-0.131394000
H	5.410545000	-0.808602000	-1.493717000	H	5.430688000	-0.733801000	-1.372669000
C	4.113435000	-1.565413000	0.100676000	C	4.041377000	-1.488138000	0.141218000
H	3.892792000	-2.494524000	-0.448864000	H	3.810049000	-2.391946000	-0.442695000
H	4.934192000	-1.815681000	0.785719000	H	4.797898000	-1.782165000	0.875646000
N	2.951978000	-1.075347000	0.827550000	N	2.845376000	-0.974482000	0.804470000
C	2.584097000	-1.884738000	1.879254000	C	2.506296000	-1.697779000	1.943164000
O	3.169016000	-2.948674000	2.160315000	O	3.148834000	-2.699664000	2.305174000
N	1.528026000	-1.417485000	2.642608000	N	1.432322000	-1.226790000	2.665429000
H	0.996670000	-0.6496668000	2.244228000	H	0.842531000	-0.550129000	2.182647000
C	0.880370000	-2.261552000	3.619630000	C	0.807763000	-2.061064000	3.669662000
C	3.632806000	1.368206000	-2.228217000	C	3.668643000	1.504424000	-2.069947000
H	2.839518000	1.524348000	-2.965178000	H	2.914556000	1.683593000	-2.842490000
H	4.601492000	1.446934000	-2.747822000	H	4.663437000	1.639531000	-2.526159000
C	3.491840000	2.411431000	-1.131350000	C	3.431389000	2.475693000	-0.927242000
H	4.409793000	2.451030000	-0.519988000	H	4.302770000	2.497219000	-0.251460000
H	3.406478000	3.404126000	-1.590464000	H	3.335132000	3.492417000	-1.322863000
N	2.325132000	2.093531000	-0.317600000	N	2.2255681000	2.072586000	-0.206766000
C	1.969889000	3.146176000	0.510836000	C	1.739920000	3.110866000	0.597618000
O	2.432246000	4.297182000	0.392097000	O	2.101128000	4.292953000	0.462540000
N	1.069926000	2.825778000	1.500995000	N	0.858351000	2.726640000	1.574244000
H	0.640701000	1.904798000	1.414296000	H	0.494462000	1.778053000	1.465932000
C	0.440555000	3.840724000	2.307228000	C	0.076229000	3.698235000	2.301163000
C	3.086419000	-0.961378000	-2.768543000	C	3.168575000	-0.797797000	-2.739288000
H	3.358750000	-1.967150000	-2.444459000	H	3.471238000	-1.811802000	-2.471852000
H	3.646039000	-0.726510000	-3.687229000	H	3.724920000	-0.495905000	-3.640368000
C	1.568634000	-0.927632000	-2.946740000	C	1.652537000	-0.803705000	-2.922533000
H	1.253000000	0.043320000	-3.351971000	H	1.309045000	0.173786000	-3.287868000
H	1.251003000	-1.713552000	-3.638438000	H	1.358652000	-1.567797000	-3.648131000
N	0.972070000	-1.114338000	-1.631042000	N	1.059144000	-1.060946000	-1.619007000
C	0.595425000	-2.416103000	-1.347746000	C	0.757940000	-2.387450000	-1.379236000
O	0.667500000	-3.354922000	-2.158425000	O	0.939702000	-3.305735000	-2.197049000
N	0.048173000	-2.598102000	-0.088214000	N	0.162401000	-2.635851000	-0.148834000

H	0.160293000	-1.813008000	0.541660000	H	0.195135000	-1.856193000	0.496551000	
C	0.060162000	-3.914967000	0.524880000	C	0.256945000	-3.956936000	0.447147000	
P	-1.798655000	0.093002000	-0.274768000	P	-1.657056000	0.025099000	-0.267756000	
C	-2.920327000	-1.606633000	3.908723000	C	-3.014984000	-1.707635000	3.840255000	
C	-2.256200000	-0.383580000	3.786714000	C	-2.413063000	-0.449733000	3.761575000	
C	-1.978646000	0.144166000	2.527170000	C	-2.056356000	0.083704000	2.523948000	
C	-2.374467000	-0.531368000	1.356322000	C	-2.309806000	-0.618957000	1.329878000	
C	-3.040896000	-1.760783000	1.493837000	C	-2.917714000	-1.882289000	1.425306000	
C	-3.310033000	-2.291769000	2.756445000	C	-3.262473000	-2.421125000	2.665913000	
H	-3.124926000	-2.023862000	4.891104000	H	-3.281868000	-2.129127000	4.805815000	
H	-1.939018000	0.156256000	4.675041000	H	-2.207671000	0.114995000	4.667371000	
H	-1.446246000	1.085234000	2.446107000	H	-1.576247000	1.055007000	2.480144000	
H	-3.349830000	-2.309659000	0.610582000	H	-3.121567000	-2.452259000	0.525374000	
H	-3.825267000	-3.245636000	2.837224000	H	-3.727125000	-3.402897000	2.712080000	
C	-4.936533000	-1.606806000	-3.299987000	C	-4.742440000	-1.671477000	-3.393588000	
C	-3.846061000	-2.360376000	-2.859317000	C	-3.642291000	-2.410118000	-2.952098000	
C	-2.939523000	-1.818340000	-1.947689000	C	-2.764981000	-1.870319000	-2.010506000	
C	-3.124175000	-0.519260000	-1.432060000	C	-2.985569000	-0.590683000	-1.461916000	
C	-4.216015000	0.232800000	-1.897206000	C	-4.087479000	0.145906000	-1.929955000	
C	-5.112523000	-0.306583000	-2.822079000	C	-4.955821000	-0.388872000	-2.884430000	
H	-5.636183000	-2.024283000	-4.019864000	H	-5.419594000	-2.085687000	-4.136690000	
H	-3.686506000	-3.366268000	-3.238635000	H	-3.452701000	-3.402456000	-3.353436000	
H	-2.074774000	-2.399546000	-1.638725000	H	-1.893941000	-2.441070000	-1.699952000	
H	-4.366466000	1.245870000	-1.539099000	H	-4.272123000	1.145139000	-1.549524000	
H	-5.952206000	0.291658000	-3.168509000	H	-5.803768000	0.199252000	-3.229018000	
H	0.745078000	-1.734652000	4.573705000	H	1.540155000	-2.795772000	4.008255000	
H	-0.110389000	-2.602159000	3.286618000	H	0.481135000	-1.454427000	4.521902000	
H	1.518526000	-3.132196000	3.783466000	H	-0.074895000	-2.592400000	3.284144000	
H	0.447075000	3.560212000	3.369343000	H	0.066942000	3.465983000	3.374447000	
H	1.004098000	4.768015000	2.184447000	H	0.530419000	4.680384000	2.156912000	
H	-0.601482000	4.026639000	2.007082000	H	-0.962909000	3.739543000	1.947105000	
H	-0.765285000	-3.989438000	1.241305000	H	-0.590622000	-4.111952000	1.124247000	
H	-0.075698000	-4.661115000	-0.259755000	H	0.219559000	-4.698785000	-0.352286000	
H	1.003631000	-4.113218000	1.051764000	H	1.188194000	-4.087046000	1.016023000	
C	-2.102725000	1.904025000	-0.178357000	C	-2.040661000	1.826457000	-0.210054000	
C	-1.118055000	2.742196000	-0.724516000	C	-1.140530000	2.695453000	-0.845214000	
C	-3.233152000	2.488422000	0.419266000	C	-3.179580000	2.372919000	0.405403000	
C	-1.269716000	4.129987000	-0.698654000	C	-1.375820000	4.070567000	-0.878876000	
H	-0.204367000	2.310160000	-1.121701000	H	-0.224446000	2.299240000	-1.272611000	
C	-3.391706000	3.874742000	0.435103000	C	-3.425496000	3.746827000	0.360436000	
H	-3.982842000	1.851633000	0.881078000	H	-3.873412000	1.716684000	0.922940000	
C	-2.410069000	4.696954000	-0.127466000	C	-2.523634000	4.597788000	-0.284051000	
H	-0.470091000	4.759366000	-1.077654000	H	-0.640092000	4.726849000	-1.333502000	
H	-4.271907000	4.314094000	0.898129000	H	-4.313397000	4.153085000	0.838784000	
H	-2.523788000	5.777650000	-0.097238000	H	-2.704170000	5.669554000	-0.302664000	
⁶P₃								
Mn	-1.760704000	0.243583000	-0.005029000	⁴P₃	Mn	1.755145000	0.034357000	-0.326662000
O	0.476168000	0.479456000	-0.311380000	O	-0.319326000	0.449190000	-0.214454000	
N	-4.121754000	-0.008714000	0.245721000	N	3.836471000	-0.412492000	-0.308446000	
C	-4.497309000	-0.799970000	-0.940905000	C	4.207492000	-0.656359000	1.116535000	
H	-4.637853000	-0.109824000	-1.777932000	H	4.387308000	0.307292000	1.596107000	
H	-5.454354000	-1.329090000	-0.778274000	H	5.140207000	-1.242379000	1.160257000	
C	-3.379942000	-1.785407000	-1.336559000	C	3.046530000	-1.319464000	1.873820000	
H	-3.217634000	-2.489638000	-0.507891000	H	2.822466000	-2.297390000	1.428648000	
H	-3.705924000	-2.357847000	-2.212525000	H	3.359302000	-1.474324000	2.914257000	
N	-2.135250000	-1.073810000	-1.611103000	N	1.864583000	-0.474003000	1.774166000	
C	-1.778849000	-1.008483000	-2.917981000	C	1.808051000	0.496958000	2.723068000	
O	-2.349078000	-1.534620000	-3.890558000	O	2.570013000	0.648293000	3.696936000	
N	-0.575794000	-0.283849000	-3.136112000	N	0.712009000	1.385073000	2.549103000	
H	-0.343004000	0.354928000	-2.384828000	H	0.435839000	1.455476000	1.575971000	
C	-0.321939000	0.226782000	-4.469673000	C	0.793196000	2.674435000	3.214146000	
C	-4.617549000	1.380373000	0.246947000	C	4.505552000	0.792664000	-0.861657000	

H	-4.577652000	1.743063000	1.278724000	H	4.417722000	0.738805000	-1.951607000
H	-5.671348000	1.426966000	-0.085288000	H	5.577065000	0.793981000	-0.598871000
C	-3.728849000	2.307228000	-0.601270000	C	3.791217000	2.060638000	-0.390058000
H	-3.801642000	2.000960000	-1.657382000	H	3.938158000	2.186178000	0.694314000
H	-4.109517000	3.332908000	-0.529273000	H	4.237793000	2.934447000	-0.878145000
N	-2.345640000	2.236269000	-0.151310000	N	2.373805000	1.940296000	-0.711002000
C	-1.793154000	3.403955000	0.266581000	C	1.840253000	3.027709000	-1.325359000
O	-2.307201000	4.537901000	0.238795000	O	2.418908000	4.096309000	-1.597207000
N	-0.500547000	3.245049000	0.810457000	N	0.473470000	2.881963000	-1.658649000
H	-0.045642000	2.376033000	0.565868000	H	0.164443000	1.918898000	-1.660073000
C	0.352482000	4.402832000	0.948078000	C	-0.079247000	3.725345000	-2.697316000
C	-4.308657000	-0.714436000	1.529415000	C	4.053633000	-1.629783000	-1.149306000
H	-4.354336000	-1.789007000	1.329646000	H	4.064907000	-2.501234000	-0.489814000
H	-5.263097000	-0.425154000	2.003642000	H	5.030556000	-1.573510000	-1.654876000
C	-3.107689000	-0.476645000	2.467327000	C	2.875541000	-1.811095000	-2.115012000
H	-3.057010000	0.590016000	2.726762000	H	2.878570000	-1.000315000	-2.858240000
H	-3.250964000	-1.051961000	3.390255000	H	2.973400000	-2.766319000	-2.645043000
N	-1.879954000	-0.857905000	1.782014000	N	1.648530000	-1.746868000	-1.328265000
C	-1.447870000	-2.124307000	2.017565000	C	1.196583000	-2.951081000	-0.878341000
O	-1.811697000	-2.890020000	2.927484000	O	1.510110000	-4.074200000	-1.314938000
N	-0.428245000	-2.531328000	1.119673000	N	0.255317000	-2.832167000	0.162017000
H	-0.589497000	-2.202773000	0.171363000	H	0.461886000	-2.059842000	0.793567000
C	-0.006326000	-3.918553000	1.192092000	C	-0.142143000	-4.058258000	0.828390000
P	1.878536000	0.046789000	0.035990000	P	-1.767357000	0.046114000	-0.118568000
C	2.634648000	0.421525000	4.560401000	C	-3.105174000	-1.717186000	-4.156075000
C	1.352987000	0.186108000	4.060276000	C	-1.783511000	-1.822254000	-3.717908000
C	1.137201000	0.083480000	2.685231000	C	-1.396300000	-1.269695000	-2.495987000
C	2.223884000	0.216841000	1.804646000	C	-2.352010000	-0.608459000	-1.704536000
C	3.511137000	0.468198000	2.308561000	C	-3.677307000	-0.491612000	-2.152485000
C	3.714739000	0.565265000	3.684540000	C	-4.052121000	-1.048382000	-3.375206000
H	2.794294000	0.500346000	5.632760000	H	-3.398888000	-2.150310000	-5.108949000
H	0.509220000	0.077074000	4.734954000	H	-1.043979000	-2.338757000	-4.322950000
H	0.129862000	-0.099307000	2.311064000	H	-0.360025000	-1.348391000	-2.162014000
H	4.348789000	0.602505000	1.629903000	H	-4.410695000	0.042850000	-1.555827000
H	4.710866000	0.762037000	4.071714000	H	-5.078064000	-0.954115000	-3.721010000
C	4.776094000	2.898571000	-2.162119000	C	-4.250656000	3.790495000	0.969973000
C	3.453793000	3.268211000	-1.906338000	C	-2.935805000	3.913098000	0.517983000
C	2.594194000	2.385991000	-1.251574000	C	-2.192148000	2.778018000	0.186590000
C	3.056983000	1.124852000	-0.843194000	C	-2.772570000	1.505341000	0.310591000
C	4.381090000	0.751933000	-1.120158000	C	-4.088432000	1.385540000	0.788902000
C	5.238254000	1.638996000	-1.772051000	C	-4.827209000	2.524568000	1.106340000
H	5.443661000	3.586722000	-2.673749000	H	-4.823702000	4.677641000	1.227241000
H	3.086686000	4.241685000	-2.217989000	H	-2.478272000	4.893909000	0.424269000
H	1.561685000	2.663490000	-1.065126000	H	-1.165950000	2.880454000	-0.166237000
H	4.734869000	-0.237506000	-0.843154000	H	-4.526142000	0.401886000	0.936823000
H	6.261928000	1.343552000	-1.985325000	H	-5.844366000	2.424188000	1.475408000
H	0.736815000	0.495135000	-4.566773000	H	-0.179623000	3.175380000	3.150473000
H	-0.563884000	-0.557804000	-5.188482000	H	1.051335000	2.514934000	4.262486000
H	-0.927444000	1.111620000	-4.726884000	H	1.555969000	3.339029000	2.778717000
H	1.155471000	4.192184000	1.664185000	H	0.151680000	3.381912000	-3.720246000
H	0.820220000	4.737430000	0.002858000	H	-1.170716000	3.777542000	-2.593859000
H	-0.253164000	5.232316000	1.317416000	H	0.343226000	4.724933000	-2.581431000
H	0.834236000	-4.069854000	0.510603000	H	-0.876404000	-3.817608000	1.599771000
H	0.314160000	-4.142290000	2.212164000	H	-0.595359000	-4.741043000	0.104741000
H	-0.804358000	-4.634115000	0.940132000	H	0.701100000	-4.593342000	1.291644000
C	2.289385000	-1.642481000	-0.476843000	C	-2.187311000	-1.152161000	1.179234000
C	3.238529000	-2.415922000	0.208745000	C	-3.166438000	-2.138180000	0.986881000
C	1.668107000	-2.152565000	-1.629406000	C	-1.570984000	-1.011243000	2.434725000
C	3.582696000	-3.681795000	-0.266592000	C	-3.543234000	-2.965911000	2.045400000
H	3.691960000	-2.040273000	1.121278000	H	-3.622999000	-2.269198000	0.010633000
C	2.011156000	-3.424902000	-2.088557000	C	-1.944402000	-1.854787000	3.481319000
H	0.913792000	-1.569146000	-2.160103000	H	-0.805365000	-0.253085000	2.592836000

