

Deciphering the Mechanistic Insights and Reactivity Trend of High-Valent Mn/Fe/Co-oxo Species toward C-H Bond Activation and Oxygen Atom Transfer

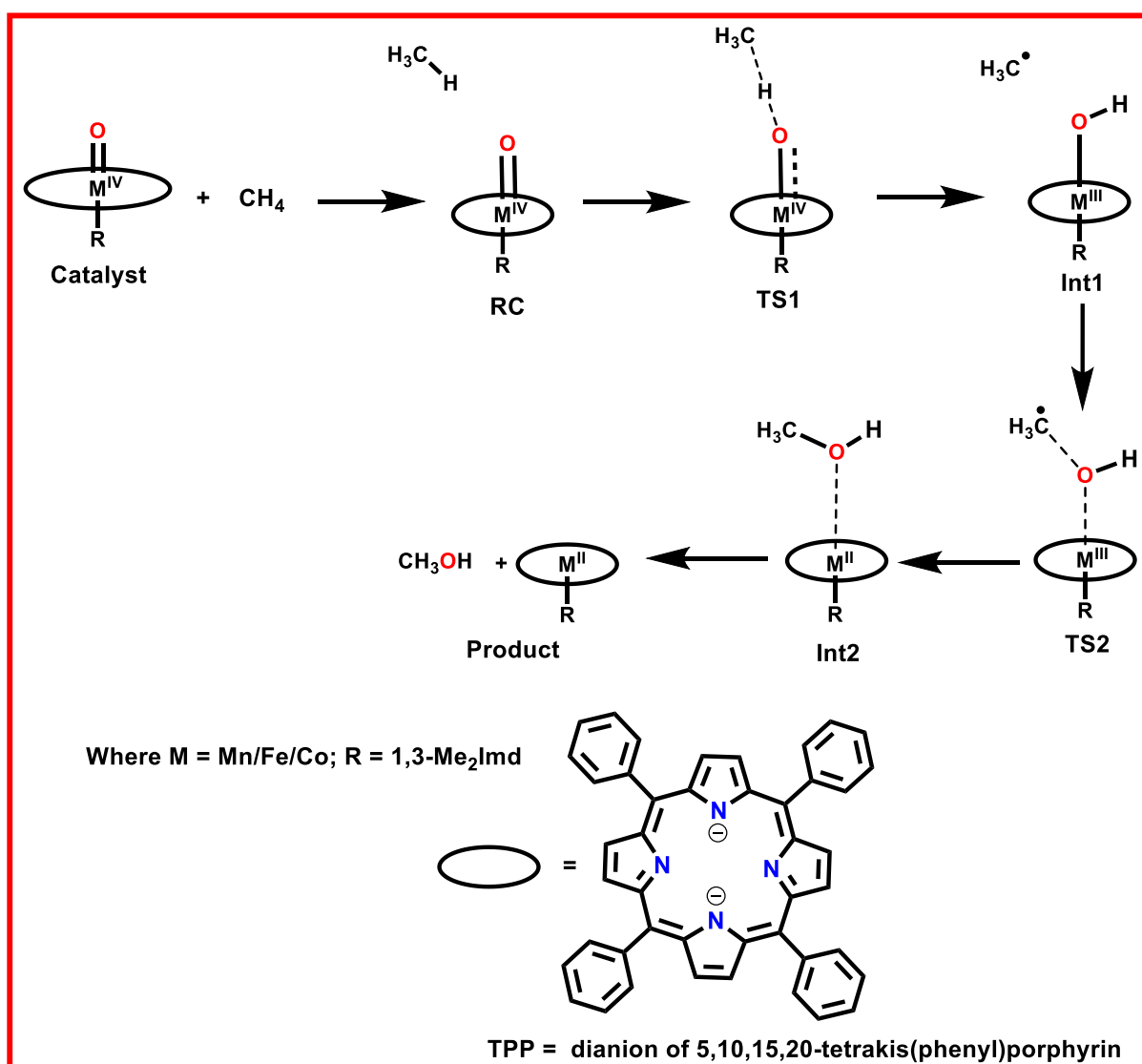
Mukhtar Ahmed,¹ Manjeet Kumar,² Mursaleem Ansari,^{3*} Manoj Kumar Gupta^{1*} and Azaj Ansari^{1*}

¹Department of Chemistry, Central University of Haryana, Mahendergarh, Haryana 123031, India

²Department of Chemistry, Indian Institute of Technology Bombay, Mumbai 400076, India

³Institut de Química Computacional i Catàlisi and Department of Chemistry, University of Girona, 17003 Girona, Spain

Corresponding authors: Mursaleem Ansari (mansaribhu@gmail.com), Manoj Kumar Gupta (mkgupta@cuh.ac.in) and Azaj Ansari (ajaz.alam2@gmail.com)



Scheme S1. Schematic mechanism adopted for the methane hydroxylation by species 1-3.

Table S1. Computed relative energy (ΔG in kJ/mol) for **1** with substrates CH₄, CHD and SMe₂.

1							
Spin states (CH ₄)	Relative energies (kJ/mol)		Spin states (CHD)	Relative energies (kJ/mol)		Spin states (SMe ₂)	Relative energies (kJ/mol)
⁴ R-1 _{hs}	0		⁴ R-1 _{hs}	0		⁴ R-1 _{hs}	0
² R-1 _{ls}	51.0		² R-1 _{ls}	51.0		² R-1 _{ls}	51.0
⁴ RC-1 _{hs}	0		⁴ RC _{hs}	0.0		⁴ RC _{hs}	0.0
² RC-1 _{ls}	48.4		² RC _{ls}	25.4		² RC _{ls}	42.2
⁴ TS1-1 _{hs}	0		⁴ TS1-1 _{hs}	0.0		⁴ TS-1 _{hs}	39.9
² TS1-1 _{ls}	54.1		² TS1-1 _{ls}	11.3		² TS-1 _{ls}	0.0
⁶ INT1-1 _{hs}	110.3		⁶ INT1-1 _{hs}	20.7		⁶ INT-1 _{hs}	0.0
⁴ INT1-1 _{hs}	30.6		⁴ INT1-1 _{hs}	25.2		⁴ INT-1 _{is}	12.1
⁴ INT1-1 _{is}	0.80		⁴ INT1-1 _{is}	0.0		² INT-1 _{ls}	53.1
² INT1-1 _{is}	0		² INT1-1 _{is}	1.2		⁶ P-1 _{hs}	0.0
² INT1-1 _{ls}	50.9		² INT1-1 _{ls}	53.7		⁴ P-1 _{is}	47.7
⁶ TS2-1 _{hs}	7.2		⁶ TS2-1 _{hs}	19.1		² P-1 _{ls}	95.2
⁴ TS2-1 _{hs}	68.0		⁴ TS2-1 _{hs}	21.2			
⁴ TS2-1 _{is}	29.4		⁴ TS2-1 _{is}	11.6			
² TS2-1 _{is}	0		² TS2-1 _{is}	0.0			
² TS2-1 _{ls}	40.1		² TS2-1 _{ls}	39.4			
⁶ INT2-1 _{hs}	0.0		⁶ INT2-1 _{hs}	0.0			
⁴ INT2-1 _{is}	57.1		⁴ INT2-1 _{is}	22.4			
² INT2-1 _{ls}	85.1		² INT2-1 _{ls}	49.4			
⁶ P-1 _{hs}	0.0		⁶ P-1 _{hs}	0.0			
⁴ P-1 _{is}	47.2		⁴ P-1 _{is}	60.4			
² P-1 _{ls}	95.2		² P-1 _{ls}	94.4			

Table S2. Computed relative energy (ΔG in kJ/mol) for **2** with substrates CH₄, CHD and SMe₂.

2					
Spin states (CH ₄)	Relative energies (kJ/mol)		Spin states (CHD)	Relative energies (kJ/mol)	
⁵ R-2 _{hs}	52.9		⁵ R-2 _{hs}	52.9	
³ R-2 _{is}	0		³ R-2 _{is}	0	
¹ R-2 _{ls}	125.0		¹ R-2 _{ls}	125.0	
⁵ RC-2 _{hs}	57.8		⁵ RC-2 _{hs}	52.3	
³ RC-2 _{is}	0.0		³ RC-2 _{is}	0.0	
¹ RC-2 _{ls}	126.6		¹ RC-2 _{ls}	111.8	
⁵ TS1-2 _{hs}	63.1		⁵ TS1-2 _{hs}	62.6	
³ TS1-2 _{is}	0.0		³ TS1-2 _{is}	0.0	
¹ TS1-2 _{ls}	95.5		¹ TS1-2 _{ls}	84.3	
⁷ INT1-2 _{hs}	46.9		⁷ INT1-2 _{hs}	45.2	
⁵ INT1-2 _{hs}	46.6		⁵ INT1-2 _{hs}	46.1	
⁵ INT1-2 _{is}	49.1		⁵ INT1-2 _{is}	47.3	
³ INT1-2 _{is}	49.6		³ INT1-2 _{is}	48.7	
³ INT1-2 _{ls}	2.2		³ INT1-2 _{ls}	0.0	
¹ INT1-2 _{ls}	0.0		¹ INT1-2 _{ls}	2.7	
⁷ TS2-2 _{hs}	85.7		⁷ TS2-2 _{hs}	58.6	
⁵ TS2-2 _{hs}	34.4		⁵ TS2-2 _{hs}	31.8	
⁵ TS2-2 _{is}	57.5		⁵ TS2-2 _{is}	66.4	
³ TS2-2 _{is}	64.2		³ TS2-2 _{is}	36.8	
³ TS2-2 _{ls}	18.6		³ TS2-2 _{ls}	27.8	
¹ TS2-2 _{ls}	0.0		¹ TS2-2 _{ls}	0.0	
⁵ INT2-2 _{hs}	11.7		⁵ INT2-2 _{hs}	14.4	
³ INT2-2 _{is}	24.2		³ INT2-2 _{is}	27.2	
¹ INT2-2 _{ls}	0.0		¹ INT2-2 _{ls}	0.0	
⁵ P-2 _{hs}	0.0		⁵ P-2 _{hs}	0.0	
³ P-2 _{is}	7.5		³ P-2 _{is}	25.7	
¹ P-2 _{ls}	13.3		¹ P-2 _{ls}	22.1	

Table S3. Computed relative energy (ΔG in kJ/mol) for **3** with substrates CH₄, CHD and SMe₂.

3					
Spin states (CH ₄)	Relative energies (kJ/mol)		Spin states (CHD)	Relative energies (kJ/mol)	
⁶ R-3 _{hs}	123.2		⁶ R-3 _{hs}	123.2	
⁴ R-3 _{is}	59.3		⁴ R-3 _{is}	59.3	
² R-3 _{ls}	0.0		² R-3 _{ls}	0.0	
⁶ RC-3 _{hs}	135.4		⁶ RC-3 _{hs}	152.0	
⁴ RC-3 _{is}	54.5		⁴ RC-3 _{is}	76.2	
² RC-3 _{ls}	0.0		² RC-3 _{ls}	0.0	
⁶ TS1-3 _{hs}	131.3		⁶ TS1-3 _{hs}	147.6	
⁴ TS1-3 _{is}	89.4		⁴ TS1-3 _{is}	82.7	
² TS1-3 _{ls}	0.0		² TS1-3 _{ls}	0.0	
⁶ INT1-3 _{hs}	154.7		⁶ INT1-3 _{hs}	120.8	
⁴ INT1-3 _{hs}	128.5		⁴ INT1-3 _{hs}	123.4	
⁴ INT1-3 _{is}	92.3		⁴ INT1-3 _{is}	88.6	
² INT1-3 _{ls}	0.0		² INT1-3 _{ls}	0.0	
⁶ TS2-3 _{hs}	153.2		⁶ TS2-3 _{hs}	127.8	
⁴ TS2-3 _{hs}	152.8		⁴ TS2-3 _{hs}	176.6	
⁴ TS2-3 _{is}	84.8		⁴ TS2-3 _{is}	74.1	
² TS2-3 _{ls}	0.0		² TS2-3 _{ls}	0.0	
⁴ INT2-3 _{hs}	12.3		⁴ INT2-3 _{hs}	18.3	
² INT2-3 _{ls}	0.0		² INT2-3 _{ls}	0.0	
⁴ P-3 _{hs}	7.2		⁴ P-3 _{hs}	57.4	
² P-3 _{ls}	0.0		² P-3 _{ls}	0.0	

Table S4: Computed salient bond parameters of manganese species (**1**). *Given bond length in Å and angle in °.*

	Spin states	Mn-O	O-H	H-C _{CH4}	Mn-O-H	O-H-C _{CH4}	Mn-C _{NHC}	Mn-N1	Mn-N2	Mn-N3	Mn-N4
CH ₄	⁴ R-1 _{hs}	1.686					2.274	2.003	1.998	2.003	1.998
	² R-1 _{ls}	1.707					2.246	2.015	2.007	2.015	2.007
	⁴ RC-1 _{hs}	1.688					2.263	2.001	1.996	2.001	1.994
	² RC-1 _{ls}	1.710					2.235	2.013	2.007	2.015	2.005
	⁴ TS1-1 _{hs}	1.838	1.122	1.433	114.1	176.3	2.162	1.998	1.987	2.008	2.004
	² TS1-1 _{ls}	1.799	1.090	1.489	116.1	173.9	2.191	2.011	2.012	2.009	2.003
	⁶ INT1-1 _{hs}	1.837	0.981		114.2		2.203	2.121	2.051	2.123	2.061
	⁴ INT1-1 _{hs}	1.834	0.985		114.4		2.205	2.122	2.053	2.123	2.057
	⁴ INT1-1 _{is}	1.838	0.981		113.9		2.186	2.011	2.005	2.012	2.012
	² INT1-1 _{is}	1.833	0.984		113.9		2.188	2.010	2.007	2.011	2.009
	² INT1-1 _{ls}	1.825	0.985		114.8		2.187	2.006	2.011	2.011	2.012
				O-C _{CH3}		Mn-O-C _{CH3}					
	⁶ TS2-1 _{hs}	1.887	0.982	2.354	114.3	129.7	2.230	2.111	2.080	2.127	2.076
	⁴ TS2-1 _{hs}	1.916	0.981	2.229	112.7	120.7	2.120	1.991	1.996	2.004	1.991
	⁴ TS2-1 _{is}	1.916	0.981	2.229	112.7	120.7	2.120	1.991	1.996	2.004	1.991
	² TS2-1 _{is}	1.868	0.978	2.305	113.6	118.4	2.152	2.017	2.011	2.006	2.001
	² TS2-1 _{ls}	1.851	0.977	2.404	114.8	117.8	2.161	2.019	2.014	2.006	2.000
	⁶ INT2-1 _{hs}						2.218	2.134	2.164	2.146	2.142
	⁴ INT2-1 _{is}						2.327	2.013	1.997	2.029	1.987
	² INT2-1 _{ls}						2.028	1.975	2.003	1.971	2.011
	⁶ P-1 _{hs}						2.232	2.137	2.146	2.137	2.146
	⁴ P-1 _{is}						2.253	1.987	2.018	1.987	2.018
	² P-1 _{ls}						1.970	1.989	1.996	1.989	1.996
CHD				H-C _{CHD}		O-H-C _{CHD}					
	⁴ RC _{hs}	1.684					2.264	2.005	2.001	2.004	1.988
	² RC _{ls}	1.707					2.321	2.011	2.011	2.003	2.002
	⁴ TS1-1 _{hs}	1.770	1.236	1.327	120.0	169.7	2.184	1.996	1.990	1.984	1.982
	² TS1-1 _{ls}	1.758	1.392	1.206	118.4	168.4	2.212	2.016	2.010	2.010	1.993
	⁶ INT1-1 _{hs}	1.838	0.979		114.5		2.188	2.117	2.045	2.122	2.063
	⁴ INT1-1 _{hs}	1.838	0.979		113.8		2.187	2.115	2.047	2.119	2.066

	⁴ INT1-1 _{is}	1.842	0.978		114.3		2.175	2.011	1.997	2.015	2.009
	² INT1-1 _{is}	1.842	0.979		114.0		2.175	2.011	1.997	2.014	2.011
	² INT1-1 _{is}	1.831	0.979		114.8		2.171	2.009	1.995	2.013	2.011
	⁶ TS2-1 _{hs}	1.942	1.509	1.203	137.8	179.5	2.248	2.128	2.057	2.121	2.053
	⁴ TS2-1 _{hs}	1.934	1.590	1.177	128.1	172.7	2.265	2.144	1.982	2.129	1.975
	⁴ TS2-1 _{is}	1.908	1.454	1.226	128.0	176.7	2.135	2.009	2.007	1.997	1.987
	² TS2-1 _{is}	1.887	1.542	1.192	128.4	170.4	2.138	2.011	2.001	2.011	1.986
	² TS2-1 _{is}	1.879	1.580	1.181	126.7	168.4	2.141	2.013	2.005	2.008	1.983
	⁶ INT2-1 _{hs}	2.425					2.319	2.121	2.142	2.137	2.125
	⁴ INT2-1 _{is}	2.334					2.361	2.011	1.976	2.015	1.991
	² INT2-1 _{is}	2.093					2.025	1.967	1.989	1.969	2.008
	⁶ P-1 _{hs}	3.156					2.223	2.129	2.167	2.147	2.137
	⁴ P-1 _{is}	2.499					2.335	2.011	1.975	2.022	1.999
	² P-1 _{is}	2.152					2.022	1.977	2.002	1.975	2.009
			O-S		Mn-O-S						
SMe₂	⁴ RC _{hs}	1.691	3.952		118.2		2.259	2.001	1.994	2.001	1.996
	² RC _{is}	1.721	4.019		117.8		2.225	2.015	2.004	2.013	2.005
	⁴ TS-1 _{hs}	1.917	2.023		139.6		2.386	2.015	1.982	2.024	2.000
	² TS-1 _{is}	1.898	1.874		122.9		2.108	2.004	1.987	2.017	1.988
	⁶ INT-1 _{hs}	2.361	1.697		133.2		2.375	2.113	2.113	2.126	2.123
	⁴ INT-1 _{is}	2.264	1.705		132.5		2.364	2.014	1.979	2.021	1.998
	² INT-1 _{is}	2.053	1.714		132.1		2.055	1.969	2.005	1.972	2.001
	⁶ P-1 _{hs}						2.232	2.137	2.146	2.137	2.146
	⁴ P-1 _{is}						2.253	1.987	2.018	1.987	2.018
	² P-1 _{is}						1.971	1.989	1.996	1.989	1.996

Table S5: Computed salient bond parameters of iron species (**2**). Given bond length in Å and angle in °.

	Spin states	Fe-O	O-H	H-C _{CH4}	Fe-O-H	O-H-C _{CH4}	Fe-C _{NHC}	Fe-N1	Fe-N2	Fe-N3	Fe-N4
CH ₄	⁵ R-2 _{hs}	1.662					2.208	2.072	2.051	2.072	2.052
	³ R-2 _{is}	1.672					2.180	1.988	1.984	1.988	1.983
	¹ R-2 _{ls}	1.671					2.178	1.982	1.987	1.981	1.987
	⁵ RC-2 _{hs}	1.663					2.203	2.069	2.048	2.071	2.049
	³ RC-2 _{is}	1.672					2.177	1.985	1.982	1.987	1.981
	¹ RC-2 _{ls}	1.674					2.167	1.993	1.991	1.969	1.978
	⁵ TS1-2 _{hs}	1.805	1.108	1.462	113.7	174.6	2.135	2.097	2.024	2.100	2.022
	³ TS1-2 _{is}	1.810	1.103	1.471	112.4	177.3	2.112	1.986	1.981	1.982	1.977
	¹ TS1-2 _{ls}	1.873	1.032	1.525	109.2	117.2	2.061	2.009	1.980	1.964	2.003
	⁷ INT1-2 _{hs}	1.876			123.8		2.471	2.076	2.055	2.086	2.081
	⁵ INT1-2 _{hs}	1.871			124.0		2.473	2.076	2.056	2.087	2.081
	⁵ INT1-2 _{is}	1.914			119.3		2.486	2.007	1.996	2.014	2.009
	³ INT1-2 _{is}	1.908			119.4		2.487	2.007	1.996	2.015	2.008
	³ INT1-2 _{ls}	1.834			109.8		2.107	1.984	1.978	1.985	1.982
	¹ INT1-2 _{ls}	1.836			109.7		2.106	1.984	1.978	1.985	1.982
				O-C _{CH3}		Fe-O- C _{CH3}					
	⁷ TS2-2 _{hs}	1.970		2.177		121.2	2.368	2.082	2.072	2.060	2.050
	⁵ TS2-2 _{hs}	1.913		2.159		120.1	2.457	2.061	2.077	2.087	2.073
	⁵ TS2-2 _{is}	1.869		2.446		126.3	2.160	2.093	2.042	2.109	2.036
	³ TS2-2 _{is}	1.851		2.406		118.9	2.102	2.111	2.029	2.092	2.016
	³ TS2-2 _{ls}	1.901		2.165		140.5	2.153	1.998	1.988	1.988	1.988
	¹ TS2-2 _{ls}	1.856		2.456		125.2	2.087	1.986	1.969	1.986	1.986
	⁵ INT2-2 _{hs}						2.225	2.089	2.112	2.104	2.081
	³ INT2-2 _{is}						2.251	1.985	2.047	1.994	2.031
	¹ INT2-2 _{ls}						1.989	1.985	1.998	1.991	1.983
	⁵ P-2 _{hs}						2.164	2.109	2.093	2.109	2.093
	³ P-2 _{is}						2.237	2.001	2.015	2.001	2.015
	¹ P-2 _{ls}						1.939	1.981	1.988	1.981	1.988
				H-C _{CHD}		O-H-C _{CHD}					
CHD	⁵ RC-2 _{hs}	1.662					2.199	2.073	2.048	2.074	2.051

	³ RC-2 _{is}	1.671					2.166	1.984	1.979	1.987	1.979
	¹ RC-2 _{ls}	1.698					2.133	2.008	1.993	1.945	1.976
	⁵ TS1-2 _{hs}	1.752	1.298	1.265	119.6	164.1	2.149	2.084	2.031	2.081	2.036
	³ TS1-2 _{is}	1.763	1.297	1.266	117.7	167.3	2.129	1.984	1.977	1.976	1.976
	¹ TS1-2 _{ls}	1.764	1.297	1.266	117.7	167.2	2.129	1.983	1.977	1.976	1.976
	⁷ INT1-2 _{hs}	1.888					2.447	2.081	2.054	2.081	2.077
	⁵ INT1-2 _{hs}	1.888					2.447	2.081	2.054	2.081	2.077
	⁵ INT1-2 _{is}	1.908					2.479	2.003	1.993	2.003	2.007
	³ INT1-2 _{is}	1.906					2.479	2.002	1.992	2.004	2.007
	³ INT1-2 _{ls}	1.851					2.100	1.987	1.980	1.989	1.985
	¹ INT1-2 _{ls}	1.851					2.101	1.987	1.979	1.989	1.986
				H-C_{MHD}		O-H-C_{MHD}					
	⁷ TS2-2 _{hs}	1.978	1.473	1.221	123.5	175.8	2.360	2.079	2.068	2.054	2.042
	⁵ TS2-2 _{hs}	1.925	1.781	1.137	121.5	166.8	2.424	2.086	2.079	2.074	2.045
	⁵ TS2-2 _{is}	1.998	1.537	1.194	122.1	176.7	2.439	2.003	1.988	1.993	1.983
	³ TS2-2 _{is}	1.956	1.744	1.142	124.1	172.9	2.486	2.007	1.999	1.999	1.978
	³ TS2-2 _{ls}	1.886	1.458	1.223	128.2	176.3	2.069	1.977	1.975	1.973	1.973
	¹ TS2-2 _{ls}	1.871	1.667	1.159	125.2	164.1	2.075	1.974	1.972	1.977	1.966
	⁵ INT2-2 _{hs}	2.346					2.242	2.089	2.076	2.110	2.110
	³ INT2-2 _{is}	2.359					2.346	1.991	2.009	1.996	2.014
	¹ INT2-2 _{ls}	2.103					1.989	1.983	1.977	1.987	1.993
	⁵ P-2 _{hs}						2.162	2.110	2.084	2.119	2.111
	³ P-2 _{is}						2.262	1.998	2.007	2.100	2.011
	¹ P-2 _{ls}						1.984	1.993	1.982	1.980	1.998
			O-S		Fe-O-S						
SMe₂	⁵ RC-2 _{hs}	1.664					2.196	2.071	2.046	2.072	2.051
	³ RC-2 _{is}	1.672					2.171	1.985	1.981	1.987	1.981
	¹ RC-2 _{ls}	1.684					2.147	2.007	1.997	1.961	1.965
	⁵ TS-2 _{hs}	1.838	2.069		139.4		2.469	2.082	2.070	2.082	2.086
	³ TS-2 _{is}	1.921	1.951		139.4		2.327	2.001	1.988	2.007	2.005
	¹ TS-2 _{ls}	1.678	3.119		124.6		2.166	1.995	1.982	1.955	1.992
	⁵ INT-2 _{hs}	2.264					2.301	2.079	2.071	2.085	2.101
	³ INT-2 _{is}	2.326					2.338	2.014	1.981	2.016	1.999

	¹ INT-2 _{ls}	2.056					2.003	1.979	1.979	1.986	1.984
	⁵ P-2 _{hs}						2.164	2.109	2.093	2.109	2.093
	³ P-2 _{is}						2.237	2.001	2.015	2.001	2.015
	¹ P-2 _{ls}						1.939	1.981	1.988	1.981	1.988

Table S6: Computed salient bond parameters of cobalt species (**3**). Given bond length in Å and angle in °.

	Spin states	Co-O	O-H	H-C _{CH4}	Co-O-H	O-H-C _{CH4}	Co-C _{NHC}	Co-N1	Co-N2	Co-N3	Co-N4
CH ₄	⁶ R-3 _{hs}	1.924					2.276	2.097	2.033	2.066	2.068
	⁴ R-3 _{is}	1.699					2.115	2.103	1.992	2.103	1.992
	² R-3 _{is}	1.854					2.058	1.960	1.954	1.960	1.954
	⁶ RC-3 _{hs}	1.924					2.271	2.061	2.067	2.101	2.028
	⁴ RC-3 _{is}	1.702					2.110	2.102	1.989	2.103	1.989
	² RC-3 _{is}	1.858					2.054	1.960	1.954	1.963	1.953
	⁶ TS1-3 _{hs}	1.901	1.167	1.366	113.3	176.7	2.346	2.056	2.034	2.076	2.070
	⁴ TS1-3 _{is}	1.807	1.127	1.425	113.4	173.6	2.132	2.101	1.967	2.116	1.971
	² TS1-3 _{is}	1.887	1.118	1.425	110.0	178.2	2.049	1.957	1.952	1.957	1.951
	⁶ INT1-3 _{hs}	1.925					2.338	2.051	2.054	2.061	2.064
	⁴ INT1-3 _{hs}	1.850					2.377	2.065	2.037	2.077	2.072
	⁴ INT1-3 _{is}	1.826					2.135	2.101	1.961	2.115	1.971
	² INT1-3 _{is}	1.891					2.048	1.958	1.950	1.961	1.954
				O-C _{CH3}		Co-O-C _{CH3}					
	⁶ TS2-3 _{hs}	1.845		2.477		135.5	2.139	2.107	1.997	2.094	1.996
	⁴ TS2-3 _{hs}	1.845		2.477		135.5	2.139	2.107	1.997	2.094	1.996
	⁴ TS2-3 _{is}	1.845		2.477		135.5	2.139	2.107	1.997	2.094	1.996
	² TS2-3 _{is}	1.931		2.274		137.5	2.070	1.966	1.961	1.962	1.964
	⁴ INT2-3 _{hs}						2.213	2.079	2.074	2.083	2.108
	² INT2-3 _{is}						2.235	1.994	1.996	1.981	1.993
	⁴ P-3 _{hs}						2.1482	2.083	2.085	2.083	2.085
	² P-3 _{is}						2.177	1.985	1.989	1.985	1.989
				H-C _{CHD}		O-H-C _{CHD}					
CHD	⁶ RC-3 _{hs}	1.993					2.244	2.046	2.066	2.119	2.055
	⁴ RC-3 _{is}	1.698					2.105	2.103	1.989	2.103	1.991
	² RC-3 _{is}	1.857					2.047	1.950	1.951	1.950	1.951
	⁶ TS1-3 _{hs}	1.926	1.378	1.224	112.8	165.4	2.325	2.060	2.059	2.049	2.054
	⁴ TS1-3 _{is}	1.762	1.357	1.229	117.3	160.8	2.123	2.102	1.970	2.100	1.984

	² TS1-3 _{ls}	1.869	1.347	1.219	114.4	166.5	2.053	1.954	1.948	1.953	1.951
	⁶ INT1-3 _{hs}	1.851					2.371	2.076	2.033	2.071	2.073
	⁴ INT1-3 _{hs}	1.850					2.369	2.076	2.034	2.072	2.071
	⁴ INT1-3 _{is}	1.840					2.133	2.105	1.959	2.109	1.968
	² INT1-3 _{ls}	1.900					2.044	1.963	1.948	1.964	1.959
				H-C_{MHD}							
	⁶ TS2-3 _{hs}	1.967	1.527	1.192	120.4	178.7	2.298	2.101	2.099	2.032	2.017
	⁴ TS2-3 _{hs}	1.874	1.673	1.151	131.7	172.5	2.158	2.102	1.986	2.085	1.988
	⁴ TS2-3 _{is}	1.876	1.651	1.155	133.1	170.8	2.151	2.099	1.989	2.089	1.990
	² TS2-3 _{ls}	1.919	1.541	1.190	120.6	170.8	2.001	1.947	1.953	1.953	1.944
	⁴ INT2-3 _{hs}	2.279					2.213	2.086	2.082	2.073	2.083
	² INT2-3 _{is}	2.031					1.941	1.945	1.951	1.954	1.951
	⁴ P-3 _{hs}	2.195					2.294	2.061	2.084	2.085	2.066
	² P-3 _{ls}	3.024					2.165	1.980	1.955	1.987	1.983
SMe₂			O-S		Co-O-S						
	⁶ RC-3 _{hs}	1.914					2.270	2.071	2.064	2.093	2.026
	⁴ RC-3 _{is}	1.706					2.105	2.101	1.984	2.105	1.986
	² RC-3 _{ls}	1.859					2.041	1.963	1.953	1.961	1.953
	⁶ TS-3 _{hs}	1.969	1.968		129.4		2.180	1.976	1.973	1.976	1.993
	⁴ TS-3 _{is}	1.813	2.138		130.6		2.217	2.081	2.029	2.090	2.065
	² TS-3 _{ls}	1.969	1.968		129.4		2.180	1.976	1.993	1.976	1.973
	⁴ INT-3 _{hs}	2.222					2.263	2.083	2.069	2.077	2.088
	² INT-3 _{is}	2.309					2.253	1.976	1.977	1.979	1.992
	⁴ P-3 _{hs}						2.148	2.083	2.085	2.083	2.085
	² P-3 _{ls}						2.177	1.985	1.989	1.985	1.989

Table S7. Mulliken spin density of the species **1** along with respective intermediates and transition states in the C-H bond activation and OAT.

Mulliken spin density					
CH ₄	Spin states	Mn	O	C _{CH4}	H _{CH4}
	⁴ R-1 _{hs}	2.339	0.788		
	² R-1 _{ls}	1.728	-0.643		
	⁴ RC-1 _{hs}	2.352	0.770		
	² RC-1 _{ls}	1.733	-0.641		
	⁴ TS1-1 _{hs}	2.008	0.514	0.703	-0.070
	² TS1-1 _{ls}	-0.059	0.440	0.777	-0.062
	⁶ INT1-1 _{hs}	3.850	0.041	1.126	0.012
	⁴ INT1-1 _{hs}	3.841	-0.012	0.011	0.005
	⁴ INT1-1 _{is}	1.942	0.147	1.128	0.009
	² INT1-1 _{is}	1.933	0.090	-1.111	0.006
	² INT1-1 _{ls}	-0.038	0.104	1.107	-0.007
	⁶ TS2-1 _{hs}	4.098	-0.097	0.982	0.024
	⁴ TS2-1 _{hs}	3.655	0.042	-0.791	0.004
	⁴ TS2-1 _{is}	2.178	0.038	0.816	0.008
	² TS2-1 _{is}	1.906	0.110	-0.871	-0.009
	² TS2-1 _{ls}	0.236	-0.106	-0.971	0.050
	⁶ INT2-1 _{hs}	4.758	0.002		
	⁴ INT2-1 _{is}	3.770	0.025		
	² INT2-1 _{ls}	1.739	-0.005		
	⁶ P-1 _{hs}	4.743			
	⁴ P-1 _{is}	3.649			
	² P-1 _{ls}	1.360			
CHD		Mn	O	C _{CHD}	H _{CHD}
	⁴ R-1 _{hs}	2.339	0.788		
	² R-1 _{ls}	1.728	-0.643		
	⁴ RC _{hs}	2.352	0.775		
	² RC _{ls}	1.721	-0.634		
	⁴ TS1-1 _{hs}	2.249	0.548	0.318	-0.059
	² TS1-1 _{ls}	1.833	-0.436	-0.255	0.053
	⁶ INT1-1 _{hs}	3.850	0.021	-0.250	0.009
	⁴ INT1-1 _{hs}	3.848	0.009	0.250	0.007
	⁴ INT1-1 _{is}	1.954	0.116	0.607	0.007
	² INT1-1 _{is}	1.953	0.104	-0.604	0.005
	² INT1-1 _{ls}	-0.044	0.056	0.607	-0.003
	⁶ TS2-1 _{hs}	4.157	-0.076	-0.086	0.073
	⁴ TS2-1 _{hs}	3.803	0.048	0.050	-0.052
	⁴ TS2-1 _{is}	2.044	0.040	-0.022	0.048
	² TS2-1 _{is}	1.935	0.060	0.052	-0.058
	² TS2-1 _{ls}	0.083	0.031	-0.063	0.061
	⁶ INT2-1 _{hs}	4.752	0.014		
	⁴ INT2-1 _{is}	3.761	0.027		
	² INT2-1 _{ls}	1.800	-0.005		
	⁶ P-1 _{hs}	4.753	0.005		
	⁴ P-1 _{is}	3.733	0.022		
	² P-1 _{ls}	1.643	-0.006		
SMe ₂		Mn	O	S _{SMe2}	

	⁴R-1_{hs}	2.339	0.788		
	²R-1_{ls}	1.728	-0.643		
	⁴RC_{hs}	2.404	0.713		
	²RC_{ls}	1.768	-0.671		
	⁴TS-1_{hs}	3.336	0.100	0.095	
	²TS-1_{ls}	1.699	-0.042	-0.122	
	⁶INT-1_{hs}	4.730			
	⁴INT-1_{is}	3.763			
	²INT-1_{ls}	1.869			
	⁶P-1_{hs}	4.743			
	⁴P-1_{is}	3.649			
	²P-1_{ls}	1.360			

Table S8. Mulliken spin density of the species **2** along with respective intermediates and transition states in the C-H bond activation and OAT.

	Mulliken spin density				
	Spin states	Fe	O	C _{CH4}	H _{CH4}
CH ₄	⁵ R-2 _{hs}	2.950	0.805		
	³ R-2 _{is}	1.047	1.034		
	¹ R-2 _{ls}	0.000	0.000		
	⁵ RC-2 _{hs}	2.958	0.788		
	³ RC-2 _{is}	1.065	1.013		
	¹ RC-2 _{ls}	0.000	0.000		
	⁵ TS1-2 _{hs}	2.796	0.435	0.746	- 0.066
	³ TS1-2 _{is}	0.919	0.550	0.761	-0.073
	¹ TS1-2 _{ls}	0.000	0.000	0	0
	⁷ INT1-2 _{hs}	4.062	0.427	1.125	- 0.066
	⁵ INT1-2 _{hs}	4.052	0.383	-1.115	-0.073
	⁵ INT1-2 _{is}	2.599	0.397	1.130	0.000
	³ INT1-2 _{is}	2.588	0.354	-1.123	0.010
	³ INT1-2 _{ls}	0.917	0.206	1.118	0.001
	¹ INT1-2 _{ls}	0.913	0.138	-1.125	0.007
	⁷ TS2-2 _{hs}	4.120	0.266	0.725	0.005
	⁵ TS2-2 _{hs}	4.020	0.367	- 1.009	-0.008
	⁵ TS2-2 _{is}	3.031	-0.072	1.013	-0.006
	³ TS2-2 _{is}	2.623	0.110	- 0.976	
	³ TS2-2 _{ls}	1.310	-0.018	0.862	
	¹ TS2-2 _{ls}	0.778	0.178	-0.993	
	⁵ INT2-2 _{hs}	3.777			
	³ INT2-2 _{is}	2.056			
	¹ INT2-2 _{ls}	0.0			
	⁵ P-2 _{hs}	3.735			
	³ P-2 _{is}	2.005			
	¹ P-2 _{ls}	0.0			
CHD		Fe	O	C _{CHD}	H _{CHD}
	⁵ R-2 _{hs}	2.950	0.805		
	³ R-2 _{is}	1.047	1.034		
	¹ R-2 _{ls}	0.000	0.000		
	⁵ RC-2 _{hs}	2.947	0.806		
	³ RC-2 _{is}	1.040	1.036		
	¹ RC-2 _{ls}	0.000	0.000		
	⁵ TS1-2 _{hs}	2.836	0.594	0.312	-0.058
	³ TS1-2 _{is}	0.942	0.750	0.334	-0.069
	¹ TS1-2 _{ls}	0.000	0.000	0.000	0.000
	⁷ INT1-2 _{hs}	4.070	0.374	0.606	0.007
	⁵ INT1-2 _{hs}	4.069	0.373	-0.605	0.006
	⁵ INT1-2 _{is}	2.590	0.386	0.0601	0.003
	³ INT1-2 _{is}	2.587	0.376	-0.600	0.004
	³ INT1-2 _{ls}	0.941	0.135	0.606	-0.006
	¹ INT1-2 _{ls}	0.940	0.135	-0.606	-0.006
	⁷ TS2-2 _{hs}	4.113	0.224	-0.009	0.037
	⁵ TS2-2 _{hs}	4.056	0.318	0.095	-0.063
	⁵ TS2-2 _{is}	2.715	0.225	-0.022	0.042
	³ TS2-2 _{is}	2.621	0.278	0.084	-0.060

	³ TS2-2 _{ls}	1.041	0.063	-0.022	0.048
	¹ TS2-2 _{ls}	0.863	0.119	0.078	-0.069
	⁵ INT2-2 _{hs}	3.781	0.022		
	³ INT2-2 _{is}	2.060	0.022		
	¹ INT2-2 _{ls}	0.000	0.000		
	⁵ P-2 _{hs}	3.737	0.006		
	³ P-2 _{is}	1.996	0.009		
	¹ P-2 _{ls}	0.000	0.000		
SMe ₂		Fe	O	S_{SMe2}	
	⁵ R-2 _{hs}	2.950	0.805		
	³ R-2 _{is}	1.047	1.034		
	¹ R-2 _{ls}	0.000	0.000		
	⁵ RC-2 _{hs}	2.982	0.756		
	³ RC-2 _{is}	1.090	0.986		
	¹ RC-2 _{ls}	0.000	0.000		
	⁵ TS-2 _{hs}	3.780	0.094	- 0.189	
	³ TS-2 _{is}	1.701	0.194	0.189	
	¹ TS-2 _{ls}	0.000	0.000	0.000	
	⁵ INT-2 _{hs}	3.776			
	³ INT-2 _{is}	2.079			
	¹ INT-2 _{ls}	0.0			
	⁵ P-2 _{hs}	3.735			
	³ P-2 _{is}	2.005			
	¹ P-2 _{ls}	0.000			

Table S9. Mulliken spin density of the species **3** along with respective intermediates and transition states in the C-H bond activation and OAT.

	Mulliken spin density				
	Spin states	Co	O	C _{CH4}	H _{CH4}
CH ₄	⁶ R-3 _{hs}	2.803	1.576		
	⁴ R-3 _{is}	1.610	1.178		
	² R-3 _{is}	-0.061	1.048		
	⁶ RC-3 _{hs}	2.800	1.614		
	⁴ RC-3 _{is}	1.615	1.168		
	² RC-3 _{is}	-0.054	1.044		
	⁶ TS1-3 _{hs}	2.856	1.002	0.676	-0.070
	⁴ TS1-3 _{is}	1.630	0.625	0.726	-0.071
	² TS1-3 _{is}	-0.027	0.457	0.726	-0.083
	⁶ INT1-3 _{hs}	2.878	0.610	1.115	-0.011
	⁴ INT1-3 _{hs}	2.889	0.484	-1.098	-0.006
	⁴ INT1-3 _{is}	1.641	0.237	1.125	-0.004
	² INT1-3 _{is}	0.002	0.025	1.133	-0.001
	⁶ TS2-3 _{hs}	2.898	0.536	1.114	
	⁴ TS2-3 _{hs}	2.819	0.316	-0.871	
	⁴ TS2-3 _{is}	1.913	0.025	1.016	
	² TS2-3 _{is}	0.262	0.027	0.917	
	⁴ INT2-3 _{hs}	2.681			
	² INT2-3 _{is}	0.946			
	⁴ P-3 _{hs}	2.663			
	² P-3 _{is}	0.944			
CHD		Co	O	C _{CHD}	H _{CHD}
	⁶ R-3 _{hs}	2.803	1.576		
	⁴ R-3 _{is}	1.610	1.178		
	² R-3 _{is}	-0.061	1.048		
	⁶ RC-3 _{hs}	2.739	1.638		
	⁴ RC-3 _{is}	1.601	1.177		
	² RC-3 _{is}	-0.052	1.036		
	⁶ TS1-3 _{hs}	2.796	1.290	0.314	-0.068
	⁴ TS1-3 _{is}	1.612	0.840	0.303	-0.063
	² TS1-3 _{is}	-0.040	0.716	0.306	-0.074
	⁶ INT1-3 _{hs}	2.892	0.518	0.615	0.001
	⁴ INT1-3 _{hs}	2.893	0.507	-0.608	-0.001
	⁴ INT1-3 _{is}	1.657	0.194	0.607	-0.006
	² INT1-3 _{is}	0.001	-0.001	0.610	0.001
	⁶ TS2-3 _{hs}	2.822	0.272	-0.012	0.040
	⁴ TS2-3 _{hs}	1.946	0.045	-0.090	0.066
	⁴ TS2-3 _{is}	1.967	0.031	-0.091	0.066
	² TS2-3 _{is}	-0.003	0.041	-0.032	0.047
	⁴ INT2-3 _{hs}	2.688	0.026		
	² INT2-3 _{is}	-0.004	-0.001		
	⁴ P-3 _{hs}	2.679	0.024		
	² P-3 _{is}	0.936	0.009		
SMe ₂		Co	O	S _{SMe2}	
	⁶ R-3 _{hs}	2.803	1.576		
	⁴ R-3 _{is}	1.610	1.178		

	² R-3 _{ls}	-0.061	1.048		
	⁶ RC-3 _{hs}	2.826	1.482		
	⁴ RC-3 _{is}	1.625	1.156		
	² RC-3 _{ls}	-0.038	1.028		
	⁶ TS-3 _{hs}	2.766	1.210	0.523	
	⁴ TS-3 _{is}	2.231	0.417	0.137	
	² TS-3 _{ls}	0.598	0.226	0.161	
	⁴ INT-3 _{hs}	2.678			
	² INT-3 _{ls}	0.936			
	⁴ P-3 _{hs}	2.663			
	² P-3 _{ls}	0.944			

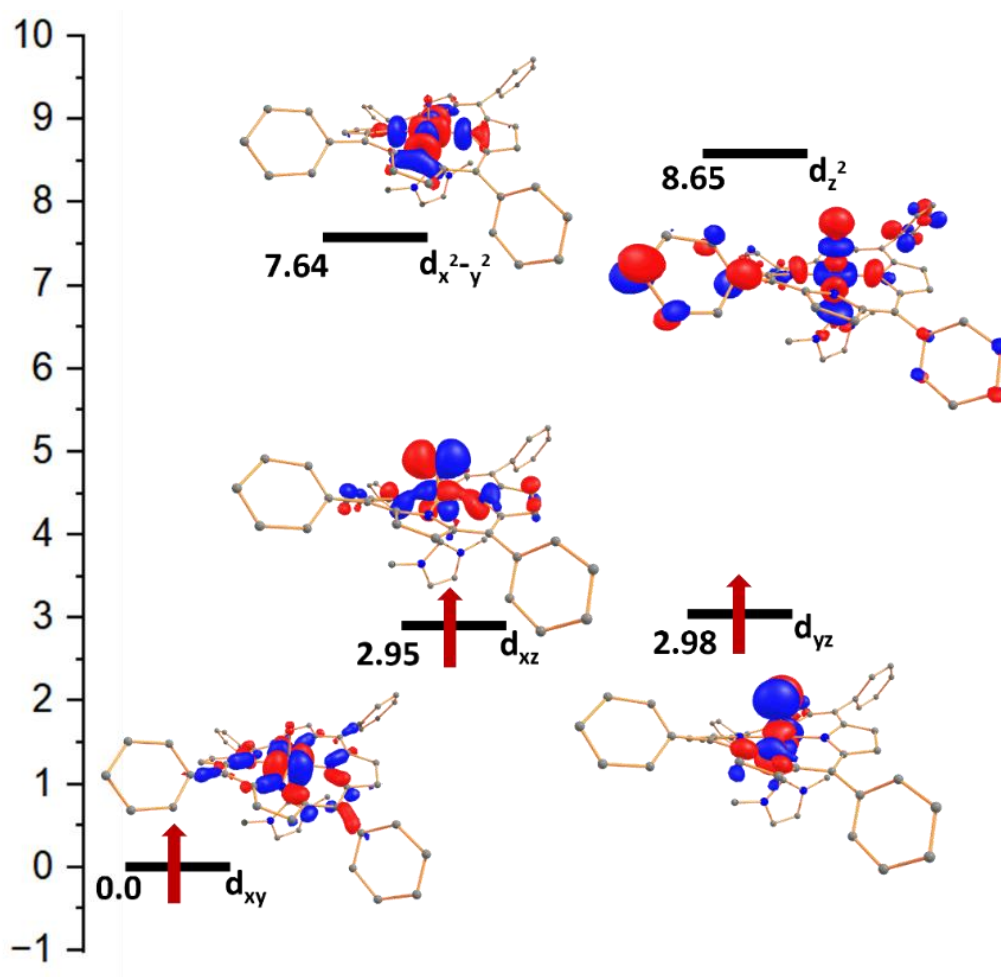


Fig. S1. DFT computed frontier *d*-based qualitative molecular orbital diagram of ⁴**R-1** (energies are given in eV).

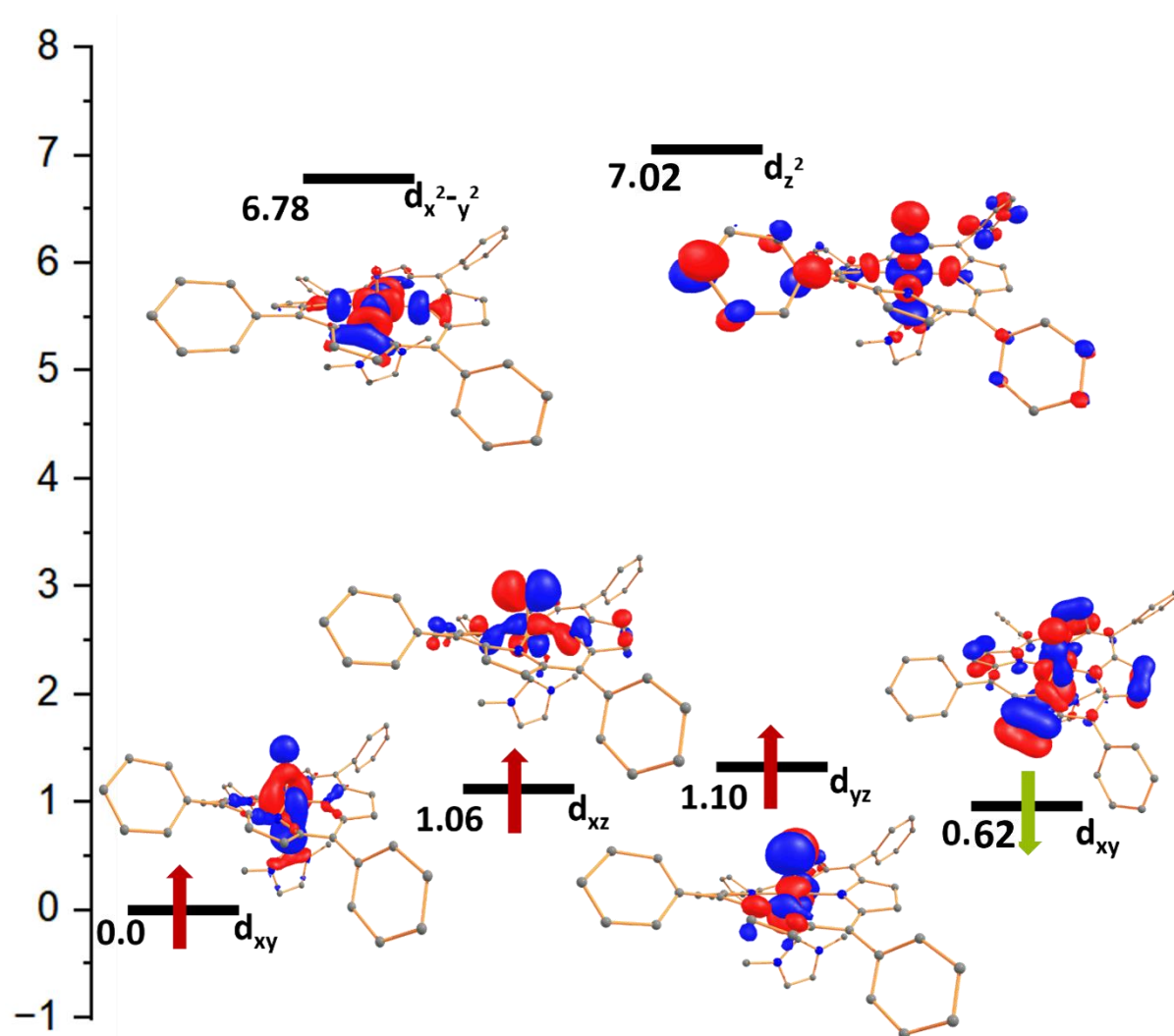


Fig. S2. DFT computed frontier d -based qualitative molecular orbital diagram of $^3\text{R-2}$ (energies are given in eV).

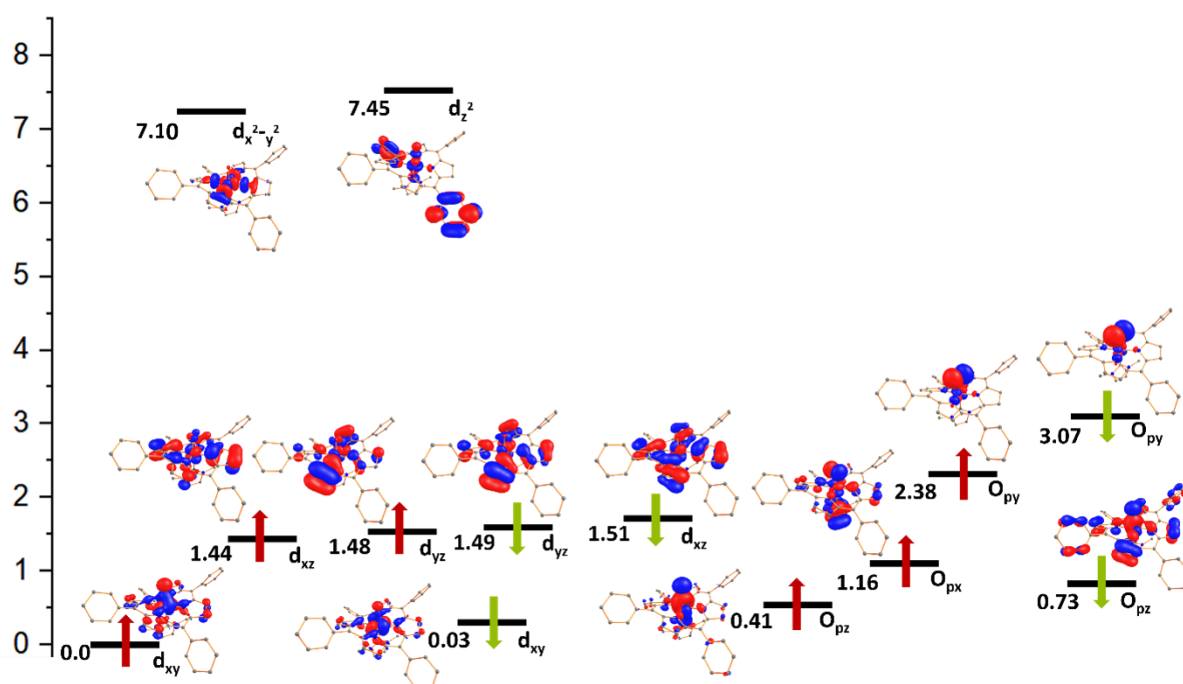


Fig. S3. DFT computed frontier *d*-based qualitative molecular orbital diagram of ²**R-3** (energies are given in eV).

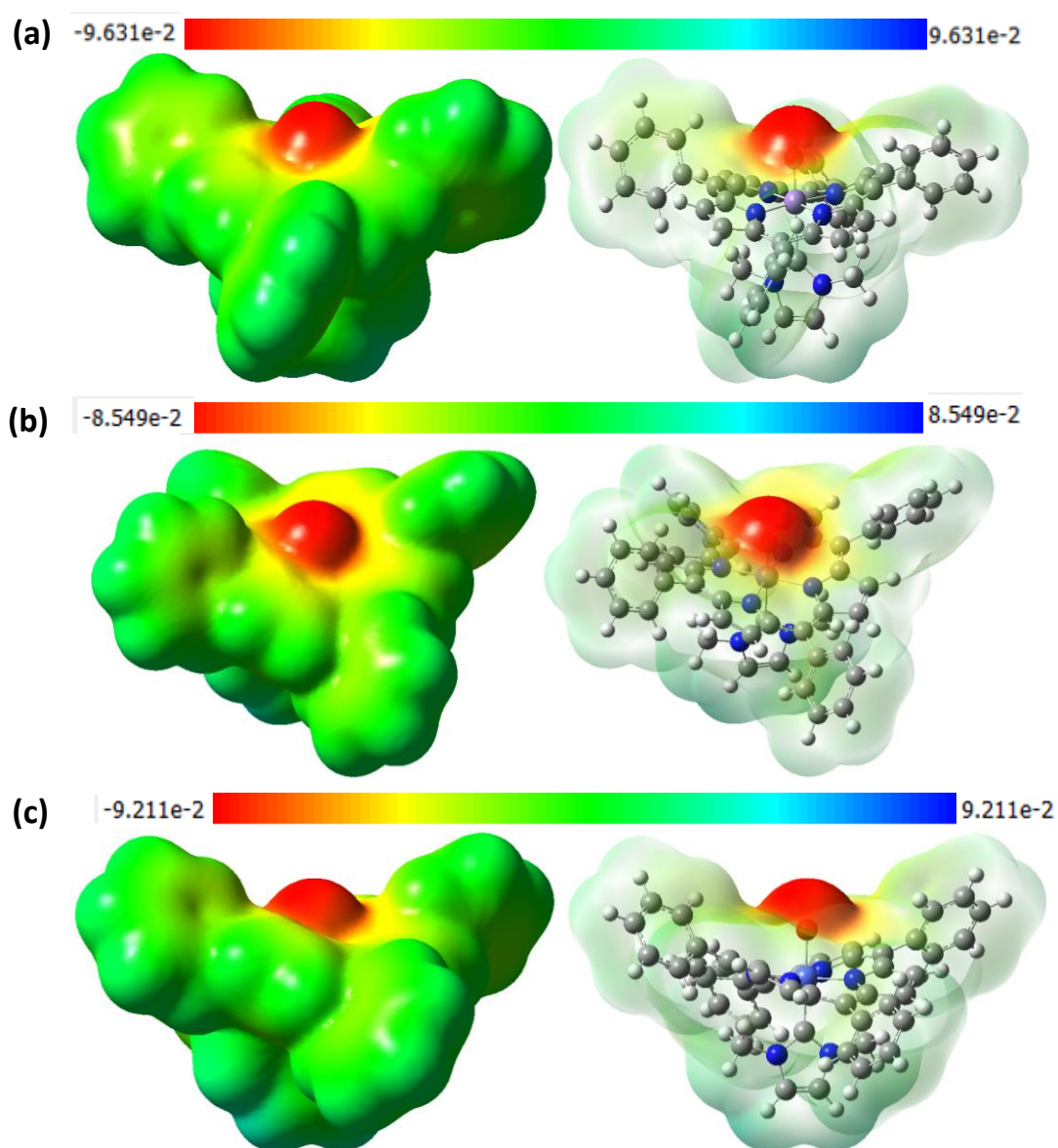
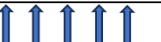


Fig. S4. Computed molecular electrostatic potential (MEP) maps of species (a) **1** (b) **2** and (c) **3**.

Table S10. Possible interactions of Mn/Fe/Co(III)-OH with $\cdot\text{CH}_3$ and MHD molecules.

	Valence electrons (Metals)	CH_3/MHD radical	Possible Interactions	Relative energies (kJ/mol) with CH_4/CHD
Species 1				
$^6\text{INT1-1}_{\text{hs}}$			Ferromagnetic	110.3/20.7
$^4\text{INT1-1}_{\text{hs}}$			Anti-ferromagnetic	30.6/25.2
$^4\text{INT1-1}_{\text{is}}$			Ferromagnetic	0.80/0.0
$^2\text{INT1-1}_{\text{is}}$			Anti-ferromagnetic	0.0/1.2
$^2\text{INT1-1}_{\text{ls}}$			Ferromagnetic	50.9/53.7
Species 2				
$^7\text{INT1-2}_{\text{hs}}$			Ferromagnetic	46.9/45.2
$^5\text{INT1-2}_{\text{hs}}$			Anti-ferromagnetic	46.6/46.1
$^5\text{INT1-2}_{\text{is}}$			Ferromagnetic	49.1/47.3
$^3\text{INT1-2}_{\text{is}}$			Anti-ferromagnetic	49.6/48.7
$^3\text{INT1-2}_{\text{ls}}$			Ferromagnetic	2.2/0.0
$^1\text{INT1-2}_{\text{ls}}$			Anti-ferromagnetic	0.0/2.7
Species 3				
$^6\text{INT1-3}_{\text{hs}}$			Ferromagnetic	154.7/120.8
$^4\text{INT1-3}_{\text{hs}}$			Anti-ferromagnetic	128.5/123.4
$^4\text{INT1-3}_{\text{is}}$			Ferromagnetic	92.3/88.6
$^2\text{INT1-3}_{\text{ls}}$			Ferromagnetic	0.0/0.0

Table S11. Possible interactions of INT1 of species 1-3 with $\cdot\text{CH}_3$ and MHD molecule in second transition state (TS2-1/2/3).

	Valence electrons (Metals)	CH_3/MHD radical	Possible interactions	Relative energies (kJ/mol) with CH_4/CHD
Species 1				
$^6\text{TS2-1}_{\text{hs}}$			Ferromagnetic	7.2/19.1
$^4\text{TS2-1}_{\text{hs}}$			Anti-ferromagnetic	68.0/21.2
$^4\text{TS2-1}_{\text{is}}$			Ferromagnetic	29.4/11.6
$^2\text{TS2-1}_{\text{is}}$			Anti-ferromagnetic	0.0/0.0
$^2\text{TS2-1}_{\text{ls}}$			Ferromagnetic	40.1/39.4
Species 2				
$^7\text{TS2-2}_{\text{hs}}$			Ferromagnetic	85.7/58.6
$^5\text{TS2-2}_{\text{hs}}$			Anti-ferromagnetic	34.4/31.8
$^5\text{TS2-2}_{\text{is}}$			Ferromagnetic	57.5/66.4
$^3\text{TS2-2}_{\text{is}}$			Anti-ferromagnetic	64.2/36.8
$^3\text{TS2-2}_{\text{ls}}$			Ferromagnetic	18.6/27.8
$^1\text{TS2-2}_{\text{ls}}$			Anti-ferromagnetic	0.0/0.0
Species 3				
$^6\text{TS2-3}_{\text{hs}}$			Ferromagnetic	153.2/127.8
$^4\text{TS2-3}_{\text{hs}}$			Anti-ferromagnetic	152.8/176.6
$^4\text{TS2-3}_{\text{is}}$			Ferromagnetic	84.8/74.1
$^2\text{TS2-3}_{\text{ls}}$			Ferromagnetic	0.0/0.0

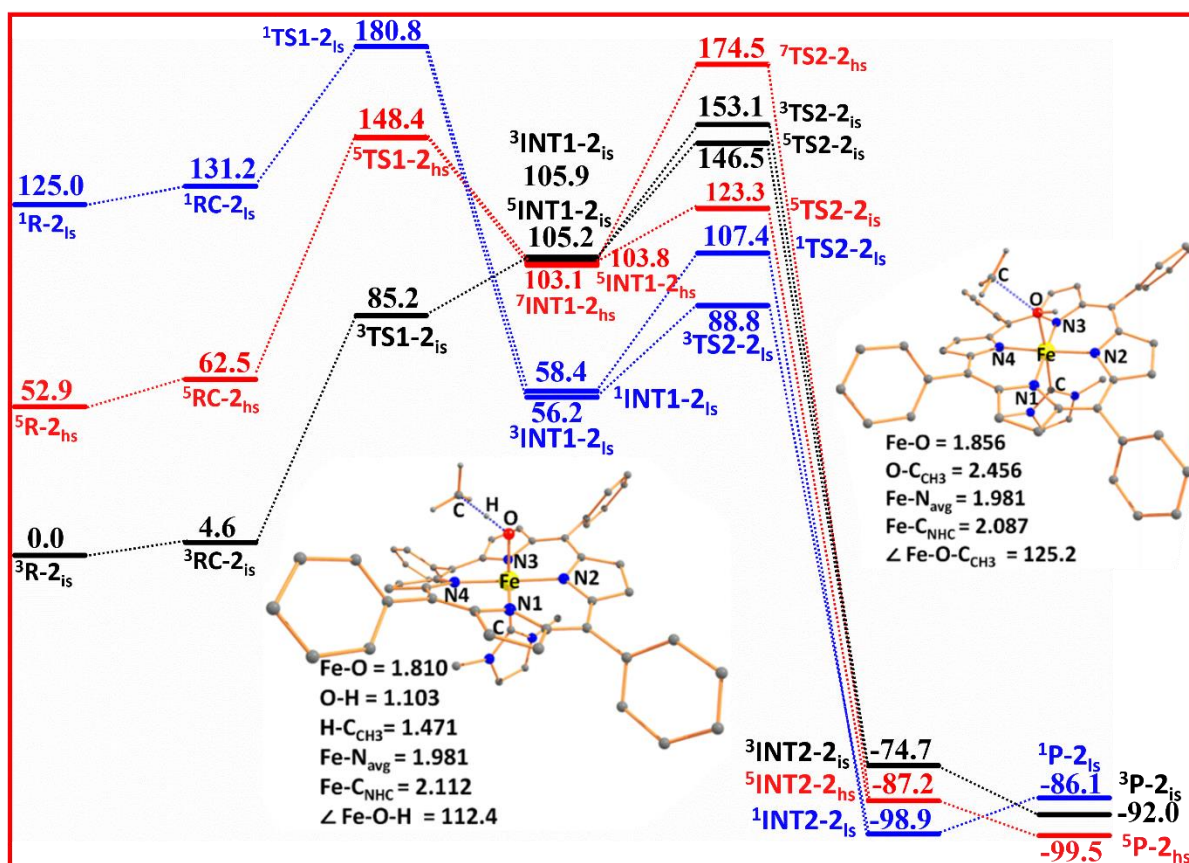


Fig. S5. The key geometric parameters of the transition states ($^3TS1-2_{is}$ and $^3TS2-2_{is}$) and energy profile (ΔG in kJ/mol) for C-H bond activation of CH₄ by **2** (given bond lengths are in Å and bond angle in °).

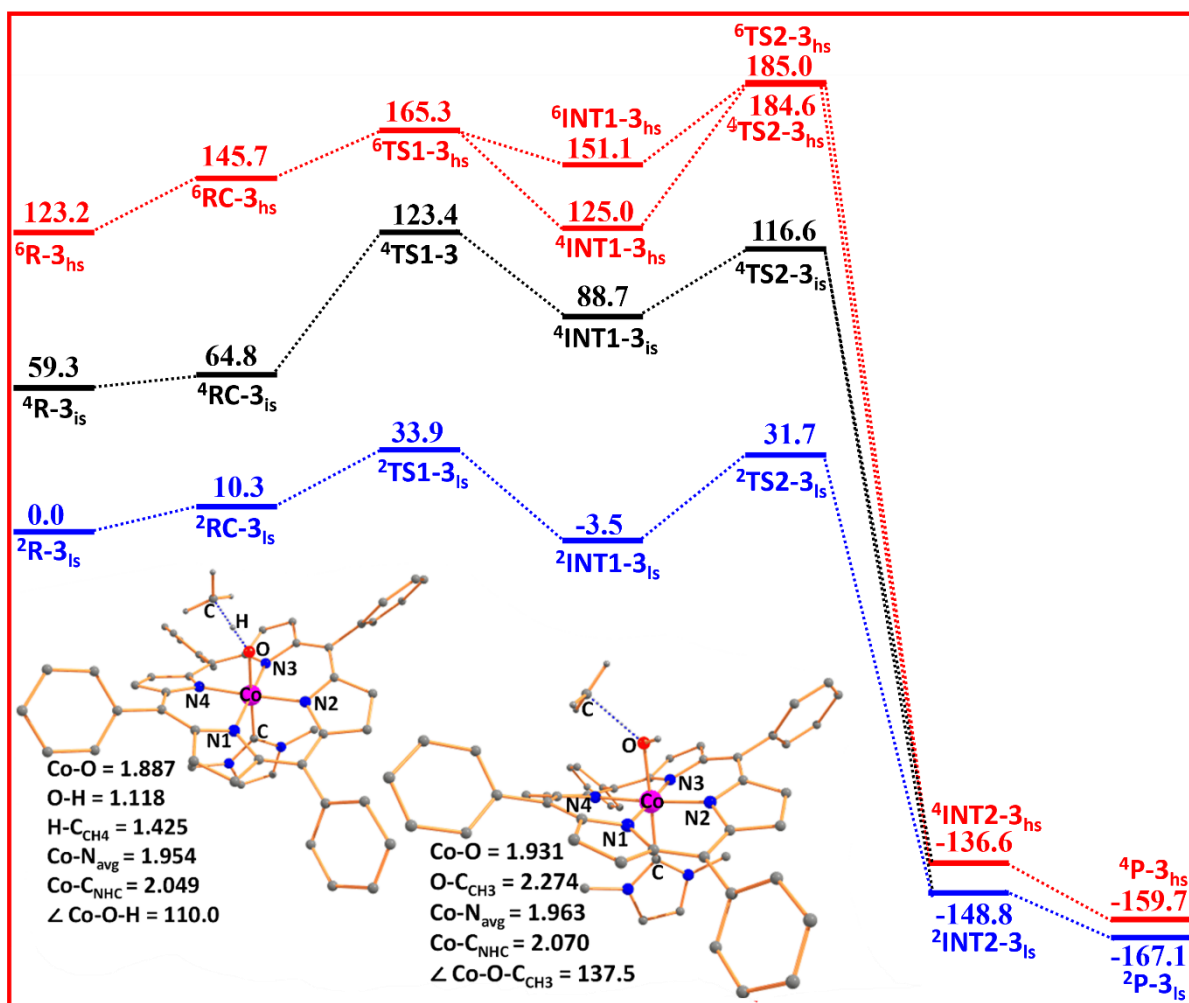
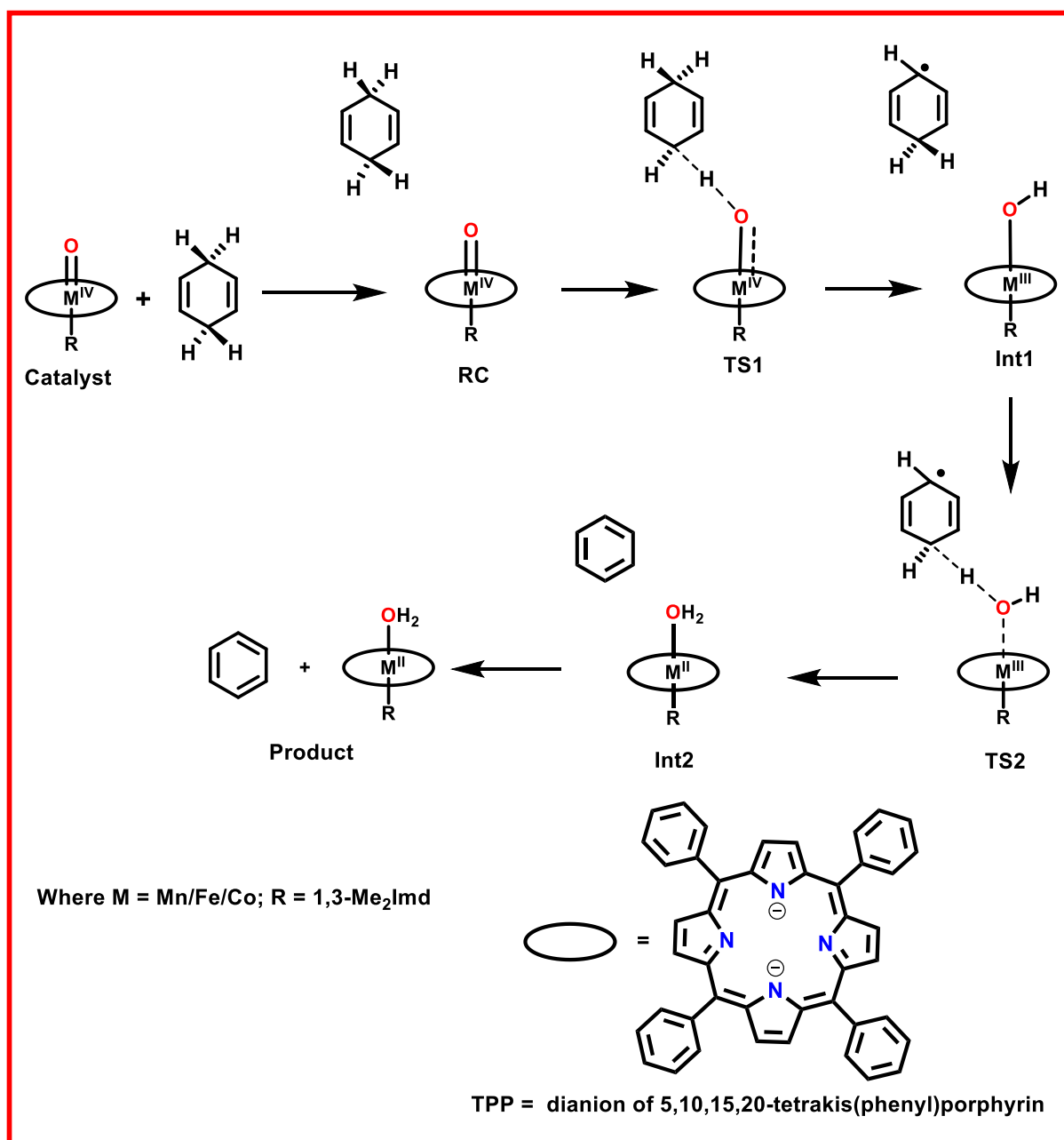


Fig. S6. The key geometric parameters of the transition states ($^2\text{TS1-3}_{\text{ls}}$ and $^2\text{TS2-3}_{\text{ls}}$) and energy profile (ΔG in kJ/mol) for C-H bond activation of CH_4 by **3** (given bond lengths are in Å and bond angle in $^\circ$).



Scheme S2. Schematic mechanism adopted for the C-H bond activation reaction of CHD by species 1-3.