C	2.971073000	-4.185948000	-1.416923000	C	-2.933308000	-2.824018000	3.293823000
H	4.313414000	-4.279849000	0.270885000	H	-4.299211000	-3.730714000	1.889518000
H	1.516999000	-3.820357000	-2.971238000	H	-1.454698000	-1.751589000	4.445333000
H	3.231920000	-5.176666000	-1.779750000	H	-3.220110000	-3.475575000	4.115209000
²P₃				⁶RC₄			
Mn	-1.802983000	0.128472000	0.205337000	Mn	-1.950038000	0.265323000	0.185028000
O	0.295709000	0.453772000	0.098293000	N	-3.226848000	1.494734000	1.443819000
N	-3.895029000	-0.269149000	0.275866000	C	-3.664140000	0.663415000	2.593922000
C	-4.285692000	-0.667460000	-1.104884000	H	-4.560598000	0.123471000	2.282120000
H	-4.438286000	0.240913000	-1.692854000	H	-3.931236000	1.303649000	3.449941000
H	-5.236056000	-1.227157000	-1.085979000	C	-2.594259000	-0.365053000	2.953493000
C	-3.140598000	-1.451004000	-1.757307000	H	-1.760250000	0.125460000	3.484997000
H	-2.970203000	-2.387015000	-1.208633000	H	-3.003744000	-1.094911000	3.661236000
H	-3.411579000	-1.697248000	-2.790134000	N	-2.154367000	-1.010999000	1.725727000
N	-1.937752000	-0.631153000	-1.692546000	C	-1.689612000	-2.299371000	1.894585000
C	-1.649128000	0.037144000	-2.844252000	O	-1.585260000	-2.862367000	3.001842000
O	-2.208698000	-0.094250000	-3.948274000	N	-1.355553000	-2.939958000	0.718159000
N	-0.556769000	0.930817000	-2.728213000	H	-1.171424000	-2.298397000	-0.066956000
H	-0.388166000	1.230725000	-1.775186000	C	-0.615641000	-4.178710000	0.788475000
C	-0.434397000	1.980843000	-3.722096000	C	-4.364775000	1.988949000	0.633239000
C	-4.542231000	0.994945000	0.706883000	H	-3.972566000	2.740635000	-0.051484000
H	-4.462574000	1.040951000	1.797505000	H	-5.120511000	2.467256000	1.276092000
H	-5.612517000	0.996550000	0.436838000	C	-4.993734000	0.873050000	-0.210563000
C	-3.795415000	2.197086000	0.132036000	H	-5.584200000	0.178439000	0.409110000
H	-3.933198000	2.232489000	-0.960440000	H	-5.705438000	1.282563000	-0.940946000
H	-4.217826000	3.122687000	0.539696000	N	-3.942806000	0.132444000	-0.848366000
N	-2.383224000	2.057465000	0.471080000	C	-4.320607000	-0.665023000	-1.946198000
C	-1.811932000	3.183930000	0.978958000	O	-5.474680000	-0.758653000	-2.380468000
O	-2.354819000	4.291616000	1.143016000	N	-3.229019000	-1.302636000	-2.440932000
N	-0.453537000	3.023888000	1.329731000	H	-2.305400000	-1.155317000	-1.924588000
H	-0.178256000	2.054724000	1.418019000	C	-3.357244000	-2.200658000	-3.558604000
C	0.129931000	3.941288000	2.285154000	C	-2.295304000	2.582651000	1.833256000
C	-4.131329000	-1.377873000	1.247832000	H	-1.543824000	2.128635000	2.485484000
H	-4.172731000	-2.318437000	0.692849000	H	-2.818615000	3.359073000	2.415385000
H	-5.100588000	-1.241378000	1.753290000	C	-1.609857000	3.175716000	0.597891000
C	-2.945036000	-1.472849000	2.213286000	H	-2.248998000	3.934735000	0.120645000
H	-2.925027000	-0.586109000	2.863990000	H	-0.716214000	3.724900000	0.925038000
H	-3.046421000	-2.363303000	2.845509000	N	-1.283594000	2.098024000	-0.325073000
N	-1.7371169000	-1.517122000	1.400537000	C	-0.680304000	2.539650000	-1.484928000
C	-1.262659000	-2.769463000	1.145879000	O	-0.382668000	3.734129000	-1.688559000
O	-1.544892000	-3.814033000	1.762414000	N	-0.446979000	1.556514000	-2.417003000
N	-0.333741000	-2.799397000	0.090874000	H	-0.585330000	0.592517000	-2.083691000
H	-0.544317000	-2.117236000	-0.636104000	C	0.382770000	1.824453000	-3.563906000
C	0.073067000	-4.103895000	-0.393344000	P	4.057926000	-0.510947000	0.081823000
P	1.740627000	0.041876000	0.135525000	C	1.279284000	-0.740005000	3.831646000
C	2.861528000	-1.076845000	4.459199000	C	2.457961000	-1.746489000	3.753876000
C	1.560523000	-1.240590000	3.979237000	C	3.494985000	-1.326569000	2.698444000
C	1.240245000	-0.886535000	2.667519000	C	2.876071000	-1.368362000	1.270997000
C	2.242061000	-0.367560000	1.829044000	C	1.378321000	-0.963016000	1.333183000
C	3.546608000	-0.191506000	2.316617000	C	1.095714000	-0.001655000	2.490751000
C	3.854684000	-0.548776000	3.629203000	H	1.448009000	-0.017281000	4.641059000
H	3.103142000	-1.354551000	5.482125000	H	2.935685000	-1.857104000	4.735279000
H	0.785757000	-1.648724000	4.621813000	H	3.849098000	-0.313277000	2.936690000
H	0.220874000	-1.008008000	2.295344000	H	0.996546000	-0.573218000	0.392624000
H	4.314985000	0.236036000	1.678926000	H	1.758954000	0.869525000	2.432646000
H	4.864391000	-0.408280000	4.005771000	C	2.360453000	-3.512250000	-2.423403000
C	4.316766000	3.593364000	-1.326655000	C	3.831225000	-3.330887000	-2.018055000
C	2.992616000	3.787426000	-0.929569000	C	4.328084000	-1.921148000	-2.372922000
C	2.220853000	2.710330000	-0.487812000	C	3.482078000	-0.807727000	-1.705346000
C	2.781223000	1.423409000	-0.443313000	C	1.991254000	-1.021574000	-2.057455000
C	4.107800000	1.229791000	-0.863787000	C	1.475684000	-2.439346000	-1.776261000
C	4.874390000	2.312269000	-1.294312000	H	2.007535000	-4.515527000	-2.150917000

H	4.911905000	4.435496000	-1.670472000	H	3.935424000	-3.494350000	-0.935795000
H	2.550573000	4.779193000	-0.964253000	H	5.385406000	-1.808856000	-2.106209000
H	1.188767000	2.868562000	-0.175535000	H	1.343645000	-0.299785000	-1.563260000
H	4.533643000	0.229983000	-0.875659000	H	1.432059000	-2.614018000	-0.698628000
H	5.899567000	2.154117000	-1.618288000	H	0.430114000	-4.049181000	1.117742000
H	0.550783000	2.451859000	-3.629036000	H	-1.094831000	-4.855124000	1.500587000
H	-0.533361000	1.538804000	-4.715091000	H	-0.601942000	-4.646104000	-0.201310000
H	-1.203799000	2.763912000	-3.628092000	H	-2.373592000	-2.351491000	-4.011096000
H	-0.121178000	3.710083000	3.334404000	H	-3.753989000	-3.179491000	-3.250816000
H	1.222851000	3.935505000	2.186902000	H	-4.050310000	-1.786772000	-4.298793000
H	-0.247333000	4.942148000	2.067950000	H	0.117595000	1.146068000	-4.382596000
H	0.823631000	-3.973078000	-1.175732000	H	0.225771000	2.856637000	-3.885440000
H	0.508386000	-4.679571000	0.427541000	H	1.459165000	1.698185000	-3.359003000
H	-0.761929000	-4.698293000	-0.796320000	C	3.700457000	1.322477000	0.318796000
C	2.230676000	-1.334618000	-0.944309000	C	4.897036000	2.148160000	-0.239353000
C	3.157869000	-2.305550000	-0.538876000	C	2.383714000	1.940323000	-0.192149000
C	1.723790000	-1.355150000	-2.255136000	C	4.543811000	3.640976000	-0.447440000
C	3.593603000	-3.276956000	-1.441606000	H	5.236965000	1.726031000	-1.195054000
H	3.528377000	-2.312715000	0.481389000	C	2.180852000	3.351368000	0.407583000
C	2.155289000	-2.338740000	-3.145120000	H	2.419824000	2.008109000	-1.285678000
H	0.992321000	-0.609091000	-2.568924000	C	3.517108000	4.109281000	0.591033000
C	3.095599000	-3.292623000	-2.746060000	H	4.119424000	3.787852000	-1.448809000
H	4.309115000	-4.029030000	-1.120386000	H	1.500192000	3.906203000	-0.244711000
H	1.749895000	-2.358180000	-4.152739000	H	3.356580000	5.191809000	0.518746000
H	3.429463000	-4.054557000	-3.445671000	H	4.258024000	-1.798307000	-3.465202000
				H	4.462151000	-4.085078000	-2.507045000
				H	1.887487000	-0.833166000	-3.137883000
				H	2.285084000	-3.438838000	-3.519210000
				H	0.439882000	-2.507050000	-2.122922000
				H	3.927002000	3.926326000	1.594440000
				H	5.456113000	4.249616000	-0.407558000
				H	1.680068000	3.256659000	1.380096000
				H	0.075885000	0.381047000	2.401016000
				H	4.380264000	-1.971361000	2.737281000
				H	0.358239000	-1.286944000	4.062280000
				H	2.070590000	-2.737733000	3.485599000
				H	0.788078000	-1.863538000	1.513750000
				H	5.745364000	2.052504000	0.449274000
				H	1.509478000	1.334461000	0.038011000
				H	3.788876000	0.141864000	-2.168623000
				H	2.923953000	-2.415928000	0.944573000
				H	3.710036000	1.435720000	1.412326000
O	-1.091601000	-0.723519000	-0.958406000				
⁴RC₄				²RC₄			
Mn	-2.060017000	0.421229000	-0.009997000	Mn	2.255795000	-0.284844000	-0.013109000
N	-3.206177000	1.793140000	1.179018000	N	3.213408000	-1.843269000	1.147057000
C	-3.702888000	1.070202000	2.372126000	C	3.754472000	-1.181333000	2.347378000
H	-4.624451000	0.560650000	2.088073000	H	4.641968000	-0.622569000	2.045784000
H	-3.936256000	1.779385000	3.181317000	H	4.048471000	-1.921502000	3.109453000
C	-2.682318000	0.025500000	2.796134000	C	2.715124000	-0.202478000	2.864566000
H	-1.838030000	0.503088000	3.319354000	H	1.907857000	-0.724467000	3.399664000
H	-3.127685000	-0.664993000	3.518930000	H	3.166095000	0.470700000	3.599127000
N	-2.234576000	-0.689570000	1.602700000	N	2.203323000	0.552452000	1.722168000
C	-1.863974000	-2.001230000	1.852230000	C	1.710436000	1.802347000	2.099432000
O	-1.812822000	-2.484939000	2.997807000	O	1.582609000	2.121200000	3.296975000
N	-1.561075000	-2.753930000	0.738240000	N	1.394115000	2.678393000	1.095076000
H	-1.287478000	-2.187443000	-0.068001000	H	1.287312000	2.247374000	0.171248000
C	-0.908279000	-4.030983000	0.926516000	C	0.644102000	3.870005000	1.421326000
C	-4.294849000	2.215065000	0.268611000	C	4.250396000	-2.388329000	0.253098000
H	-3.866245000	2.895468000	-0.466936000	H	3.743114000	-2.991846000	-0.501751000
H	-5.084857000	2.745893000	0.822319000	H	4.952680000	-3.035588000	0.803239000
C	-4.835066000	0.988450000	-0.451169000	C	4.960487000	-1.232992000	-0.435070000

H	-5.464138000	0.377751000	0.212212000	H	5.707479000	-0.769025000	0.225211000
H	-5.489970000	1.305805000	-1.271349000	H	5.524038000	-1.602166000	-1.299037000
N	-3.707444000	0.218118000	-0.970274000	N	3.950199000	-0.258453000	-0.846665000
C	-4.117696000	-0.892051000	-1.709825000	C	4.496505000	0.717248000	-1.704799000
O	-5.322642000	-1.145406000	-1.864289000	O	5.709328000	0.730779000	-1.969075000
N	-3.126065000	-1.631670000	-2.303417000	N	3.615380000	1.610840000	-2.234658000
H	-2.185690000	-1.416895000	-1.971219000	H	2.658554000	1.567902000	-1.865077000
C	-3.405565000	-2.983659000	-2.733306000	C	4.082710000	2.763560000	-2.963430000
C	-2.249099000	2.869085000	1.507420000	C	2.151147000	-2.811010000	1.474065000
H	-1.533485000	2.447470000	2.219438000	H	1.539766000	-2.367979000	2.260520000
H	-2.757771000	3.715243000	1.996929000	H	2.576668000	-3.748875000	1.866662000
C	-1.517908000	3.306951000	0.243765000	C	1.298287000	-3.056539000	0.241042000
H	-2.118120000	4.028672000	-0.329849000	H	1.751044000	-3.818473000	-0.407469000
H	-0.607077000	3.849731000	0.524205000	H	0.328273000	-3.472249000	0.542360000
N	-1.202456000	2.121503000	-0.549447000	N	1.134591000	-1.794792000	-0.482753000
C	-0.530752000	2.452126000	-1.720453000	C	0.473997000	-2.003561000	-1.693792000
O	-0.167847000	3.616260000	-1.976409000	O	0.032745000	-3.125817000	-2.010875000
N	-0.304648000	1.415766000	-2.585246000	N	0.334288000	-0.931236000	-2.524864000
H	-0.500970000	0.483984000	-2.214546000	H	0.653277000	-0.028075000	-2.167380000
C	0.559844000	1.589005000	-3.725550000	C	-0.408302000	-1.056822000	-3.753466000
P	4.027995000	-0.643946000	0.239440000	P	-4.115624000	0.658843000	0.270459000
C	1.126229000	-0.441628000	3.890689000	C	-1.092579000	-0.112331000	3.760101000
C	2.258834000	-1.501569000	3.938879000	C	-2.161052000	0.992328000	3.958928000
C	3.347434000	-1.222290000	2.889243000	C	-3.300261000	0.870161000	2.934516000
C	2.772478000	-1.357482000	1.448910000	C	-2.771614000	1.135584000	1.495514000
C	1.293510000	-0.887382000	1.425231000	C	-1.326225000	0.587177000	1.349972000
C	1.013503000	0.181351000	2.484864000	C	-1.044027000	-0.585616000	2.291978000
H	1.306245000	0.342279000	4.638248000	H	-1.298004000	-0.964782000	4.421345000
H	2.700239000	-1.547292000	4.942172000	H	-2.560023000	0.963336000	4.980483000
H	3.744167000	-0.210057000	3.053068000	H	-3.733928000	-0.137677000	3.007047000
H	0.963250000	-0.556510000	0.444853000	H	-1.068879000	0.325607000	0.326921000
H	1.713881000	1.017643000	2.375523000	H	-1.770778000	-1.389782000	2.121420000
C	2.275363000	-3.735425000	-2.107796000	C	-2.207815000	3.912613000	-1.728488000
C	3.739011000	-3.590652000	-1.664769000	C	-3.658273000	3.824528000	-1.229568000
C	4.312193000	-2.233759000	-2.100827000	C	-4.365133000	2.588584000	-1.806717000
C	3.497959000	-1.040187000	-1.542144000	C	-3.632218000	1.267473000	-1.462929000
C	2.011702000	-1.209849000	-1.935155000	C	-2.153665000	1.377462000	-1.908132000
C	1.420102000	-2.579372000	-1.572881000	C	-1.432545000	2.631897000	-1.393725000
H	1.866112000	-4.698362000	-1.775906000	H	-1.705194000	4.786988000	-1.295143000
H	3.801783000	-3.679583000	-0.570690000	H	-3.664822000	3.771742000	-0.131688000
H	5.364290000	-2.149088000	-1.805369000	H	-5.405332000	2.547162000	-1.463831000
H	1.387872000	-0.421165000	-1.518600000	H	-1.585873000	0.486874000	-1.642555000
H	1.330090000	-2.673466000	-0.487839000	H	-1.299462000	2.569562000	-0.311978000
H	0.125916000	-3.943843000	1.299622000	H	-0.390174000	3.658238000	1.739355000
H	-1.465782000	-4.625432000	1.653922000	H	1.130785000	4.404484000	2.241008000
H	-0.883496000	-4.562083000	-0.029892000	H	0.605359000	4.516863000	0.539927000
H	-2.744398000	-3.259232000	-3.562773000	H	3.363281000	3.031103000	-3.746011000
H	-3.268409000	-3.716583000	-1.922165000	H	4.227298000	3.645126000	-2.317986000
H	-4.442159000	-3.036181000	-3.071576000	H	5.042936000	2.524920000	-3.425970000
H	0.298495000	0.860885000	-4.500502000	H	-0.175638000	-0.204648000	-4.399124000
H	0.432824000	2.599300000	-4.120526000	H	-0.134729000	-1.983704000	-4.266008000
H	1.626605000	1.457127000	-3.480805000	H	-1.497609000	-1.078733000	-3.594717000
C	3.746789000	1.217431000	0.330145000	C	-3.958850000	-1.211533000	0.108208000
C	4.999227000	1.943737000	-0.244054000	C	-5.270788000	-1.769378000	-0.521405000
C	2.476891000	1.850194000	-0.273066000	C	-2.746559000	-1.848195000	-0.597930000
C	4.721517000	3.426834000	-0.588239000	C	-5.099914000	-3.199119000	-1.085961000
H	5.3555757000	1.429283000	-1.146978000	H	-5.618221000	-1.108313000	-1.326943000
C	2.322077000	3.314233000	0.201510000	C	-2.693645000	-3.367071000	-0.314858000
H	2.546988000	1.823615000	-1.366914000	H	-2.822478000	-1.675108000	-1.678112000
C	3.685681000	4.025085000	0.371278000	C	-4.102798000	-4.002659000	-0.242638000
H	4.335361000	3.505529000	-1.612518000	H	-4.729176000	-3.150484000	-2.117964000
H	1.691197000	3.842343000	-0.519168000	H	-2.076153000	-3.834144000	-1.085983000

H	3.578288000	5.103832000	0.205529000	H	-4.070032000	-5.048836000	-0.570301000
H	4.283008000	-2.186207000	-3.200656000	H	-4.392885000	2.691193000	-2.902851000
H	4.348279000	-4.405732000	-2.077000000	H	-4.213518000	4.732806000	-1.498541000
H	1.953689000	-1.096766000	-3.029319000	H	-2.151704000	1.416613000	-3.009113000
H	2.238091000	-3.739697000	-3.207684000	H	-2.216925000	4.062818000	-2.818784000
H	0.397429000	-2.635080000	-1.960596000	H	-0.420101000	2.657216000	-1.810488000
H	4.053834000	3.907739000	1.400278000	H	-4.461387000	-4.018702000	0.796280000
H	5.658961000	3.996796000	-0.567972000	H	-6.074981000	-3.700376000	-1.133414000
H	1.784056000	3.323988000	1.158616000	H	-2.171212000	-3.531601000	0.636607000
H	0.014355000	0.592169000	2.320335000	H	-0.061661000	-0.994168000	2.044523000
H	4.197497000	-1.902257000	3.014727000	H	-4.115130000	1.566687000	3.162076000
H	0.175035000	-0.924396000	4.140941000	H	-0.116652000	0.297469000	4.039491000
H	1.834691000	-2.494780000	3.743642000	H	-1.684888000	1.973882000	3.839807000
H	0.656814000	-1.744496000	1.659202000	H	-0.634522000	1.386428000	1.614500000
H	5.815694000	1.870473000	0.484580000	H	-6.061808000	-1.755707000	0.238183000
H	1.569251000	1.304472000	-0.022037000	H	-1.803118000	-1.403998000	-0.289301000
H	3.863814000	-0.139076000	-2.056327000	H	-4.093685000	0.482420000	-2.080758000
H	2.786366000	-2.429568000	1.209453000	H	-2.724321000	2.227519000	1.385855000
H	3.723838000	1.411686000	1.411723000	H	-3.931159000	-1.544930000	1.155785000
O	-1.028154000	-0.589350000	-0.869122000	O	1.404553000	0.884383000	-0.886472000
⁶TS₄				⁴TS₄			
Mn	-1.779734000	-0.433321000	-0.086537000	Mn	1.878472000	0.221290000	-0.126506000
O	-0.449713000	-0.112898000	1.034346000	N	3.672632000	0.208691000	-1.380884000
N	-3.407218000	-0.830761000	-1.426322000	C	3.463119000	-0.780066000	-2.474760000
C	-3.695687000	0.411291000	-2.192546000	H	3.824096000	-1.754667000	-2.143699000
H	-4.367441000	1.023589000	-1.588609000	H	4.029578000	-0.482215000	-3.370408000
H	-4.204902000	0.164009000	-3.137961000	C	1.958674000	-0.913574000	-2.713239000
C	-2.401707000	1.202387000	-2.401819000	H	1.549170000	0.019798000	-3.121933000
H	-1.754630000	0.681657000	-3.126838000	H	1.763231000	-1.723095000	-3.424542000
H	-2.629130000	2.191576000	-2.813404000	N	1.322305000	-1.170271000	-1.427840000
N	-1.736112000	1.314515000	-1.116990000	C	1.310344000	-2.508345000	-1.052591000
C	-1.518547000	2.591451000	-0.657934000	O	1.752116000	-3.426329000	-1.765053000
O	-1.846782000	3.637456000	-1.253255000	N	0.702568000	-2.755404000	0.160772000
N	-0.856695000	2.630324000	0.553628000	H	0.517689000	-1.931281000	0.720527000
H	-0.625412000	1.719116000	0.960384000	C	1.008612000	-3.973068000	0.890030000
C	-0.866229000	3.822716000	1.360781000	C	4.780137000	-0.179757000	-0.469495000
C	-4.543378000	-1.265518000	-0.572127000	H	5.053198000	0.702978000	0.112375000
H	-4.299137000	-2.262573000	-0.204137000	H	5.657566000	-0.496073000	-1.055474000
H	-5.466733000	-1.329320000	-1.169643000	C	4.314528000	-1.266844000	0.493066000
C	-4.722690000	-0.343181000	0.636566000	H	4.146809000	-2.212910000	-0.048695000
H	-5.166887000	0.621582000	0.341606000	H	5.108224000	-1.469208000	1.222076000
H	-5.453692000	-0.792338000	1.326303000	N	3.100798000	-0.808050000	1.152049000
N	-3.435140000	-0.136548000	1.256295000	C	2.823419000	-1.459211000	2.325150000
C	-3.474158000	0.560042000	2.445854000	O	3.577675000	-2.295972000	2.860786000
O	-4.490476000	1.084089000	2.929895000	N	1.597935000	-1.149073000	2.899019000
N	-2.241392000	0.594968000	3.068762000	H	1.064015000	-0.411250000	2.449561000
H	-1.447856000	0.257279000	2.504578000	C	1.319713000	-1.509792000	4.266706000
C	-2.012398000	1.482283000	4.179256000	C	3.807783000	1.587486000	-1.908002000
C	-2.896642000	-1.917276000	-2.297729000	H	3.077841000	1.690383000	-2.716886000
H	-2.133307000	-1.465995000	-2.938226000	H	4.814150000	1.739576000	-2.331616000
H	-3.699490000	-2.301441000	-2.948488000	C	3.482028000	2.611959000	-0.831534000
C	-2.259912000	-3.033709000	-1.470077000	H	4.297968000	2.665793000	-0.091847000
H	-3.032475000	-3.728614000	-1.100957000	H	3.434504000	3.609674000	-1.285592000
H	-1.620254000	-3.640664000	-2.125526000	N	2.214829000	2.248812000	-0.211749000
N	-1.506045000	-2.438352000	-0.376481000	C	1.649194000	3.298016000	0.478525000
C	-0.658171000	-3.326341000	0.242875000	O	2.147335000	4.435121000	0.556632000
O	-0.481013000	-4.501313000	-0.141864000	N	0.422191000	3.012321000	1.066263000
N	0.002350000	-2.821770000	1.344894000	H	0.240552000	2.008518000	1.148156000
H	-0.048082000	-1.800920000	1.453524000	C	-0.086283000	3.889417000	2.095880000
C	1.073965000	-3.568892000	1.952543000	P	-1.803371000	-0.322163000	-0.415504000
P	1.937582000	0.756872000	-0.209441000	C	-3.793837000	1.058770000	3.554769000
C	4.170253000	-0.847125000	3.619607000	C	-2.820819000	-0.139113000	3.656125000

C	2.917591000	0.035968000	3.838853000	C	-1.957072000	-0.237091000	2.393911000
C	2.071204000	0.110142000	2.562636000	C	-2.818956000	-0.608331000	1.152222000
C	2.831842000	0.873584000	1.448405000	C	-4.250992000	-0.010348000	1.301063000
C	4.359175000	0.555211000	1.513114000	C	-4.230910000	1.305309000	2.091145000
C	4.624244000	-0.819530000	2.143437000	H	-3.311440000	1.962238000	3.947243000
H	3.953949000	-1.881961000	3.911317000	H	-2.186108000	-0.039208000	4.544265000
H	2.319493000	-0.352992000	4.671016000	H	-1.450194000	0.720334000	2.239567000
H	1.831372000	-0.905642000	2.237505000	H	-4.733839000	0.126592000	0.333768000
H	4.829802000	0.623408000	0.528896000	H	-3.534864000	1.999940000	1.606920000
H	4.076894000	-1.583148000	1.579216000	C	-3.817952000	-3.895234000	-1.426237000
C	1.344980000	3.952243000	-2.466323000	C	-2.304738000	-3.630464000	-1.402895000
C	1.273068000	2.502936000	-2.974085000	C	-1.946125000	-2.448038000	-2.310289000
C	2.619780000	1.782589000	-2.798788000	C	-2.682604000	-1.153029000	-1.896174000
C	3.093753000	1.782114000	-1.326419000	C	-4.206753000	-1.419463000	-1.890946000
C	3.210192000	3.253367000	-0.863143000	C	-4.619997000	-2.638168000	-1.048539000
C	1.890038000	4.023935000	-1.030088000	H	-4.079990000	-4.723149000	-0.754708000
H	0.344806000	4.396092000	-2.491768000	H	-1.963895000	-3.414808000	-0.382120000
H	0.489726000	1.970360000	-2.420471000	H	-0.867625000	-2.283983000	-2.315727000
H	2.575056000	0.765577000	-3.199515000	H	-4.765965000	-0.530183000	-1.585648000
H	3.560565000	3.315735000	0.174271000	H	-4.471214000	-2.424838000	0.014384000
H	1.139645000	3.596613000	-0.360319000	H	0.159253000	-4.244997000	1.527022000
H	0.016586000	3.840885000	2.010479000	H	1.178284000	-4.771578000	0.165930000
H	-0.846407000	4.696148000	0.704362000	H	1.898899000	-3.865162000	1.523879000
H	-1.762718000	3.898873000	1.997455000	H	1.677435000	-0.766324000	4.999028000
H	-1.710593000	2.494551000	3.864065000	H	0.239831000	-1.634156000	4.411978000
H	-2.941654000	1.576563000	4.746465000	H	1.822277000	-2.455411000	4.481984000
H	-1.225543000	1.079250000	4.826959000	H	0.400074000	3.748690000	3.075869000
H	1.163838000	-3.304170000	3.012444000	H	0.078665000	4.925854000	1.793340000
H	0.857854000	-4.635639000	1.862787000	H	-1.162804000	3.720197000	2.223314000
H	2.058196000	-3.393668000	1.479248000	C	-1.962009000	1.486456000	-0.855491000
C	2.173280000	-0.983192000	-0.858436000	C	-0.870576000	1.837968000	-1.909594000
C	1.151748000	-1.272004000	-2.007282000	C	-3.312967000	2.059408000	-1.327585000
C	3.582253000	-1.431387000	-1.296114000	C	-1.140925000	3.190174000	-2.609504000
C	1.616608000	-2.407734000	-2.940866000	H	-0.794526000	1.044823000	-2.665434000
H	0.942227000	-0.373816000	-2.595565000	C	-3.263154000	3.607923000	-1.304585000
C	3.614227000	-2.965823000	-1.482126000	H	-3.514179000	1.705629000	-2.346980000
H	3.845425000	-0.935546000	-2.238197000	C	-1.857177000	4.151152000	-1.654219000
C	2.319006000	-3.510193000	-2.139366000	H	-1.758288000	3.046018000	-3.508008000
H	2.297751000	-2.021105000	-3.713180000	H	-4.009451000	4.003022000	-2.007059000
H	4.493352000	-3.232499000	-2.084220000	H	-1.934493000	5.156373000	-2.085720000
H	2.553849000	-4.367300000	-2.782113000	H	-2.242482000	-2.695849000	-3.342289000
H	3.383687000	2.309361000	-3.392368000	H	-1.750580000	-4.521579000	-1.719322000
H	0.976444000	2.488458000	-4.030944000	H	-4.501130000	-1.617818000	-2.934215000
H	3.991194000	3.730685000	-1.475796000	H	-4.106896000	-4.211382000	-2.440122000
H	1.997919000	4.535002000	-3.135510000	H	-5.695208000	-2.822371000	-1.175379000
H	2.030797000	5.071217000	-0.732543000	H	-1.248138000	4.239940000	-0.747266000
H	1.622169000	-3.880338000	-1.378229000	H	-0.190752000	3.618530000	-2.948843000
H	0.747860000	-2.814989000	-3.472332000	H	-3.555738000	3.963284000	-0.308080000
H	3.753799000	-3.440500000	-0.502185000	H	-5.214960000	1.788452000	2.060647000
H	5.686262000	-1.082052000	2.063194000	H	-1.156950000	-0.970689000	2.509011000
H	1.106778000	0.587312000	2.738761000	H	-4.673943000	0.876354000	4.184648000
H	4.985895000	-0.503830000	4.269103000	H	-3.384819000	-1.073205000	3.784708000
H	3.220813000	1.052341000	4.126256000	H	-4.880436000	-0.730360000	1.843451000
H	4.854652000	1.318926000	2.128924000	H	0.094388000	1.883186000	-1.405354000
H	0.208595000	-1.561329000	-1.545799000	H	-4.149759000	1.718184000	-0.716746000
H	4.349825000	-1.139243000	-0.577215000	H	-2.488735000	-0.410534000	-2.681429000
H	4.091767000	1.324661000	-1.288833000	H	-2.914129000	-1.701092000	1.160856000
H	2.715549000	1.941704000	1.676834000	H	-1.681774000	2.000502000	0.070293000
H	1.871080000	-1.608372000	-0.011439000	O	0.430538000	0.288545000	0.775218000
²T₄				⁶P₄			
Mn	1.885585000	0.135188000	-0.195193000	Mn	-1.741075000	-0.302372000	-0.302365000
N	3.652707000	-0.013001000	-1.452614000	O	0.398829000	0.349093000	-0.021037000