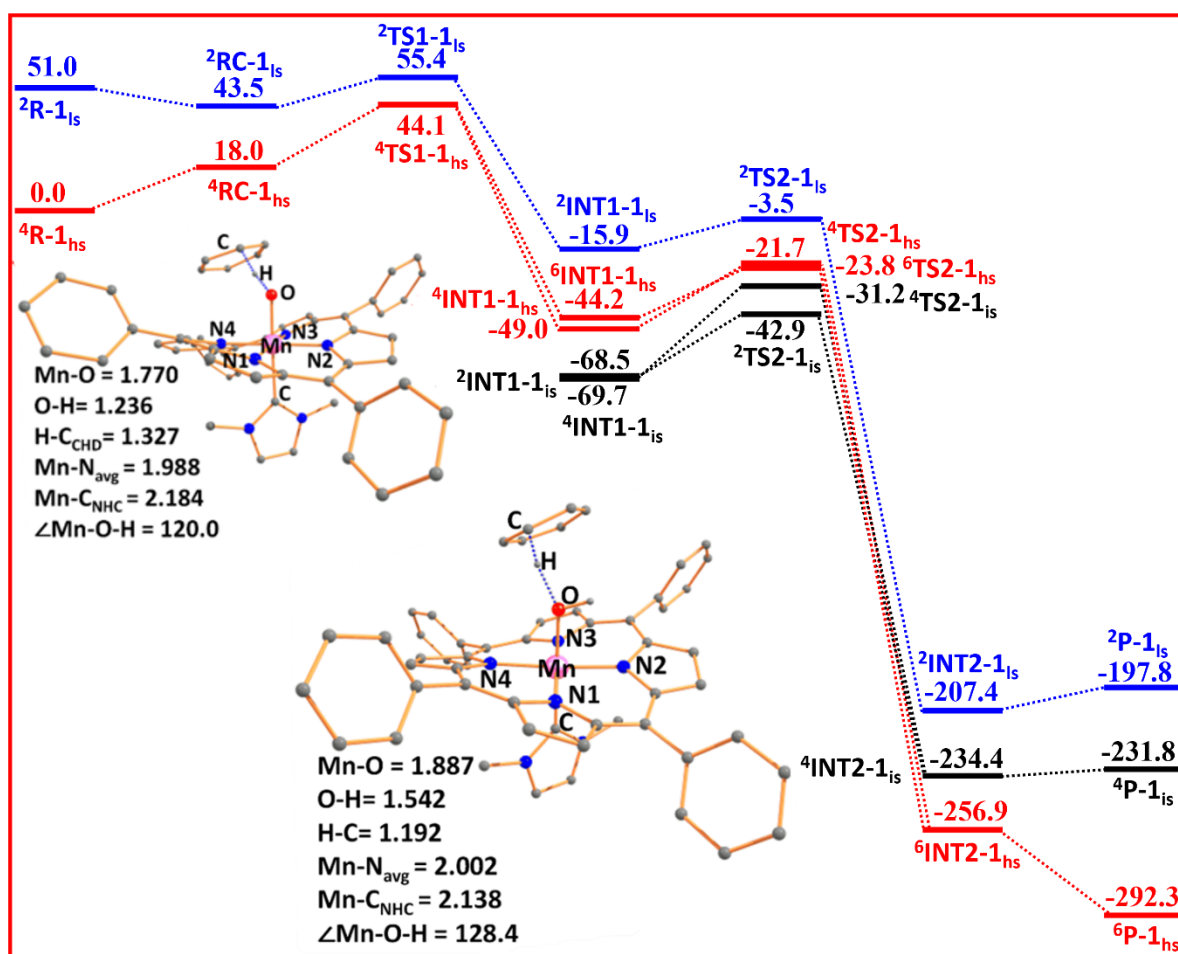


Fig.S7. The key geometric parameters of the transition states ($^4\text{TS1-1}_{\text{hs}}$ and $^2\text{TS2-1}_{\text{is}}$) and energy profile (ΔG in kJ/mol) for C-H bond activation of CHD by **1** (given bond lengths are in Å and bond angle in °).

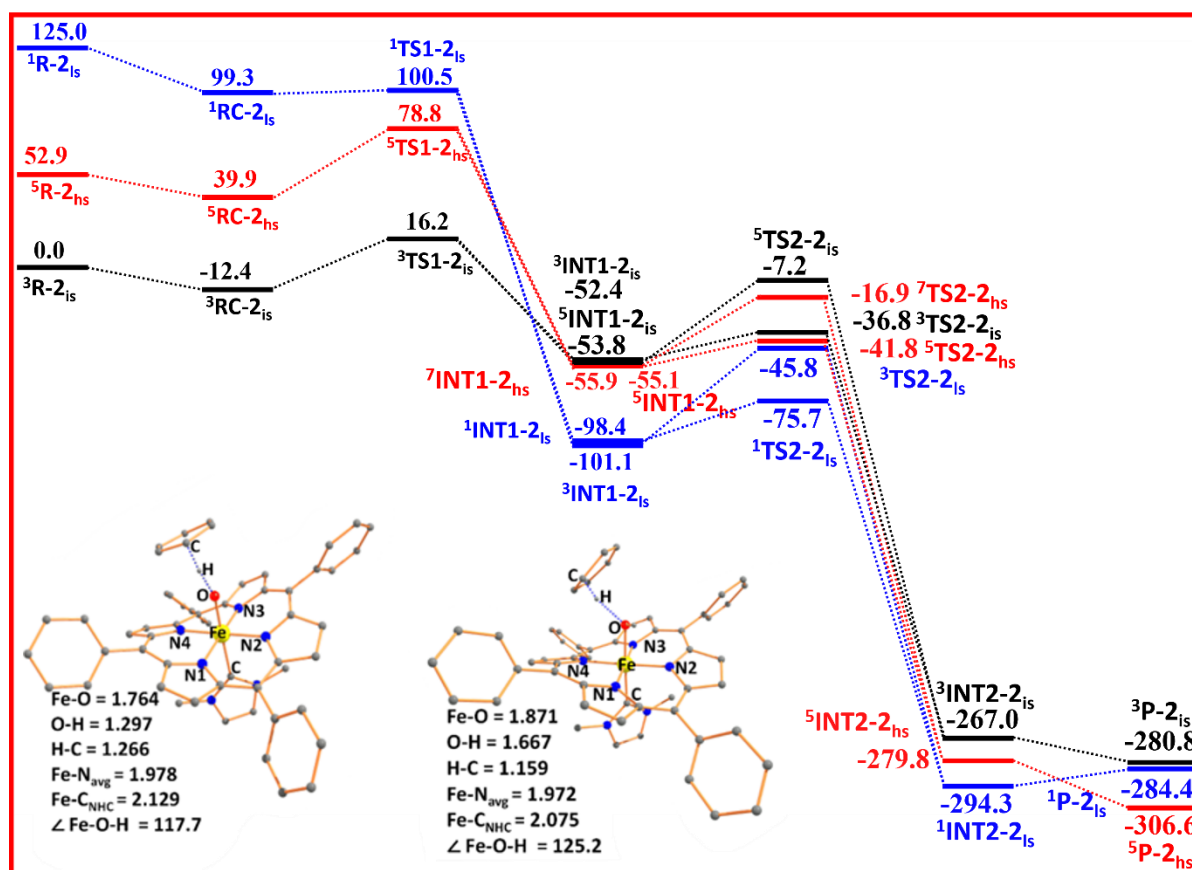


Fig. S8. The key geometric parameters of the transition states (³TS1-2_{is} and ¹TS2-2_{is}) and energy profile (ΔG in kJ mol⁻¹) for C-H bond activation of CHD by 2 (given bond lengths are in Å and bond angle in °).

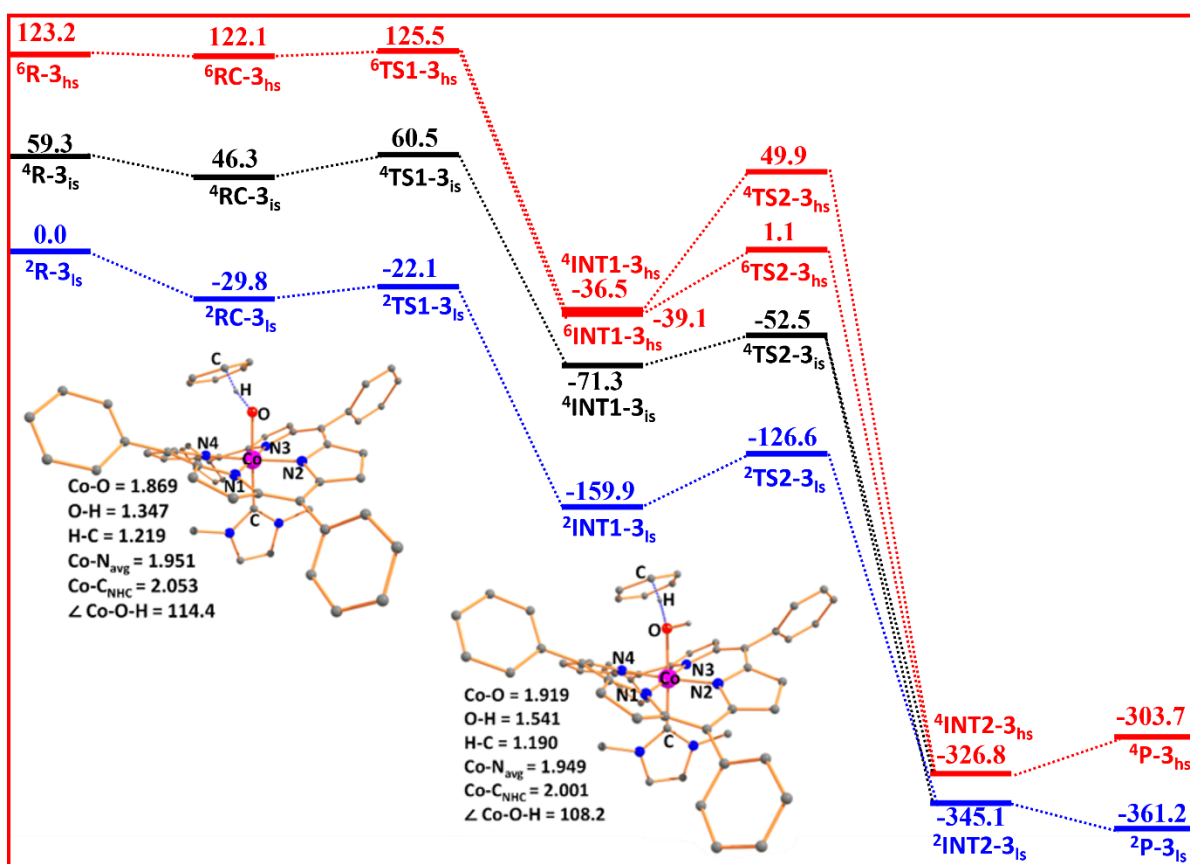
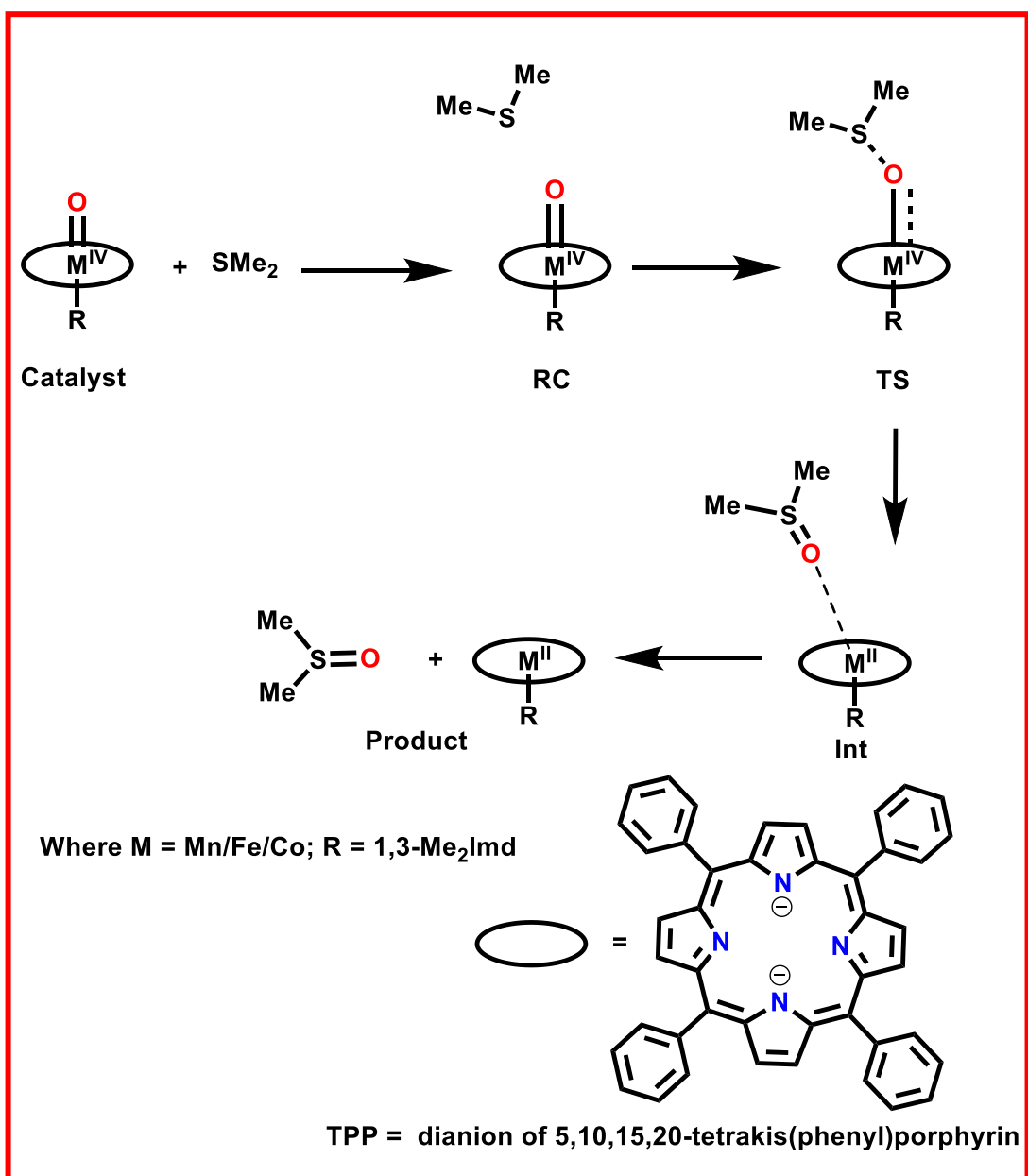


Fig. S9. The key geometric parameters of the transition states (²TS1-3_{ls} and ²TS2-3_{ls}) and energy profile (ΔG in kJ mol⁻¹) for C-H bond activation of CHD by **3** (given bond lengths are in Å and bond angle in °).



Scheme S3. Schematic mechanism adopted for the oxygen atom transfer reaction in SMe_2 by species 1-3.

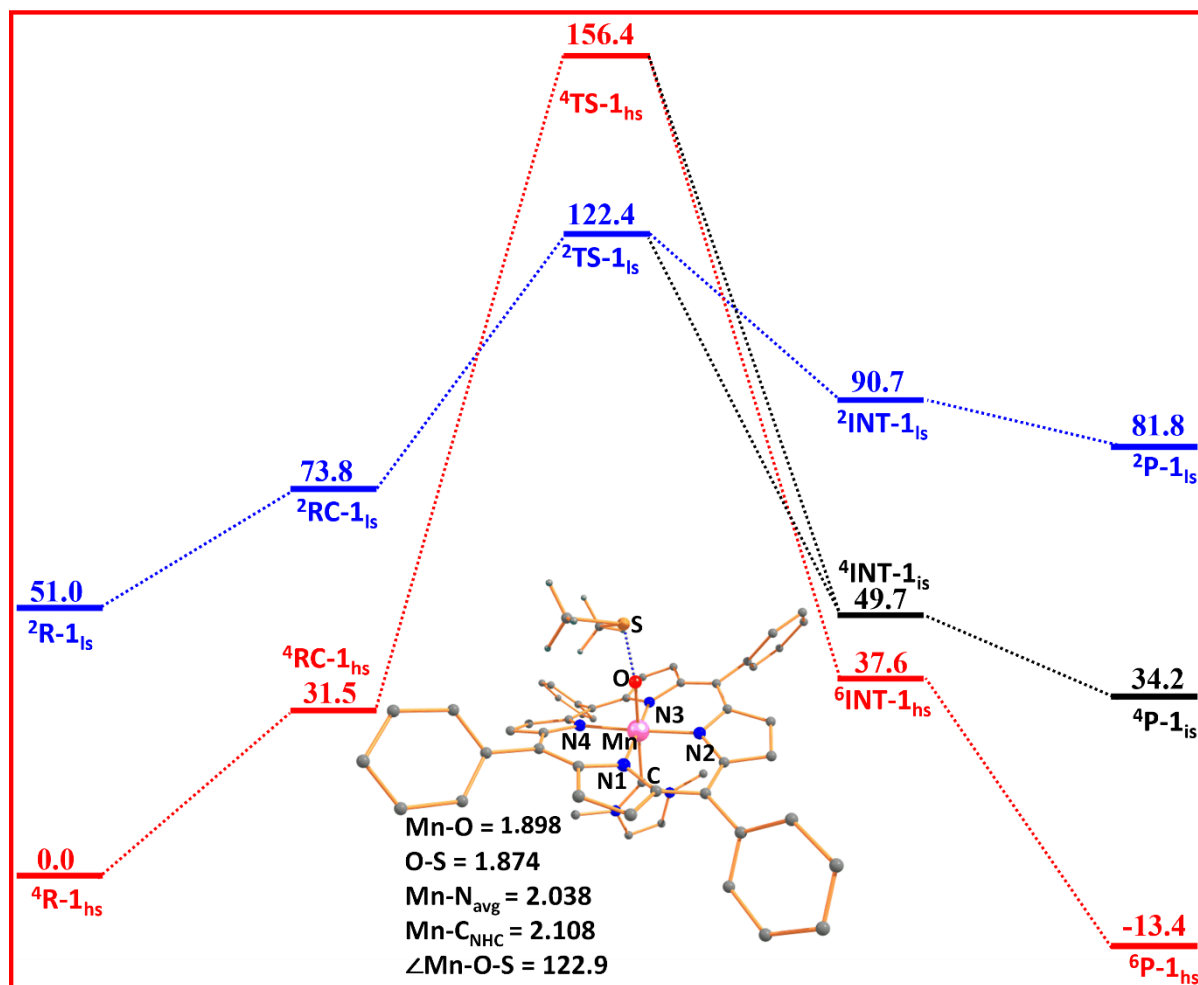


Fig. S10. The key geometric parameters of the transition state ($^{2}\text{TS-1}_{\text{ls}}$) and energy profile (ΔG in kJ/mol) for OAT in SMe_2 by **1** (given bond lengths are in Å and bond angle in °).

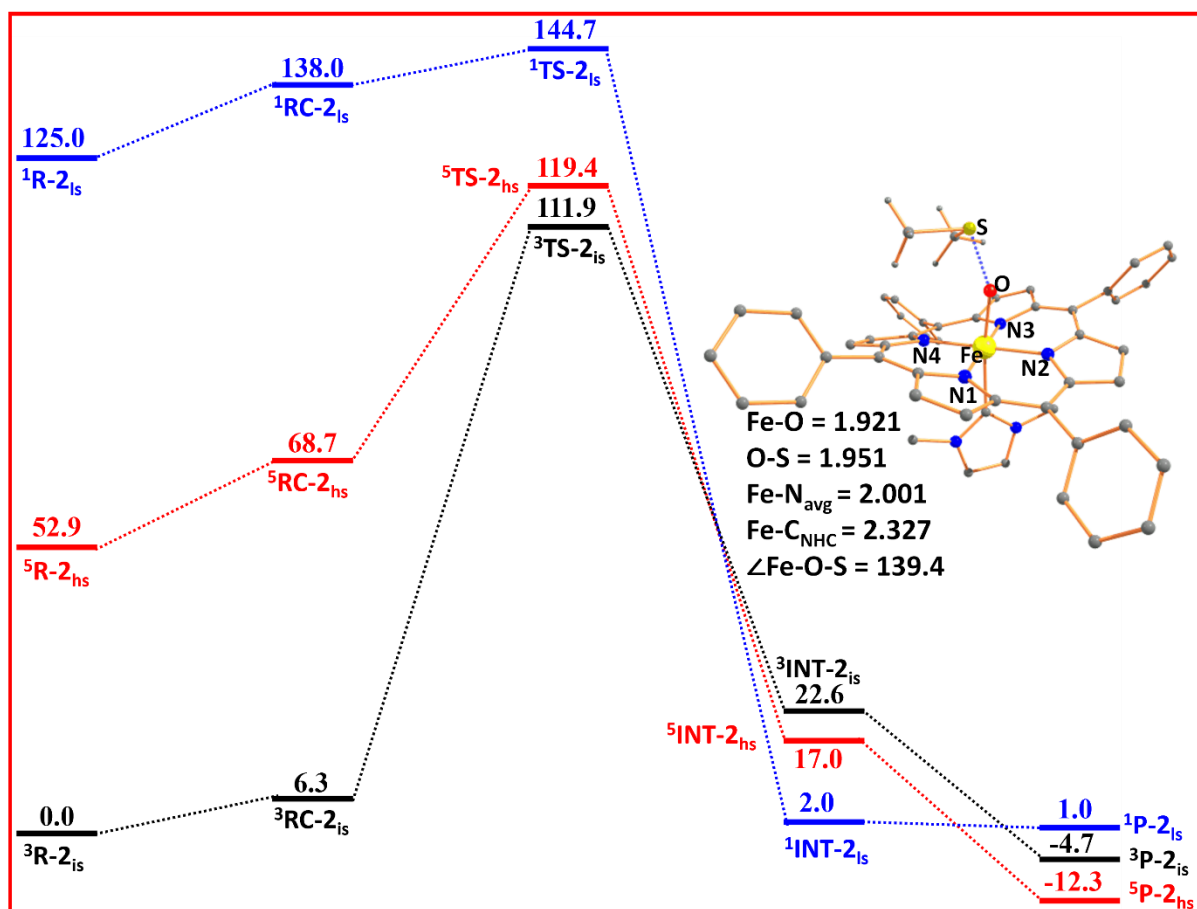


Fig. S11. The key geometric parameters of the transition state (³TS-2_{is}) and energy profile (ΔG in kJ/mol) for OAT in SMe₂ by **2** (given bond lengths are in Å and bond angle in °).

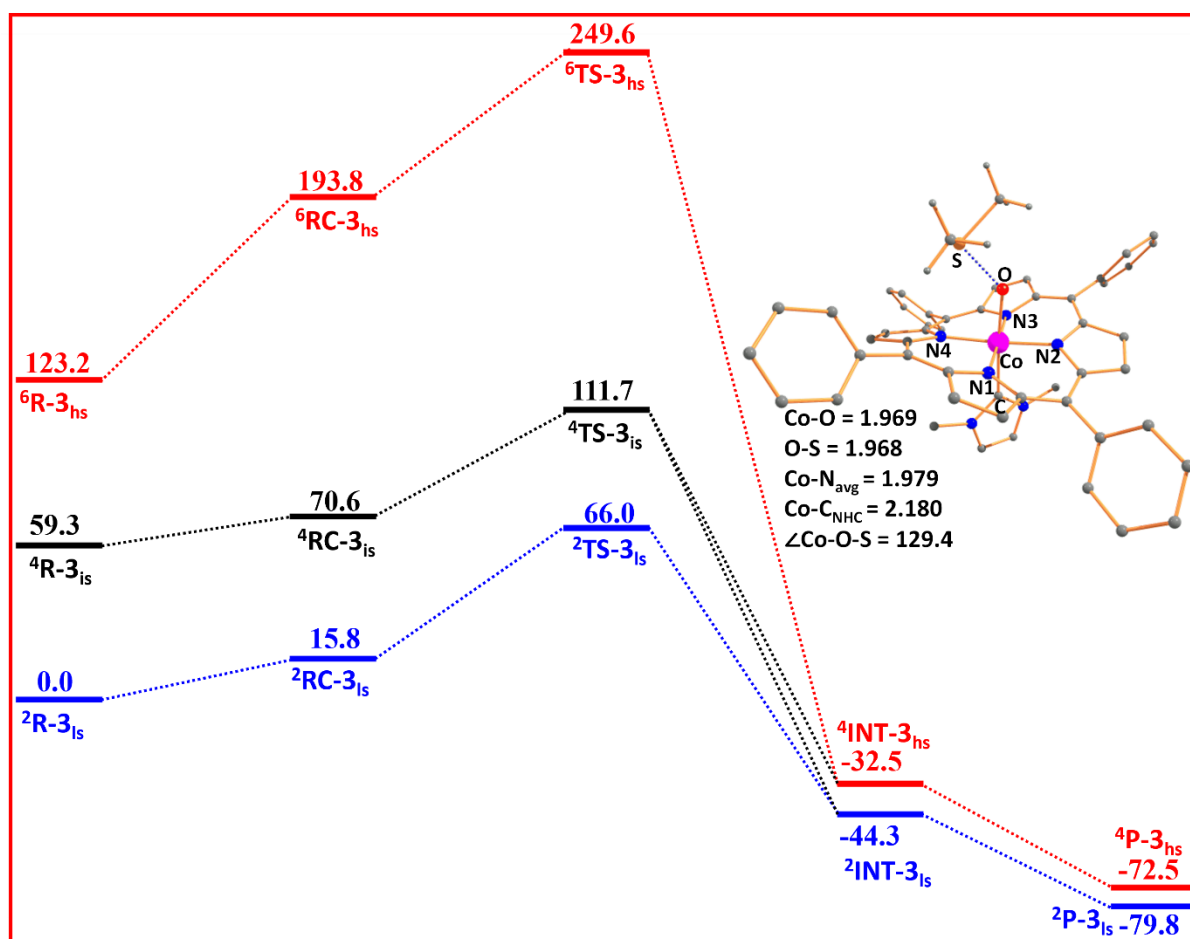


Fig. S12. The key geometric parameters of the transition states and energy profile (ΔG in kJ mol⁻¹) for OAT in SMe₂ by **3** (given bond lengths are in Å and bond angle in °).

Table S12. Computed relative deformation energies in each fragment with respect to the catalyst and interaction energy in the reorganization TSs. (Note: - All energies (in kJ/mol) have been calculated using C-H activation of (CH₄, CHD) and OAT(SMe₂) transition state and reactant from the ground spin state energetics.

Species	ΔE_{def}	ΔE_{int}	ΔE_{act}	$\Delta E^\ddagger$
CH ₄				
1	100.9	24.4	125.2	125.3
2	101.9	-16.6	85.3	85.3
3	61.1	-27.2	34.0	33.9
CHD				
1	30.4	13.7	44.1	44.1
2	-0.43	16.6	16.2	28.7
3	-27.8	5.6	-22.3	7.7
SMe ₂				
1	133.4	-11.1	122.3	122.5
2	46.5	65.4	111.9	112.0
3	-14.2	80.2	66.0	66.1

Where, ΔE_{def} , ΔE_{int} , ΔE_{act} , and $\Delta E^\ddagger$ are a deformation, interaction, activation strain energy and barrier height of the HAA/OAT, respectively.

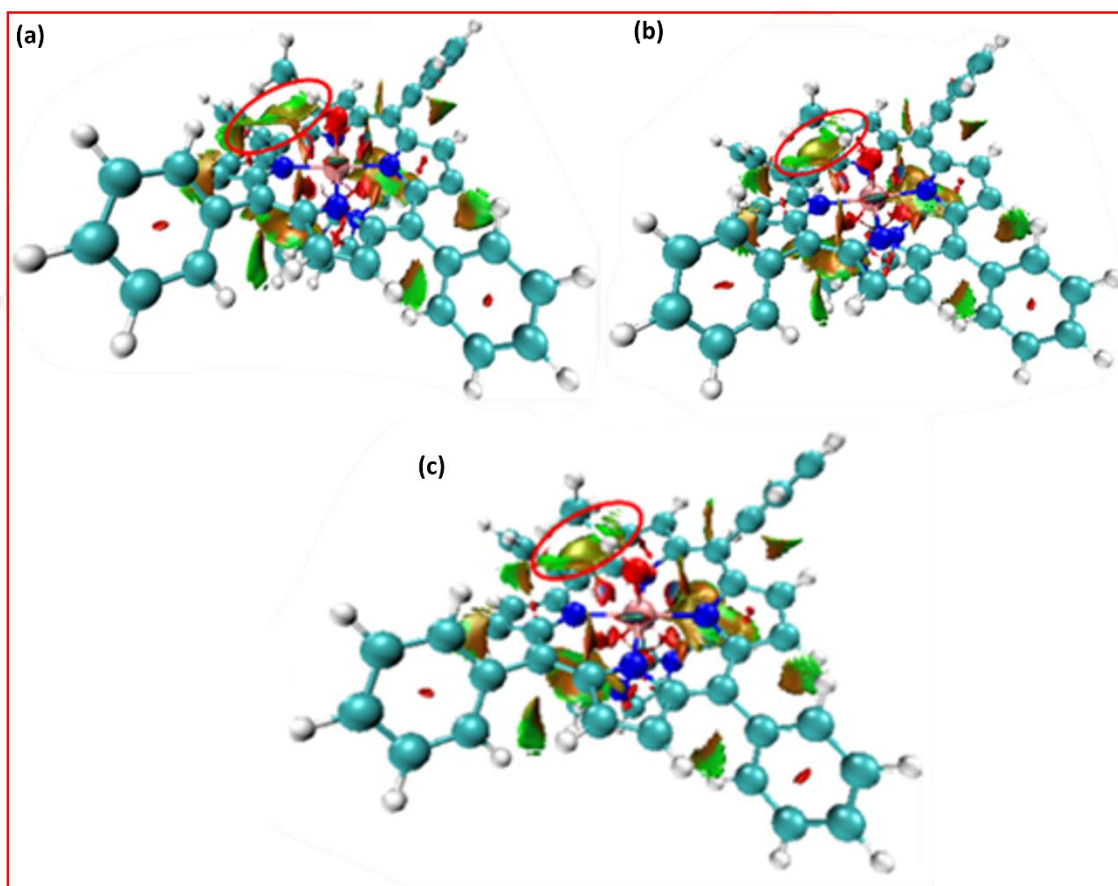


Fig. S13. NCI surfaces of the transition states of (a) $^4\text{TS1-1}_{\text{hs}}$ (b) $^3\text{TS1-2}_{\text{is}}$ and (c) $^2\text{TS1-3}_{\text{ls}}$ with substrate CH₄.

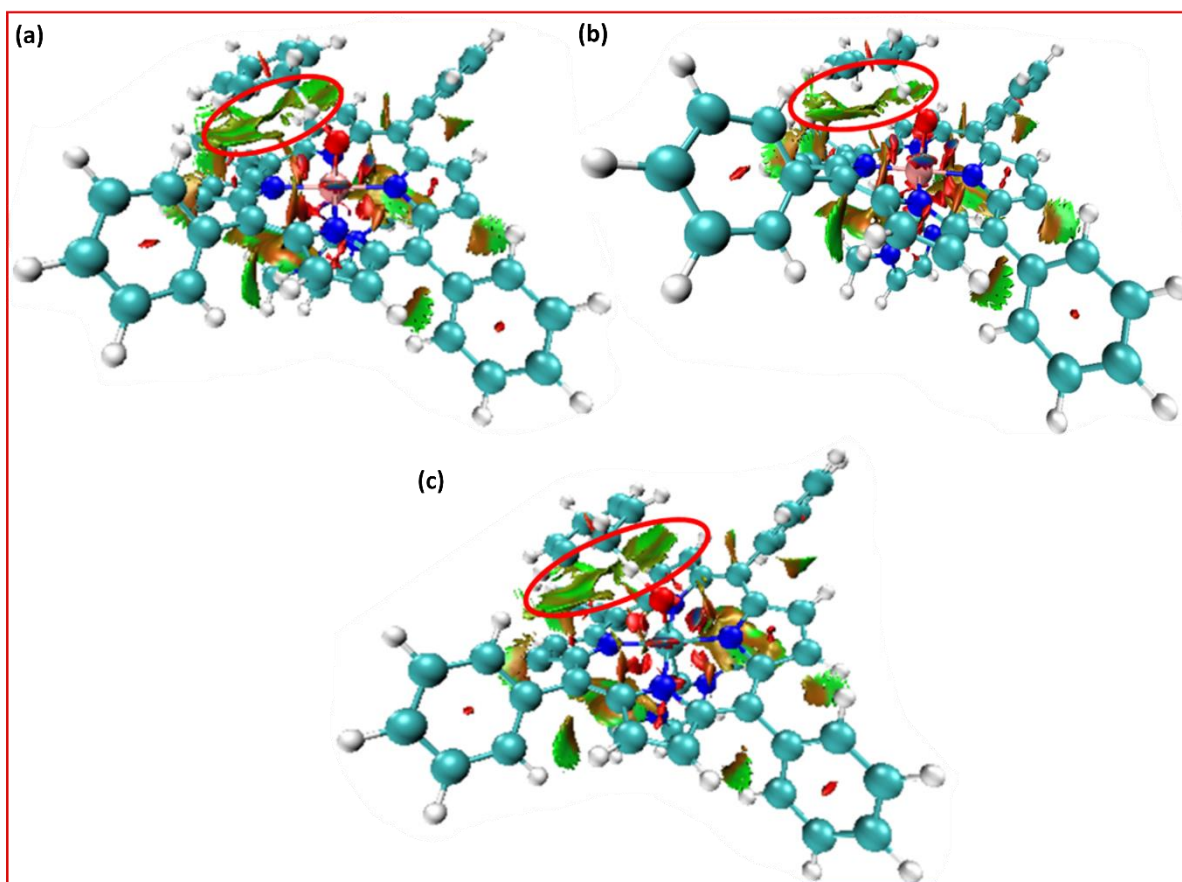


Fig. S14. NCI surfaces of the transition states of (a) ${}^4\text{TS1-1}_{\text{hs}}$ (b) ${}^3\text{TS1-2}_{\text{is}}$ and (c) ${}^2\text{TS1-3}_{\text{ls}}$ with substrate CHD.

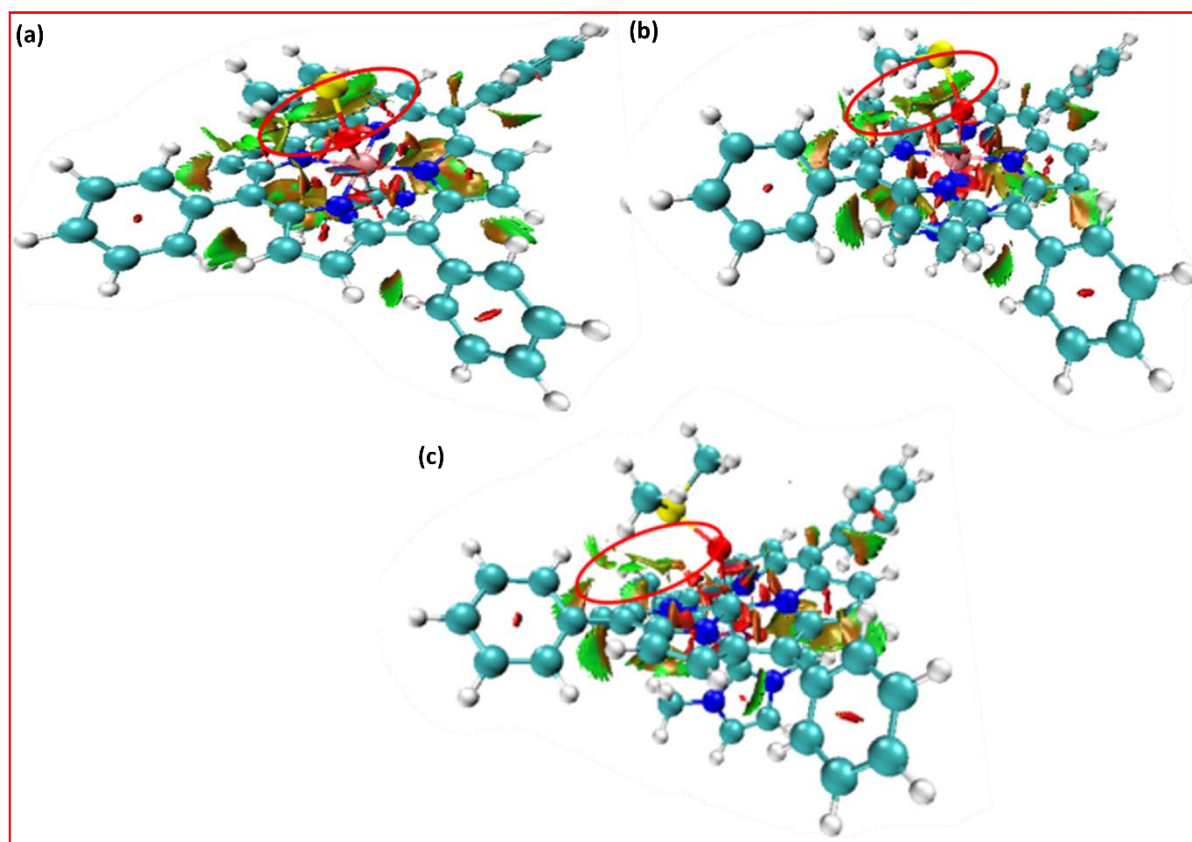


Fig. S15. NCI surfaces of the transition states of (a) ${}^4\text{TS1-1}_{\text{hs}}$ (b) ${}^3\text{TS1-2}_{\text{is}}$ and (c) ${}^2\text{TS1-3}_{\text{ls}}$ with substrate SMe_2 .

Table S13. Calculated percentage buried volume (%V_{bur}) and quadrant-wise steric analysis for **1-3** and transition states (TS1) for CH₄, CHD and SMe₂. The quadrant values represent localized %V_{bur} in the southwest (SW), northwest (NW), northeast (NE) and southeast (SE) hemispheres, relative to the metal-oxo bond.

	Species	%V _{Free}	%V _{Bur}	Quadrant (%V _{Bur})
Reactant	1	10.1	89.9	SW = 93.2; NW = 86.7 NE = 93.2; SE = 86.7
	2	13.8	86.2	SW = 83.7; NW = 88.7 NE = 83.7; SE = 88.7
	3	7.9	92.1	SW = 93.8; NW = 90.4 NE = 93.8; SE = 90.4
TS1 (CH ₄)	1	6.5	93.5	SW = 94.9; NW = 96.7 NE = 94.6; SE = 87.7
	2	5.8	94.2	SW = 95.7; NW = 97.6 NE = 95.4; SE = 88.3
	3	5.0	95.0	SW = 98.0; NW = 96.7 NE = 91.6; SE = 93.7
(TS1) CHD	1	5.5	94.5	SW = 89.4; NW = 97.5 NE = 97.6; SE = 93.6
	2	5.4	94.6	SW = 88.3; NW = 96.5 NE = 97.9; SE = 95.9
	3	4.7	95.3	SW = 92.1; NW = 93.4 NE = 98.2; SE = 97.5
TS (SMe ₂)	1	4.6	95.4	SW = 96.2; NW = 89.5 NE = 98.3; SE = 97.6
	2	4.5	95.5	SW = 93.7; NW = 92.2 NE = 99.0; SE = 97.0
	3	5.1	94.9	SW = 96.6; NW = 89.5 NE = 99.4; SE = 94.0

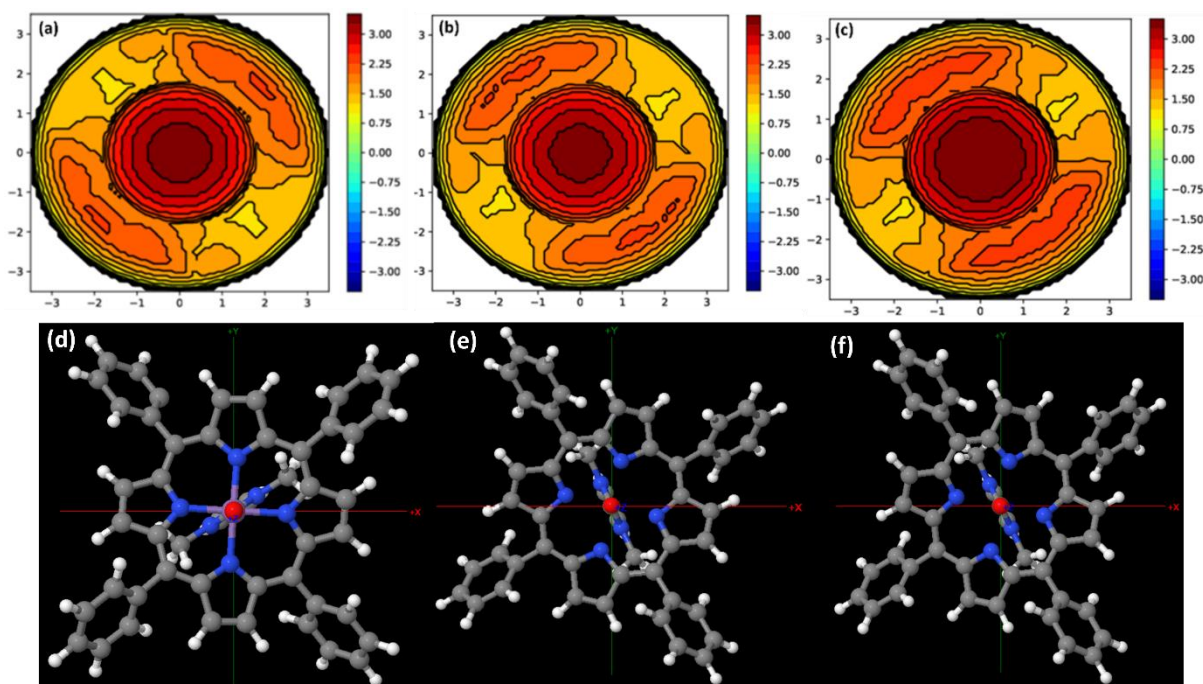


Fig. S16. Steric contour maps generated *via* SambVca 2.1 for the reactants (a) ${}^4\text{R-1}_{\text{hs}}$ (b) ${}^3\text{R-2}_{\text{is}}$ and (c) ${}^2\text{R-3}_{\text{is}}$ along with the orientation (d-f) used for quadrant-specific steric analysis.

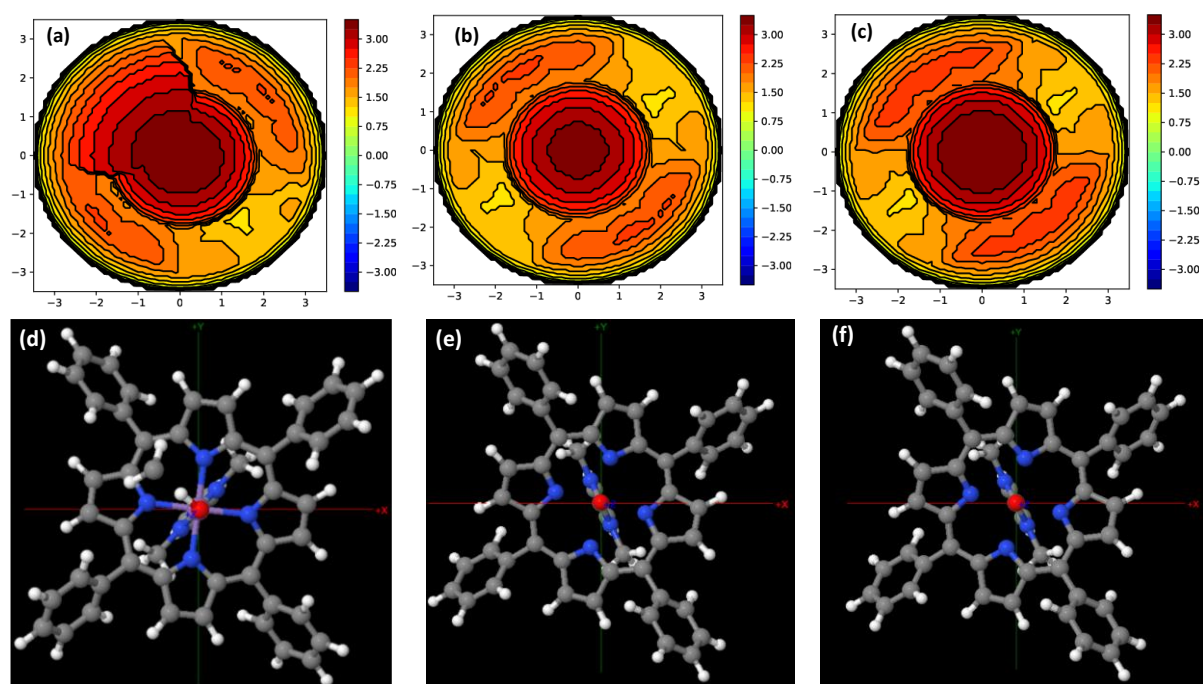


Fig. S17. Steric contour maps generated *via* SambVca 2.1 for the transition states of C-H bond activation of CH_4 by (a) **1** (b) **2** and (c) **3**. Optimized structures of transition states of species 1-3 (d-f) used for $\%V_{\text{bur}}$ analysis. Coordinate axes define the orientation used for quadrant-specific steric analysis.

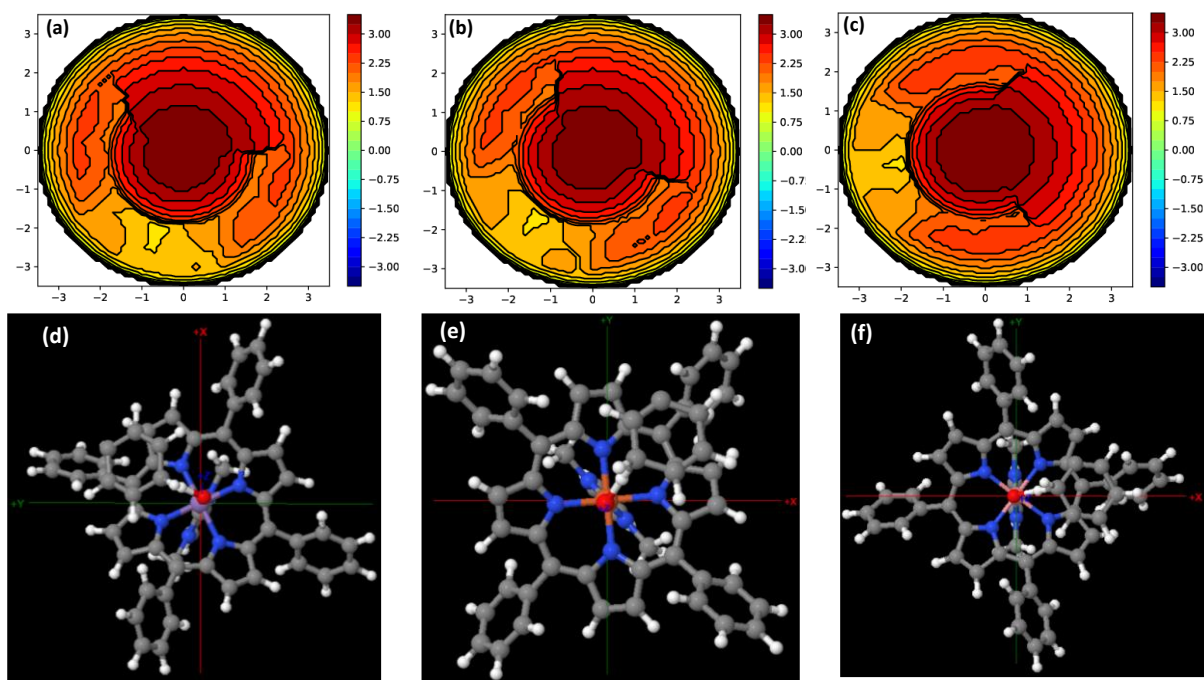


Fig. S18. Steric contour maps generated *via* SambVca 2.1 for the transition states for hydrogen abstraction of CHD by (a) **1** (b) **2** and (c) **3**. Optimized structures of transition state of species **1-3** (d-f) used for %V_{bur} analysis. Coordinate axis defines the orientation used for quadrant-specific steric analysis.

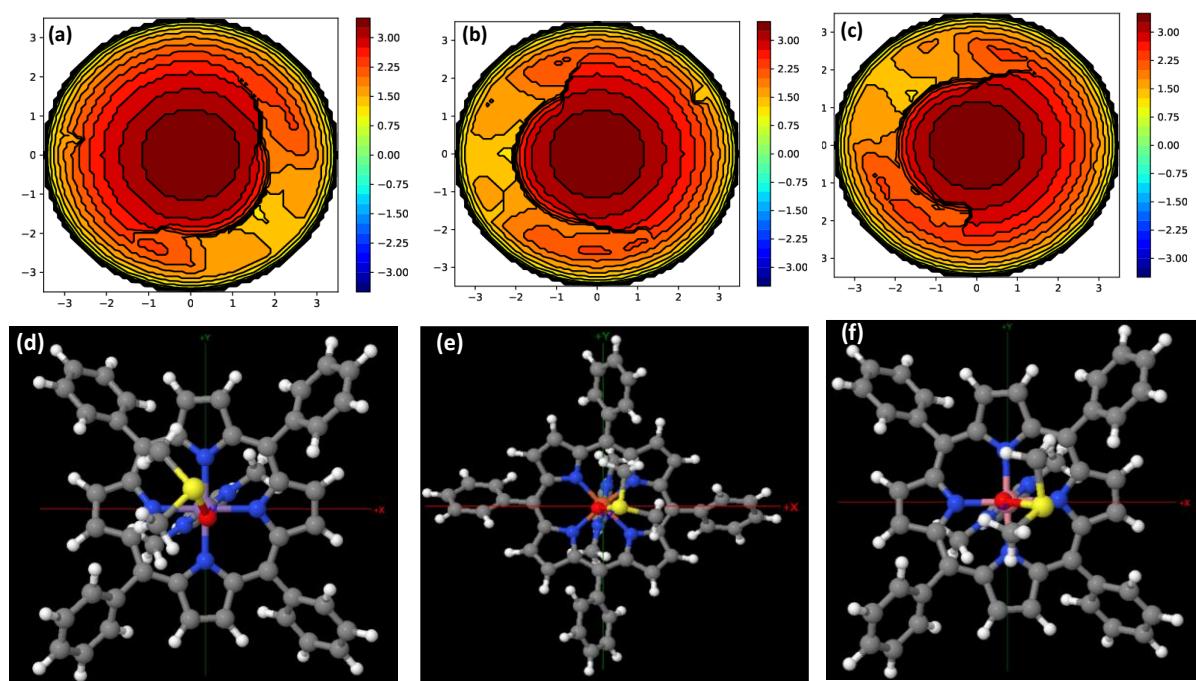


Fig. S19. Steric contour maps generated *via* SambVca 2.1 for the transition states for oxygen atom transfer in SMe₂ by (a) **1** (b) **2** and (c) **3**. Optimized structures of transition state of species **1-3** (d-f) used for %V_{bur} analysis.

Table S14: Electron density properties at the BCPs of interest in the transition states of species **1-3** with substrates (CH₄, CHD and SMe₂). Parameters include the electron density (ρ), Laplacian of the density ($\nabla^2\rho$), kinetic energy density ($G(r)$), potential energy density ($V(r)$), and total energy density ($H(r)$) in atomic units (a.u.).

CH ₄							
	Bonds	BCPs	ρ (a.u.)	$\nabla^2\rho$ (a.u.)	$G(r)$ (a.u.)	$V(r)$ (a.u.)	$H(r)$ (a.u.)
1	Mn-O	185	0.1328	0.6619	0.2045	-0.2434	-0.0389
	O-H	182	0.209	-0.482	0.0918	-0.304	-0.212
	C-H _{CH4}	178	0.109	-0.0172	0.0433	-0.0909	-0.0476
2	Fe-O	182	0.1263	0.6395	0.1977	-0.2356	-0.0379
	O-H	184	0.2226	-0.6048	0.0899	-0.3312	-0.2412
	C-H _{CH4}	181	0.0995	0.0083	0.0422	-0.0823	-0.0401
3	Co-O	174	0.1036	0.4881	0.1405	-0.1589	-0.0184
	O-H	182	0.2116	-0.4833	0.0936	-0.3081	-0.2144
	C-H _{CH4}	190	0.1112	-0.0187	0.0443	-0.0934	-0.0490
CHD							
1	Mn-O	205	0.1467	0.7157	0.2318	-0.2846	-0.0528
	O-H	214	0.1527	-0.0225	0.0907	-0.1872	-0.0964
	H-H _{CHD}	218	0.1441	-0.1430	0.0446	-0.1249	-0.0803
2	Fe-O	206	0.1429	0.7137	0.2309	-0.2834	-0.0524
	O-H	216	0.1294	0.1234	0.0867	-0.1427	-0.0559
	H-H _{CHD}	219	0.1658	-0.2339	0.0448	-0.1482	-0.1033
3	Co-O	205	0.1080	0.5110	0.1492	-0.1707	-0.0214
	O-H	215	0.1105	0.1989	0.0820	-0.1144	-0.0323
	H-H _{CHD}	220	0.1867	-0.3345	0.0446	-0.1728	-0.1282
SMe ₂							
1	Mn-O	193	0.0946	0.5283	0.1473	-0.1625	-0.0152
	O-S	195	0.1203	0.1315	0.0706	-0.1104	-0.0398
2	Fe-O	202	0.0938	0.4810	0.1332	-0.1462	-0.0129
	O-S	203	0.1087	0.1959	0.0788	-0.1092	-0.0303
3	Co-O	190	0.0796	0.4583	0.1162	-0.1179	-0.0016
	O-S	186	0.0996	0.1828	0.0670	-0.0890	-0.0219

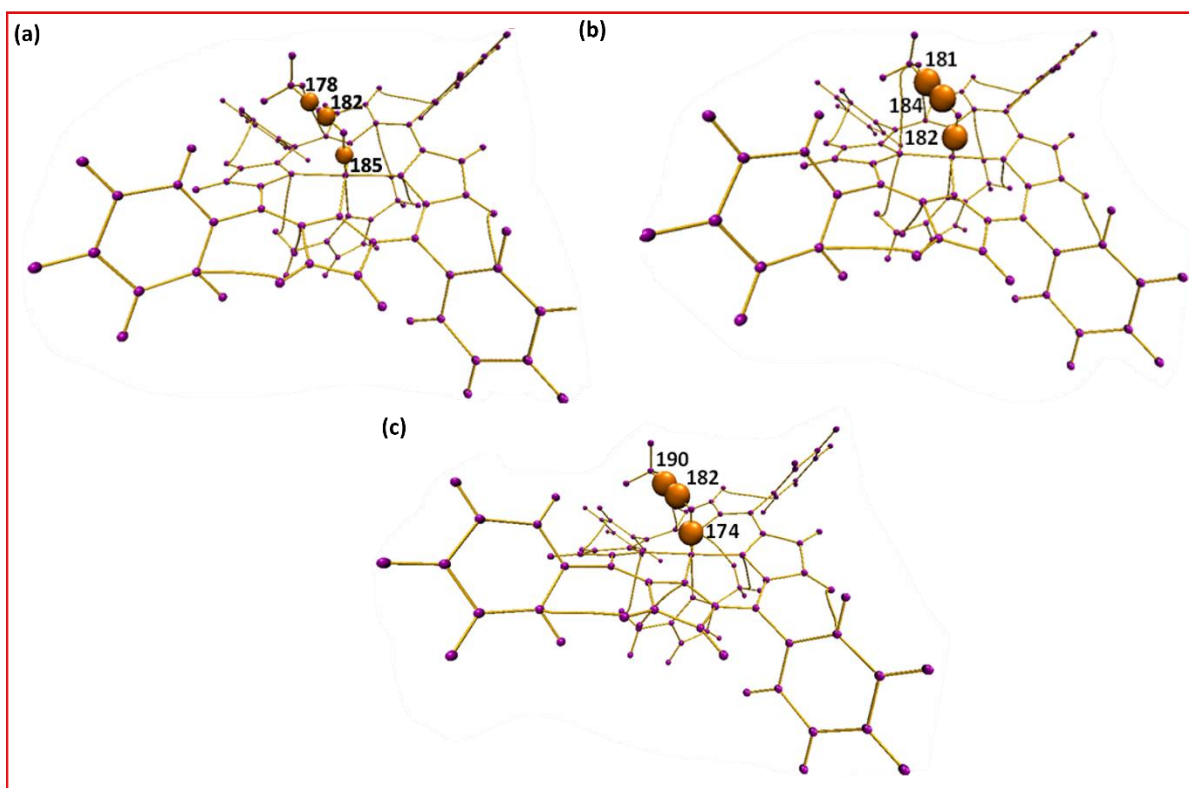


Fig. S20. Molecular graphs showing the BCPs (orange spheres) derived from QTAIM analysis in the transition states of (a) ${}^4\text{TS1-1}_{\text{hs}}$ (b) ${}^3\text{TS1-2}_{\text{is}}$ and (c) ${}^2\text{TS1-3}_{\text{is}}$ with substrate CH_4 . The labelled BCPs correspond to M-O, O-H and H- C_{CH_4} interactions relevant to the HAA and OAT process.

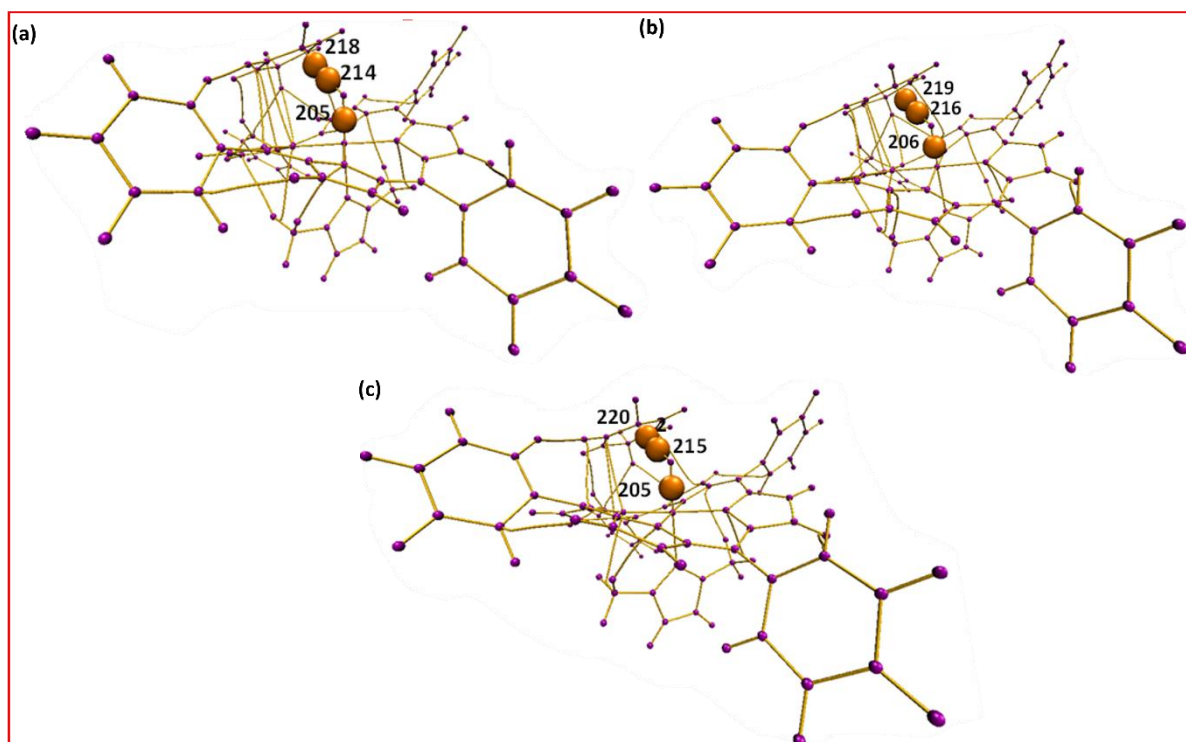


Fig. S21. Molecular graphs showing the BCPs (orange spheres) derived from QTAIM analysis in the transition states of (a) ${}^4\text{TS1-1}_{\text{hs}}$ (b) ${}^3\text{TS1-2}_{\text{is}}$ and (c) ${}^2\text{TS1-3}_{\text{ls}}$ with substrate CHD. The labelled BCPs correspond to M-O, O-H_{CHD} and H-C_{MHD} interactions relevant to the HAA process.

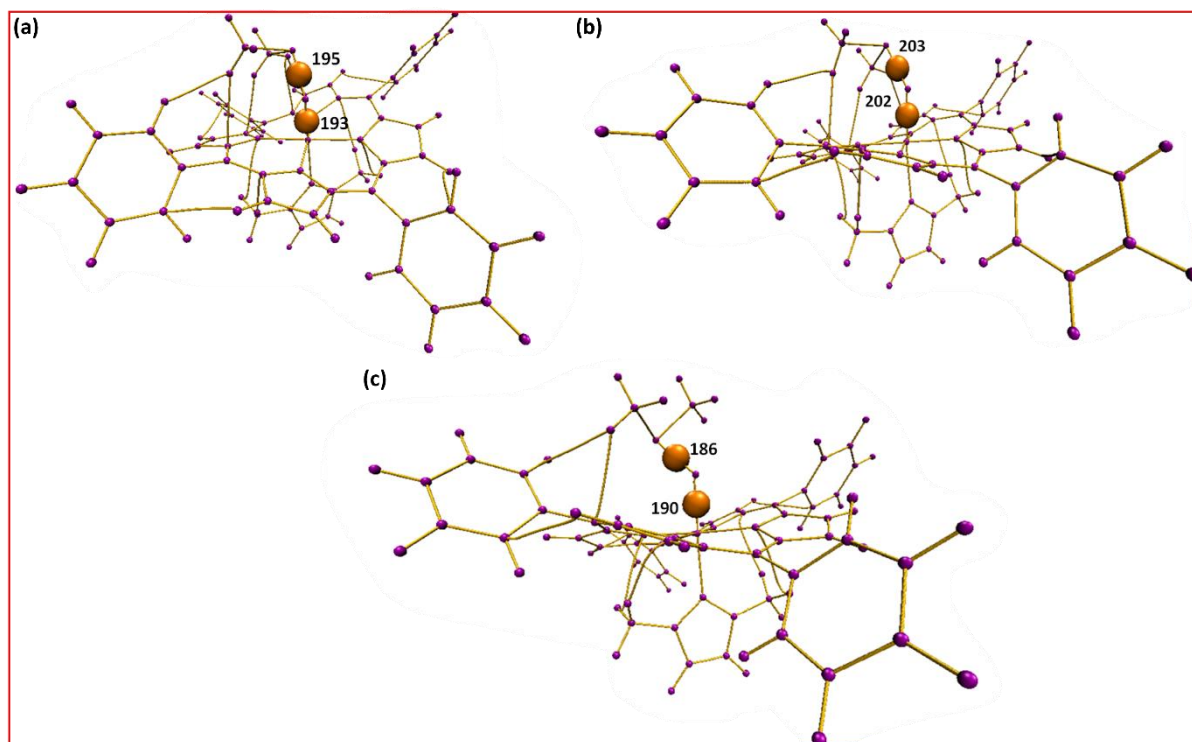


Fig. S22. Molecular graphs showing the BCPs (orange spheres) derived from QTAIM analysis in the transition states of (a) ${}^2\text{TS-1}_{\text{hs}}$, (b) ${}^3\text{TS-2}_{\text{is}}$ and (c) ${}^2\text{TS-3}_{\text{ls}}$ with substrate SMe_2 . The labelled BCPs correspond to M-O and O-S interactions relevant to the oxygen atom transfer (OAT) process.

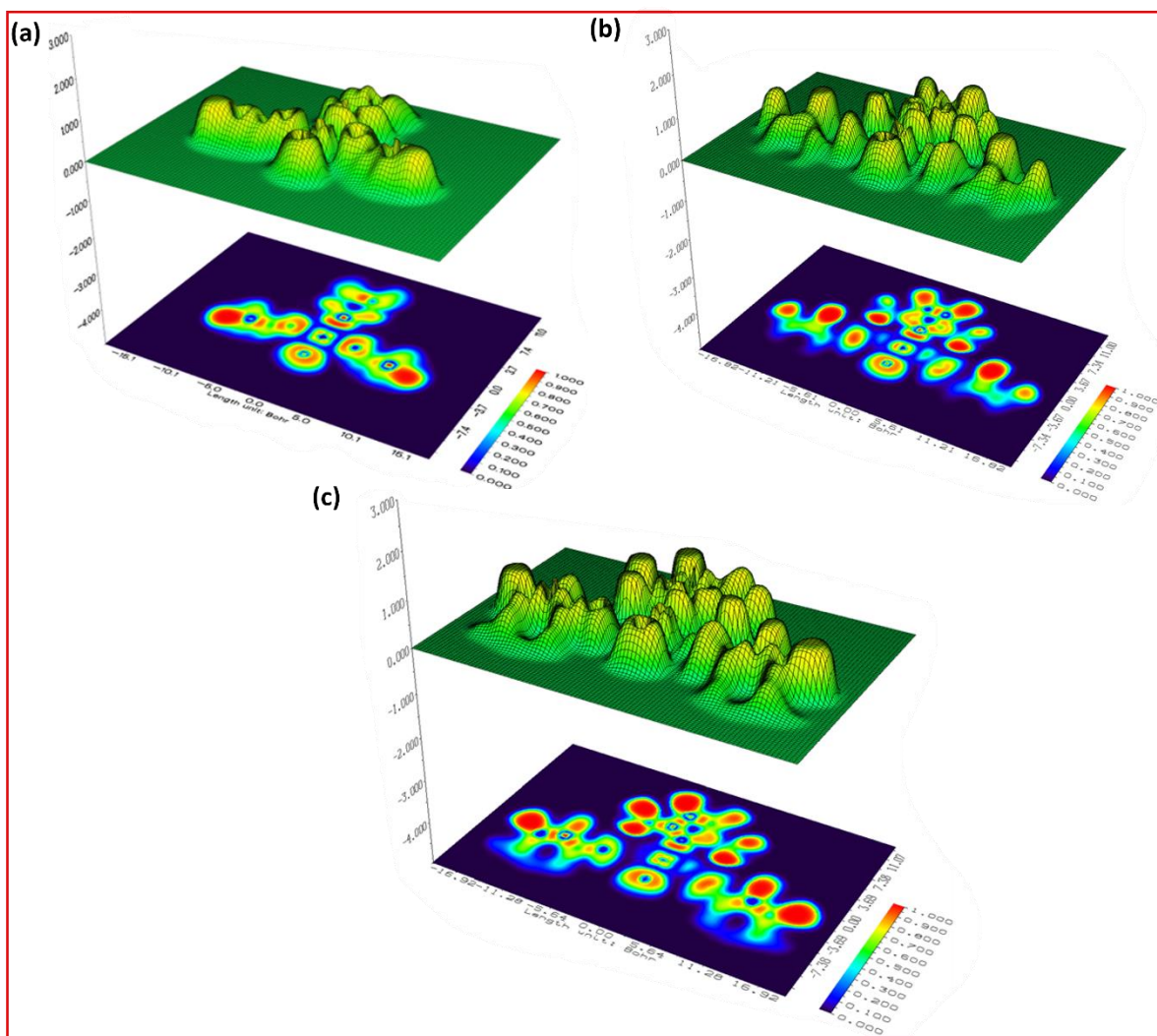


Fig. S23. ELF surface and contour plots for the transition states of (a) $^4\text{TS1-1}_{\text{hs}}$ (b) $^3\text{TS1-2}_{\text{is}}$ and (c) $^2\text{TS1-3}_{\text{is}}$ with substrate CH₄.

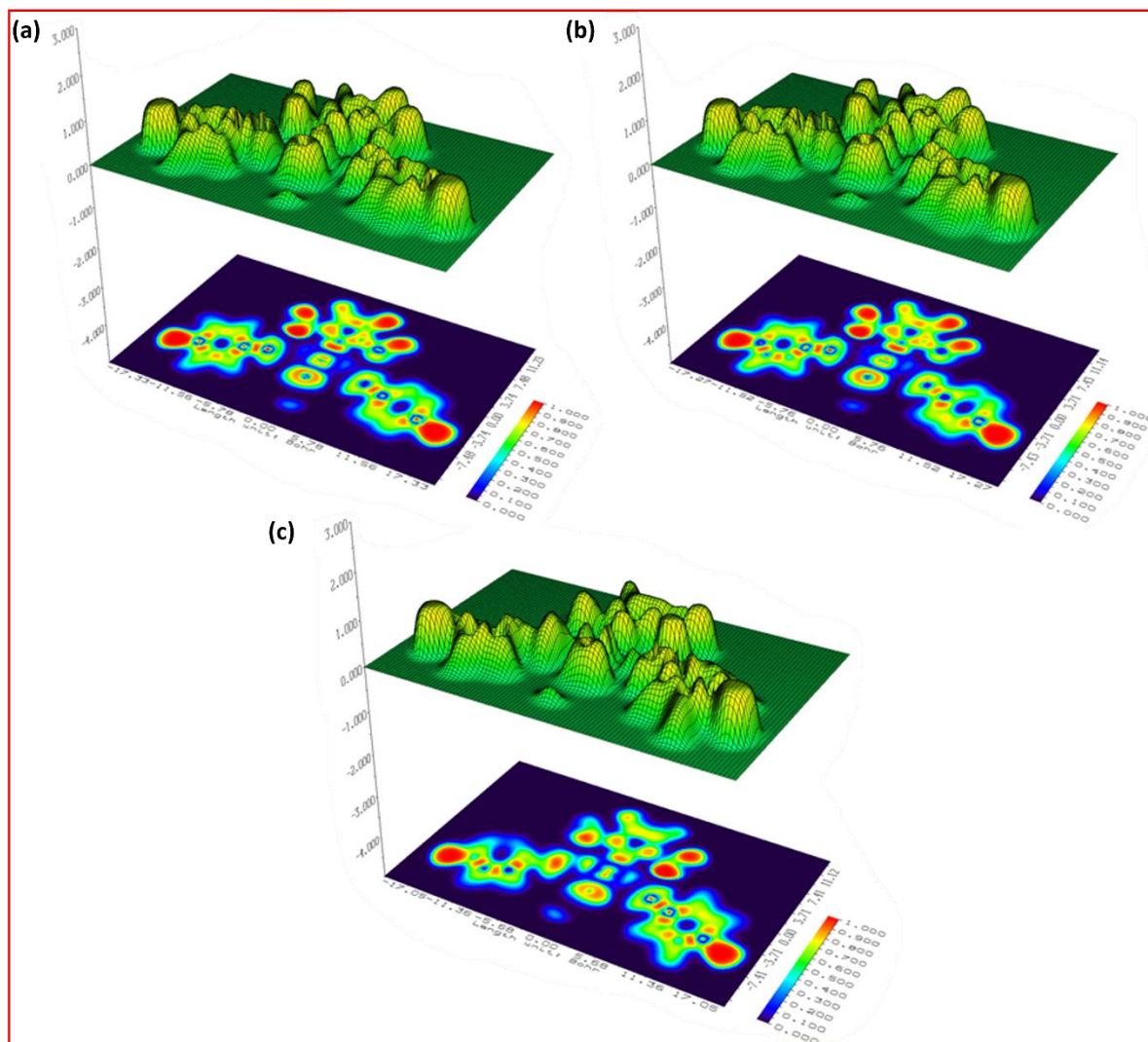


Fig. S24. ELF surface and contour plots for the transition states of (a) $^4\text{TS1-1}_{\text{hs}}$, (b) $^3\text{TS1-2}_{\text{is}}$ and (c) $^2\text{TS1-3}_{\text{hs}}$ with substrate CHD.

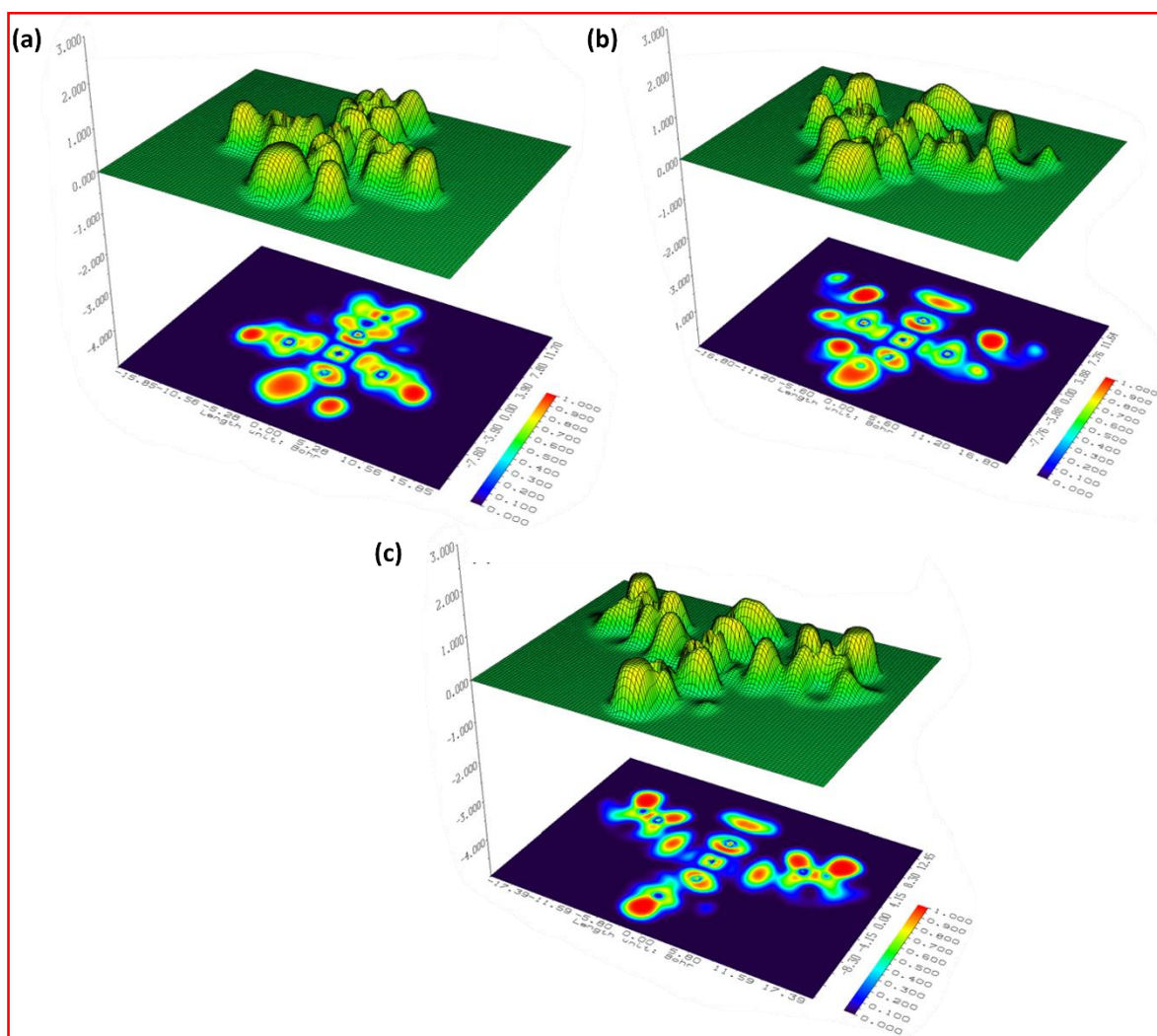


Fig. S25. ELF surface and contour plots for the transition states of (a) $^2\text{TS-1}_{\text{hs}}$, (b) $^3\text{TS-2}_{\text{is}}$ and (c) $^2\text{TS-3}_{\text{is}}$ with substrate SMe_2 .

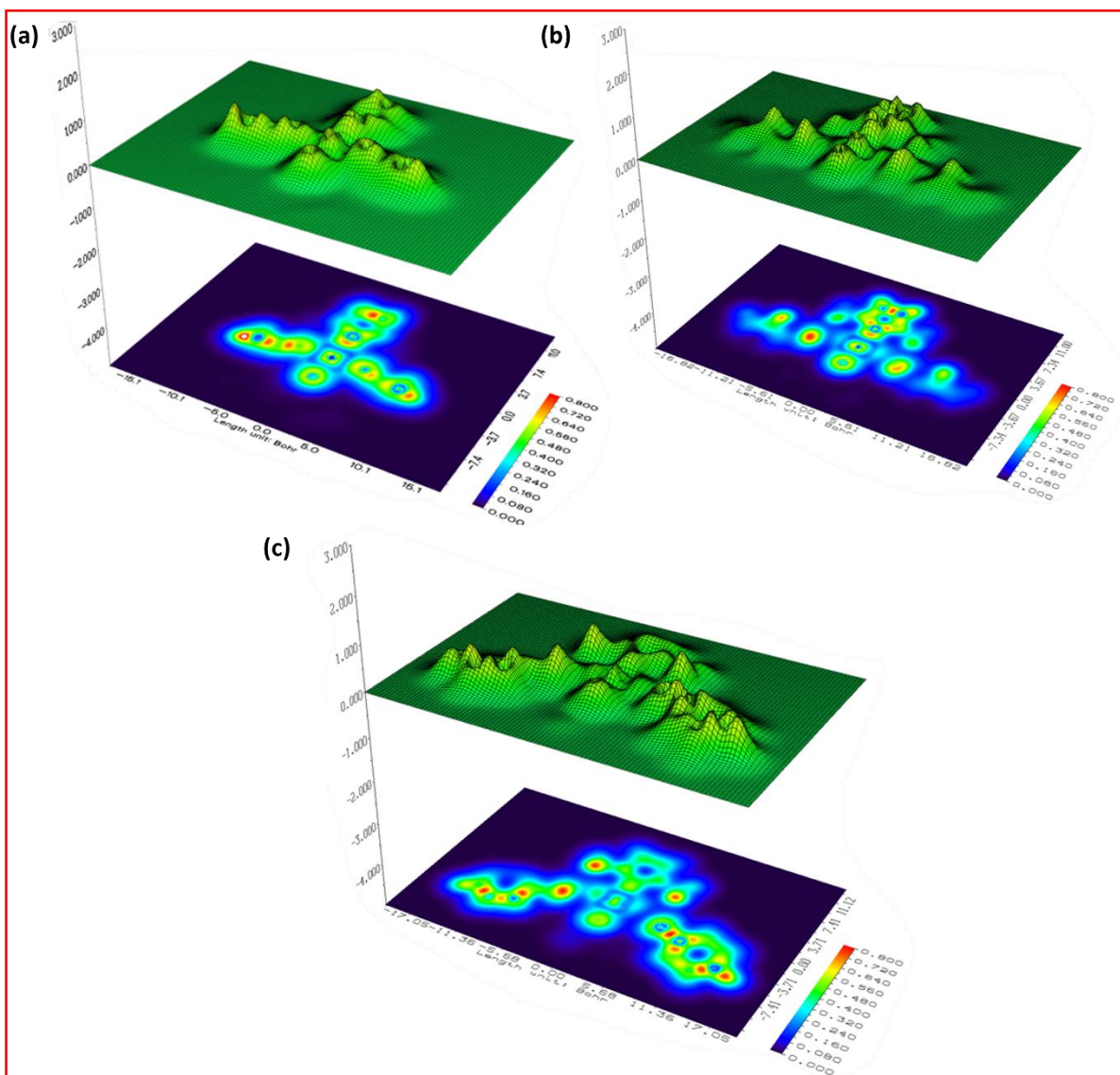


Fig. S26. LOL surface and contour plots for the transition states of (a) $^4\text{TS1-1}_{\text{hs}}$ (b) $^3\text{TS1-2}_{\text{is}}$ and (c) $^2\text{TS1-3}_{\text{is}}$ with substrate CH_4 .

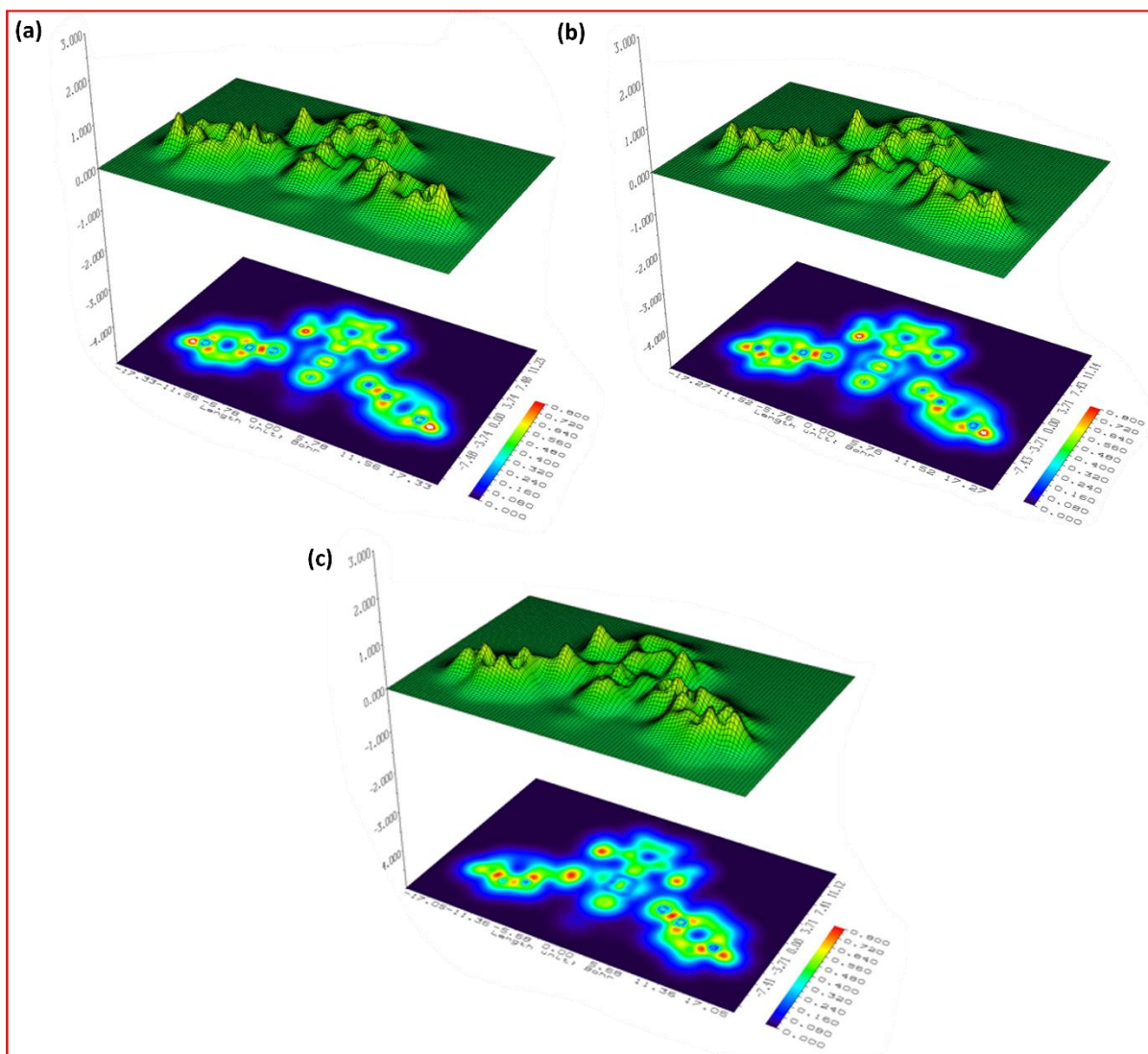


Fig. S27. LOL surface and contour plots for the transition states of (a) ${}^4\text{TS1-1}_{\text{hs}}$ (b) ${}^3\text{TS1-2}_{\text{is}}$ and (c) ${}^2\text{TS1-3}_{\text{is}}$ with substrate CHD.

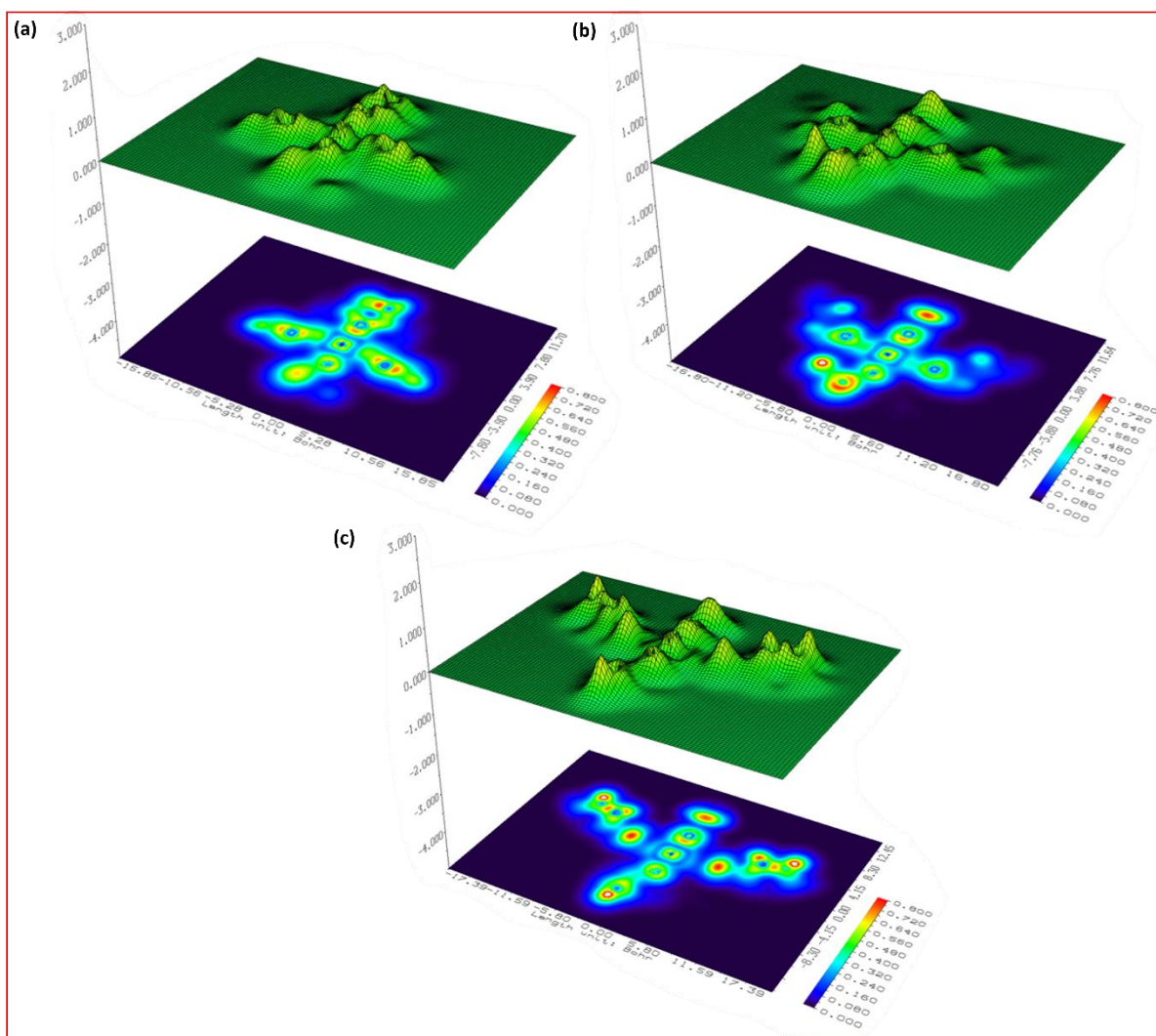


Fig. S28. LOL surface and contour plots for the transition states of (a) ${}^4\text{TS1-1}_{\text{hs}}$ (b) ${}^3\text{TS1-2}_{\text{is}}$ and (c) ${}^2\text{TS1-3}_{\text{is}}$ with substrate SMe_2 .

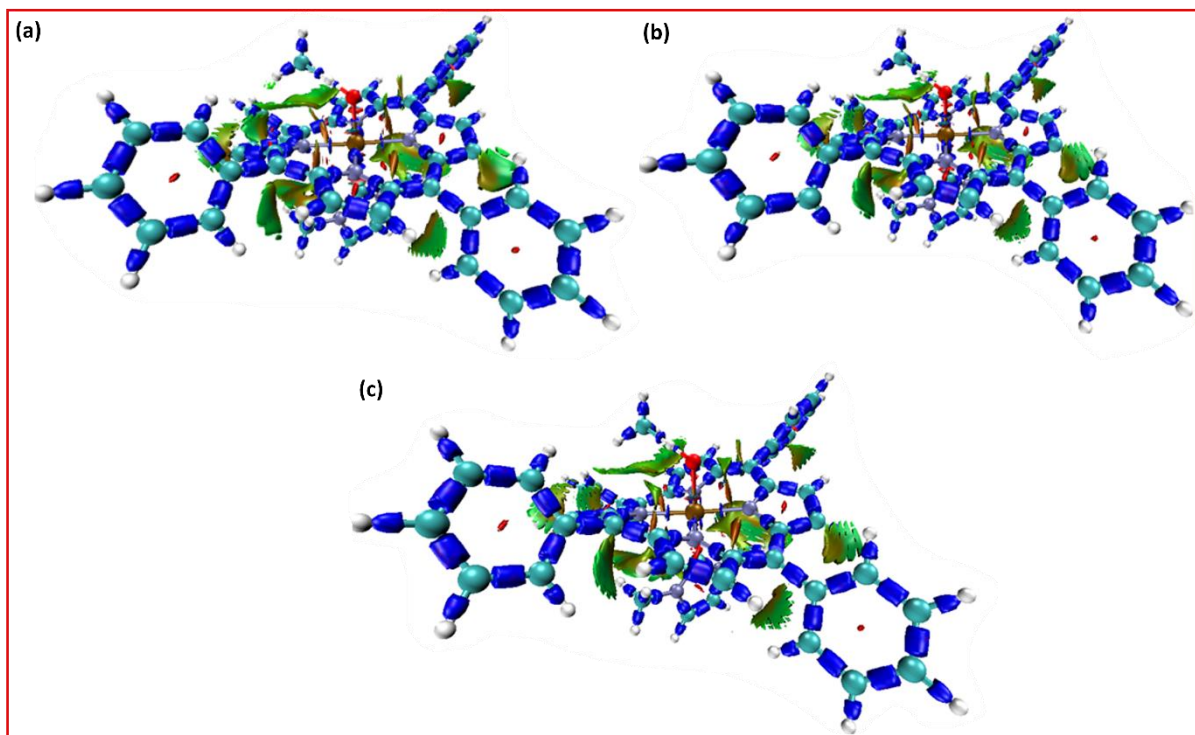


Fig. S29. IRI analysis of the transition states of (a) ${}^4\text{TS1-1}_{\text{hs}}$ (b) ${}^3\text{TS1-2}_{\text{is}}$ and (c) ${}^2\text{TS1-3}_{\text{ls}}$ with substrate CH_4 (isosurface value = 1.0 a.u.), highlighting weak noncovalent interactions (green) and strong covalent regions (blue).

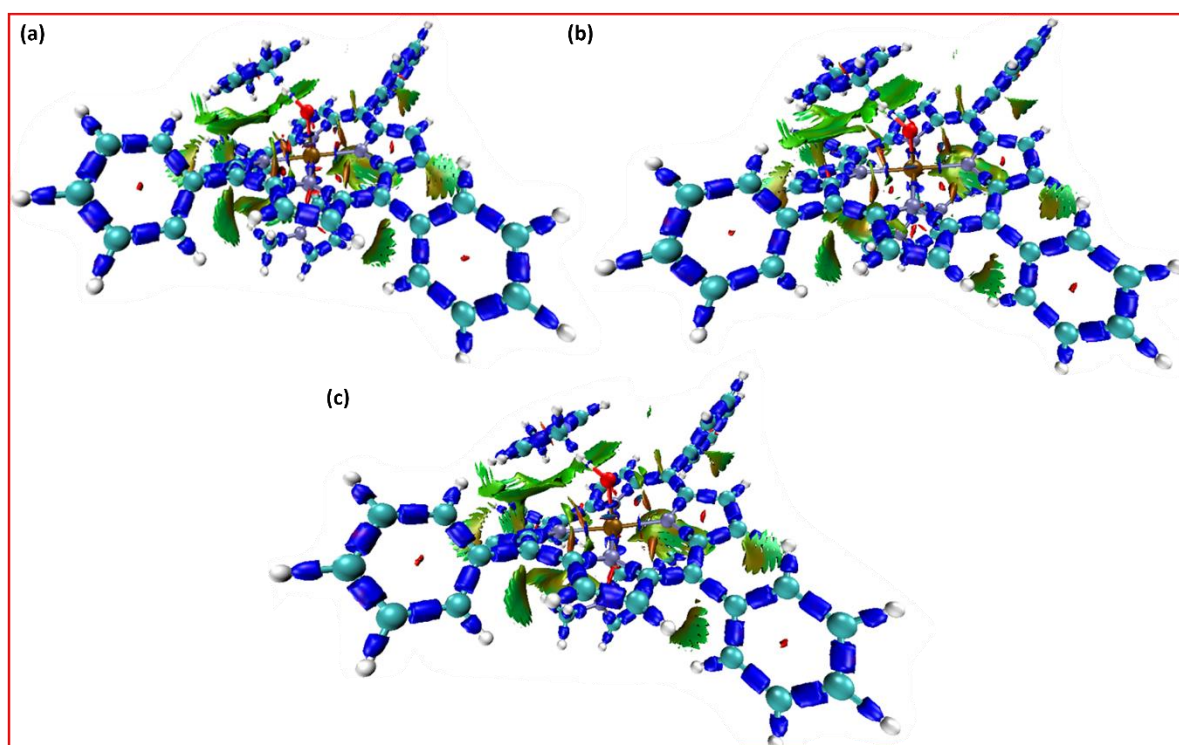


Fig. S30. IRI analysis of the transition states of (a) $^4\text{TS1-1}_{\text{hs}}$ (b) $^3\text{TS1-2}_{\text{is}}$ and (c) $^2\text{TS1-3}_{\text{ls}}$ with substrate CHD (isosurface value = 1.0 a.u.), highlighting weak noncovalent interactions (green) and strong covalent regions (blue).

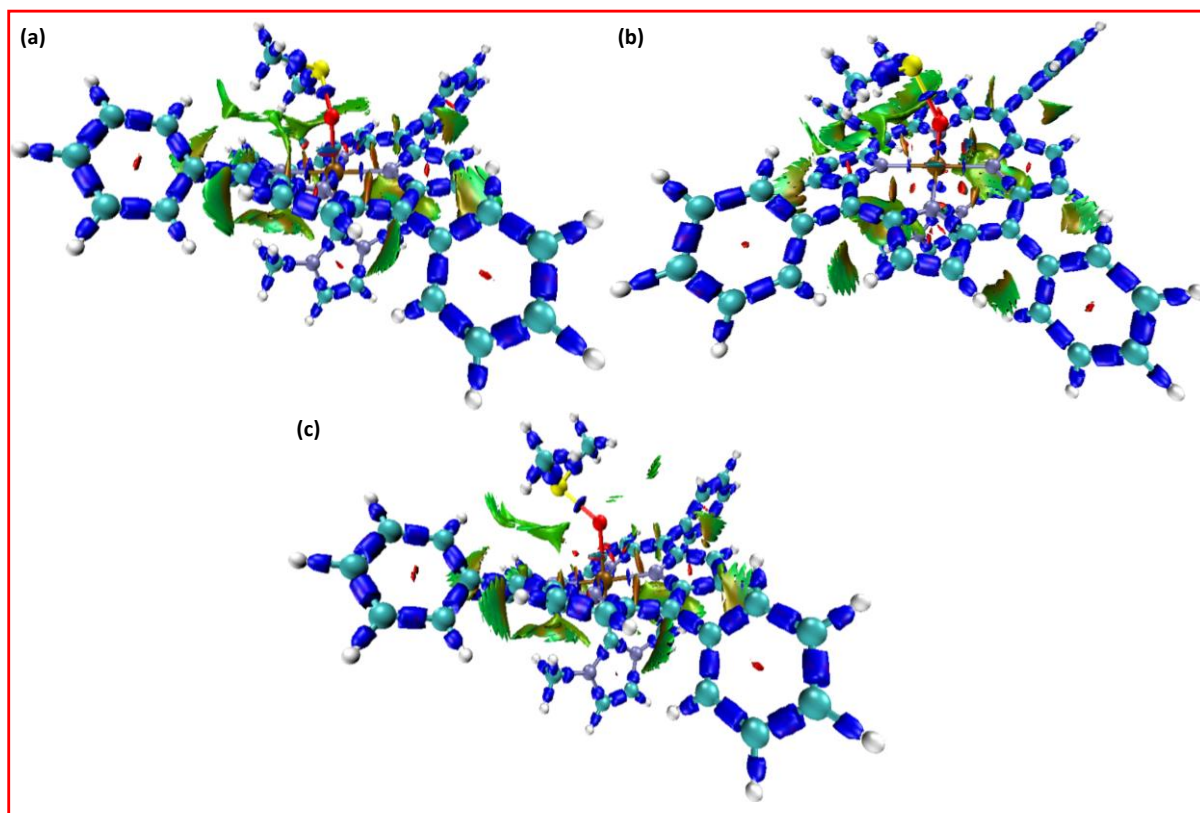


Fig. S31. IRI analysis of the transition states of (a) $^4\text{TS1-1}_{\text{hs}}$ (b) $^3\text{TS1-2}_{\text{is}}$ and (c) $^2\text{TS1-3}_{\text{ls}}$ with substrate SMe_2 (isosurface value = 1.0 a.u.), highlighting weak noncovalent interactions (green) and strong covalent regions (blue).

The source of stabilizing energy between methane and porphyrin ring

The stabilization energy of methane remains nearly same in both the gas phase (porphyrin environment) and the solvent phase after applying Gibbs free energy corrections. For subsequent analysis, solvent-phase optimized structures were employed to determine bond distances, Mulliken charge distributions and electrostatic interactions.

(1) UB3LYP computed data for species 1, 2 and 3.

Distances(Å)

Distances	1	2	3
O-H1	1.222	1.103	1.118
O-H2	2.965	2.984	2.982
O-H3	3.005	3.003	2.976
O-H4	3.007	3.002	2.994
O-C	2.554	2.574	2.543
M-O	1.838	1.810	1.887

Mulliken Charge Densities

Atoms	1	2	3
O	-0.462	-0.428	-0.459
C	-0.527	-0.459	-0.452
H1	0.203	0.188	0.173
H2	0.131	0.137	0.134
H3	0.125	0.139	0.136
H4	0.124	0.141	0.138

(2) Stabilization Energy by methane

Evaluated as $E_{ts1} - (E_R + E_{CH4})$ neglecting counterpoise corrections.

	Stabilization Energy (kJ/mol)
⁴ TS1-1 _{hs}	24.3 kJ/mol
³ TS1-2 _{is}	-16.6 kJ/mol
² TS1-3 _{ls}	-27.1 kJ/mol

(3) Electrostatic Interaction

Evaluated (general equation) in kcal/mol from

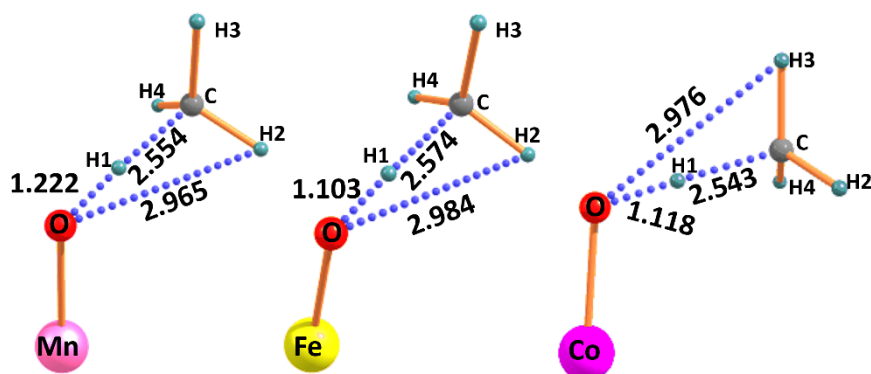
$$E_{el} = 332 \cdot \sum_{A,B} q_A \cdot q_B / R_{AB}$$

where the distance between two-point charges R_{AB} is in Å.

In our case, we include the interactions between C, H1, and one shorted distance H2/H3 atom from the O atom.

Evaluated in kJ/mol from

$$E_{el} = 1388 \cdot q_O \left(\frac{q_C}{R_{OC}} + \sum_n^4 \frac{q_H}{R_{OH}} \right)$$



	Electrostatic Interaction (kJ/mol)
⁴ TS1-1 _{hs}	-2.6
³ TS1-2 _{is}	-21.9
² TS1-3 _{is}	-14.0

Reaction Coordinates

C-H bond activation of methane by species 1

⁴R-1_{hs}

Mn	0.000003000	0.000097000	-0.389937000
O	-0.000024000	0.000183000	-2.076601000
C	0.000055000	-0.000271000	1.884255000
C	0.679403000	-0.005974000	4.087829000
H	1.392039000	-0.007227000	4.894804000
C	-0.679317000	0.002954000	4.087829000
H	-1.391961000	0.003303000	4.894798000
C	-2.486012000	-0.004089000	2.356473000
H	-3.085578000	0.270581000	3.229001000
H	-2.647176000	0.719583000	1.562820000
H	-2.781457000	-0.995745000	2.007215000
C	2.486126000	0.003348000	2.356513000
H	3.085784000	-0.271124000	3.229038000
H	2.647709000	-0.720136000	1.562756000
H	2.781109000	0.995189000	2.007421000
N	1.075105000	-0.009986000	2.747280000
N	-1.074998000	0.008561000	2.747281000
N	-1.612362000	-1.179043000	-0.334074000
N	1.203810000	-1.599142000	-0.305264000
N	1.612346000	1.179203000	-0.333892000
N	-1.203812000	1.599316000	-0.305014000
C	-2.899992000	-0.800169000	-0.651447000
C	-1.641476000	-2.513153000	0.029769000
C	0.802340000	-2.896474000	-0.065625000
C	2.521526000	-1.639361000	-0.734296000
C	2.899982000	0.800368000	-0.651291000
C	1.641465000	2.513257000	0.030181000
C	-0.802338000	2.896635000	-0.065287000
C	-2.521532000	1.639582000	-0.734056000
C	-3.785412000	-1.927048000	-0.433908000
H	-4.854137000	-1.901842000	-0.576258000
C	-3.020723000	-2.965170000	0.024034000
H	-3.350267000	-3.950255000	0.311634000
C	1.911292000	-3.789919000	-0.343235000
H	1.866239000	-4.864020000	-0.258207000
C	2.950655000	-3.023010000	-0.790718000
H	3.917774000	-3.355871000	-1.130930000
C	3.785416000	1.927188000	-0.433510000
H	4.854149000	1.901972000	-0.575801000
C	3.020723000	2.965252000	0.024557000
H	3.350257000	3.950289000	0.312331000
C	-1.911282000	3.790106000	-0.342821000
H	-1.866224000	4.864200000	-0.257693000
C	-2.950656000	3.023236000	-0.790346000
H	-3.917780000	3.356128000	-1.130515000
C	-3.329577000	0.509744000	-0.934160000
C	-0.509192000	-3.323813000	0.213833000
C	3.329574000	-0.509497000	-0.934225000
C	0.509184000	3.323926000	0.214239000
C	-4.745998000	0.686797000	-1.359320000
C	-5.218580000	0.012655000	-2.502520000
H	-4.528859000	-0.606719000	-3.066120000
C	-6.549153000	0.148359000	-2.911637000
H	-6.894701000	-0.371321000	-3.799937000
C	-7.431604000	0.956555000	-2.182584000
H	-8.464160000	1.062427000	-2.500469000
C	-6.974819000	1.625539000	-1.039531000
H	-7.655252000	2.245186000	-0.463334000
C	-5.644070000	1.489794000	-0.629955000
H	-5.293431000	1.996325000	0.263050000
C	-0.688035000	-4.756246000	0.586893000
C	-1.467718000	-5.633838000	-0.190942000
H	-1.950003000	-5.256739000	-1.086111000
C	-1.602012000	-6.978758000	0.170267000

H	-2.201320000	-7.643434000	-0.444344000
C	-0.954769000	-7.470858000	1.311329000
H	-1.058726000	-8.514873000	1.589996000
C	-0.166590000	-6.609825000	2.086195000
H	0.340981000	-6.984036000	2.970053000
C	-0.032460000	-5.265202000	1.724926000
H	0.578243000	-4.594447000	2.320624000
C	4.745993000	-0.686462000	-1.359415000
C	5.218558000	-0.012114000	-2.502503000
H	4.528821000	0.607343000	-3.065993000
C	6.549131000	-0.147721000	-2.911650000
H	6.894664000	0.372119000	-3.799862000
C	7.431603000	-0.956020000	-2.182737000
H	8.464159000	-1.061818000	-2.500645000
C	6.974840000	-1.625198000	-1.039790000
H	7.655291000	-2.244924000	-0.463699000
C	5.644091000	-1.489550000	-0.630183000
H	5.293474000	-1.996231000	0.262746000
C	0.688017000	4.756355000	0.587366000
C	1.467657000	5.633958000	-0.190514000
H	1.949947000	5.256841000	-1.085671000
C	1.601920000	6.978887000	0.170671000
H	2.201189000	7.643579000	-0.443960000
C	0.954680000	7.470975000	1.311742000
H	1.058591000	8.514999000	1.590394000
C	0.166540000	6.609932000	2.086634000
H	-0.341014000	6.984149000	2.970498000
C	0.032435000	5.265298000	1.725383000
H	-0.578249000	4.594539000	2.321097000

²R-1_s

Mn	-0.000016000	0.000159000	-0.358858000
O	-0.000025000	0.000386000	-2.066437000
C	0.000050000	-0.000429000	1.887236000
C	0.678347000	-0.034101000	4.089623000
H	1.390709000	-0.064667000	4.896076000
C	-0.678416000	0.029504000	4.089628000
H	-1.390834000	0.058765000	4.896081000
C	-2.487131000	0.103117000	2.371013000
H	-3.066993000	0.383227000	3.254963000
H	-2.624937000	0.849753000	1.595217000
H	-2.824749000	-0.868221000	2.005011000
C	2.487228000	-0.104309000	2.371025000
H	3.067280000	-0.383837000	3.255030000
H	2.625726000	-0.850899000	1.595288000
H	2.824069000	0.867265000	2.004971000
N	1.074258000	-0.053587000	2.750410000
N	-1.074211000	0.051360000	2.750421000
N	-1.674321000	-1.107600000	-0.320211000
N	1.126531000	-1.668811000	-0.278489000
N	1.674297000	1.107898000	-0.319936000
N	-1.126580000	1.669132000	-0.278110000
C	-2.947585000	-0.657284000	-0.604177000
C	-1.767606000	-2.451135000	-0.003636000
C	0.658313000	-2.952532000	-0.089726000
C	2.451505000	-1.765930000	-0.674785000
C	2.947556000	0.657628000	-0.603973000
C	1.767581000	2.451387000	-0.003157000
C	-0.658331000	2.952845000	-0.089292000
C	-2.451539000	1.766298000	-0.674437000
C	-3.885954000	-1.744414000	-0.410246000
H	-4.954135000	-1.663542000	-0.535213000
C	-3.166621000	-2.835256000	-0.002319000
H	-3.541779000	-3.811531000	0.258576000
C	1.728579000	-3.893762000	-0.361574000
H	1.629803000	-4.966414000	-0.309045000
C	2.817065000	-3.167049000	-0.756493000
H	3.775085000	-3.538477000	-1.082407000
C	3.885930000	1.744717000	-0.409829000

H	4.954111000	1.663854000	-0.534794000	H	-1.849616000	2.419180000	3.346755000
C	3.166604000	2.835479000	-0.001679000	H	-1.293037000	2.412591000	1.655729000
H	3.541755000	3.811692000	0.259459000	H	-2.548322000	1.267484000	2.174308000
C	-1.728561000	3.894102000	-0.361185000	N	-0.588717000	0.838255000	2.843708000
H	-1.629752000	4.966751000	-0.308664000	N	0.962975000	-0.650842000	2.813814000
C	-2.817075000	3.167427000	-0.756088000	N	2.045200000	-0.202236000	-0.313017000
H	-3.775083000	3.538885000	-1.082004000	N	0.273449000	2.022931000	-0.261271000
C	-3.316701000	0.676292000	-0.863529000	N	-1.912631000	0.271956000	-0.156722000
C	-0.677060000	-3.323082000	0.158704000	N	-0.143269000	-1.954105000	-0.168375000
C	3.316669000	-0.675894000	-0.863644000	C	2.716738000	-1.361936000	-0.638095000
C	0.677043000	3.323335000	0.159218000	C	2.987659000	0.758901000	0.005587000
C	-4.729688000	0.927326000	-1.263712000	C	1.457892000	2.703164000	-0.075401000
C	-5.256433000	0.290229000	-2.404587000	C	-0.677296000	2.939012000	-0.684661000
H	-4.609374000	-0.357777000	-2.986314000	C	-2.609792000	1.414114000	-0.487371000
C	-6.585452000	0.496629000	-2.788394000	C	-2.827244000	-0.674901000	0.265396000
H	-6.972329000	0.003801000	-3.675006000	C	-1.312167000	-2.624993000	0.123860000
C	-7.413052000	1.340977000	-2.036379000	C	0.773085000	-2.886679000	-0.629356000
H	-8.444391000	1.501912000	-2.334520000	C	4.139289000	-1.139093000	-0.471902000
C	-6.902521000	1.975047000	-0.896105000	H	4.898824000	-1.888124000	-0.630608000
H	-7.540174000	2.623151000	-0.302489000	C	4.303502000	0.147785000	-0.036370000
C	-5.573380000	1.768051000	-0.511931000	H	5.226143000	0.646449000	0.212349000
H	-5.181092000	2.249080000	0.377942000	C	1.245870000	4.105641000	-0.381467000
C	-0.932847000	-4.756052000	0.482207000	H	2.012500000	4.862959000	-0.338249000
C	-1.749815000	-5.564826000	-0.331467000	C	-0.050695000	4.241778000	-0.793863000
H	-2.203850000	-5.131927000	-1.216206000	H	-0.541665000	5.136178000	-1.141702000
C	-1.957939000	-6.912401000	-0.018475000	C	-4.016399000	1.197914000	-0.213119000
H	-2.585235000	-7.523127000	-0.660578000	H	-4.788032000	1.938154000	-0.353251000
C	-1.348704000	-7.476775000	1.110056000	C	-4.144508000	-0.068418000	0.289689000
H	-1.509772000	-8.522849000	1.351420000	H	-5.045480000	-0.560381000	0.618432000
C	-0.524929000	-6.685121000	1.921009000	C	-1.125709000	-4.036174000	-0.155292000
H	-0.046924000	-7.115373000	2.795843000	H	-1.888721000	-4.788602000	-0.034793000
C	-0.317329000	-5.337744000	1.607922000	C	0.138376000	-4.189948000	-0.652734000
H	0.320773000	-4.720907000	2.232480000	H	0.602686000	-5.096315000	-1.006108000
C	4.729656000	-0.926857000	-1.263875000	C	2.126345000	-2.615570000	-0.884346000
C	5.256373000	-0.289621000	-2.404688000	C	2.717241000	2.126804000	0.176208000
H	4.609297000	0.358452000	-2.986320000	C	-2.043742000	2.655664000	-0.832321000
C	6.585383000	-0.495969000	-2.788548000	C	-2.548046000	-2.037876000	0.448579000
H	6.972240000	-0.003030000	-3.675107000	C	3.024401000	-3.716530000	-1.330267000
C	7.413006000	-1.340404000	-2.036653000	C	3.792270000	-3.557242000	-2.500696000
H	8.444339000	-1.501298000	-2.334837000	H	3.692655000	-2.638974000	-3.069757000
C	6.902501000	-1.974621000	-0.896450000	C	4.657966000	-4.568762000	-2.928973000
H	7.540168000	-2.622796000	-0.302928000	H	5.236317000	-4.433291000	-3.837634000
C	5.573364000	-1.767681000	-0.512226000	C	4.774176000	-5.755212000	-2.192588000
H	5.181101000	-2.248825000	0.377596000	H	5.445638000	-6.540597000	-2.525365000
C	0.932866000	4.756289000	0.482804000	C	4.021307000	-5.921618000	-1.022832000
C	1.749818000	5.565103000	-0.330854000	H	4.114409000	-6.833625000	-0.441039000
H	2.203788000	5.132259000	-1.215652000	C	3.155683000	-4.909871000	-0.593880000
C	1.957973000	6.912651000	-0.017789000	H	2.583464000	-5.031728000	0.319658000
H	2.585233000	7.523419000	-0.659886000	C	3.833695000	3.060020000	0.499712000
C	1.348807000	7.476959000	1.110818000	C	4.980386000	3.157000000	-0.312028000
H	1.509903000	8.523016000	1.352241000	H	5.052850000	2.536571000	-1.198592000
C	0.525075000	6.685265000	1.921766000	C	6.003464000	4.057353000	0.004181000
H	0.047130000	7.115461000	2.796659000	H	6.877564000	4.124782000	-0.636205000
C	0.317430000	5.337907000	1.608593000	C	5.895538000	4.879990000	1.133169000
H	-0.320654000	4.721049000	2.233148000	H	6.689583000	5.578917000	1.376912000
*RC-1_{hs}				C	4.753648000	4.801201000	1.941238000
Mn	0.062715000	0.032679000	-0.293853000	H	4.660573000	5.437802000	2.815834000
O	-0.006893000	-0.003142000	-1.981019000	C	3.730697000	3.901268000	1.624830000
C	0.156009000	0.078455000	1.966863000	H	2.842834000	3.837594000	2.245663000
C	-0.255714000	0.586454000	4.177642000	C	-2.976254000	3.730439000	-1.270329000
H	-0.744293000	1.090230000	4.994054000	C	-3.818112000	3.508309000	-2.378170000
C	0.726396000	-0.352310000	4.158652000	H	-3.749931000	2.562075000	-2.904571000
H	1.273118000	-0.827791000	4.954908000	C	-4.716947000	4.493465000	-2.799409000
C	1.983982000	-1.618252000	2.405325000	H	-5.352612000	4.309410000	-3.659961000
H	2.263262000	-2.210350000	3.281476000	C	-4.792907000	5.715677000	-2.118240000
H	1.577641000	-2.273253000	1.640061000	H	-5.490066000	6.480649000	-2.445682000
H	2.866274000	-1.107925000	2.013223000	C	-3.966627000	5.944253000	-1.010219000
C	-1.638777000	1.791030000	2.476560000	H	-4.028317000	6.884242000	-0.470266000
				C	-3.067741000	4.958885000	-0.587982000
				H	-2.439305000	5.128737000	0.279802000

C	-3.653794000	-2.960623000	0.833220000
C	-4.816438000	-3.075241000	0.046748000
H	-4.899666000	-2.479536000	-0.855409000
C	-5.832637000	-3.966786000	0.406983000
H	-6.720049000	-4.050065000	-0.212936000
C	-5.700757000	-4.760822000	1.553927000
H	-6.489687000	-5.452830000	1.831854000
C	-4.541901000	-4.663912000	2.335605000
H	-4.430948000	-5.279441000	3.223121000
C	-3.524961000	-3.773260000	1.975414000
H	-2.623677000	-3.695587000	2.575093000
C	-2.958009000	-1.484953000	-2.912772000
H	-1.979076000	-1.030940000	-2.723296000
H	-2.982644000	-2.488891000	-2.473800000
H	-3.735226000	-0.866319000	-2.448944000
H	-3.138396000	-1.554566000	-3.991777000

²RC-1_h

Mn	0.065328000	0.027255000	-0.266003000
O	0.000051000	-0.001119000	-1.974548000
C	0.148451000	0.062330000	1.968096000
C	-0.247041000	0.581000000	4.178098000
H	-0.717938000	1.101521000	4.994210000
C	0.698878000	-0.393536000	4.158712000
H	1.226282000	-0.891228000	4.954239000
C	1.910289000	-1.707316000	2.416793000
H	2.174693000	-2.292167000	3.302295000
H	1.475360000	-2.361166000	1.667270000
H	2.806396000	-1.234658000	2.010617000
C	-1.579314000	1.846525000	2.490058000
H	-1.780661000	2.455995000	3.375556000
H	-1.199617000	2.478973000	1.693516000
H	-2.501435000	1.363656000	2.161693000
N	-0.568921000	0.848037000	2.845523000
N	0.926640000	-0.698369000	2.814954000
N	2.043644000	-0.308725000	-0.298856000
N	0.386089000	2.014606000	-0.229548000
N	-1.908414000	0.365821000	-0.154027000
N	-0.251050000	-1.957991000	-0.147319000
C	2.654086000	-1.511111000	-0.591698000
C	3.040532000	0.611269000	-0.027269000
C	1.610101000	2.634255000	-0.088870000
C	-0.527773000	2.984267000	-0.613645000
C	-2.540873000	1.555135000	-0.449505000
C	-2.882008000	-0.544172000	0.214410000
C	-1.463829000	-2.571047000	0.090426000
C	0.632450000	-2.938837000	-0.570395000
C	4.088212000	-1.357381000	-0.450901000
H	4.808082000	-2.147633000	-0.594073000
C	4.323496000	-0.065255000	-0.064956000
H	5.273697000	0.393286000	0.156060000
C	1.462239000	4.048586000	-0.377487000
H	2.267729000	4.765576000	-0.360197000
C	0.159193000	4.255480000	-0.736320000
H	-0.296578000	5.176548000	-1.061906000
C	-3.961816000	1.406020000	-0.207413000
H	-4.691858000	2.190086000	-0.331234000
C	-4.166138000	0.128670000	0.240677000
H	-5.097871000	-0.325246000	0.537156000
C	-1.339517000	-3.991056000	-0.178984000
H	-2.143448000	-4.704579000	-0.091527000
C	-0.063665000	-4.210139000	-0.618807000
H	0.368036000	-5.139413000	-0.953700000
C	2.001557000	-2.738660000	-0.813110000
C	2.845937000	1.994945000	0.126890000
C	-1.908725000	2.774606000	-0.758393000
C	-2.679407000	-1.924123000	0.378487000
C	2.844577000	-3.893642000	-1.230674000
C	3.625048000	-3.803746000	-2.400148000

H	3.577437000	-2.895157000	-2.991061000
C	4.438322000	-4.869227000	-2.799456000
H	5.027107000	-4.785947000	-3.707764000
C	4.488501000	-6.042541000	-2.035019000
H	5.119161000	-6.869787000	-2.345471000
C	3.722165000	-6.141175000	-0.866356000
H	3.763716000	-7.042920000	-0.262946000
C	2.909567000	-5.075029000	-0.466457000
H	2.326290000	-5.145284000	0.445655000
C	4.020979000	2.870339000	0.402748000
C	5.143963000	2.894116000	-0.446789000
H	5.152716000	2.258347000	-1.325431000
C	6.225273000	3.739896000	-0.176999000
H	7.079950000	3.750455000	-0.846467000
C	6.200704000	4.581006000	0.943279000
H	7.039616000	5.237902000	1.151036000
C	5.084052000	4.574724000	1.789486000
H	5.055659000	5.225601000	2.658097000
C	4.003164000	3.729037000	1.519374000
H	3.135037000	3.722480000	2.170631000
C	-2.782686000	3.909826000	-1.165761000
C	-3.632753000	3.769811000	-2.280732000
H	-3.615390000	2.838448000	-2.836961000
C	-4.476211000	4.815021000	-2.670746000
H	-5.119006000	4.693050000	-3.537086000
C	-4.487622000	6.017429000	-1.951194000
H	-5.141766000	6.828947000	-2.254470000
C	-3.652264000	6.165490000	-0.836289000
H	-3.663524000	7.089997000	-0.266944000
C	-2.809342000	5.119641000	-0.445376000
H	-2.172971000	5.228099000	0.426620000
C	-3.843279000	-2.791573000	0.718569000
C	-4.990077000	-2.830589000	-0.098033000
H	-5.018468000	-2.216493000	-0.991327000
C	-6.063101000	-3.669505000	0.221759000
H	-6.937375000	-3.693726000	-0.421577000
C	-6.005432000	-4.486532000	1.358612000
H	-6.838221000	-5.137770000	1.605361000
C	-4.863935000	-4.464697000	2.170944000
H	-4.810375000	-5.097731000	3.051495000
C	-3.790604000	-3.626488000	1.851060000
H	-2.902915000	-3.607476000	2.475261000
C	-3.020755000	-1.225946000	-2.996595000
H	-2.023072000	-0.800214000	-2.850388000
H	-3.053797000	-2.223433000	-2.545189000
H	-3.758399000	-0.580333000	-2.507104000
H	-3.243207000	-1.299260000	-4.067195000

⁴TS1-1_h

Mn	0.051252000	0.021518000	-0.206239000
O	0.032230000	-0.026855000	-2.044394000
C	0.114278000	0.069290000	1.954715000
C	-0.281819000	0.612742000	4.156568000
H	-0.754736000	1.140687000	4.966702000
C	0.670705000	-0.355332000	4.148120000
H	1.202697000	-0.839288000	4.949042000
C	1.886315000	-1.686302000	2.418915000
H	2.134669000	-2.277344000	3.305030000
H	1.461563000	-2.334608000	1.658608000
H	2.790219000	-1.213924000	2.029252000
C	-1.632655000	1.841875000	2.452876000
H	-1.840464000	2.460472000	3.330498000
H	-1.261553000	2.468075000	1.647536000
H	-2.549298000	1.343755000	2.131100000
N	-0.609683000	0.860192000	2.821126000
N	0.898674000	-0.677036000	2.807880000
N	2.009592000	-0.307921000	-0.277865000
N	0.361143000	1.995680000	-0.220014000
N	-1.925851000	0.353093000	-0.174847000

N	-0.276270000	-1.958709000	-0.130491000
C	2.618955000	-1.503296000	-0.607463000
C	3.007709000	0.601868000	0.021065000
C	1.576691000	2.618086000	-0.034134000
C	-0.540226000	2.962852000	-0.644800000
C	-2.553196000	1.530318000	-0.521207000
C	-2.906756000	-0.548352000	0.201353000
C	-1.484337000	-2.573847000	0.127788000
C	0.597692000	-2.931420000	-0.585248000
C	4.054324000	-1.353821000	-0.463020000
H	4.773587000	-2.140020000	-0.630104000
C	4.291120000	-0.074614000	-0.039301000
H	5.242432000	0.377568000	0.189909000
C	1.437022000	4.031429000	-0.333132000
H	2.241722000	4.748356000	-0.291301000
C	0.149206000	4.234543000	-0.744509000
H	-0.294526000	5.153338000	-1.092630000
C	-3.980441000	1.382260000	-0.315782000
H	-4.709149000	2.159146000	-0.484870000
C	-4.193561000	0.120260000	0.170264000
H	-5.131520000	-0.324959000	0.460000000
C	-1.364400000	-3.990945000	-0.157990000
H	-2.165166000	-4.706501000	-0.058886000
C	-0.099253000	-4.202091000	-0.633401000
H	0.325319000	-5.127047000	-0.988859000
C	1.965123000	-2.724949000	-0.842817000
C	2.809388000	1.979891000	0.205253000
C	-1.913159000	2.748017000	-0.829637000
C	-2.701400000	-1.923230000	0.404729000
C	2.802177000	-3.871501000	-1.293486000
C	3.568036000	-3.755159000	-2.470333000
H	3.512482000	-2.833337000	-3.039657000
C	4.376266000	-4.811389000	-2.903151000
H	4.954040000	-4.707809000	-3.816437000
C	4.435897000	-6.001287000	-2.165479000
H	5.062756000	-6.821291000	-2.501853000
C	3.684313000	-6.126016000	-0.989694000
H	3.733843000	-7.040770000	-0.406784000
C	2.876526000	-5.069346000	-0.556257000
H	2.305195000	-5.159671000	0.361587000
C	3.973600000	2.854471000	0.523694000
C	5.114648000	2.902573000	-0.300423000
H	5.146090000	2.287057000	-1.192830000
C	6.184524000	3.748711000	0.010752000
H	7.053583000	3.778193000	-0.639400000
C	6.130016000	4.566679000	1.146967000
H	6.960082000	5.223955000	1.386694000
C	4.994486000	4.537437000	1.967214000
H	4.942316000	5.171152000	2.847374000
C	3.925234000	3.691038000	1.656038000
H	3.042229000	3.666697000	2.286660000
C	-2.777199000	3.876737000	-1.274878000
C	-3.589149000	3.725687000	-2.416187000
H	-3.549731000	2.790757000	-2.965185000
C	-4.422703000	4.764885000	-2.841935000
H	-5.035887000	4.634484000	-3.728293000
C	-4.462019000	5.972390000	-2.131996000
H	-5.108475000	6.779312000	-2.462777000
C	-3.664438000	6.131634000	-0.991314000
H	-3.697342000	7.060395000	-0.429805000
C	-2.831397000	5.091708000	-0.564958000
H	-2.223874000	5.208714000	0.326209000
C	-3.858710000	-2.788879000	0.770732000
C	-5.015028000	-2.854874000	-0.030330000
H	-5.063129000	-2.258504000	-0.934938000
C	-6.077739000	-3.694604000	0.319961000
H	-6.959415000	-3.738876000	-0.312045000
C	-6.000005000	-4.487146000	1.472780000
H	-6.824653000	-5.139273000	1.743229000
C	-4.848766000	-4.439755000	2.269981000

H	-4.779070000	-5.054113000	3.162503000
C	-3.786150000	-3.600294000	1.919428000
H	-2.890785000	-3.561993000	2.531538000
C	-2.093809000	-1.102525000	-2.966007000
H	-0.898510000	-0.476990000	-2.482264000
H	-2.079729000	-2.067248000	-2.459196000
H	-2.887164000	-0.427882000	-2.644458000
H	-1.918623000	-1.139310000	-4.042273000

²TS1-1_{hs}

Mn	-0.021709000	0.031416000	-0.228913000
C	-0.076316000	0.128832000	1.959661000
C	-0.710677000	-0.137914000	4.158631000
H	-1.332294000	-0.488082000	4.964600000
C	0.429627000	0.599171000	4.157649000
H	1.005524000	1.022036000	4.962714000
C	2.012476000	1.492146000	2.450022000
H	2.391753000	1.989570000	3.346933000
H	2.769858000	0.812739000	2.056856000
H	1.774550000	2.238956000	1.697881000
C	-2.183448000	-1.203956000	2.452158000
H	-2.563813000	-1.688437000	3.355883000
H	-2.955322000	-0.562376000	2.023345000
H	-1.903838000	-1.962337000	1.727354000
N	-1.004342000	-0.417394000	2.822167000
N	0.802950000	0.752937000	2.820482000
N	0.065619000	2.042074000	-0.258132000
N	-2.031972000	0.107859000	-0.236266000
N	-0.108821000	-1.968408000	-0.151454000
N	1.985054000	-0.046258000	-0.169589000
C	1.182178000	2.800679000	-0.543154000
C	-0.973494000	2.916642000	-0.006058000
C	-2.800023000	1.243240000	-0.088432000
C	-2.880319000	-0.917332000	-0.612788000
C	-1.218664000	-2.744040000	-0.441288000
C	0.923209000	-2.833797000	0.171074000
C	2.753590000	-1.169352000	0.061446000
C	2.843915000	0.964851000	-0.572478000
C	0.847926000	4.207591000	-0.411313000
H	1.542510000	5.020907000	-0.550163000
C	-0.467419000	4.277584000	-0.045721000
H	-1.047031000	5.161734000	0.164631000
C	-4.188241000	0.919496000	-0.366856000
H	-5.000575000	1.628632000	-0.345980000
C	-4.230693000	-0.398904000	-0.726049000
H	-5.088197000	-0.967533000	-1.047435000
C	-0.883851000	-4.140574000	-0.247537000
H	-1.571503000	-4.961203000	-0.377372000
C	0.420534000	-4.193076000	0.162900000
H	0.993878000	-5.067559000	0.424514000
C	4.146277000	-0.856367000	-0.198389000
H	4.959801000	-1.559862000	-0.117260000
C	4.195633000	0.443107000	-0.623002000
H	5.061282000	0.997048000	-0.948124000
C	2.478091000	2.304270000	-0.779446000
C	-2.322744000	2.548940000	0.132801000
C	-2.507012000	-2.264160000	-0.744177000
C	2.269217000	-2.463695000	0.327894000
C	3.522597000	3.289388000	-1.180149000
C	3.342669000	4.065757000	-2.341857000
H	2.448330000	3.914749000	-2.937148000
C	4.302370000	5.007471000	-2.727265000
H	4.151286000	5.591801000	-3.629716000
C	5.457384000	5.192829000	-1.955866000
H	6.202628000	5.923215000	-2.255302000
C	5.643958000	4.432195000	-0.794217000
H	6.531310000	4.577261000	-0.185435000
C	4.683471000	3.490893000	-0.408636000
H	4.821099000	2.909254000	0.496833000

C	-3.340604000	3.606411000	0.397228000
C	-3.500658000	4.709273000	-0.463878000
H	-2.866716000	4.788471000	-1.340295000
C	-4.474963000	5.679839000	-0.207123000
H	-4.588615000	6.520489000	-0.884773000
C	-5.310581000	5.562064000	0.911305000
H	-6.066868000	6.315263000	1.109400000
C	-5.168919000	4.463166000	1.768835000
H	-5.814029000	4.363066000	2.636486000
C	-4.194261000	3.493199000	1.511774000
H	-4.081434000	2.639268000	2.171994000
C	-3.536750000	-3.269698000	-1.132314000
C	-3.324104000	-4.095201000	-2.253730000
H	-2.414183000	-3.968512000	-2.830888000
C	-4.271929000	-5.054168000	-2.625647000
H	-4.095215000	-5.676200000	-3.497745000
C	-5.448752000	-5.207277000	-1.880680000
H	-6.185248000	-5.950519000	-2.169841000
C	-5.668847000	-4.396810000	-0.759343000
H	-6.573877000	-4.515672000	-0.171298000
C	-4.719829000	-3.438618000	-0.387229000
H	-4.883887000	-2.817320000	0.486908000
C	3.280129000	-3.513950000	0.643254000
C	3.458828000	-4.635586000	-0.189628000
H	2.842278000	-4.734876000	-1.076511000
C	4.428344000	-5.599051000	0.108560000
H	4.556313000	-6.454888000	-0.547192000
C	5.241048000	-5.454470000	1.240673000
H	5.993836000	-6.201908000	1.471169000
C	5.081193000	-4.336454000	2.069885000
H	5.708806000	-4.215878000	2.947675000
C	4.110874000	-3.373839000	1.771578000
H	3.983835000	-2.505309000	2.409734000
O	-0.008014000	0.029068000	-2.028373000
H	0.495657000	-0.813192000	-2.504327000
C	1.244909000	-1.995543000	-3.013235000
H	0.626411000	-2.822931000	-2.670340000
H	2.198767000	-1.873158000	-2.503764000
H	1.236256000	-1.791528000	-4.083698000

⁶INT1-I_{hs}

Mn	0.074717000	0.006742000	-0.125628000
O	0.063069000	-0.017382000	-1.963230000
C	0.131541000	0.016165000	2.077256000
C	-0.212648000	0.577830000	4.281398000
H	-0.607806000	1.162700000	5.093900000
C	0.566106000	-0.534539000	4.268028000
H	0.994790000	-1.115221000	5.066421000
C	1.574420000	-2.022056000	2.540778000
H	1.744702000	-2.628630000	3.434507000
H	1.035456000	-2.607043000	1.802106000
H	2.532064000	-1.702921000	2.126700000
C	-1.291096000	2.056059000	2.588586000
H	-1.405138000	2.680923000	3.478682000
H	-0.792776000	2.622365000	1.808555000
H	-2.273581000	1.735171000	2.238544000
N	-0.466444000	0.901260000	2.947605000
N	0.765378000	-0.864527000	2.926523000
N	2.000334000	-0.695798000	-0.189960000
N	0.764310000	2.011752000	-0.077107000
N	-1.864705000	0.703102000	-0.117185000
N	-0.634821000	-1.992234000	-0.021248000
C	2.368184000	-2.001252000	-0.435674000
C	3.139921000	0.065352000	-0.023419000
C	2.091866000	2.359839000	-0.106585000
C	0.017377000	3.100556000	-0.477556000
C	-2.249671000	2.012939000	-0.336230000
C	-2.992368000	-0.050652000	0.162194000
C	-1.961397000	-2.347605000	0.035616000

C	0.094075000	-3.085863000	-0.440830000
C	3.817441000	-2.086763000	-0.343473000
H	4.392107000	-2.992939000	-0.452941000
C	4.287472000	-0.830538000	-0.063994000
H	5.313453000	-0.536119000	0.087782000
C	2.195066000	3.760650000	-0.502886000
H	3.120765000	4.300631000	-0.626916000
C	0.926025000	4.207223000	-0.752151000
H	0.631297000	5.178925000	-1.115894000
C	-3.684269000	2.100112000	-0.132971000
H	-4.264380000	3.006684000	-0.204385000
C	-4.133113000	0.846259000	0.199324000
H	-5.144697000	0.554707000	0.432444000
C	-2.080684000	-3.753736000	-0.332271000
H	-3.008870000	-4.300572000	-0.391874000
C	-0.824132000	-4.199379000	-0.644415000
H	-0.545115000	-5.177563000	-1.003125000
C	1.497180000	-3.104276000	-0.620943000
C	3.192982000	1.479122000	0.044095000
C	-1.392263000	3.116983000	-0.583511000
C	-3.049131000	-1.463555000	0.239627000
C	2.128914000	-4.401324000	-0.996718000
C	2.958997000	-4.484973000	-2.132476000
H	3.113655000	-3.594593000	-2.732492000
C	3.563617000	-5.694915000	-2.488160000
H	4.194315000	-5.742427000	-3.370605000
C	3.350166000	-6.843945000	-1.714953000
H	3.818859000	-7.783241000	-1.991691000
C	2.527952000	-6.773732000	-0.582684000
H	2.362801000	-7.657941000	0.025560000
C	1.923983000	-5.563324000	-0.226632000
H	1.292991000	-5.505391000	0.654135000
C	4.533236000	2.127478000	0.153577000
C	5.558714000	1.872605000	-0.778028000
H	5.366802000	1.186432000	-1.595643000
C	6.799615000	2.508746000	-0.666383000
H	7.575991000	2.305166000	-1.397579000
C	7.036417000	3.416081000	0.374834000
H	7.999424000	3.909931000	0.460183000
C	6.020278000	3.688022000	1.300270000
H	6.193949000	4.392365000	2.108208000
C	4.779587000	3.051940000	1.187961000
H	3.988697000	3.262016000	1.900720000
C	-2.048515000	4.409075000	-0.931184000
C	-2.960221000	4.481015000	-2.003513000
H	-3.160775000	3.584133000	-2.579962000
C	-3.588314000	5.687161000	-2.329651000
H	-4.281837000	5.724648000	-3.164137000
C	-3.317163000	6.845627000	-1.589373000
H	-3.803585000	7.782301000	-1.843259000
C	-2.413810000	6.787853000	-0.520004000
H	-2.203113000	7.679318000	0.062986000
C	-1.787147000	5.580871000	-0.193288000
H	-1.093994000	5.532671000	0.639886000
C	-4.388930000	-2.101039000	0.400547000
C	-5.434750000	-1.845736000	-0.508493000
H	-5.253198000	-1.174043000	-1.341136000
C	-6.676996000	-2.471405000	-0.359791000
H	-7.470002000	-2.269400000	-1.073429000
C	-6.894028000	-3.367121000	0.695824000
H	-7.858250000	-3.852735000	0.810015000
C	-5.857016000	-3.639166000	1.597956000
H	-6.016007000	-4.335061000	2.416137000
C	-4.614494000	-3.013916000	1.448979000
H	-3.807322000	-3.223279000	2.143491000
H	-0.832522000	0.032334000	-2.360746000
C	-3.059676000	-0.416854000	-3.073368000
H	-2.728548000	-1.306554000	-2.549356000
H	-3.367250000	0.452913000	-2.503498000
H	-3.090007000	-0.402454000	-4.157584000

⁴INT1-1_{hs}

Mn	0.067994000	0.006181000	-0.125963000
O	0.055779000	-0.015098000	-1.959801000
C	0.130418000	0.016070000	2.078578000
C	-0.199005000	0.587699000	4.282611000
H	-0.581502000	1.181194000	5.094922000
C	0.558433000	-0.539308000	4.269637000
H	0.977397000	-1.126828000	5.068195000
C	1.533040000	-2.049571000	2.542548000
H	1.687325000	-2.661492000	3.435559000
H	0.982842000	-2.620816000	1.801472000
H	2.498650000	-1.751331000	2.131263000
C	-1.253616000	2.082500000	2.589115000
H	-1.357245000	2.709426000	3.479041000
H	-0.745377000	2.639883000	1.809049000
H	-2.241233000	1.778479000	2.238454000
N	-0.449305000	0.913615000	2.948708000
N	0.748754000	-0.875158000	2.928247000
N	1.983310000	-0.731695000	-0.187720000
N	0.797505000	1.997522000	-0.076150000
N	-1.855340000	0.736302000	-0.112464000
N	-0.675743000	-1.980070000	-0.022298000
C	2.327762000	-2.043261000	-0.433697000
C	3.136381000	0.008543000	-0.020869000
C	2.130879000	2.321856000	-0.104418000
C	0.070473000	3.099288000	-0.476666000
C	-2.215973000	2.052193000	-0.337853000
C	-2.997987000	0.002612000	0.158884000
C	-2.008184000	-2.312281000	0.034319000
C	0.034333000	-3.086731000	-0.440926000
C	3.775378000	-2.155129000	-0.341335000
H	4.333818000	-3.071356000	-0.451071000
C	4.267871000	-0.907718000	-0.061557000
H	5.298930000	-0.631623000	0.090217000
C	2.259463000	3.720850000	-0.499991000
H	3.194693000	4.244411000	-0.623066000
C	0.998708000	4.190013000	-0.749961000
H	0.721385000	5.167061000	-1.113098000
C	-3.650151000	2.164576000	-0.144856000
H	-4.214322000	3.080680000	-0.221931000
C	-4.123220000	0.919329000	0.186020000
H	-5.141351000	0.646407000	0.413061000
C	-2.151908000	-3.716232000	-0.333243000
H	-3.089285000	-4.247213000	-0.392797000
C	-0.903155000	-4.183959000	-0.644561000
H	-0.641207000	-5.167113000	-1.002550000
C	1.436979000	-3.130309000	-0.619698000
C	3.215453000	1.421114000	0.046662000
C	-1.338585000	3.140404000	-0.583937000
C	-3.080328000	-1.408903000	0.236930000
C	2.045455000	-4.438795000	-0.994500000
C	2.874576000	-4.538330000	-2.129673000
H	3.045925000	-3.651315000	-2.730141000
C	3.457245000	-5.759355000	-2.484180000
H	4.087526000	-5.818948000	-3.366192000
C	3.222431000	-6.903789000	-1.710331000
H	3.674101000	-7.851652000	-1.986167000
C	2.401060000	-6.817801000	-0.578552000
H	2.219565000	-7.698416000	0.030254000
C	1.819097000	-5.596323000	-0.223680000
H	1.188855000	-5.526222000	0.656734000
C	4.567361000	2.044827000	0.156514000
C	5.587831000	1.772455000	-0.775615000
H	5.383407000	1.090530000	-1.593749000
C	6.839970000	2.386141000	-0.663656000
H	7.612398000	2.169424000	-1.395259000
C	7.093303000	3.287948000	0.378489000
H	8.065060000	3.764314000	0.464072000

C	6.082501000	3.577087000	1.304537000
H	6.269038000	4.277314000	2.113183000
C	4.830546000	2.963525000	1.191878000
H	4.043746000	3.186964000	1.905110000
C	-1.970531000	4.444456000	-0.932559000
C	-2.876189000	4.534766000	-2.008551000
H	-3.090421000	3.642738000	-2.587590000
C	-3.481182000	5.752636000	-2.334903000
H	-4.170457000	5.804128000	-3.172162000
C	-3.192413000	6.904650000	-1.591216000
H	-3.660945000	7.850368000	-1.845228000
C	-2.294585000	6.828680000	-0.518359000
H	-2.070220000	7.715140000	0.067166000
C	-1.691028000	5.610001000	-0.191512000
H	-1.002038000	5.547773000	0.644197000
C	-4.431291000	-2.023152000	0.395773000
C	-5.472232000	-1.750008000	-0.513647000
H	-5.280932000	-1.078112000	-1.343713000
C	-6.724650000	-2.355651000	-0.367194000
H	-7.513602000	-2.139555000	-1.081175000
C	-6.957173000	-3.249174000	0.686932000
H	-7.929202000	-3.719320000	0.799494000
C	-5.925649000	-3.538699000	1.589897000
H	-6.096694000	-4.232795000	2.407169000
C	-4.673109000	-2.933343000	1.443015000
H	-3.870213000	-3.156505000	2.138152000
H	-0.843408000	-0.002032000	-2.362049000
C	-2.910438000	-0.351453000	-3.066837000
H	-2.782886000	-1.292660000	-2.544012000
H	-3.275538000	0.513612000	-2.524759000
H	-2.723096000	-0.291567000	-4.133675000

⁴INT1-1_{is}

Mn	-0.063729000	0.032048000	-0.215539000
C	-0.117558000	0.050242000	1.970521000
C	-0.409253000	-0.566397000	4.169470000
H	-0.677252000	-1.227255000	4.975708000
C	0.060572000	0.707691000	4.169755000
H	0.287326000	1.383499000	4.976241000
C	0.740630000	2.391168000	2.459480000
H	0.709563000	3.027447000	3.348309000
H	1.765751000	2.319263000	2.092062000
H	0.111543000	2.821306000	1.686245000
C	-1.003276000	-2.280944000	2.458267000
H	-1.010645000	-2.903269000	3.357465000
H	-2.011393000	-2.215748000	2.045243000
H	-0.341524000	-2.722432000	1.719791000
N	-0.511731000	-0.952312000	2.831155000
N	0.232311000	1.068604000	2.831564000
N	-1.193769000	1.688791000	-0.246732000
N	-1.714695000	-1.114772000	-0.223137000
N	1.074622000	-1.626711000	-0.157492000
N	1.595699000	1.169737000	-0.159956000
C	-0.752528000	2.963603000	-0.540574000
C	-2.551548000	1.766811000	-0.006847000
C	-3.010095000	-0.667479000	-0.081397000
C	-1.776019000	-2.443500000	-0.605998000
C	0.650550000	-2.911866000	-0.441808000
C	2.412776000	-1.701266000	0.190214000
C	2.882897000	0.728697000	0.077573000
C	1.679348000	2.492286000	-0.560865000
C	-1.865599000	3.888918000	-0.425246000
H	-1.797564000	4.954950000	-0.574031000
C	-2.962704000	3.158911000	-0.062080000
H	-3.958437000	3.520954000	0.136615000
C	-3.925744000	-1.759146000	-0.364039000
H	-5.001160000	-1.679132000	-0.346518000
C	-3.167613000	-2.838310000	-0.723391000
H	-3.511701000	-3.806819000	-1.048560000