C	3.426307000	-1.099210000	-2.445761000	N	-3.820151000	-0.801496000	-1.245705000
H	3.859346000	-2.022584000	-2.056251000	C	-4.200614000	0.315425000	-2.134415000
H	3.926165000	-0.858528000	-3.396451000	H	-4.784627000	1.035636000	-1.559535000
C	1.920018000	-1.317586000	-2.585555000	H	-4.827521000	-0.045630000	-2.969436000
H	1.462023000	-0.465368000	-3.109374000	C	-2.950099000	1.067055000	-2.628211000
H	1.719726000	-2.227045000	-3.161699000	H	-2.367495000	0.420677000	-3.301477000
N	1.363682000	-1.413115000	-1.245584000	H	-3.283324000	1.942937000	-3.202051000
C	1.124061000	-2.685412000	-0.771405000	N	-2.102502000	1.435723000	-1.503517000
O	1.345653000	-3.727379000	-1.413551000	C	-2.544987000	2.535522000	-0.827165000
N	0.546302000	-2.716297000	0.487123000	O	-3.561418000	3.206436000	-1.095370000
H	0.480504000	-1.809085000	0.932656000	N	-1.709522000	2.918830000	0.240295000
C	0.744843000	-3.865713000	1.349454000	H	-1.045592000	2.202348000	0.509445000
C	4.760044000	-0.330245000	-0.520556000	C	-2.304771000	3.632560000	1.361757000
H	5.060772000	0.596234000	-0.028074000	C	-4.686450000	-0.927061000	-0.055429000
H	5.626917000	-0.732729000	-1.068585000	H	-4.530494000	-1.919448000	0.374407000
C	4.246705000	-1.295740000	0.539776000	H	-5.751027000	-0.839854000	-0.336238000
H	4.047467000	-2.285936000	0.098497000	C	-4.319535000	0.112685000	1.016973000
H	5.008894000	-1.447397000	1.311054000	H	-4.489729000	1.127328000	0.624725000
N	3.038249000	-0.717181000	1.112524000	H	-4.994807000	-0.006367000	1.874832000
C	2.747431000	-1.174384000	2.379445000	N	-2.929776000	-0.080563000	1.415395000
O	3.433759000	-2.025733000	2.976068000	C	-2.621394000	0.302054000	2.667580000
N	1.647273000	-0.598157000	2.991097000	O	-3.348950000	0.888890000	3.490520000
H	1.004463000	-0.120129000	2.360711000	N	-1.276237000	-0.021174000	3.029875000
C	1.106029000	-1.211568000	4.182847000	H	-0.965900000	-0.850500000	2.537299000
C	3.769537000	1.315059000	-2.089867000	C	-0.976346000	-0.046736000	4.451099000
H	2.996745000	1.360328000	-2.864159000	C	-3.547145000	-2.046425000	-1.977006000
H	4.752047000	1.433991000	-2.576950000	H	-2.977034000	-1.760603000	-2.868668000
C	3.506651000	2.417625000	-1.073814000	H	-4.480814000	-2.526986000	-2.326251000
H	4.366966000	2.536916000	-0.396775000	C	-2.720472000	-3.054296000	-1.171367000
H	3.417205000	3.377263000	-1.598480000	H	-3.345251000	-3.516880000	-0.393129000
N	2.285922000	2.100004000	-0.340498000	H	-2.451576000	-3.882815000	-1.846482000
C	1.816513000	3.192551000	0.370476000	N	-1.541792000	-2.429796000	-0.576587000
O	2.392286000	4.293337000	0.401375000	C	-0.877190000	-3.285371000	0.236137000
N	0.605793000	2.994524000	1.012112000	O	-1.143885000	-4.485162000	0.426642000
H	0.333509000	2.009943000	1.078660000	N	0.256788000	-2.718991000	0.889509000
C	0.189463000	3.906503000	2.052044000	H	0.263335000	-1.706551000	0.893592000
P	-1.753029000	-0.258109000	-0.439686000	C	0.717761000	-3.351638000	2.111355000
C	-3.806394000	1.137960000	3.505341000	P	1.853790000	0.471285000	-0.429365000
C	-2.830500000	-0.055025000	3.627824000	C	4.391953000	-0.553062000	3.261791000
C	-1.942748000	-0.153745000	2.382375000	C	3.066795000	0.203784000	3.519514000
C	-2.776854000	-0.535220000	1.125758000	C	2.153105000	0.134341000	2.292408000
C	-4.214264000	0.057120000	1.248454000	C	2.781902000	0.922111000	1.107048000
C	-4.215205000	1.376652000	2.032676000	C	4.334096000	0.804272000	1.118901000
H	-3.336224000	2.044884000	3.904778000	C	4.787483000	-0.511727000	1.767301000
H	-2.211837000	0.049903000	4.526680000	H	4.292618000	-1.597752000	3.579648000
H	-1.434373000	0.803760000	2.234746000	H	2.556208000	-0.211525000	4.394823000
H	-4.682289000	0.187562000	0.273622000	H	2.023331000	-0.919245000	2.023301000
H	-3.512337000	2.071953000	1.559392000	H	4.760458000	0.912455000	0.119959000
C	-3.763328000	-3.842833000	-1.439720000	H	4.322631000	-1.350336000	1.235507000
C	-2.252499000	-3.567414000	-1.419766000	C	2.570408000	4.570814000	-1.087986000
C	-1.905938000	-2.384677000	-2.331956000	C	1.210786000	3.897578000	-0.854131000
C	-2.647351000	-1.092300000	-1.917288000	C	0.981273000	2.757824000	-1.851840000
C	-4.169158000	-1.370664000	-1.910360000	C	2.102368000	1.692747000	-1.803707000
C	-4.572293000	-2.589503000	-1.062974000	C	3.496416000	2.356437000	-1.945092000
H	-4.018741000	-4.670183000	-0.764846000	C	3.719956000	3.554103000	-1.005199000
H	-1.911369000	-3.343524000	-0.401125000	H	2.736332000	5.380762000	-0.366426000
H	-0.827739000	-2.220658000	-2.341189000	H	1.152713000	3.510966000	0.171955000
H	-4.736235000	-0.484583000	-1.610084000	H	0.000889000	2.291956000	-1.710284000
H	-4.419969000	-2.372012000	-0.001347000	H	4.305120000	1.624719000	-1.838760000
H	-0.117335000	-3.990123000	2.016311000	H	3.816007000	3.210634000	0.029846000
H	0.830944000	-4.751931000	0.718067000	H	-1.528554000	4.193993000	1.896990000
H	1.650727000	-3.768588000	1.964329000	H	-3.034917000	4.336896000	0.959514000

H	0.457039000	-0.495591000	4.698576000	H	-2.809985000	2.966430000	2.074649000
H	0.518038000	-2.123115000	3.980465000	H	-1.438939000	-0.889818000	4.990947000
H	1.927724000	-1.494513000	4.843785000	H	0.108840000	-0.095803000	4.599919000
H	0.658934000	3.699766000	3.028011000	H	-1.359344000	0.872301000	4.897503000
H	0.462034000	4.923205000	1.760719000	H	0.199665000	-2.995183000	3.017319000
H	-0.898705000	3.849868000	2.179205000	H	0.526087000	-4.421366000	2.014024000
C	-1.913991000	1.550079000	-0.886639000	H	1.794921000	-3.192238000	2.252298000
C	-0.825406000	1.894519000	-1.945067000	C	2.424839000	-1.143895000	-1.088747000
C	-3.262098000	2.127741000	-1.360386000	C	1.387766000	-1.658591000	-2.132896000
C	-1.082642000	3.253675000	-2.637596000	C	3.842129000	-1.254686000	-1.683595000
H	-0.767822000	1.104668000	-2.706979000	C	1.944674000	-2.854399000	-2.943851000
C	-3.205562000	3.676293000	-1.336677000	H	1.108735000	-0.856034000	-2.827343000
H	-3.461941000	1.775228000	-2.380462000	C	4.216643000	-2.750574000	-1.844032000
C	-1.795061000	4.212887000	-1.677839000	H	3.851398000	-0.754286000	-2.660167000
H	-1.699332000	3.120511000	-3.538106000	C	2.979684000	-3.634615000	-2.126256000
H	-3.944831000	4.075767000	-2.044019000	H	2.416097000	-2.504487000	-3.873208000
H	-1.864152000	5.221778000	-2.102167000	H	4.946626000	-2.851363000	-2.657281000
H	-2.204896000	-2.636256000	-3.362522000	H	3.282726000	-4.552298000	-2.643416000
H	-1.685137000	-4.450931000	-1.731567000	H	0.987017000	3.179856000	-2.868310000
H	-4.461912000	-1.576487000	-2.952788000	H	0.390447000	4.616121000	-0.935076000
H	-4.054039000	-4.163680000	-2.451797000	H	3.559619000	2.723366000	-2.979343000
H	-5.647090000	-2.780014000	-1.184882000	H	2.572432000	5.033588000	-2.086044000
H	-1.187902000	4.292507000	-0.768421000	H	4.675847000	4.032284000	-1.255769000
H	-0.128694000	3.677380000	-2.972103000	H	2.512387000	-3.946138000	-1.184536000
H	-3.502842000	4.033201000	-0.342077000	H	1.113962000	-3.503831000	-3.239297000
H	-5.200387000	1.855681000	1.980232000	H	4.716850000	-3.098472000	-0.931450000
H	-1.147996000	-0.887228000	2.520480000	H	5.870108000	-0.640378000	1.653404000
H	-4.697816000	0.953047000	4.118363000	H	1.151099000	0.518418000	2.495119000
H	-3.392252000	-0.991253000	3.749348000	H	5.192929000	-0.116730000	3.871477000
H	-4.849195000	-0.663397000	1.783558000	H	3.271143000	1.256734000	3.754535000
H	0.144055000	1.922466000	-1.448098000	H	4.742865000	1.638704000	1.702888000
H	-4.102110000	1.789974000	-0.752532000	H	0.469449000	-1.948590000	-1.619548000
H	-2.461228000	-0.348790000	-2.703723000	H	4.601543000	-0.757451000	-1.076570000
H	-2.867143000	-1.628197000	1.139469000	H	1.967383000	1.046601000	-2.681121000
H	-1.631123000	2.064234000	0.038706000	H	2.513665000	1.975321000	1.250788000
O	0.387454000	0.300747000	0.691575000	H	2.352972000	-1.811245000	-0.220407000
⁴P₄		²P₄		²P₄		²P₄	
Mn	1.772389000	0.411352000	-0.427438000	Mn	1.933567000	-0.154007000	-0.242773000
O	-0.277623000	-0.103560000	-0.189926000	O	-0.169092000	-0.025764000	0.155892000
N	3.536338000	0.892341000	-1.474536000	N	3.802814000	-0.256746000	-1.108385000
C	3.942652000	-0.284769000	-2.299630000	C	4.138456000	-1.683476000	-1.345417000
H	4.746284000	-0.799718000	-1.769173000	H	4.621095000	-2.059422000	-0.441101000
H	4.340375000	0.052543000	-3.269943000	H	4.852491000	-1.781219000	-2.180713000
C	2.772494000	-1.265224000	-2.453644000	C	2.865945000	-2.500292000	-1.574022000
H	2.060845000	-0.859286000	-3.198313000	H	2.456145000	-2.279552000	-2.578197000
H	3.133463000	-2.227036000	-2.838070000	H	3.103534000	-3.571083000	-1.574687000
N	2.127349000	-1.413417000	-1.161952000	N	1.920366000	-2.157274000	-0.522175000
C	2.018781000	-2.665721000	-0.649429000	C	1.189603000	-3.195014000	-0.043661000
O	2.407610000	-3.720150000	-1.193691000	O	1.171627000	-4.360457000	-0.492403000
N	1.346739000	-2.710750000	0.586461000	N	0.361402000	-2.856998000	1.045707000
H	1.242218000	-1.802690000	1.023295000	H	0.680810000	-2.030232000	1.538542000
C	1.719527000	-3.753125000	1.529833000	C	-0.091093000	-3.938181000	1.898558000
C	4.544076000	1.208549000	-0.426648000	C	4.726322000	0.394931000	-0.148234000
H	4.321468000	2.203603000	-0.039608000	H	4.574610000	1.471649000	-0.229934000
H	5.554208000	1.223600000	-0.868325000	H	5.778028000	0.170317000	-0.395434000
C	4.450156000	0.220032000	0.739736000	C	4.372709000	-0.033294000	1.275038000
H	4.709266000	-0.797459000	0.403519000	H	4.717341000	-1.064952000	1.462642000
H	5.210715000	0.492922000	1.487556000	H	4.909963000	0.599919000	1.992503000
N	3.105835000	0.281653000	1.281462000	N	2.929822000	0.072758000	1.433559000
C	2.932856000	-0.424928000	2.407506000	C	2.508697000	0.119289000	2.719099000
O	3.760042000	-1.131756000	3.014417000	O	3.237957000	0.179061000	3.726381000
N	1.588633000	-0.331589000	2.905572000	N	1.099877000	0.075346000	2.878527000

H	1.185086000	0.555958000	2.628929000	H	0.568335000	0.229348000	2.028960000
C	1.392706000	-0.656514000	4.307849000	C	0.533969000	0.622142000	4.094857000
C	3.120671000	2.063779000	-2.277991000	C	3.626261000	0.498037000	-2.366883000
H	2.440218000	1.680490000	-3.047667000	H	2.979767000	-0.116658000	-3.003654000
H	3.983172000	2.524882000	-2.791783000	H	4.585938000	0.626636000	-2.899231000
C	2.385869000	3.099324000	-1.416207000	C	2.962435000	1.859437000	-2.106115000
H	3.105633000	3.698670000	-0.839817000	H	3.721501000	2.613657000	-1.850679000
H	1.893727000	3.819784000	-2.090368000	H	2.518194000	2.216277000	-3.049449000
N	1.435997000	2.423000000	-0.538855000	N	1.979291000	1.717940000	-1.035175000
C	0.852200000	3.257999000	0.356464000	C	1.604765000	2.913136000	-0.514163000
O	1.055373000	4.480041000	0.467181000	O	1.841594000	4.035246000	-1.010403000
N	-0.109144000	2.626509000	1.187454000	N	0.872820000	2.833722000	0.690329000
H	-0.054344000	1.616890000	1.133506000	H	1.093960000	1.992827000	1.206961000
C	-0.333902000	3.182288000	2.507738000	C	0.822363000	4.028301000	1.514916000
P	-1.743707000	-0.323411000	-0.475008000	P	-1.576003000	0.052790000	-0.387846000
C	-3.995543000	-0.246080000	3.531844000	C	-4.579994000	-1.094566000	3.130956000
C	-2.580965000	-0.874821000	3.543633000	C	-3.081386000	-1.489826000	3.189729000
C	-1.798002000	-0.496716000	2.281902000	C	-2.217234000	-0.665763000	2.226500000
C	-2.461462000	-1.129034000	1.024631000	C	-2.645975000	-0.934977000	0.762321000
C	-4.009648000	-1.183984000	1.176787000	C	-4.202265000	-0.923402000	0.617627000
C	-4.522252000	-0.062639000	2.090953000	C	-4.911820000	-0.323434000	1.841215000
H	-3.976888000	0.727575000	4.036050000	H	-4.849079000	-0.477578000	3.996828000
H	-2.032899000	-0.558084000	4.437250000	H	-2.695730000	-1.391800000	4.210615000
H	-1.779776000	0.596893000	2.199652000	H	-2.290276000	0.401919000	2.473421000
H	-4.517403000	-1.159197000	0.210701000	H	-4.529936000	-0.403972000	-0.285115000
H	-4.188794000	0.903386000	1.694189000	H	-4.613732000	0.723006000	1.959262000
C	-2.333676000	-4.297744000	-1.905608000	C	-2.751964000	-3.280024000	-2.903355000
C	-0.989730000	-3.628094000	-1.596803000	C	-1.455880000	-3.161762000	-2.093212000
C	-0.861158000	-2.283649000	-2.322873000	C	-0.759882000	-1.828987000	-2.384657000
C	-2.024492000	-1.309074000	-2.020317000	C	-1.641962000	-0.584699000	-2.128587000
C	-3.396423000	-2.005045000	-2.208255000	C	-3.023923000	-0.739738000	-2.814393000
C	-3.503894000	-3.378101000	-1.522605000	C	-3.693730000	-2.107846000	-2.589711000
H	-2.422994000	-5.255423000	-1.377570000	H	-3.260298000	-4.230727000	-2.697863000
H	-0.875015000	-3.469166000	-0.518333000	H	-1.671381000	-3.238521000	-1.020997000
H	0.091358000	-1.813165000	-2.070661000	H	0.169397000	-1.757652000	-1.818117000
H	-4.223752000	-1.352938000	-1.905467000	H	-3.707746000	0.071036000	-2.534863000
H	-3.514297000	-3.258296000	-0.434135000	H	-4.018092000	-2.200311000	-1.550290000
H	0.875917000	-3.984704000	2.193281000	H	-0.871710000	-3.569187000	2.573412000
H	1.977599000	-4.647888000	0.959980000	H	-0.501377000	-4.732064000	1.270998000
H	2.576380000	-3.455829000	2.151897000	H	0.708259000	-4.384530000	2.512944000
H	1.771584000	0.112852000	5.001415000	H	0.344379000	1.708438000	4.041227000
H	0.327112000	-0.810792000	4.512845000	H	-0.412884000	0.126362000	4.339888000
H	1.936194000	-1.579267000	4.516384000	H	1.249287000	0.446117000	4.899992000
H	0.425492000	2.882078000	3.249773000	H	1.806760000	4.346192000	1.892214000
H	-0.303156000	4.269879000	2.419593000	H	0.414253000	4.858835000	0.935031000
H	-1.318317000	2.881352000	2.888193000	H	0.167672000	3.838306000	2.372982000
C	-2.513077000	1.319487000	-0.769484000	C	-2.070503000	1.837946000	-0.468767000
C	-1.668448000	2.093246000	-1.822945000	C	-1.479396000	2.544945000	-1.712545000
C	-4.001680000	1.446088000	-1.142410000	C	-3.559194000	2.220866000	-0.301398000
C	-2.348730000	3.427211000	-2.227291000	C	-1.484638000	4.086671000	-1.538122000
H	-1.539643000	1.479916000	-2.724432000	H	-2.081280000	2.266936000	-2.588699000
C	-4.456926000	2.913677000	-0.924597000	C	-3.826888000	3.696664000	-0.700353000
H	-4.120997000	1.165971000	-2.197069000	H	-4.2066689000	1.573809000	-0.902078000
C	-3.301247000	3.920641000	-1.132581000	C	-2.5667799000	4.556177000	-0.546967000
H	-2.919178000	3.298582000	-3.158116000	H	-1.673549000	4.545302000	-2.517645000
H	-5.282502000	3.139859000	-1.611556000	H	-4.148550000	3.741040000	-1.749759000
H	-3.704471000	4.909721000	-1.379495000	H	-2.798258000	5.615831000	-0.708603000
H	-0.867880000	-2.465039000	-3.408048000	H	-0.489078000	-1.808394000	-3.451191000
H	-0.140489000	-4.259930000	-1.874036000	H	-0.761984000	-3.980819000	-2.300628000
H	-3.520671000	-2.160176000	-3.289585000	H	-2.852692000	-0.623622000	-3.894053000
H	-2.392327000	-4.524772000	-2.981132000	H	-2.510687000	-3.277399000	-3.977101000
H	-4.464784000	-3.837106000	-1.790199000	H	-4.603086000	-2.164154000	-3.202646000