C	1.750910000	-3.831167000	-0.226743000	H	0.573137000	1.290474000	4.975363000
H	1.691459000	-4.900871000	-0.350915000	C	1.177122000	2.209406000	2.455033000
C	2.822247000	-3.091013000	0.196498000	H	1.255744000	2.845985000	3.340719000
H	3.802405000	-3.446481000	0.470684000	H	2.174544000	1.955409000	2.091663000
C	3.811559000	1.814568000	-0.174394000	H	0.636427000	2.739123000	1.676997000
H	4.883883000	1.738955000	-0.085795000	C	-1.384797000	-2.068742000	2.460906000
C	3.074515000	2.885437000	-0.601748000	H	-1.516953000	-2.671815000	3.363473000
H	3.437590000	3.848437000	-0.922473000	H	-2.358306000	-1.819956000	2.035539000
C	0.582310000	3.343089000	-0.775290000	H	-0.808838000	-2.631838000	1.732596000
C	-3.412340000	0.664737000	0.132976000	N	-0.658925000	-0.851684000	2.832798000
C	-0.670933000	-3.297307000	-0.743984000	N	0.441316000	0.999714000	2.830627000
C	3.267395000	-0.597720000	0.348760000	N	-0.863755000	1.876855000	-0.243331000
C	0.826753000	4.753781000	-1.189973000	N	-1.887901000	-0.784429000	-0.218080000
C	0.222805000	5.251264000	-2.361472000	N	0.760762000	-1.796404000	-0.162118000
H	-0.396243000	4.584675000	-2.952648000	N	1.784126000	0.855475000	-0.167588000
C	0.423936000	6.576418000	-2.761326000	C	-0.198152000	3.049510000	-0.538272000
H	-0.043315000	6.940923000	-3.670999000	C	-2.183036000	2.201894000	0.003459000
C	1.229753000	7.429164000	-1.995163000	C	-3.079237000	-0.107283000	-0.075192000
H	1.386337000	8.457564000	-2.305604000	C	-2.191982000	-2.077628000	-0.605784000
C	1.830497000	6.947734000	-0.824645000	C	0.108189000	-2.982065000	-0.447730000
H	2.448292000	7.604990000	-0.220135000	C	2.064258000	-2.115169000	0.179786000
C	1.628498000	5.622412000	-0.424543000	C	2.969939000	0.187605000	0.065716000
H	2.083582000	5.252366000	0.488284000	C	2.106224000	2.140798000	-0.569673000
C	-4.862588000	0.901499000	0.387085000	C	-1.121896000	4.163133000	-0.416781000
C	-5.648961000	1.677756000	-0.485976000	H	-0.859696000	5.198756000	-0.564842000
H	-5.184390000	2.113895000	-1.363604000	C	-2.332392000	3.646114000	-0.048147000
C	-7.012764000	1.868451000	-0.238970000	H	-3.243750000	4.184333000	0.156339000
H	-7.605668000	2.464571000	-0.925934000	C	-4.179572000	-1.010959000	-0.362996000
C	-7.615645000	1.281857000	0.881622000	H	-5.221978000	-0.734806000	-0.346324000
H	-8.674228000	1.429420000	1.071755000	C	-3.632273000	-2.209573000	-0.726200000
C	-6.846004000	0.498303000	1.751420000	H	-4.148214000	-3.096755000	-1.056029000
H	-7.306066000	0.038220000	2.620730000	C	1.022856000	-4.087040000	-0.239691000
C	-5.482368000	0.308278000	1.504130000	H	0.768628000	-5.127596000	-0.365688000
H	-4.882429000	-0.299026000	2.174361000	C	2.212897000	-3.556407000	0.181181000
C	-0.890260000	-4.718048000	-1.137275000	H	3.111496000	-4.086803000	0.452223000
C	-0.221151000	-5.245005000	-2.259344000	C	4.080325000	1.085562000	-0.191341000
H	0.428199000	-4.592938000	-2.834060000	H	5.121197000	0.815532000	-0.107188000
C	-0.397051000	-6.580763000	-2.634740000	C	3.549431000	2.272898000	-0.616649000
H	0.120582000	-6.967715000	-3.507104000	H	4.080533000	3.153825000	-0.939209000
C	-1.242955000	-7.415399000	-1.892308000	C	1.182715000	3.178175000	-0.778389000
H	-1.380287000	-8.452079000	-2.183611000	C	-3.230574000	1.275510000	0.143829000
C	-1.909219000	-6.904829000	-0.770628000	C	-1.262062000	-3.119228000	-0.746371000
H	-2.559220000	-7.547604000	-0.184665000	C	3.106798000	-1.186712000	0.337521000
C	-1.732330000	-5.568761000	-0.395349000	C	1.680838000	4.521125000	-1.190847000
H	-2.239366000	-5.175337000	0.479466000	C	1.180585000	5.121594000	-2.362907000
C	4.706455000	-0.837211000	0.657656000	H	0.451492000	4.580156000	-2.956489000
C	5.516077000	-1.608524000	-0.198574000	C	1.621613000	6.388073000	-2.760375000
H	5.075693000	-2.030173000	-1.096328000	H	1.231386000	6.832932000	-3.670611000
C	6.871389000	-1.803591000	0.088333000	C	2.567609000	7.078458000	-1.990988000
H	7.484421000	-2.395299000	-0.584690000	H	2.910085000	8.061316000	-2.299578000
C	7.440442000	-1.226639000	1.231619000	C	3.067002000	6.494638000	-0.819463000
H	8.492425000	-1.377898000	1.452984000	H	3.792415000	7.027740000	-0.212303000
C	6.646633000	-0.447505000	2.083612000	C	2.625195000	5.228074000	-0.421816000
H	7.081457000	0.005152000	2.969629000	H	3.001816000	4.780285000	0.491927000
C	5.291251000	-0.252397000	1.796692000	C	-4.612927000	1.771856000	0.401742000
H	4.672029000	0.351302000	2.452578000	C	-5.244010000	2.685264000	-0.464720000
O	-0.038016000	0.036314000	-2.053913000	H	-4.708214000	3.034636000	-1.340483000
H	0.776298000	-0.350361000	-2.440905000	C	-6.549920000	3.120483000	-0.214773000
C	2.895709000	-1.307166000	-3.015789000	H	-7.023656000	3.819906000	-0.896830000
H	2.547232000	-2.195467000	-2.501081000	C	-7.250266000	2.645680000	0.901970000
H	3.150770000	-0.423866000	-2.441155000	H	-8.264022000	2.982968000	1.094442000
H	2.987920000	-1.299923000	-4.096591000	C	-6.637381000	1.727447000	1.764685000
² INT1-I _{is}				H	-7.174289000	1.352279000	2.630711000
				C	-5.331496000	1.292995000	1.514466000
				H	-4.853153000	0.580005000	2.178329000
Mn	-0.054191000	0.039714000	-0.216697000	C	-1.739739000	-4.475232000	-1.138837000
C	-0.096484000	0.065761000	1.970810000	C	-1.179908000	-5.118593000	-2.260167000
C	-0.474756000	-0.496573000	4.170997000	H	-0.420597000	-4.599502000	-2.835623000
H	-0.851668000	-1.100709000	4.978171000	C	-1.600587000	-6.398876000	-2.634273000
C	0.219729000	0.670442000	4.169620000	H	-1.163743000	-6.876025000	-3.506174000

C	-2.587101000	-7.061152000	-1.891645000
H	-2.914516000	-8.054551000	-2.182138000
C	-3.147044000	-6.434686000	-0.770595000
H	-3.904991000	-6.945091000	-0.184073000
C	-2.724747000	-5.154583000	-0.396188000
H	-3.148672000	-4.673807000	0.479113000
C	4.478043000	-1.682897000	0.648824000
C	5.133183000	-2.598101000	-0.197809000
H	4.623591000	-2.943350000	-1.091222000
C	6.430109000	-3.034859000	0.092867000
H	6.924059000	-3.735848000	-0.573074000
C	7.095911000	-2.559370000	1.230394000
H	8.102619000	-2.898050000	1.454770000
C	6.458527000	-1.638712000	2.072658000
H	6.969467000	-1.263366000	2.954149000
C	5.161507000	-1.202407000	1.781934000
H	4.663593000	-0.487987000	2.429685000
O	-0.036177000	0.036225000	-2.050598000
H	0.698057000	-0.490371000	-2.442420000
C	2.455792000	-1.714491000	-3.027860000
H	2.052650000	-2.586895000	-2.526232000
H	2.991339000	-0.968454000	-2.451812000
H	2.361480000	-1.608395000	-4.103329000

³INT1-1_g

Mn	-0.053759000	0.041984000	-0.226403000
C	-0.101666000	0.068385000	1.960794000
C	-0.490608000	-0.489426000	4.161565000
H	-0.875047000	-1.089829000	4.967998000
C	0.213537000	0.671529000	4.161472000
H	0.570125000	1.288957000	4.967834000
C	1.190712000	2.200376000	2.450172000
H	1.268138000	2.838411000	3.334968000
H	2.188820000	1.936787000	2.095430000
H	0.661193000	2.733400000	1.666886000
C	-1.409427000	-2.054947000	2.451276000
H	-1.541905000	-2.659315000	3.352993000
H	-2.383360000	-1.798780000	2.030946000
H	-0.840531000	-2.620559000	1.719511000
N	-0.673719000	-0.843970000	2.822894000
N	0.441402000	0.998280000	2.822760000
N	-0.828948000	1.889426000	-0.258233000
N	-1.897727000	-0.749872000	-0.217617000
N	0.730105000	-1.810349000	-0.175487000
N	1.798211000	0.821111000	-0.158844000
C	-0.141394000	3.049089000	-0.554202000
C	-2.140004000	2.241075000	-0.003409000
C	-3.076467000	-0.051572000	-0.066261000
C	-2.227422000	-2.037271000	-0.607000000
C	0.056829000	-2.983331000	-0.464868000
C	2.024820000	-2.154989000	0.174551000
C	2.970387000	0.131815000	0.081096000
C	2.145853000	2.098723000	-0.564789000
C	-1.043061000	4.181161000	-0.430302000
H	-0.760593000	5.211354000	-0.579101000
C	-2.261428000	3.688376000	-0.055699000
H	-3.160890000	4.244436000	0.153662000
C	-4.193524000	-0.935033000	-0.347712000
H	-5.230762000	-0.640575000	-0.323843000
C	-3.669822000	-2.142677000	-0.717649000
H	-4.203952000	-3.019420000	-1.046396000
C	0.950119000	-4.106462000	-0.256470000
H	0.676394000	-5.141704000	-0.385478000
C	2.147107000	-3.599359000	0.172215000
H	3.033809000	-4.146930000	0.448207000
C	4.097954000	1.008696000	-0.171064000
H	5.133208000	0.719777000	-0.080743000
C	3.591010000	2.204079000	-0.603905000
H	4.140018000	3.073593000	-0.927397000

C	1.242486000	3.151312000	-0.787048000
C	-3.202389000	1.334571000	0.149288000
C	-1.316754000	-3.094557000	-0.758548000
C	3.081540000	-1.246113000	0.347073000
C	1.766862000	4.482995000	-1.203104000
C	1.281162000	5.087358000	-2.379286000
H	0.544377000	4.556425000	-2.972850000
C	1.746046000	6.344024000	-2.780680000
H	1.366772000	6.791894000	-3.694064000
C	2.701720000	7.020690000	-2.011062000
H	3.062779000	7.995916000	-2.322673000
C	3.186582000	6.433165000	-0.835291000
H	3.919209000	6.955952000	-0.227822000
C	2.720941000	5.176418000	-0.433707000
H	3.086075000	4.726274000	0.483510000
C	-4.573496000	1.855819000	0.417191000
C	-5.194224000	2.780702000	-0.444588000
H	-4.658863000	3.120096000	-1.324531000
C	-6.489784000	3.240261000	-0.184594000
H	-6.955620000	3.948428000	-0.863067000
C	-7.190192000	2.778705000	0.937648000
H	-8.195919000	3.134932000	1.137958000
C	-6.587843000	1.849244000	1.795768000
H	-7.124861000	1.484300000	2.666085000
C	-5.292261000	1.390528000	1.535575000
H	-4.821999000	0.669019000	2.195995000
C	-1.820315000	-4.440217000	-1.154318000
C	-1.275345000	-5.089462000	-2.279566000
H	-0.508006000	-4.582256000	-2.854984000
C	-1.719885000	-6.360630000	-2.657157000
H	-1.294127000	-6.842305000	-3.532047000
C	-2.715830000	-7.007948000	-1.913961000
H	-3.061846000	-7.994236000	-2.207101000
C	-3.260877000	-6.375888000	-0.788712000
H	-4.025764000	-6.875036000	-0.201516000
C	-2.814691000	-5.104939000	-0.410840000
H	-3.226825000	-4.620304000	0.467922000
C	4.441143000	-1.766793000	0.668689000
C	5.087699000	-2.691572000	-0.174102000
H	4.580209000	-3.025976000	-1.072767000
C	6.374025000	-3.151791000	0.127179000
H	6.861490000	-3.860032000	-0.535864000
C	7.037899000	-2.690454000	1.271646000
H	8.036400000	-3.047371000	1.504273000
C	6.409379000	-1.760267000	2.110098000
H	6.918938000	-1.395716000	2.996899000
C	5.122933000	-1.300522000	1.808748000
H	4.631878000	-0.578666000	2.453470000
O	-0.024575000	0.039062000	-2.052073000
H	0.635741000	-0.572461000	-2.454209000
C	2.419730000	-1.709141000	-3.029170000
H	2.030861000	-2.594288000	-2.538145000
H	2.945443000	-0.963175000	-2.444460000
H	2.335714000	-1.597912000	-4.105023000

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Mn	0.026008000	0.026494000	-0.078804000
O	-0.147636000	-0.109750000	-1.953104000
C	0.110235000	0.107667000	2.148796000
C	-0.394133000	0.518629000	4.355696000
H	-0.985012000	0.894120000	5.173296000
C	0.790052000	-0.147453000	4.332196000
H	1.445049000	-0.466364000	5.124696000
C	2.298749000	-1.087540000	2.572496000
H	2.752302000	-1.541286000	3.457996000
H	2.040998000	-1.863257000	1.856996000
H	3.004274000	-0.391168000	2.115896000
C	-2.040067000	1.342861000	2.664296000
H	-2.417901000	1.857983000	3.551896000

H	-1.843333000	2.066797000	1.878696000
H	-2.780300000	0.622000000	2.313496000
N	-0.792085000	0.667758000	3.025396000
N	1.080874000	-0.390447000	2.988396000
N	2.088265000	0.201728000	-0.287904000
N	-0.166213000	2.128956000	-0.120204000
N	-2.043447000	-0.144538000	-0.044504000
N	0.244426000	-2.087577000	0.023296000
C	2.980528000	-0.843660000	-0.437204000
C	2.805943000	1.373397000	-0.112104000
C	0.887072000	3.012216000	-0.172804000
C	-1.322695000	2.806029000	-0.452104000
C	-2.937618000	0.875550000	-0.283004000
C	-2.745525000	-1.317012000	0.137496000
C	-0.822454000	-2.956433000	0.028796000
C	1.365403000	-2.779239000	-0.390804000
C	4.325799000	-0.313794000	-0.305504000
H	5.229009000	-0.902286000	-0.344704000
C	4.219134000	1.035640000	-0.082904000
H	5.022960000	1.734881000	0.083496000
C	0.369297000	4.328983000	-0.524304000
H	0.970783000	5.214589000	-0.658104000
C	-0.979745000	4.197819000	-0.715404000
H	-1.674799000	4.960543000	-1.029304000
C	-4.284592000	0.336585000	-0.159904000
H	-5.193307000	0.909578000	-0.256104000
C	-4.167723000	-1.000153000	0.116696000
H	-4.966051000	-1.706695000	0.278496000
C	-0.343982000	-4.281087000	-0.352604000
H	-0.964765000	-5.158187000	-0.447604000
C	0.991854000	-4.168518000	-0.625504000
H	1.655506000	-4.938832000	-0.985704000
C	2.652684000	-2.217954000	-0.568504000
C	2.260265000	2.680073000	-0.058204000
C	-2.616179000	2.235547000	-0.518404000
C	-2.189345000	-2.617691000	0.193996000
C	3.774784000	-3.148016000	-0.880504000
C	4.619262000	-2.907089000	-1.983104000
H	4.429441000	-2.040528000	-2.607504000
C	5.678383000	-3.771531000	-2.277104000
H	6.313047000	-3.573036000	-3.135404000
C	5.914820000	-4.895107000	-1.474004000
H	6.736203000	-5.567072000	-1.702704000
C	5.084139000	-5.146139000	-0.373904000
H	5.264160000	-6.010697000	0.257796000
C	4.025918000	-4.280297000	-0.079604000
H	3.385757000	-4.469491000	0.775496000
C	3.209636000	3.828166000	0.027896000
C	4.250090000	3.995531000	-0.907404000
H	4.359056000	3.270595000	-1.706804000
C	5.120942000	5.086750000	-0.821704000
H	5.912679000	5.202494000	-1.555704000
C	4.965348000	6.034500000	0.198396000
H	5.640821000	6.881782000	0.264296000
C	3.928700000	5.885434000	1.129196000
H	3.800235000	6.615876000	1.922196000
C	3.058147000	4.794115000	1.042696000
H	2.253209000	4.675875000	1.760696000
C	-3.752685000	3.147114000	-0.840904000
C	-4.595773000	2.874086000	-1.936204000
H	-4.395355000	1.998621000	-2.544604000
C	-5.666700000	3.719831000	-2.242504000
H	-6.301772000	3.497336000	-3.094504000
C	-5.914834000	4.855011000	-1.459304000
H	-6.745521000	5.512180000	-1.697604000
C	-5.083842000	5.137643000	-0.367304000
H	-5.272160000	6.012304000	0.247996000
C	-4.013316000	4.290698000	-0.060904000
H	-3.371246000	4.505191000	0.786996000
C	-3.136817000	-3.768786000	0.286096000

C	-4.136881000	-3.968663000	-0.685504000
H	-4.212855000	-3.268238000	-1.510404000
C	-5.003135000	-5.063983000	-0.602604000
H	-5.764181000	-5.207238000	-1.363604000
C	-4.880831000	-5.981123000	0.449796000
H	-5.552805000	-6.831506000	0.513496000
C	-3.881672000	-5.799345000	1.415096000
H	-3.778601000	-6.507579000	2.231696000
C	-3.014819000	-4.704225000	1.331296000
H	-2.237173000	-4.561176000	2.074596000
H	0.681620000	0.062782000	-2.451004000
C	-1.704527000	-1.322348000	-3.238204000
H	-1.302722000	-2.236877000	-2.821704000
H	-2.438746000	-0.760011000	-2.678304000
H	-1.394118000	-0.985648000	-4.220704000

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Mn	-0.002272000	0.045001000	-0.184100000
O	-0.055032000	-0.063170000	-2.096600000
C	0.008155000	0.093095000	1.936100000
C	-0.654164000	0.240361000	4.134500000
H	-1.355897000	0.361549000	4.941700000
C	0.688623000	0.036119000	4.133300000
H	1.396875000	-0.052373000	4.939100000
C	2.476967000	-0.246670000	2.410800000
H	3.027984000	-0.577775000	3.295500000
H	2.537246000	-1.008203000	1.639400000
H	2.909682000	0.683791000	2.037900000
C	-2.457744000	0.457658000	2.419400000
H	-2.996838000	0.830057000	3.295100000
H	-2.525242000	1.185196000	1.616400000
H	-2.898966000	-0.485898000	2.092000000
N	-1.053846000	0.272882000	2.796400000
N	1.076975000	-0.050796000	2.794300000
N	1.760943000	0.975726000	-0.296100000
N	-0.935599000	1.803717000	-0.219500000
N	-1.762687000	-0.885826000	-0.200400000
N	0.950054000	-1.718026000	-0.121400000
C	2.979620000	0.391752000	-0.606400000
C	2.011273000	2.295588000	0.058300000
C	-0.345618000	3.036891000	-0.012400000
C	-2.230575000	2.029833000	-0.669000000
C	-2.971578000	-0.327258000	-0.570600000
C	-2.005109000	-2.191292000	0.187700000
C	0.352979000	-2.937396000	0.111300000
C	2.225617000	-1.964831000	-0.623000000
C	4.032761000	1.369270000	-0.407400000
H	5.083653000	1.173689000	-0.551900000
C	3.446397000	2.519994000	0.041200000
H	3.931607000	3.442326000	0.316800000
C	-1.302445000	4.072220000	-0.323400000
H	-1.099860000	5.130008000	-0.269700000
C	-2.446288000	3.452553000	-0.761800000
H	-3.348231000	3.918451000	-1.124700000
C	-4.024318000	-1.304476000	-0.356800000
H	-5.072919000	-1.123396000	-0.533700000
C	-3.439841000	-2.430699000	0.150800000
H	-3.923047000	-3.346232000	0.450800000
C	1.282798000	-3.989510000	-0.228400000
H	1.064015000	-5.043490000	-0.162900000
C	2.418729000	-3.391138000	-0.714100000
H	3.301562000	-3.873127000	-1.102200000
C	3.195466000	-0.972467000	-0.861400000
C	1.022411000	3.268735000	0.253800000
C	-3.193631000	1.023565000	-0.876500000
C	-1.012642000	-3.156941000	0.411900000
C	4.557542000	-1.377721000	-1.306700000
C	5.126671000	-0.783935000	-2.450800000
H	4.547576000	-0.050315000	-3.001800000

C	6.411476000	-1.136246000	-2.876400000	C	2.979540000	0.392232000	-0.606408000
H	6.830232000	-0.673777000	-3.764900000	C	2.010897000	2.295986000	0.058323000
C	7.153451000	-2.086956000	-2.163100000	C	-0.346161000	3.036833000	-0.012362000
H	8.150299000	-2.361707000	-2.493500000	C	-2.230964000	2.029377000	-0.669022000
C	6.602323000	-2.678551000	-1.018900000	C	-2.971532000	-0.327826000	-0.570652000
H	7.175320000	-3.407468000	-0.453800000	C	-2.004681000	-2.191667000	0.187749000
C	5.317518000	-2.325541000	-0.593300000	C	0.353532000	-2.937292000	0.111387000
H	4.896171000	-2.773708000	0.300100000	C	2.225981000	-1.964433000	-0.622998000
C	1.414682000	4.662618000	0.603100000	C	4.032483000	1.370039000	-0.407398000
C	2.329088000	5.396813000	-0.177400000	H	5.083412000	1.174642000	-0.551999000
H	2.757832000	4.934875000	-1.059900000	C	3.445902000	2.520597000	0.041156000
C	2.665415000	6.711527000	0.163100000	H	3.930957000	3.443020000	0.316696000
H	3.367520000	7.264139000	-0.453700000	C	-1.303187000	4.071928000	-0.323361000
C	2.087751000	7.319446000	1.285400000	H	-1.100788000	5.129791000	-0.269527000
H	2.348115000	8.340003000	1.548100000	C	-2.446908000	3.452134000	-0.761772000
C	1.165555000	6.604856000	2.061500000	H	-3.348934000	3.917818000	-1.124567000
H	0.710012000	7.069708000	2.930600000	C	-4.024126000	-1.305209000	-0.356800000
C	0.830529000	5.290341000	1.721400000	H	-5.072673000	-1.124304000	-0.533714000
H	0.115221000	4.734037000	2.318400000	C	-3.439377000	-2.431329000	0.150776000
C	-4.556521000	1.404519000	-1.340600000	H	-3.922496000	-3.346959000	0.450792000
C	-5.096760000	0.791418000	-2.488200000	C	1.283484000	-3.989266000	-0.228321000
H	-4.493060000	0.067284000	-3.025000000	H	1.064971000	-5.043296000	-0.162831000
C	-6.382180000	1.116428000	-2.933600000	C	2.419358000	-3.390688000	-0.714127000
H	-6.779944000	0.639648000	-3.824200000	H	3.302232000	-3.872579000	-1.102137000
C	-7.151960000	2.057754000	-2.237400000	C	3.195651000	-0.971946000	-0.861433000
H	-8.149420000	2.310806000	-2.583300000	C	1.021831000	3.268953000	0.253775000
C	-6.628222000	2.668665000	-1.090400000	C	-3.193797000	1.022934000	-0.876469000
H	-7.222823000	3.390794000	-0.539000000	C	-1.012052000	-3.157154000	0.411961000
C	-5.342802000	2.343154000	-0.644600000	C	4.557798000	-1.376932000	-1.306687000
H	-4.942446000	2.805733000	0.251300000	C	5.126816000	-0.783082000	-2.450854000
C	-1.396008000	-4.541029000	0.804500000	H	4.547535000	-0.049591000	-3.001908000
C	-2.309731000	-5.306024000	0.052800000	C	6.411676000	-1.135174000	-2.876499000
H	-2.746693000	-4.875283000	-0.841300000	H	6.830321000	-0.672634000	-3.765027000
C	-2.632453000	-6.612646000	0.434900000	C	7.153802000	-2.085658000	-2.163176000
H	-3.334472000	-7.188958000	-0.160200000	H	8.150734000	-2.360248000	-2.493538000
C	-2.041168000	-7.182873000	1.569700000	C	6.602770000	-2.677367000	-1.018878000
H	-2.291329000	-8.197235000	1.864600000	H	7.175921000	-3.406183000	-0.453842000
C	-1.117557000	-6.438784000	2.316200000	C	5.317929000	-2.324563000	-0.593291000
H	-0.650398000	-6.874642000	3.194300000	H	4.896670000	-2.772757000	0.300090000
C	-0.796335000	-5.132461000	1.934600000	C	1.413860000	4.662817000	0.603081000
H	-0.080314000	-4.552957000	2.508600000	C	2.328090000	5.397259000	-0.177385000
H	0.701821000	0.393112000	-2.523600000	H	2.756813000	4.935403000	-1.059958000
C	-0.252221000	-2.033161000	-3.121300000	C	2.664124000	6.711974000	0.163096000
H	0.705265000	-2.421691000	-2.798800000	H	3.366160000	7.264706000	-0.453792000
H	-1.123511000	-2.195380000	-2.503400000	C	2.086432000	7.319792000	1.285386000
H	-0.372000000	-1.634395000	-4.121300000	H	2.346621000	8.340456000	1.548138000
⁴TS2-1_{is}				C	1.164380000	6.605002000	2.061582000
Mn	-0.002257000	0.044949000	-0.184084000	H	0.708821000	7.069815000	2.930718000
O	-0.055056000	-0.063248000	-2.096547000	C	0.829678000	5.290490000	1.721431000
C	0.008159000	0.093106000	1.936067000	H	0.114441000	4.733990000	2.318491000
C	-0.654237000	0.240419000	4.134479000	C	-4.556760000	1.403705000	-1.340596000
H	-1.355942000	0.361455000	4.941711000	C	-5.096848000	0.790523000	-2.488272000
C	0.688628000	0.036428000	4.133293000	H	-4.493010000	0.066475000	-3.025057000
H	1.396865000	-0.051937000	4.939073000	C	-6.382344000	1.115314000	-2.933676000
C	2.476972000	-0.246218000	2.410757000	H	-6.780021000	0.638427000	-3.824272000
H	3.028046000	-0.577271000	3.295502000	C	-7.152295000	2.056464000	-2.237495000
H	2.537380000	-1.007675000	1.639347000	H	-8.149785000	2.309323000	-2.583334000
H	2.909615000	0.684413000	2.037932000	C	-6.628702000	2.667384000	-1.090440000
C	-2.457872000	0.457291000	2.419379000	H	-7.223490000	3.389368000	-0.539054000
H	-2.997011000	0.829533000	3.295144000	C	-5.343241000	2.342117000	-0.644610000
H	-2.525430000	1.184811000	1.616444000	H	-4.942973000	2.804742000	0.251288000
H	-2.898853000	-0.486366000	2.092004000	C	-1.395148000	-4.541231000	0.804519000
N	-1.053935000	0.272776000	2.796353000	C	-2.308721000	-5.306426000	0.052815000
N	1.076992000	-0.050523000	2.794349000	H	-2.745820000	-4.875844000	-0.841272000
N	1.760769000	0.976033000	-0.296068000	C	-2.631263000	-6.613085000	0.434945000
N	-0.935928000	1.803495000	-0.219533000	H	-3.333108000	-7.189535000	-0.160131000
N	-1.762491000	-0.886104000	-0.200425000	C	-2.039865000	-7.183216000	1.569847000
N	0.950323000	-1.717878000	-0.121389000	H	-2.289895000	-8.197651000	1.864741000
				C	-1.116430000	-6.438980000	2.316323000
				H	-0.649227000	-6.874676000	3.194389000

C	-0.795381000	-5.132557000	1.934730000
H	-0.079502000	-4.552921000	2.508725000
H	0.701577000	0.393476000	-2.523662000
C	-0.251904000	-2.033166000	-3.121534000
H	0.705239000	-2.421808000	-2.798219000
H	-1.123720000	-2.195181000	-2.504379000
H	-0.370756000	-1.634365000	-4.121599000

²TS2-1_{is}

Mn	-0.003707000	0.032497000	-0.181902000
O	-0.075000000	-0.009416000	-2.048102000
C	0.004376000	0.126898000	1.968298000
C	-0.664443000	0.234979000	4.167098000
H	-1.372656000	0.308653000	4.974198000
C	0.689276000	0.125720000	4.164898000
H	1.403382000	0.091348000	4.969498000
C	2.489909000	-0.056359000	2.446098000
H	3.059858000	-0.333257000	3.337498000
H	2.597246000	-0.829440000	1.691498000
H	2.863040000	0.891208000	2.053498000
C	-2.479559000	0.321155000	2.456998000
H	-3.043316000	0.639855000	3.338298000
H	-2.601089000	1.052734000	1.664498000
H	-2.848286000	-0.648410000	2.117198000
N	-1.065944000	0.236207000	2.829598000
N	1.080588000	0.058690000	2.826298000
N	1.717208000	1.069603000	-0.280902000
N	-1.042415000	1.761612000	-0.211002000
N	-1.720224000	-0.996209000	-0.181202000
N	1.043598000	-1.678017000	-0.115302000
C	2.973400000	0.551827000	-0.544902000
C	1.880868000	2.417533000	0.010998000
C	-0.517841000	3.029005000	-0.068302000
C	-2.360941000	1.907177000	-0.614802000
C	-2.967914000	-0.492432000	-0.496502000
C	-1.884287000	-2.327639000	0.152698000
C	0.513223000	-2.940211000	0.069098000
C	2.354728000	-1.846683000	-0.548602000
C	3.961014000	1.594303000	-0.374202000
H	5.024738000	1.459293000	-0.491802000
C	3.295112000	2.730385000	0.005998000
H	3.719340000	3.692360000	0.244298000
C	-1.542917000	0.011022000	-0.377702000
H	-1.393207000	5.079049000	-0.366802000
C	-2.661994000	3.321023000	-0.749002000
H	-3.600365000	3.723656000	-1.094802000
C	-3.958629000	-1.529908000	-0.300802000
H	-5.019751000	-1.403298000	-0.446702000
C	-3.298430000	-2.647291000	0.138098000
H	-3.723460000	-3.601266000	0.405098000
C	1.523400000	-3.935131000	-0.238802000
H	1.366090000	-5.001259000	-0.198102000
C	2.640081000	-3.264632000	-0.652202000
H	3.567256000	-3.684967000	-1.006902000
C	3.273143000	-0.807519000	-0.768402000
C	0.834702000	3.344446000	0.161598000
C	-3.271253000	0.852514000	-0.783902000
C	-0.834722000	-3.249052000	0.326298000
C	4.669702000	-1.141170000	-1.165402000
C	5.241395000	-0.541068000	-2.305202000
H	4.640572000	0.146725000	-2.891002000
C	6.557146000	-0.828134000	-2.682302000
H	6.977363000	-0.361759000	-3.568102000
C	7.328605000	-1.719096000	-1.924602000
H	8.349645000	-1.943114000	-2.217402000
C	6.775012000	-2.316895000	-0.784802000
H	7.369433000	-3.000089000	-0.185702000
C	5.459360000	-2.028229000	-0.407402000
H	5.034941000	-2.480505000	0.482598000

C	1.158948000	4.772004000	0.443298000
C	2.017615000	5.516357000	-0.389002000
H	2.454301000	5.036035000	-1.257802000
C	2.289775000	6.861106000	-0.115502000
H	2.949076000	7.420923000	-0.771802000
C	1.703364000	7.488401000	0.991598000
H	1.914078000	8.532239000	1.202598000
C	0.837493000	6.762447000	1.820098000
H	0.376208000	7.241865000	2.678198000
C	0.566333000	5.417898000	1.546398000
H	-0.105766000	4.852479000	2.183998000
C	-4.667808000	1.160365000	-1.202502000
C	-5.213696000	0.527868000	-2.336902000
H	-4.592573000	-0.161421000	-2.899102000
C	-6.527742000	0.789834000	-2.737802000
H	-6.929655000	0.299162000	-3.619002000
C	-7.321302000	1.686292000	-2.009702000
H	-8.341138000	1.889910000	-2.320902000
C	-6.791715000	2.316487000	-0.876002000
H	-7.403337000	3.004978000	-0.300702000
C	-5.477468000	2.054021000	-0.474902000
H	-5.070553000	2.532593000	0.409698000
C	-1.155069000	-4.669209000	0.645598000
C	-2.008432000	-5.437961000	-0.170002000
H	-2.443413000	-4.981838000	-1.052502000
C	-2.275593000	-6.776308000	0.137198000
H	-2.930690000	-7.355625000	-0.506302000
C	-1.689187000	-7.372904000	1.261298000
H	-1.896202000	-8.411941000	1.498298000
C	-0.828021000	-6.622750000	2.072998000
H	-0.366640000	-7.078368000	2.943898000
C	-0.561959000	-5.284303000	1.765698000
H	0.105836000	-4.699784000	2.390398000
H	0.731038000	0.338428000	-2.479402000
C	-0.073234000	-2.060116000	-3.100902000
H	0.900525000	-2.394242000	-2.765302000
H	-0.944994000	-2.283171000	-2.502802000
H	-0.196810000	-1.636438000	-4.090202000

²TS2-1_{is}

Mn	-0.003301000	0.032705000	-0.193502000
O	-0.076096000	0.001693000	-2.043402000
C	0.009583000	0.122108000	1.966298000
C	-0.648045000	0.284094000	4.167398000
H	-1.348567000	0.410973000	4.974698000
C	0.693891000	0.076826000	4.164898000
H	1.404006000	-0.007651000	4.969398000
C	2.475746000	-0.237565000	2.446798000
H	3.023401000	-0.557671000	3.337798000
H	2.528080000	-1.014456000	1.690498000
H	2.917986000	0.681111000	2.057098000
C	-2.453082000	0.496381000	2.458398000
H	-2.992643000	0.851988000	3.340798000
H	-2.523510000	1.236769000	1.667898000
H	-2.890619000	-0.443394000	2.116798000
N	-1.049049000	0.310624000	2.829798000
N	1.078308000	-0.021407000	2.825998000
N	1.792241000	0.941116000	-0.283802000
N	-0.910914000	1.837048000	-0.203302000
N	-1.790746000	-0.865504000	-0.189502000
N	0.915607000	-1.749135000	-0.119302000
C	3.005847000	0.332426000	-0.546502000
C	2.055411000	2.273062000	0.006798000
C	-0.292426000	3.061155000	-0.064502000
C	-2.213656000	2.079323000	-0.608102000
C	-2.997549000	-0.269613000	-0.497902000
C	-2.053018000	-2.181949000	0.141398000
C	0.293818000	-2.968243000	0.068598000
C	2.213153000	-2.014711000	-0.541602000

C	4.070079000	1.299911000	-0.376702000
H	5.120717000	1.085393000	-0.493002000
C	3.490275000	2.481210000	0.001998000
H	3.984014000	3.409296000	0.240898000
C	-1.240908000	4.116491000	-0.374002000
H	-1.012191000	5.170331000	-0.364802000
C	-2.409104000	3.511289000	-0.743502000
H	-3.314985000	3.982332000	-1.089502000
C	-4.064282000	-1.232198000	-0.302702000
H	-5.113318000	-1.025379000	-0.444402000
C	-3.488481000	-2.396298000	0.129298000
H	-3.982121000	-3.317083000	0.394798000
C	1.230603000	-4.035281000	-0.225702000
H	0.996185000	-5.086922000	-0.181002000
C	2.396302000	-3.449979000	-0.634302000
H	3.292786000	-3.938724000	-0.980302000
C	3.205885000	-1.045639000	-0.763502000
C	1.081837000	3.274593000	0.158698000
C	-3.200685000	1.094552000	-0.779602000
C	-1.075446000	-3.176580000	0.317598000
C	4.575461000	-1.482802000	-1.154402000
C	5.191066000	-0.934295000	-2.297202000
H	4.642641000	-0.209490000	-2.889702000
C	6.483233000	-1.318672000	-2.669102000
H	6.937859000	-0.890693000	-3.557302000
C	7.186795000	-2.257450000	-1.902902000
H	8.189347000	-2.557076000	-2.191702000
C	6.589290000	-2.804853000	-0.760002000
H	7.131715000	-3.524659000	-0.154402000
C	5.297423000	-2.418677000	-0.387702000
H	4.839895000	-2.832056000	0.504798000
C	1.512195000	4.674868000	0.435698000
C	2.421178000	5.350625000	-0.401702000
H	2.817867000	4.836594000	-1.270402000
C	2.793349000	6.672190000	-0.133402000
H	3.490161000	7.179710000	-0.793602000
C	2.258733000	7.344597000	0.973398000
H	2.546955000	8.370547000	1.180298000
C	1.344247000	6.687439000	1.807098000
H	0.922757000	7.202466000	2.665098000
C	0.972775000	5.365975000	1.538498000
H	0.262564000	4.854052000	2.179698000
C	-4.570757000	1.507315000	-1.195002000
C	-5.164955000	0.919212000	-2.329002000
H	-4.598528000	0.186310000	-2.893902000
C	-6.456517000	1.279488000	-2.726702000
H	-6.895938000	0.821612000	-3.607602000
C	-7.178982000	2.231963000	-1.995802000
H	-8.181431000	2.511990000	-2.304602000
C	-6.601284000	2.819263000	-0.862602000
H	-7.158310000	3.550867000	-0.285102000
C	-5.309621000	2.458187000	-0.464502000
H	-4.866298000	2.903564000	0.419898000
C	-1.501105000	-4.568854000	0.637998000
C	-2.402983000	-5.274010000	-0.182502000
H	-2.795667000	-4.789378000	-1.069702000
C	-2.771055000	-6.587974000	0.125898000
H	-3.462363000	-7.119093000	-0.521402000
C	-2.239145000	-7.222782000	1.256098000
H	-2.524469000	-8.242831000	1.493998000
C	-1.331164000	-6.536225000	2.072898000
H	-0.911780000	-7.022152000	2.948698000
C	-0.963792000	-5.222261000	1.764398000
H	-0.259384000	-4.686839000	2.392698000
H	0.748256000	0.276636000	-2.492002000
C	-0.203125000	-2.141629000	-3.124902000
H	0.747040000	-2.518065000	-2.767302000
H	-1.086005000	-2.256982000	-2.513002000
H	-0.285002000	-1.698343000	-4.110002000

⁶INT2-1_{hs}

Mn	-0.043307000	0.016145000	0.248135000
O	0.764301000	0.533837000	-3.061526000
C	-0.060309000	0.018992000	2.466829000
C	-0.752691000	-0.096945000	4.649086000
H	-1.462048000	-0.194918000	5.453143000
C	0.602727000	0.059693000	4.660759000
H	1.301266000	0.131050000	5.477000000
C	2.385266000	0.307586000	2.865374000
H	3.059808000	0.177773000	3.715551000
H	2.609278000	-0.434792000	2.098044000
H	2.518293000	1.303786000	2.435122000
C	-2.510927000	-0.287937000	2.824049000
H	-3.199665000	-0.134138000	3.658815000
H	-2.709430000	0.444962000	2.040988000
H	-2.649886000	-1.289113000	2.406945000
N	-1.135960000	-0.116583000	3.305282000
N	1.003741000	0.126098000	3.323621000
N	1.578894000	1.326133000	-0.332305000
N	-1.361616000	1.613723000	-0.266915000
N	-1.632130000	-1.307447000	-0.310577000
N	1.311130000	-1.586362000	-0.206461000
C	2.922783000	0.988168000	-0.290929000
C	1.490138000	2.704327000	-0.179552000
C	-1.001424000	2.940821000	-0.394265000
C	-2.718366000	1.523035000	-0.521051000
C	-2.971297000	-0.968791000	-0.346978000
C	-1.550349000	-2.683388000	-0.177117000
C	0.948301000	-2.914452000	-0.334554000
C	2.670395000	-1.500353000	-0.454343000
C	3.701424000	2.186464000	-0.049095000
H	4.774081000	2.217552000	0.060751000
C	2.823205000	3.236453000	0.028560000
H	3.055513000	4.273443000	0.212612000
C	-2.177904000	3.719054000	-0.750438000
H	-2.180287000	4.778575000	-0.951811000
C	-3.228990000	2.849431000	-0.834476000
H	-4.246261000	3.070866000	-1.115928000
C	-3.766036000	-2.171999000	-0.162847000
H	-4.843039000	-2.204292000	-0.114053000
C	-2.894500000	-3.222655000	-0.050539000
H	-3.136066000	-4.262282000	0.104083000
C	2.124321000	-3.693779000	-0.686173000
H	2.126971000	-4.754206000	-0.883139000
C	3.178461000	-2.826050000	-0.766549000
H	4.196515000	-3.049770000	-1.043521000
C	3.443677000	-0.318092000	-0.422538000
C	0.302952000	3.466099000	-0.253401000
C	-3.488180000	0.338793000	-0.494750000
C	-0.358616000	-3.441428000	-0.217207000
C	4.923513000	-0.456111000	-0.530259000
C	5.645222000	0.271036000	-1.498250000
H	5.102819000	0.921699000	-2.175741000
C	7.034765000	0.147066000	-1.596236000
H	7.572801000	0.708958000	-2.353498000
C	7.729689000	-0.707018000	-0.729484000
H	8.808155000	-0.803923000	-0.806865000
C	7.024031000	-1.437450000	0.235804000
H	7.555182000	-2.098859000	0.913618000
C	5.634538000	-1.312353000	0.334300000
H	5.086117000	-1.874814000	1.082853000
C	0.434147000	4.951757000	-0.229997000
C	1.270462000	5.621648000	-1.144984000
H	1.816034000	5.039246000	-1.879538000
C	1.383436000	7.015595000	-1.121232000
H	2.026299000	7.515580000	-1.839186000
C	0.660742000	7.765768000	-0.183952000
H	0.747993000	8.847739000	-0.166653000
C	-0.178607000	7.111939000	0.727763000

H	-0.740722000	7.685871000	1.458253000
C	-0.291645000	5.718098000	0.703590000
H	-0.939759000	5.208163000	1.408724000
C	-4.966765000	0.478204000	-0.631891000
C	-5.669362000	-0.227559000	-1.628812000
H	-5.114283000	-0.866146000	-2.307515000
C	-7.056540000	-0.099634000	-1.752953000
H	-7.579691000	-0.645310000	-2.532228000
C	-7.768128000	0.737767000	-0.883514000
H	-8.844642000	0.837991000	-0.981090000
C	-7.081458000	1.447482000	0.110351000
H	-7.625411000	2.096569000	0.789904000
C	-5.694307000	1.318182000	0.234563000
H	-5.160334000	1.865861000	1.004252000
C	-0.482611000	-4.928369000	-0.197944000
C	-1.282496000	-5.606036000	-1.139262000
H	-1.811106000	-5.028927000	-1.890231000
C	-1.384702000	-7.000908000	-1.118966000
H	-2.000151000	-7.506354000	-1.856892000
C	-0.686449000	-7.744893000	-0.158643000
H	-0.765036000	-8.827537000	-0.143781000
C	0.117175000	-7.083672000	0.779563000
H	0.660395000	-7.652720000	1.527925000
C	0.218989000	-5.688869000	0.758627000
H	0.839887000	-5.173130000	1.483714000
H	1.014376000	0.749560000	-2.133529000
C	0.560431000	-0.896150000	-3.216935000
H	-0.210964000	-1.275003000	-2.533225000
H	0.232104000	-1.046674000	-4.249132000
H	1.485964000	-1.467000000	-3.049017000

⁴INT2-1_h

Mn	-0.010223000	0.026549000	-0.202981000
O	0.225950000	-0.106386000	-2.545599000
C	-0.029197000	0.108025000	2.122684000
C	-0.726539000	0.208215000	4.311305000
H	-1.442962000	0.245856000	5.114330000
C	0.635769000	0.193976000	4.321987000
H	1.340123000	0.223889000	5.135959000
C	2.438957000	0.118500000	2.551506000
H	3.067193000	-0.154888000	3.404000000
H	2.557081000	-0.614347000	1.755022000
H	2.733487000	1.101639000	2.174880000
C	-2.503374000	0.125105000	2.514263000
H	-3.149449000	0.413677000	3.348095000
H	-2.627599000	0.826587000	1.690718000
H	-2.771471000	-0.876698000	2.168872000
N	-1.110658000	0.156746000	2.967616000
N	1.039589000	0.130093000	2.984479000
N	1.594318000	1.209008000	-0.331770000
N	-1.211929000	1.636882000	-0.339893000
N	-1.600266000	-1.161602000	-0.295839000
N	1.211642000	-1.593885000	-0.216267000
C	2.923069000	0.813189000	-0.536696000
C	1.620666000	2.573676000	-0.006649000
C	-0.812139000	2.957410000	-0.197068000
C	-2.545552000	1.656993000	-0.748468000
C	-2.923987000	-0.775497000	-0.540067000
C	-1.633113000	-2.511574000	0.086820000
C	0.801766000	-2.909848000	-0.061339000
C	2.541362000	-1.629094000	-0.645085000
C	3.790746000	1.948756000	-0.283442000
H	4.867330000	1.913193000	-0.338282000
C	3.005729000	3.001432000	0.081885000
H	3.322995000	3.990788000	0.369580000
C	-1.903167000	3.818397000	-0.531050000
H	-1.858427000	4.895987000	-0.529497000
C	-2.965971000	3.014288000	-0.898662000
H	-3.940120000	3.327939000	-1.237614000

C	-3.796959000	-1.897490000	-0.249597000
H	-4.872481000	-1.863053000	-0.323576000
C	-3.020603000	-2.934440000	0.173549000
H	-3.343917000	-3.909725000	0.499597000
C	1.879095000	-3.782769000	-0.402422000
H	1.825525000	-4.859943000	-0.389971000
C	2.946056000	-2.990290000	-0.790785000
H	3.913967000	-3.316992000	-1.135734000
C	3.368764000	-0.483207000	-0.784074000
C	0.507663000	3.398388000	0.095992000
C	-3.369376000	0.507726000	-0.842720000
C	-0.524728000	-3.336670000	0.231338000
C	4.809581000	-0.674091000	-1.109673000
C	5.393502000	0.029170000	-2.182329000
H	4.770388000	0.694040000	-2.771800000
C	6.750183000	-0.122187000	-2.487592000
H	7.179353000	0.425504000	-3.321148000
C	7.551086000	-0.982449000	-1.725455000
H	8.603540000	-1.102931000	-1.962711000
C	6.984671000	-1.685354000	-0.653428000
H	7.600414000	-2.346474000	-0.051026000
C	5.628726000	-1.531711000	-0.347936000
H	5.192356000	-2.069342000	0.486803000
C	0.680896000	4.844174000	0.409546000
C	1.518628000	5.676398000	-0.358549000
H	2.047628000	5.251801000	-1.205019000
C	1.656637000	7.034469000	-0.050675000
H	2.303568000	7.660932000	-0.657478000
C	0.952435000	7.588250000	1.026076000
H	1.058204000	8.642240000	1.263914000
C	0.103997000	6.774462000	1.789330000
H	-0.448389000	7.196304000	2.623656000
C	-0.032260000	5.417350000	1.481658000
H	-0.691303000	4.784466000	2.066885000
C	-4.810601000	0.682344000	-1.177608000
C	-5.378913000	-0.037635000	-2.246865000
H	-4.742342000	-0.696718000	-2.827937000
C	-6.735578000	0.096348000	-2.560679000
H	-7.154132000	-0.462461000	-3.392261000
C	-7.550384000	0.953659000	-1.809866000
H	-8.602915000	1.059874000	-2.053762000
C	-6.998419000	1.672698000	-0.741159000
H	-7.625019000	2.332345000	-0.148365000
C	-5.642190000	1.537358000	-0.427477000
H	-5.215926000	2.088062000	0.404123000
C	-0.703241000	-4.773114000	0.580794000
C	-1.544741000	-5.622887000	-0.164168000
H	-2.077725000	-5.218157000	-1.017828000
C	-1.683070000	-6.973097000	0.176088000
H	-2.333388000	-7.612715000	-0.413147000
C	-0.975237000	-7.502468000	1.262712000
H	-1.081408000	-8.550404000	1.525741000
C	-0.122865000	-6.671850000	2.003189000
H	0.432260000	-7.074512000	2.845139000
C	0.013716000	-5.322635000	1.663114000
H	0.675906000	-4.677066000	2.230586000
H	1.116298000	0.276466000	-2.673555000
C	0.119552000	-1.447589000	-3.127253000
H	0.919173000	-2.098805000	-2.758876000
H	-0.843204000	-1.827312000	-2.785497000
H	0.138208000	-1.389240000	-4.221789000

²INT2-1_h

Mn	0.006874000	0.016264000	-0.113905000
O	0.055291000	-0.037787000	-2.235688000
C	-0.024540000	0.106203000	1.911900000
C	-0.711984000	0.216556000	4.102359000
H	-1.428526000	0.254115000	4.904552000
C	0.646053000	0.215996000	4.108446000

H	1.355414000	0.259857000	4.916714000	C	-7.363311000	1.131764000	-2.197709000
C	2.469090000	0.139066000	2.405000000	H	-8.389163000	1.259261000	-2.529320000
H	3.049813000	-0.112007000	3.297277000	C	-6.901389000	1.805944000	-1.060087000
H	2.640966000	-0.610838000	1.638720000	H	-7.571462000	2.452434000	-0.501296000
H	2.774202000	1.119055000	2.031909000	C	-5.579430000	1.640859000	-0.632248000
C	-2.520739000	0.097561000	2.386827000	H	-5.225524000	2.152147000	0.256657000
H	-3.114396000	0.376606000	3.262024000	C	-0.804039000	-4.729987000	0.755528000
H	-2.708314000	0.801779000	1.582282000	C	-1.623822000	-5.591479000	0.000013000
H	-2.795754000	-0.908311000	2.063086000	H	-2.122312000	-5.204043000	-0.881721000
N	-1.107100000	0.149254000	2.765380000	C	-1.783853000	-6.931720000	0.367313000
N	1.052060000	0.144584000	2.775138000	H	-2.415090000	-7.581870000	-0.231060000
N	1.627160000	1.181144000	-0.292616000	C	-1.123313000	-7.438893000	1.494328000
N	-1.123805000	1.630560000	-0.244650000	H	-1.248035000	-8.479271000	1.778404000
N	-1.633773000	-1.139845000	-0.223181000	C	-0.297222000	-6.595648000	2.248758000
N	1.142054000	-1.595048000	-0.148566000	H	0.220135000	-6.980004000	3.122720000
C	2.916575000	0.757304000	-0.601870000	C	-0.139046000	-5.255200000	1.881468000
C	1.715676000	2.525344000	0.062299000	H	0.499598000	-4.597573000	2.462330000
C	-0.712492000	2.941491000	-0.024876000	H	0.839604000	0.487733000	-2.488715000
C	-2.452266000	1.692395000	-0.692002000	C	-0.015969000	-1.321390000	-2.941665000
C	-2.910502000	-0.734356000	-0.571493000	H	0.881807000	-1.917068000	-2.751017000
C	-1.718408000	-2.465256000	0.178364000	H	-0.886232000	-1.823864000	-2.523414000
C	0.714388000	-2.901089000	0.098249000	H	-0.151425000	-1.139396000	-4.013051000
C	2.469109000	-1.677527000	-0.594103000	⁶P-1_{hs}			
C	3.828701000	1.846467000	-0.405875000	C	-0.000345000	-0.000821000	2.280707000
H	4.896560000	1.787949000	-0.547282000	C	-0.678372000	-0.075794000	4.470814000
C	3.094340000	2.926686000	0.039816000	H	-1.383186000	-0.156182000	5.280825000
H	3.462805000	3.904763000	0.304052000	C	0.677664000	0.073124000	4.470859000
C	-1.810383000	3.843590000	-0.333898000	H	1.382475000	0.153035000	5.280921000
H	-1.748171000	4.918742000	-0.272723000	C	2.451303000	0.277420000	2.663906000
C	-2.849000000	3.087812000	-0.786249000	H	3.125477000	0.180234000	3.518763000
H	-3.801720000	3.431168000	-1.155974000	H	2.676161000	-0.493824000	1.925843000
C	-3.827481000	-1.817549000	-0.346106000	H	2.584799000	1.255663000	2.194996000
H	-4.892540000	-1.767560000	-0.509506000	C	-2.451997000	-0.279146000	2.663731000
C	-3.098531000	-2.873891000	0.157861000	H	-3.126115000	-0.183141000	3.518762000
H	-3.466490000	-3.842330000	0.455875000	H	-2.677074000	0.492937000	1.926585000
C	1.804358000	-3.816126000	-0.193171000	H	-2.585322000	-1.256847000	2.193673000
H	1.736575000	-4.889111000	-0.105743000	N	-1.070617000	-0.116861000	3.129807000
C	2.852120000	-3.078256000	-0.657403000	N	1.069932000	0.114814000	3.129881000
H	3.804245000	-3.439140000	-1.011681000	N	1.687826000	1.213997000	-0.484813000
C	3.299903000	-0.586753000	-0.850319000	N	-1.228977000	1.689061000	-0.406029000
C	0.592981000	3.363455000	0.246182000	N	-1.687758000	-1.213726000	-0.485154000
C	-3.286374000	0.595113000	-0.889921000	N	1.229088000	-1.688756000	-0.406287000
C	-0.593742000	-3.304493000	0.375726000	C	3.002287000	0.787396000	-0.505768000
C	4.705720000	-0.814393000	-1.288388000	C	1.694313000	2.592999000	-0.359203000
C	5.197657000	-0.164692000	-2.438264000	C	-0.786971000	2.995168000	-0.490080000
H	4.532125000	0.487089000	-2.994896000	C	-2.596092000	1.692266000	-0.616244000
C	6.519019000	-0.347889000	-2.857615000	C	-3.002224000	-0.787119000	-0.506055000
H	6.876232000	0.157335000	-3.749910000	C	-1.694219000	-2.592720000	-0.359647000
C	7.378927000	-1.182787000	-2.131481000	C	0.787098000	-2.994888000	-0.490328000
H	8.404833000	-1.326203000	-2.456178000	C	2.596224000	-1.691970000	-0.616332000
C	6.907120000	-1.825890000	-0.979909000	C	3.873280000	1.938989000	-0.331791000
H	7.570113000	-2.463601000	-0.402882000	H	4.949820000	1.902249000	-0.276164000
C	5.585487000	-1.639663000	-0.560313000	C	3.071408000	3.044697000	-0.232697000
H	5.225974000	-2.124431000	0.341009000	H	3.380313000	4.067202000	-0.083670000
C	0.795089000	4.795898000	0.600563000	C	-1.923534000	3.859059000	-0.774548000
C	1.616125000	5.646452000	-0.165930000	H	-1.867952000	4.925314000	-0.927839000
H	2.117783000	5.245615000	-1.039815000	C	-3.030461000	3.060445000	-0.858360000
C	1.771014000	6.993308000	0.178856000	H	-4.040025000	3.358457000	-1.093491000
H	2.403006000	7.634765000	-0.428074000	C	-3.873194000	-1.938740000	-0.332090000
C	1.103614000	7.518282000	1.293530000	H	-4.949729000	-1.902032000	-0.276349000
H	1.223989000	8.563846000	1.559945000	C	-3.071301000	-3.044446000	-0.233142000
C	0.275473000	6.686114000	2.058081000	H	-3.380174000	-4.066976000	-0.084212000
H	-0.247860000	7.084505000	2.922176000	C	1.923726000	-3.858776000	-0.774578000
C	0.122720000	5.339085000	1.713592000	H	1.868217000	-4.925048000	-0.927781000
H	-0.517793000	4.690297000	2.302351000	C	3.030652000	-3.060143000	-0.858283000
C	-4.692327000	0.804951000	-1.337762000	H	4.040259000	-3.358160000	-1.093217000
C	-5.172804000	0.124212000	-2.473889000	C	3.436291000	-0.554932000	-0.611407000
H	-4.497115000	-0.530723000	-3.013876000	C	0.554469000	3.429594000	-0.382012000
C	-6.494010000	0.287832000	-2.902007000				
H	-6.843884000	-0.239446000	-3.784396000				

C	-3.436195000	0.555240000	-0.611476000	C	-1.509325000	-2.624084000	-0.107316000
C	-0.554340000	-3.429304000	-0.382435000	C	0.939422000	-2.871384000	-0.237417000
C	4.906338000	-0.789858000	-0.713457000	C	2.623106000	-1.487559000	-0.787795000
C	5.669318000	-0.166664000	-1.720926000	C	2.885784000	0.959103000	-0.683858000
H	5.167315000	0.480408000	-2.432238000	C	1.509343000	2.624193000	-0.107386000
C	7.048281000	-0.382653000	-1.811431000	C	-0.939408000	2.871470000	-0.237366000
H	7.618392000	0.101024000	-2.598759000	C	-2.623111000	1.487651000	-0.787689000
C	7.691315000	-1.227234000	-0.896684000	C	-3.691547000	-2.108289000	-0.426476000
H	8.761414000	-1.395635000	-0.967810000	H	-4.767550000	-2.132482000	-0.494621000
C	6.944335000	-1.854683000	0.108942000	C	-2.844385000	-3.129252000	-0.037274000
H	7.435135000	-2.507958000	0.824093000	H	-3.113052000	-4.133574000	0.247053000
C	5.565576000	-1.637178000	0.199314000	C	2.107605000	-3.684655000	-0.522953000
H	4.985039000	-2.120397000	0.978371000	H	2.114964000	-4.762593000	-0.492992000
C	0.780340000	4.904702000	-0.340543000	C	3.114225000	-2.849315000	-0.895657000
C	1.605783000	5.542275000	-1.287721000	H	4.106336000	-3.114949000	-1.223025000
H	2.078130000	4.943046000	-2.058661000	C	3.691571000	2.108352000	-0.426461000
C	1.805618000	6.926121000	-1.246609000	H	4.767573000	2.132529000	-0.494640000
H	2.439869000	7.400795000	-1.989132000	C	2.844412000	3.129323000	-0.037263000
C	1.181503000	7.699386000	-0.258789000	H	3.113115000	4.133606000	0.247156000
H	1.335996000	8.773521000	-0.227492000	C	-2.107601000	3.684742000	-0.522855000
C	0.353804000	7.078490000	0.686018000	H	-2.114960000	4.762679000	-0.492860000
H	-0.132409000	7.670114000	1.455847000	C	-3.114254000	2.849406000	-0.895489000
C	0.154589000	5.694585000	0.644243000	H	-4.106362000	3.115055000	-1.222849000
H	-0.485535000	5.209892000	1.374004000	C	-3.391411000	0.341323000	-0.933889000
C	-4.906230000	0.790223000	-0.713508000	C	-0.324766000	-3.388365000	0.023301000
C	-5.669254000	0.167123000	-1.721007000	C	3.391431000	-0.341228000	-0.933926000
H	-5.167285000	-0.479904000	-2.432383000	C	0.324787000	3.388471000	0.023315000
C	-7.048207000	0.383178000	-1.811491000	C	-4.839371000	0.455466000	-1.265358000
H	-7.618344000	-0.100417000	-2.598850000	C	-5.367761000	-0.251947000	-2.363463000
C	-7.691200000	1.227722000	-0.896684000	H	-4.699813000	-0.861830000	-2.962519000
H	-8.761292000	1.396177000	-0.967798000	C	-6.727305000	-0.170001000	-2.680225000
C	-6.944185000	1.855081000	0.108975000	H	-7.114937000	-0.715806000	-3.535028000
H	-7.434958000	2.508329000	0.824167000	C	-7.586524000	0.616918000	-1.901323000
C	-5.565436000	1.637519000	0.199324000	H	-8.641979000	0.680652000	-2.147205000
H	-4.984873000	2.120658000	0.978408000	C	-7.075713000	1.317179000	-0.800916000
C	-0.780237000	-4.904424000	-0.341058000	H	-7.736283000	1.920115000	-0.185114000
C	-1.605515000	-5.541906000	-1.288438000	C	-5.715449000	1.233933000	-0.484076000
H	-2.077724000	-4.942606000	-2.059410000	H	-5.321258000	1.765954000	0.375387000
C	-1.805362000	-6.925757000	-1.247463000	C	-0.431315000	-4.841695000	0.335353000
H	-2.439472000	-7.400377000	-1.990138000	C	-1.200276000	-5.714632000	-0.459242000
C	-1.181435000	-7.699097000	-0.259589000	H	-1.730570000	-5.314715000	-1.316622000
H	-1.335939000	-8.773234000	-0.228398000	C	-1.270657000	-7.079098000	-0.159565000
C	-0.353905000	-7.078286000	0.685418000	H	-1.862946000	-7.738026000	-0.787286000
H	0.132147000	-7.669981000	1.455295000	C	-0.570437000	-7.597794000	0.937997000
C	-0.154667000	-5.694377000	0.643780000	H	-0.625475000	-8.656974000	1.169755000
H	0.485333000	-5.209742000	1.373690000	C	0.204431000	-6.741719000	1.731270000
Mn	0.000032000	0.000095000	0.048112000	H	0.750875000	-7.135062000	2.583217000

⁴P-1_s

C	-0.000058000	-0.000159000	2.009412000	C	5.367828000	0.252237000	-2.363354000
C	0.677389000	0.072930000	4.201492000	H	4.699893000	0.862202000	-2.962343000
H	1.383290000	0.154079000	5.010471000	C	6.727384000	0.170340000	-2.680070000
C	-0.677374000	-0.074384000	4.201502000	H	7.115062000	0.716261000	-3.534780000
H	-1.383225000	-0.155927000	5.010486000	C	7.586572000	-0.616691000	-1.901237000
C	-2.455939000	-0.288087000	2.414335000	H	8.642035000	-0.680381000	-2.147086000
H	-3.122289000	-0.094035000	3.259286000	C	7.075731000	-1.317092000	-0.800942000
H	-2.664015000	0.417386000	1.610938000	H	7.736282000	-1.920105000	-0.185192000
H	-2.614838000	-1.303818000	2.042335000	C	5.715445000	-1.233888000	-0.484142000
C	2.455803000	0.287867000	2.414298000	H	5.321222000	-1.766027000	0.375238000
H	3.122251000	0.093733000	3.259154000	C	0.431304000	4.841776000	0.335464000
H	2.664024000	-0.417310000	1.610714000	C	1.200226000	5.714825000	-0.459034000
H	2.614401000	1.303758000	2.042549000	H	1.730490000	5.315040000	-1.316494000
N	1.070461000	0.112653000	2.860398000	C	1.270608000	7.079257000	-0.159195000
N	-1.070533000	-0.113371000	2.860404000	H	1.862880000	7.738265000	-0.786854000
N	-1.547565000	-1.276374000	-0.470350000	C	0.570416000	7.597803000	0.938455000
N	1.267273000	-1.521339000	-0.411775000	H	0.625459000	8.656949000	1.170355000
N	1.547583000	1.276467000	-0.470446000	C	-0.204427000	6.741621000	1.731634000
N	-1.267261000	1.521441000	-0.411729000	H	-0.750866000	7.134858000	2.583631000
C	-2.885771000	-0.959017000	-0.683866000	C	-0.273306000	5.376935000	1.431756000

H	-0.871730000	4.709325000	2.043249000
Mn	0.000008000	0.000064000	-0.244168000

²P-1_h

C	0.000348000	-0.000093000	1.802783000
C	-0.657495000	-0.164481000	4.007460000
H	-1.347983000	-0.336772000	4.815018000
C	0.658879000	0.163653000	4.007305000
H	1.349539000	0.335910000	4.814721000
C	2.425271000	0.599342000	2.299108000
H	2.936610000	0.959848000	3.196296000
H	2.946715000	-0.276225000	1.905733000
H	2.424172000	1.383780000	1.547811000
C	-2.424286000	-0.599896000	2.299550000
H	-2.935397000	-0.960747000	3.196732000
H	-2.945954000	0.275664000	1.906513000
H	-2.423142000	-1.384083000	1.547977000
N	-1.048250000	-0.263252000	2.669509000
N	1.049243000	0.262835000	2.669251000
N	0.570211000	1.905025000	-0.342798000
N	-1.892972000	0.570350000	-0.387610000
N	-0.570361000	-1.904963000	-0.342951000
N	1.892815000	-0.570349000	-0.388102000
C	1.844879000	2.388882000	-0.625562000
C	-0.213649000	3.017221000	-0.039255000
C	-2.381411000	1.857463000	-0.186387000
C	-2.983435000	-0.207168000	-0.784692000
C	-1.845045000	-2.388822000	-0.625681000
C	0.213537000	-3.017133000	-0.039627000
C	2.381269000	-1.857408000	-0.186845000
C	2.983263000	0.207228000	-0.785145000
C	1.866943000	3.824517000	-0.438328000
H	2.739545000	4.444860000	-0.568166000
C	0.615481000	4.204762000	-0.044175000
H	0.273688000	5.197435000	0.200060000
C	-3.800652000	1.885414000	-0.471581000
H	-4.415670000	2.770094000	-0.423456000
C	-4.159637000	0.630741000	-0.876392000
H	-5.129044000	0.296726000	-1.209069000
C	-1.866997000	-3.824515000	-0.438813000
H	-2.739554000	-4.444882000	-0.568829000
C	-0.615513000	-4.204750000	-0.044718000
H	-0.273649000	-5.197453000	0.199288000
C	3.800539000	-1.885333000	-0.471997000
H	4.415528000	-2.770031000	-0.423908000
C	4.159510000	-0.630652000	-0.876777000
H	5.128903000	-0.296556000	-1.209441000
C	2.968834000	1.601236000	-0.917078000
C	-1.607384000	2.994506000	0.090861000
C	-2.969059000	-1.601177000	-0.916836000
C	1.607279000	-2.994460000	0.090430000
C	4.226435000	2.312016000	-1.290231000
C	4.248248000	3.156003000	-2.417183000
H	3.345242000	3.261146000	-3.009437000
C	5.412164000	3.846458000	-2.771174000
H	5.412836000	4.487924000	-3.647126000
C	6.574546000	3.707953000	-2.001273000
H	7.478195000	4.243361000	-2.275613000
C	6.563215000	2.876804000	-0.873566000
H	7.457079000	2.771622000	-0.266157000
C	5.398540000	2.186670000	-0.520379000
H	5.385865000	1.549283000	0.357406000
C	-2.337410000	4.256785000	0.405666000
C	-2.228020000	5.399070000	-0.409913000
H	-1.591944000	5.359560000	-1.287497000
C	-2.939144000	6.564845000	-0.104847000
H	-2.847249000	7.435119000	-0.747560000
C	-3.776333000	6.606824000	1.017748000
H	-4.328390000	7.511412000	1.253373000

C	-3.901349000	5.472903000	1.831087000
H	-4.549529000	5.496560000	2.701911000
C	-3.189570000	4.308138000	1.525534000
H	-3.284242000	3.426628000	2.151430000
C	-4.226651000	-2.311897000	-1.289988000
C	-4.248427000	-3.155968000	-2.416902000
H	-3.345378000	-3.261190000	-3.009073000
C	-5.412342000	-3.846368000	-2.770978000
H	-5.412930000	-4.487871000	-3.646905000
C	-6.574797000	-3.707758000	-2.001206000
H	-7.478463000	-4.243108000	-2.275593000
C	-6.563499000	-2.876561000	-0.873532000
H	-7.457411000	-2.771274000	-0.266211000
C	-5.398820000	-2.186489000	-0.520254000
H	-5.386205000	-1.549128000	0.357546000
C	2.337275000	-4.256714000	0.405357000
C	2.228053000	-5.399038000	-0.410157000
H	1.592149000	-5.359607000	-1.287871000
C	2.939109000	-6.564802000	-0.104868000
H	2.847305000	-7.435118000	-0.747543000
C	3.776074000	-6.606723000	1.017887000
H	4.328071000	-7.511298000	1.253693000
C	3.900933000	-5.472739000	1.831178000
H	4.548947000	-5.496337000	2.702126000
C	3.189217000	-4.308001000	1.525407000
H	3.283746000	-3.426450000	2.151277000
Mn	-0.000011000	0.000029000	-0.167867000

C-H bond activation of methane by species 2

⁵R-2_{hs}

C	-0.000040000	-0.000217000	1.906352000
C	0.677989000	-0.026373000	4.107041000
H	1.391230000	-0.050202000	4.912727000
C	-0.678097000	0.024096000	4.107057000
H	-1.391345000	0.047188000	4.912758000
C	-2.493497000	0.085615000	2.405987000
H	-3.061958000	0.358848000	3.299381000
H	-2.645461000	0.836167000	1.637820000
H	-2.830505000	-0.886046000	2.041563000
C	2.493450000	-0.086268000	2.406003000
H	3.061940000	-0.359568000	3.299360000
H	2.645681000	-0.836574000	1.637648000
H	2.830194000	0.885580000	2.041849000
N	1.075571000	-0.042381000	2.768551000
N	-1.075650000	0.041251000	2.768573000
N	-1.722108000	-1.115189000	-0.267556000
N	1.152221000	-1.719192000	-0.198043000
N	1.722271000	1.115178000	-0.267109000
N	-1.152431000	1.719394000	-0.197576000
C	-2.985466000	-0.642311000	-0.546635000
C	-1.804495000	-2.467162000	-0.004395000
C	0.647702000	-2.994199000	-0.081331000
C	2.471511000	-1.807195000	-0.603538000
C	2.985594000	0.642431000	-0.546415000
C	1.804520000	2.467204000	-0.004064000
C	-0.647779000	2.994342000	-0.080815000
C	-2.471656000	1.807430000	-0.603170000
C	-3.927103000	-1.738876000	-0.390288000
H	-4.995477000	-1.656123000	-0.513353000
C	-3.209606000	-2.847456000	-0.027108000
H	-3.590478000	-3.832512000	0.189478000
C	1.708429000	-3.940132000	-0.396292000
H	1.593453000	-5.012606000	-0.401926000
C	2.814544000	-3.213619000	-0.743931000
H	3.767793000	-3.588512000	-1.080739000
C	3.927147000	1.739085000	-0.390273000
H	4.995505000	1.656444000	-0.513542000
C	3.209597000	2.847626000	-0.027069000

H	3.590422000	3.832730000	0.189378000
C	-1.708483000	3.940334000	-0.395690000
H	-1.593489000	5.012808000	-0.401211000
C	-2.814634000	3.213886000	-0.743404000
H	-3.767851000	3.588858000	-1.080214000
C	-3.338249000	0.707515000	-0.778073000
C	-0.706668000	-3.345695000	0.125635000
C	3.338252000	-0.707354000	-0.778113000
C	0.706655000	3.345705000	0.126061000
C	-4.752926000	0.975555000	-1.163707000
C	-5.306421000	0.343689000	-2.294902000
H	-4.679231000	-0.318320000	-2.882483000
C	-6.636249000	0.573049000	-2.662338000
H	-7.043681000	0.083655000	-3.541620000
C	-7.438008000	1.436622000	-1.904163000
H	-8.469944000	1.615421000	-2.189787000
C	-6.900379000	2.067653000	-0.774675000
H	-7.517441000	2.731830000	-0.177096000
C	-5.570456000	1.837700000	-0.406965000
H	-5.156160000	2.318396000	0.473076000
C	-0.982166000	-4.792777000	0.366838000
C	-1.792478000	-5.546535000	-0.504325000
H	-2.226516000	-5.060234000	-1.371130000
C	-2.019566000	-6.906943000	-0.269957000
H	-2.641248000	-7.474578000	-0.955573000
C	-1.436370000	-7.539083000	0.836188000
H	-1.612252000	-8.595013000	1.016715000
C	-0.619083000	-6.802489000	1.703594000
H	-0.161020000	-7.285613000	2.561327000
C	-0.392102000	-5.442315000	1.468718000
H	0.241868000	-4.868187000	2.136640000
C	4.752935000	-0.975441000	-1.163729000
C	5.306484000	-0.343546000	-2.294879000
H	4.679339000	0.318515000	-2.882447000
C	6.636318000	-0.572934000	-2.662282000
H	7.043798000	-0.083514000	-3.541527000
C	7.438019000	-1.436571000	-1.904123000
H	8.469957000	-1.615396000	-2.189724000
C	6.900331000	-2.067636000	-0.774683000
H	7.517347000	-2.731871000	-0.177123000
C	5.570404000	-1.837653000	-0.407004000
H	5.156060000	-2.318380000	0.472996000
C	0.982227000	4.792803000	0.367189000
C	1.792337000	5.546535000	-0.504174000
H	2.226205000	5.060202000	-1.371048000
C	2.019473000	6.906952000	-0.269886000
H	2.641002000	7.474573000	-0.955652000
C	1.436527000	7.539108000	0.836382000
H	1.612446000	8.595042000	1.016849000
C	0.619445000	6.802528000	1.703995000
H	0.161578000	7.285666000	2.561824000
C	0.392412000	5.442347000	1.469195000
H	-0.241416000	4.868231000	2.137263000
O	0.000003000	0.000758000	-1.963900000
Fe	-0.000055000	0.000363000	-0.302007000