H	-2.728634000	4.041261000	-0.205534000	H	-2.193389000	4.477713000	0.482321000
H	-1.578905000	4.178496000	-2.431345000	H	-0.492913000	4.419239000	-1.223177000
H	-4.858628000	3.021409000	0.090965000	H	-4.659480000	4.092957000	-0.106467000
H	-5.618197000	-0.034106000	2.083438000	H	-5.995223000	-0.312293000	1.670697000
H	-0.756071000	-0.816840000	2.336798000	H	-1.171310000	-0.944604000	2.339253000
H	-4.686223000	-0.878820000	4.103244000	H	-5.202940000	-1.995944000	3.190908000
H	-2.653392000	-1.968766000	3.601211000	H	-2.965923000	-2.547266000	2.920865000
H	-4.281884000	-2.148272000	1.624374000	H	-4.547165000	-1.958681000	0.507147000
H	-0.668164000	2.266295000	-1.423200000	H	-0.454475000	2.210290000	-1.893802000
H	-4.649899000	0.777315000	-0.572847000	H	-3.849844000	2.068133000	0.741626000
H	-1.971083000	-0.511504000	-2.773102000	H	-1.128643000	0.243583000	-2.629670000
H	-2.079511000	-2.154122000	0.949700000	H	-2.277664000	-1.945015000	0.543591000
H	-2.341109000	1.822387000	0.191810000	H	-1.497219000	2.224819000	0.384069000
⁶RC₅				⁴RC₅			
Mn	-0.234805000	-0.478399000	-0.066745000	Mn	-0.349913000	-0.427734000	-0.170462000
O	0.059820000	0.462028000	1.356219000	O	-0.001813000	0.318035000	1.294773000
N	-0.794101000	-1.701378000	-1.781765000	N	-0.595544000	-1.325070000	-2.126624000
C	0.521659000	-2.196717000	-2.252750000	C	0.756046000	-1.775721000	-2.513866000
H	1.037229000	-1.333184000	-2.685296000	H	1.325876000	-0.877592000	-2.769483000
H	0.395404000	-2.948244000	-3.050165000	H	0.714828000	-2.419535000	-3.407515000
C	1.352269000	-2.745020000	-1.091504000	C	1.428143000	-2.476330000	-1.342441000
H	1.053254000	-3.782070000	-0.862179000	H	1.092048000	-3.522461000	-1.262836000
H	2.4011137000	-2.814564000	-1.409000000	H	2.507415000	-2.532593000	-1.525299000
N	1.200414000	-1.870730000	0.062902000	N	1.146610000	-1.730338000	-0.118805000
C	2.145026000	-2.104584000	1.046978000	C	1.958666000	-2.159298000	0.933982000
O	3.069094000	-2.929979000	0.922777000	O	2.891330000	-2.965334000	0.774808000
N	1.983640000	-1.355264000	2.189566000	N	1.651161000	-1.643089000	2.163693000
H	1.311209000	-0.579824000	2.116714000	H	1.006714000	-0.847903000	2.151132000
C	3.063023000	-1.277987000	3.142157000	C	2.568218000	-1.822858000	3.262558000
C	-1.471845000	-0.837845000	-2.782599000	C	-1.133630000	-0.291954000	-3.044806000
H	-2.539664000	-0.839653000	-2.559350000	H	-2.221332000	-0.296001000	-2.958674000
H	-1.337107000	-1.247696000	-3.795729000	H	-0.867954000	-0.530242000	-4.086272000
C	-0.972114000	0.602029000	-2.674595000	C	-0.618364000	1.069346000	-2.601620000
H	0.047728000	0.678121000	-3.091214000	H	0.451236000	1.169706000	-2.850982000
H	-1.605317000	1.268669000	-3.269992000	H	-1.145953000	1.871718000	-3.124769000
N	-0.973291000	0.986311000	-1.274016000	N	-0.821900000	1.187330000	-1.162850000
C	-1.347554000	2.300630000	-1.021763000	C	-1.362260000	2.397664000	-0.744176000
O	-1.759639000	3.089137000	-1.889042000	O	-1.690044000	3.307956000	-1.522904000
N	-1.217926000	2.648164000	0.300365000	N	-1.509892000	2.519747000	0.616560000
H	-0.659914000	1.990297000	0.870115000	H	-0.952678000	1.857549000	1.160623000
C	-1.376118000	4.019708000	0.710347000	C	-1.819308000	3.814213000	1.176960000
C	-1.670388000	-2.780953000	-1.268734000	C	-1.545182000	-2.432170000	-1.878783000
H	-1.051743000	-3.418439000	-0.635409000	H	-0.998758000	-3.229878000	-1.373790000
H	-2.065403000	-3.392374000	-2.095932000	H	-1.944736000	-2.826352000	-2.826305000
C	-2.808489000	-2.212490000	-0.411591000	C	-2.651722000	-1.935198000	-0.961217000
H	-3.617697000	-1.773844000	-1.013046000	H	-3.344235000	-1.268108000	-1.494804000
H	-3.292957000	-3.025114000	0.152312000	H	-3.257260000	-2.784292000	-0.623685000
N	-2.261306000	-1.221553000	0.475973000	N	-2.041361000	-1.264665000	0.183841000
C	-3.186191000	-0.598174000	1.328854000	C	-2.981995000	-0.899223000	1.147543000
O	-4.406826000	-0.797055000	1.294875000	O	-4.188781000	-1.140860000	0.989501000
N	-2.539912000	0.239561000	2.187052000	N	-2.489533000	-0.333863000	2.297562000
H	-1.509925000	0.365710000	2.030803000	H	-1.519241000	-0.025923000	2.229046000
C	-3.274036000	1.125662000	3.053571000	C	-3.382929000	0.429666000	3.140422000
H	2.677495000	-0.933838000	4.108315000	H	2.054471000	-1.598669000	4.202978000
H	3.510524000	-2.267494000	3.265447000	H	2.918007000	-2.858196000	3.281981000
H	3.869317000	-0.589497000	2.834461000	H	3.458667000	-1.176502000	3.194573000
H	-1.719528000	4.061913000	1.751021000	H	-2.149278000	3.688583000	2.213514000
H	-0.440642000	4.599515000	0.639413000	H	-0.964215000	4.510232000	1.165926000
H	-2.114339000	4.502542000	0.065824000	H	-2.623143000	4.277408000	0.600028000
H	-2.757340000	1.227412000	4.014083000	H	-2.988355000	0.469915000	4.161700000
H	-3.370077000	2.125918000	2.606622000	H	-3.521112000	1.461271000	2.778339000
H	-4.276069000	0.720794000	3.213489000	H	-4.359009000	-0.059111000	3.153788000

P	3.666410000	2.152615000	-0.477740000	P	3.744248000	2.141069000	-0.096253000
C	2.906712000	2.124418000	1.217885000	C	3.135231000	1.627845000	1.584017000
H	3.618608000	1.694881000	1.931239000	H	3.856151000	0.945503000	2.046528000
H	2.701127000	3.153105000	1.536332000	H	3.049021000	2.509605000	2.228639000
H	1.972503000	1.547996000	1.251191000	H	2.159342000	1.133329000	1.523517000
C	2.155009000	2.596771000	-1.468520000	C	2.181667000	2.915509000	-0.741397000
H	1.846882000	3.626457000	-1.260282000	H	1.975924000	3.850190000	-0.209256000
H	2.373246000	2.528015000	-2.539888000	H	2.289186000	3.160402000	-1.803487000
H	1.315096000	1.935553000	-1.232123000	H	1.322053000	2.249243000	-0.617004000
C	3.704993000	0.329971000	-0.843008000	C	3.627528000	0.499754000	-0.964931000
H	4.045157000	0.167176000	-1.872064000	H	3.802863000	0.634618000	-2.038327000
H	4.401306000	-0.188213000	-0.176444000	H	4.386108000	-0.190618000	-0.582512000
H	2.720519000	-0.130603000	-0.712087000	H	2.648481000	0.035803000	-0.808501000
²RC₅				⁶TS₅			
Mn	-0.753455000	-0.045051000	-0.173269000	Mn	0.569493000	0.266703000	-0.162076000
O	-0.314674000	0.095713000	1.445192000	O	-0.821826000	0.047891000	0.896489000
N	-1.165940000	-0.313844000	-2.264833000	N	2.265127000	0.523892000	-1.446768000
C	0.095150000	-0.802722000	-2.847588000	C	3.407958000	0.740981000	-0.521302000
H	0.789140000	0.038619000	-2.863856000	H	3.257726000	1.718777000	-0.061529000
H	-0.052853000	-1.144535000	-3.885011000	H	4.357003000	0.762892000	-1.080811000
C	0.662477000	-1.907165000	-1.966859000	C	3.431324000	-0.318601000	0.583035000
H	0.223242000	-2.884395000	-2.216958000	H	3.830911000	-1.276838000	0.216956000
H	1.735600000	-2.014157000	-2.166026000	H	4.141302000	0.000552000	1.362784000
N	0.419348000	-1.564227000	-0.565387000	N	2.088846000	-0.483045000	1.098128000
C	0.996058000	-2.492523000	0.290618000	C	1.984120000	-1.436547000	2.092892000
O	1.744467000	-3.395167000	-0.134188000	O	2.914596000	-2.173802000	2.459680000
N	0.696163000	-2.375417000	1.624107000	N	0.729405000	-1.475183000	2.664485000
H	0.258694000	-1.485973000	1.884626000	H	0.009396000	-0.897991000	2.206617000
C	1.506008000	-3.080445000	2.590825000	C	0.345634000	-2.583077000	3.500495000
C	-1.555766000	1.017604000	-2.763393000	C	1.943725000	1.722129000	-2.259479000
H	-2.566227000	1.216938000	-2.402392000	H	1.160236000	1.421072000	-2.960296000
H	-1.569580000	1.041183000	-3.865150000	H	2.821709000	2.038527000	-2.846409000
C	-0.609771000	2.057637000	-2.181940000	C	1.418212000	2.851247000	-1.375981000
H	0.347175000	2.078751000	-2.724004000	H	2.249086000	3.379226000	-0.882540000
H	-1.036661000	3.058990000	-2.308111000	H	0.945800000	3.610145000	-2.017585000
N	-0.403091000	1.745931000	-0.768360000	N	0.485759000	2.291296000	-0.407789000
C	0.231579000	2.799943000	-0.102066000	C	-0.018467000	3.247247000	0.445338000
O	0.638984000	3.804836000	-0.712810000	O	0.278953000	4.454265000	0.378601000
N	0.380845000	2.678278000	1.247953000	N	-0.918485000	2.770733000	1.386656000
H	0.212707000	1.743112000	1.632218000	H	-0.959761000	1.746450000	1.466878000
C	1.185249000	3.648559000	1.951656000	C	-1.242664000	3.582188000	2.535674000
C	-2.253810000	-1.308091000	-2.306741000	C	2.416964000	-0.696541000	-2.277916000
H	-1.814782000	-2.274959000	-2.058782000	H	2.930708000	-1.445205000	-1.673547000
H	-2.697806000	-1.374243000	-3.313127000	H	3.035469000	-0.480216000	-3.163844000
C	-3.289088000	-0.951639000	-1.251417000	C	1.045010000	-1.259862000	-2.654809000
H	-3.983769000	-0.179445000	-1.614426000	H	0.557508000	-0.598570000	-3.391489000
H	-3.913316000	-1.825338000	-1.032504000	H	1.158574000	-2.241176000	-3.128396000
N	-2.587160000	-0.494590000	-0.053253000	N	0.242930000	-1.346740000	-1.449994000
C	-3.466214000	-0.273922000	1.012544000	C	-0.409691000	-2.547140000	-1.257691000
O	-4.678156000	-0.527590000	0.906554000	O	-0.324192000	-3.546151000	-1.992142000
N	-2.926442000	0.245862000	2.155753000	N	-1.221064000	-2.528880000	-0.141049000
H	-1.903676000	0.261760000	2.197994000	H	-1.182159000	-1.683918000	0.442393000
C	-3.710379000	0.293643000	3.365323000	C	-1.825909000	-3.737748000	0.351392000
H	0.965436000	-3.146114000	3.540897000	P	-3.252217000	-0.088262000	-0.184054000
H	1.712100000	-4.088053000	2.223046000	C	-4.810252000	-0.806728000	-0.938442000
H	2.475348000	-2.589843000	2.777826000	H	-5.488452000	-1.143300000	-0.146920000
H	1.146559000	3.428645000	3.022807000	H	-5.344246000	-0.087972000	-1.574874000
H	2.238391000	3.647142000	1.630989000	H	-4.542025000	-1.679933000	-1.542106000
H	0.802920000	4.660512000	1.782631000	H	-0.072098000	-3.427971000	2.927121000
H	-3.698806000	-0.654937000	3.927575000	H	1.230735000	-2.946200000	4.028335000
H	-3.328546000	1.083652000	4.021278000	H	-0.408949000	-2.263867000	4.228543000
H	-4.749680000	0.510860000	3.108205000	H	-2.236364000	3.314156000	2.915402000

P	4.256153000	0.561139000	0.212971000	H	-0.522590000	3.472955000	3.364216000
C	3.125299000	0.390037000	1.679105000	H	-1.245703000	4.632121000	2.234265000
H	3.654125000	-0.124229000	2.489481000	H	-2.711047000	-3.485860000	0.943643000
H	2.840741000	1.381329000	2.041265000	H	-2.114015000	-4.367955000	-0.494173000
H	2.206974000	-0.155148000	1.441956000	H	-1.139853000	-4.325442000	0.983272000
C	3.005181000	0.986118000	-1.093739000	C	-3.941656000	1.464514000	0.551982000
H	2.658075000	2.018355000	-0.986883000	H	-4.519477000	1.237483000	1.453663000
H	3.463317000	0.886212000	-2.084458000	H	-3.103719000	2.115573000	0.818430000
H	2.139129000	0.321931000	-1.022933000	H	-4.589634000	1.993512000	-0.158706000
C	4.516395000	-1.238638000	-0.190626000	C	-2.451691000	0.589404000	-1.698750000
H	5.032047000	-1.322219000	-1.154230000	H	-1.770755000	1.392746000	-1.401569000
H	5.167548000	-1.691155000	0.565715000	H	-1.841779000	-0.188738000	-2.166559000
H	3.589253000	-1.820706000	-0.236545000	H	-3.191190000	0.970400000	-2.413806000
⁴TS₅				²TS₅			
Mn	-0.040240000	-0.511252000	-0.165624000	Mn	0.131393000	-0.526438000	-0.190656000
O	0.741740000	0.771004000	0.679429000	O	0.652321000	1.091368000	0.509666000
N	-0.947419000	-2.130784000	-1.304818000	N	-0.452969000	-2.340447000	-1.175828000
C	-1.826405000	-2.837502000	-0.337939000	C	-1.086451000	-3.178898000	-0.127769000
H	-1.186520000	-3.456119000	0.294384000	H	-0.287670000	-3.631636000	0.463457000
H	-2.527541000	-3.494523000	-0.876191000	H	-1.682443000	-3.984337000	-0.585572000
C	-2.549761000	-1.827236000	0.545240000	C	-1.916988000	-2.284925000	0.783763000
H	-3.300611000	-1.268547000	-0.036492000	H	-2.817756000	-1.926919000	0.259619000
H	-3.109051000	-2.363006000	1.322276000	H	-2.270946000	-2.857446000	1.647774000
N	-1.554503000	-0.940734000	1.129876000	N	-1.066424000	-1.177918000	1.202489000
C	-2.021436000	-0.226484000	2.205948000	C	-1.458266000	-0.591347000	2.384079000
O	-3.183232000	-0.325938000	2.649946000	O	-2.452037000	-0.963676000	3.040661000
N	-1.093874000	0.608956000	2.809144000	N	-0.662654000	0.448821000	2.832721000
H	-0.265687000	0.810476000	2.252612000	H	-0.047070000	0.863802000	2.127016000
C	-1.527806000	1.594851000	3.769580000	C	-1.167793000	1.308529000	3.878381000
C	0.177975000	-2.964144000	-1.789975000	C	0.805438000	-2.908593000	-1.706536000
H	0.627364000	-2.429971000	-2.632615000	H	1.065010000	-2.322669000	-2.593902000
H	-0.194186000	-3.933580000	-2.159522000	H	0.661442000	-3.957283000	-2.015799000
C	1.228907000	-3.136052000	-0.705051000	C	1.925438000	-2.764908000	-0.686242000
H	0.883103000	-3.849296000	0.060780000	H	1.804547000	-3.494456000	0.130173000
H	2.124095000	-3.597248000	-1.142312000	H	2.882786000	-3.014965000	-1.160221000
N	1.528024000	-1.830942000	-0.127405000	N	1.923354000	-1.394084000	-0.184589000
C	2.651654000	-1.876851000	0.670918000	C	3.103625000	-1.082997000	0.472690000
O	3.340422000	-2.899104000	0.837568000	O	4.042289000	-1.884286000	0.620039000
N	3.002189000	-0.673150000	1.269027000	N	3.196549000	0.223274000	0.919557000
H	2.239807000	0.008367000	1.285689000	H	2.296828000	0.716712000	0.953123000
C	3.910220000	-0.706686000	2.394818000	C	4.214631000	0.560409000	1.887573000
C	-1.711744000	-1.532581000	-2.433432000	C	-1.408713000	-1.987104000	-2.262120000
H	-2.721031000	-1.299308000	-2.093375000	H	-2.424309000	-2.037607000	-1.867938000
H	-1.776007000	-2.246153000	-3.269550000	H	-1.320619000	-2.701247000	-3.095546000
C	-1.045604000	-0.208537000	-2.804039000	C	-1.161836000	-0.534404000	-2.670013000
H	-0.049114000	-0.389787000	-3.228488000	H	-0.187007000	-0.444138000	-3.169033000
H	-1.652019000	0.314994000	-3.550842000	H	-1.939427000	-0.210340000	-3.370786000
N	-0.896328000	0.589792000	-1.591329000	N	-1.153561000	0.284973000	-1.462876000
C	-2.043849000	1.310651000	-1.260652000	C	-2.418366000	0.690959000	-1.056029000
O	-3.097681000	1.264505000	-1.916965000	O	-3.469760000	0.380613000	-1.641288000
N	-1.904219000	2.124000000	-0.160579000	N	-2.416441000	1.516143000	0.052481000
H	-1.051154000	1.983086000	0.369408000	H	-1.525856000	1.548533000	0.536068000
C	-3.082537000	2.573603000	0.558781000	C	-3.608165000	1.608260000	0.879269000
P	1.700877000	2.520016000	-0.727105000	P	0.690394000	2.619884000	-0.929844000
C	1.835515000	4.047789000	-1.808121000	C	-0.027665000	3.879631000	-2.137784000
H	1.636450000	4.943345000	-1.210147000	H	-0.667920000	4.581465000	-1.594690000
H	2.823549000	4.149876000	-2.277806000	H	0.743509000	4.442121000	-2.683549000
H	1.073910000	3.996388000	-2.592704000	H	-0.655033000	3.339117000	-2.852420000
H	-1.748275000	2.575694000	3.315096000	H	-1.912403000	2.042607000	3.523221000
H	-2.444043000	1.231451000	4.238913000	H	-1.654612000	0.697989000	4.641718000

H	-0.762890000	1.745207000	4.541805000	H	-0.336942000	1.859398000	4.333588000
H	4.746452000	-1.368908000	2.160253000	H	5.155940000	0.086173000	1.600144000
H	4.294217000	0.302013000	2.586457000	H	4.354176000	1.647764000	1.910410000
H	3.444610000	-1.078939000	3.322449000	H	3.974048000	0.225371000	2.910275000
H	-2.840628000	3.479641000	1.125579000	H	-3.624934000	2.573408000	1.399499000
H	-3.861624000	2.809002000	-0.168659000	H	-4.481024000	1.542936000	0.227421000
H	-3.466952000	1.815432000	1.254377000	H	-3.659003000	0.806515000	1.628213000
C	3.191632000	2.769697000	0.345421000	C	1.805389000	3.710813000	0.054459000
H	2.978037000	3.488425000	1.142749000	H	1.216312000	4.340622000	0.728322000
H	3.446907000	1.8091118000	0.797383000	H	2.463673000	3.081583000	0.656086000
H	4.055414000	3.126004000	-0.229826000	H	2.412193000	4.357297000	-0.590043000
C	2.361054000	1.262126000	-1.902860000	C	1.864899000	1.754684000	-2.044307000
H	2.512023000	0.318849000	-1.370840000	H	2.533521000	1.136171000	-1.441107000
H	1.622692000	1.093001000	-2.690017000	H	1.297739000	1.096875000	-2.707596000
H	3.307575000	1.586515000	-2.352715000	H	2.443957000	2.461124000	-2.650665000
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⁶P₅				⁴P₅			
Mn	-0.023996000	-0.471933000	0.067756000	Mn	-0.149013000	0.571255000	0.008341000
O	1.163471000	1.428711000	0.620915000	O	-0.649249000	-1.505613000	0.139386000
N	-1.199739000	-2.417010000	-0.657771000	N	0.348594000	2.545912000	-0.423312000
C	-2.266144000	-2.520170000	0.356117000	C	0.925213000	3.068522000	0.843145000
H	-1.834744000	-2.991822000	1.243753000	H	0.091373000	3.206840000	1.536964000
H	-3.090315000	-3.165260000	-0.000496000	H	1.401003000	4.048424000	0.671811000
C	-2.802699000	-1.140370000	0.777536000	C	1.904000000	2.062657000	1.449864000
H	-3.293840000	-0.671362000	-0.089816000	H	2.833866000	2.032331000	0.858113000
H	-3.565261000	-1.287510000	1.550974000	H	2.201052000	2.419445000	2.446456000
N	-1.740017000	-0.268460000	1.268320000	N	1.264502000	0.754995000	1.502748000
C	-1.881450000	0.175316000	2.551886000	C	1.938660000	-0.135660000	2.271157000
O	-2.748913000	-0.171944000	3.373058000	O	2.970702000	0.095572000	2.933096000
N	-0.943582000	1.162540000	2.900375000	N	1.414275000	-1.441845000	2.238735000
H	-0.175190000	1.286385000	2.252061000	H	0.484003000	-1.531445000	1.854077000
C	-0.650151000	1.393446000	4.296697000	C	1.812780000	-2.393442000	3.247748000
C	-0.195167000	-3.493172000	-0.600389000	C	-0.907316000	3.231387000	-0.820194000
H	0.345428000	-3.489013000	-1.552027000	H	-1.091956000	2.959983000	-1.862831000
H	-0.676046000	-4.483315000	-0.491339000	H	-0.777547000	4.325655000	-0.773483000
C	0.832419000	-3.252684000	0.513484000	C	-2.095187000	2.772620000	0.010527000
H	0.326432000	-3.318825000	1.489305000	H	-2.060549000	3.227906000	1.014862000
H	1.586320000	-4.047053000	0.475117000	H	-3.016184000	3.158028000	-0.447967000
N	1.454982000	-1.940399000	0.379234000	N	-2.094521000	1.312532000	0.096128000
C	2.793794000	-1.955546000	0.171720000	C	-3.259758000	0.852193000	0.626374000
O	3.531227000	-2.945872000	0.018982000	O	-4.266670000	1.538023000	0.882044000
N	3.363859000	-0.651545000	0.121192000	N	-3.296166000	-0.542687000	0.873314000
H	2.809066000	0.010623000	0.652101000	H	-2.371622000	-0.927575000	1.029481000
C	4.795971000	-0.551429000	0.329188000	C	-4.310632000	-1.008683000	1.802529000
C	-1.676400000	-2.135112000	-2.027769000	C	1.321715000	2.569931000	-1.554061000
H	-2.695470000	-1.742890000	-1.977386000	H	2.327181000	2.418607000	-1.161567000
H	-1.708349000	-3.059318000	-2.630086000	H	1.286094000	3.555584000	-2.047236000
C	-0.804847000	-1.045239000	-2.682941000	C	1.037876000	1.400635000	-2.507813000
H	0.228196000	-1.408863000	-2.774796000	H	0.031939000	1.506081000	-2.940783000
H	-1.188925000	-0.834662000	-3.688765000	H	1.767407000	1.438853000	-3.327122000
N	-0.812324000	0.141947000	-1.830970000	N	1.106343000	0.152714000	-1.756935000
C	-1.911957000	0.925163000	-2.014649000	C	2.399164000	-0.260272000	-1.589526000
O	-2.696479000	0.892945000	-2.980193000	O	3.405790000	0.254791000	-2.115477000
N	-2.121127000	1.865528000	-0.969891000	N	2.539441000	-1.405505000	-0.776684000
H	-1.920283000	1.442337000	-0.059322000	H	1.805806000	-1.475465000	-0.078832000
C	-3.401090000	2.558684000	-0.986524000	C	3.851363000	-1.647905000	-0.187335000
P	1.642998000	2.447090000	-0.399325000	P	-1.126473000	-2.231155000	-1.114814000
C	0.462317000	3.788849000	-0.649060000	C	0.153787000	-3.274973000	-1.848774000
H	0.320423000	4.333001000	0.289688000	H	0.372386000	-4.108534000	-1.174134000
H	0.798054000	4.483174000	-1.425969000	H	-0.177920000	-3.671784000	-2.813876000
H	-0.495174000	3.323080000	-0.932996000	H	1.068238000	-2.681609000	-1.962157000

H	-0.295206000	2.420691000	4.449559000	H	1.713732000	-3.417641000	2.865763000
H	-1.572789000	1.247953000	4.861738000	H	2.859047000	-2.202171000	3.493722000
H	0.110251000	0.706628000	4.708889000	H	1.232088000	-2.322331000	4.184968000
H	5.165325000	0.417317000	-0.032612000	H	-4.348519000	-2.104782000	1.783800000
H	5.105473000	-0.664750000	1.382205000	H	-4.140101000	-0.686603000	2.842720000
H	5.278919000	-1.348200000	-0.238665000	H	-5.279576000	-0.610588000	1.496545000
H	-3.415919000	3.294716000	-0.175495000	H	3.920571000	-2.695021000	0.130730000
H	-3.525783000	3.072519000	-1.942338000	H	4.612356000	-1.448574000	-0.943096000
H	-4.262134000	1.884562000	-0.865245000	H	4.043228000	-1.011092000	0.687259000
C	3.193866000	3.223330000	0.160954000	C	-2.495216000	-3.356246000	-0.701055000
H	3.960555000	2.451700000	0.273231000	H	-3.348605000	-2.747669000	-0.391839000
H	3.546621000	3.973055000	-0.554352000	H	-2.771554000	-3.977013000	-1.559204000
H	3.037181000	3.701984000	1.131998000	H	-2.199052000	-4.005723000	0.127946000
C	1.994312000	1.708664000	-2.004299000	C	-1.759190000	-1.130061000	-2.396555000
H	1.047244000	1.282922000	-2.366500000	H	-0.895511000	-0.640210000	-2.851634000
H	2.405272000	2.433375000	-2.713878000	H	-2.346184000	-1.678362000	-3.140163000
H	2.694142000	0.881494000	-1.839783000	H	-2.369479000	-0.366800000	-1.902152000
²P₅				⁶R_S			
Mn	-0.088516000	0.577311000	-0.061617000	Mn	0.136724000	-0.447175000	-0.479168000
O	-0.721636000	-1.505536000	0.106058000	N	-0.307694000	-2.100796000	1.015361000
N	0.500260000	2.535295000	-0.509174000	C	0.910382000	-2.911662000	0.864976000
C	1.106030000	3.050589000	0.743091000	H	0.855034000	-3.373052000	-0.125962000
H	0.286721000	3.265551000	1.433530000	H	0.970130000	-3.717501000	1.617674000
H	1.653836000	3.988823000	0.550471000	C	2.172675000	-2.039003000	0.932107000
C	2.002718000	1.987856000	1.372833000	H	2.404556000	-1.761245000	1.969137000
H	2.920225000	1.858328000	0.774666000	H	3.029051000	-2.632807000	0.583509000
H	2.334958000	2.336147000	2.359778000	N	2.003420000	-0.832984000	0.129850000
N	1.250303000	0.744505000	1.460867000	C	3.012651000	0.084400000	0.216090000
C	1.794784000	-0.151843000	2.320167000	O	3.977104000	0.010178000	0.985043000
O	2.796603000	0.036507000	3.040763000	N	2.840682000	1.185703000	-0.649520000
N	1.173041000	-1.414351000	2.322288000	H	2.441036000	0.894829000	-1.542208000
H	0.264492000	-1.457801000	1.882160000	C	3.957355000	2.112311000	-0.756245000
C	1.423423000	-2.324182000	3.414576000	C	-1.556121000	-2.735705000	0.530407000
C	-0.728869000	3.262104000	-0.8999955000	H	-2.387332000	-2.360102000	1.130634000
H	-0.952788000	2.966629000	-1.929527000	H	-1.511017000	-3.829247000	0.653607000
H	-0.557456000	4.352700000	-0.891968000	C	-1.823523000	-2.325159000	-0.929523000
C	-1.911104000	2.877401000	-0.021230000	H	-1.100568000	-2.809175000	-1.594835000
H	-1.831978000	3.364548000	0.964708000	H	-2.834110000	-2.639105000	-1.211670000
H	-2.830620000	3.278473000	-0.468624000	N	-1.678231000	-0.875111000	-1.075055000
N	-1.959601000	1.422142000	0.115924000	C	-2.822293000	-0.145926000	-0.838636000
C	-3.159616000	1.012739000	0.620226000	O	-3.894277000	-0.640590000	-0.448424000
O	-4.138625000	1.743183000	0.856734000	N	-2.710571000	1.205890000	-1.124266000
N	-3.264858000	-0.377156000	0.859033000	H	-1.767024000	1.552485000	-1.246836000
H	-2.360255000	-0.814672000	0.991704000	C	-3.646330000	2.146541000	-0.528838000
C	-4.295101000	-0.803478000	1.788746000	C	-0.456979000	-1.392707000	2.303686000
C	1.473887000	2.496792000	-1.635201000	H	0.539239000	-1.215640000	2.712553000
H	2.475750000	2.350832000	-1.230247000	H	-1.016842000	-2.007489000	3.026720000
H	1.457254000	3.452809000	-2.184611000	C	-1.134468000	-0.033197000	2.093058000
C	1.170920000	1.281230000	-2.515886000	H	-2.187670000	-0.174983000	1.805573000
H	0.182901000	1.400272000	-2.985996000	H	-1.139650000	0.524317000	3.037579000
H	1.923173000	1.217230000	-3.311410000	N	-0.405740000	0.693759000	1.066150000
N	1.156968000	0.089624000	-1.672807000	C	-0.569377000	2.039240000	1.047372000
C	2.412950000	-0.427244000	-1.489310000	O	-1.278904000	2.706126000	1.818176000
O	3.452684000	-0.020675000	-2.041600000	N	0.130775000	2.660626000	-0.012152000
N	2.459029000	-1.547234000	-0.637382000	H	1.041040000	2.231464000	-0.185701000
H	1.693525000	-1.566945000	0.028282000	C	0.156560000	4.113354000	-0.018735000
C	3.732952000	-1.852371000	0.002904000	H	3.646746000	2.975043000	-1.353674000
P	-1.207851000	-2.215974000	-1.146773000	H	4.236920000	2.451496000	0.242872000
C	0.031596000	-3.325188000	-1.856722000	H	4.850308000	1.663202000	-1.214894000
H	0.180663000	-4.179329000	-1.188955000	H	-3.305873000	2.498124000	0.453512000
H	-0.283965000	-3.688400000	-2.840180000	H	-3.775510000	3.012153000	-1.189480000
H	0.980245000	-2.781204000	-1.925644000	H	-4.606100000	1.639119000	-0.419714000