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C	-0.000042000	-0.000197000	1.826739000
C	-0.678748000	0.012762000	4.028561000
H	-1.391881000	0.023856000	4.834793000
C	0.678512000	-0.016802000	4.028579000
H	1.391598000	-0.029112000	4.834835000
C	2.492378000	-0.035526000	2.317518000
H	3.072551000	-0.315798000	3.201294000
H	2.656584000	-0.765127000	1.531287000
H	2.807871000	0.950597000	1.971684000
C	-2.492496000	0.035054000	2.317460000
H	-3.072414000	0.316331000	3.201090000
H	-2.655869000	0.764501000	1.530932000

H	-2.809000000	-0.950895000	1.972023000
N	-1.075968000	0.024608000	2.689183000
N	1.075829000	-0.026301000	2.689213000
N	1.608848000	1.160541000	-0.322848000
N	-1.176750000	1.601516000	-0.288805000
N	-1.608820000	-1.160467000	-0.323045000
N	1.176594000	-1.601301000	-0.288863000
C	2.888977000	0.773294000	-0.658392000
C	1.659873000	2.492494000	0.044343000
C	-0.771395000	2.895076000	-0.040838000
C	-2.489736000	1.657119000	-0.731253000
C	-2.888949000	-0.773179000	-0.658632000
C	-1.659920000	-2.492385000	0.044229000
C	0.771308000	-2.894865000	-0.040770000
C	2.489620000	-1.656934000	-0.731246000
C	3.790205000	1.889284000	-0.449919000
H	4.856320000	1.853429000	-0.608854000
C	3.042944000	2.931778000	0.025591000
H	3.386271000	3.911157000	0.316475000
C	-1.869830000	3.800050000	-0.321504000
H	-1.816605000	4.873200000	-0.228741000
C	-2.909072000	3.043928000	-0.786192000
H	-3.868967000	3.385644000	-1.137837000
C	-3.790221000	-1.889121000	-0.450119000
H	-4.856334000	-1.853234000	-0.609054000
C	-3.043011000	-2.931608000	0.025482000
H	-3.386397000	-3.910933000	0.316468000
C	1.869750000	-3.799840000	-0.321380000
H	1.816513000	-4.872984000	-0.228570000
C	2.908961000	-3.043743000	-0.786151000
H	3.868839000	-3.385465000	-1.137825000
C	3.305321000	-0.537605000	-0.951597000
C	0.539943000	3.313536000	0.247192000
C	-3.305333000	0.537750000	-0.951744000
C	-0.540004000	-3.313394000	0.247264000
C	4.711783000	-0.725275000	-1.403335000
C	5.168826000	-0.052262000	-2.553631000
H	4.473770000	0.573854000	-3.103090000
C	6.490778000	-0.196050000	-2.987201000
H	6.823742000	0.323330000	-3.880511000
C	7.380850000	-1.011674000	-2.275931000
H	8.406720000	-1.123984000	-2.612730000
C	6.940255000	-1.679262000	-1.125738000
H	7.626883000	-2.304193000	-0.562706000
C	5.618205000	-1.534999000	-0.691640000
H	5.281022000	-2.039610000	0.207563000
C	0.728184000	4.738311000	0.641117000
C	1.518111000	5.622971000	-0.118468000
H	2.002122000	5.257261000	-1.017371000
C	1.659576000	6.961157000	0.264328000
H	2.266958000	7.631040000	-0.336597000
C	1.008933000	7.440377000	1.408906000
H	1.118473000	8.479227000	1.704254000
C	0.209754000	6.573078000	2.165307000
H	-0.301084000	6.937275000	3.051489000
C	0.068767000	5.235182000	1.782561000
H	-0.550495000	4.559667000	2.363892000
C	-4.711758000	0.725460000	-1.403551000
C	-5.168819000	0.052384000	-2.553808000
H	-4.473808000	-0.573876000	-3.103161000
C	-6.490730000	0.196283000	-2.987464000
H	-6.823710000	-0.323163000	-3.880729000
C	-7.380737000	1.012110000	-2.276342000
H	-8.406573000	1.124514000	-2.613213000
C	-6.940110000	1.679801000	-1.126221000
H	-7.626680000	2.304912000	-0.563317000
C	-5.618102000	1.535423000	-0.692033000
H	-5.280892000	2.040130000	0.207108000
C	-0.728142000	-4.738103000	0.641458000
C	-1.517606000	-5.623128000	-0.118191000

H	-2.001308000	-5.257776000	-1.017402000
C	-1.658951000	-6.961239000	0.264909000
H	-2.265964000	-7.631405000	-0.336073000
C	-1.008645000	-7.440028000	1.409856000
H	-1.118092000	-8.478822000	1.705438000
C	-0.209903000	-6.572379000	2.166314000
H	0.300681000	-6.936245000	3.052777000
C	-0.069030000	-5.234560000	1.783261000
H	0.549886000	-4.558772000	2.364641000
O	-0.000025000	0.000267000	-2.025338000
Fe	-0.000069000	0.000237000	-0.353750000

¹R-2_h

C	0.000358000	-0.001254000	1.809421000
C	-0.678390000	0.009784000	4.011995000
H	-1.391012000	0.022549000	4.818683000
C	0.679083000	-0.026115000	4.011882000
H	1.391676000	-0.043974000	4.818498000
C	2.493402000	-0.052137000	2.303307000
H	3.071178000	-0.325549000	3.190819000
H	2.656465000	-0.790210000	1.524935000
H	2.813619000	0.928957000	1.948275000
C	-2.492592000	0.048681000	2.303597000
H	-3.069489000	0.324563000	3.190929000
H	-2.653046000	0.786839000	1.524862000
H	-2.815944000	-0.931599000	1.948987000
N	-1.075596000	0.026459000	2.673364000
N	1.076364000	-0.034004000	2.673195000
N	1.640230000	1.122458000	-0.350249000
N	-1.142336000	1.617014000	-0.266934000
N	-1.640336000	-1.121274000	-0.350652000
N	1.142194000	-1.616198000	-0.268399000
C	2.906447000	0.708371000	-0.693493000
C	1.724458000	2.449493000	0.025815000
C	-0.702003000	2.897405000	-0.002631000
C	-2.453428000	1.711288000	-0.710726000
C	-2.906589000	-0.706993000	-0.693709000
C	-1.724552000	-2.448647000	0.024430000
C	0.701966000	-2.896698000	-0.004131000
C	2.453541000	-1.710077000	-0.711624000
C	3.835849000	1.804023000	-0.494394000
H	4.899545000	1.743794000	-0.662323000
C	3.116917000	2.860661000	-0.007069000
H	3.485215000	3.830586000	0.285102000
C	-1.780591000	3.830323000	-0.261113000
H	-1.701567000	4.900226000	-0.151632000
C	-2.838366000	3.107111000	-0.738089000
H	-3.789308000	3.478424000	-1.083694000
C	-3.835899000	-1.802807000	-0.495354000
H	-4.899598000	-1.742481000	-0.663221000
C	-3.116956000	-2.859772000	-0.008710000
H	-3.485268000	-3.829904000	0.282768000
C	1.780884000	-3.829282000	-0.262212000
H	1.702137000	-4.899211000	-0.152769000
C	2.838676000	-3.105816000	-0.738871000
H	3.789789000	-3.476995000	-1.084147000
C	3.291883000	-0.615795000	-0.967390000
C	0.623489000	3.286518000	0.264314000
C	-3.291971000	0.617266000	-0.966937000
C	-0.623552000	-3.285857000	0.262450000
C	4.687855000	-0.841983000	-1.431828000
C	5.144568000	-0.193255000	-2.596263000
H	4.455461000	0.439788000	-3.145260000
C	6.457802000	-0.370094000	-3.043729000
H	6.790379000	0.130769000	-3.947687000
C	7.339546000	-1.194802000	-2.332542000
H	8.358686000	-1.332764000	-2.680084000
C	6.899539000	-1.837931000	-1.168266000
H	7.580234000	-2.469138000	-0.605014000

C	5.586226000	-1.660708000	-0.720114000
H	5.250878000	-2.145059000	0.190825000
C	0.845183000	4.701106000	0.676783000
C	1.639455000	5.582692000	-0.081901000
H	2.101051000	5.222640000	-0.994762000
C	1.813138000	6.911534000	0.319737000
H	2.423397000	7.579308000	-0.280632000
C	1.190830000	7.384616000	1.482488000
H	1.325366000	8.416288000	1.792326000
C	0.387532000	6.520648000	2.238376000
H	-0.101431000	6.880118000	3.138721000
C	0.214463000	5.192045000	1.836948000
H	-0.407892000	4.519091000	2.418005000
C	-4.687912000	0.843774000	-1.431270000
C	-5.144883000	0.195251000	-2.595714000
H	-4.455969000	-0.437885000	-3.144843000
C	-6.458121000	0.372427000	-3.043033000
H	-6.790905000	-0.128269000	-3.947006000
C	-7.339601000	1.197281000	-2.331688000
H	-8.358747000	1.335498000	-2.679112000
C	-6.899324000	1.840238000	-1.167417000
H	-7.579814000	2.471576000	-0.604067000
C	-5.586008000	1.662682000	-0.719412000
H	-5.250418000	2.146923000	0.191494000
C	-0.845419000	-4.700580000	0.674413000
C	-1.639504000	-5.581872000	-0.084795000
H	-2.100800000	-5.221497000	-0.997683000
C	-1.813443000	-6.910815000	0.316407000
H	-2.423566000	-7.578366000	-0.284349000
C	-1.191571000	-7.384280000	1.479237000
H	-1.326306000	-8.416025000	1.788743000
C	-0.388485000	-6.520585000	2.235664000
H	0.100119000	-6.880348000	3.136087000
C	-0.215183000	-5.191874000	1.834682000
H	0.406976000	-4.519118000	2.416182000
O	-0.000459000	0.003302000	-2.040266000
Fe	0.000248000	-0.000318000	-0.368970000

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Fe	0.071824000	0.016716000	-0.211611000
O	0.017063000	0.008989000	-1.873726000
C	0.152855000	0.029746000	1.990457000
C	-0.172785000	0.588558000	4.199810000
H	-0.565780000	1.169202000	5.016395000
C	0.617682000	-0.514407000	4.178454000
H	1.061872000	-1.089649000	4.972324000
C	1.631422000	-1.989727000	2.449077000
H	1.796463000	-2.600939000	3.340749000
H	1.108773000	-2.576209000	1.700814000
H	2.591865000	-1.658575000	2.050905000
C	-1.293680000	2.053506000	2.529464000
H	-1.378762000	2.684751000	3.418465000
H	-0.832485000	2.619370000	1.727513000
H	-2.286461000	1.721955000	2.220679000
N	-0.445514000	0.908816000	2.868225000
N	0.806130000	-0.843123000	2.834403000
N	2.014562000	-0.633618000	-0.239585000
N	0.698744000	1.988241000	-0.145863000
N	-1.868595000	0.665834000	-0.099935000
N	-0.552842000	-1.954289000	-0.077309000
C	2.421661000	-1.917373000	-0.527713000
C	3.130544000	0.143377000	-0.005284000
C	2.013081000	2.388655000	-0.079416000
C	-0.067113000	3.065311000	-0.554293000
C	-2.297797000	1.942723000	-0.383331000
C	-2.964217000	-0.106519000	0.226047000
C	-1.860417000	-2.352697000	0.081964000
C	0.182350000	-3.037197000	-0.524249000
C	3.869116000	-1.973496000	-0.405057000

H	4.464974000	-2.862351000	-0.540485000
C	4.300338000	-0.722145000	-0.052260000
H	5.313692000	-0.409243000	0.141284000
C	2.082472000	3.799604000	-0.431259000
H	2.992518000	4.376579000	-0.479585000
C	0.815048000	4.204425000	-0.751742000
H	0.504997000	5.174976000	-1.104724000
C	-3.732509000	2.001289000	-0.158282000
H	-4.337883000	2.887145000	-0.268686000
C	-4.135019000	0.756606000	0.248566000
H	-5.131570000	0.444477000	0.516266000
C	-1.955373000	-3.765846000	-0.252827000
H	-2.867171000	-4.341753000	-0.234821000
C	-0.712130000	-4.176618000	-0.650952000
H	-0.426845000	-5.151335000	-1.013220000
C	1.576985000	-3.031731000	-0.740534000
C	3.137615000	1.551001000	0.111685000
C	-1.472681000	3.053643000	-0.677743000
C	-2.967010000	-1.512614000	0.344838000
C	2.234823000	-4.304187000	-1.151853000
C	3.047693000	-4.337063000	-2.302338000
H	3.164382000	-3.429826000	-2.885579000
C	3.684074000	-5.519254000	-2.694017000
H	4.300177000	-5.528192000	-3.587867000
C	3.521593000	-6.689833000	-1.941203000
H	4.014769000	-7.607721000	-2.245662000
C	2.719563000	-6.668841000	-0.792607000
H	2.595435000	-7.569552000	-0.199075000
C	2.083279000	-5.486316000	-0.400786000
H	1.470285000	-5.466387000	0.494150000
C	4.444807000	2.241765000	0.314153000
C	5.526602000	2.055503000	-0.568677000
H	5.403988000	1.393098000	-1.418538000
C	6.735777000	2.729952000	-0.368715000
H	7.556765000	2.579520000	-1.063054000
C	6.883420000	3.607863000	0.713186000
H	7.821722000	4.131738000	0.866866000
C	5.810426000	3.811770000	1.590785000
H	5.915240000	4.493039000	2.429709000
C	4.601712000	3.136893000	1.390740000
H	3.767350000	3.293371000	2.066750000
C	-2.162005000	4.312854000	-1.076835000
C	-3.050226000	4.309940000	-2.170884000
H	-3.200550000	3.385709000	-2.718808000
C	-3.717796000	5.478329000	-2.551698000
H	-4.392375000	5.459886000	-3.402118000
C	-3.511797000	6.670224000	-1.844223000
H	-4.029312000	7.577362000	-2.140420000
C	-2.634866000	6.684589000	-0.751651000
H	-2.476836000	7.602024000	-0.192803000
C	-1.967452000	5.515856000	-0.370291000
H	-1.297267000	5.523134000	0.482848000
C	-4.265677000	-2.198148000	0.609571000
C	-5.377844000	-2.014450000	-0.235516000
H	-5.280187000	-1.362225000	-1.095843000
C	-6.579534000	-2.686149000	0.013292000
H	-7.425147000	-2.539580000	-0.651743000
C	-6.688683000	-3.556263000	1.106047000
H	-7.621500000	-4.077606000	1.297419000
C	-5.584934000	-3.756420000	1.945697000
H	-5.660545000	-4.431995000	2.792348000
C	-4.383035000	-3.085302000	1.697002000
H	-3.524350000	-3.238868000	2.342667000
C	-3.170349000	-0.639147000	-3.008778000
H	-2.120090000	-0.450786000	-2.765279000
H	-3.454383000	-1.627494000	-2.630845000
H	-3.789676000	0.126109000	-2.527438000
H	-3.317467000	-0.606130000	-4.094335000

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Fe	0.069119000	0.023968000	-0.261272000
O	0.004903000	0.001464000	-1.932119000
C	0.154767000	0.057029000	1.914254000
C	-0.172654000	0.627095000	4.121796000
H	-0.573675000	1.205673000	4.936120000
C	0.639157000	-0.461069000	4.105686000
H	1.097607000	-1.020797000	4.902709000
C	1.679418000	-1.922128000	2.372226000
H	1.850316000	-2.540364000	3.258073000
H	1.177013000	-2.510979000	1.611501000
H	2.636450000	-1.566860000	1.985420000
C	-1.336204000	2.048083000	2.435018000
H	-1.432099000	2.693483000	3.312781000
H	-0.898438000	2.611972000	1.617888000
H	-2.322605000	1.685217000	2.139741000
N	-0.456548000	0.931271000	2.787996000
N	0.827749000	-0.796306000	2.762608000
N	1.976810000	-0.513027000	-0.296195000
N	0.591359000	1.939389000	-0.247659000
N	-1.833952000	0.562036000	-0.155290000
N	-0.449627000	-1.891985000	-0.151738000
C	2.456576000	-1.760144000	-0.635355000
C	3.063321000	0.278519000	0.026355000
C	1.863529000	2.430892000	-0.052704000
C	-0.197245000	2.992006000	-0.686798000
C	-2.342166000	1.795210000	-0.501488000
C	-2.891014000	-0.219134000	0.271154000
C	-1.705275000	-2.375550000	0.145843000
C	0.302584000	-2.956610000	-0.624649000
C	3.896970000	-1.771354000	-0.473984000
H	4.525488000	-2.631019000	-0.644818000
C	4.265366000	-0.533176000	-0.023308000
H	5.255593000	-0.191132000	0.230093000
C	1.878687000	3.847561000	-0.364569000
H	2.754575000	4.474789000	-0.314542000
C	0.625277000	4.181000000	-0.795994000
H	0.283977000	5.137425000	-1.157316000
C	-3.766823000	1.810437000	-0.235595000
H	-4.409338000	2.662789000	-0.389969000
C	-4.096036000	0.587970000	0.283261000
H	-5.064224000	0.249939000	0.615226000
C	-1.746824000	-3.797445000	-0.136527000
H	-2.618417000	-4.420058000	-0.010999000
C	-0.528213000	-4.144544000	-0.649186000
H	-0.215980000	-5.109498000	-1.014130000
C	1.677858000	-2.902257000	-0.895166000
C	3.015907000	1.669003000	0.211213000
C	-1.588055000	2.928528000	-0.855435000
C	-2.833196000	-1.604960000	0.475391000
C	2.387144000	-4.122863000	-1.367963000
C	3.162750000	-4.065981000	-2.542807000
H	3.207759000	-3.132566000	-3.093906000
C	3.853067000	-5.193937000	-2.998087000
H	4.438942000	-5.134594000	-3.910137000
C	3.784108000	-6.397888000	-2.284529000
H	4.318989000	-7.273727000	-2.638431000
C	3.023619000	-6.464163000	-1.109800000
H	2.974706000	-7.390069000	-0.544758000
C	2.333698000	-5.335795000	-0.654004000
H	1.757852000	-5.382422000	0.264209000
C	4.260401000	2.413702000	0.552587000
C	5.419416000	2.332668000	-0.243394000
H	5.405217000	1.711960000	-1.132519000
C	6.566965000	3.059593000	0.091298000
H	7.449585000	2.990607000	-0.537178000
C	6.574189000	3.885165000	1.223309000
H	7.464886000	4.449489000	1.481467000
C	5.422716000	3.984621000	2.015254000
H	5.418672000	4.625302000	2.891854000

C	4.275649000	3.257593000	1.680580000
H	3.380536000	3.332330000	2.289728000
C	-2.334607000	4.130527000	-1.317969000
C	-3.188657000	4.029800000	-2.434164000
H	-3.265533000	3.077548000	-2.948427000
C	-3.915925000	5.138689000	-2.878566000
H	-4.562729000	5.045744000	-3.745506000
C	-3.806241000	6.366503000	-2.212265000
H	-4.370094000	7.227431000	-2.557693000
C	-2.967467000	6.476150000	-1.095487000
H	-2.886333000	7.420946000	-0.566558000
C	-2.240222000	5.367029000	-0.650479000
H	-1.603253000	5.447580000	0.224002000
C	-4.063991000	-2.339995000	0.881043000
C	-5.242606000	-2.278093000	0.112612000
H	-5.246410000	-1.683293000	-0.793930000
C	-6.379824000	-2.997539000	0.495352000
H	-7.278817000	-2.945194000	-0.111180000
C	-6.355907000	-3.794528000	1.647557000
H	-7.238806000	-4.352753000	1.943206000
C	-5.183803000	-3.874581000	2.411142000
H	-5.156184000	-4.494064000	3.302453000
C	-4.046285000	-3.155955000	2.028290000
H	-3.134535000	-3.216303000	2.614021000
C	-3.147106000	-1.066419000	-2.885853000
H	-2.111195000	-0.760746000	-2.707538000
H	-3.321600000	-2.038102000	-2.411028000
H	-3.819069000	-0.320626000	-2.446022000
H	-3.336423000	-1.145175000	-3.962505000

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Fe	0.052409000	0.018902000	-0.265107000
O	0.032325000	0.052419000	-1.939447000
C	0.158690000	0.084888000	1.898737000
C	0.748052000	-0.324840000	4.088210000
H	1.298598000	-0.796299000	4.884026000
C	-0.226063000	0.621187000	4.106275000
H	-0.702811000	1.137809000	4.921443000
C	-1.624365000	1.819823000	2.427776000
H	-1.836058000	2.424180000	3.314390000
H	-1.280426000	2.463888000	1.625148000
H	-2.532520000	1.302191000	2.114323000
C	1.974992000	-1.634382000	2.359471000
H	2.237405000	-2.213916000	3.249199000
H	1.560510000	-2.296905000	1.606914000
H	2.869028000	-1.148528000	1.964547000
N	0.969474000	-0.641877000	2.746491000
N	-0.573042000	0.860481000	2.774998000
N	-1.902486000	0.309197000	-0.172839000
N	-0.192713000	-1.930352000	-0.128488000
N	2.023755000	-0.259242000	-0.320802000
N	0.310060000	1.994954000	-0.214426000
C	-2.568345000	1.460948000	-0.526346000
C	-2.848465000	-0.601913000	0.254736000
C	-1.372602000	-2.574098000	0.188284000
C	0.693945000	-2.893817000	-0.591452000
C	2.664398000	-1.422837000	-0.672791000
C	2.994574000	0.670842000	-0.000873000
C	1.509137000	2.643015000	-0.011695000
C	-0.605175000	2.938212000	-0.654594000
C	-3.985914000	1.285249000	-0.277149000
H	-4.735601000	2.042772000	-0.442124000
C	-4.152730000	0.033157000	0.247918000
H	-5.069351000	-0.430134000	0.575307000
C	-1.218427000	-3.992811000	-0.060988000
H	-1.995246000	-4.726225000	0.085721000
C	0.032388000	-4.181622000	-0.579669000
H	0.470190000	-5.102537000	-0.928838000
C	4.096783000	-1.238672000	-0.536455000

H	4.834351000	-2.003000000	-0.723820000
C	4.298198000	0.034139000	-0.078010000
H	5.235748000	0.506771000	0.165775000
C	1.338177000	4.053328000	-0.302706000
H	2.123898000	4.789458000	-0.240824000
C	0.053971000	4.225174000	-0.740180000
H	-0.406696000	5.133212000	-1.093876000
C	-1.970011000	2.688891000	-0.858086000
C	-2.599875000	-1.961063000	0.491577000
C	2.040658000	-2.661901000	-0.903064000
C	2.757423000	2.036093000	0.221527000
C	-2.863410000	3.780089000	-1.332405000
C	-3.677065000	3.565584000	-2.462853000
H	-3.612634000	2.613504000	-2.979082000
C	-4.543670000	4.564364000	-2.918010000
H	-5.157778000	4.385300000	-3.795147000
C	-4.615574000	5.793511000	-2.248990000
H	-5.287872000	6.569044000	-2.602571000
C	-3.817977000	6.014899000	-1.118676000
H	-3.877623000	6.960016000	-0.587479000
C	-2.951570000	5.015783000	-0.662401000
H	-2.347678000	5.179975000	0.223637000
C	-3.721020000	-2.850836000	0.905084000
C	-4.886304000	-2.970829000	0.123225000
H	-4.960908000	-2.402288000	-0.797277000
C	-5.917970000	-3.832037000	0.512013000
H	-6.807342000	-3.919343000	-0.104556000
C	-5.799021000	-4.591506000	1.683565000
H	-6.599737000	-5.260322000	1.983684000
C	-4.637696000	-4.490357000	2.461007000
H	-4.536531000	-5.079556000	3.367395000
C	-3.605861000	-3.629325000	2.072468000
H	-2.702724000	-3.548576000	2.668979000
C	2.895930000	-3.781408000	-1.383394000
C	3.622131000	-3.633983000	-2.581746000
H	3.519154000	-2.712067000	-3.144336000
C	4.451652000	-4.660584000	-3.044340000
H	4.997959000	-4.533694000	-3.973869000
C	4.573387000	-5.850738000	-2.314874000
H	5.216898000	-6.647802000	-2.674099000
C	3.863092000	-6.005212000	-1.117141000
H	3.961906000	-6.919679000	-0.540127000
C	3.033717000	-4.978304000	-0.653914000
H	2.496685000	-5.090506000	0.281948000
C	3.891827000	2.936885000	0.570774000
C	5.039687000	3.037950000	-0.239069000
H	5.100009000	2.444251000	-1.144589000
C	6.079151000	3.909673000	0.102802000
H	6.953795000	3.980566000	-0.536502000
C	5.986816000	4.700299000	1.255775000
H	6.793400000	5.377400000	1.519198000
C	4.843793000	4.618468000	2.061979000
H	4.762341000	5.231000000	2.954764000
C	3.804699000	3.746861000	1.720112000
H	2.915784000	3.681312000	2.339299000
C	-2.839636000	-1.373291000	-2.923023000
H	-1.927382000	-0.789801000	-2.757611000
H	-3.001214000	-1.524374000	-3.996479000
H	-2.736691000	-2.344569000	-2.427099000
H	-3.690539000	-0.833113000	-2.492132000

⁵TS1-2_{is}

Fe	0.048680000	0.000980000	-0.121014000
O	0.074848000	-0.074821000	-1.925089000
C	0.124016000	0.023721000	2.013117000
C	0.543301000	-0.531851000	4.205704000
H	0.940317000	-1.131882000	5.006121000
C	-0.161657000	0.627799000	4.214389000
H	-0.510020000	1.245233000	5.024145000

C	-1.167436000	2.155997000	2.524957000
H	-1.236456000	2.785479000	3.416542000
H	-0.644693000	2.694605000	1.741562000
H	-2.170313000	1.894342000	2.183953000
C	1.435712000	-2.103011000	2.491716000
H	1.545882000	-2.718658000	3.388838000
H	0.865314000	-2.648372000	1.747045000
H	2.421523000	-1.858611000	2.092656000
N	0.709362000	-0.887498000	2.865620000
N	-0.409730000	0.953859000	2.879362000
N	-1.798285000	0.825913000	-0.125758000
N	-0.784868000	-1.924105000	-0.019751000
N	1.895664000	-0.822731000	-0.206317000
N	0.876639000	1.927813000	-0.107364000
C	-2.094541000	2.145247000	-0.413227000
C	-2.981030000	0.168500000	0.170733000
C	-2.127951000	-2.188841000	0.094864000
C	-0.153863000	-3.068653000	-0.464711000
C	2.173633000	-2.141981000	-0.494217000
C	3.088351000	-0.160866000	0.011681000
C	2.222813000	2.192399000	-0.050590000
C	0.228353000	3.070701000	-0.526604000
C	-3.521624000	2.341929000	-0.234350000
H	-4.033504000	3.283189000	-0.356999000
C	-4.057998000	1.143235000	0.154248000
H	-5.087930000	0.933333000	0.393628000
C	-2.359649000	-3.584247000	-0.252855000
H	-3.325385000	-4.065014000	-0.265369000
C	-1.152539000	-4.115578000	-0.620626000
H	-0.957146000	-5.111212000	-0.986168000
C	3.610718000	-2.339777000	-0.388000000
H	4.114334000	-3.283451000	-0.525682000
C	4.166930000	-1.137583000	-0.045798000
H	5.208097000	-0.924573000	0.134811000
C	2.439440000	3.587355000	-0.411921000
H	3.404030000	4.067215000	-0.468125000
C	1.218990000	4.117553000	-0.731607000
H	1.008166000	5.111282000	-1.093798000
C	-1.169134000	3.182304000	-0.678542000
C	-3.143959000	-1.227810000	0.305204000
C	1.234090000	-3.181228000	-0.690457000
C	3.250238000	1.237377000	0.128619000
C	-1.730966000	4.503774000	-1.076800000
C	-2.591033000	4.603447000	-2.188471000
H	-2.818893000	3.706802000	-2.755155000
C	-3.133557000	5.836330000	-2.564719000
H	-3.788430000	5.895294000	-3.428652000
C	-2.827151000	6.993054000	-1.835518000
H	-3.247409000	7.950275000	-2.128014000
C	-1.975370000	6.906961000	-0.726535000
H	-1.739174000	7.797218000	-0.151504000
C	-1.433991000	5.673424000	-0.349838000
H	-0.782413000	5.603364000	0.514749000
C	-4.517702000	-1.766124000	0.529227000
C	-5.576041000	-1.479066000	-0.355037000
H	-5.385563000	-0.844244000	-1.213676000
C	-6.848814000	-2.020170000	-0.145021000
H	-7.651269000	-1.793609000	-0.840424000
C	-7.084977000	-2.863112000	0.949096000
H	-8.072660000	-3.283555000	1.110965000
C	-6.037015000	-3.166814000	1.828073000
H	-6.210571000	-3.822450000	2.675988000
C	-4.764394000	-2.625652000	1.617363000
H	-3.948589000	-2.861297000	2.293081000
C	1.771328000	-4.505776000	-1.111831000
C	2.565109000	-4.609634000	-2.271584000
H	2.760427000	-3.714334000	-2.852212000
C	3.082207000	-5.844912000	-2.674873000
H	3.685570000	-5.907760000	-3.575278000
C	2.816842000	-6.998869000	-1.925422000

H	3.217616000	-7.957799000	-2.239054000
C	2.031995000	-6.907994000	-0.768383000
H	1.828827000	-7.796126000	-0.177627000
C	1.515395000	-5.672333000	-0.364639000
H	0.915360000	-5.598566000	0.536276000
C	4.626904000	1.782991000	0.314853000
C	5.668586000	1.494616000	-0.588261000
H	5.463759000	0.855890000	-1.440474000
C	6.943974000	2.039439000	-0.404704000
H	7.733253000	1.811829000	-1.114679000
C	7.199730000	2.886943000	0.681430000
H	8.189551000	3.309865000	0.822570000
C	6.168362000	3.191777000	1.579332000
H	6.356747000	3.850789000	2.421480000
C	4.893175000	2.647193000	1.395026000
H	4.090288000	2.883472000	2.085920000
C	-2.258416000	-0.222604000	-2.988183000
H	-0.933017000	-0.079895000	-2.386872000
H	-2.773614000	0.689291000	-2.690543000
H	-2.007885000	-0.309309000	-4.045617000
H	-2.606373000	-1.135204000	-2.505717000

³TS1-2_{is}

Fe	0.046084000	0.008311000	-0.191115000
O	0.066965000	0.002589000	-2.001821000
C	0.114156000	0.020339000	1.920241000
C	0.424266000	-0.596147000	4.116113000
H	0.717946000	-1.250460000	4.918736000
C	-0.092216000	0.658964000	4.122034000
H	-0.348112000	1.321309000	4.930973000
C	-0.843630000	2.321107000	2.420319000
H	-0.792345000	2.970410000	3.298993000
H	-0.264093000	2.758146000	1.613701000
H	-1.883612000	2.214674000	2.105385000
C	1.089727000	-2.277510000	2.397405000
H	1.081001000	-2.916885000	3.284781000
H	0.468998000	-2.721775000	1.626017000
H	2.112871000	-2.178306000	2.029636000
N	0.543267000	-0.971949000	2.775244000
N	-0.274666000	1.021270000	2.784529000
N	-1.659216000	1.008827000	-0.175600000
N	-0.968511000	-1.694721000	-0.140790000
N	1.753933000	-0.994192000	-0.251666000
N	1.060963000	1.715430000	-0.208808000
C	-1.813443000	2.330834000	-0.541045000
C	-2.900873000	0.541368000	0.218360000
C	-2.310340000	-1.845885000	0.138966000
C	-0.506028000	-2.914297000	-0.614162000
C	1.889628000	-2.318242000	-0.606316000
C	3.010541000	-0.521796000	0.074276000
C	2.414091000	1.865146000	-0.002883000
C	0.577620000	2.929236000	-0.669750000
C	-3.192695000	2.722150000	-0.329874000
H	-3.584415000	3.710665000	-0.510650000
C	-3.851050000	1.635601000	0.179909000
H	-4.884423000	1.571013000	0.479749000
C	-2.709697000	-3.207384000	-0.156867000
H	-3.712623000	-3.588854000	-0.047744000
C	-1.612061000	-3.850157000	-0.659938000
H	-1.551919000	-4.860407000	-1.031108000
C	3.277822000	-2.711910000	-0.449032000
H	3.659069000	-3.704037000	-0.632647000
C	3.958912000	-1.620247000	0.013973000
H	5.004281000	-1.553222000	0.268019000
C	2.799987000	3.226613000	-0.325109000
H	3.807893000	3.606492000	-0.269735000
C	1.680339000	3.866601000	-0.776430000
H	1.601692000	4.873724000	-1.152561000
C	-0.778403000	3.225249000	-0.870880000

C	-3.211124000	-0.808786000	0.439317000
C	0.839700000	-3.214215000	-0.876414000
C	3.328567000	0.831208000	0.267895000
C	-1.172551000	4.579945000	-1.348007000
C	-1.986355000	4.707550000	-2.490999000
H	-2.291689000	3.809430000	-3.017516000
C	-2.385338000	5.968119000	-2.946961000
H	-3.005763000	6.048215000	-3.834294000
C	-1.980885000	7.124134000	-2.266131000
H	-2.289650000	8.102699000	-2.620455000
C	-1.178104000	7.009766000	-1.123705000
H	-0.869643000	7.900089000	-0.584094000
C	-0.780085000	5.748758000	-0.667146000
H	-0.170535000	5.658960000	0.225726000
C	-4.592967000	-1.199362000	0.835392000
C	-5.715311000	-0.833843000	0.066832000
H	-5.567392000	-0.253116000	-0.837010000
C	-7.001044000	-1.233768000	0.446264000
H	-7.854484000	-0.948423000	-0.161224000
C	-7.186889000	-2.012714000	1.595942000
H	-8.184809000	-2.323744000	1.888991000
C	-6.076624000	-2.395306000	2.360162000
H	-6.211673000	-3.002885000	3.249847000
C	-4.791185000	-1.994695000	1.980854000
H	-3.927849000	-2.290252000	2.568311000
C	1.208384000	-4.573757000	-1.359820000
C	1.970064000	-4.710354000	-2.537281000
H	2.253896000	-3.815755000	-3.081515000
C	2.345473000	-5.974972000	-3.002073000
H	2.925808000	-6.062398000	-3.915447000
C	1.969826000	-7.125523000	-2.295900000
H	2.260793000	-8.107103000	-2.656953000
C	1.219736000	-7.001958000	-1.119091000
H	0.934950000	-7.888019000	-0.559778000
C	0.844807000	-5.737051000	-0.653792000
H	0.277041000	-5.640067000	0.265521000
C	4.722592000	1.226747000	0.613243000
C	5.823382000	0.844045000	-0.177814000
H	5.651031000	0.247170000	-1.066610000
C	7.119663000	1.247297000	0.160154000
H	7.955785000	0.948532000	-0.464720000
C	7.338336000	2.046278000	1.290124000
H	8.344532000	2.359532000	1.550748000
C	6.249757000	2.445894000	2.076420000
H	6.409684000	3.069093000	2.951073000
C	4.953831000	2.042443000	1.738431000
H	4.107249000	2.351833000	2.342917000
C	-2.284688000	-0.429576000	-2.956026000
H	-0.933618000	-0.169478000	-2.435140000
H	-2.106339000	-0.419247000	-4.031572000
H	-2.854896000	0.408730000	-2.558670000
H	-2.514644000	-1.401364000	-2.521524000

¹TS1-2_s

Fe	0.025400000	0.020305000	-0.145104000
O	0.007691000	0.111004000	-2.016704000
C	0.014493000	0.095404000	1.914596000
C	0.662307000	-0.057436000	4.122296000
H	1.353222000	-0.215271000	4.932396000
C	-0.654224000	0.271042000	4.114196000
H	-1.349940000	0.450977000	4.915696000
C	-2.409462000	0.682479000	2.395796000
H	-2.902704000	1.137433000	3.259696000
H	-2.400327000	1.387380000	1.572696000
H	-2.949878000	-0.218772000	2.098196000
C	2.431549000	-0.511171000	2.430096000
H	2.914488000	-0.930426000	3.317596000
H	2.420918000	-1.253972000	1.640296000
H	2.984867000	0.368681000	2.095196000

N	1.056516000	-0.158799000	2.786196000
N	-1.032832000	0.363907000	2.773196000
N	-1.826229000	-0.739967000	-0.238004000
N	0.769869000	-1.798126000	-0.135104000
N	1.850429000	0.785475000	-0.219704000
N	-0.747673000	1.873733000	-0.223304000
C	-2.985094000	-0.046775000	-0.549004000
C	-2.206411000	-2.012702000	0.150296000
C	0.063378000	-2.972291000	0.065996000
C	2.044603000	-2.164107000	-0.573804000
C	3.006992000	0.105883000	-0.526804000
C	2.216908000	2.079709000	0.115296000
C	-0.048482000	3.044898000	-0.037404000
C	-2.008705000	2.221116000	-0.688304000
C	-4.129515000	-0.900081000	-0.306204000
H	-5.157442000	-0.600677000	-0.436004000
C	-3.653703000	-2.094537000	0.164796000
H	-4.225924000	-2.950190000	0.484596000
C	0.911383000	-4.102412000	-0.250404000
H	0.599179000	-5.133541000	-0.200304000
C	2.111137000	-3.606401000	-0.680104000
H	2.961889000	-4.161522000	-1.040804000
C	4.149111000	0.977889000	-0.327104000
H	5.177638000	0.683385000	-0.465104000
C	3.666899000	2.178644000	0.113696000
H	4.230718000	3.054296000	0.391696000
C	-0.891486000	4.173020000	-0.390104000
H	-0.579382000	5.204849000	-0.357204000
C	-2.080939000	3.664509000	-0.828104000
H	-2.926190000	4.207231000	-1.219104000
C	-3.071621000	1.321917000	-0.866904000
C	-1.311912000	-3.080619000	0.338896000
C	3.099620000	-1.271509000	-0.800204000
C	1.324109000	3.151026000	0.256196000
C	-4.399169000	1.839094000	-1.301604000
C	-5.054715000	1.257233000	-2.405004000
H	-4.563240000	0.450878000	-2.939304000
C	-6.313358000	1.711616000	-2.811904000
H	-6.799415000	1.255070000	-3.668604000
C	-6.942855000	2.755257000	-2.120804000
H	-7.919887000	3.108266000	-2.436104000
C	-6.305409000	3.337416000	-1.017404000
H	-6.791483000	4.138371000	-0.468404000
C	-5.047266000	2.881733000	-0.610204000
H	-4.562407000	3.321879000	0.254496000
C	-1.832787000	-4.424568000	0.711596000
C	-2.850428000	-5.061562000	-0.026304000
H	-3.264074000	-4.561401000	-0.895004000
C	-3.309409000	-6.332305000	0.336096000
H	-4.089765000	-6.809378000	-0.249204000
C	-2.755148000	-6.995053000	1.438896000
H	-3.111156000	-7.981787000	1.718696000
C	-1.733205000	-6.379158000	2.173396000
H	-1.295658000	-6.886418000	3.027996000
C	-1.275823000	-5.108116000	1.811596000
H	-0.485468000	-4.627242000	2.378796000
C	4.417769000	-1.795486000	-1.253104000
C	5.028619000	-1.256029000	-2.402404000
H	4.512446000	-0.474277000	-2.949904000
C	6.273562000	-1.723714000	-2.835904000
H	6.726523000	-1.301471000	-3.727704000
C	6.932556000	-2.736452000	-2.126104000
H	7.898690000	-3.099262000	-2.462804000
C	6.339606000	-3.274307000	-0.976404000
H	6.849478000	-4.050160000	-0.413404000
C	5.094963000	-2.805923000	-0.542604000
H	4.643100000	-3.212065000	0.356096000
C	1.846882000	4.509775000	0.575096000
C	2.834124000	5.130267000	-0.215004000
H	3.230274000	4.600803000	-1.074404000

C	3.281704000	6.421208000	0.085796000
H	4.037361000	6.887678000	-0.539004000
C	2.747340000	7.116958000	1.178196000
H	3.094346000	8.119291000	1.409496000
C	1.756896000	6.514666000	1.965096000
H	1.334946000	7.048127000	2.811496000
C	1.308616000	5.224725000	1.663296000
H	0.537559000	4.756353000	2.266596000
H	-0.726350000	-0.516965000	-2.380904000
C	-0.269632000	-1.783322000	-3.098104000
H	-0.264368000	-1.400022000	-4.113104000
H	-1.169184000	-2.300006000	-2.760004000
H	0.667909000	-2.224335000	-2.755204000

⁷INT1-2_{hs}

Fe	0.064174000	0.041433000	-0.377753000
O	-0.011558000	-0.024208000	-2.251954000
C	0.091818000	0.077465000	2.093281000
C	0.764437000	-0.155990000	4.291971000
H	1.432322000	-0.434294000	5.089450000
C	-0.467428000	0.417985000	4.309614000
H	-1.093841000	0.735558000	5.125867000
C	-2.147582000	1.126436000	2.589758000
H	-2.587302000	1.607707000	3.468087000
H	-1.995284000	1.866046000	1.807730000
H	-2.822026000	0.349857000	2.222993000
C	2.356061000	-0.946832000	2.524475000
H	2.836021000	-1.395519000	3.398995000
H	2.166218000	-1.714993000	1.779419000
H	3.013413000	-0.186823000	2.096764000
N	1.085527000	-0.356859000	2.945563000
N	-0.857521000	0.553594000	2.973190000
N	-1.980549000	-0.303673000	-0.212246000
N	0.426149000	-2.001487000	-0.152789000
N	2.091491000	0.378232000	-0.327161000
N	-0.309278000	2.078491000	-0.221538000
C	-2.964762000	0.644039000	-0.394799000
C	-2.582334000	-1.503945000	0.108853000
C	-0.544789000	-2.970270000	-0.012235000
C	1.610282000	-2.621717000	-0.503785000
C	3.065507000	-0.579599000	-0.512053000
C	2.707615000	1.592524000	-0.100166000
C	0.662897000	3.051354000	-0.166343000
C	-1.512687000	2.684048000	-0.537595000
C	-4.252831000	0.020929000	-0.145833000
H	-5.203270000	0.529312000	-0.187598000
C	-4.016343000	-1.287879000	0.190234000
H	-4.742958000	-2.038310000	0.457621000
C	0.056496000	-4.268558000	-0.279582000
H	-0.473558000	-5.207849000	-0.262672000
C	1.368953000	-4.052700000	-0.602175000
H	2.102338000	-4.786657000	-0.895479000
C	4.364357000	0.051730000	-0.352904000
H	5.311478000	-0.460735000	-0.414221000
C	4.145376000	1.375026000	-0.072852000
H	4.884993000	2.133568000	0.127421000
C	0.045244000	4.339017000	-0.448612000
H	0.573199000	5.278383000	-0.494415000
C	-1.279853000	4.110733000	-0.700375000
H	-2.027681000	4.832600000	-0.987031000
C	-2.757640000	2.025350000	-0.627959000
C	-1.923826000	-2.750290000	0.207444000
C	2.850915000	-1.967720000	-0.676119000
C	2.053095000	2.841301000	-0.008107000
C	-3.970416000	2.843988000	-0.913350000
C	-4.814209000	2.503944000	-1.989320000
H	-4.553404000	1.653487000	-2.610487000
C	-5.962358000	3.254079000	-2.263028000
H	-6.596109000	2.982279000	-3.101576000

C	-6.290131000	4.357067000	-1.463490000
H	-7.180649000	4.940301000	-1.676076000
C	-5.462589000	4.702059000	-0.386881000
H	-5.714499000	5.549737000	0.243122000
C	-4.314539000	3.951118000	-0.113186000
H	-3.678780000	4.211053000	0.726593000
C	-2.761242000	-3.962603000	0.444183000
C	-3.812012000	-4.303313000	-0.430055000
H	-4.001097000	-3.671907000	-1.292303000
C	-4.580056000	-5.450932000	-0.205889000
H	-5.382100000	-5.704517000	-0.892420000
C	-4.308252000	-6.278276000	0.892040000
H	-4.905005000	-7.168534000	1.064965000
C	-3.258194000	-5.954575000	1.761471000
H	-3.040608000	-6.592028000	2.613055000
C	-2.489278000	-4.807681000	1.537110000
H	-1.674529000	-4.552134000	2.206828000
C	4.048570000	-2.800126000	-0.983663000
C	4.843389000	-2.502286000	-2.108474000
H	4.555252000	-1.674236000	-2.747431000
C	5.976950000	-3.266029000	-2.404774000
H	6.573141000	-3.027285000	-3.280120000
C	6.338332000	-4.340031000	-1.580589000
H	7.217729000	-4.933396000	-1.810919000
C	5.559016000	-4.643130000	-0.456372000
H	5.837520000	-5.467973000	0.192515000
C	4.425558000	-3.878868000	-0.159720000
H	3.827618000	-4.105998000	0.716654000
C	2.892264000	4.061432000	0.175653000
C	3.931222000	4.381385000	-0.720085000
H	4.118142000	3.725067000	-1.563038000
C	4.699041000	5.536691000	-0.539280000
H	5.491492000	5.771719000	-1.243255000
C	4.439096000	6.394992000	0.537337000
H	5.035036000	7.291650000	0.676516000
C	3.401932000	6.092592000	1.429544000
H	3.193445000	6.752979000	2.265803000
C	2.634270000	4.937452000	1.248400000
H	1.829696000	4.699021000	1.936364000
H	-0.749943000	-0.424806000	-2.754823000
C	-2.610203000	-1.906692000	-3.122867000
H	-2.764322000	-2.037960000	-4.188681000
H	-3.221533000	-1.210517000	-2.559834000
H	-1.852195000	-2.483709000	-2.605416000

⁵INT1-2_{hs}

Fe	0.060528000	0.043395000	-0.377608000
O	-0.029158000	-0.033478000	-2.245275000
C	0.092033000	0.079296000	2.095681000
C	0.769703000	-0.142236000	4.294233000
H	1.444764000	-0.403953000	5.091292000
C	-0.478065000	0.396278000	4.312943000
H	-1.113622000	0.693303000	5.129870000
C	-2.176499000	1.062315000	2.593952000
H	-2.628438000	1.532525000	3.472086000
H	-2.044752000	1.804752000	1.810892000
H	-2.829945000	0.267345000	2.228432000
C	2.383798000	-0.882018000	2.524720000
H	2.878789000	-1.314514000	3.399016000
H	2.215414000	-1.656975000	1.781402000
H	3.017500000	-0.103650000	2.094411000
N	1.097207000	-0.329267000	2.947346000
N	-0.871008000	0.525231000	2.976670000
N	-1.972917000	-0.361298000	-0.205484000
N	0.483033000	-1.988431000	-0.153431000
N	2.078214000	0.439574000	-0.330016000
N	-0.371347000	2.068604000	-0.221687000
C	-2.984543000	0.556836000	-0.390150000
C	-2.539546000	-1.580382000	0.107937000

C	-0.459205000	-2.985440000	-0.016075000
C	1.685076000	-2.573162000	-0.504791000
C	3.080060000	-0.489451000	-0.512184000
C	2.658309000	1.671506000	-0.102973000
C	0.571765000	3.069827000	-0.168578000
C	-1.592777000	2.638410000	-0.534638000
C	-4.254241000	-0.105483000	-0.148007000
H	-5.219480000	0.373994000	-0.191837000
C	-3.979906000	-1.407952000	0.183910000
H	-4.684875000	-2.180651000	0.445865000
C	0.179920000	-4.265119000	-0.286097000
H	-0.322358000	-5.219568000	-0.271985000
C	1.485835000	-4.010341000	-0.606595000
H	2.240827000	-4.721749000	-0.900682000
C	4.359773000	0.179638000	-0.351648000
H	5.321579000	-0.304926000	-0.410841000
C	4.101768000	1.496248000	-0.073453000
H	4.818573000	2.276290000	0.127244000
C	-0.084256000	4.338622000	-0.449532000
H	0.415502000	5.293170000	-0.496859000
C	-1.402649000	4.071352000	-0.697938000
H	-2.172358000	4.770839000	-0.982201000
C	-2.818054000	1.943644000	-0.622592000
C	-1.844452000	-2.806833000	0.203406000
C	2.906313000	-1.883479000	-0.675333000
C	1.967661000	2.900733000	-0.011694000
C	-4.054480000	2.726975000	-0.905925000
C	-4.888706000	2.365492000	-1.982321000
H	-4.603612000	1.524842000	-2.606148000
C	-6.058580000	3.082469000	-2.253043000
H	-6.684793000	2.794493000	-3.091864000
C	-6.417888000	4.173146000	-1.450174000
H	-7.325352000	4.730524000	-1.660454000
C	-5.599853000	4.539308000	-0.373306000
H	-5.875902000	5.377560000	0.259186000
C	-4.430131000	3.821473000	-0.102582000
H	-3.801519000	4.097769000	0.737389000
C	-2.645134000	-4.044645000	0.435595000
C	-3.684742000	-4.414622000	-0.440052000
H	-3.894639000	-3.785704000	-1.299162000
C	-4.416780000	-5.586505000	-0.220859000
H	-5.210455000	-5.862062000	-0.908629000
C	-4.119445000	-6.409457000	0.873722000
H	-4.688029000	-7.318681000	1.042782000
C	-3.080299000	-6.056458000	1.744839000
H	-2.843045000	-6.690177000	2.593953000
C	-2.347576000	-4.885203000	1.525396000
H	-1.541397000	-4.607240000	2.196538000
C	4.128512000	-2.680966000	-0.978614000
C	4.918761000	-2.361379000	-2.100678000
H	4.609289000	-1.542771000	-2.741827000
C	6.075278000	-3.092123000	-2.391519000
H	6.667766000	-2.836998000	-3.264761000
C	6.464611000	-4.154169000	-1.564562000
H	7.361969000	-4.721719000	-1.790631000
C	5.689936000	-4.478673000	-0.443112000
H	5.989793000	-5.294291000	0.207910000
C	4.533500000	-3.747473000	-0.151991000
H	3.938814000	-3.991106000	0.722192000
C	2.770356000	4.145269000	0.170875000
C	3.800465000	4.494674000	-0.724117000
H	4.008417000	3.842549000	-1.565403000
C	4.532430000	5.673307000	-0.544929000
H	5.318234000	5.930843000	-1.248475000
C	4.244928000	6.525775000	0.529329000
H	4.812913000	7.440619000	0.667049000
C	3.216401000	6.193790000	1.420982000
H	2.986718000	6.849363000	2.255475000
C	2.484704000	5.015326000	1.241539000
H	1.686948000	4.754142000	1.929172000

H	-0.751059000	-0.474596000	-2.742484000
C	-2.486266000	-1.926551000	-3.135636000
H	-2.569271000	-1.987145000	-4.215652000
H	-3.138372000	-1.270903000	-2.569718000
H	-1.780219000	-2.556426000	-2.606482000

5INT1-2_B

Fe	0.052919000	0.039000000	-0.390482000
O	0.008213000	-0.024778000	-2.303290000
C	0.096341000	0.099124000	2.094733000
C	0.801302000	-0.060751000	4.288825000
H	1.480895000	-0.308555000	5.086735000
C	-0.435782000	0.505524000	4.305582000
H	-1.052524000	0.842830000	5.121550000
C	-2.142316000	1.134690000	2.562996000
H	-2.585916000	1.658659000	3.414568000
H	-1.999405000	1.830312000	1.738787000
H	-2.809658000	0.332368000	2.238650000
C	2.368727000	-0.889124000	2.500336000
H	2.847886000	-1.375609000	3.355026000
H	2.166580000	-1.625129000	1.725569000
H	3.032603000	-0.120725000	2.095656000
N	1.104060000	-0.302062000	2.943654000
N	-0.844458000	0.595480000	2.969716000
N	-1.910515000	-0.358572000	-0.236782000
N	0.470383000	-1.924363000	-0.215065000
N	2.009024000	0.434856000	-0.357645000
N	-0.364929000	1.999980000	-0.300852000
C	-2.937767000	0.535664000	-0.464003000
C	-2.485396000	-1.552284000	0.165912000
C	-0.441203000	-2.934143000	0.023922000
C	1.657541000	-2.527817000	-0.597542000
C	3.022442000	-0.473981000	-0.588686000
C	2.604037000	1.649851000	-0.067886000
C	0.552062000	3.020021000	-0.165818000
C	-1.573397000	2.581082000	-0.656765000
C	-4.200601000	-0.107014000	-0.168899000
H	-5.163952000	0.372718000	-0.239142000
C	-3.919542000	-1.378757000	0.254481000
H	-4.614196000	-2.136359000	0.579368000
C	0.190333000	-4.215768000	-0.223799000
H	-0.304636000	-5.169695000	-0.133638000
C	1.468793000	-3.964243000	-0.637067000
H	2.216538000	-4.677044000	-0.944750000
C	4.300037000	0.181985000	-0.401452000
H	5.258125000	-0.304227000	-0.494161000
C	4.042928000	1.476582000	-0.042722000
H	4.754793000	2.247685000	0.203320000
C	-0.095725000	4.287221000	-0.445924000
H	0.400849000	5.244372000	-0.433592000
C	-1.390780000	4.013698000	-0.783248000
H	-2.153985000	4.708274000	-1.094471000
C	-2.794307000	1.902370000	-0.764376000
C	-1.805594000	-2.770693000	0.312816000
C	2.870555000	-1.854282000	-0.801965000
C	1.930895000	2.874080000	0.060627000
C	-4.029886000	2.661000000	-1.105005000
C	-4.826738000	2.250805000	-2.191929000
H	-4.508792000	1.396705000	-2.780651000
C	-6.001214000	2.937668000	-2.516027000
H	-6.598826000	2.612980000	-3.362227000
C	-6.402362000	4.044513000	-1.756169000
H	-7.313587000	4.578044000	-2.007960000
C	-5.622517000	4.457020000	-0.667852000
H	-5.932427000	5.307049000	-0.067608000
C	-4.448117000	3.769625000	-0.343639000
H	-3.851300000	4.079859000	0.507563000
C	-2.584501000	-3.995571000	0.651685000
C	-3.645547000	-4.431271000	-0.165740000

H	-3.888142000	-3.862236000	-1.057562000
C	-4.355216000	-5.594594000	0.150722000
H	-5.166097000	-5.922418000	-0.492574000
C	-4.013121000	-6.342587000	1.285283000
H	-4.564188000	-7.245406000	1.529838000
C	-2.951634000	-5.923943000	2.098451000
H	-2.679460000	-6.500152000	2.977526000
C	-2.240880000	-4.761184000	1.781976000
H	-1.417461000	-4.432299000	2.407818000
C	4.088154000	-2.633081000	-1.160902000
C	4.829237000	-2.285101000	-2.307430000
H	4.481755000	-1.463291000	-2.924673000
C	5.985975000	-2.992551000	-2.650888000
H	6.540932000	-2.716362000	-3.542158000
C	6.424288000	-4.057324000	-1.852372000
H	7.322019000	-4.606239000	-2.119275000
C	5.699168000	-4.408082000	-0.706001000
H	6.038279000	-5.225108000	-0.076381000
C	4.542458000	-3.700541000	-0.362208000
H	3.987758000	-3.962739000	0.532642000
C	2.712349000	4.111838000	0.340332000
C	3.769967000	4.522841000	-0.493934000
H	4.017349000	3.923394000	-1.363320000
C	4.479157000	5.697322000	-0.220227000
H	5.287207000	6.003403000	-0.877567000
C	4.140162000	6.483758000	0.888751000
H	4.690482000	7.395410000	1.099762000
C	3.082621000	6.090832000	1.719581000
H	2.812371000	6.695884000	2.579681000
C	2.373559000	4.916663000	1.445778000
H	1.553578000	4.608261000	2.086289000
H	-0.667767000	-0.577392000	-2.749524000
C	-2.494676000	-2.184329000	-3.033495000
H	-2.663792000	-2.383060000	-4.086470000
H	-3.087027000	-1.440876000	-2.512692000
H	-1.719020000	-2.716851000	-2.495201000

³INT1-2_h

Fe	0.051547000	0.038777000	-0.388914000
O	-0.004981000	-0.033995000	-2.295447000
C	0.097047000	0.101890000	2.097210000
C	0.803035000	-0.053078000	4.291357000
H	1.485063000	-0.294333000	5.089198000
C	-0.440309000	0.499337000	4.308476000
H	-1.060931000	0.828693000	5.124756000
C	-2.153376000	1.111220000	2.565971000
H	-2.602808000	1.630228000	3.417526000
H	-2.018286000	1.808290000	1.741663000
H	-2.811682000	0.301459000	2.241551000
C	2.379492000	-0.862581000	2.501766000
H	2.865127000	-1.342700000	3.356399000
H	2.184564000	-1.601730000	1.728068000
H	3.034269000	-0.087302000	2.095386000
N	1.108855000	-0.289202000	2.945938000
N	-0.849538000	0.586552000	2.972569000
N	-1.907395000	-0.377162000	-0.232855000
N	0.488271000	-1.920941000	-0.211605000
N	2.003836000	0.453340000	-0.359011000
N	-0.384518000	1.996314000	-0.299677000
C	-2.943181000	0.506966000	-0.462449000
C	-2.471520000	-1.577519000	0.164899000
C	-0.413865000	-2.939472000	0.025332000
C	1.681127000	-2.513003000	-0.594420000
C	3.025821000	-0.445899000	-0.589516000
C	2.587501000	1.674304000	-0.070681000
C	0.522655000	3.025147000	-0.165052000
C	-1.598913000	2.565888000	-0.653256000
C	-4.200257000	-0.149166000	-0.172931000
H	-5.168288000	0.320706000	-0.245341000

C	-3.907702000	-1.418999000	0.248452000
H	-4.595827000	-2.184103000	0.569656000
C	0.229982000	-4.215100000	-0.222684000
H	-0.255981000	-5.173754000	-0.133737000
C	1.506215000	-3.951208000	-0.634706000
H	2.260918000	-4.656614000	-0.942483000
C	4.297174000	0.222485000	-0.404188000
H	5.259838000	-0.254536000	-0.497139000
C	4.027932000	1.514985000	-0.046801000
H	4.732558000	2.293161000	0.197800000
C	-0.137923000	4.286311000	-0.442726000
H	0.349227000	5.248282000	-0.430187000
C	-1.430745000	4.000448000	-0.778282000
H	-2.201331000	4.687841000	-1.087296000
C	-2.813058000	1.875217000	-0.761215000
C	-1.780340000	-2.789469000	0.311751000
C	2.887258000	-1.828077000	-0.800328000
C	1.903098000	2.892145000	0.058943000
C	-4.055884000	2.622189000	-1.101525000
C	-4.847330000	2.206883000	-2.190412000
H	-4.520020000	1.357677000	-2.781063000
C	-6.028466000	2.882593000	-2.513786000
H	-6.621920000	2.554138000	-3.361459000
C	-6.441659000	3.983167000	-1.751268000
H	-7.358092000	4.507986000	-2.002466000
C	-5.667042000	4.400766000	-0.661158000
H	-5.986136000	5.246036000	-0.059011000
C	-4.485976000	3.724529000	-0.337691000
H	-3.892873000	4.038656000	0.514691000
C	-2.547833000	-4.022483000	0.647425000
C	-3.602360000	-4.468278000	-0.172939000
H	-3.849825000	-3.900340000	-1.064024000
C	-4.300484000	-5.639481000	0.140127000
H	-5.106406000	-5.974814000	-0.505513000
C	-3.953100000	-6.385482000	1.274364000
H	-4.495071000	-7.294482000	1.516303000
C	-2.898103000	-5.956668000	2.090688000
H	-2.621897000	-6.531202000	2.969599000
C	-2.198970000	-4.786004000	1.777549000
H	-1.380478000	-4.449362000	2.405709000
C	4.112261000	-2.595461000	-1.158645000
C	4.849734000	-2.241938000	-2.305799000
H	4.494063000	-1.424538000	-2.924226000
C	6.013431000	-2.938383000	-2.648216000
H	6.565580000	-2.658076000	-3.539944000
C	6.462393000	-3.997444000	-1.848004000
H	7.365584000	-4.537747000	-2.114059000
C	5.740799000	-4.353675000	-0.701094000
H	6.088029000	-5.166336000	-0.070252000
C	4.577091000	-3.657186000	-0.358385000
H	4.024852000	-3.923555000	0.536761000
C	2.673281000	4.137205000	0.337518000
C	3.725317000	4.558399000	-0.498700000
H	3.977019000	3.961253000	-1.368440000
C	4.423573000	5.739728000	-0.226378000
H	5.227378000	6.053611000	-0.885240000
C	4.079050000	6.522865000	0.883229000
H	4.620836000	7.439856000	1.093179000
C	3.027023000	6.119641000	1.716130000
H	2.752568000	6.722025000	2.576770000
C	2.328859000	4.938645000	1.443686000
H	1.513132000	4.622286000	2.085746000
H	-0.686049000	-0.586756000	-2.736820000
C	-2.437795000	-2.157427000	-3.047219000
H	-2.553149000	-2.300064000	-4.116382000
H	-3.068005000	-1.453719000	-2.515724000
H	-1.692243000	-2.721506000	-2.498648000

³INT1-2_h

Fe	0.065764000	0.004345000	-0.179945000	H	-3.860571000	-2.412690000	2.605397000
O	0.070363000	-0.015665000	-2.014136000	C	1.393068000	-4.530106000	-1.355251000
C	0.134801000	0.014264000	1.925924000	C	2.134345000	-4.638019000	-2.548570000
C	0.482803000	-0.588316000	4.119816000	H	2.367577000	-3.733925000	-3.101122000
H	0.810914000	-1.228295000	4.920647000	C	2.553086000	-5.887233000	-3.018036000
C	-0.094577000	0.640005000	4.128991000	H	3.116852000	-5.953222000	-3.943515000
H	-0.379059000	1.288547000	4.939546000	C	2.242180000	-7.050110000	-2.300705000
C	-0.930016000	2.266099000	2.431244000	H	2.566888000	-8.019731000	-2.665313000
H	-0.909417000	2.915448000	3.311135000	C	1.513063000	-6.954435000	-1.108167000
H	-0.372062000	2.731706000	1.625323000	H	1.278427000	-7.849878000	-0.540562000
H	-1.963744000	2.110902000	2.116429000	C	1.094478000	-5.704941000	-0.638274000
C	1.222667000	-2.234152000	2.396991000	H	0.542296000	-5.628802000	0.292496000
H	1.254808000	-2.871103000	3.285553000	C	4.698932000	1.403716000	0.568681000
H	0.617123000	-2.710773000	1.632830000	C	5.799533000	1.067561000	-0.243532000
H	2.235566000	-2.084982000	2.018209000	H	5.634728000	0.467100000	-1.131352000
N	0.615643000	-0.956559000	2.778219000	C	7.084610000	1.521175000	0.072506000
N	-0.299827000	0.994027000	2.792675000	H	7.920481000	1.258042000	-0.568519000
N	-1.684476000	0.935511000	-0.175359000	C	7.291729000	2.324846000	1.201340000
N	-0.886562000	-1.736683000	-0.126409000	H	8.289200000	2.677281000	1.444924000
N	1.808656000	-0.929759000	-0.258232000	C	6.202541000	2.678411000	2.008598000
N	1.008337000	1.750494000	-0.197801000	H	6.353372000	3.304984000	2.882458000
C	-1.892411000	2.253672000	-0.530626000	C	4.917758000	2.224600000	1.692494000
C	-2.903607000	0.422415000	0.234827000	H	4.070528000	2.498368000	2.313049000
C	-2.221020000	-1.940337000	0.160667000	H	-0.854469000	-0.081902000	-2.351165000
C	-0.377556000	-2.940200000	-0.592614000	C	-3.031626000	-0.341622000	-2.950785000
C	1.992100000	-2.246668000	-0.615888000	H	-2.909294000	-0.380605000	-4.027905000
C	3.049464000	-0.409240000	0.050939000	H	-3.266073000	0.596433000	-2.460596000
C	2.357291000	1.952250000	-0.008059000	H	-2.948246000	-1.247203000	-2.360788000
C	0.474408000	2.945073000	-0.655045000	¹INT1-2_h			
C	-3.283913000	2.591264000	-0.306431000	Fe	0.067593000	0.004199000	-0.179702000
H	-3.714023000	3.565140000	-0.479012000	O	0.070493000	-0.015801000	-2.015302000
C	-3.895337000	1.478532000	0.206451000	C	0.137593000	0.014400000	1.926098000
H	-4.923320000	1.371746000	0.513107000	C	0.485997000	-0.588298000	4.119898000
C	-2.565659000	-3.319276000	-0.122317000	H	0.814801000	-1.228096000	4.920498000
H	-3.551703000	-3.740167000	-0.004405000	C	-0.092711000	0.639398000	4.129298000
C	-1.444057000	-3.921321000	-0.623442000	H	-0.377815000	1.287497000	4.939998000
H	-1.343682000	-4.931562000	-0.985864000	C	-0.929321000	2.265193000	2.431898000
C	3.397517000	-2.586197000	-0.477903000	H	-0.908226000	2.914793000	3.311598000
H	3.814322000	-3.562769000	-0.667345000	H	-0.372324000	2.730797000	1.625298000
C	4.040935000	-1.469254000	-0.023232000	H	-1.963320000	2.109387000	2.118098000
H	5.086026000	-1.360868000	0.217263000	C	1.228007000	-2.232793000	2.396598000
C	2.686904000	3.327938000	-0.331631000	H	1.262111000	-2.869493000	3.285298000
H	3.680027000	3.746062000	-0.286693000	H	0.622510000	-2.710597000	1.633098000
C	1.538843000	3.924522000	-0.770319000	H	2.240306000	-2.082087000	2.016798000
H	1.417742000	4.927812000	-1.145392000	N	0.619299000	-0.956097000	2.778198000
C	-0.892196000	3.189547000	-0.854295000	N	-0.298113000	0.993597000	2.792998000
C	-3.160395000	-0.937816000	0.459477000	N	-1.684113000	0.932988000	-0.174102000
C	0.976306000	-3.185258000	-0.869253000	N	-0.882396000	-1.738007000	-0.125502000
C	3.316003000	0.954491000	0.245055000	N	1.811599000	-0.927289000	-0.259102000
C	-1.339429000	4.531767000	-1.319839000	N	1.007682000	1.751705000	-0.199202000
C	-2.162625000	4.637649000	-2.458332000	C	-1.894221000	2.251087000	-0.528302000
H	-2.434852000	3.733159000	-2.992126000	C	-2.901910000	0.418381000	0.238398000
C	-2.612633000	5.885495000	-2.901583000	C	-2.216495000	-1.943415000	0.162198000
H	-3.239679000	5.948993000	-3.785597000	C	-0.371988000	-2.941003000	-0.591802000
C	-2.250618000	7.050440000	-2.212183000	C	1.996607000	-2.244088000	-0.616502000
H	-2.599010000	8.019230000	-2.556457000	C	3.051996000	-0.404982000	0.048898000
C	-1.438688000	6.957569000	-1.074259000	C	2.356581000	1.955414000	-0.011002000
H	-1.162775000	7.854573000	-0.528136000	C	0.471574000	2.945402000	-0.656402000
C	-0.989860000	5.709194000	-0.630382000	C	-3.285723000	2.586978000	-0.301102000
H	-0.373174000	5.635350000	0.259045000	H	-3.717430000	3.560275000	-0.473102000
C	-4.531501000	-1.377988000	0.840616000	C	-3.894916000	1.473374000	0.212498000
C	-5.649209000	-1.069701000	0.040837000	H	-4.922516000	1.364568000	0.519598000
H	-5.500924000	-0.501847000	-0.871465000	C	-2.559486000	-3.322717000	-0.120602000
C	-6.926273000	-1.513650000	0.399996000	H	-3.544883000	-3.744924000	-0.002102000
H	-7.776939000	-1.273164000	-0.230379000	C	-1.437382000	-3.923310000	-0.622302000
C	-7.106285000	-2.279404000	1.559588000	H	-1.335876000	-4.933409000	-0.984702000
H	-8.097483000	-2.624416000	1.837093000	C	3.402609000	-2.581579000	-0.479402000
C	-5.999105000	-2.605487000	2.353978000	H	3.820616000	-3.557677000	-0.668802000
H	-6.130152000	-3.203077000	3.251000000				
C	-4.722004000	-2.161223000	1.994977000				

C	4.044902000	-1.463575000	-0.025702000	C	-2.364063000	0.267223000	2.619532000
H	5.090002000	-1.353569000	0.213798000	H	-2.929211000	0.548531000	3.512505000
C	2.683972000	3.331316000	-0.335902000	H	-2.493952000	1.025375000	1.851541000
H	3.676669000	3.750822000	-0.292402000	H	-2.726623000	-0.690983000	2.242391000
C	1.534668000	3.926109000	-0.773502000	C	2.580058000	-0.147518000	2.474301000
H	1.411762000	4.929008000	-1.149002000	H	3.192772000	-0.424320000	3.336841000
C	-0.895627000	3.188293000	-0.853402000	H	2.641310000	-0.926155000	1.718305000
C	-3.156901000	-0.942221000	0.462198000	H	2.942187000	0.792770000	2.053762000
C	0.982113000	-3.184195000	-0.869002000	N	1.191726000	-0.015828000	2.918786000
C	3.316887000	0.959220000	0.241998000	N	-0.948263000	0.176895000	2.980607000
C	-1.345336000	4.529890000	-1.318102000	N	-1.779328000	-0.991332000	-0.191237000
C	-2.171237000	4.634685000	-2.454802000	N	1.042622000	-1.797141000	-0.176613000
H	-2.443631000	3.729883000	-2.987802000	N	1.827076000	0.999661000	-0.335189000
C	-2.623544000	5.881982000	-2.897202000	N	-0.989342000	1.806348000	-0.148924000
H	-3.252645000	5.944678000	-3.779902000	C	-3.022603000	-0.416431000	-0.358849000
C	-2.261252000	7.047485000	-2.208902000	C	-1.957106000	-2.337202000	0.100329000
H	-2.611458000	8.015882000	-2.552502000	C	0.447385000	-3.040679000	-0.055277000
C	-1.446651000	6.955690000	-1.072702000	C	2.359781000	-1.984772000	-0.570470000
H	-1.170557000	7.852992000	-0.527402000	C	3.064002000	0.420537000	-0.556447000
C	-0.995543000	5.707793000	-0.629602000	C	2.020717000	2.343857000	-0.053868000
H	-0.376943000	5.634897000	0.258498000	C	-0.388691000	3.051094000	-0.057462000
C	-4.527998000	-1.384130000	0.841798000	C	-2.324115000	1.990810000	-0.464346000
C	-5.644400000	-1.077937000	0.039398000	C	-4.028260000	-1.426035000	-0.130363000
H	-5.494904000	-0.511436000	-0.873502000	H	-5.092839000	-1.256464000	-0.168128000
C	-6.921597000	-1.523245000	0.396698000	C	-3.375018000	-2.598313000	0.182278000
H	-7.771399000	-1.284551000	-0.235602000	H	-3.820545000	-3.548647000	0.428927000
C	-7.102792000	-2.287946000	1.556798000	C	1.437206000	-4.056418000	-0.373191000
H	-8.094090000	-2.633953000	1.832798000	H	1.245685000	-5.117827000	-0.384626000
C	-5.996790000	-2.611739000	2.353598000	C	2.595132000	-3.412570000	-0.712539000
H	-6.128787000	-3.208540000	3.251098000	H	3.518430000	-3.856516000	-1.048696000
C	-4.719593000	-2.166231000	1.996598000	C	4.080666000	1.433550000	-0.382322000
H	-3.858892000	-2.415926000	2.608898000	H	5.142492000	1.265529000	-0.468922000
C	1.400622000	-4.528592000	-1.354702000	C	3.441712000	2.605612000	-0.047282000
C	2.141623000	-4.635787000	-2.548302000	H	3.898097000	3.555968000	0.179351000
H	2.373117000	-3.731586000	-3.101302000	C	-1.398200000	4.065198000	-0.312037000
C	2.562131000	-5.884585000	-3.017502000	H	-1.212230000	5.127673000	-0.326696000
H	3.125531000	-5.949981000	-3.943202000	C	-2.572211000	3.418589000	-0.589486000
C	2.253338000	-7.047687000	-2.299502000	H	-3.515378000	3.862043000	-0.865777000
H	2.579544000	-8.016885000	-2.663902000	C	-3.281533000	0.962133000	-0.585317000
C	1.524637000	-6.952691000	-1.106702000	C	-0.919241000	-3.297802000	0.177348000
H	1.291743000	-7.848293000	-0.538602000	C	3.314212000	-0.964057000	-0.745875000
C	1.104329000	-5.703694000	-0.637102000	C	0.989362000	3.306726000	0.087417000
H	0.552529000	-5.628097000	0.293898000	C	-4.684605000	1.328715000	-0.923084000
C	4.699484000	1.410529000	0.564298000	C	-5.316725000	0.721003000	-2.027416000
C	5.799986000	1.075236000	-0.248402000	H	-4.756455000	0.004904000	-2.620249000
H	5.635390000	0.474035000	-1.135702000	C	-6.635351000	1.043875000	-2.362952000
C	7.084683000	1.530744000	0.066598000	H	-7.103372000	0.571791000	-3.221544000
H	7.920385000	1.268250000	-0.574802000	C	-7.349303000	1.977059000	-1.599197000
C	7.291478000	2.335346000	1.194798000	H	-8.373583000	2.226374000	-1.858552000
H	8.288576000	2.689252000	1.437598000	C	-6.734103000	2.584000000	-0.496106000
C	6.202276000	2.687939000	2.002598000	H	-7.283705000	3.300568000	0.106964000
H	6.352872000	3.315240000	2.875898000	C	-5.415144000	2.261266000	-0.160282000
C	4.917879000	2.232330000	1.687498000	H	-4.942915000	2.720975000	0.701661000
H	4.070777000	2.505325000	2.308498000	C	-1.297704000	-4.720607000	0.419118000
H	-0.853406000	-0.086406000	-2.349302000	C	-2.213496000	-5.391268000	-0.415149000
C	-3.106405000	-0.345221000	-2.941702000	H	-2.651125000	-4.856671000	-1.251093000
H	-3.012905000	-0.386420000	-4.021702000	C	-2.542384000	-6.730947000	-0.183533000
H	-3.319711000	0.595078000	-2.446202000	H	-3.244555000	-7.234155000	-0.841242000
H	-2.993499000	-1.247120000	-2.350902000	C	-1.958950000	-7.426027000	0.884223000
⁷TS2-2_{hs}				H	-2.214253000	-8.465921000	1.063082000
Fe	0.019407000	-0.011298000	-0.276010000	C	-1.040222000	-6.772750000	1.716036000
O	0.000709000	0.013373000	-2.246214000	H	-0.582960000	-7.304286000	2.545101000
C	0.095021000	0.057323000	2.090410000	C	-0.711555000	-5.433010000	1.483915000
C	0.841115000	0.059778000	4.269497000	H	-0.000452000	-4.922956000	2.125497000
H	1.576225000	0.022622000	5.055194000	C	4.713395000	-1.352363000	-1.079599000
C	-0.512794000	0.178802000	4.308706000	C	5.360487000	-0.782439000	-2.194642000
H	-1.197304000	0.259844000	5.135729000	H	4.815451000	-0.073616000	-2.809007000
				C	6.677826000	-1.127496000	-2.512401000
				H	7.156384000	-0.683569000	-3.380049000
				C	7.376091000	-2.048630000	-1.720097000