H	1.241050000	-3.358131000	3.095033000	H	0.715596000	4.545616000	0.825885000
H	2.469314000	-2.218229000	3.708720000	H	0.610300000	4.458145000	-0.953831000
H	0.805513000	-2.130479000	4.309633000	H	-0.865495000	4.492462000	0.043159000
H	-4.397285000	-1.894943000	1.748587000	S	1.187254000	-1.179935000	-2.429353000
H	-4.095123000	-0.514924000	2.833824000				
H	-5.242170000	-0.343417000	1.501522000				
H	3.736688000	-2.898437000	0.331467000				
H	4.530341000	-1.700180000	-0.725853000				
H	3.922404000	-1.217303000	0.879324000				
C	-2.649444000	-3.256644000	-0.761659000				
H	-3.462485000	-2.595629000	-0.449939000				
H	-2.961003000	-3.846198000	-1.629733000				
H	-2.405313000	-3.934238000	0.061741000				
C	-1.756508000	-1.086095000	-2.444347000				
H	-0.862934000	-0.630017000	-2.875243000				
H	-2.346030000	-1.601952000	-3.208713000				
H	-2.348899000	-0.300672000	-1.962760000				
⁴R_S				²R_S			
Mn	0.229745000	-0.395173000	-0.511963000	Mn	0.175624000	-0.366010000	-0.446351000
N	0.070462000	-2.290974000	0.631917000	N	-0.273336000	-2.219792000	0.723516000
C	1.327558000	-2.990032000	0.322954000	C	0.933695000	-3.041421000	0.564803000
H	1.244233000	-3.333176000	-0.714156000	H	0.901288000	-3.451358000	-0.449796000
H	1.461601000	-3.877824000	0.963054000	H	0.943254000	-3.887198000	1.272868000
C	2.499581000	-2.035746000	0.453695000	C	2.168728000	-2.183527000	0.713005000
H	2.797843000	-1.926977000	1.506582000	H	2.376467000	-1.972831000	1.773098000
H	3.376335000	-2.472904000	-0.041208000	H	3.041314000	-2.741352000	0.356975000
N	2.158483000	-0.736658000	-0.132596000	N	2.004207000	-0.934267000	-0.042053000
C	3.250482000	0.123285000	-0.012394000	C	3.234987000	-0.255588000	-0.052564000
O	4.335897000	-0.246249000	0.469369000	O	4.262437000	-0.760216000	0.432752000
N	3.064819000	1.415650000	-0.427272000	N	3.263131000	1.005565000	-0.575296000
H	2.280124000	1.571442000	-1.059738000	H	2.467035000	1.281107000	-1.148277000
C	4.207388000	2.293931000	-0.518427000	C	4.536592000	1.650755000	-0.791455000
C	-1.121286000	-3.043217000	0.170092000	C	-1.465734000	-2.892847000	0.153608000
H	-1.969486000	-2.813896000	0.816124000	H	-2.360670000	-2.572635000	0.688486000
H	-0.928523000	-4.125542000	0.209527000	H	-1.368929000	-3.984700000	0.248647000
C	-1.459921000	-2.524764000	-1.226014000	C	-1.597966000	-2.396895000	-1.283366000
H	-0.686997000	-2.832873000	-1.944636000	H	-0.770769000	-2.775190000	-1.899403000
H	-2.421459000	-2.926021000	-1.562311000	H	-2.541299000	-2.735573000	-1.723798000
N	-1.496757000	-1.074149000	-1.162427000	N	-1.527757000	-0.949338000	-1.241647000
C	-2.731581000	-0.537640000	-0.843695000	C	-2.737158000	-0.324468000	-1.003365000
O	-3.691963000	-1.224919000	-0.448168000	O	-3.775796000	-0.946726000	-0.704042000
N	-2.826587000	0.819155000	-1.022422000	N	-2.727129000	1.044479000	-1.138379000
H	-1.976433000	1.282261000	-1.325440000	H	-1.817873000	1.448738000	-1.331857000
C	-3.848153000	1.590529000	-0.343746000	C	-3.701430000	1.861845000	-0.443378000
C	-0.052495000	-1.795075000	2.019994000	C	-0.502323000	-1.695263000	2.083520000
H	0.937482000	-1.494962000	2.364818000	H	0.466584000	-1.490029000	2.542635000
H	-0.431460000	-2.587988000	2.682816000	H	-1.035789000	-2.431067000	2.704994000
C	-0.960893000	-0.573340000	2.034388000	C	-1.271165000	-0.387925000	1.964898000
H	-1.991538000	-0.846038000	1.767827000	H	-2.282802000	-0.565941000	1.576460000
H	-0.996280000	-0.153684000	3.043611000	H	-1.380150000	0.084753000	2.943561000
N	-0.425570000	0.429362000	1.108674000	N	-0.526295000	0.497442000	1.063386000
C	-0.852511000	1.720195000	1.386082000	C	-0.638499000	1.849198000	1.398133000
O	-1.608277000	1.968055000	2.343352000	O	-1.382664000	2.240829000	2.313717000
N	-0.358344000	2.725131000	0.595398000	N	0.134223000	2.728099000	0.691247000
H	0.094148000	2.446263000	-0.269943000	H	0.536738000	2.386028000	-0.178132000
C	-0.955074000	4.040091000	0.651828000	C	-0.122584000	4.146325000	0.807540000
H	3.855946000	3.314329000	-0.700900000	H	4.359741000	2.694308000	-1.069839000
H	4.768257000	2.270457000	0.419627000	H	5.131225000	1.619372000	0.125678000
H	4.906501000	2.015325000	-1.323349000	H	5.134066000	1.173604000	-1.584277000
H	-3.537997000	1.895065000	0.665131000	H	-3.348780000	2.169764000	0.551655000
H	-4.084111000	2.487863000	-0.927148000	H	-3.929153000	2.760662000	-1.028812000
H	-4.745984000	0.974418000	-0.264078000	H	-4.615106000	1.275645000	-0.329621000

H	-0.248212000	4.777353000	0.258234000	H	0.715684000	4.696020000	0.369507000
H	-1.889934000	4.113134000	0.073221000	H	-1.048511000	4.458023000	0.299451000
H	-1.187010000	4.280578000	1.691058000	H	-0.219173000	4.414200000	1.862036000
S	0.388748000	1.077857000	-2.134594000	S	0.498190000	1.052396000	-2.049162000
⁶RC_S				⁴RC_S			
Mn	-1.707416000	-0.074308000	-0.018746000	Mn	1.570729000	0.131996000	-0.223828000
N	-0.994644000	-0.714325000	2.019255000	N	1.807817000	-1.713135000	-1.529132000
C	0.050261000	0.301440000	2.261977000	C	1.398145000	-1.163035000	-2.831451000
H	0.896597000	0.049308000	1.615885000	H	0.324518000	-0.960720000	-2.759444000
H	0.406417000	0.278590000	3.305503000	H	1.554901000	-1.883066000	-3.653821000
C	-0.450583000	1.703554000	1.896970000	C	2.134827000	0.149699000	-3.132865000
H	-1.160086000	2.072355000	2.652561000	H	3.163226000	-0.042611000	-3.466871000
H	0.399205000	2.395201000	1.919066000	H	1.635961000	0.645730000	-3.977704000
N	-1.069292000	1.682266000	0.573902000	N	2.149848000	1.004215000	-1.952338000
C	-1.408558000	2.897038000	0.068893000	C	2.927846000	2.122898000	-2.042025000
O	-1.162767000	3.988382000	0.608035000	O	3.667589000	2.400843000	-2.992735000
N	-2.109263000	2.844502000	-1.154296000	N	2.847275000	2.958006000	-0.905349000
H	-1.842710000	2.053722000	-1.739184000	H	1.896775000	2.985983000	-0.536070000
C	-2.266255000	4.095269000	-1.878505000	C	3.496409000	4.256597000	-1.004545000
C	-0.509683000	-2.109449000	1.868011000	C	0.884020000	-2.720605000	-0.955119000
H	-1.270999000	-2.781529000	2.270265000	H	1.465486000	-3.414020000	-0.344163000
H	0.422408000	-2.263681000	2.430170000	H	0.385145000	-3.293202000	-1.751721000
C	-0.330903000	-2.445918000	0.377014000	C	-0.128591000	-2.022876000	-0.036903000
H	0.544150000	-1.922072000	-0.019589000	H	-0.817858000	-1.423759000	-0.634966000
H	-0.181426000	-3.522725000	0.250332000	H	-0.707255000	-2.774853000	0.507556000
N	-1.505581000	-1.992416000	-0.365170000	N	0.558925000	-1.125483000	0.896152000
C	-2.537325000	-2.907101000	-0.546119000	C	0.998701000	-1.715274000	2.062816000
O	-2.555551000	-4.010615000	0.017936000	O	0.890340000	-2.927748000	2.309288000
N	-3.521172000	-2.478955000	-1.397720000	N	1.520654000	-0.827733000	2.990149000
H	-3.453968000	-1.521600000	-1.721932000	H	1.759739000	0.088971000	2.631974000
C	-4.843349000	-3.079960000	-1.367867000	C	2.381116000	-1.324703000	4.052781000
C	-2.185132000	-0.603079000	2.894738000	C	3.235386000	-2.070769000	-1.399231000
H	-2.269764000	0.435298000	3.218816000	H	3.809309000	-1.434221000	-2.074344000
H	-2.063848000	-1.231626000	3.790433000	H	3.405326000	-3.119616000	-1.690358000
C	-3.455946000	-0.966580000	2.119526000	C	3.719533000	-1.806188000	0.031253000
H	-3.456077000	-2.041584000	1.878668000	H	3.252199000	-2.518113000	0.728623000
H	-4.335455000	-0.787529000	2.750542000	H	4.801914000	-1.973178000	0.089966000
N	-3.492232000	-0.151862000	0.919277000	N	3.385069000	-0.436420000	0.383800000
C	-4.698616000	-0.018543000	0.312314000	C	4.082429000	0.114276000	1.407904000
O	-5.767551000	-0.536958000	0.680635000	O	4.968443000	-0.439960000	2.077660000
N	-4.644391000	0.754579000	-0.862442000	N	3.660445000	1.430581000	1.706152000
H	-3.935920000	1.485303000	-0.853776000	H	3.452797000	1.969479000	0.863083000
C	-5.897759000	1.136283000	-1.483724000	C	4.439461000	2.160476000	2.692343000
H	-2.938877000	3.931716000	-2.726058000	H	3.444950000	4.752921000	-0.030457000
H	-2.701885000	4.841485000	-1.211765000	H	4.543779000	4.114470000	-1.277305000
H	-1.315954000	4.504187000	-2.254597000	H	3.043131000	4.910732000	-1.763402000
H	-5.516405000	-2.529199000	-0.699240000	H	3.432487000	-1.368849000	3.741817000
H	-5.270014000	-3.097729000	-2.377119000	H	2.297626000	-0.675828000	4.932447000
H	-4.737651000	-4.105683000	-1.010765000	H	2.039665000	-2.326256000	4.318586000
H	-6.461528000	1.890303000	-0.910852000	H	5.469233000	2.373496000	2.366464000
H	-5.696937000	1.536492000	-2.483063000	H	3.936404000	3.107608000	2.913357000
H	-6.534766000	0.254152000	-1.571981000	H	4.506452000	1.570391000	3.608698000
S	-0.765542000	-0.179686000	-2.156962000	S	-0.200467000	1.563905000	-0.728804000
P	3.466310000	-0.8366685000	-0.067253000	P	-3.980216000	-0.635062000	1.387786000
C	3.365528000	1.003058000	0.106129000	C	-3.552684000	-1.212250000	-0.319908000
C	2.207462000	1.685112000	-0.314345000	C	-3.540508000	-2.590726000	-0.581637000
C	4.359004000	1.729637000	0.787931000	C	-3.162022000	-0.330261000	-1.341046000
C	2.059166000	3.052889000	-0.067931000	C	-3.136892000	-3.079849000	-1.826499000
H	1.394281000	1.157757000	-0.807501000	H	-3.829871000	-3.285161000	0.203211000
C	4.211364000	3.096656000	1.024452000	C	-2.754030000	-0.815415000	-2.582944000
H	5.259152000	1.226712000	1.129994000	H	-3.139900000	0.738183000	-1.157522000
C	3.060471000	3.762013000	0.597936000	C	-2.739311000	-2.191440000	-2.827636000

H	1.141431000	3.556603000	-0.352639000	H	-3.121854000	-4.151093000	-2.009379000
H	4.994996000	3.639025000	1.548446000	H	-2.421062000	-0.117598000	-3.345503000
H	2.933870000	4.822981000	0.795508000	H	-2.411031000	-2.569252000	-3.792622000
C	5.298087000	-1.097569000	-0.244493000	C	-5.173692000	0.724374000	0.978362000
C	6.098878000	-0.335306000	-1.113885000	C	-5.095740000	2.001283000	1.558371000
C	5.907952000	-2.126060000	0.488122000	C	-6.260378000	0.454893000	0.125088000
C	7.461209000	-0.596817000	-1.248273000	C	-6.064146000	2.973002000	1.292816000
H	5.648928000	0.478350000	-1.675915000	H	-4.267295000	2.250855000	2.214044000
C	7.273735000	-2.394715000	0.354415000	C	-7.223674000	1.424508000	-0.145323000
H	5.304780000	-2.721645000	1.169098000	H	-6.338595000	-0.521533000	-0.346861000
C	8.052248000	-1.630700000	-0.514574000	C	-7.131249000	2.690514000	0.440261000
H	8.064282000	0.004134000	-1.924236000	H	-5.975941000	3.956444000	1.747694000
H	7.727011000	-3.197424000	0.930309000	H	-8.046385000	1.194347000	-0.817870000
H	9.114570000	-1.835536000	-0.619804000	H	-7.880889000	3.448565000	0.229164000
C	2.943629000	-1.068636000	-1.832304000	C	-2.459331000	0.324161000	1.834201000
H	3.119368000	-2.112609000	-2.110391000	H	-2.531485000	0.676446000	2.868187000
H	1.871984000	-0.868374000	-1.937882000	H	-1.578230000	-0.321424000	1.759046000
H	3.493921000	-0.418272000	-2.519395000	H	-2.285832000	1.178237000	1.172111000
⁶Ts_s				⁴Ts_s			
Mn	1.719694000	0.038088000	-0.731913000	Mn	1.510614000	0.197274000	-0.632355000
N	3.976223000	-0.447282000	-0.433298000	N	3.753627000	-0.084474000	-0.613957000
C	4.598704000	0.846450000	-0.768300000	C	4.254109000	1.306984000	-0.566205000
H	4.599148000	0.934758000	-1.859989000	H	4.188745000	1.715453000	-1.579882000
H	5.646374000	0.882951000	-0.423601000	H	5.310020000	1.328731000	-0.250359000
C	3.799958000	2.009095000	-0.192825000	C	3.375903000	2.154687000	0.347727000
H	3.834129000	1.980052000	0.907142000	H	3.444592000	1.777956000	1.377986000
H	4.276196000	2.950869000	-0.487368000	H	3.738295000	3.186497000	0.352771000
N	2.413211000	1.965891000	-0.669159000	N	1.987588000	2.114102000	-0.121851000
C	1.793281000	3.184480000	-0.545503000	C	1.401334000	3.363566000	-0.204608000
O	2.356138000	4.239931000	-0.200144000	O	1.981907000	4.439570000	0.014742000
N	0.419821000	3.182789000	-0.778121000	N	0.047550000	3.362604000	-0.520521000
H	0.056465000	2.390632000	-1.303786000	H	-0.296074000	2.511714000	-0.956995000
C	-0.250419000	4.452161000	-0.959644000	C	-0.560898000	4.600377000	-0.964018000
C	4.289919000	-1.524988000	-1.398184000	C	4.120833000	-0.798613000	-1.868083000
H	4.227731000	-2.486508000	-0.883564000	H	4.249137000	-1.859272000	-1.641829000
H	5.310729000	-1.410660000	-1.797867000	H	5.068021000	-0.409737000	-2.271613000
C	3.213514000	-1.536648000	-2.488405000	C	2.942389000	-0.693808000	-2.830942000
H	3.257264000	-0.608710000	-3.075050000	H	2.812490000	0.344828000	-3.168255000
H	3.368630000	-2.381276000	-3.168263000	H	3.102334000	-1.325563000	-3.710861000
N	1.911681000	-1.620969000	-1.834132000	N	1.755426000	-1.111037000	-2.095769000
C	1.502292000	-2.900260000	-1.537854000	C	1.496873000	-2.458106000	-2.125128000
O	2.141881000	-3.924655000	-1.837150000	O	2.169112000	-3.289259000	-2.762007000
N	0.314716000	-2.971231000	-0.829777000	N	0.424801000	-2.849621000	-1.336429000
H	-0.266537000	-2.140649000	-0.899315000	H	-0.239824000	-2.111620000	-1.131676000
C	-0.359265000	-4.242689000	-0.692193000	C	-0.101544000	-4.190508000	-1.458152000
C	4.134886000	-0.857375000	0.982645000	C	4.102815000	-0.876897000	0.602438000
H	4.388990000	0.016512000	1.584941000	H	4.365276000	-0.193025000	1.412287000
H	4.954117000	-1.586600000	1.077418000	H	4.981485000	-1.503532000	0.392545000
C	2.798673000	-1.403044000	1.518693000	C	2.879171000	-1.680320000	1.067390000
H	2.509065000	-2.301568000	0.962124000	H	2.577502000	-2.400648000	0.300407000
H	2.927499000	-1.666688000	2.575556000	H	3.136777000	-2.224560000	1.983323000
N	1.765305000	-0.390414000	1.334418000	N	1.800038000	-0.723910000	1.282883000
C	1.762646000	0.568925000	2.307688000	C	1.849799000	-0.134533000	2.510997000
O	2.495251000	0.590816000	3.312762000	O	2.523558000	-0.509623000	3.488347000
N	0.787601000	1.570889000	2.115290000	N	1.023078000	1.005825000	2.621759000
H	0.537657000	1.686174000	1.139609000	H	1.016040000	1.530410000	1.749151000
C	0.998385000	2.854778000	2.776062000	C	1.208953000	1.840976000	3.796406000
P	-2.605415000	0.492810000	0.138261000	P	-2.365928000	0.281451000	0.327461000
C	-2.327170000	-3.275652000	2.806839000	C	-2.334149000	-3.920931000	2.246270000
C	-1.188771000	-2.557561000	2.435614000	C	-1.150983000	-3.210909000	2.031501000
C	-1.296835000	-1.432458000	1.618491000	C	-1.178160000	-1.941236000	1.454695000
C	-2.562595000	-1.004192000	1.179571000	C	-2.411150000	-1.361567000	1.092921000

C	-3.707419000	-1.726903000	1.558833000	C	-3.602693000	-2.075500000	1.323596000
C	-3.586315000	-2.858791000	2.365247000	C	-3.560058000	-3.347431000	1.891370000
H	-2.236005000	-4.159454000	3.433099000	H	-2.304890000	-4.913476000	2.688439000
H	-0.201287000	-2.873463000	2.757637000	H	-0.190562000	-3.640123000	2.301662000
H	-0.381059000	-0.917062000	1.330587000	H	-0.231567000	-1.424919000	1.288878000
H	-4.690199000	-1.407760000	1.225898000	H	-4.559802000	-1.635850000	1.062884000
H	-4.476652000	-3.413499000	2.650632000	H	-4.486517000	-3.889965000	2.062198000
C	-6.811779000	0.819057000	-1.773177000	C	-6.379119000	1.406911000	-1.642226000
C	-6.031143000	-0.329662000	-1.940863000	C	-5.816079000	0.138384000	-1.841124000
C	-4.781635000	-0.423463000	-1.335139000	C	-4.636527000	-0.219822000	-1.201627000
C	-4.293510000	0.622592000	-0.524532000	C	-3.992997000	0.675454000	-0.308520000
C	-5.083169000	1.777268000	-0.373439000	C	-4.559843000	1.962658000	-0.137109000
C	-6.330257000	1.871412000	-0.992821000	C	-5.735555000	2.314266000	-0.792657000
H	-7.783309000	0.894522000	-2.253710000	H	-7.296711000	1.686774000	-2.151634000
H	-6.393441000	-1.149843000	-2.554629000	H	-6.297163000	-0.570350000	-2.510425000
H	-4.172371000	-1.310237000	-1.486800000	H	-4.197555000	-1.195296000	-1.389438000
H	-4.728908000	2.606004000	0.231661000	H	-4.081111000	2.685567000	0.515930000
H	-6.928122000	2.769473000	-0.861007000	H	-6.157850000	3.303830000	-0.635824000
C	-2.390025000	1.873827000	1.320065000	C	-1.954801000	1.476838000	1.626691000
H	-2.214384000	2.811768000	0.787375000	H	-1.634866000	2.421572000	1.175818000
H	-3.253388000	1.966697000	1.987074000	H	-2.802925000	1.624272000	2.301604000
H	-1.495983000	1.647367000	1.911251000	H	-1.099245000	1.074904000	2.183531000
H	0.034398000	4.971734000	-1.888579000	H	-1.647058000	4.466215000	-1.007336000
H	-1.333056000	4.284372000	-0.980457000	H	-0.323095000	5.395664000	-0.254415000
H	-0.003872000	5.115855000	-0.127610000	H	-0.212430000	4.929577000	-1.956041000
H	0.384229000	-5.013564000	-0.478840000	H	-0.714714000	-4.340036000	-2.361940000
H	-1.071226000	-4.186452000	0.136829000	H	0.732675000	-4.893340000	-1.508742000
H	-0.902271000	-4.549899000	-1.601286000	H	-0.714509000	-4.415340000	-0.579666000
H	0.040038000	3.378434000	2.877408000	H	0.421409000	2.602178000	3.821150000
H	1.408155000	2.661464000	3.768229000	H	1.139938000	1.220529000	4.691919000
H	1.688239000	3.504140000	2.221064000	H	2.185542000	2.348202000	3.822147000
S	-0.577867000	0.165698000	-1.614464000	S	-0.759083000	0.283296000	-1.266988000
⁶P_s							
Mn	1.585638000	0.133365000	-0.510161000	⁴P_s	Mn	1.585963000	0.146835000
N	3.944839000	-0.216466000	-0.375776000	N	3.782798000	-0.198954000	
C	4.448787000	1.166524000	-0.418628000	C	4.339027000	1.168935000	
H	4.471081000	1.473246000	-1.469534000	H	4.288946000	1.490284000	
H	5.481943000	1.228027000	-0.029744000	H	5.397967000	1.180649000	
C	3.542166000	2.146675000	0.337231000	C	3.504091000	2.139566000	
H	3.543238000	1.879274000	1.406336000	H	3.587786000	1.867394000	
H	3.968218000	3.152940000	0.261397000	H	3.912028000	3.150344000	
N	2.173318000	2.138085000	-0.186350000	N	2.103479000	2.099915000	
C	1.628034000	3.376612000	-0.365726000	C	1.535781000	3.338355000	
O	2.186474000	4.472658000	-0.187619000	O	2.097984000	4.433735000	
N	0.268669000	3.351098000	-0.740725000	N	0.169370000	3.314130000	
H	-0.033378000	2.480387000	-1.162135000	H	-0.126417000	2.449343000	
C	-0.284475000	4.540967000	-1.358910000	C	-0.407216000	4.516463000	
C	4.289518000	-1.023000000	-1.563155000	C	4.111234000	-1.027838000	
H	4.264792000	-2.078941000	-1.284050000	H	4.169259000	-2.073100000	
H	5.307435000	-0.788221000	-1.921854000	H	5.090806000	-0.738749000	
C	3.228639000	-0.842283000	-2.663425000	C	2.967465000	-0.935098000	
H	3.234822000	0.196581000	-3.021355000	H	2.906685000	0.087450000	
H	3.483248000	-1.497031000	-3.506716000	H	3.148591000	-1.622418000	
N	1.903334000	-1.138122000	-2.128201000	N	1.725446000	-1.255502000	
C	1.633413000	-2.473212000	-2.055339000	C	1.408008000	-2.581840000	
O	2.367335000	-3.399830000	-2.449330000	O	1.994700000	-3.468942000	
N	0.416276000	-2.764122000	-1.416277000	N	0.344110000	-2.917941000	
H	-0.260541000	-2.012074000	-1.458154000	H	-0.250785000	-2.129297000	
C	-0.124158000	-4.102722000	-1.499285000	C	-0.345580000	-4.172981000	
C	4.155093000	-0.925229000	0.905908000	C	4.089467000	-0.911155000	
H	4.393488000	-0.193978000	1.683497000	H	4.358677000	-0.178024000	
H	5.007831000	-1.619763000	0.831522000	H	4.953996000	-1.577598000	

C	2.860618000	-1.644659000	1.338768000	C	2.837025000	-1.651079000	1.242721000	
H	2.582300000	-2.397224000	0.591184000	H	2.513826000	-2.400346000	0.511746000	
H	3.031672000	-2.150001000	2.297052000	H	3.076147000	-2.154748000	2.187305000	
N	1.790926000	-0.651030000	1.435914000	N	1.779121000	-0.657509000	1.403569000	
C	1.769455000	0.017352000	2.621917000	C	1.852786000	0.016126000	2.584019000	
O	2.319529000	-0.323897000	3.682942000	O	2.492893000	-0.315176000	3.598900000	
N	1.000669000	1.208304000	2.573524000	N	1.078854000	1.203928000	2.593789000	
H	1.159016000	1.702740000	1.693758000	H	1.161781000	1.677013000	1.692780000	
C	1.074831000	2.077930000	3.736564000	C	1.272089000	2.094974000	3.726211000	
P	-2.394731000	0.285957000	0.033546000	P	-2.264250000	0.308014000	0.132748000	
C	-2.303965000	-3.905657000	1.974652000	C	-2.365870000	-3.830397000	2.181985000	
C	-1.169160000	-3.092035000	1.956341000	C	-1.198996000	-3.063689000	2.147389000	
C	-1.221819000	-1.820234000	1.388119000	C	-1.196588000	-1.805896000	1.545859000	
C	-2.427077000	-1.351457000	0.836591000	C	-2.380383000	-1.307075000	0.972765000	
C	-3.563061000	-2.176593000	0.843010000	C	-3.548729000	-2.085188000	0.993993000	
C	-3.499372000	-3.447857000	1.414992000	C	-3.538952000	-3.341225000	1.602157000	
H	-2.255900000	-4.898537000	2.414225000	H	-2.359836000	-4.812239000	2.648286000	
H	-0.227227000	-3.439965000	2.368847000	H	-0.273780000	-3.440386000	2.572525000	
H	-0.301672000	-1.234399000	1.363742000	H	-0.250960000	-1.257549000	1.494607000	
H	-4.492974000	-1.834472000	0.400878000	H	-4.461012000	-1.720936000	0.533135000	
H	-4.381950000	-4.081925000	1.416357000	H	-4.445797000	-3.940047000	1.614178000	
C	-6.798258000	1.365653000	-0.958210000	C	-6.557354000	1.473497000	-1.190240000	
C	-5.858510000	1.259620000	-1.983985000	C	-5.554454000	1.307555000	-2.146111000	
C	-4.533960000	0.926344000	-1.692415000	C	-4.263351000	0.946492000	-1.755608000	
C	-4.138124000	0.699434000	-0.368520000	C	-3.963701000	0.751275000	-0.401265000	
C	-5.091068000	0.807400000	0.659596000	C	-4.979662000	0.920221000	0.555674000	
C	-6.413132000	1.136893000	0.365766000	C	-6.268776000	1.277047000	0.162924000	
H	-7.828258000	1.625814000	-1.186899000	H	-7.561219000	1.755529000	-1.496201000	
H	-6.153537000	1.436798000	-3.014336000	H	-5.774015000	1.459613000	-3.199066000	
H	-3.796400000	0.844654000	-2.485482000	H	-3.477669000	0.819554000	-2.494447000	
H	-4.805571000	0.619096000	1.690927000	H	-4.768742000	0.759414000	1.609175000	
H	-7.141345000	1.216121000	1.168123000	H	-7.046048000	1.403404000	0.911432000	
C	-1.893886000	1.481660000	1.296457000	C	-1.824314000	1.515556000	1.404810000	
H	-1.632260000	2.424257000	0.805369000	H	-1.537309000	2.454426000	0.920846000	
H	-2.696343000	1.633392000	2.023723000	H	-2.663630000	1.666702000	2.089399000	
H	-0.991695000	1.125407000	1.816088000	H	-0.947134000	1.156701000	1.963694000	
H	-1.374865000	4.447419000	-1.413141000	H	-1.498158000	4.415598000	-1.257941000	
H	-0.026024000	5.406814000	-0.746682000	H	-0.140456000	5.368094000	-0.599822000	
H	0.097302000	4.730734000	-2.375977000	H	-0.052486000	4.737482000	-2.248802000	
H	-0.873556000	-4.242623000	-0.712754000	H	-0.938996000	-4.410641000	-0.519712000	
H	-0.591523000	-4.333617000	-2.471973000	H	-1.018288000	-4.171450000	-2.284545000	
H	0.690768000	-4.814355000	-1.353044000	H	0.398818000	-4.955222000	-1.569582000	
H	0.376169000	2.910544000	3.601065000	H	0.560138000	2.924212000	3.651240000	
H	0.795658000	1.514046000	4.629390000	H	1.091837000	1.546594000	4.653460000	
H	2.080899000	2.487329000	3.910041000	H	2.289198000	2.510369000	3.785095000	
S	-1.197562000	0.298974000	-1.593841000	S	-0.981514000	0.223904000	-1.436880000	
PCy₃								
P	-0.121462000	0.039829000	-0.969043000	PPh₃	P	-0.000810000	-0.000504000	-1.265798000
C	-1.781992000	-0.119860000	-0.043660000	C	1.315658000	-1.009722000	-0.440129000	
C	-2.869555000	0.624665000	-0.853868000	C	1.630614000	-2.249160000	-1.020767000	
C	-2.252228000	-1.563904000	0.225379000	C	2.005638000	-0.612669000	0.714992000	
H	-1.672799000	0.377661000	0.931526000	C	2.598060000	-3.077872000	-0.453553000	
C	-4.231093000	0.608925000	-0.143509000	H	1.114175000	-2.565615000	-1.923615000	
H	-2.966180000	0.136953000	-1.833813000	C	2.981818000	-1.437845000	1.276449000	
H	-2.566185000	1.656013000	-1.060164000	H	1.779866000	0.342759000	1.177108000	
C	-3.620762000	-1.594456000	0.927877000	C	3.278754000	-2.672126000	0.696444000	
H	-2.323909000	-2.109858000	-0.726738000	H	2.826657000	-4.034937000	-0.913767000	
H	-1.528220000	-2.102830000	0.843528000	H	3.509231000	-1.115534000	2.169971000	
C	-4.689697000	-0.827179000	0.140065000	H	4.038799000	-3.312389000	1.134796000	
H	-4.976864000	1.137282000	-0.749712000	C	0.215044000	1.643239000	-0.439676000	
H	-4.151197000	1.158811000	0.805452000	C	-0.462106000	2.037570000	0.724301000	
H	-3.932820000	-2.634037000	1.086147000	C	1.120845000	2.540781000	-1.028234000	

H	-3.516436000	-1.143698000	1.925287000	C	-0.232116000	3.294068000	1.287538000
H	-5.641122000	-0.828891000	0.685284000	H	-1.169672000	1.361261000	1.192925000
H	-4.872544000	-1.340895000	-0.814541000	C	1.358232000	3.791772000	-0.459388000
C	0.841384000	-1.483970000	-0.386069000	H	1.643122000	2.256753000	-1.938455000
C	2.032217000	-1.798085000	-1.319445000	C	0.680105000	4.172325000	0.700606000
C	1.279222000	-1.522681000	1.090025000	H	-0.765164000	3.585095000	2.188467000
H	0.121971000	-2.300099000	-0.539393000	H	2.065163000	4.471912000	-0.925955000
C	2.683001000	-3.142621000	-0.955319000	H	0.857310000	5.149376000	1.140754000
H	2.789353000	-1.007345000	-1.247008000	C	-1.532593000	-0.635632000	-0.440000000
H	1.695829000	-1.807607000	-2.362224000	C	-2.763130000	-0.285865000	-1.019525000
C	1.927695000	-2.870424000	1.447312000	C	-1.534775000	-1.432009000	0.715138000
H	2.007583000	-0.723370000	1.278555000	C	-3.965195000	-0.705895000	-0.451202000
H	0.426869000	-1.326359000	1.751010000	H	-2.778310000	0.319060000	-1.922752000
C	3.110503000	-3.180731000	0.518804000	C	-2.738262000	-1.862092000	1.277206000
H	3.543759000	-3.332477000	-1.607911000	H	-0.594402000	-1.717379000	1.175572000
H	1.962933000	-3.952334000	-1.142084000	C	-3.955316000	-1.498296000	0.698619000
H	2.253862000	-2.866452000	2.494597000	H	-4.908165000	-0.422581000	-0.910069000
H	1.176455000	-3.667880000	1.355022000	H	-2.723895000	-2.479848000	2.170868000
H	3.545457000	-4.156331000	0.766346000	H	-4.890206000	-1.833803000	1.138226000
H	3.899943000	-2.433192000	0.683260000				
C	0.662494000	1.443107000	0.040057000				
C	2.111347000	1.713492000	-0.415601000				
C	-0.167999000	2.740747000	-0.048433000				
H	0.684217000	1.135647000	1.095396000				
C	2.758445000	2.868618000	0.365130000				
H	2.110147000	1.954108000	-1.487925000				
H	2.723164000	0.814222000	-0.299782000				
C	0.483712000	3.893835000	0.732419000				
H	-0.275628000	3.031420000	-1.103162000				
H	-1.178644000	2.577594000	0.338077000				
C	1.922709000	4.150638000	0.268563000				
H	3.776179000	3.043596000	-0.004217000				
H	2.853631000	2.578901000	1.421477000				
H	-0.122192000	4.802002000	0.627658000				
H	0.490103000	3.642716000	1.802760000				
H	2.379380000	4.953318000	0.859809000				
H	1.909413000	4.495269000	-0.775233000				
PPhMe₂				PM₃			
P	-1.645426000	-0.665815000	-0.000376000	P	-0.000048000	-0.000152000	-0.612352000
C	0.159918000	-0.231921000	-0.000257000	C	1.134313000	-1.180198000	0.283333000
C	0.641725000	1.087087000	0.000253000	H	0.896334000	-2.208587000	-0.004799000
C	1.090932000	-1.280563000	-0.000552000	H	2.171138000	-0.983342000	-0.005698000
C	2.010885000	1.349412000	0.000466000	H	1.048854000	-1.090369000	1.372600000
H	-0.054590000	1.921481000	0.000457000	C	-1.589420000	-0.391987000	0.283338000
C	2.463984000	-1.022385000	-0.000333000	H	-2.360638000	0.328813000	-0.004690000
H	0.734954000	-2.307452000	-0.000976000	H	-1.938053000	-1.388061000	-0.005784000
C	2.926169000	0.293312000	0.000171000	H	-1.468884000	-0.363018000	1.372608000
H	2.365540000	2.376457000	0.000864000	C	0.455149000	1.572399000	0.283178000
H	3.169794000	-1.848193000	-0.000570000	H	1.464745000	1.880365000	-0.005285000
H	3.993080000	0.497405000	0.000350000	H	-0.233743000	2.372121000	-0.005219000
C	-2.249166000	0.386696000	1.419200000	H	0.420716000	1.453075000	1.372449000
H	-3.341644000	0.334133000	1.459915000				
H	-1.854545000	-0.010611000	2.358262000				
H	-1.951703000	1.436606000	1.329442000				
C	-2.249502000	0.388468000	-1.418520000				
H	-1.855062000	-0.007483000	-2.358218000				
H	-3.341986000	0.335940000	-1.459056000				
H	-1.952117000	1.438301000	-1.327392000				