H	8.398417000	-2.317473000	-1.967190000
C	6.746779000	-2.618943000	-0.605849000
H	7.283394000	-3.326398000	0.019172000
C	5.429733000	-2.271691000	-0.287408000
H	4.946140000	-2.704038000	0.582201000
C	1.383466000	4.728373000	0.309156000
C	2.252156000	5.399804000	-0.573730000
H	2.642101000	4.866636000	-1.433949000
C	2.595993000	6.738390000	-0.358271000
H	3.261022000	7.241905000	-1.053317000
C	2.074993000	7.432030000	0.742184000
H	2.341985000	8.471020000	0.908719000
C	1.203670000	6.778217000	1.623197000
H	0.795244000	7.308497000	2.478149000
C	0.860198000	5.439484000	1.407286000
H	0.186224000	4.928458000	2.086930000
H	0.425594000	0.785983000	-2.672488000
C	-1.822944000	-0.399734000	-3.362280000
H	-2.357033000	0.486889000	-3.047066000
H	-1.350713000	-0.433301000	-4.336452000
H	-1.930649000	-1.308983000	-2.789862000

⁵TS2-2_{hs}

Fe	0.021689000	0.023955000	-0.333982000
O	0.002817000	-0.022574000	-2.246526000
C	0.126183000	0.013435000	2.121675000
C	0.863553000	-0.052980000	4.310869000
H	1.595131000	-0.117426000	5.098353000
C	-0.489058000	0.075446000	4.348479000
H	-1.175788000	0.139459000	5.175394000
C	-2.329041000	0.238014000	2.653998000
H	-2.892264000	0.529962000	3.545086000
H	-2.438685000	1.001170000	1.887670000
H	-2.713272000	-0.709899000	2.271606000
C	2.606740000	-0.209686000	2.516295000
H	3.223085000	-0.476719000	3.379515000
H	2.679551000	-0.989282000	1.761869000
H	2.959983000	0.732632000	2.092647000
N	1.217696000	-0.090533000	2.958474000
N	-0.917529000	0.115983000	3.017820000
N	-1.782404000	-0.986983000	-0.185274000
N	1.049051000	-1.790654000	-0.235249000
N	1.846549000	1.017202000	-0.305665000
N	-0.984468000	1.816647000	-0.182246000
C	-3.026917000	-0.413604000	-0.329468000
C	-1.949513000	-2.339447000	0.039682000
C	0.462298000	-3.034158000	-0.120698000
C	2.383217000	-1.968334000	-0.561548000
C	3.081984000	0.442542000	-0.511617000
C	2.024615000	2.365849000	-0.082165000
C	-0.390945000	3.059914000	-0.115620000
C	-2.332478000	1.993359000	-0.443006000
C	-4.034635000	-1.442766000	-0.139440000
H	-5.100041000	-1.277154000	-0.170053000
C	-3.376368000	-2.617652000	0.112378000
H	-3.812223000	-3.581638000	0.320607000
C	1.471036000	-4.045977000	-0.389180000
H	1.291826000	-5.109579000	-0.393983000
C	2.639890000	-3.393992000	-0.679702000
H	3.583790000	-3.833570000	-0.959953000
C	4.099736000	1.472185000	-0.360613000
H	5.162945000	1.306930000	-0.435920000
C	3.454299000	2.644510000	-0.073388000
H	3.898638000	3.607731000	0.119972000
C	-1.411655000	4.070067000	-0.341672000
H	-1.231078000	5.133045000	-0.368656000
C	-2.594186000	3.416983000	-0.564778000
H	-3.551317000	3.853227000	-0.802174000
C	-3.291863000	0.960572000	-0.521941000

C	-0.912295000	-3.296964000	0.091652000
C	3.338472000	-0.934789000	-0.697384000
C	0.991739000	3.323707000	0.023402000
C	-4.709391000	1.338568000	-0.789982000
C	-5.381241000	0.792939000	-1.901791000
H	-4.840758000	0.120826000	-2.560895000
C	-6.713813000	1.129138000	-2.162656000
H	-7.216051000	0.706957000	-3.027720000
C	-7.396780000	2.013507000	-1.316980000
H	-8.430913000	2.273990000	-1.520197000
C	-6.738355000	2.560403000	-0.207634000
H	-7.263252000	3.241263000	0.455629000
C	-5.405645000	2.224714000	0.053895000
H	-4.895346000	2.639913000	0.916869000
C	-1.290570000	-4.726315000	0.299711000
C	-2.181760000	-5.383868000	-0.570372000
H	-2.598341000	-4.835637000	-1.408515000
C	-2.516392000	-6.727268000	-0.369214000
H	-3.200471000	-7.219949000	-1.053401000
C	-1.962517000	-7.438479000	0.703344000
H	-2.221868000	-8.481087000	0.858839000
C	-1.068429000	-6.797710000	1.571217000
H	-0.634996000	-7.341821000	2.404869000
C	-0.734336000	-5.454370000	1.369666000
H	-0.042909000	-4.953955000	2.039668000
C	4.749550000	-1.321810000	-0.988298000
C	5.418625000	-0.777363000	-2.102190000
H	4.884055000	-0.088967000	-2.748264000
C	6.746249000	-1.121490000	-2.376981000
H	7.243970000	-0.697685000	-3.243803000
C	7.430070000	-2.014869000	-1.541736000
H	8.460143000	-2.282624000	-1.755505000
C	6.777318000	-2.559290000	-0.427965000
H	7.303007000	-3.245253000	0.229353000
C	5.449881000	-2.214139000	-0.153056000
H	4.946004000	-2.627228000	0.714487000
C	1.380108000	4.753226000	0.207921000
C	2.228052000	5.406349000	-0.707643000
H	2.600111000	4.854824000	-1.564287000
C	2.573011000	6.750142000	-0.527878000
H	3.222336000	7.239963000	-1.247096000
C	2.073232000	7.465787000	0.568098000
H	2.340766000	8.508732000	0.706749000
C	1.221842000	6.829402000	1.480989000
H	0.829894000	7.377176000	2.332606000
C	0.877016000	5.485721000	1.300841000
H	0.218190000	4.988432000	2.005201000
H	0.243687000	-0.843531000	-2.719842000
C	-2.155696000	-0.421940000	-3.483280000
H	-2.381951000	0.568731000	-3.116741000
H	-1.711119000	-0.548214000	-4.464011000
H	-2.372210000	-1.280912000	-2.860665000

⁵TS2-2_{is}

Fe	0.038660000	0.021907000	-0.090470000
O	-0.157954000	-0.035448000	-1.948293000
C	0.145031000	0.050218000	2.067018000
C	0.655037000	-0.463727000	4.251466000
H	1.136407000	-1.011387000	5.043260000
C	-0.200206000	0.590929000	4.277177000
H	-0.620537000	1.148653000	5.096237000
C	-1.410126000	1.985400000	2.598810000
H	-1.551532000	2.604912000	3.488922000
H	-0.969047000	2.583026000	1.807145000
H	-2.373842000	1.595942000	2.266332000
C	1.741815000	-1.871337000	2.499162000
H	1.995044000	-2.453223000	3.389736000
H	1.227335000	-2.506658000	1.784297000
H	2.654861000	-1.478509000	2.049218000

C	-0.776272000	-7.504571000	-1.909050000
H	-0.854728000	-8.541684000	-2.220143000
C	-1.473081000	-7.052984000	-0.780623000
H	-2.088356000	-7.741590000	-0.209376000
C	-1.372103000	-5.716385000	-0.380273000
H	-1.904776000	-5.367221000	0.498131000
C	4.830353000	-0.580992000	0.504280000
C	5.638070000	-1.323736000	-0.378803000
H	5.178934000	-1.792702000	-1.242176000
C	7.014875000	-1.440596000	-0.160213000
H	7.623330000	-2.011540000	-0.854945000
C	7.610106000	-0.812123000	0.941693000
H	8.678780000	-0.902513000	1.110003000
C	6.819304000	-0.060341000	1.820469000
H	7.273078000	0.432643000	2.674912000
C	5.442727000	0.056496000	1.601065000
H	4.826533000	0.640260000	2.277249000
C	0.551691000	4.803159000	-1.054867000
C	-0.117754000	5.307004000	-2.188109000
H	-0.726445000	4.630864000	-2.779188000
C	0.002575000	6.651777000	-2.552440000
H	-0.515278000	7.019445000	-3.433008000
C	0.794395000	7.520372000	-1.789540000
H	0.889046000	8.564051000	-2.072682000
C	1.462253000	7.033570000	-0.658181000
H	2.070888000	7.701601000	-0.056272000
C	1.340203000	5.688779000	-0.293462000
H	1.849046000	5.313548000	0.588109000
C	-4.924755000	0.564396000	0.310520000
C	-5.707531000	1.330367000	-0.575571000
H	-5.225734000	1.814659000	-1.417912000
C	-7.088406000	1.451752000	-0.387538000
H	-7.676636000	2.040963000	-1.084459000
C	-7.713669000	0.804344000	0.686341000
H	-8.785511000	0.898005000	0.830934000
C	-6.948431000	0.029391000	1.567688000
H	-7.425401000	-0.478289000	2.400584000
C	-5.567812000	-0.091520000	1.378996000
H	-4.971499000	-0.692915000	2.057449000
H	-0.488923000	0.608791000	-2.346863000
C	2.049602000	0.418063000	-3.101426000
H	1.595511000	0.174419000	-4.054176000
H	2.474204000	-0.368143000	-2.494146000
H	2.146449000	1.448677000	-2.784080000

³TS2-2_h

Fe	-0.024600000	-0.000903000	-0.168901000
O	0.149403000	-0.042588000	-2.061301000
C	-0.088600000	-0.007208000	1.983499000
C	-0.767526000	0.303834000	4.161799000
H	-1.430354000	0.627078000	4.946199000
C	0.440926000	-0.314964000	4.202999000
H	1.049153000	-0.636812000	5.030899000
C	2.117695000	-1.125822000	2.533399000
H	2.492238000	-1.641190000	3.422499000
H	1.964656000	-1.844935000	1.734599000
H	2.844231000	-0.377160000	2.210399000
C	-2.324194000	1.111303000	2.375699000
H	-2.763138000	1.628665000	3.233599000
H	-2.111955000	1.828020000	1.588299000
H	-3.025131000	0.361543000	2.002399000
N	-1.074441000	0.484508000	2.810099000
N	0.839542000	-0.497930000	2.875199000
N	1.941774000	0.296263000	-0.143601000
N	-0.317067000	1.965972000	-0.183601000
N	-1.982674000	-0.308869000	-0.321501000
N	0.260067000	-1.978879000	-0.143301000
C	2.896154000	-0.645256000	-0.459401000
C	2.606576000	1.457219000	0.197099000

C	0.636652000	2.932653000	0.061099000
C	-1.445622000	2.616277000	-0.660601000
C	-2.930155000	0.641451000	-0.653901000
C	-2.669577000	-1.463927000	0.030399000
C	-0.701551000	-2.946960000	0.053199000
C	1.419122000	-2.625981000	-0.544901000
C	4.215806000	-0.072344000	-0.262701000
H	5.143350000	-0.601766000	-0.413601000
C	4.038397000	1.206841000	0.185899000
H	4.796937000	1.921705000	0.460799000
C	0.088241000	4.237107000	-0.253001000
H	0.631063000	5.165452000	-0.171101000
C	-1.175242000	4.038800000	-0.735501000
H	-1.860505000	4.779742000	-1.114201000
C	-4.254207000	0.076939000	-0.479701000
H	-5.175552000	0.611961000	-0.647801000
C	-4.095099000	-1.200547000	-0.018301000
H	-4.865439000	-1.905012000	0.250399000
C	-0.128741000	-4.251612000	-0.209701000
H	-0.669162000	-5.182958000	-0.145901000
C	1.161942000	-4.050203000	-0.617501000
H	1.873605000	-4.791343000	-0.943901000
C	2.660069000	-2.000576000	-0.745501000
C	1.990671000	2.706367000	0.368499000
C	-2.681570000	2.001172000	-0.914901000
C	-2.072971000	-2.710776000	0.266999000
C	3.820037000	-2.811578000	-1.209501000
C	4.503605000	-2.431620000	-2.381701000
H	4.151232000	-1.566350000	-2.934301000
C	5.603467000	-3.168027000	-2.834401000
H	6.114942000	-2.867384000	-3.743701000
C	6.040963000	-4.292490000	-2.121701000
H	6.894811000	-4.863418000	-2.473401000
C	5.372295000	-4.675047000	-0.951401000
H	5.711868000	-5.539318000	-0.388501000
C	4.272033000	-3.939340000	-0.498101000
H	3.761057000	-4.226783000	0.414899000
C	2.814770000	3.892437000	0.735199000
C	3.923337000	4.293031000	-0.035801000
H	4.182085000	3.723353000	-0.921601000
C	4.668941000	5.422494000	0.318399000
H	5.516616000	5.720466000	-0.291201000
C	4.315677000	6.175964000	1.445499000
H	4.894003000	7.053013000	1.719099000
C	3.206509000	5.795670000	2.212599000
H	2.923360000	6.376446000	3.085199000
C	2.461605000	4.665907000	1.858299000
H	1.600730000	4.368534000	2.448499000
C	-3.830940000	2.830775000	-1.373201000
C	-4.533410000	2.473216000	-2.540901000
H	-4.206536000	1.603743000	-3.101501000
C	-5.626574000	3.228523000	-2.977901000
H	-6.150649000	2.942679000	-3.884801000
C	-6.040469000	4.353688000	-2.252601000
H	-6.888118000	4.940817000	-2.592201000
C	-5.355699000	4.714746000	-1.084901000
H	-5.677072000	5.578619000	-0.510901000
C	-4.263235000	3.958339000	-0.647901000
H	-3.741258000	4.230183000	0.263499000
C	-2.919572000	-3.884848000	0.617599000
C	-4.004938000	-4.287640000	-0.185001000
H	-4.229985000	-3.727559000	-1.086001000
C	-4.771043000	-5.406604000	0.158499000
H	-5.600118000	-5.706075000	-0.475401000
C	-4.462181000	-6.147778000	1.306699000
H	-5.056607000	-7.016429000	1.571899000
C	-3.376813000	-5.765387000	2.105999000
H	-3.128565000	-6.336066000	2.995799000
C	-2.611508000	-4.646222000	1.762699000
H	-1.769433000	-4.346851000	2.378199000

H	-0.566951000	-0.585649000	-2.461601000
C	1.672706000	-0.070760000	-3.599701000
H	1.835296000	-1.141946000	-3.575501000
H	2.291952000	0.564393000	-2.981301000
H	1.116768000	0.367893000	-4.420301000

¹TS2-2_{ts}

Fe	0.028055000	-0.000465000	-0.167288000
O	0.069593000	-0.103412000	-2.020391000
C	0.106882000	0.021430000	1.918535000
C	0.786187000	-0.230458000	4.104162000
H	1.460650000	-0.510506000	4.894831000
C	-0.449891000	0.328067000	4.131937000
H	-1.078911000	0.628572000	4.952005000
C	-2.161770000	1.037091000	2.467001000
H	-2.548850000	1.543565000	3.355860000
H	-2.058723000	1.754963000	1.659942000
H	-2.852615000	0.247085000	2.166341000
C	2.401091000	-0.983731000	2.363391000
H	2.842545000	-1.459691000	3.243704000
H	2.249761000	-1.729018000	1.589239000
H	3.071338000	-0.204316000	1.996172000
N	1.110933000	-0.414292000	2.757625000
N	-0.849802000	0.478658000	2.801523000
N	-1.880995000	-0.481154000	-0.126774000
N	0.516637000	-1.925586000	-0.183501000
N	1.948226000	0.501814000	-0.245021000
N	-0.448954000	1.927297000	-0.225975000
C	-2.935425000	0.350080000	-0.449834000
C	-2.420993000	-1.706181000	0.234115000
C	-0.323907000	-2.985525000	0.061922000
C	1.701763000	-2.448576000	-0.674361000
C	2.983101000	-0.339300000	-0.604165000
C	2.506641000	1.721629000	0.095720000
C	0.400625000	2.994936000	-0.000180000
C	-1.665511000	2.455447000	-0.636078000
C	-4.181588000	-0.352991000	-0.225450000
H	-5.161540000	0.071610000	-0.375428000
C	-3.866760000	-1.601047000	0.239375000
H	-4.545059000	-2.386408000	0.531159000
C	0.352113000	-4.227271000	-0.272910000
H	-0.090561000	-5.207594000	-0.193586000
C	1.581619000	-3.893788000	-0.764532000
H	2.338502000	-4.554323000	-1.155832000
C	4.241249000	0.359475000	-0.430919000
H	5.212747000	-0.071603000	-0.614481000
C	3.951494000	1.610864000	0.042527000
H	4.644783000	2.393752000	0.304461000
C	-0.299931000	4.232327000	-0.284293000
H	0.138231000	5.215258000	-0.211752000
C	-1.554093000	3.899017000	-0.715500000
H	-2.334902000	4.562281000	-1.051611000
C	-2.844539000	1.710582000	-0.789982000
C	-1.688005000	-2.891259000	0.392728000
C	2.869630000	-1.708161000	-0.906862000
C	1.775540000	2.905977000	0.281207000
C	-4.092979000	2.387151000	-1.241481000
C	-4.773679000	1.899241000	-2.375106000
H	-4.357248000	1.053213000	-2.912334000
C	-5.958355000	2.502808000	-2.809526000
H	-6.466401000	2.118988000	-3.688969000
C	-6.485865000	3.600511000	-2.116796000
H	-7.405666000	4.068433000	-2.453837000
C	-5.821297000	4.089451000	-0.984383000
H	-6.229594000	4.933012000	-0.435945000
C	-4.636015000	3.486617000	-0.549341000
H	-4.128250000	3.855546000	0.335714000
C	-2.382547000	-4.152912000	0.774989000
C	-3.461970000	-4.667237000	0.030839000
H	-3.801166000	-4.126996000	-0.846160000

C	-4.074026000	-5.870054000	0.399786000
H	-4.900308000	-6.255893000	-0.189461000
C	-3.614315000	-6.583022000	1.514888000
H	-4.089192000	-7.516927000	1.799196000
C	-2.533212000	-6.087817000	2.255848000
H	-2.168078000	-6.636209000	3.118946000
C	-1.921531000	-4.885518000	1.886607000
H	-1.080967000	-4.499564000	2.454237000
C	4.096063000	-2.400121000	-1.392709000
C	4.742626000	-1.935758000	-2.555138000
H	4.314780000	-1.093697000	-3.088839000
C	5.909139000	-2.551949000	-3.019274000
H	6.389751000	-2.185491000	-3.921209000
C	6.453192000	-3.641715000	-2.326617000
H	7.358508000	-4.120726000	-2.686438000
C	5.823413000	-4.108350000	-1.165419000
H	6.244671000	-4.945632000	-0.617192000
C	4.656571000	-3.491546000	-0.701285000
H	4.176280000	-3.843782000	0.205514000
C	2.479656000	4.168089000	0.643297000
C	3.536032000	4.682952000	-0.132982000
H	3.848699000	4.143445000	-1.020234000
C	4.160126000	5.884895000	0.218133000
H	4.968357000	6.270668000	-0.395709000
C	3.735672000	6.596854000	1.347700000
H	4.219730000	7.530082000	1.618340000
C	2.678102000	6.100956000	2.121502000
H	2.340664000	6.648128000	2.996547000
C	2.054740000	4.899246000	1.770321000
H	1.232952000	4.512203000	2.364052000
H	0.272219000	0.783158000	-2.391755000
C	-1.903056000	-0.205164000	-3.480614000
H	-2.114395000	0.850106000	-3.357173000
H	-2.290966000	-0.914498000	-2.763766000
H	-1.272304000	-0.546425000	-4.291844000

⁵INT2-2

Fe	-0.025700000	0.026830000	0.008893000
O	0.024193000	0.043269000	-2.391753000
C	-0.008661000	0.070098000	2.234101000
C	0.674854000	0.161404000	4.430828000
H	1.382839000	0.260057000	5.236086000
C	-0.674728000	-0.016953000	4.436387000
H	-1.376387000	-0.112950000	5.247469000
C	-2.455162000	-0.261836000	2.661614000
H	-3.119409000	-0.076084000	3.510442000
H	-2.676648000	0.440575000	1.860010000
H	-2.604823000	-1.279547000	2.291486000
C	2.439923000	0.405464000	2.639578000
H	3.109240000	0.268660000	3.493580000
H	2.671369000	-0.328087000	1.868906000
H	2.571764000	1.408100000	2.224931000
N	1.060610000	0.208864000	3.087088000
N	-1.071493000	-0.065857000	3.095910000
N	-1.586446000	-1.320544000	-0.266945000
N	1.366511000	-1.540289000	-0.178981000
N	1.565830000	1.366081000	-0.359057000
N	-1.384805000	1.596216000	-0.226493000
C	-2.924358000	-1.008483000	-0.391178000
C	-1.481320000	-2.681668000	-0.040063000
C	1.024034000	-2.879366000	-0.183540000
C	2.709313000	-1.447690000	-0.506038000
C	2.912087000	1.052328000	-0.431109000
C	1.457794000	2.731420000	-0.130865000
C	-1.046505000	2.932205000	-0.266345000
C	-2.726696000	1.490177000	-0.540720000
C	-3.703049000	-2.214772000	-0.179851000
H	-4.780570000	-2.266315000	-0.185631000
C	-2.819738000	-3.237682000	0.055498000

H	-3.053068000	-4.269123000	0.266462000
C	2.202836000	-3.665619000	-0.526752000
H	2.219346000	-4.739160000	-0.630914000
C	3.228869000	-2.789285000	-0.740686000
H	4.236188000	-3.019427000	-1.050117000
C	3.682954000	2.257712000	-0.204821000
H	4.760205000	2.307958000	-0.174372000
C	2.792760000	3.282288000	0.001274000
H	3.021665000	4.313059000	0.220539000
C	-2.233195000	3.710248000	-0.611505000
H	-2.252730000	4.781004000	-0.740594000
C	-3.256224000	2.826284000	-0.796921000
H	-4.266900000	3.044078000	-1.104056000
C	-3.461564000	0.288077000	-0.588027000
C	-0.271471000	-3.416085000	-0.009701000
C	3.450744000	-0.249263000	-0.587128000
C	0.250284000	3.470086000	-0.108179000
C	-4.931195000	0.379414000	-0.823271000
C	-5.535426000	-0.350387000	-1.866268000
H	-4.909578000	-0.967303000	-2.502229000
C	-6.914476000	-0.275694000	-2.086831000
H	-7.361135000	-0.839455000	-2.900216000
C	-7.716725000	0.529614000	-1.267399000
H	-8.787123000	0.588107000	-1.438839000
C	-7.128956000	1.258889000	-0.225433000
H	-7.744152000	1.880276000	0.418377000
C	-5.749673000	1.183354000	-0.005246000
H	-5.293234000	1.743224000	0.804325000
C	-0.361512000	-4.899204000	0.134199000
C	-1.131638000	-5.679656000	-0.750426000
H	-1.671410000	-5.186258000	-1.551522000
C	-1.193545000	-7.070089000	-0.610031000
H	-1.787655000	-7.655576000	-1.305189000
C	-0.482688000	-7.707337000	0.415597000
H	-0.530213000	-8.786505000	0.523930000
C	0.293102000	-6.943638000	1.297691000
H	0.846570000	-7.429295000	2.095708000
C	0.353990000	-5.553403000	1.156679000
H	0.953088000	-4.957775000	1.837562000
C	4.922291000	-0.349751000	-0.801194000
C	5.549150000	0.379266000	-1.831916000
H	4.939341000	1.005087000	-2.474927000
C	6.931048000	0.297591000	-2.030577000
H	7.393927000	0.862008000	-2.834372000
C	7.715295000	-0.515133000	-1.201225000
H	8.787899000	-0.579562000	-1.355598000
C	7.106224000	-1.242956000	-0.170438000
H	7.707341000	-1.868662000	0.482385000
C	5.724373000	-1.159359000	0.028395000
H	5.252656000	-1.715986000	0.831232000
C	0.344918000	4.953676000	0.021914000
C	1.131697000	5.722105000	-0.858793000
H	1.677750000	5.218879000	-1.649392000
C	1.200385000	7.113221000	-0.729329000
H	1.806941000	7.689136000	-1.421727000
C	0.479992000	7.763609000	0.281267000
H	0.532788000	8.843357000	0.381121000
C	-0.312468000	7.012223000	1.159147000
H	-0.873507000	7.507999000	1.945570000
C	-0.380104000	5.621325000	1.029191000
H	-0.991785000	5.035473000	1.707320000
H	0.821309000	0.610264000	-2.430333000
C	0.228851000	-1.241429000	-3.054707000
H	0.182052000	-1.125155000	-4.145021000
H	-0.590563000	-1.873328000	-2.710827000
H	1.179645000	-1.698816000	-2.760526000

³INT2-2

Fe	-0.014657000	0.026917000	-0.127304000
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O	0.075642000	0.003549000	-2.549277000
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H	1.371712000	0.270541000	5.131777000
C	-0.689517000	0.043525000	4.325902000
H	-1.396315000	-0.023995000	5.135567000
C	-2.469002000	-0.175602000	2.549824000
H	-3.129440000	0.047092000	3.392975000
H	-2.668804000	0.513802000	1.732299000
H	-2.646271000	-1.196821000	2.202362000
C	2.443536000	0.355949000	2.541333000
H	3.104526000	0.166650000	3.392132000
H	2.644968000	-0.363159000	1.749950000
H	2.617980000	1.363987000	2.156244000
N	1.056410000	0.202429000	2.981266000
N	-1.081488000	-0.008992000	2.984068000
N	-1.564061000	-1.275075000	-0.299923000
N	1.277351000	-1.490552000	-0.213442000
N	1.549530000	1.325907000	-0.371285000
N	-1.290399000	1.541165000	-0.278263000
C	-2.893919000	-0.965525000	-0.504570000
C	-1.511198000	-2.619596000	0.031142000
C	0.952273000	-2.833374000	-0.074270000
C	2.623048000	-1.449688000	-0.583212000
C	2.886923000	1.008719000	-0.537226000
C	1.494323000	2.678965000	-0.068449000
C	-0.968765000	2.885478000	-0.170788000
C	-2.635099000	1.487909000	-0.636782000
C	-3.706114000	-2.136550000	-0.263524000
H	-4.782431000	-2.165461000	-0.327586000
C	-2.855551000	-3.149206000	0.099316000
H	-3.113724000	-4.158031000	0.378901000
C	2.115698000	-3.650295000	-0.372581000
H	2.123818000	-4.728764000	-0.365536000
C	3.128320000	-2.805697000	-0.716083000
H	4.124105000	-3.063945000	-1.038211000
C	3.694113000	2.184110000	-0.312120000
H	4.771571000	2.211023000	-0.354630000
C	2.837117000	3.206289000	0.010060000
H	3.092068000	4.220762000	0.271654000
C	-2.140050000	3.694479000	-0.471490000
H	-2.150554000	4.772786000	-0.487328000
C	-3.150501000	2.839843000	-0.788923000
H	-4.149488000	3.085661000	-1.110563000
C	-3.401922000	0.323806000	-0.755552000
C	-0.324938000	-3.364418000	0.160738000
C	3.394352000	-0.290507000	-0.739869000
C	0.307288000	3.424449000	0.048527000
C	-4.854322000	0.434299000	-1.072338000
C	-5.392600000	-0.271835000	-2.165962000
H	-4.728215000	-0.873869000	-2.776853000
C	-6.756619000	-0.195332000	-2.465767000
H	-7.152498000	-0.740355000	-3.317314000
C	-7.609054000	0.585987000	-1.674395000
H	-8.667771000	0.645944000	-1.906948000
C	-7.087261000	1.287597000	-0.579669000
H	-7.742497000	1.887890000	0.044337000
C	-5.722889000	1.210290000	-0.280397000
H	-5.318742000	1.746090000	0.572049000
C	-0.415647000	-4.822789000	0.456613000
C	-1.172845000	-5.695807000	-0.348785000
H	-1.703371000	-5.293591000	-1.205033000
C	-1.231917000	-7.063678000	-0.061460000
H	-1.815949000	-7.722486000	-0.696973000
C	-0.531173000	-7.584901000	1.034200000
H	-0.576978000	-8.646501000	1.256629000
C	0.232993000	-6.728478000	1.837848000
H	0.779641000	-7.124232000	2.688468000
C	0.291615000	-5.361039000	1.549874000
H	0.882398000	-4.693373000	2.168408000

C	4.848996000	-0.415050000	-1.039761000
C	5.408319000	0.276038000	-2.132867000
H	4.759142000	0.881722000	-2.756706000
C	6.775398000	0.186631000	-2.414441000
H	7.186421000	0.721598000	-3.265167000
C	7.611359000	-0.593960000	-1.605163000
H	8.672454000	-0.664265000	-1.823277000
C	7.069702000	-1.280304000	-0.510302000
H	7.712141000	-1.878728000	0.128579000
C	5.702527000	-1.189175000	-0.229032000
H	5.283833000	-1.711575000	0.624566000
C	0.398158000	4.887193000	0.320742000
C	1.156598000	5.746416000	-0.498143000
H	1.684246000	5.330293000	-1.349523000
C	1.218677000	7.118267000	-0.231094000
H	1.803104000	7.766530000	-0.877001000
C	0.519993000	7.657049000	0.857373000
H	0.568095000	8.721752000	1.063981000
C	-0.245458000	6.814291000	1.674138000
H	-0.790781000	7.223772000	2.519097000
C	-0.307188000	5.442906000	1.406462000
H	-0.899021000	4.785801000	2.035245000
H	0.941200000	0.458609000	-2.578940000
C	0.147835000	-1.334069000	-3.133784000
H	0.193796000	-1.276009000	-4.228806000
H	-0.771871000	-1.831126000	-2.823788000
H	1.004508000	-1.895086000	-2.745200000

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Fe	-0.004576000	0.024554000	-0.080009000
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C	0.691615000	0.006398000	4.113800000
H	1.401235000	-0.087923000	4.917726000
C	-0.647172000	0.224208000	4.117621000
H	-1.346753000	0.351792000	4.925746000
C	-2.452640000	0.461587000	2.418005000
H	-2.978761000	0.845624000	3.297145000
H	-2.519353000	1.185329000	1.612721000
H	-2.910280000	-0.478299000	2.101750000
C	2.475828000	-0.300337000	2.403039000
H	3.011697000	-0.655073000	3.288592000
H	2.532027000	-1.051092000	1.622214000
H	2.930848000	0.627679000	2.050020000
N	1.077543000	-0.087626000	2.774215000
N	-1.049792000	0.263305000	2.780277000
N	-1.764384000	-0.883314000	-0.190734000
N	0.907948000	-1.742935000	-0.158576000
N	1.765093000	0.935384000	-0.260321000
N	-0.901977000	1.790206000	-0.215562000
C	-2.975011000	-0.305136000	-0.527132000
C	-2.032241000	-2.198784000	0.160907000
C	0.309546000	-2.971480000	0.051969000
C	2.200278000	-2.001375000	-0.607763000
C	2.981452000	0.344854000	-0.570797000
C	2.035266000	2.259171000	0.065051000
C	-0.307898000	3.023045000	-0.027961000
C	-2.196524000	2.035314000	-0.655341000
C	-4.041685000	-1.267020000	-0.324741000
H	-5.089523000	-1.065811000	-0.483543000
C	-3.467424000	-2.417910000	0.140394000
H	-3.961157000	-3.334482000	0.420527000
C	1.247034000	-4.031896000	-0.269439000
H	1.024287000	-5.085871000	-0.212820000
C	2.393679000	-3.436590000	-0.712868000
H	3.286847000	-3.916503000	-1.079416000
C	4.045828000	1.310996000	-0.389685000
H	5.094676000	1.105758000	-0.536175000
C	3.469051000	2.473766000	0.044444000

H	3.963308000	3.395832000	0.305207000
C	-1.255968000	4.076510000	-0.350636000
H	-1.037101000	5.132048000	-0.311118000
C	-2.401727000	3.469075000	-0.775388000
H	-3.300912000	3.937536000	-1.141880000
C	-3.177928000	1.051007000	-0.839931000
C	-1.051991000	-3.188191000	0.333712000
C	3.182813000	-1.023739000	-0.832776000
C	1.055408000	3.249056000	0.235468000
C	-4.543269000	1.452328000	-1.283021000
C	-5.117756000	0.848938000	-2.418997000
H	-4.540628000	0.110432000	-2.965609000
C	-6.405455000	1.195746000	-2.840713000
H	-6.828894000	0.724752000	-3.722679000
C	-7.145308000	2.150886000	-2.131077000
H	-8.144727000	2.420987000	-2.457856000
C	-6.588743000	2.752305000	-0.994726000
H	-7.159634000	3.485093000	-0.432402000
C	-5.301021000	2.403966000	-0.573200000
H	-4.874874000	2.860062000	0.313971000
C	-1.457950000	-4.577446000	0.689853000
C	-2.384458000	-5.306440000	-0.080799000
H	-2.818327000	-4.842837000	-0.959973000
C	-2.729898000	-6.616939000	0.266583000
H	-3.442032000	-7.165291000	-0.342717000
C	-2.149951000	-7.225907000	1.387178000
H	-2.417683000	-8.243182000	1.655648000
C	-1.217132000	-6.516162000	2.154785000
H	-0.760336000	-6.981341000	3.023118000
C	-0.872972000	-5.205824000	1.807217000
H	-0.149850000	-4.652568000	2.397629000
C	4.547148000	-1.443226000	-1.261449000
C	5.137233000	-0.864910000	-2.402838000
H	4.574881000	-0.126788000	-2.965544000
C	6.424818000	-1.230259000	-2.808868000
H	6.859526000	-0.777169000	-3.694694000
C	7.150044000	-2.180548000	-2.078155000
H	8.149259000	-2.465417000	-2.392599000
C	6.579070000	-2.756993000	-0.935924000
H	7.138893000	-3.484864000	-0.356407000
C	5.291931000	-2.389306000	-0.529924000
H	4.855680000	-2.824852000	0.362527000
C	1.462905000	4.643286000	0.568137000
C	2.384560000	5.360106000	-0.219653000
H	2.810509000	4.883571000	-1.095769000
C	2.733102000	6.675407000	0.105732000
H	3.440918000	7.214329000	-0.516875000
C	2.161160000	7.301398000	1.221025000
H	2.431115000	8.322466000	1.472355000
C	1.232979000	6.603876000	2.005328000
H	0.782100000	7.082469000	2.869459000
C	0.885727000	5.288730000	1.679848000
H	0.165931000	4.745182000	2.283178000
H	0.861987000	0.431726000	-2.431288000
C	-0.219383000	-1.232167000	-2.929250000
H	-0.326177000	-1.020487000	-3.999099000
H	-1.148407000	-1.630157000	-2.524474000
H	0.592609000	-1.943534000	-2.748909000

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C	-0.000015000	-0.000121000	2.155835000
C	-0.677237000	-0.072336000	4.350511000
H	-1.383662000	-0.151804000	5.159173000
C	0.677285000	0.071613000	4.350504000
H	1.383743000	0.150852000	5.159160000
C	2.454914000	0.265663000	2.557163000
H	3.122879000	0.103367000	3.407440000
H	2.660246000	-0.470383000	1.780387000
H	2.616175000	1.265489000	2.145539000

C	-2.454939000	-0.266005000	2.557200000
H	-3.122857000	-0.103815000	3.407532000
H	-2.660288000	0.470152000	1.780528000
H	-2.616226000	-1.265773000	2.145460000
N	-1.070689000	-0.109866000	3.008884000
N	1.070691000	0.109433000	3.008876000
N	1.619964000	1.250272000	-0.450107000
N	-1.290030000	1.633043000	-0.353137000
N	-1.619983000	-1.250196000	-0.450163000
N	1.289987000	-1.632998000	-0.353230000
C	2.950292000	0.877306000	-0.545606000
C	1.586639000	2.625414000	-0.254505000
C	-0.893937000	2.956701000	-0.375456000
C	-2.644154000	1.602584000	-0.641598000
C	-2.950319000	-0.877239000	-0.545580000
C	-1.586645000	-2.625334000	-0.254506000
C	0.893923000	-2.956672000	-0.375547000
C	2.644111000	-1.602517000	-0.641672000
C	3.782362000	2.048180000	-0.356386000
H	4.860829000	2.046681000	-0.350025000
C	2.947242000	3.116522000	-0.157982000
H	3.226175000	4.140499000	0.032205000
C	-2.045155000	3.794382000	-0.685939000
H	-2.014999000	4.866810000	-0.797349000
C	-3.113526000	2.963895000	-0.864356000
H	-4.118444000	3.233701000	-1.147876000
C	-3.782373000	-2.048101000	-0.356223000
H	-4.860839000	-2.046613000	-0.349753000
C	-2.947234000	-3.116434000	-0.157838000
H	-3.226149000	-4.140402000	0.032421000
C	2.045167000	-3.794335000	-0.685946000
H	2.015049000	-4.866771000	-0.797298000
C	3.113508000	-2.963814000	-0.864418000
H	4.118439000	-3.233604000	-1.147910000
C	3.437467000	-0.440975000	-0.699159000
C	0.425357000	3.429207000	-0.226723000
C	-3.437516000	0.441051000	-0.699115000
C	-0.425364000	-3.429150000	-0.226790000
C	4.905734000	-0.606680000	-0.901263000
C	5.565465000	0.064527000	-1.949931000
H	4.984182000	0.693678000	-2.615589000
C	6.943669000	-0.081280000	-2.138138000
H	7.433393000	0.438602000	-2.955890000
C	7.689228000	-0.901539000	-1.280958000
H	8.758820000	-1.015518000	-1.427551000
C	7.045773000	-1.574106000	-0.233780000
H	7.616902000	-2.207081000	0.438667000
C	5.667560000	-1.426734000	-0.045459000
H	5.168245000	-1.942810000	0.767918000
C	0.598407000	4.907140000	-0.108144000
C	1.391655000	5.629408000	-1.021065000
H	1.885101000	5.094292000	-1.825204000
C	1.532332000	7.016360000	-0.905030000
H	2.142635000	7.557430000	-1.621741000
C	0.878982000	7.707563000	0.123882000
H	0.987654000	8.784055000	0.213101000
C	0.080811000	7.001905000	1.033871000
H	-0.428817000	7.529881000	1.834194000
C	-0.059123000	5.615047000	0.917251000
H	-0.676621000	5.064477000	1.619345000
C	-4.905769000	0.606762000	-0.901231000
C	-5.56514000	-0.064510000	-1.949859000
H	-4.984235000	-0.693718000	-2.615466000
C	-6.943708000	0.081316000	-2.138096000
H	-7.433435000	-0.438619000	-2.955813000
C	-7.689262000	0.901662000	-1.280994000
H	-8.758848000	1.015660000	-1.427618000
C	-7.045803000	1.574299000	-0.233863000
H	-7.616924000	2.207339000	0.438527000
C	-5.667598000	1.426910000	-0.045510000

H	-5.168290000	1.943026000	0.767844000
C	-0.598409000	-4.907090000	-0.108248000
C	-1.391728000	-5.629313000	-1.021143000
H	-1.885269000	-5.094150000	-1.825194000
C	-1.532366000	-7.016274000	-0.905172000
H	-2.142723000	-7.557321000	-1.621853000
C	-0.878901000	-7.707523000	0.123634000
H	-0.987541000	-8.784024000	0.212797000
C	-0.080652000	-7.001910000	1.033585000
H	0.429061000	-7.529931000	1.833825000
C	0.059251000	-5.615041000	0.917031000
H	0.676816000	-5.064500000	1.619088000
Fe	0.000035000	0.000028000	-0.008243000

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C	-0.000031000	-0.000784000	2.009700000
C	0.679226000	0.050554000	4.209990000
H	1.387202000	0.109351000	5.019353000
C	-0.678934000	-0.054439000	4.210044000
H	-1.386771000	-0.114137000	5.019461000
C	-2.461411000	-0.205132000	2.425988000
H	-3.119953000	0.017040000	3.270608000
H	-2.641054000	0.503722000	1.620001000
H	-2.660869000	-1.214994000	2.057951000
C	2.461382000	0.203409000	2.425773000
H	3.120111000	-0.018602000	3.270287000
H	2.641307000	-0.505172000	1.619598000
H	2.660306000	1.213443000	2.057945000
N	1.071576000	0.077896000	2.867887000
N	-1.071503000	-0.080339000	2.867973000
N	-1.556746000	-1.259666000	-0.453542000
N	1.268234000	-1.537680000	-0.405719000
N	1.556644000	1.260002000	-0.453395000
N	-1.268315000	1.538055000	-0.405410000
C	-2.889458000	-0.936958000	-0.655968000
C	-1.521539000	-2.616389000	-0.155568000
C	0.932108000	-2.875170000	-0.262990000
C	2.617507000	-1.510387000	-0.753722000
C	2.889357000	0.937306000	-0.655781000
C	1.521450000	2.616699000	-0.155224000
C	-0.932192000	2.875530000	-0.262529000
C	-2.617619000	1.510778000	-0.753319000
C	-3.711608000	-2.107259000	-0.443508000
H	-4.787544000	-2.124733000	-0.512985000
C	-2.872111000	-3.132792000	-0.102572000
H	-3.138440000	-4.145582000	0.153456000
C	2.091023000	-3.702904000	-0.538372000
H	2.089902000	-4.781342000	-0.524888000
C	3.116744000	-2.867328000	-0.869800000
H	4.115584000	-3.133110000	-1.175573000
C	3.711516000	2.107563000	-0.443137000
H	4.787449000	2.125041000	-0.512630000
C	2.872024000	3.133058000	-0.102055000
H	3.138367000	4.145809000	0.154115000
C	-2.091132000	3.703283000	-0.537771000
H	-2.090010000	4.781718000	-0.524169000
C	-3.116879000	2.867739000	-0.869173000
H	-4.115744000	3.133542000	-1.174854000
C	-3.395112000	0.353784000	-0.883475000
C	-0.354048000	-3.385243000	-0.031110000
C	3.395021000	-0.353375000	-0.883607000
C	0.353988000	3.385571000	-0.030692000
C	-4.849144000	0.481802000	-1.187392000
C	-5.402229000	-0.196014000	-2.291334000
H	-4.749227000	-0.792427000	-2.919875000
C	-6.767922000	-0.100794000	-2.578281000
H	-7.175555000	-0.624700000	-3.437434000
C	-7.606554000	0.671931000	-1.764175000
H	-8.666434000	0.746455000	-1.986857000

C	-7.069570000	1.346192000	-0.659636000
H	-7.714115000	1.939820000	-0.018410000
C	-5.703707000	1.249909000	-0.372925000
H	-5.287805000	1.764519000	0.486897000
C	-0.470629000	-4.844168000	0.254773000
C	-1.221947000	-5.701648000	-0.572116000
H	-1.727672000	-5.287010000	-1.437430000
C	-1.304357000	-7.070412000	-0.294633000
H	-1.883060000	-7.717841000	-0.946425000
C	-0.633107000	-7.607157000	0.811958000
H	-0.696782000	-8.669470000	1.026398000
C	0.125329000	-6.765845000	1.636604000
H	0.649691000	-7.173948000	2.495362000
C	0.207498000	-5.397459000	1.358535000
H	0.794625000	-4.741814000	1.993261000
C	4.849050000	-0.481333000	-1.187512000
C	5.402172000	0.196720000	-2.291304000
H	4.749179000	0.793273000	-2.919722000
C	6.767864000	0.101551000	-2.578238000
H	7.175518000	0.625635000	-3.437274000
C	7.606479000	-0.671345000	-1.764267000
H	8.666362000	-0.745821000	-1.986937000
C	7.069467000	-1.345821000	-0.659881000
H	7.713987000	-1.939585000	-0.018752000
C	5.703591000	-1.249595000	-0.373185000
H	5.287679000	-1.764393000	0.486523000
C	0.470677000	4.844455000	0.255314000
C	1.222025000	5.701926000	-0.571546000
H	1.727639000	5.287318000	-1.436939000
C	1.304599000	7.070656000	-0.293944000
H	1.883326000	7.718080000	-0.945724000
C	0.633513000	7.607373000	0.812755000
H	0.697328000	8.669655000	1.027298000
C	-0.124921000	6.766060000	1.637404000
H	-0.649153000	7.174141000	2.496252000
C	-0.207253000	5.397708000	1.359221000
H	-0.794366000	4.742060000	1.993962000
Fe	-0.000054000	0.000205000	-0.227704000

'P-2

C	0.000093000	-0.000151000	1.784321000
C	0.657145000	0.167785000	3.987568000
H	1.347129000	0.344962000	4.794419000
C	-0.656581000	-0.168981000	3.987609000
H	-1.346445000	-0.346449000	4.794498000
C	-2.421033000	-0.616274000	2.283215000
H	-2.928706000	-0.973607000	3.183776000
H	-2.947313000	0.253922000	1.885656000
H	-2.416395000	-1.405421000	1.537318000
C	2.421259000	0.615953000	2.283059000
H	2.928918000	0.973383000	3.183588000
H	2.947692000	-0.254135000	1.885454000
H	2.416405000	1.405109000	1.537177000
N	1.046815000	0.269333000	2.649197000
N	-1.046487000	-0.269941000	2.649262000
N	-0.588985000	-1.890474000	-0.342207000
N	1.877139000	-0.590100000	-0.386172000
N	0.588928000	1.890527000	-0.342134000
N	-1.877191000	0.590132000	-0.386086000
C	-1.864498000	-2.360830000	-0.626415000
C	0.175979000	-3.010588000	-0.033155000
C	2.352578000	-1.878496000	-0.184510000
C	2.974893000	0.169582000	-0.786687000
C	1.864422000	2.360891000	-0.626394000
C	-0.176013000	3.010648000	-0.033019000
C	-2.352614000	1.878549000	-0.184388000
C	-2.974956000	-0.169516000	-0.786585000
C	-1.909530000	-3.797271000	-0.436165000
H	-2.789700000	-4.406469000	-0.568168000

C	-0.665385000	-4.191100000	-0.034174000
H	-0.337232000	-5.186180000	0.219017000
C	3.771681000	-1.928940000	-0.473730000
H	4.375644000	-2.821228000	-0.424087000
C	4.143900000	-0.680687000	-0.884214000
H	5.114713000	-0.359350000	-1.225247000
C	1.909456000	3.797338000	-0.436192000
H	2.789615000	4.406541000	-0.568271000
C	0.665355000	4.191149000	-0.034056000
H	0.337215000	5.186224000	0.219177000
C	-3.771712000	1.929009000	-0.473617000
H	-4.375692000	2.821284000	-0.423940000
C	-4.143935000	0.680766000	-0.884150000
H	-5.114754000	0.359473000	-1.225198000
C	-2.978922000	-1.562659000	-0.926501000
C	1.568930000	-3.006013000	0.103251000
C	2.978831000	1.562713000	-0.926545000
C	-1.568960000	3.006050000	0.103416000
C	-4.240141000	-2.258649000	-1.312978000
C	-4.258338000	-3.103839000	-2.439368000
H	-3.349829000	-3.219184000	-3.021223000
C	-5.425532000	-3.781748000	-2.806344000
H	-5.423008000	-4.423969000	-3.681748000
C	-6.595227000	-3.629835000	-2.050128000
H	-7.501461000	-4.155554000	-2.334488000
C	-6.587741000	-2.797999000	-0.922901000
H	-7.487252000	-2.682803000	-0.325719000
C	-5.419792000	-2.120315000	-0.556717000
H	-5.410131000	-1.483443000	0.321484000
C	2.284949000	-4.271817000	0.433409000
C	2.162974000	-5.424003000	-0.366511000
H	1.527478000	-5.389683000	-1.244705000
C	2.862610000	-6.592668000	-0.046441000
H	2.761297000	-7.470441000	-0.677430000
C	3.700651000	-6.628084000	1.075732000
H	4.243691000	-7.535016000	1.322982000
C	3.838567000	-5.484477000	1.873284000
H	4.487779000	-5.502880000	2.743459000
C	3.138634000	-4.316664000	1.552610000
H	3.243267000	-3.427635000	2.166159000
C	4.240040000	2.258765000	-1.313035000
C	4.258174000	3.104026000	-2.439357000
H	3.349658000	3.219365000	-3.021205000
C	5.425333000	3.782034000	-2.806278000
H	5.422792000	4.424316000	-3.681637000
C	6.595030000	3.630137000	-2.050062000
H	7.501226000	4.155940000	-2.334389000
C	6.587600000	2.798221000	-0.922894000
H	7.487113000	2.683058000	-0.325711000
C	5.419687000	2.120442000	-0.556765000
H	5.410048000	1.483499000	0.321389000
C	-2.284957000	4.271865000	0.433623000
C	-2.162965000	5.424065000	-0.366285000
H	-1.527485000	5.389739000	-1.244490000
C	-2.862573000	6.592743000	-0.046193000
H	-2.761261000	7.470520000	-0.677176000
C	-3.700586000	6.628158000	1.076003000
H	-4.243599000	7.535099000	1.323279000
C	-3.838484000	5.484552000	1.873563000
H	-4.487658000	5.502963000	2.743766000
C	-3.138581000	4.316728000	1.552864000
H	-3.243213000	3.427698000	2.166409000
Fe	-0.000014000	0.000024000	-0.154686000

C-H bond activation of methane by species 3

⁶R-3_{hs}

C	0.023608000	-0.018940000	2.021024000
C	-0.652295000	-0.129947000	4.219761000
H	-1.362685000	-0.184633000	5.026886000

C	0.707361000	-0.096148000	4.218239000	H	-7.261059000	0.150393000	-3.247795000
H	1.421300000	-0.108989000	5.023967000	C	-7.552889000	1.427994000	-1.530407000
C	2.502102000	0.030579000	2.466285000	H	-8.603182000	1.608053000	-1.737563000
H	3.128262000	-0.148220000	3.344695000	C	-6.944049000	2.016335000	-0.413973000
H	2.690121000	-0.737235000	1.719637000	H	-7.523659000	2.648668000	0.251755000
H	2.737168000	1.008728000	2.042735000	C	-5.590699000	1.784187000	-0.147409000
C	-2.454209000	-0.100070000	2.470864000	H	-5.119853000	2.232020000	0.721518000
H	-3.074295000	0.091022000	3.351134000	C	-0.953967000	-4.823932000	0.156631000
H	-2.621007000	0.677990000	1.730297000	C	-1.758748000	-5.552849000	-0.740807000
H	-2.717129000	-1.068652000	2.040525000	H	-2.184624000	-5.042402000	-1.597896000
N	-1.049380000	-0.078626000	2.880797000	C	-1.992195000	-6.918053000	-0.543985000
N	1.099144000	-0.029697000	2.878277000	H	-2.609360000	-7.465760000	-1.249627000
N	1.703373000	1.139460000	-0.394266000	C	-1.421444000	-7.580368000	0.550929000
N	-1.186341000	1.725942000	-0.195982000	H	-1.602049000	-8.640058000	0.702476000
N	-1.700445000	-1.129574000	-0.408259000	C	-0.611214000	-6.868584000	1.445422000
N	1.159929000	-1.712876000	-0.252277000	H	-0.164137000	-7.374775000	2.295629000
C	2.988907000	0.670140000	-0.564189000	C	-0.378296000	-5.503537000	1.248331000
C	1.769507000	2.498668000	-0.142135000	H	0.248869000	-4.948275000	1.938178000
C	-0.689419000	3.010152000	-0.132196000	O	0.066798000	0.080659000	-2.175445000
C	-2.522483000	1.802767000	-0.534242000	Co	-0.027279000	0.016008000	-0.254893000
C	-2.992700000	-0.654932000	-0.577435000				
C	-1.775434000	-2.495229000	-0.170238000				
C	0.676789000	-2.997630000	-0.185318000				
C	2.504298000	-1.784535000	-0.578396000				
C	3.912425000	1.770742000	-0.378956000				
H	4.987073000	1.690639000	-0.423005000				
C	3.166491000	2.886388000	-0.092435000				
H	3.529047000	3.875685000	0.136414000				
C	-1.773741000	3.944804000	-0.401762000				
H	-1.667903000	5.017553000	-0.436246000				
C	-2.890801000	3.204519000	-0.669908000				
H	-3.864705000	3.563811000	-0.961520000				
C	-3.914761000	-1.758961000	-0.409256000				
H	-4.989232000	-1.677066000	-0.543994000				
C	-3.172627000	-2.878833000	-0.134112000				
H	-3.538785000	-3.870668000	0.077421000				
C	1.764390000	-3.929875000	-0.452822000				
H	1.662009000	-5.003036000	-0.486868000				
C	2.878568000	-3.185219000	-0.716811000				
H	3.855054000	-3.540433000	-1.004643000				
C	3.368368000	-0.683304000	-0.729561000				
C	0.667848000	3.375571000	-0.006838000				
C	-3.380671000	0.696927000	-0.711480000				
C	-0.678747000	-3.371633000	-0.044879000				
C	4.808230000	-0.946281000	-1.011401000				
C	5.435406000	-0.339701000	-2.117879000				
H	4.846705000	0.299953000	-2.766842000				
C	6.789884000	-0.564978000	-2.383814000				
H	7.254591000	-0.095556000	-3.245419000				
C	7.543291000	-1.398929000	-1.546967000				
H	8.594487000	-1.574138000	-1.753697000				
C	6.932324000	-2.004799000	-0.441165000				
H	7.511115000	-2.645862000	0.216867000				
C	5.577751000	-1.779051000	-0.175216000				
H	5.105405000	-2.240327000	0.685782000				
C	0.949570000	4.827603000	0.188548000				
C	1.754279000	5.549003000	-0.715222000				
H	2.175759000	5.032474000	-1.570771000				
C	1.993086000	6.914212000	-0.525929000				
H	2.609616000	7.456270000	-1.236435000				
C	1.428755000	7.583813000	0.567967000				
H	1.613827000	8.643537000	0.713741000				
C	0.619525000	6.879354000	1.469102000				
H	0.177917000	7.391151000	2.318777000				
C	0.380593000	5.514303000	1.279335000				
H	-0.245627000	4.964465000	1.974299000				
C	-4.819943000	0.962520000	-0.993506000				
C	-5.444754000	0.374828000	-2.111462000				
H	-4.854984000	-0.255116000	-2.768956000				
C	-6.798244000	0.605720000	-0.377630000				

C	-4.167393000	2.432752000	-1.199287000
C	-4.872304000	1.993246000	-2.337591000
H	-4.471965000	1.164367000	-2.911624000
C	-6.061037000	2.618261000	-2.727642000
H	-6.586783000	2.270905000	-3.611746000
C	-6.568463000	3.693428000	-1.985842000
H	-7.490872000	4.178965000	-2.288982000
C	-5.878715000	4.137742000	-0.850139000
H	-6.269526000	4.964894000	-0.265231000
C	-4.690162000	3.512041000	-0.459802000
H	-4.160327000	3.848142000	0.425266000
C	-2.469538000	-4.222602000	0.394845000
C	-3.486185000	-4.669345000	-0.471850000
H	-3.738775000	-4.069413000	-1.339329000
C	-4.148319000	-5.878368000	-0.233310000
H	-4.924744000	-6.210155000	-0.915886000
C	-3.802014000	-6.666324000	0.872382000
H	-4.315491000	-7.605015000	1.056005000
C	-2.783507000	-6.239544000	1.734525000
H	-2.506105000	-6.845877000	2.591500000
C	-2.121731000	-5.030668000	1.495373000
H	-1.330179000	-4.698000000	2.159077000
C	4.167557000	-2.432773000	-1.199320000
C	4.872388000	-1.993408000	-2.337729000
H	4.471952000	-1.164672000	-2.911900000
C	6.061160000	-2.618388000	-2.727720000
H	6.586835000	-2.271150000	-3.611912000
C	6.568716000	-3.693373000	-1.985746000
H	7.491157000	-4.178881000	-2.288837000
C	5.879062000	-4.137537000	-0.849928000
H	6.269984000	-4.964534000	-0.264877000
C	4.690470000	-3.511872000	-0.459653000
H	4.160723000	-3.847840000	0.425516000
C	2.469620000	4.222604000	0.395048000
C	3.485691000	4.669813000	-0.472091000
H	3.737904000	4.070200000	-1.339896000
C	4.147694000	5.878916000	-0.233595000
H	4.923665000	6.211056000	-0.916514000
C	3.801812000	6.666515000	0.872482000
H	4.315180000	7.605274000	1.056068000
C	2.783831000	6.239314000	1.735035000
H	2.506738000	6.845381000	2.592298000
C	2.122182000	5.030360000	1.495922000
H	1.331031000	4.697375000	2.159943000
O	0.000162000	0.000325000	-1.932304000
Co	-0.000020000	0.000369000	-0.233426000

³R-3_h

C	0.000087000	0.000263000	1.813073000
C	-0.667592000	0.123212000	4.009378000
H	-1.369549000	0.248199000	4.815758000
C	0.667953000	-0.122218000	4.009347000
H	1.369980000	-0.247029000	4.815694000
C	2.456647000	-0.429331000	2.293403000
H	2.982839000	-0.817820000	3.169913000
H	2.499109000	-1.159422000	1.491768000
H	2.929080000	0.498826000	1.965195000
C	-2.456430000	0.429956000	2.293519000
H	-2.982531000	0.818710000	3.169968000
H	-2.498945000	1.159822000	1.491682000
H	-2.928916000	-0.498282000	1.965618000
N	-1.059561000	0.197309000	2.670184000
N	1.059807000	-0.196608000	2.670136000
N	1.732708000	0.900754000	-0.312668000
N	-0.901082000	1.740910000	-0.271177000
N	-1.732741000	-0.900853000	-0.312225000
N	0.901051000	-1.740990000	-0.270714000
C	2.925585000	0.334828000	-0.708320000
C	2.003665000	2.193764000	0.098977000

C	-0.325390000	2.955841000	0.026023000
C	-2.165076000	1.997726000	-0.778196000
C	-2.925658000	-0.335054000	-0.707944000
C	-2.003661000	-2.193726000	0.099869000
C	0.325388000	-2.955821000	0.026955000
C	2.164993000	-1.997973000	-0.777775000
C	3.994610000	1.289144000	-0.498197000
H	5.035790000	1.095384000	-0.702339000
C	3.435481000	2.413795000	0.045737000
H	3.936320000	3.316354000	0.356117000
C	-1.262555000	4.018492000	-0.283328000
H	-1.055017000	5.070090000	-0.163032000
C	-2.373064000	3.431716000	-0.822501000
H	-3.251598000	3.916134000	-1.216568000
C	-3.994662000	-1.289307000	-0.497429000
H	-5.035859000	-1.095617000	-0.701548000
C	-3.435481000	-2.413777000	0.046826000
H	-3.936289000	-3.316239000	0.357540000
C	1.262518000	-4.018575000	-0.282142000
H	1.054988000	-5.070133000	-0.161475000
C	2.372959000	-3.431982000	-0.821653000
H	3.251437000	-3.916536000	-1.215675000
C	3.128953000	-1.016001000	-1.037761000
C	1.026485000	3.168565000	0.347147000
C	-3.129055000	1.015671000	-1.037783000
C	-1.026454000	-3.168439000	0.348282000
C	4.466985000	-1.401726000	-1.562520000
C	4.956798000	-0.782452000	-2.729489000
H	4.331869000	-0.053563000	-3.234593000
C	6.218930000	-1.110055000	-3.235175000
H	6.577214000	-0.629813000	-4.140489000
C	7.015979000	-2.058376000	-2.580290000
H	7.995405000	-2.313196000	-2.973070000
C	6.543535000	-2.673443000	-1.413530000
H	7.160422000	-3.400142000	-0.893560000
C	5.281145000	-2.345897000	-0.907376000
H	4.922269000	-2.809659000	0.005260000
C	1.418230000	4.531797000	0.798012000
C	2.343702000	5.319469000	0.085890000
H	2.782686000	4.924484000	-0.823530000
C	2.673716000	6.605555000	0.526602000
H	3.383783000	7.201784000	-0.038272000
C	2.079539000	7.130189000	1.681962000
H	2.335739000	8.128757000	2.022051000
C	1.145907000	6.362273000	2.390210000
H	0.676776000	6.763277000	3.283534000
C	0.816286000	5.076406000	1.949730000
H	0.093098000	4.477352000	2.493805000
C	-4.467138000	1.401248000	-1.562521000
C	-4.957122000	0.781560000	-2.729198000
H	-4.332287000	0.052454000	-3.234106000
C	-6.219306000	1.109027000	-3.234844000
H	-6.577727000	0.628461000	-4.139931000
C	-7.016231000	2.057627000	-2.580210000
H	-7.995696000	2.312341000	-2.972960000
C	-6.543611000	2.673112000	-1.413742000
H	-7.160399000	3.400035000	-0.893969000
C	-5.281169000	2.345702000	-0.907628000
H	-4.922150000	2.809799000	0.004782000
C	-1.418146000	-4.531515000	0.799667000
C	-2.343671000	-5.319451000	0.087909000
H	-2.782743000	-4.924795000	-0.821612000
C	-2.673628000	-6.605385000	0.529110000
H	-3.383737000	-7.201826000	-0.035487000
C	-2.079341000	-7.129597000	1.684604000
H	-2.335498000	-8.128046000	2.025074000
C	-1.145656000	-6.361416000	2.392495000
H	-0.676440000	-6.762094000	3.285920000
C	-0.816090000	-5.075702000	1.951525000
H	-0.092861000	-4.476442000	2.495317000

O	-0.000102000	-0.000326000	-2.100013000
Co	-0.000014000	-0.000037000	-0.245467000

⁶RC-3_{hs}

Co	0.051281000	0.074313000	-0.155602000
O	0.071792000	0.018317000	-2.079602000
C	0.137289000	0.032231000	2.113498000
C	-0.414181000	0.376418000	4.321998000
H	-0.983664000	0.783702000	5.139798000
C	0.662488000	-0.454462000	4.300798000
H	1.224682000	-0.912148000	5.096698000
C	2.105299000	-1.486368000	2.522198000
H	2.519301000	-1.989284000	3.400298000
H	1.752750000	-2.227240000	1.807498000
H	2.877774000	-0.874310000	2.053698000
C	-1.827917000	1.533530000	2.598098000
H	-2.156031000	2.091363000	3.479598000
H	-1.487158000	2.226299000	1.832698000
H	-2.659697000	0.944760000	2.205398000
N	-0.716240000	0.664557000	2.988198000
N	0.982729000	-0.652297000	2.954598000
N	2.098923000	-0.132569000	-0.354102000
N	0.213161000	2.129246000	-0.135102000
N	-1.970449000	0.218801000	-0.241402000
N	-0.098292000	-2.020117000	-0.120602000
C	2.804162000	-1.303826000	-0.530502000
C	3.005815000	0.887716000	-0.128702000
C	1.405320000	2.822889000	-0.116902000
C	-0.789219000	3.015242000	-0.476302000
C	-2.689888000	1.389454000	-0.428802000
C	-2.873542000	-0.796083000	0.044498000
C	-1.276050000	-2.718958000	-0.014302000
C	0.892191000	-2.916715000	-0.486802000
C	4.216504000	-1.022837000	-0.374202000
H	5.003254000	-1.758577000	-0.428502000
C	4.338531000	0.316487000	-0.099302000
H	5.244820000	0.862972000	0.107498000
C	1.136335000	4.221834000	-0.419502000
H	1.888278000	4.991388000	-0.493002000
C	-0.203988000	4.334561000	-0.662402000
H	-0.745468000	5.215251000	-0.968702000
C	-4.094330000	1.104968000	-0.219702000
H	-4.885079000	1.836906000	-0.267802000
C	-4.203659000	-0.224855000	0.097898000
H	-5.102348000	-0.767438000	0.343998000
C	-1.023763000	-4.125006000	-0.300302000
H	-1.777706000	-4.896260000	-0.311702000
C	0.300761000	-4.241536000	-0.613402000
H	0.827242000	-5.128529000	-0.927602000
C	2.249726000	-2.598239000	-0.679002000
C	2.696134000	2.263453000	-0.008302000
C	-2.153851000	2.682763000	-0.614102000
C	-2.561463000	-2.162620000	0.172898000
C	3.200051000	-3.702845000	-0.990702000
C	4.045233000	-3.614172000	-2.114902000
H	3.974155000	-2.740687000	-2.754302000
C	4.951742000	-4.637388000	-2.410102000
H	5.588725000	-4.556058000	-3.285402000
C	5.032872000	-5.766971000	-1.584802000
H	5.736134000	-6.561428000	-1.814302000
C	4.201492000	-5.864941000	-0.461302000
H	4.264069000	-6.733028000	0.187798000
C	3.294783000	-4.841626000	-0.166402000
H	2.656998000	-4.912356000	0.708498000
C	3.826038000	3.225383000	0.144098000
C	4.891030000	3.263100000	-0.777502000
H	4.884771000	2.573899000	-1.614902000
C	5.931542000	4.186012000	-0.629102000
H	6.740138000	4.206177000	-1.353302000

C	5.924858000	5.090411000	0.441198000
H	6.732312000	5.806976000	0.555098000
C	4.867462000	5.068195000	1.360198000
H	4.854620000	5.765793000	2.192098000
C	3.826850000	4.145683000	1.211198000
H	3.005354000	4.125716000	1.919898000
C	-3.119075000	3.777267000	-0.916002000
C	-3.998252000	3.664587000	-2.011602000
H	-3.944371000	2.778798000	-2.635602000
C	-4.917359000	4.679200000	-2.297802000
H	-5.581638000	4.578564000	-3.150602000
C	-4.975592000	5.825088000	-1.493402000
H	-5.688153000	6.613043000	-1.716302000
C	-4.108817000	5.947765000	-0.399402000
H	-4.152997000	6.828956000	0.233598000
C	-3.190510000	4.932452000	-0.112602000
H	-2.525329000	5.022188000	0.739998000
C	-3.676767000	-3.125247000	0.405298000
C	-4.778352000	-3.197572000	-0.469902000
H	-4.806486000	-2.540678000	-1.331602000
C	-5.804764000	-4.122181000	-0.248702000
H	-6.642954000	-4.170252000	-0.937202000
C	-5.746586000	-4.992469000	0.847798000
H	-6.543340000	-5.709932000	1.018098000
C	-4.650898000	-4.936246000	1.719598000
H	-4.597361000	-5.608535000	2.570498000
C	-3.624186000	-4.012637000	1.497898000
H	-2.772395000	-3.966863000	2.168898000
C	-2.770071000	-1.633562000	-3.184302000
H	-1.788654000	-1.226962000	-2.922002000
H	-3.546303000	-0.989921000	-2.755402000
H	-2.879764000	-1.669485000	-4.274002000
H	-2.864765000	-2.643082000	-2.770902000

⁴RC-3_{is}

Co	0.075098000	0.007598000	-0.139397000
O	0.031398000	0.012297000	-1.841297000
C	0.140498000	0.004898000	1.969603000
C	-0.070804000	0.621897000	4.174103000
H	-0.340206000	1.271696000	4.988503000
C	0.480500000	-0.617601000	4.156503000
H	0.796402000	-1.269500000	4.952303000
C	1.177505000	-2.276199000	2.441803000
H	1.225106000	-2.893199000	3.343403000
H	0.540206000	-2.758101000	1.708303000
H	2.181304000	-2.150896000	2.033903000
C	-0.864509000	2.286195000	2.507903000
H	-0.851411000	2.902895000	3.410903000
H	-0.274310000	2.766297000	1.734803000
H	-1.893109000	2.164492000	2.165703000
N	-0.271505000	0.988997000	2.842303000
N	0.603201000	-0.981201000	2.814403000
N	1.778201000	-1.016697000	-0.235097000
N	1.138592000	1.820901000	-0.094397000
N	-1.631805000	1.029293000	-0.117997000
N	-0.987297000	-1.804906000	-0.033397000
C	1.894605000	-2.363397000	-0.529897000
C	3.047699000	-0.512594000	0.002903000
C	2.503392000	1.925405000	-0.032397000
C	0.635589000	3.031899000	-0.520197000
C	-1.769209000	2.372592000	-0.414997000
C	-2.882204000	0.526389000	0.205503000
C	-2.345397000	-1.909410000	0.119703000
C	-0.513893000	-3.016704000	-0.488797000
C	3.291406000	-2.736293000	-0.413497000
H	3.673009000	-3.734992000	-0.553997000
C	3.989903000	-1.616391000	-0.051797000
H	5.046702000	-1.538488000	0.145703000
C	2.890388000	3.284906000	-0.388897000

H	3.906387000	3.644809000	-0.436497000	C	-0.800965000	-0.327860000	4.083053000
C	1.744286000	3.955503000	-0.718697000	H	-1.428201000	-0.715285000	4.867314000
H	1.654783000	4.966302000	-1.083797000	C	0.335556000	0.413946000	4.123680000
C	-3.156410000	2.744888000	-0.213497000	H	0.897395000	0.813183000	4.950407000
H	-3.547913000	3.741887000	-0.337697000	C	1.913944000	1.410383000	2.465327000
C	-3.827607000	1.627486000	0.203803000	H	2.523327000	1.499105000	3.369119000
H	-4.869807000	1.548183000	0.467103000	H	2.483569000	0.903448000	1.693248000
C	-2.756093000	-3.266711000	-0.215197000	H	1.631935000	2.405454000	2.115441000
H	-3.773391000	-3.625514000	-0.197897000	C	-2.240208000	-1.350010000	2.317411000
C	-1.634091000	-3.938507000	-0.617697000	H	-2.918648000	-1.429058000	3.171485000
H	-1.569088000	-4.949307000	-0.987897000	H	-2.747885000	-0.853842000	1.496590000
C	0.845108000	-3.288800000	-0.737397000	H	-1.930759000	-2.348709000	2.002916000
C	3.397995000	0.847607000	0.140703000	N	-1.081789000	-0.554370000	2.733122000
C	-0.736012000	3.299095000	-0.690697000	N	0.725062000	0.620530000	2.797743000
C	-3.224800000	-0.832812000	0.357603000	N	0.587350000	1.853680000	-0.203494000
C	1.226212000	-4.661399000	-1.172897000	N	-1.907707000	0.662292000	-0.244989000
C	2.004112000	-4.846697000	-2.333197000	N	-0.702010000	-1.832222000	-0.229512000
H	2.303910000	-3.975396000	-2.905697000	N	1.790718000	-0.639939000	-0.088666000
C	2.375416000	-6.129796000	-2.747497000	C	1.859398000	2.254485000	-0.552722000
H	2.968516000	-6.253894000	-3.648397000	C	-0.116194000	2.985905000	0.169686000
C	1.977319000	-7.251997000	-2.008697000	C	-2.330495000	1.944116000	0.026725000
H	2.264722000	-8.247996000	-2.331097000	C	-2.984865000	-0.019600000	-0.788271000
C	1.207219000	-7.080999000	-0.850997000	C	-1.943220000	-2.238842000	-0.671526000
H	0.902021000	-7.944700000	-0.267897000	C	-0.029927000	-2.958554000	0.212035000
C	0.837115000	-5.797500000	-0.435997000	C	2.190081000	-1.918659000	0.230781000
H	0.250215000	-5.663202000	0.466503000	C	2.909611000	0.037082000	-0.545806000
C	4.832194000	1.207212000	0.339903000	C	1.975723000	3.684161000	-0.354702000
C	5.835696000	0.792915000	-0.557597000	H	2.874518000	4.253891000	-0.530077000
H	5.557697000	0.190114000	-1.415097000	C	0.777880000	4.126149000	0.138432000
C	7.168794000	1.169018000	-0.361397000	H	0.513327000	5.130053000	0.428118000
H	7.928195000	0.846221000	-1.067097000	C	-3.728789000	2.074090000	-0.335462000
C	7.521992000	1.971420000	0.731603000	H	-4.301706000	2.983256000	-0.243003000
H	8.556591000	2.263723000	0.882403000	C	-4.115959000	0.882246000	-0.880948000
C	6.530991000	2.401417000	1.623803000	H	-5.072566000	0.630591000	-1.309105000
H	6.795489000	3.026917000	2.471003000	C	-2.075635000	-3.665397000	-0.462023000
C	5.198192000	2.025313000	1.426903000	H	-2.958276000	-4.238350000	-0.698149000
H	4.426391000	2.358810000	2.113103000	C	-0.919109000	-4.099757000	0.127214000
C	-1.147416000	4.664994000	-1.118897000	H	-0.677740000	-5.099394000	0.449967000
C	-1.993416000	4.831091000	-2.233897000	C	3.614200000	-2.050181000	-0.010830000
H	-2.322514000	3.950691000	-2.775697000	H	4.177453000	-2.957923000	0.137487000
C	-2.393920000	6.106890000	-2.643197000	C	4.045006000	-0.863558000	-0.533548000
H	-3.039620000	6.216088000	-3.509097000	H	5.032049000	-0.616013000	-0.888133000
C	-1.957823000	7.240792000	-1.944697000	C	2.947781000	1.408135000	-0.823560000
H	-2.267826000	8.231091000	-2.263297000	C	-1.503719000	3.028908000	0.366591000
C	-1.120223000	7.088694000	-0.831997000	C	-3.004317000	-1.396142000	-1.043573000
H	-0.785326000	7.961495000	-0.279697000	C	1.338398000	-2.999034000	0.516482000
C	-0.720819000	5.812495000	-0.421697000	C	4.203723000	2.037706000	-1.311715000
H	-0.082019000	5.692997000	0.447003000	C	4.177356000	2.799149000	-2.497123000
C	-4.647399000	-1.191316000	0.628303000	H	3.242393000	2.886234000	-3.039943000
C	-5.689000000	-0.780319000	-0.226497000	C	5.338086000	3.415950000	-2.974835000
H	-5.446002000	-0.187219000	-1.100597000	H	5.302139000	3.990932000	-3.894919000
C	-7.011899000	-1.156223000	0.030503000	C	6.544347000	3.286313000	-2.273718000
H	-7.801900000	-0.836926000	-0.642297000	H	7.445756000	3.763682000	-2.645189000
C	-7.316096000	-1.953624000	1.141803000	C	6.580309000	2.539461000	-1.089041000
H	-8.342996000	-2.245227000	1.339603000	H	7.508615000	2.444155000	-0.533941000
C	-6.286595000	-2.379921000	1.991103000	C	5.419201000	1.922797000	-0.610507000
H	-6.513293000	-3.001922000	2.851703000	H	5.443408000	1.358779000	0.315865000
C	-4.963696000	-2.005217000	1.733403000	C	-2.168757000	4.295231000	0.778333000
H	-4.162295000	-2.336415000	2.386003000	C	-2.007539000	5.494637000	0.057609000
C	-3.213102000	-0.207612000	-2.988497000	H	-1.383087000	5.497154000	-0.828848000
H	-2.157101000	-0.284809000	-2.713097000	C	-2.665758000	6.661954000	0.459231000
H	-3.315302000	-0.192812000	-4.079397000	H	-2.535901000	7.575992000	-0.112092000
H	-3.754799000	-1.067014000	-2.579597000	C	-3.502085000	6.649875000	1.583290000
H	-3.622104000	0.716787000	-2.565497000	H	-4.013020000	7.556194000	1.893040000
²RC-3_h				C	-3.682445000	5.459228000	2.299368000
Co	-0.061286000	0.011437000	-0.143350000	H	-4.333037000	5.439892000	3.168428000
O	0.004218000	-0.001090000	-2.000769000	C	-3.024204000	4.292322000	1.897905000
C	-0.143554000	0.026672000	1.909339000	H	-3.161909000	3.366809000	2.447768000
				C	-4.222947000	-2.034729000	-1.610601000
				C	-4.112934000	-2.825955000	-2.771201000

H	-3.140823000	-2.930363000	-3.241374000
C	-5.237494000	-3.454736000	-3.315265000
H	-5.136562000	-4.053650000	-4.215085000
C	-6.490778000	-3.307952000	-2.706007000
H	-7.363775000	-3.795474000	-3.128691000
C	-6.610587000	-2.531383000	-1.546152000
H	-7.576060000	-2.422828000	-1.061310000
C	-5.485838000	-1.902721000	-1.001339000
H	-5.575474000	-1.315966000	-0.093310000
C	1.967689000	-4.260861000	0.993156000
C	1.862503000	-5.467881000	0.274863000
H	1.310447000	-5.479758000	-0.658359000
C	2.485042000	-6.631166000	0.740053000
H	2.399624000	-7.551228000	0.170028000
C	3.229598000	-6.607426000	1.926695000
H	3.713078000	-7.510613000	2.285723000
C	3.354523000	-5.409084000	2.641775000
H	3.934468000	-5.380500000	3.559248000
C	2.731762000	-4.246260000	2.176854000
H	2.826886000	-3.314819000	2.725682000
C	2.879990000	-0.492823000	-3.844184000
H	1.947620000	-0.269127000	-3.312605000
H	3.375372000	-1.340239000	-3.356737000
H	2.666070000	-0.745048000	-4.889624000
H	3.545278000	0.377532000	-3.807583000

⁶TS1-3_{hs}

Co	0.042759000	0.060378000	-0.280757000
O	0.029027000	0.030973000	-2.180650000
C	0.023795000	0.037326000	2.065255000
C	0.694118000	-0.140152000	4.264160000
H	1.389694000	-0.317121000	5.066627000
C	-0.621503000	0.200263000	4.272576000
H	-1.307505000	0.374177000	5.083899000
C	-2.377484000	0.659248000	2.548695000
H	-2.893862000	1.046619000	3.431642000
H	-2.346962000	1.425998000	1.779357000
H	-2.910324000	-0.214075000	2.167763000
C	2.436419000	-0.563127000	2.516548000
H	2.983237000	-0.903759000	3.400272000
H	2.414600000	-1.355355000	1.773179000
H	2.932831000	0.312627000	2.094842000
N	1.068722000	-0.235723000	2.920727000
N	-1.010675000	0.306450000	2.934044000
N	-1.898787000	-0.657759000	-0.225764000
N	0.766030000	-1.882368000	-0.153627000
N	1.955518000	0.754860000	-0.288031000
N	-0.694610000	1.978232000	-0.196193000
C	-3.035703000	0.087979000	-0.436481000
C	-2.278896000	-1.953502000	0.061100000
C	-0.007095000	-3.015459000	-0.022424000
C	2.041678000	-2.273429000	-0.508855000
C	3.093794000	-0.003484000	-0.492794000
C	2.345874000	2.060633000	-0.058198000
C	0.075570000	3.116597000	-0.122312000
C	-1.986436000	2.358405000	-0.527686000
C	-4.194888000	-0.764561000	-0.238960000
H	-5.221099000	-0.440498000	-0.311918000
C	-3.731017000	-2.010503000	0.095742000
H	-4.314610000	-2.884248000	0.337698000
C	0.821492000	-4.179804000	-0.297995000
H	0.473571000	-5.200786000	-0.289480000
C	2.070696000	-3.722952000	-0.620744000
H	2.926166000	-4.305841000	-0.922410000
C	4.255190000	0.854299000	-0.337173000
H	5.279928000	0.526103000	-0.412201000
C	3.798981000	2.111606000	-0.042061000
H	4.388001000	2.991524000	0.161267000
C	-0.764482000	4.271452000	-0.404854000

H	-0.417102000	5.292040000	-0.438741000
C	-2.020095000	3.804861000	-0.678493000
H	-2.884128000	4.377939000	-0.974344000
C	-3.084658000	1.486161000	-0.654591000
C	-1.405255000	-3.056659000	0.180059000
C	3.141295000	-1.401374000	-0.675082000
C	1.478083000	3.167963000	0.045896000
C	-4.421056000	2.070855000	-0.963242000
C	-5.162875000	1.600139000	-2.064539000
H	-4.734887000	0.823100000	-2.688979000
C	-6.424184000	2.129648000	-2.355918000
H	-6.978135000	1.760596000	-3.213621000
C	-6.968622000	3.137753000	-1.549183000
H	-7.947301000	3.549292000	-1.775597000
C	-6.242997000	3.610974000	-0.448091000
H	-6.661286000	4.386239000	0.186710000
C	-4.981744000	3.080781000	-0.156960000
H	-4.422100000	3.439836000	0.700369000
C	-2.001807000	-4.403774000	0.416438000
C	-2.966155000	-4.941713000	-0.458116000
H	-3.277603000	-4.358916000	-1.318348000
C	-3.502413000	-6.214191000	-0.234481000
H	-4.240099000	-6.616042000	-0.922352000
C	-3.080649000	-6.973387000	0.865086000
H	-3.496592000	-7.961075000	1.038128000
C	-2.114429000	-6.453234000	1.736335000
H	-1.781159000	-7.035996000	2.589700000
C	-1.577835000	-5.181049000	1.511806000
H	-0.828268000	-4.774583000	2.182953000
C	4.471013000	-1.997264000	-0.990640000
C	5.196589000	-1.553647000	-2.113924000
H	4.761039000	-0.788593000	-2.747892000
C	6.451068000	-2.094814000	-2.413606000
H	6.992688000	-1.746457000	-3.287680000
C	7.004413000	-3.087676000	-1.594117000
H	7.977753000	-3.508157000	-1.827126000
C	6.294743000	-3.533992000	-0.471533000
H	6.720310000	-4.296985000	0.173264000
C	5.040425000	-2.992295000	-0.171881000
H	4.493716000	-3.330344000	0.702216000
C	2.077773000	4.520242000	0.241801000
C	3.036629000	5.036621000	-0.651557000
H	3.340981000	4.434629000	-1.500943000
C	3.577568000	6.312488000	-0.460157000
H	4.310811000	6.696894000	-1.162624000
C	3.166106000	7.097427000	0.625108000
H	3.585569000	8.087788000	0.772677000
C	2.205521000	6.599055000	1.515034000
H	1.880053000	7.201330000	2.357855000
C	1.664966000	5.323248000	1.323178000
H	0.920066000	4.933966000	2.009687000
C	-1.320003000	-1.917453000	-3.074466000
H	-0.592983000	-0.851683000	-2.625306000
H	-1.161547000	-1.880661000	-4.153768000
H	-2.333463000	-1.688165000	-2.744875000
H	-0.859210000	-2.764350000	-2.566574000

⁴TS1-3_{is}

Co	-0.052782000	-0.000069000	-0.130805000
C	-0.119568000	0.002253000	2.000851000
C	-0.460331000	0.612176000	4.192253000
H	-0.779451000	1.258222000	4.991703000
C	0.100182000	-0.623731000	4.203328000
H	0.375237000	-1.275425000	5.014470000
C	0.905882000	-2.268961000	2.516607000
H	0.905298000	-2.897165000	3.411840000
H	0.316595000	-2.745284000	1.739921000
H	1.930767000	-2.131925000	2.168462000
C	-1.168350000	2.270927000	2.474958000

H	-1.216418000	2.892956000	3.373185000
H	-0.534524000	2.750546000	1.736209000
H	-2.172457000	2.139798000	2.068748000
N	-0.587797000	0.980096000	2.850995000
N	0.301385000	-0.982155000	2.868456000
N	1.652761000	-0.988059000	-0.126870000
N	1.006142000	1.829108000	-0.025005000
N	-1.752205000	0.989054000	-0.206069000
N	-1.096207000	-1.824058000	-0.103786000
C	1.804167000	-2.334452000	-0.421240000
C	2.906968000	-0.477867000	0.188720000
C	2.363091000	1.953179000	0.105642000
C	0.511907000	3.030318000	-0.482386000
C	-1.883268000	2.333013000	-0.508067000
C	-3.017199000	0.477229000	0.033236000
C	-2.457902000	-1.949866000	-0.021741000
C	-0.585315000	-3.029506000	-0.529822000
C	3.194428000	-2.693556000	-0.230685000
H	3.592790000	-3.687727000	-0.355476000
C	3.859710000	-1.570149000	0.179327000
H	4.902611000	-1.482990000	0.437023000
C	2.754326000	3.313030000	-0.244530000
H	3.767282000	3.684790000	-0.243829000
C	1.617036000	3.967475000	-0.633714000
H	1.532393000	4.975273000	-1.008454000
C	-3.284105000	2.694117000	-0.391887000
H	-3.674336000	3.688825000	-0.536458000
C	-3.971272000	1.570984000	-0.023469000
H	-5.026875000	1.482666000	0.175231000
C	-2.832863000	-3.314108000	-0.372674000
H	-3.844740000	-3.687070000	-0.406307000
C	-1.682318000	-3.969741000	-0.715779000
H	-1.582657000	-4.979975000	-1.080045000
C	0.787821000	-3.276542000	-0.701540000
C	3.251580000	0.881996000	0.332402000
C	-0.852171000	3.275774000	-0.723363000
C	-3.360309000	-0.884244000	0.167506000
C	1.217878000	-4.637168000	-1.129115000
C	2.053429000	-4.796232000	-2.252628000
H	2.362767000	-3.914020000	-2.803219000
C	2.468701000	-6.067633000	-2.660970000
H	3.106270000	-6.171405000	-3.533608000
C	2.057195000	-7.204652000	-1.952730000
H	2.378454000	-8.191754000	-2.270316000
C	1.229430000	-7.059818000	-0.831762000
H	0.913016000	-7.935000000	-0.272346000
C	0.815638000	-5.787728000	-0.422730000
H	0.183736000	-5.673377000	0.451682000
C	4.675557000	1.248176000	0.584424000
C	5.711486000	0.837476000	-0.277318000
H	5.466063000	0.228809000	-1.140831000
C	7.034583000	1.223778000	-0.038462000
H	7.819561000	0.903265000	-0.716655000
C	7.345176000	2.033341000	1.062293000
H	8.372044000	2.333543000	1.246479000
C	6.321766000	2.459947000	1.918738000
H	6.553335000	3.091023000	2.771420000
C	4.998826000	2.073884000	1.678920000
H	4.202099000	2.405320000	2.336948000
C	-1.256592000	4.637575000	-1.171584000
C	-2.034808000	4.797649000	-2.335495000
H	-2.319466000	3.914904000	-2.898132000
C	-2.424623000	6.070337000	-2.764584000
H	-3.017962000	6.175545000	-3.667708000
C	-2.045027000	7.206670000	-2.037559000
H	-2.347120000	8.194535000	-2.371325000
C	-1.274456000	7.060441000	-0.876665000
H	-0.983658000	7.935160000	-0.302761000
C	-0.885571000	5.787355000	-0.446891000
H	-0.297901000	5.671757000	0.457738000

C	-4.789582000	-1.256198000	0.377547000
C	-5.802757000	-0.854126000	-0.514528000
H	-5.535857000	-0.250871000	-1.375327000
C	-7.130739000	-1.242931000	-0.308683000
H	-7.897909000	-0.929417000	-1.010118000
C	-7.468933000	-2.045906000	0.788754000
H	-8.499618000	-2.347861000	0.947060000
C	-6.467986000	-2.463730000	1.675497000
H	-6.720781000	-3.089690000	2.525953000
C	-5.140208000	-2.075182000	1.468852000
H	-4.360601000	-2.399422000	2.150679000
O	-0.069406000	0.107035000	-1.934573000
C	2.256445000	-0.046080000	-2.966009000
H	0.947707000	-0.029156000	-2.400850000
H	2.043312000	0.072620000	-4.029064000
H	2.660554000	-1.012276000	-2.667026000
H	2.710522000	0.815981000	-2.478097000

²TS1-3_k

Co	-0.046700000	-0.001655000	-0.149265000
O	-0.066975000	0.008172000	-2.036199000
C	-0.118203000	-0.019507000	1.899236000
C	-0.368879000	0.619238000	4.092833000
H	-0.579230000	1.302437000	4.897551000
C	-0.032486000	-0.696208000	4.094064000
H	0.118555000	-1.392860000	4.900554000
C	0.507615000	-2.435174000	2.386378000
H	0.359938000	-3.076585000	3.259797000
H	-0.115907000	-2.785973000	1.570185000
H	1.555838000	-2.466405000	2.082848000
C	-0.770887000	2.389129000	2.378330000
H	-0.647753000	3.023849000	3.260500000
H	-0.108713000	2.731541000	1.590005000
H	-1.805358000	2.439653000	2.032016000
N	-0.415087000	1.018087000	2.754500000
N	0.115595000	-1.072151000	2.756248000
N	1.502824000	-1.188523000	-0.162395000
N	1.144845000	1.551194000	-0.131942000
N	-1.594938000	1.185325000	-0.238437000
N	-1.237261000	-1.553906000	-0.219329000
C	1.511629000	-2.499838000	-0.584625000
C	2.777842000	-0.886467000	0.281014000
C	2.481290000	1.546418000	0.201666000
C	0.855653000	2.799361000	-0.660232000
C	-1.580424000	2.499946000	-0.645009000
C	-2.890846000	0.879497000	0.130209000
C	-2.588136000	-1.550978000	0.039457000
C	-0.919562000	-2.797972000	-0.737514000
C	2.827716000	-3.060523000	-0.359200000
H	3.103903000	-4.079715000	-0.578739000
C	3.592515000	-2.083716000	0.220196000
H	4.616554000	-2.155041000	0.548871000
C	3.055862000	2.839975000	-0.110629000
H	4.093062000	3.098508000	0.033327000
C	2.068408000	3.591749000	-0.685921000
H	2.147028000	4.587791000	-1.090275000
C	-2.905990000	3.062983000	-0.477727000
H	-3.167858000	4.086093000	-0.696643000
C	-3.700487000	2.081290000	0.048142000
H	-4.739674000	2.150535000	0.325723000
C	-3.145094000	-2.845580000	-0.306186000
H	-4.188573000	-3.104456000	-0.219448000
C	-2.128725000	-3.593572000	-0.830344000
H	-2.184202000	-4.587880000	-1.242715000
C	0.385735000	-3.250487000	-0.963984000
C	3.239794000	0.412165000	0.539265000
C	-0.436598000	3.253673000	-0.955458000
C	-3.363925000	-0.421501000	0.354180000
C	0.620983000	-4.615040000	-1.508656000

C	1.424257000	-4.773204000	-2.655357000	N	2.052515000	0.495339000	-0.342213000
H	1.833551000	-3.888465000	-3.131477000	N	-0.445901000	2.030268000	-0.223525000
C	1.678742000	-6.044890000	-3.178807000	C	-3.001009000	0.452271000	-0.443364000
H	2.292424000	-6.147953000	-4.068420000	C	-2.491673000	-1.651546000	0.116968000
C	1.139068000	-7.181598000	-2.562233000	C	-0.369408000	-2.983696000	0.023263000
H	1.335791000	-8.168707000	-2.968920000	C	1.748455000	-2.510409000	-0.523664000
C	0.346909000	-7.037482000	-1.415761000	C	3.078228000	-0.392230000	-0.562672000
H	-0.064808000	-7.914273000	-0.925112000	C	2.596833000	1.736412000	-0.095197000
C	0.092576000	-5.765535000	-0.891776000	C	0.466408000	3.059621000	-0.139780000
H	-0.506390000	-5.655339000	0.005903000	C	-1.673378000	2.567393000	-0.570158000
C	4.636894000	0.637265000	1.000849000	C	-4.251723000	-0.242758000	-0.190381000
C	5.746914000	0.145212000	0.286865000	H	-5.230859000	0.205723000	-0.251661000
H	5.579571000	-0.413756000	-0.627120000	C	-3.937954000	-1.524163000	0.182225000
C	7.049346000	0.397689000	0.730710000	H	-4.618753000	-2.310942000	0.465572000
H	7.893715000	0.016815000	0.164351000	C	0.302846000	-4.245105000	-0.248182000
C	7.265733000	1.152560000	1.891103000	H	-0.170048000	-5.213856000	-0.212596000
H	8.276920000	1.348829000	2.233757000	C	1.590603000	-3.953172000	-0.606728000
C	6.169894000	1.660891000	2.600859000	H	2.359481000	-4.643459000	-0.914698000
H	6.329027000	2.251837000	3.497730000	C	4.343099000	0.312775000	-0.4111031000
C	4.867752000	1.408089000	2.157124000	H	5.317726000	-0.140808000	-0.499430000
H	4.015278000	1.801759000	2.701363000	C	4.048717000	1.611127000	-0.094348000
C	-0.641309000	4.620021000	-1.507449000	H	4.742468000	2.409995000	0.113178000
C	-1.389181000	4.780620000	-2.690904000	C	-0.219531000	4.309772000	-0.429535000
H	-1.778796000	3.896845000	-3.185005000	H	0.253966000	5.278333000	-0.456944000
C	-1.614182000	6.053173000	-3.225630000	C	-1.520674000	4.005452000	-0.720347000
H	-2.185257000	6.158193000	-4.142951000	H	-2.302012000	4.683154000	-1.024861000
C	-1.099970000	7.188099000	-2.584418000	C	-2.876021000	1.840003000	-0.685954000
H	-1.273893000	8.175838000	-2.999933000	C	-1.757948000	-2.849064000	0.250751000
C	-0.363626000	7.041546000	-1.401612000	C	2.943746000	-1.789178000	-0.727995000
H	0.026910000	7.917118000	-0.891824000	C	1.864901000	2.936937000	0.028086000
C	-0.138858000	5.768850000	-0.865991000	C	-4.130536000	2.582222000	-0.996066000
H	0.415068000	5.657132000	0.059968000	C	-4.938966000	2.180746000	-2.078041000
C	-4.776715000	-0.652467000	0.761612000	H	-4.618898000	1.341877000	-2.687141000
C	-5.862730000	-0.146411000	0.021012000	C	-6.128328000	2.855399000	-2.371691000
H	-5.666056000	0.426045000	-0.878604000	H	-6.734296000	2.536724000	-3.214282000
C	-7.179041000	-0.401927000	0.420142000	C	-6.533594000	3.942813000	-1.586429000
H	-8.004276000	-0.010039000	-0.166541000	H	-7.456362000	4.467111000	-1.814452000
C	-7.433760000	-1.173425000	1.561652000	C	-5.741938000	4.348049000	-0.503870000
H	-8.455709000	-1.371643000	1.869536000	H	-6.053890000	5.183460000	0.115556000
C	-6.361990000	-1.695701000	2.297459000	C	-4.552794000	3.672550000	-0.210231000
H	-6.550474000	-2.299563000	3.179950000	H	-3.945463000	3.978356000	0.635095000
C	-5.046078000	-1.440162000	1.898415000	C	-2.510672000	-4.107620000	0.525075000
H	-4.212318000	-1.844564000	2.463422000	C	-3.544454000	-4.541132000	-0.327947000
C	2.316689000	0.219219000	-2.899093000	H	-3.788854000	-3.945009000	-1.201030000
H	0.976587000	0.090520000	-2.430513000	C	-4.228800000	-5.733551000	-0.069209000
H	2.176780000	0.215780000	-3.981282000	H	-5.018351000	-6.057656000	-0.740336000
H	2.816434000	-0.660056000	-2.493310000	C	-3.888658000	-6.514551000	1.043424000
H	2.644503000	1.169525000	-2.478840000	H	-4.419884000	-7.439962000	1.243303000
INT1-3_{ns}				C	-2.854631000	-6.098543000	1.892540000
Co	0.050254000	0.040085000	-0.280774000	H	-2.583927000	-6.699577000	2.755320000
O	0.062887000	-0.035384000	-2.204649000	C	-2.169656000	-4.906742000	1.633336000
C	0.112956000	0.103312000	2.056503000	H	-1.367309000	-4.580666000	2.287236000
C	0.811117000	-0.050009000	4.251136000	C	4.181751000	-2.548728000	-1.061493000
H	1.500652000	-0.269658000	5.048397000	C	4.936120000	-2.201286000	-2.199805000
C	-0.457760000	0.436868000	4.268013000	H	4.585711000	-1.392026000	-2.831691000
H	-1.100479000	0.722320000	5.083364000	C	6.109910000	-2.892541000	-2.516965000
C	-2.197289000	0.990691000	2.549291000	H	6.674538000	-2.616396000	-3.402201000
H	-2.669833000	1.442900000	3.425944000	C	6.552924000	-3.941504000	-1.700329000
H	-2.107428000	1.733084000	1.760583000	H	7.464013000	-4.477886000	-1.946702000
H	-2.809360000	0.159843000	2.192431000	C	5.814329000	-4.292939000	-0.562778000
C	2.441542000	-0.768087000	2.487068000	H	6.155923000	-5.098245000	0.080482000
H	2.945868000	-1.182879000	3.364625000	C	4.640484000	-3.601551000	-0.245561000
H	2.294282000	-1.551783000	1.748299000	H	4.073958000	-3.865517000	0.641322000
H	3.055295000	0.024503000	2.053958000	C	2.619201000	4.205780000	0.245195000
N	1.139208000	-0.248796000	2.906130000	C	3.637206000	4.619788000	-0.635801000
N	-0.864430000	0.524015000	2.932558000	H	3.874074000	3.999464000	-1.493335000
N	-1.960244000	-0.426356000	-0.235136000	C	4.320625000	5.821704000	-0.422336000
N	0.537348000	-1.958671000	-0.145115000	H	5.097579000	6.129152000	-1.115598000
				C	3.995755000	6.633126000	0.672847000
				H	4.526021000	7.566067000	0.837064000

C	2.978313000	6.236763000	1.550752000
H	2.719302000	6.860515000	2.400923000
C	2.294908000	5.035303000	1.336811000
H	1.505240000	4.724986000	2.013366000
H	-0.735119000	-0.494739000	-2.567850000
C	-2.352133000	-2.007641000	-3.108844000
H	-2.314504000	-1.958084000	-4.191957000
H	-3.097552000	-1.444928000	-2.558290000
H	-1.681029000	-2.668069000	-2.571097000

⁴INT1-3_{ss}

Co	0.069615000	0.039570000	-0.307761000
O	-0.053449000	-0.028559000	-2.153112000
C	0.079491000	0.066288000	2.069504000
C	0.721985000	-0.225706000	4.266314000
H	1.365462000	-0.553884000	5.064688000
C	-0.467723000	0.430148000	4.281181000
H	-1.076334000	0.784948000	5.095357000
C	-2.086002000	1.271449000	2.569222000
H	-2.482573000	1.778985000	3.453232000
H	-1.880237000	2.002223000	1.792226000
H	-2.818965000	0.550460000	2.202494000
C	2.271886000	-1.111262000	2.513401000
H	2.710735000	-1.588098000	3.394482000
H	2.040626000	-1.866421000	1.767961000
H	2.981100000	-0.395403000	2.093481000
N	1.037752000	-0.439694000	2.921300000
N	-0.841043000	0.601078000	2.944597000
N	-1.988804000	-0.166029000	-0.189979000
N	0.286037000	-2.018461000	-0.123203000
N	2.097537000	0.233540000	-0.296095000
N	-0.162112000	2.088416000	-0.191366000
C	-2.904953000	0.842573000	-0.397006000
C	-2.678880000	-1.321654000	0.115344000
C	-0.749004000	-2.919871000	0.009227000
C	1.419701000	-2.719710000	-0.486894000
C	3.005175000	-0.785508000	-0.499580000
C	2.803105000	1.401973000	-0.081595000
C	0.870588000	2.995120000	-0.139811000
C	-1.318609000	2.775002000	-0.520266000
C	-4.237663000	0.309508000	-0.177392000
H	-5.150562000	0.880598000	-0.240748000
C	-4.097133000	-1.011051000	0.166109000
H	-4.878680000	-1.709013000	0.420558000
C	-0.242254000	-4.256006000	-0.270149000
H	-0.837266000	-5.155719000	-0.259817000
C	1.080137000	-4.129804000	-0.597241000
H	1.758947000	-4.910097000	-0.902460000
C	4.346454000	-0.245951000	-0.360600000
H	5.255260000	-0.821545000	-0.439047000
C	4.222863000	1.087813000	-0.074701000
H	5.015829000	1.793108000	0.115694000
C	0.345662000	4.321694000	-0.430458000
H	0.937989000	5.221866000	-0.478817000
C	-0.989649000	4.182433000	-0.689531000
H	-1.684807000	4.951209000	-0.986912000
C	-2.603230000	2.205188000	-0.630557000
C	-2.110344000	-2.609472000	0.224186000
C	2.699550000	-2.153819000	-0.670742000
C	2.242471000	2.692772000	0.017980000
C	-3.752441000	3.102617000	-0.941284000
C	-4.596208000	2.817646000	-2.033119000
H	-4.380469000	1.950624000	-2.648622000
C	-5.687389000	3.640936000	-2.328646000
H	-6.321774000	3.410038000	-3.178938000
C	-5.957177000	4.764295000	-1.535825000
H	-6.803482000	5.404253000	-1.765231000
C	-5.128640000	5.056212000	-0.444369000
H	-5.335637000	5.919971000	0.180160000

C	-4.037821000	4.231778000	-0.148879000
H	-3.401072000	4.451086000	0.701659000
C	-3.028440000	-3.763611000	0.452693000
C	-4.092178000	-4.034846000	-0.430221000
H	-4.237195000	-3.389571000	-1.290370000
C	-4.933679000	-5.131809000	-0.217067000
H	-5.744840000	-5.331047000	-0.910777000
C	-4.723520000	-5.978916000	0.879165000
H	-5.376546000	-6.830386000	1.043782000
C	-3.661976000	-5.725140000	1.757869000
H	-3.491679000	-6.378303000	2.608334000
C	-2.820025000	-4.628548000	1.544189000
H	-1.995332000	-4.428148000	2.220421000
C	3.833561000	-3.062579000	-1.002281000
C	4.631244000	-2.809447000	-2.136023000
H	4.390750000	-1.958249000	-2.764169000
C	5.707769000	-3.643797000	-2.453593000
H	6.307018000	-3.437567000	-3.335137000
C	6.008145000	-4.746209000	-1.642503000
H	6.843269000	-5.394444000	-1.889203000
C	5.225067000	-5.006490000	-0.510198000
H	5.456540000	-5.853569000	0.128484000
C	4.149017000	-4.171068000	-0.192146000
H	3.548602000	-4.365122000	0.690434000
C	3.163605000	3.852280000	0.200194000
C	4.214490000	4.106479000	-0.702625000
H	4.350682000	3.443251000	-1.549905000
C	5.059685000	5.206696000	-0.523624000
H	5.860679000	5.391077000	-1.233036000
C	4.866283000	6.075848000	0.558219000
H	5.521990000	6.929979000	0.696262000
C	3.817750000	5.839867000	1.457176000
H	3.660048000	6.509411000	2.297315000
C	2.972793000	4.739613000	1.277683000
H	2.158703000	4.553239000	1.970582000
H	-0.847609000	-0.442693000	-2.568886000
C	-2.547790000	-1.659017000	-3.107278000
H	-2.497732000	-1.621127000	-4.190380000
H	-3.214425000	-0.997582000	-2.565030000
H	-1.999091000	-2.419793000	-2.563172000

⁴INT1-3_{ss}

Co	-0.072768000	0.001999000	-0.130212000
C	-0.152368000	-0.012361000	2.003424000
C	-0.553772000	0.561612000	4.194011000
H	-0.925122000	1.179325000	4.993317000
C	0.095125000	-0.630595000	4.204955000
H	0.410301000	-1.264121000	5.015902000
C	1.029682000	-2.205274000	2.516039000
H	1.071442000	-2.836085000	3.408407000
H	0.479226000	-2.719075000	1.734704000
H	2.043221000	-1.992473000	2.172886000
C	-1.363721000	2.173384000	2.476047000
H	-1.460155000	2.788620000	3.375032000
H	-0.759849000	2.696787000	1.741995000
H	-2.353508000	1.973854000	2.062436000
N	-0.696984000	0.925202000	2.853359000
N	0.332136000	-0.967399000	2.870569000
N	1.693149000	-0.874015000	-0.133768000
N	0.861243000	1.895783000	0.000870000
N	-1.824398000	0.881347000	-0.214594000
N	-0.986800000	-1.889337000	-0.109326000
C	1.938472000	-2.209992000	-0.419293000
C	2.903956000	-0.285669000	0.218587000
C	2.206682000	2.105874000	0.147802000
C	0.297762000	3.065676000	-0.456616000
C	-2.042492000	2.211971000	-0.518906000
C	-3.054456000	0.286433000	0.012297000
C	-2.338343000	-2.100063000	-0.037707000

C	-0.398769000	-3.059185000	-0.537268000
C	3.343817000	-2.477495000	-0.196548000
H	3.808037000	-3.443975000	-0.310418000
C	3.924432000	-1.313349000	0.230658000
H	4.953696000	-1.156607000	0.509809000
C	2.514001000	3.490362000	-0.188475000
H	3.501390000	3.925163000	-0.173300000
C	1.341739000	4.073091000	-0.587739000
H	1.196863000	5.075696000	-0.957862000
C	-3.465674000	2.479641000	-0.418726000
H	-3.919124000	3.446244000	-0.569222000
C	-4.079727000	1.313935000	-0.054831000
H	-5.128814000	1.155156000	0.134072000
C	-2.625029000	-3.483895000	-0.394706000
H	-3.611396000	-3.919207000	-0.435970000
C	-1.433771000	-4.065101000	-0.733003000
H	-1.269591000	-5.065478000	-1.101073000
C	0.987978000	-3.218094000	-0.704179000
C	3.159120000	1.092237000	0.373138000
C	-1.074831000	3.221990000	-0.719395000
C	-3.308694000	-1.094410000	0.144717000
C	1.509999000	-4.546659000	-1.127766000
C	2.376097000	-4.647056000	-2.235069000
H	2.639033000	-3.744109000	-2.776181000
C	2.880172000	-5.887268000	-2.639120000
H	3.540154000	-5.946069000	-3.499178000
C	2.528802000	-7.051416000	-1.942640000
H	2.919034000	-8.014476000	-2.256735000
C	1.671755000	-6.964863000	-0.837751000
H	1.401945000	-7.860964000	-0.287109000
C	1.169223000	-5.723892000	-0.432747000
H	0.515726000	-5.654069000	0.430324000
C	4.559180000	1.542849000	0.621633000
C	5.604315000	1.212776000	-0.263397000
H	5.379394000	0.613348000	-1.139405000
C	6.904309000	1.675921000	-0.034853000
H	7.697378000	1.418811000	-0.730449000
C	7.180617000	2.481650000	1.077992000
H	8.189675000	2.841292000	1.254136000
C	6.145820000	2.828642000	1.956512000
H	6.350956000	3.457089000	2.817870000
C	4.845449000	2.366322000	1.727204000
H	4.039235000	2.636094000	2.401779000
C	-1.561547000	4.552467000	-1.178481000
C	-2.326192000	4.655433000	-2.357830000
H	-2.538357000	3.753613000	-2.922245000
C	-2.792663000	5.897465000	-2.799972000
H	-3.374058000	5.959514000	-3.714778000
C	-2.504986000	7.059037000	-2.070695000
H	-2.866587000	8.023180000	-2.414539000
C	-1.749111000	6.969047000	-0.894446000
H	-1.529577000	7.863346000	-0.319041000
C	-1.283099000	5.726647000	-0.451635000
H	-0.706575000	5.653831000	0.464569000
C	-4.712064000	-1.558705000	0.346405000
C	-5.743180000	-1.227811000	-0.554198000
H	-5.510751000	-0.611241000	-1.415591000
C	-7.043862000	-1.703377000	-0.356195000
H	-7.824996000	-1.443862000	-1.064237000
C	-7.336034000	-2.523258000	0.741963000
H	-8.345515000	-2.892434000	0.894245000
C	-6.315954000	-2.870630000	1.637244000
H	-6.532653000	-3.509071000	2.488393000
C	-5.015459000	-2.395416000	1.438349000
H	-4.221026000	-2.665090000	2.126829000
O	-0.056202000	0.097157000	-1.954433000
H	0.814419000	-0.200673000	-2.305447000
C	3.069412000	0.122983000	-2.989940000
H	3.071492000	0.130762000	-4.074704000
H	3.393199000	-0.757655000	-2.446281000

H	2.755079000	1.003051000	-2.440631000
²INT1-3_k			
Co	-0.070058000	0.001569000	-0.142747000
O	-0.069442000	0.018665000	-2.034201000
C	-0.148535000	-0.012635000	1.904219000
C	-0.452411000	0.614207000	4.094842000
H	-0.719083000	1.281562000	4.896153000
C	-0.009542000	-0.669219000	4.102804000
H	0.197275000	-1.347322000	4.912731000
C	0.672486000	-2.365537000	2.403197000
H	0.560093000	-3.018842000	3.273084000
H	0.091467000	-2.760252000	1.576198000
H	1.725248000	-2.315528000	2.117307000
C	-0.999685000	2.335869000	2.372085000
H	-0.941145000	2.979622000	3.254351000
H	-0.362009000	2.734627000	1.590016000
H	-2.031286000	2.296800000	2.015837000
N	-0.530438000	1.001296000	2.754475000
N	0.169537000	-1.038118000	2.766865000
N	1.579899000	-1.046643000	-0.149030000
N	0.991974000	1.648874000	-0.127576000
N	-1.710151000	1.052659000	-0.243928000
N	-1.121660000	-1.649338000	-0.215332000
C	1.702850000	-2.358739000	-0.555539000
C	2.818543000	-0.639458000	0.316951000
C	2.322720000	1.759170000	0.216169000
C	0.599700000	2.869526000	-0.653813000
C	-1.802638000	2.362465000	-0.653616000
C	-2.978902000	0.637862000	0.109401000
C	-2.471598000	-1.758648000	0.019562000
C	-0.694118000	-2.860300000	-0.732736000
C	3.056310000	-2.806865000	-0.303299000
H	3.419835000	-3.801559000	-0.507873000
C	3.728466000	-1.765093000	0.279961000
H	4.750971000	-1.746235000	0.620965000
C	2.786353000	3.097274000	-0.093199000
H	3.796521000	3.444297000	0.057558000
C	1.740318000	3.763342000	-0.670745000
H	1.735146000	4.764248000	-1.070841000
C	-3.173522000	2.811856000	-0.501156000
H	-3.519272000	3.808819000	-0.724553000
C	-3.887222000	1.767058000	0.017817000
H	-4.931361000	1.747867000	0.284560000
C	-2.914932000	-3.093575000	-0.339312000
H	-3.934919000	-3.437633000	-0.270998000
C	-1.832219000	-3.752961000	-0.848213000
H	-1.798775000	-4.746708000	-1.264355000
C	0.647041000	-3.202906000	-0.942326000
C	3.170047000	0.694539000	0.566635000
C	-0.725217000	3.211290000	-0.955616000
C	-3.343978000	-0.699008000	0.324472000
C	1.002534000	-4.545496000	-1.475645000
C	1.836929000	-4.643490000	-2.606868000
H	2.180519000	-3.730940000	-3.082627000
C	2.204764000	-5.892628000	-3.116976000
H	2.841102000	-5.949648000	-3.994743000
C	1.748789000	-7.066565000	-2.502560000
H	2.033471000	-8.036278000	-2.898888000
C	0.926114000	-6.981914000	-1.371745000
H	0.578535000	-7.886959000	-0.882801000
C	0.558755000	-5.732486000	-0.860997000
H	-0.063862000	-5.666821000	0.024783000
C	4.549454000	1.033339000	1.011472000
C	5.679112000	0.646169000	0.264368000
H	5.534260000	0.093594000	-0.657772000
C	6.965562000	0.999911000	0.684943000
H	7.826134000	0.700359000	0.094605000
C	7.143701000	1.752285000	1.853602000

H	8.142441000	2.027093000	2.178444000
C	6.025839000	2.157122000	2.594994000
H	6.155945000	2.745799000	3.498021000
C	4.739191000	1.803501000	2.174695000
H	3.869096000	2.116217000	2.743220000
C	-1.041134000	4.555656000	-1.508972000
C	-1.785194000	4.653056000	-2.701677000
H	-2.090726000	3.739714000	-3.201137000
C	-2.112134000	5.902588000	-3.238187000
H	-2.678705000	5.959918000	-4.162504000
C	-1.705732000	7.076378000	-2.589576000
H	-1.959146000	8.046217000	-3.006407000
C	-0.974164000	6.991823000	-1.397713000
H	-0.666941000	7.896910000	-0.882482000
C	-0.646985000	5.742202000	-0.860542000
H	-0.096135000	5.676644000	0.071677000
C	-4.738858000	-1.049358000	0.708024000
C	-5.851054000	-0.632107000	-0.049014000
H	-5.688197000	-0.041564000	-0.943655000
C	-7.147864000	-0.997757000	0.327447000
H	-7.993124000	-0.673166000	-0.271692000
C	-7.356083000	-1.793139000	1.461937000
H	-8.362871000	-2.077076000	1.752158000
C	-6.256671000	-2.228226000	2.213541000
H	-6.408628000	-2.849949000	3.090654000
C	-4.960180000	-1.862487000	1.837226000
H	-4.104989000	-2.199222000	2.414438000
H	0.872161000	0.044893000	-2.316798000
C	3.241862000	0.138076000	-2.853619000
H	3.282226000	0.194853000	-3.936084000
H	3.325514000	-0.819671000	-2.353034000
H	3.084995000	1.036722000	-2.268261000

⁶TS2-3_{hs}

Co	-0.031099000	0.000801000	-0.119998000
O	0.116706000	-0.036178000	-1.959198000
C	-0.091300000	0.003992000	2.018702000
C	-0.784840000	0.282891000	4.194002000
H	-1.470380000	0.557292000	4.977102000
C	0.473134000	-0.226126000	4.236302000
H	1.111071000	-0.483633000	5.064002000
C	2.204235000	-0.928575000	2.587302000
H	2.624698000	-1.361014000	3.499502000
H	2.104348000	-1.701689000	1.832102000
H	2.862521000	-0.140179000	2.219102000
C	-2.418935000	0.936054000	2.428602000
H	-2.912496000	1.353283000	3.310702000
H	-2.279349000	1.717575000	1.688102000
H	-3.035420000	0.139365000	2.010002000
N	-1.114260000	0.417444000	2.843802000
N	0.880958000	-0.391667000	2.910902000
N	1.921640000	0.417484000	-0.105698000
N	-0.500396000	2.041433000	-0.090098000
N	-1.974937000	-0.428681000	-0.284098000
N	0.423699000	-2.055133000	-0.034998000
C	2.938770000	-0.478668000	-0.363998000
C	2.491161000	1.652067000	0.146502000
C	0.422658000	3.050267000	0.027802000
C	-1.678076000	2.596662000	-0.544698000
C	-2.990468000	0.474571000	-0.558998000
C	-2.561659000	-1.658566000	-0.002998000
C	-0.498254000	-3.066167000	0.028402000
C	1.627978000	-2.602659000	-0.423398000
C	4.209971000	0.206516000	-0.209098000
H	5.176538000	-0.258344000	-0.321498000
C	3.938083000	1.500877000	0.139502000
H	4.645269000	2.284679000	0.357102000
C	-0.207725000	4.314475000	-0.329498000
H	0.290936000	5.271148000	-0.342298000

C	-1.491084000	4.031089000	-0.708998000
H	-2.232284000	4.716381000	-1.088498000
C	-4.262870000	-0.203013000	-0.409398000
H	-5.226038000	0.265747000	-0.534098000
C	-4.002683000	-1.493476000	-0.034398000
H	-4.718970000	-2.266480000	0.192202000
C	0.156129000	-4.328972000	-0.288898000
H	-0.336432000	-5.288244000	-0.327898000
C	1.457487000	-4.038383000	-0.597198000
H	2.224086000	-4.720272000	-0.929898000
C	2.815172000	-1.866586000	-0.595998000
C	1.804283000	2.879967000	0.258302000
C	-2.860070000	1.866690000	-0.773698000
C	-1.891680000	-2.887969000	0.172002000
C	4.047378000	-2.596807000	-1.006798000
C	4.757418000	-2.189104000	-2.154098000
H	4.375998000	-1.356360000	-2.736398000
C	5.920416000	-2.860036000	-2.546598000
H	6.451969000	-2.538458000	-3.436998000
C	6.394674000	-3.946967000	-1.799898000
H	7.297749000	-4.466536000	-2.105298000
C	5.697033000	-4.360068000	-0.657198000
H	6.061855000	-5.197315000	-0.069798000
C	4.533636000	-3.690137000	-0.264098000
H	3.996382000	-4.002315000	0.625502000
C	2.590402000	4.124981000	0.500802000
C	3.634744000	4.525333000	-0.355298000
H	3.877234000	3.907168000	-1.212898000
C	4.337272000	5.711735000	-0.118898000
H	5.135129000	6.007951000	-0.793198000
C	4.004454000	6.523086000	0.974002000
H	4.549420000	7.444266000	1.155902000
C	2.958909000	6.142635000	1.825402000
H	2.691719000	6.767496000	2.672202000
C	2.256781000	4.956333000	1.588202000
H	1.444125000	4.659415000	2.243302000
C	-4.083878000	2.608313000	-1.188198000
C	-4.810619000	2.205407000	-2.326598000
H	-4.453596000	1.357259000	-2.901198000
C	-5.967118000	2.888139000	-2.716698000
H	-6.509272000	2.567161000	-3.600898000
C	-6.420878000	3.987074000	-1.974998000
H	-7.318055000	4.517743000	-2.278398000
C	-5.710337000	4.395577000	-0.838798000
H	-6.059860000	5.240526000	-0.253198000
C	-4.554538000	3.711544000	-0.448398000
H	-4.009683000	4.020923000	0.437202000
C	-2.694101000	-4.123786000	0.401602000
C	-3.721743000	-4.522535000	-0.475898000
H	-3.93932000	-3.908967000	-1.343098000
C	-4.439072000	-5.701739000	-0.248298000
H	-5.223129000	-5.996353000	-0.939198000
C	-4.138255000	-6.508495000	0.857202000
H	-4.694722000	-7.424076000	1.032302000
C	-3.109810000	-6.130346000	1.730302000
H	-2.867720000	-6.751311000	2.587402000
C	-2.393281000	-4.951142000	1.502102000
H	-1.594124000	-4.655826000	2.174102000
H	-0.734455000	-0.304201000	-2.371998000
C	1.987717000	-0.112206000	-3.581998000
H	1.470166000	0.239719000	-4.467498000
H	2.027571000	-1.170001000	-3.357598000
H	2.386514000	0.595652000	-2.869098000

⁴TS2-3_{hs}

Co	-0.031099000	0.000801000	-0.119998000
O	0.116706000	-0.036178000	-1.959198000
C	-0.091300000	0.003992000	2.018702000
C	-0.784840000	0.282891000	4.194002000

H	-1.470380000	0.557292000	4.977102000
C	0.473134000	-0.226126000	4.236302000
H	1.111071000	-0.483633000	5.064002000
C	2.204235000	-0.928575000	2.587302000
H	2.624698000	-1.361014000	3.499502000
H	2.104348000	-1.701689000	1.832102000
H	2.862521000	-0.140179000	2.219102000
C	-2.418935000	0.936054000	2.428602000
H	-2.912496000	1.353283000	3.310702000
H	-2.279349000	1.717575000	1.688102000
H	-3.035420000	0.139365000	2.010002000
N	-1.114260000	0.417444000	2.843802000
N	0.880958000	-0.391667000	2.910902000
N	1.921640000	0.417484000	-0.105698000
N	-0.500396000	2.041433000	-0.090098000
N	-1.974937000	-0.428681000	-0.284098000
N	0.423699000	-2.055133000	-0.034998000
C	2.938770000	-0.478668000	-0.363998000
C	2.491161000	1.652067000	0.146502000
C	0.422658000	3.050267000	0.027802000
C	-1.678076000	2.596662000	-0.544698000
C	-2.990468000	0.474571000	-0.558998000
C	-2.561659000	-1.658566000	-0.002998000
C	-0.498254000	-3.066167000	0.028402000
C	1.627978000	-2.602659000	-0.423398000
C	4.209971000	0.206516000	-0.209098000
H	5.176538000	-0.258344000	-0.321498000
C	3.938083000	1.500877000	0.139502000
H	4.645269000	2.284679000	0.357102000
C	-0.207725000	4.314475000	-0.329498000
H	0.290936000	5.271148000	-0.342298000
C	-1.491084000	4.031089000	-0.708998000
H	-2.232284000	4.716381000	-1.088498000
C	-4.262870000	-0.203013000	-0.409398000
H	-5.226038000	0.265747000	-0.534098000
C	-4.002683000	-1.493476000	-0.034398000
H	-4.718970000	-2.266480000	0.192202000
C	0.156129000	-4.328972000	-0.288898000
H	-0.336432000	-5.288244000	-0.327898000
C	1.457487000	-4.038383000	-0.597198000
H	2.224086000	-4.720272000	-0.929898000
C	2.815172000	-1.866586000	-0.595998000
C	1.804283000	2.879967000	0.258302000
C	-2.860070000	1.866690000	-0.773698000
C	-1.891680000	-2.887969000	0.172002000
C	4.047378000	-2.596807000	-1.006798000
C	4.757418000	-2.189104000	-2.154098000
H	4.375998000	-1.356360000	-2.736398000
C	5.920416000	-2.860036000	-2.546598000
H	6.451969000	-2.538458000	-3.436998000
C	6.394674000	-3.946967000	-1.799898000
H	7.297749000	-4.466536000	-2.105298000
C	5.697033000	-4.360068000	-0.657198000
H	6.061855000	-5.197315000	-0.069798000
C	4.533636000	-3.690137000	-0.264098000
H	3.996382000	-4.002315000	0.625502000
C	2.590402000	4.124981000	0.500802000
C	3.634744000	4.525333000	-0.355298000
H	3.877234000	3.907168000	-1.212898000
C	4.337272000	5.711735000	-0.118898000
H	5.135129000	6.007951000	-0.793198000
C	4.004454000	6.523086000	0.974002000
H	4.549420000	7.444266000	1.155902000
C	2.958909000	6.142635000	1.825402000
H	2.691719000	6.767496000	2.672202000
C	2.256781000	4.956333000	1.588202000
H	1.444125000	4.659415000	2.243302000
C	-4.083878000	2.608313000	-1.188198000
C	-4.810619000	2.205407000	-2.326598000
H	-4.453596000	1.357259000	-2.901198000

C	-5.967118000	2.888139000	-2.716698000
H	-6.509272000	2.567161000	-3.600898000
C	-6.420878000	3.987074000	-1.974998000
H	-7.318055000	4.517743000	-2.278398000
C	-5.710337000	4.395577000	-0.838798000
H	-6.059860000	5.240526000	-0.253198000
C	-4.554538000	3.711544000	-0.448398000
H	-4.009683000	4.020923000	0.437202000
C	-2.694101000	-4.123786000	0.401602000
C	-3.721743000	-4.522535000	-0.475898000
H	-3.939932000	-3.908967000	-1.343098000
C	-4.439072000	-5.701739000	-0.248298000
H	-5.223129000	-5.996353000	-0.939198000
C	-4.138255000	-6.508495000	0.857202000
H	-4.694722000	-7.424076000	1.032302000
C	-3.109810000	-6.130346000	1.730302000
H	-2.867720000	-6.751311000	2.587402000
C	-2.393281000	-4.951142000	1.502102000
H	-1.594124000	-4.655826000	2.174102000
H	-0.734455000	-0.304201000	-2.371998000
C	1.987717000	-0.112206000	-3.581998000
H	1.470166000	0.239719000	-4.467498000
H	2.027571000	-1.170001000	-3.357598000
H	2.386514000	0.595652000	-2.869098000

⁴TS2-3_{is}

Co	-0.031072000	0.000840000	-0.119982000
O	0.116688000	-0.036296000	-1.959224000
C	-0.091246000	0.004076000	2.018745000
C	-0.784867000	0.282652000	4.194025000
H	-1.470495000	0.556832000	4.977106000
C	0.473233000	-0.225864000	4.236326000
H	1.111287000	-0.483122000	5.064046000
C	2.204603000	-0.927641000	2.587258000
H	2.625212000	-1.360045000	3.499491000
H	2.105005000	-1.700711000	1.832009000
H	2.862652000	-0.139004000	2.219209000
C	-2.419230000	0.935350000	2.428648000
H	-2.912748000	1.352740000	3.310722000
H	-2.279945000	1.716611000	1.687867000
H	-3.035541000	0.138390000	2.010388000
N	-1.114339000	0.417167000	2.843801000
N	0.881113000	-0.391202000	2.910937000
N	1.921481000	0.418201000	-0.105725000
N	-0.501122000	2.041238000	-0.090228000
N	-1.974753000	-0.429408000	-0.284017000
N	0.424513000	-2.054884000	-0.034903000
C	2.938993000	-0.477569000	-0.364021000
C	2.490567000	1.653016000	0.146553000
C	0.421585000	3.050404000	0.027714000
C	-1.678970000	2.596042000	-0.544852000
C	-2.990644000	0.473459000	-0.558962000
C	-2.561044000	-1.659406000	-0.002725000
C	-0.497111000	-3.066236000	0.028492000
C	1.628909000	-2.601997000	-0.423384000
C	4.209923000	0.208112000	-0.209064000
H	5.176632000	-0.256423000	-0.321387000
C	3.937492000	1.502324000	0.139613000
H	4.644415000	2.286362000	0.357282000
C	-0.209298000	4.314381000	-0.329728000
H	0.289019000	5.271183000	-0.342586000
C	-1.492491000	4.030510000	-0.709254000
H	-2.233961000	4.715482000	-1.088884000
C	-4.262827000	-0.204579000	-0.409209000
H	-5.226140000	0.263833000	-0.533912000
C	-4.002181000	-1.494858000	-0.034120000
H	-4.718096000	-2.268144000	0.192583000
C	0.157648000	-4.328875000	-0.289003000
H	-0.334574000	-5.288220000	-0.328099000

C	1.458911000	-4.037750000	-0.597354000	H	-2.091372000	1.864529000	1.543188000
H	2.225658000	-4.719324000	-0.930268000	H	-3.030387000	0.424378000	1.992294000
C	2.815843000	-1.865565000	-0.596052000	N	-1.063506000	0.511281000	2.764307000
C	1.803229000	2.880628000	0.258259000	N	0.830061000	-0.515197000	2.821144000
C	-2.860785000	1.865675000	-0.773798000	N	1.910645000	0.314729000	-0.132191000
C	-1.890568000	-2.888584000	0.172212000	N	-0.344129000	1.936971000	-0.181313000
C	4.048270000	-2.595321000	-1.006878000	N	-1.957241000	-0.325673000	-0.281266000
C	4.758286000	-2.187212000	-2.154068000	N	0.285423000	-1.939958000	-0.167143000
H	4.376567000	-1.354562000	-2.736357000	C	2.876784000	-0.591924000	-0.503851000
C	5.921421000	-2.857716000	-2.546641000	C	2.558183000	1.469251000	0.262647000
H	6.452919000	-2.535945000	-3.437064000	C	0.578392000	2.913847000	0.116089000
C	6.396063000	-3.944679000	-1.800159000	C	-1.454167000	2.570889000	-0.716131000
H	7.299293000	-4.463869000	-2.105535000	C	-2.911251000	0.592134000	-0.673495000
C	5.698462000	-4.358130000	-0.657503000	C	-2.628351000	-1.472293000	0.116027000
H	6.063578000	-5.195334000	-0.070228000	C	-0.646951000	-2.920985000	0.099922000
C	4.534906000	-3.688557000	-0.264293000	C	1.431198000	-2.575785000	-0.620573000
H	3.997726000	-4.001042000	0.625237000	C	4.186670000	-0.008784000	-0.287378000
C	2.588839000	4.125972000	0.500911000	H	5.120486000	-0.514798000	-0.475199000
C	3.633135000	4.526612000	-0.355156000	C	3.991998000	1.241047000	0.233323000
H	3.875930000	3.908598000	-1.212638000	H	4.740772000	1.952576000	0.541185000
C	4.335281000	5.713329000	-0.118629000	C	0.028822000	4.213352000	-0.223011000
H	5.133036000	6.009811000	-0.792837000	H	0.554952000	5.147920000	-0.108419000
C	4.002027000	6.524587000	0.974183000	C	-1.200462000	3.997976000	-0.778612000
H	4.546652000	7.445911000	1.156129000	H	-1.875773000	4.728390000	-1.193483000
C	2.956494000	6.143794000	1.825419000	C	-4.227689000	0.018460000	-0.485881000
H	2.688958000	6.768585000	2.672233000	H	-5.153513000	0.531255000	-0.693787000
C	2.254834000	4.957163000	1.588247000	C	-4.055681000	-1.231377000	0.045169000
H	1.442163000	4.660038000	2.243260000	H	-4.818378000	-1.933718000	0.339899000
C	-4.084857000	2.606753000	-1.188324000	C	-0.068352000	-4.219836000	-0.179597000
C	-4.811464000	2.203463000	-2.326602000	H	-0.590643000	-5.157556000	-0.072711000
H	-4.454257000	1.355294000	-2.901065000	C	1.191550000	-4.004115000	-0.666984000
C	-5.968180000	2.885760000	-2.716877000	H	1.896697000	-4.737153000	-1.023891000
H	-6.510312000	2.564381000	-3.600966000	C	2.659325000	-1.937100000	-0.841498000
C	-6.422323000	3.984662000	-1.975387000	C	1.923616000	2.702626000	0.468255000
H	-7.319631000	4.514951000	-2.278810000	C	-2.674817000	1.940369000	-0.991266000
C	-5.711796000	4.393645000	-0.839248000	C	-2.009329000	-2.704269000	0.372706000
H	-6.061619000	5.238580000	-0.253835000	C	3.819927000	-2.713560000	-1.357821000
C	-4.555806000	3.709976000	-0.448716000	C	4.471867000	-2.278124000	-2.528975000
H	-4.011089000	4.019683000	0.436849000	H	4.090004000	-1.403467000	-3.045651000
C	-2.692593000	-4.124743000	0.401816000	C	5.574231000	-2.978083000	-3.030657000
C	-3.720193000	-4.523747000	-0.475544000	H	6.060548000	-2.635494000	-3.938920000
H	-3.938661000	-3.910242000	-1.342760000	C	6.046388000	-4.119486000	-2.369092000
C	-4.437043000	-5.703282000	-0.247910000	H	6.902284000	-4.661788000	-2.758938000
H	-5.221061000	-5.998142000	-0.938752000	C	5.409937000	-4.556112000	-1.199628000
C	-4.135837000	-6.509946000	0.857516000	H	5.776879000	-5.433462000	-0.675497000
H	-4.691903000	-7.425711000	1.032645000	C	4.306931000	-3.857519000	-0.696927000
C	-3.107441000	-6.131469000	1.730465000	H	3.822722000	-4.185091000	0.217028000
H	-2.864966000	-6.752373000	2.587581000	C	2.712708000	3.889542000	0.899341000
C	-2.391281000	-4.952032000	1.502288000	C	3.840088000	4.336064000	0.182598000
H	-1.592139000	-4.656470000	2.174243000	H	4.141168000	3.802498000	-0.712062000
H	-0.734486000	-0.304496000	-2.372029000	C	4.548133000	5.468410000	0.599108000
C	1.987509000	-0.112852000	-3.582209000	H	5.410802000	5.802472000	0.030751000
H	1.469333000	0.238084000	-4.467656000	C	4.137797000	6.179216000	1.734623000
H	2.028283000	-1.170418000	-3.357155000	H	4.687206000	7.058504000	2.056336000
H	2.386195000	0.595745000	-2.869925000	C	3.008489000	5.754180000	2.446791000
² TS2-3 _s				H	2.680339000	6.302571000	3.324607000
				C	2.300893000	4.621716000	2.030341000
				H	1.424168000	4.289124000	2.576780000
Co	-0.028485000	0.000771000	-0.134005000	C	-3.818026000	2.730065000	-1.525426000
C	-0.090344000	-0.000064000	1.935363000	C	-4.471484000	2.299562000	-2.697156000
C	-0.756483000	0.317574000	4.113898000	H	-4.109250000	1.408586000	-3.199080000
H	-1.410824000	0.651099000	4.900925000	C	-5.558825000	3.012370000	-3.212405000
C	0.438473000	-0.326779000	4.149748000	H	-6.044575000	2.671068000	-4.121393000
H	1.042524000	-0.663342000	4.974752000	C	-6.016297000	4.166229000	-2.562258000
C	2.097870000	-1.165806000	2.480505000	H	-6.859601000	4.720486000	-2.962397000
H	2.449197000	-1.706199000	3.364206000	C	-5.381517000	4.598545000	-1.390477000
H	1.938914000	-1.865801000	1.666781000	H	-5.737857000	5.484678000	-0.873968000
H	2.844816000	-0.427169000	2.181760000	C	-4.294213000	3.885077000	-0.874939000
C	-2.305712000	1.162558000	2.342575000	H	-3.812245000	4.210677000	0.040605000
H	-2.716133000	1.700204000	3.202077000	C	-2.822005000	-3.881273000	0.785072000

C	-3.924830000	-4.327751000	0.030866000
H	-4.189289000	-3.800908000	-0.879334000
C	-4.656958000	-5.450259000	0.431910000
H	-5.500046000	-5.784108000	-0.165231000
C	-4.295913000	-6.151334000	1.589974000
H	-4.864024000	-7.022887000	1.899954000
C	-3.192094000	-5.725909000	2.340811000
H	-2.902816000	-6.266052000	3.237186000
C	-2.460517000	-4.603207000	1.939850000
H	-1.604151000	-4.269829000	2.517156000
O	0.083432000	0.031698000	-2.061790000
H	-0.501986000	-0.684883000	-2.394152000
C	1.697498000	-0.157497000	-3.653208000
H	2.304853000	0.477436000	-3.024231000
H	1.115698000	0.278004000	-4.456076000
H	1.787704000	-1.233169000	-3.566935000

⁴INT2-3_{hs}

Co	-0.010093000	0.015246000	-0.021916000
O	-0.129712000	-0.108773000	-2.393263000
C	-0.035758000	0.065628000	2.191276000
C	-0.745105000	0.032575000	4.380707000
H	-1.460796000	-0.054409000	5.180438000
C	0.600342000	0.242654000	4.396152000
H	1.289223000	0.382378000	5.211784000
C	2.400364000	0.462991000	2.646339000
H	3.047266000	0.342355000	3.519945000
H	2.659053000	-0.276084000	1.890743000
H	2.531859000	1.461838000	2.224113000
C	-2.482338000	-0.315109000	2.586554000
H	-3.158194000	-0.182884000	3.436050000
H	-2.730034000	0.396510000	1.801941000
H	-2.581887000	-1.328083000	2.190010000
N	-1.111545000	-0.070477000	3.036559000
N	1.012207000	0.255717000	3.061048000
N	1.521919000	1.388970000	-0.286188000
N	-1.432647000	1.516977000	-0.237631000
N	-1.551365000	-1.385557000	-0.350836000
N	1.397813000	-1.510315000	-0.196657000
C	2.871325000	1.124501000	-0.395559000
C	1.372501000	2.749579000	-0.103682000
C	-1.135614000	2.862145000	-0.246900000
C	-2.769406000	1.382181000	-0.563443000
C	-2.905618000	-1.115597000	-0.443561000
C	-1.408755000	-2.742814000	-0.103400000
C	1.101807000	-2.858331000	-0.200014000
C	2.748955000	-1.377062000	-0.466386000
C	3.611626000	2.365133000	-0.223103000
H	4.686662000	2.453595000	-0.228831000
C	2.692532000	3.359608000	-0.023950000
H	2.886698000	4.404632000	0.158293000
C	-2.338547000	3.612684000	-0.587148000
H	-2.387971000	4.684815000	-0.694919000
C	-3.336098000	2.703809000	-0.797830000
H	-4.349887000	2.898849000	-1.109594000
C	-3.646290000	-2.341176000	-0.208590000
H	-4.721947000	-2.422321000	-0.192437000
C	-2.729641000	-3.334557000	0.020835000
H	-2.929503000	-4.368427000	0.254156000
C	2.315948000	-3.607785000	-0.489780000
H	2.372842000	-4.681142000	-0.581415000
C	3.321989000	-2.698627000	-0.669414000
H	4.348054000	-2.897705000	-0.935169000
C	3.452679000	-0.155461000	-0.541712000
C	0.142278000	3.443228000	-0.076322000
C	-3.478877000	0.163094000	-0.628321000
C	-0.180531000	-3.438375000	-0.047505000
C	4.927776000	-0.212395000	-0.752564000
C	5.526373000	0.497382000	-1.812564000

H	4.893826000	1.077098000	-2.476580000
C	6.909991000	0.455381000	-2.012299000
H	7.351807000	1.004204000	-2.838434000
C	7.723083000	-0.297423000	-1.154726000
H	8.797027000	-0.330758000	-1.309671000
C	7.141299000	-1.006391000	-0.095434000
H	7.764720000	-1.586631000	0.578159000
C	5.757504000	-0.962896000	0.104050000
H	5.305764000	-1.506714000	0.927072000
C	0.181803000	4.929561000	0.057914000
C	0.909159000	5.731126000	-0.843652000
H	1.450199000	5.251845000	-1.652353000
C	0.923363000	7.123737000	-0.711537000
H	1.483849000	7.726068000	-1.420098000
C	0.207368000	7.741236000	0.322619000
H	0.217905000	8.822072000	0.424253000
C	-0.526400000	6.955764000	1.221341000
H	-1.084282000	7.426203000	2.025410000
C	-0.540497000	5.563455000	1.088181000
H	-1.108153000	4.951097000	1.781132000
C	-4.952210000	0.218098000	-0.848591000
C	-5.549603000	-0.531597000	-1.881556000
H	-4.915797000	-1.134897000	-2.522796000
C	-6.932682000	-0.495836000	-2.085840000
H	-7.373329000	-1.074678000	-2.891868000
C	-7.746805000	0.289930000	-1.259322000
H	-8.820358000	0.318604000	-1.417983000
C	-7.166585000	1.038066000	-0.226458000
H	-7.790852000	1.643991000	0.423313000
C	-5.783357000	1.001120000	-0.022588000
H	-5.333319000	1.575294000	0.780400000
C	-0.225909000	-4.920241000	0.122297000
C	-0.970134000	-5.739354000	-0.749704000
H	-1.519366000	-5.277093000	-1.562923000
C	-0.994789000	-7.127883000	-0.581659000
H	-1.569006000	-7.743226000	-1.267679000
C	-0.272624000	-7.724804000	0.460194000
H	-0.291391000	-8.802457000	0.590111000
C	0.476750000	-6.922528000	1.330876000
H	1.038024000	-7.376631000	2.141912000
C	0.500737000	-5.534404000	1.162046000
H	1.078579000	-4.909090000	1.834520000
H	-0.780954000	-0.837297000	-2.303571000
C	1.051728000	-0.513769000	-3.144785000
H	0.842799000	-0.518087000	-4.222332000
H	1.414034000	-1.496865000	-2.824272000
H	1.811722000	0.233878000	-2.915975000

²INT2-3_k

Co	-0.026581000	0.008852000	-0.156375000
C	-0.016800000	-0.023056000	2.078410000
C	-0.705274000	-0.076259000	4.281940000
H	-1.419496000	-0.106667000	5.087439000
C	0.655034000	-0.053523000	4.287631000
H	1.363109000	-0.052190000	5.099110000
C	2.452706000	0.032925000	2.524792000
H	3.085882000	-0.230002000	3.377424000
H	2.611905000	-0.677510000	1.716401000
H	2.709854000	1.034761000	2.171597000

C	-2.489462000	-0.092681000	2.503378000
H	-3.127092000	0.177508000	3.350461000
H	-2.628687000	0.621654000	1.695309000
H	-2.756834000	-1.090310000	2.145242000
N	-1.093211000	-0.054515000	2.937423000
N	1.053273000	-0.024001000	2.946076000
N	1.559445000	1.210130000	-0.280411000
N	-1.230677000	1.577725000	-0.257056000
N	-1.601930000	-1.208202000	-0.304785000
N	1.179657000	-1.571546000	-0.312324000
C	2.874738000	0.849688000	-0.510765000
C	1.573991000	2.553742000	0.065979000
C	-0.861855000	2.894753000	-0.069825000
C	-2.559492000	1.593437000	-0.657938000
C	-2.911656000	-0.843079000	-0.555052000
C	-1.622758000	-2.555343000	0.028030000
C	0.812703000	-2.894293000	-0.119430000
C	2.525542000	-1.585671000	-0.667168000
C	3.742188000	1.985142000	-0.265759000
H	4.817445000	1.965876000	-0.347095000
C	2.945118000	3.023000000	0.127040000
H	3.247908000	4.015672000	0.418468000
C	-1.984762000	3.765883000	-0.367262000
H	-1.952648000	4.843120000	-0.325303000
C	-3.016879000	2.967521000	-0.764364000
H	-3.994502000	3.268686000	-1.104274000
C	-3.783730000	-1.978537000	-0.330606000
H	-4.857461000	-1.957136000	-0.429843000
C	-2.994709000	-3.022208000	0.066528000
H	-3.303961000	-4.017292000	0.342650000
C	-4.799314000	0.625014000	-1.188728000
C	-5.316909000	-0.052205000	-2.310266000
H	-4.648898000	-0.670006000	-2.901113000
C	-6.664592000	0.073598000	-2.662696000
H	-7.044531000	-0.449875000	-3.534759000
C	-7.520852000	0.876159000	-1.897150000
H	-8.566946000	0.974223000	-2.170330000
C	-7.019618000	1.549343000	-0.775314000
H	-7.678695000	2.165301000	-0.170944000
C	-5.671600000	1.422989000	-0.423215000
H	-5.284705000	1.934929000	0.451489000
C	-0.633867000	-4.802475000	0.504134000
C	-1.426503000	-5.671065000	-0.270873000
H	-1.941225000	-5.278216000	-1.141059000
C	-1.539795000	-7.024910000	0.063491000

C	1.943941000	-3.758380000	-0.391250000
H	1.916843000	-4.835592000	-0.344097000
C	2.985521000	-2.957235000	-0.763206000
H	3.973605000	-3.257840000	-1.072100000
C	3.337001000	-0.447977000	-0.783994000
C	0.434771000	3.357383000	0.207572000
C	-3.365403000	0.459519000	-0.818441000
C	-0.482318000	-3.359674000	0.161763000
C	4.779205000	-0.609412000	-1.124009000
C	5.322190000	0.080655000	-2.225641000
H	4.669939000	0.712644000	-2.819538000
C	6.676556000	-0.043384000	-2.552098000
H	7.075841000	0.491594000	-3.408379000
C	7.514809000	-0.858121000	-1.779664000
H	8.566054000	-0.955337000	-2.032372000
C	6.988986000	-1.543364000	-0.676494000
H	7.634278000	-2.167735000	-0.065973000
C	5.634320000	-1.418076000	-0.350442000
H	5.228668000	-1.938900000	0.510373000
C	0.588496000	4.800062000	0.548729000
C	1.382565000	5.666404000	-0.227464000
H	1.897198000	5.270998000	-1.096483000
C	1.494942000	7.021211000	0.102883000
H	2.106549000	7.675896000	-0.510561000
C	0.811215000	7.535469000	1.212428000
H	0.898110000	8.587029000	1.467861000
C	0.009681000	6.685903000	1.986370000
H	-0.525255000	7.076776000	2.846616000
C	-0.102483000	5.331585000	1.655395000
H	-0.723008000	4.669491000	2.250371000
H	-2.151047000	-7.681173000	-0.548595000
C	-0.858341000	-7.535889000	1.175886000
H	-0.946287000	-8.586526000	1.434668000
C	-0.058516000	-6.683968000	1.949034000
H	0.473982000	-7.072046000	2.812057000
C	0.054208000	-5.330626000	1.614335000
H	0.672359000	-4.666422000	2.209425000
O	-0.226813000	-0.131971000	-2.607183000
H	-0.243221000	-1.103382000	-2.495646000
C	0.960618000	0.294496000	-3.341273000
H	1.024710000	1.372901000	-3.192054000
H	0.860913000	0.072232000	-4.412188000
H	1.864300000	-0.174350000	-2.939286000

⁴P-3_{hs}

C	0.000030000	-0.000093000	2.109996000
C	-0.678282000	-0.068632000	4.300827000
H	-1.384459000	-0.143922000	5.110096000
C	0.678500000	0.068173000	4.300787000
H	1.384736000	0.143363000	5.110014000
H	-3.124143000	-0.069400000	3.353270000
H	-2.648532000	0.458826000	1.713208000
H	-2.623865000	-1.266807000	2.120748000
N	-1.070946000	-0.104998000	2.961092000
N	1.071065000	0.104712000	2.961028000
N	1.573539000	1.307556000	-0.445153000
N	-1.332486000	1.565179000	-0.380962000
N	-1.573559000	-1.307517000	-0.445186000
N	1.332459000	-1.565137000	-0.381030000
C	2.913215000	0.988651000	-0.575030000
C	1.496388000	2.675376000	-0.234026000
C	-0.991621000	2.903751000	-0.352324000
C	-2.684551000	1.493480000	-0.678732000
C	-2.913234000	-0.988609000	-0.575066000
C	-1.496409000	-2.675342000	-0.234098000
C	0.991597000	-2.903710000	-0.352419000
C	2.684524000	-1.493432000	-0.678796000
C	3.710231000	2.187884000	-0.388413000
H	4.787943000	2.225195000	-0.408615000
C	2.841437000	3.219851000	-0.157636000
H	3.084850000	4.251160000	0.041988000
C	-2.169280000	3.704375000	-0.647451000
H	-2.181317000	4.780471000	-0.720734000
C	-3.203589000	2.838322000	-0.866150000
H	-4.215502000	3.078713000	-1.150804000
C	-3.710251000	-2.187846000	-0.388481000
H	-4.787963000	-2.225156000	-0.408688000
C	-2.841458000	-3.219819000	-0.157725000
H	-3.084872000	-4.251134000	0.041871000
C	2.169253000	-3.704328000	-0.647577000
H	2.181290000	-4.780421000	-0.720889000
C	3.203562000	-2.838269000	-0.866258000
H	4.215474000	-3.078652000	-1.150921000
C	3.441126000	-0.307491000	-0.750541000
C	0.306407000	3.429188000	-0.179258000
C	-3.441147000	0.307539000	-0.750532000
C	-0.306428000	-3.429153000	-0.179353000
C	4.910842000	-0.422272000	-0.977515000
C	5.524012000	0.265802000	-2.043154000

C	2.456048000	0.258803000	2.508688000
H	3.124294000	0.069156000	3.353050000
H	2.648579000	-0.458978000	1.712986000
H	2.623883000	1.266625000	2.120643000
C	-2.455967000	-0.259015000	2.508846000
H	4.906044000	0.866918000	-2.701701000
C	6.903204000	0.172556000	-2.256265000
H	7.356903000	0.704599000	-3.086880000
C	7.696221000	-0.610134000	-1.406668000
H	8.766605000	-0.683228000	-1.572345000
C	7.099335000	-1.297880000	-0.341896000
H	7.707454000	-1.901506000	0.325107000
C	5.719983000	-1.203412000	-0.129046000
H	5.256660000	-1.731442000	0.697866000
C	0.413678000	4.908396000	-0.010866000
C	1.167297000	5.697937000	-0.901281000
H	1.678778000	5.214575000	-1.726639000
C	1.246021000	7.084888000	-0.736078000
H	1.826468000	7.678283000	-1.436001000
C	0.569026000	7.708713000	0.320257000
H	0.629607000	8.785160000	0.447494000
C	-0.190626000	6.935593000	1.208080000
H	-0.718652000	7.411062000	2.029154000
C	-0.268804000	5.548923000	1.042123000
H	-0.856629000	4.946297000	1.726767000
C	-4.910862000	0.422328000	-0.977507000
C	-5.524028000	-0.265709000	-2.043173000
H	-4.906058000	-0.866802000	-2.701738000
C	-6.903219000	-0.172454000	-2.256286000
H	-7.356916000	-0.704468000	-3.086920000
C	-7.696239000	0.610207000	-1.406664000
H	-8.766623000	0.683307000	-1.572343000
C	-7.099356000	1.297916000	-0.341867000
H	-7.707477000	1.901520000	0.325154000
C	-5.720006000	1.203440000	-0.129015000
H	-5.256684000	1.731441000	0.697917000
C	-0.413694000	-4.908366000	-0.010995000
C	-1.167317000	-5.697888000	-0.901422000
H	-1.678805000	-5.214510000	-1.726766000
C	-1.246036000	-7.084843000	-0.736251000
H	-1.826486000	-7.678224000	-1.436183000
C	-0.569032000	-7.708691000	0.320065000
H	-0.629609000	-8.785141000	0.447278000
C	0.190624000	-6.935589000	1.207901000

H	0.718658000	-7.411076000	2.028960000
C	0.268797000	-5.548915000	1.041975000
H	0.856625000	-4.946303000	1.726629000
Co	-0.000012000	0.000028000	-0.038257000

²P-3_{Is}

C	0.000089000	-0.000034000	1.942220000
C	0.679702000	0.035545000	4.145754000
H	1.389850000	0.076915000	4.954257000
C	-0.679088000	-0.036007000	4.145880000
H	-1.389075000	-0.077517000	4.954517000
C	-2.468369000	-0.151869000	2.374204000
H	-3.113084000	0.097868000	3.221982000
H	-2.640661000	0.550288000	1.561608000
H	-2.696061000	-1.162037000	2.024030000
C	2.468611000	0.151795000	2.373702000
H	3.113534000	-0.097870000	3.221343000
H	2.640802000	-0.550347000	1.561065000
H	2.696125000	1.161982000	2.023468000
N	1.073216000	0.053813000	2.802884000
N	-1.072876000	-0.054012000	2.803085000
N	-1.538762000	-1.247383000	-0.424267000
N	1.249834000	-1.532754000	-0.410890000
N	1.538702000	1.247414000	-0.424283000
N	-1.249898000	1.532783000	-0.410823000
C	-2.860981000	-0.929216000	-0.683443000
C	-1.518495000	-2.594608000	-0.087487000
C	0.922329000	-2.863111000	-0.214818000
C	2.585955000	-1.512466000	-0.798697000
C	2.860920000	0.929246000	-0.683466000
C	1.518442000	2.594632000	-0.087473000
C	-0.922386000	2.863138000	-0.214749000
C	-2.586024000	1.512500000	-0.798615000
C	-3.695092000	-2.092615000	-0.462467000
H	-4.767981000	-2.107926000	-0.570079000
C	-2.873906000	-3.106563000	-0.056618000
H	-3.150418000	-4.110880000	0.220363000
C	2.072263000	-3.698224000	-0.500131000
H	2.072979000	-4.775629000	-0.451671000
C	3.083086000	-2.870996000	-0.895437000
H	4.071692000	-3.144467000	-1.226750000
C	3.695035000	2.092639000	-0.462474000
H	4.767924000	2.107949000	-0.570092000
C	2.873855000	3.106583000	-0.056606000

H	3.150371000	4.110895000	0.220392000
C	-2.072327000	3.698254000	-0.500028000
H	-2.073042000	4.775659000	-0.451556000
C	-3.083157000	2.871032000	-0.895326000
H	-4.071768000	3.144507000	-1.226619000
C	-3.359494000	0.355187000	-0.951230000
C	-0.358301000	-3.364547000	0.063062000
C	3.359428000	-0.355152000	-0.951282000
C	0.358251000	3.364570000	0.063106000
C	-4.800327000	0.476455000	-1.312702000
C	-5.306027000	-0.217057000	-2.429682000
H	-4.625842000	-0.818249000	-3.023920000
C	-6.659259000	-0.130630000	-2.772736000
H	-7.029998000	-0.666347000	-3.641257000
C	-7.532862000	0.648141000	-2.002287000
H	-8.583118000	0.715822000	-2.268461000
C	-7.043582000	1.336493000	-0.884421000
H	-7.715916000	1.933693000	-0.275900000
C	-5.690120000	1.249231000	-0.541503000
H	-5.312391000	1.772576000	0.330449000
C	-0.469853000	-4.811108000	0.405174000
C	-1.224734000	-5.703330000	-0.380533000
H	-1.738876000	-5.326068000	-1.257839000
C	-1.298561000	-7.060468000	-0.048704000
H	-1.880426000	-7.735289000	-0.669144000
C	-0.614284000	-7.550760000	1.071288000
H	-0.671334000	-8.604065000	1.327859000
C	0.149372000	-6.674957000	1.854206000
H	0.684757000	-7.047242000	2.722376000
C	0.222893000	-5.318239000	1.521951000
H	0.814299000	-4.636070000	2.123923000
C	4.800259000	-0.476414000	-1.312764000
C	5.305955000	0.217122000	-2.429731000
H	4.625768000	0.818326000	-3.023954000
C	6.659186000	0.130703000	-2.772791000
H	7.029922000	0.666437000	-3.641302000
C	7.532793000	-0.648083000	-2.002361000
H	8.583047000	-0.715757000	-2.268539000
C	7.043517000	-1.336457000	-0.884507000
H	7.715854000	-1.933668000	-0.275999000
C	5.690056000	-1.249203000	-0.541582000
H	5.312331000	-1.772566000	0.330361000
C	0.469813000	4.811129000	0.405227000
C	1.224680000	5.703354000	-0.380491000
H	1.738803000	5.326095000	-1.257809000

C	1.298515000	7.060490000	-0.048657000
H	1.880368000	7.735314000	-0.669105000
C	0.614261000	7.550778000	1.071351000
H	0.671317000	8.604082000	1.327926000
C	-0.149382000	6.674972000	1.854279000
H	-0.684749000	7.047253000	2.722461000
C	-0.222911000	5.318256000	1.522019000
H	-0.814307000	4.636085000	2.123999000
Co	-0.000024000	0.000015000	-0.235483000

C-H bond activation of CHD by species 1

***RC-1_{hs}**

Mn	-0.126368000	0.038267000	-0.080591000
O	-0.025846000	-0.050144000	1.598085000
C	-0.274703000	0.143656000	-2.337600000
C	-1.082499000	0.092698000	-4.496321000
H	-1.827696000	-0.037893000	-5.262280000
C	0.231660000	0.430736000	-4.568384000
H	0.866538000	0.647055000	-5.410512000
C	2.104308000	0.758628000	-2.940711000
H	2.566959000	1.200185000	-3.827887000
H	2.147397000	1.466508000	-2.117956000
H	2.641692000	-0.150495000	-2.662542000
C	-2.715064000	-0.436783000	-2.675542000
H	-3.281157000	-0.822959000	-3.528079000
H	-2.640008000	-1.205398000	-1.911808000
H	-3.226076000	0.435589000	-2.262212000
N	-1.372717000	-0.080825000	-3.140151000
N	0.705881000	0.458046000	-3.253867000
N	1.715588000	-0.722145000	-0.272010000
N	-0.924232000	-1.799724000	-0.174273000
N	-1.969256000	0.804615000	0.018759000
N	0.663510000	1.879706000	-0.119924000
C	2.897965000	-0.058984000	-0.017161000
C	2.032486000	-2.003556000	-0.687803000
C	-0.240793000	-2.960306000	-0.471498000
C	-2.162748000	-2.161466000	0.333659000
C	-3.108862000	0.119367000	0.385301000
C	-2.333113000	2.109123000	-0.262506000
C	-0.046466000	3.055254000	-0.247857000
C	1.961012000	2.210531000	0.243667000
C	4.005086000	-0.937015000	-0.338289000
H	5.045379000	-0.663603000	-0.263860000

C	3.475617000	-2.116392000	-0.785265000
H	4.005960000	-2.988782000	-1.130595000
C	-1.084692000	-4.097290000	-0.155180000
H	-0.789961000	-5.127919000	-0.272576000
C	-2.246561000	-3.607819000	0.373016000
H	-3.083590000	-4.166294000	0.759528000
C	-4.245599000	1.011928000	0.278996000
H	-5.266806000	0.727827000	0.477948000
C	-3.776688000	2.220387000	-0.159140000
H	-4.345511000	3.111392000	-0.369808000
C	0.833998000	4.170420000	0.043329000
H	0.530380000	5.205157000	0.040322000
C	2.052009000	3.650596000	0.381887000
H	2.932535000	4.185366000	0.698748000
C	3.028224000	1.302194000	0.312236000
C	1.115489000	-3.057258000	-0.833021000
C	-3.198547000	-1.262725000	0.628987000
C	-1.435407000	3.173649000	-0.442834000
C	4.395286000	1.804156000	0.626218000
C	5.141523000	1.210427000	1.663510000
H	4.691896000	0.408509000	2.235545000
C	6.434046000	1.655770000	1.958286000
H	6.990657000	1.192107000	2.766851000
C	7.006621000	2.698936000	1.218868000
H	8.009597000	3.044912000	1.448444000
C	6.278329000	3.290679000	0.178511000
H	6.718972000	4.091500000	-0.407559000
C	4.985489000	2.845363000	-0.116789000
H	4.427106000	3.293410000	-0.931863000
C	1.608312000	-4.401156000	-1.249999000
C	2.614487000	-5.076238000	-0.532341000
H	3.041037000	-4.605102000	0.346452000
C	3.044220000	-6.346559000	-0.930966000
H	3.816218000	-6.856050000	-0.362581000
C	2.471234000	-6.966351000	-2.049317000
H	2.804397000	-7.952632000	-2.356957000
C	1.460289000	-6.309726000	-2.763330000
H	1.008700000	-6.784809000	-3.628912000
C	1.030844000	-5.039624000	-2.364718000
H	0.246463000	-4.527951000	-2.913222000
C	-4.499143000	-1.784921000	1.132672000
C	-5.030702000	-1.282419000	2.336665000
H	-4.465706000	-0.537288000	2.886783000
C	-6.257837000	-1.745791000	2.822053000
H	-6.649518000	-1.354952000	3.756084000

C	-6.976329000	-2.715691000	2.110352000
H	-7.928436000	-3.075569000	2.487752000
C	-6.460769000	-3.217194000	0.908045000
H	-7.016699000	-3.961411000	0.345936000
C	-5.233321000	-2.753889000	0.422231000
H	-4.839023000	-3.132061000	-0.515140000
C	-1.965882000	4.541731000	-0.707332000
C	-2.879701000	5.163326000	0.165379000
H	-3.204900000	4.631873000	1.053002000
C	-3.345654000	6.456878000	-0.093148000
C	1.475263000	-1.922664000	3.532797000
C	2.558128000	-0.872180000	3.425050000
C	2.366093000	0.402969000	3.784402000
H	0.516975000	1.431317000	3.514010000
H	1.904707000	-2.881347000	3.866629000
H	-0.313749000	-2.275300000	4.815717000
H	-0.665292000	0.048848000	5.469954000
H	3.161006000	1.136762000	3.665502000
H	3.511621000	-1.196084000	3.008861000
H	1.052773000	-2.092891000	2.527882000
H	1.217838000	1.641434000	5.128052000

³RC-1_h

Mn	0.342062000	0.027101000	-0.074321000
C	0.652007000	0.034011000	2.135609000
C	0.660930000	0.645700000	4.357072000
H	0.466900000	1.288456000	5.198383000
C	1.240123000	-0.579901000	4.277300000
H	1.652986000	-1.223415000	5.034979000
C	1.773911000	-2.220912000	2.476232000
H	2.326872000	-2.663824000	3.309239000
H	0.971168000	-2.892747000	2.167723000
H	2.449456000	-2.061930000	1.640765000
C	-0.344481000	2.285567000	2.769451000
H	-0.648638000	2.727564000	3.722279000
H	0.339656000	2.959801000	2.251971000
H	-1.223720000	2.123226000	2.152527000
N	0.308970000	1.004852000	3.053721000
N	1.228422000	-0.937760000	2.927029000
N	2.316455000	-0.299725000	-0.276845000
N	0.655708000	2.014284000	-0.065219000
N	-1.605486000	0.349373000	0.259371000
N	0.039902000	-1.951135000	0.020551000
C	2.902468000	-1.496988000	-0.636140000

H	-4.044663000	6.924172000	0.593662000
C	-2.901600000	7.153451000	-1.224761000
H	-3.262859000	8.157561000	-1.423893000
C	-1.982521000	6.550155000	-2.093334000
H	-1.630492000	7.084862000	-2.970272000
C	-1.516601000	5.256875000	-1.834566000
H	-0.802262000	4.786109000	-2.502288000
C	0.165580000	-0.220276000	4.819678000
C	0.358370000	-1.495653000	4.460738000
C	1.046860000	0.905222000	4.326426000
C	3.328919000	0.625696000	-0.106288000
C	1.884951000	2.640123000	-0.045836000
C	-0.299467000	2.979276000	-0.333253000
C	-2.273505000	1.546742000	0.082339000
C	-2.521705000	-0.567537000	0.744988000
C	-1.125440000	-2.578745000	0.406830000
C	0.884370000	-2.921758000	-0.494055000
C	4.343608000	-1.335419000	-0.631765000
H	5.050272000	-2.121050000	-0.847706000
C	4.606609000	-0.042518000	-0.270135000
H	5.570440000	0.422175000	-0.140215000
C	1.699287000	4.055377000	-0.306776000
H	2.497480000	4.777726000	-0.372190000
C	0.363429000	4.255198000	-0.522480000
H	-0.128829000	5.175220000	-0.792380000
C	-3.648348000	1.386892000	0.512595000
H	-4.389859000	2.169361000	0.503851000
C	-3.788677000	0.102090000	0.958385000
H	-4.669380000	-0.354407000	1.379198000
C	-1.017244000	-3.996217000	0.121420000
H	-1.796012000	-4.720021000	0.302275000
C	0.200925000	-4.199180000	-0.468840000
H	0.601084000	-5.123228000	-0.853581000
C	2.230183000	-2.718090000	-0.836979000
C	3.139992000	2.009352000	0.053419000
C	-1.689289000	2.773335000	-0.289116000
C	-2.293061000	-1.945975000	0.875125000
C	3.036997000	-3.863615000	-1.344661000
C	3.708450000	-3.751680000	-2.578042000
H	3.605874000	-2.833750000	-3.147195000
C	4.485217000	-4.807246000	-3.066489000
H	4.989130000	-4.707397000	-4.022891000
C	4.608354000	-5.991675000	-2.328016000
H	5.210896000	-6.811179000	-2.707211000
C	3.951948000	-6.111747000	-1.096124000

H	4.051281000	-7.022407000	-0.513216000
C	3.174865000	-5.055827000	-0.607834000
H	2.675878000	-5.142690000	0.351590000
C	4.331171000	2.893735000	0.204494000
C	5.361733000	2.917335000	-0.755066000
H	5.284803000	2.274215000	-1.624928000
C	6.459622000	3.770927000	-0.602395000
H	7.241879000	3.781047000	-1.355194000
C	6.543891000	4.619933000	0.508997000
H	7.395609000	5.282731000	0.626039000
C	5.519357000	4.613604000	1.464635000
H	5.575898000	5.270279000	2.327474000
C	4.421930000	3.760033000	1.311486000
H	3.624911000	3.753074000	2.048040000
C	-2.607964000	3.924095000	-0.518375000
C	-3.649689000	3.812460000	-1.460686000
H	-3.762121000	2.887663000	-2.015835000
C	-4.533106000	4.875483000	-1.674698000
H	-5.326089000	4.773582000	-2.409441000
C	-4.396420000	6.066171000	-0.948954000
H	-5.082255000	6.890863000	-1.116712000
C	-3.372996000	6.183329000	0.000631000
H	-3.268841000	7.096350000	0.579121000
C	-2.489329000	5.120585000	0.216362000
H	-1.707155000	5.205825000	0.963244000
C	-3.361506000	-2.825220000	1.429371000
C	-4.662125000	-2.860079000	0.889293000
H	-4.896973000	-2.230720000	0.040441000
C	-5.634366000	-3.712940000	1.423036000
H	-6.629334000	-3.730655000	0.988777000
C	-5.324844000	-4.550547000	2.502204000
H	-6.080080000	-5.212532000	2.914303000
C	-4.032261000	-4.532438000	3.042585000
H	-3.782523000	-5.178752000	3.878580000
C	-3.060778000	-3.679722000	2.509281000
H	-2.058529000	-3.662727000	2.925058000
O	0.178650000	0.040828000	-1.774424000
C	-4.982083000	-0.884364000	-2.396211000
C	-3.630247000	-1.553803000	-2.273235000
C	-2.490443000	-1.002428000	-2.709487000
C	-2.423876000	0.342279000	-3.392314000
C	-3.785470000	0.944857000	-3.636448000
C	-4.927719000	0.405058000	-3.185377000
H	-5.710029000	-1.573033000	-2.859534000
H	-3.605655000	-2.521776000	-1.778138000

H	-1.540399000	-1.505646000	-2.556035000
H	-1.800669000	1.015021000	-2.782459000
H	-3.816583000	1.871275000	-4.209079000
H	-5.879687000	0.893582000	-3.388729000
H	-1.875564000	0.249351000	-4.344540000
H	-5.384947000	-0.673888000	-1.387840000

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Mn	0.304545000	0.009704000	-0.055094000
O	0.253672000	0.010958000	-1.824418000
C	0.517894000	0.011755000	2.119097000
C	0.630232000	0.691709000	4.316496000
H	0.619648000	1.402065000	5.125243000
C	0.770958000	-0.659206000	4.307563000
H	0.915975000	-1.366134000	5.106341000
C	0.844662000	-2.461988000	2.577205000
H	0.730077000	-3.078510000	3.473252000
H	0.073184000	-2.721795000	1.858547000
H	1.826693000	-2.640422000	2.134113000
C	0.280689000	2.487532000	2.613105000
H	0.595693000	3.110352000	3.455236000
H	0.886505000	2.721146000	1.743219000
H	-0.769739000	2.682795000	2.386824000
N	0.480281000	1.084401000	2.983659000
N	0.699743000	-1.057756000	2.969746000
N	1.658539000	-1.444646000	-0.165945000
N	1.744399000	1.388733000	-0.150533000
N	-1.052757000	1.448377000	0.083540000
N	-1.122933000	-1.355789000	0.129338000
C	1.402326000	-2.756167000	-0.499729000
C	3.015925000	-1.322070000	0.070839000
C	3.096704000	1.149512000	-0.036638000
C	1.579937000	2.682966000	-0.617605000
C	-0.870725000	2.762606000	-0.296976000
C	-2.315020000	1.337411000	0.639966000
C	-2.405150000	-1.126896000	0.583610000
C	-1.060501000	-2.668557000	-0.318170000
C	2.638863000	-3.507515000	-0.417145000
H	2.724823000	-4.567148000	-0.599905000
C	3.621140000	-2.638620000	-0.022934000
H	4.660337000	-2.857877000	0.160724000
C	3.818038000	2.348452000	-0.423809000
H	4.892805000	2.434829000	-0.445386000
C	2.890040000	3.271559000	-0.819932000

H	3.069518000	4.257163000	-1.218058000
C	-2.052858000	3.517079000	0.062372000
H	-2.175927000	4.576272000	-0.099828000
C	-2.918593000	2.654439000	0.679928000
H	-3.883197000	2.883690000	1.101692000
C	-3.181223000	-2.339853000	0.421772000
H	-4.226320000	-2.432930000	0.670817000
C	-2.371553000	-3.266770000	-0.174687000
H	-2.634287000	-4.262480000	-0.492789000
C	0.125804000	-3.328602000	-0.670797000
C	3.700845000	-0.101183000	0.196673000
C	0.341573000	3.335911000	-0.728378000
C	-2.938913000	0.120590000	0.960783000
C	0.070373000	-4.740411000	-1.141456000
C	0.659555000	-5.079539000	-2.375621000
H	1.126447000	-4.296598000	-2.963959000
C	0.634102000	-6.398505000	-2.840074000
H	1.085109000	-6.640939000	-3.797376000
C	0.024275000	-7.402687000	-2.076482000
H	0.003860000	-8.426367000	-2.437177000
C	-0.555451000	-7.079211000	-0.842779000
H	-1.018810000	-7.854034000	-0.239527000
C	-0.529950000	-5.759881000	-0.377822000
H	-0.964769000	-5.512100000	0.584618000
C	5.173744000	-0.105624000	0.425886000
C	6.058843000	-0.776956000	-0.439687000
H	5.657461000	-1.304962000	-1.297666000
C	7.439003000	-0.745334000	-0.212935000
H	8.107827000	-1.262662000	-0.893962000
C	7.958845000	-0.037142000	0.878550000
H	9.030041000	-0.012500000	1.052825000
C	7.089032000	0.645789000	1.738759000
H	7.484024000	1.200505000	2.584431000
C	5.709158000	0.614325000	1.511708000
H	5.031321000	1.144538000	2.173042000
C	0.290793000	4.744134000	-1.208215000
C	-0.566553000	5.083229000	-2.273644000
H	-1.154350000	4.299932000	-2.741128000
C	-0.650670000	6.402066000	-2.731054000
H	-1.310693000	6.644004000	-3.558353000
C	0.117940000	7.406725000	-2.128229000
H	0.053251000	8.430555000	-2.483151000
C	0.967848000	7.083300000	-1.062411000
H	1.557555000	7.858404000	-0.582407000
C	1.051595000	5.764099000	-0.604604000

H	1.696268000	5.516511000	0.231937000
C	-4.279628000	0.117192000	1.609265000
C	-5.379887000	0.814532000	1.072922000
H	-5.252484000	1.363271000	0.148064000
C	-6.627730000	0.773435000	1.703726000
H	-7.466183000	1.310497000	1.270824000
C	-6.801709000	0.030611000	2.878711000
H	-7.771098000	-0.001278000	3.366238000
C	-5.718392000	-0.676943000	3.415992000
H	-5.844270000	-1.258078000	4.324483000
C	-4.470620000	-0.634908000	2.785799000
H	-3.628396000	-1.180846000	3.198387000
C	-3.979024000	1.048690000	-2.261552000
C	-2.751164000	1.287850000	-2.769275000
C	-4.567141000	-0.340928000	-2.160228000
C	-1.859423000	0.217158000	-3.242705000
C	-2.466728000	-1.123686000	-3.298080000
C	-3.686897000	-1.396428000	-2.789314000
H	-4.744265000	-0.595338000	-1.100179000
H	-1.247903000	0.481939000	-4.113724000
H	-2.376227000	2.308234000	-2.809223000
H	-4.591804000	1.876670000	-1.910179000
H	-4.078206000	-2.410606000	-2.815931000
H	-1.873950000	-1.922398000	-3.738486000
H	-0.828393000	0.115126000	-2.413502000
H	-5.572471000	-0.360287000	-2.621446000

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Mn	-0.278692000	0.002721000	0.033201000
C	-0.575375000	0.009382000	2.225880000
C	-0.923558000	-0.671097000	4.398554000
H	-1.078400000	-1.383702000	5.190358000
C	-0.831387000	0.684171000	4.413068000
H	-0.896403000	1.394684000	5.219131000
C	-0.478439000	2.492354000	2.726874000
H	-0.285985000	3.062122000	3.640439000
H	0.358083000	2.606448000	2.044311000
H	-1.388912000	2.860741000	2.250253000
C	-0.786877000	-2.477458000	2.679790000
H	-1.197229000	-3.053445000	3.514068000
H	-1.417625000	-2.604973000	1.805478000
H	0.221871000	-2.828875000	2.454888000
N	-0.767866000	-1.065387000	3.067615000
N	-0.618004000	1.081217000	3.091043000

N	-1.364898000	1.690416000	-0.076857000
N	-1.954263000	-1.108799000	-0.118091000
N	0.801122000	-1.666117000	0.185404000
N	1.381895000	1.104624000	0.301120000
C	-0.865997000	2.951559000	-0.320670000
C	-2.734075000	1.799161000	0.064963000
C	-3.243252000	-0.623781000	-0.107759000
C	-2.005530000	-2.416406000	-0.570975000
C	0.383486000	-2.932985000	-0.171463000
C	2.071363000	-1.781321000	0.727858000
C	2.621196000	0.629449000	0.670515000
C	1.544683000	2.419323000	-0.105622000
C	-1.957069000	3.906491000	-0.270394000
H	-1.848349000	4.972215000	-0.396738000
C	-3.098898000	3.204514000	0.007657000
H	-4.094827000	3.594896000	0.141262000
C	-4.148661000	-1.671103000	-0.549232000
H	-5.216086000	-1.556125000	-0.653127000
C	-3.384489000	-2.758083000	-0.870426000
H	-3.715608000	-3.697985000	-1.281785000
C	1.411026000	-3.886343000	0.191230000
H	1.337260000	-4.952976000	0.048886000
C	2.426145000	-3.184881000	0.787934000
H	3.336590000	-3.578439000	1.210013000
C	3.605505000	1.680098000	0.494335000
H	4.661103000	1.571039000	0.686289000
C	2.951074000	2.766336000	-0.018824000
H	3.375324000	3.712071000	-0.315231000
C	0.495290000	3.295612000	-0.430777000
C	-3.629367000	0.714546000	0.107417000
C	-0.902111000	-3.283825000	-0.632633000
C	2.928704000	-0.703659000	1.003601000
C	0.814077000	4.695613000	-0.827421000
C	0.320609000	5.204667000	-2.045034000
H	-0.270083000	4.553995000	-2.681148000
C	0.596570000	6.519645000	-2.433445000
H	0.215323000	6.892851000	-3.379020000
C	1.367378000	7.350946000	-1.609775000
H	1.582262000	8.371348000	-1.911647000
C	1.856666000	6.858669000	-0.392763000
H	2.445290000	7.499881000	0.256420000
C	1.580094000	5.543542000	-0.004070000
H	1.947341000	5.166091000	0.944446000
C	-5.090134000	0.980449000	0.240944000
C	-5.778207000	1.819522000	-0.657170000

H	-5.229722000	2.282491000	-1.470082000
C	-7.153513000	2.036330000	-0.520490000
H	-7.669108000	2.680972000	-1.225780000
C	-7.867018000	1.413224000	0.511878000
H	-8.934411000	1.581407000	0.616400000
C	-7.196483000	0.565379000	1.403278000
H	-7.742680000	0.075367000	2.203607000
C	-5.821363000	0.349005000	1.266442000
H	-5.297806000	-0.308826000	1.952726000
C	-1.092342000	-4.679464000	-1.114343000
C	-0.275122000	-5.176936000	-2.149343000
H	0.467156000	-4.519833000	-2.590697000
C	-0.422546000	-6.489290000	-2.609229000
H	0.210467000	-6.852615000	-3.412957000
C	-1.388139000	-7.330503000	-2.040541000
H	-1.503944000	-8.348945000	-2.398032000
C	-2.201525000	-6.850490000	-1.005621000
H	-2.944285000	-7.499703000	-0.551930000
C	-2.052860000	-5.538087000	-0.544708000
H	-2.671634000	-5.171062000	0.267198000
C	4.302229000	-0.972228000	1.512781000
C	5.187547000	-1.834083000	0.835049000
H	4.855194000	-2.318737000	-0.075796000
C	6.484933000	-2.046427000	1.313375000
H	7.155272000	-2.708864000	0.774255000
C	6.923594000	-1.397061000	2.474790000
H	7.930802000	-1.561483000	2.844808000
C	6.056670000	-0.529113000	3.151746000
H	6.389317000	-0.020063000	4.051264000
C	4.759606000	-0.317133000	2.672968000
H	4.085445000	0.356323000	3.192124000
O	-0.183389000	0.085144000	-1.720814000
C	4.114379000	0.870824000	-3.078982000
C	2.979184000	1.015782000	-4.065523000
C	1.920889000	0.184931000	-4.083271000
C	1.757984000	-0.922142000	-3.100937000
C	2.981604000	-1.235055000	-2.319710000
C	4.049298000	-0.415624000	-2.290597000
H	5.083503000	0.945056000	-3.602347000
H	3.043722000	1.838472000	-4.774810000
H	1.115153000	0.336944000	-4.796760000
H	0.898011000	-0.519970000	-2.356058000
H	2.970934000	-2.145063000	-1.726245000
H	4.911653000	-0.658705000	-1.674533000
H	1.268581000	-1.811131000	-3.520557000

H	4.101278000	1.723575000	-2.375579000
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⁶INT1-1_{hs}

Mn	0.316743000	0.019692000	0.151073000
C	0.519015000	-0.034540000	2.329163000
C	0.352463000	0.483908000	4.562433000
H	0.040691000	1.063518000	5.414007000
C	1.078429000	-0.660362000	4.469107000
H	1.534344000	-1.279387000	5.222349000
C	1.898709000	-2.143556000	2.638771000
H	2.095412000	-2.786176000	3.501393000
H	1.288895000	-2.679070000	1.917514000
H	2.842364000	-1.853493000	2.174025000
C	-0.777069000	2.047164000	2.978812000
H	-0.801627000	2.658169000	3.885384000
H	-0.312474000	2.608420000	2.174241000
H	-1.794187000	1.771702000	2.695561000
N	0.022329000	0.852565000	3.257573000
N	1.170026000	-0.963874000	3.109734000
N	2.196711000	-0.755582000	-0.069683000
N	1.066134000	1.999611000	0.182706000
N	-1.599724000	0.772647000	0.287514000
N	-0.463045000	-1.952004000	0.244513000
C	2.493820000	-2.061616000	-0.392111000
C	3.371863000	-0.037628000	0.023535000
C	2.401366000	2.295263000	0.052568000
C	0.332870000	3.113215000	-0.176838000
C	-1.951099000	2.098501000	0.130381000
C	-2.718023000	0.062957000	0.696459000
C	-1.789353000	-2.259888000	0.418617000
C	0.181483000	-3.055746000	-0.276058000
C	3.941322000	-2.199892000	-0.418716000
H	4.471638000	-3.120208000	-0.606633000
C	4.478633000	-0.970674000	-0.136894000
H	5.523819000	-0.717104000	-0.061348000
C	2.527193000	3.689246000	-0.359143000
H	3.461267000	4.193848000	-0.551309000
C	1.260681000	4.181657000	-0.524681000
H	0.978696000	5.160786000	-0.878399000
C	-3.344901000	2.244994000	0.504457000
H	-3.888041000	3.176925000	0.507676000
C	-3.801195000	1.010852000	0.890372000
H	-4.784821000	0.767947000	1.258020000
C	-2.000092000	-3.643043000	0.010683000

H	-2.951258000	-4.152547000	0.019186000
C	-0.797597000	-4.121747000	-0.439843000
H	-0.595540000	-5.093669000	-0.861717000
C	1.566234000	-3.121298000	-0.559531000
C	3.477857000	1.372725000	0.112219000
C	-1.080204000	3.173644000	-0.189600000
C	-2.815468000	-1.347321000	0.778242000
C	2.113013000	-4.422161000	-1.039978000
C	2.852727000	-4.482149000	-2.238191000
H	3.003511000	-3.569368000	-2.804672000
C	3.373079000	-5.696467000	-2.697007000
H	3.933987000	-5.724862000	-3.626173000
C	3.164781000	-6.873900000	-1.966340000
H	3.567906000	-7.816633000	-2.323073000
C	2.432952000	-6.827383000	-0.772474000
H	2.272932000	-7.733994000	-0.196704000
C	1.912922000	-5.612651000	-0.313459000
H	1.351495000	-5.573930000	0.614185000
C	4.844398000	1.974001000	0.126429000
C	5.783890000	1.705644000	-0.888389000
H	5.504694000	1.042808000	-1.700011000
C	7.050255000	2.299534000	-0.864417000
H	7.759444000	2.086555000	-1.658492000
C	7.398660000	3.177085000	0.171015000
H	8.381453000	3.637946000	0.188333000
C	6.468469000	3.462565000	1.179018000
H	6.728916000	4.144474000	1.982852000
C	5.202048000	2.869098000	1.154087000
H	4.476895000	3.090132000	1.930676000
C	-1.727920000	4.469412000	-0.532876000
C	-2.727650000	4.511006000	-1.526868000
H	-2.997712000	3.589180000	-2.032362000
C	-3.350721000	5.717047000	-1.861870000
H	-4.113090000	5.732679000	-2.634979000
C	-2.988371000	6.903563000	-1.209877000
H	-3.471533000	7.839966000	-1.471128000
C	-1.999386000	6.874198000	-0.217686000
H	-1.719497000	7.787600000	0.298454000
C	-1.376096000	5.668045000	0.118823000
H	-0.618222000	5.642194000	0.894684000
C	-4.118295000	-1.956509000	1.172102000
C	-5.335003000	-1.608873000	0.550453000
H	-5.325229000	-0.875490000	-0.245347000
C	-6.535332000	-2.216029000	0.933677000
H	-7.459804000	-1.938894000	0.436152000

C	-6.545450000	-3.187553000	1.942825000
H	-7.477480000	-3.659103000	2.238457000
C	-5.342744000	-3.550729000	2.563093000
H	-5.339416000	-4.303586000	3.345474000
C	-4.143103000	-2.943280000	2.179856000
H	-3.210260000	-3.222887000	2.657968000
O	0.215141000	0.056882000	-1.684194000
H	-0.559895000	0.538811000	-2.039001000
C	-2.294016000	-1.335236000	-3.057701000
C	-1.782907000	-0.176442000	-3.876424000
C	-2.462271000	1.014515000	-3.960314000
C	-3.716357000	1.199036000	-3.311109000
C	-4.287973000	0.124670000	-2.572203000
C	-3.647062000	-1.081684000	-2.448104000
H	-2.315481000	-2.258992000	-3.667282000
H	-0.819987000	-0.298431000	-4.361836000
H	-2.041020000	1.833588000	-4.537923000
H	-5.255905000	0.274147000	-2.099909000
H	-4.094649000	-1.886906000	-1.874380000
H	-4.245251000	2.142414000	-3.400745000
H	-1.553550000	-1.551113000	-2.263913000

⁴INT1-1_{hs}

Mn	0.329237000	0.023830000	0.137772000
C	0.541393000	-0.037940000	2.313966000
C	0.336265000	0.440598000	4.552844000
H	-0.015989000	0.987093000	5.410503000
C	1.140103000	-0.649203000	4.447457000
H	1.637344000	-1.243678000	5.194250000
C	2.067247000	-2.047605000	2.601658000
H	2.324141000	-2.674704000	3.459848000
H	1.492977000	-2.627883000	1.885530000
H	2.979407000	-1.682693000	2.127602000
C	-0.897381000	1.940466000	2.986689000
H	-0.952290000	2.545591000	3.895887000
H	-0.480397000	2.533975000	2.179502000
H	-1.897073000	1.598727000	2.713506000
N	-0.016732000	0.801322000	3.251804000
N	1.254742000	-0.929120000	3.084858000
N	2.261907000	-0.610739000	-0.096900000
N	0.930865000	2.051886000	0.183617000
N	-1.638356000	0.636994000	0.286342000
N	-0.302331000	-1.997624000	0.209878000
C	2.654413000	-1.889321000	-0.426397000

C	3.381161000	0.190988000	0.002510000
C	2.241081000	2.445732000	0.052665000
C	0.116920000	3.114097000	-0.158862000
C	-2.086828000	1.935311000	0.146933000
C	-2.700907000	-0.158159000	0.687378000
C	-1.602833000	-2.402410000	0.381461000
C	0.420380000	-3.047934000	-0.318869000
C	4.108277000	-1.921095000	-0.451497000
H	4.704838000	-2.799170000	-0.642604000
C	4.553683000	-0.657361000	-0.162184000
H	5.577479000	-0.328604000	-0.083228000
C	2.262915000	3.849493000	-0.342825000
H	3.156661000	4.423320000	-0.532360000
C	0.963112000	4.250650000	-0.497093000
H	0.609535000	5.211236000	-0.837008000
C	-3.486652000	1.974244000	0.525988000
H	-4.096719000	2.863545000	0.541189000
C	-3.850069000	0.705178000	0.896167000
H	-4.812621000	0.385629000	1.260783000
C	-1.712650000	-3.794191000	-0.037232000
H	-2.624048000	-4.371788000	-0.031287000
C	-0.478815000	-4.180866000	-0.490928000
H	-0.206435000	-5.132298000	-0.919938000
C	1.806385000	-3.012703000	-0.600380000
C	3.382953000	1.604570000	0.101416000
C	-1.297357000	3.074046000	-0.162505000
C	-2.692576000	-1.572458000	0.754492000
C	2.447216000	-4.269459000	-1.081858000
C	3.196329000	-4.273336000	-2.275624000
H	3.283786000	-3.350965000	-2.839864000
C	3.806568000	-5.445670000	-2.732988000
H	4.373563000	-5.431276000	-3.658773000
C	3.680296000	-6.636587000	-2.005360000
H	4.153207000	-7.546756000	-2.360948000
C	2.939795000	-6.645689000	-0.816026000
H	2.842664000	-7.562552000	-0.242431000
C	2.330080000	-5.472866000	-0.358437000
H	1.762482000	-5.476820000	0.566292000
C	4.701586000	2.304563000	0.117200000
C	5.657028000	2.109549000	-0.899473000
H	5.426489000	1.430493000	-1.712994000
C	6.876053000	2.795334000	-0.875382000
H	7.597748000	2.637552000	-1.671107000
C	7.160063000	3.693543000	0.161953000
H	8.105956000	4.226024000	0.179291000

C	6.212674000	3.906351000	1.171955000
H	6.422948000	4.603467000	1.977438000
C	4.993701000	3.220790000	1.146974000
H	4.255096000	3.385924000	1.924758000
C	-2.036863000	4.326958000	-0.479420000
C	-3.044206000	4.315837000	-1.466416000
H	-3.254789000	3.386248000	-1.984976000
C	-3.751961000	5.481184000	-1.776390000
H	-4.519322000	5.456845000	-2.544396000
C	-3.468336000	6.678785000	-1.106006000
H	-4.017132000	7.583682000	-1.348010000
C	-2.472915000	6.701223000	-0.120093000
H	-2.253602000	7.622868000	0.410497000
C	-1.765053000	5.535744000	0.191595000
H	-1.001762000	5.549488000	0.962428000
C	-3.941139000	-2.282774000	1.156066000
C	-5.188124000	-2.025954000	0.551064000
H	-5.243897000	-1.288761000	-0.238645000
C	-6.333479000	-2.726545000	0.943086000
H	-7.282372000	-2.518023000	0.458157000
C	-6.257053000	-3.702536000	1.945024000
H	-7.146466000	-4.246436000	2.247649000
C	-5.022807000	-3.975507000	2.549367000
H	-4.952345000	-4.730671000	3.326377000
C	-3.878156000	-3.274841000	2.157226000
H	-2.921264000	-3.484640000	2.623444000
O	0.213537000	0.072924000	-1.696809000
H	-0.570772000	0.556220000	-2.030962000
C	-2.287889000	-1.264798000	-3.109638000
C	-1.925724000	0.021977000	-3.808600000
C	-2.757076000	1.115657000	-3.804734000
C	-4.029789000	1.074828000	-3.169040000
C	-4.454065000	-0.121603000	-2.525346000
C	-3.657123000	-1.237160000	-2.485323000
H	-2.205624000	-2.118193000	-3.810973000
H	-0.954216000	0.066444000	-4.291242000
H	-2.443585000	2.030794000	-4.301200000
H	-5.433958000	-0.139896000	-2.054389000
H	-3.991741000	-2.134667000	-1.974201000
H	-4.679235000	1.943981000	-3.187166000
H	-1.517635000	-1.473597000	-2.342502000

⁴INT1-1_{is}

Mn	0.322705000	0.028920000	0.045182000
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C	0.583881000	0.018727000	2.204847000
C	0.476729000	0.567834000	4.436290000
H	0.177682000	1.152036000	5.289423000
C	1.228968000	-0.558906000	4.336269000
H	1.725054000	-1.153782000	5.083706000
C	2.034185000	-2.042503000	2.496470000
H	2.256231000	-2.682864000	3.354804000
H	1.430301000	-2.591017000	1.780014000
H	2.966094000	-1.729315000	2.022203000
C	-0.751207000	2.071436000	2.865704000
H	-0.753249000	2.704824000	3.757247000
H	-0.343312000	2.626379000	2.026728000
H	-1.771799000	1.760494000	2.635785000
N	0.094843000	0.907291000	3.136805000
N	1.283608000	-0.881090000	2.978647000
N	2.191881000	-0.631234000	-0.196705000
N	0.956891000	1.937693000	0.006113000
N	-1.566675000	0.680489000	0.254792000
N	-0.328397000	-1.875506000	0.150385000
C	2.556346000	-1.909233000	-0.560170000
C	3.349562000	0.102336000	-0.023935000
C	2.275960000	2.338304000	0.004916000
C	0.188900000	3.039182000	-0.342455000
C	-2.013032000	1.967340000	0.032173000
C	-2.632019000	-0.045446000	0.766898000
C	-1.601101000	-2.278387000	0.490870000
C	0.324018000	-2.972154000	-0.391200000
C	4.003380000	-2.005584000	-0.553445000
H	4.561759000	-2.902604000	-0.769939000
C	4.490990000	-0.780801000	-0.182760000
H	5.522308000	-0.496040000	-0.051094000
C	2.344980000	3.748020000	-0.335281000
H	3.259307000	4.312803000	-0.426541000
C	1.068419000	4.166970000	-0.588201000
H	0.749179000	5.141147000	-0.921601000
C	-3.393176000	2.069535000	0.456867000
H	-3.984533000	2.970310000	0.413100000
C	-3.756971000	0.847663000	0.955759000
H	-4.704900000	0.572196000	1.387933000
C	-1.761387000	-3.681170000	0.157372000
H	-2.669030000	-4.246460000	0.299533000
C	-0.592452000	-4.095851000	-0.420829000
H	-0.370476000	-5.065965000	-0.835469000
C	1.682484000	-2.998703000	-0.749338000
C	3.402305000	1.500459000	0.126983000

C	-1.216882000	3.062693000	-0.361705000
C	-2.647738000	-1.441146000	0.930568000
C	2.270177000	-4.260718000	-1.277936000
C	2.966055000	-4.248346000	-2.503428000
H	3.042541000	-3.314518000	-3.050328000
C	3.538090000	-5.418828000	-3.012048000
H	4.063918000	-5.392236000	-3.961532000
C	3.427736000	-6.622911000	-2.303769000
H	3.870971000	-7.531665000	-2.698990000
C	2.744175000	-6.646659000	-1.081082000
H	2.663298000	-7.573305000	-0.520867000
C	2.172827000	-5.475738000	-0.571745000
H	1.655241000	-5.491039000	0.381600000
C	4.725390000	2.169587000	0.281441000
C	5.762556000	1.992380000	-0.655109000
H	5.591777000	1.353383000	-1.514487000
C	6.988292000	2.647544000	-0.495585000
H	7.774326000	2.504357000	-1.230760000
C	7.197285000	3.497120000	0.598778000
H	8.148493000	4.005781000	0.721178000
C	6.168465000	3.692785000	1.529566000
H	6.320492000	4.352682000	2.378336000
C	4.943197000	3.037310000	1.369926000
H	4.142498000	3.187497000	2.086992000
C	-1.929940000	4.314637000	-0.734874000
C	-2.927760000	4.270462000	-1.730512000
H	-3.142264000	3.321712000	-2.211822000
C	-3.625294000	5.427091000	-2.092399000
H	-4.385505000	5.377295000	-2.866213000
C	-3.342404000	6.647561000	-1.464394000
H	-3.883465000	7.545510000	-1.746344000
C	-2.359938000	6.701486000	-0.466943000
H	-2.143924000	7.640566000	0.033563000
C	-1.661980000	5.544882000	-0.103331000
H	-0.913439000	5.583450000	0.680861000
C	-3.860875000	-2.112651000	1.474825000
C	-5.146700000	-1.899106000	0.939442000
H	-5.258525000	-1.226901000	0.098626000
C	-6.259868000	-2.563809000	1.464643000
H	-7.241164000	-2.391291000	1.033022000
C	-6.110218000	-3.459223000	2.531451000
H	-6.974788000	-3.975293000	2.937199000
C	-4.835782000	-3.689374000	3.066431000
H	-4.709125000	-4.383206000	3.891953000
C	-3.723203000	-3.024807000	2.541358000

H	-2.734581000	-3.200870000	2.952489000
O	0.167907000	0.018614000	-1.791009000
C	-2.429010000	-1.406412000	-2.925581000
C	-2.107642000	-0.195748000	-3.765368000
C	-2.928189000	0.905112000	-3.804450000
C	-4.154865000	0.939673000	-3.082891000
C	-4.549535000	-0.193218000	-2.316575000
C	-3.762724000	-1.313408000	-2.234230000
H	-2.378827000	-2.326048000	-3.540095000
H	-1.168693000	-0.207242000	-4.310099000
H	-2.642396000	1.767673000	-4.401920000
H	-0.597464000	0.522925000	-2.133774000
H	-5.498916000	-0.159253000	-1.787153000
H	-4.075096000	-2.163483000	-1.635409000
H	-4.794112000	1.815307000	-3.130682000
H	-1.618608000	-1.533062000	-2.182562000

²INT1-1_{is}

Mn	0.327020000	0.030688000	0.039025000
C	0.585240000	0.019613000	2.199244000
C	0.456288000	0.554599000	4.433004000
H	0.139186000	1.126590000	5.287884000
C	1.238081000	-0.551544000	4.330129000
H	1.747311000	-1.136723000	5.076365000
C	2.088921000	-2.003931000	2.486032000
H	2.332071000	-2.638139000	3.343210000
H	1.499636000	-2.569462000	1.770515000
H	3.009856000	-1.662788000	2.009884000
C	-0.806287000	2.032695000	2.866254000
H	-0.823277000	2.664163000	3.759007000
H	-0.414349000	2.599684000	2.027865000
H	-1.818930000	1.695914000	2.637342000
N	0.070079000	0.890441000	3.133866000
N	1.305837000	-0.865395000	2.971198000
N	2.214308000	-0.577737000	-0.202260000
N	0.907997000	1.956501000	0.005118000
N	-1.580181000	0.629955000	0.247730000
N	-0.270738000	-1.890777000	0.135219000
C	2.615167000	-1.844204000	-0.567603000
C	3.350994000	0.187893000	-0.027250000
C	2.215729000	2.393297000	0.005175000
C	0.109958000	3.038551000	-0.337636000
C	-2.061964000	1.905537000	0.031887000
C	-2.626124000	-0.127601000	0.754635000

C	-1.532835000	-2.329684000	0.471948000
C	0.412946000	-2.968249000	-0.406425000
C	4.064392000	-1.900024000	-0.558932000
H	4.647925000	-2.780778000	-0.775805000
C	4.516973000	-0.662640000	-0.186005000
H	5.539726000	-0.349248000	-0.052493000
C	2.246004000	3.805411000	-0.329545000
H	3.144460000	4.395331000	-0.419218000
C	0.958141000	4.190665000	-0.579226000
H	0.612271000	5.157274000	-0.908030000
C	-3.444745000	1.967285000	0.456105000
H	-4.060484000	2.851695000	0.417153000
C	-3.775033000	0.733239000	0.947888000
H	-4.715422000	0.429604000	1.377527000
C	-1.653122000	-3.735946000	0.136219000
H	-2.544911000	-4.326498000	0.276016000
C	-0.471801000	-4.117042000	-0.439710000
H	-0.221828000	-5.080004000	-0.855095000
C	1.772501000	-2.957175000	-0.760858000
C	3.364749000	1.586501000	0.125320000
C	-1.296231000	3.024570000	-0.354681000
C	-2.602921000	-1.523913000	0.913477000
C	2.396396000	-4.202087000	-1.288545000
C	3.095838000	-4.169882000	-2.511590000
H	3.148405000	-3.233963000	-3.057705000
C	3.701698000	-5.323879000	-3.018766000
H	4.229845000	-5.282318000	-3.966425000
C	3.622115000	-6.530943000	-2.311424000
H	4.091570000	-7.426918000	-2.705553000
C	2.935346000	-6.574212000	-1.091088000
H	2.878191000	-7.503035000	-0.531555000
C	2.330329000	-5.419712000	-0.583157000
H	1.810366000	-5.449661000	0.368543000
C	4.669135000	2.291562000	0.279532000
C	5.708783000	2.145228000	-0.659606000
H	5.553936000	1.503342000	-1.519847000
C	6.916124000	2.833956000	-0.501233000
H	7.704280000	2.714392000	-1.238357000
C	7.103625000	3.686736000	0.594521000
H	8.040505000	4.221555000	0.715960000
C	6.071838000	3.851625000	1.527996000
H	6.207320000	4.513728000	2.377844000
C	4.864930000	3.162649000	1.369464000
H	4.061765000	3.289024000	2.088333000
C	-2.042440000	4.261474000	-0.713680000

C	-3.043131000	4.202326000	-1.705626000
H	-3.236762000	3.253521000	-2.195159000
C	-3.771196000	5.344583000	-2.052747000
H	-4.533387000	5.283318000	-2.823803000
C	-3.516557000	6.565415000	-1.413506000
H	-4.081342000	7.452203000	-1.684034000
C	-2.531637000	6.633914000	-0.419401000
H	-2.337339000	7.572942000	0.090029000
C	-1.803272000	5.491644000	-0.070432000
H	-1.052762000	5.541199000	0.711243000
C	-3.794992000	-2.230955000	1.459703000
C	-5.089093000	-2.051672000	0.931707000
H	-5.224292000	-1.380316000	0.093768000
C	-6.180550000	-2.748601000	1.460756000
H	-7.168530000	-2.602038000	1.034789000
C	-6.000727000	-3.642499000	2.524135000
H	-6.848575000	-4.183407000	2.932819000
C	-4.717662000	-3.838513000	3.051988000
H	-4.567429000	-4.530645000	3.874982000
C	-3.626789000	-3.141777000	2.523137000
H	-2.631648000	-3.291231000	2.929039000
O	0.174143000	0.021506000	-1.797264000
C	-2.415385000	-1.378825000	-2.924506000
C	-2.150293000	-0.131163000	-3.728210000
C	-3.029448000	0.923971000	-3.751832000
C	-4.264240000	0.873332000	-3.045902000
C	-4.604332000	-0.297632000	-2.311358000
C	-3.757372000	-1.374285000	-2.244723000
H	-2.311905000	-2.277394000	-3.563264000
H	-1.208268000	-0.081183000	-4.265803000
H	-2.784463000	1.815212000	-4.324878000
H	-0.583941000	0.539469000	-2.137552000
H	-5.559774000	-0.328305000	-1.792690000
H	-4.028656000	-2.253780000	-1.668724000
H	-4.949074000	1.714531000	-3.078768000
H	-1.603403000	-1.485073000	-2.179291000

²INT1-1_{is}

Mn	0.323346000	0.033482000	0.034855000
C	0.585750000	0.025321000	2.190154000
C	0.470463000	0.570384000	4.423152000
H	0.162627000	1.149010000	5.276967000
C	1.239807000	-0.544605000	4.321984000
H	1.744908000	-1.132483000	5.068927000

C	2.067522000	-2.014609000	2.483107000
H	2.302346000	-2.648904000	3.342589000
H	1.470927000	-2.575038000	1.769869000
H	2.992984000	-1.687550000	2.005826000
C	-0.782228000	2.055903000	2.857471000
H	-0.794039000	2.686128000	3.751226000
H	-0.384728000	2.620707000	2.020322000
H	-1.797775000	1.728958000	2.627627000
N	0.083169000	0.905181000	3.124320000
N	1.299417000	-0.864453000	2.964311000
N	2.199206000	-0.603317000	-0.206075000
N	0.926613000	1.949950000	0.007174000
N	-1.574494000	0.660938000	0.246154000
N	-0.297493000	-1.878697000	0.144301000
C	2.583761000	-1.875152000	-0.571239000
C	3.346215000	0.146404000	-0.029773000
C	2.240715000	2.367407000	0.011166000
C	0.145765000	3.043371000	-0.341071000
C	-2.040778000	1.940720000	0.023875000
C	-2.629099000	-0.080015000	0.759041000
C	-1.564026000	-2.298355000	0.489604000
C	0.368482000	-2.968426000	-0.395737000
C	4.032556000	-1.950229000	-0.564356000
H	4.604023000	-2.838755000	-0.781682000
C	4.501308000	-0.719570000	-0.190563000
H	5.528111000	-0.419831000	-0.056672000
C	2.292468000	3.778652000	-0.323713000
H	3.199737000	4.355446000	-0.410125000
C	1.011324000	4.182425000	-0.579856000
H	0.681177000	5.153635000	-0.911232000
C	-3.422895000	2.022850000	0.447928000
H	-4.027089000	2.915047000	0.404374000
C	-3.767948000	0.796278000	0.947471000
H	-4.711306000	0.506916000	1.380553000
C	-1.705026000	-3.703971000	0.161432000
H	-2.604103000	-4.281620000	0.308294000
C	-0.531984000	-4.104361000	-0.419149000
H	-0.297736000	-5.072780000	-0.830956000
C	1.726204000	-2.977020000	-0.758220000
C	3.378531000	1.543813000	0.128872000
C	-1.260018000	3.047892000	-0.366289000
C	-2.622940000	-1.475109000	0.927029000
C	2.330835000	-4.231771000	-1.284832000
C	3.026203000	-4.212215000	-2.510489000
H	3.089671000	-3.278485000	-3.059225000

C	3.614642000	-5.375555000	-3.016811000
H	4.139941000	-5.343524000	-3.966424000
C	3.521447000	-6.579597000	-2.306002000
H	3.977375000	-7.482830000	-2.699437000
C	2.838719000	-6.610368000	-1.083018000
H	2.771241000	-7.536827000	-0.520719000
C	2.251111000	-5.446539000	-0.575950000
H	1.734496000	-5.467055000	0.377806000
C	4.692070000	2.230702000	0.287656000
C	5.731102000	2.074537000	-0.650564000
H	5.568997000	1.438522000	-1.513832000
C	6.947400000	2.746184000	-0.487370000
H	7.735022000	2.619170000	-1.223824000
C	7.144739000	3.591498000	0.612438000
H	8.088580000	4.113044000	0.737662000
C	6.113814000	3.766162000	1.545093000
H	6.256911000	4.422589000	2.398096000
C	4.897985000	3.094204000	1.381759000
H	4.095546000	3.228086000	2.100093000
C	-1.989495000	4.290365000	-0.739052000
C	-2.985715000	4.233277000	-1.735712000
H	-3.186991000	3.281944000	-2.217496000
C	-3.698991000	5.380299000	-2.097382000
H	-4.457788000	5.320520000	-2.871886000
C	-3.433754000	6.604066000	-1.468105000
H	-3.986959000	7.494643000	-1.749865000
C	-2.453291000	6.670709000	-0.469467000
H	-2.251068000	7.612219000	0.032235000
C	-1.739659000	5.523652000	-0.106025000
H	-0.993021000	5.572010000	0.679403000
C	-3.823535000	-2.163245000	1.478732000
C	-5.114940000	-1.972207000	0.948293000
H	-5.240877000	-1.305894000	0.104856000
C	-6.215335000	-2.651245000	1.482007000
H	-7.201163000	-2.495900000	1.054178000
C	-6.047173000	-3.538791000	2.552627000
H	-6.901880000	-4.065925000	2.965004000
C	-4.766958000	-3.746513000	3.082906000
H	-4.625874000	-4.433921000	3.911459000
C	-3.667136000	-3.067613000	2.549332000
H	-2.674147000	-3.226163000	2.957032000
O	0.167096000	0.029802000	-1.790446000
H	-0.591002000	0.541802000	-2.140267000
C	-2.421747000	-1.435060000	-2.912013000
C	-2.112204000	-0.206988000	-3.730704000

C	-2.954111000	0.877951000	-3.768295000
C	-4.189904000	0.880148000	-3.062347000
C	-4.570569000	-0.268018000	-2.311616000
C	-3.762861000	-1.373215000	-2.231220000
H	-2.353693000	-2.343510000	-3.541571000
H	-1.168237000	-0.195700000	-4.266753000
H	-2.677989000	1.752546000	-4.352737000
H	-5.525577000	-0.257546000	-1.791422000
H	-4.064434000	-2.234475000	-1.642908000
H	-4.845101000	1.744020000	-3.107403000
H	-1.617086000	-1.563819000	-2.164218000

⁶TS2-1_{ss}

Mn	-0.309752000	0.002992000	0.140595000
O	-0.099086000	0.001562000	-1.790641000
C	-0.599798000	0.027773000	2.370107000
C	-0.541416000	0.620887000	4.592407000
H	-0.272360000	1.228915000	5.438981000
C	-1.274543000	-0.519914000	4.500196000
H	-1.769628000	-1.111638000	5.250887000
C	-2.012199000	-2.052710000	2.665329000
H	-2.635412000	-2.430902000	3.480444000
H	-2.640742000	-1.778622000	1.822245000
H	-1.306452000	-2.824068000	2.353246000
C	0.663497000	2.127273000	2.997407000
H	1.030672000	2.535675000	3.942924000
H	1.505499000	1.847332000	2.370331000
H	0.063083000	2.878660000	2.481566000
N	-0.139169000	0.939069000	3.293284000
N	-1.302460000	-0.865637000	3.147110000
N	-0.292349000	-2.050229000	0.113330000
N	1.788929000	0.034817000	0.448688000
N	-0.323951000	2.058181000	0.039969000
N	-2.423313000	-0.021944000	-0.110351000
C	-1.342522000	-2.856984000	-0.280425000
C	0.797549000	-2.848513000	0.406963000
C	2.571071000	-1.070563000	0.679465000
C	2.610688000	1.123484000	0.269159000
C	0.801799000	2.856815000	-0.031509000
C	-1.445259000	2.871124000	0.092892000
C	-3.220428000	1.097099000	-0.189218000
C	-3.147804000	-1.110793000	-0.547755000
C	-0.912684000	-4.242520000	-0.165546000
H	-1.531056000	-5.101676000	-0.372201000

C	0.385489000	-4.238122000	0.271219000
H	1.010562000	-5.093148000	0.474294000
C	3.965574000	-0.652491000	0.708532000
H	4.807824000	-1.310470000	0.853546000
C	3.993222000	0.687869000	0.430441000
H	4.861724000	1.315704000	0.316724000
C	0.372894000	4.243912000	0.024457000
H	1.036483000	5.094495000	0.016840000
C	-0.994209000	4.252941000	0.132507000
H	-1.635957000	5.114988000	0.220693000
C	-4.534119000	0.692948000	-0.672015000
H	-5.361521000	1.362028000	-0.851292000
C	-4.483076000	-0.656228000	-0.910906000
H	-5.264550000	-1.278818000	-1.317384000
C	-2.651845000	-2.436776000	-0.624291000
C	2.107314000	-2.408066000	0.714933000
C	2.156361000	2.434580000	-0.002004000
C	-2.790880000	2.435115000	0.007574000
C	-3.600979000	-3.494273000	-1.079953000
C	-3.282975000	-4.314541000	-2.180596000
H	-2.340922000	-4.156671000	-2.694970000
C	-4.166411000	-5.310232000	-2.610093000
H	-3.906700000	-5.928604000	-3.463959000
C	-5.385971000	-5.504252000	-1.947955000
H	-6.072225000	-6.276212000	-2.282095000
C	-5.714589000	-4.695149000	-0.852387000
H	-6.655029000	-4.842266000	-0.329871000
C	-4.829722000	-3.700651000	-0.422346000
H	-5.080663000	-3.076516000	0.429039000
C	3.147578000	-3.450965000	0.964400000
C	3.476240000	-4.396309000	-0.026456000
H	2.946814000	-4.368580000	-0.973131000
C	4.476191000	-5.348843000	0.198579000
H	4.720582000	-6.067409000	-0.577879000
C	5.168371000	-5.368529000	1.416730000
H	5.945406000	-6.106348000	1.591079000
C	4.855784000	-4.427329000	2.406455000
H	5.388627000	-4.435702000	3.352550000
C	3.855089000	-3.475609000	2.180794000
H	3.611805000	-2.742577000	2.943215000
C	3.186272000	3.489429000	-0.227721000
C	3.187514000	4.219394000	-1.432714000
H	2.438579000	3.986387000	-2.181715000
C	4.146709000	5.209953000	-1.667648000
H	4.136614000	5.758738000	-2.604530000

C	5.122543000	5.488845000	-0.701107000
H	5.868293000	6.256324000	-0.883735000
C	5.128955000	4.772553000	0.502803000
H	5.876551000	4.988402000	1.260168000
C	4.167494000	3.783299000	0.737877000
H	4.167312000	3.232859000	1.672991000
C	-3.865964000	3.470714000	0.021805000
C	-3.881481000	4.537324000	-0.898421000
H	-3.088731000	4.606643000	-1.635396000
C	-4.909645000	5.485819000	-0.876825000
H	-4.908100000	6.297537000	-1.597955000
C	-5.944729000	5.382866000	0.061852000
H	-6.742664000	6.118786000	0.077554000
C	-5.946847000	4.320835000	0.975748000
H	-6.746061000	4.232321000	1.705417000
C	-4.918676000	3.372931000	0.953365000
H	-4.917417000	2.547627000	1.657862000
H	-0.783730000	0.567472000	-2.207581000
H	1.006439000	-0.214666000	-2.795406000
C	2.537763000	0.933649000	-3.801715000
C	3.786562000	1.205872000	-3.284090000
C	1.886853000	-0.378264000	-3.600085000
C	4.529027000	0.198965000	-2.620565000
C	4.001203000	-1.114154000	-2.508100000
C	2.757305000	-1.417259000	-3.011044000
H	5.508724000	0.425357000	-2.214270000
H	1.311029000	-0.727113000	-4.472100000
H	4.213336000	2.199705000	-3.385755000
H	1.980459000	1.708492000	-4.322822000
H	4.585949000	-1.882455000	-2.010622000
H	2.355391000	-2.422459000	-2.914925000

⁴TS2-1_{ss}

Mn	-0.298170000	0.007464000	0.046791000
O	-0.254863000	0.026713000	-1.887572000
C	-0.526072000	0.015215000	2.301167000
C	-0.400910000	0.580172000	4.528696000
H	-0.110730000	1.180230000	5.373989000
C	-1.124966000	-0.567001000	4.445395000
H	-1.589291000	-1.173438000	5.203970000
C	-1.905322000	-2.083605000	2.613352000
H	-2.502969000	-2.476501000	3.440640000
H	-2.558860000	-1.804717000	1.791064000
H	-1.201476000	-2.846646000	2.276221000

C	0.733856000	2.121687000	2.916168000
H	1.115382000	2.528598000	3.856649000
H	1.566747000	1.861395000	2.268689000
H	0.110579000	2.868264000	2.420788000
N	-0.044715000	0.919559000	3.221048000
N	-1.193468000	-0.895300000	3.089251000
N	-0.241493000	-1.967354000	0.031623000
N	1.809582000	0.068328000	0.343986000
N	-0.339471000	1.989466000	0.013492000
N	-2.438931000	-0.060103000	-0.062038000
C	-1.288414000	-2.799591000	-0.359732000
C	0.834746000	-2.764952000	0.410344000
C	2.595920000	-1.005044000	0.685618000
C	2.623668000	1.158368000	0.161863000
C	0.772024000	2.817546000	-0.129230000
C	-1.474385000	2.795770000	0.143176000
C	-3.254003000	1.041008000	-0.080437000
C	-3.150419000	-1.131688000	-0.553236000
C	-0.855024000	-4.170730000	-0.186534000
H	-1.468769000	-5.035462000	-0.382513000
C	0.420979000	-4.150800000	0.309224000
H	1.034710000	-4.996419000	0.574801000
C	3.975442000	-0.563878000	0.777569000
H	4.815524000	-1.196966000	1.016339000
C	3.998792000	0.761885000	0.420379000
H	4.860525000	1.403548000	0.334499000
C	0.318285000	4.191186000	-0.048877000
H	0.967540000	5.050842000	-0.099964000
C	-1.034409000	4.177866000	0.158068000
H	-1.681549000	5.028349000	0.297943000
C	-4.568570000	0.645354000	-0.559908000
H	-5.407628000	1.311066000	-0.691333000
C	-4.496514000	-0.689640000	-0.873438000
H	-5.270853000	-1.304838000	-1.304369000
C	-2.608174000	-2.428928000	-0.699346000
C	2.130183000	-2.336372000	0.767945000
C	2.135171000	2.448963000	-0.140749000
C	-2.819343000	2.374004000	0.135918000
C	-3.509581000	-3.505355000	-1.198402000
C	-3.137040000	-4.285861000	-2.311044000
H	-2.189932000	-4.080237000	-2.798462000
C	-3.974835000	-5.300010000	-2.785903000
H	-3.674347000	-5.886743000	-3.648654000
C	-5.201368000	-5.553178000	-2.157314000
H	-5.852277000	-6.339615000	-2.526624000

C	-5.582885000	-4.784841000	-1.049474000
H	-6.528483000	-4.979163000	-0.552317000
C	-4.744377000	-3.771178000	-0.574243000
H	-5.035436000	-3.180323000	0.287894000
C	3.148299000	-3.369976000	1.118559000
C	3.524659000	-4.362874000	0.193299000
H	3.043492000	-4.382721000	-0.779131000
C	4.509711000	-5.303383000	0.514166000
H	4.790516000	-6.059123000	-0.213172000
C	5.140378000	-5.263386000	1.764682000
H	5.905975000	-5.991708000	2.013568000
C	4.780612000	-4.274721000	2.690210000
H	5.265476000	-4.236702000	3.661099000
C	3.794530000	-3.335561000	2.368662000
H	3.515421000	-2.566072000	3.081284000
C	3.127324000	3.528331000	-0.409988000
C	3.090037000	4.222097000	-1.635512000
H	2.339116000	3.944202000	-2.366961000
C	4.012518000	5.236695000	-1.911660000
H	3.972088000	5.757567000	-2.863551000
C	4.989671000	5.576586000	-0.966392000
H	5.706866000	6.362811000	-1.180749000
C	5.033439000	4.897535000	0.258214000
H	5.781028000	5.161597000	1.000152000
C	4.108501000	3.884412000	0.534577000
H	4.135367000	3.365783000	1.487175000
C	-3.896424000	3.402470000	0.232055000
C	-3.980747000	4.484080000	-0.666574000
H	-3.235887000	4.576841000	-1.449532000
C	-5.017956000	5.417781000	-0.567173000
H	-5.069539000	6.241811000	-1.272339000
C	-5.995012000	5.283341000	0.427871000
H	-6.800315000	6.007416000	0.503691000
C	-5.930880000	4.204058000	1.319117000
H	-6.686223000	4.089864000	2.090758000
C	-4.893637000	3.271271000	1.219047000
H	-4.842921000	2.431185000	1.904075000
H	-0.634008000	0.839652000	-2.276687000
H	0.925914000	-0.433162000	-2.848269000
C	2.361725000	0.709260000	-3.936710000
C	3.550618000	1.177715000	-3.424265000
C	1.833859000	-0.628361000	-3.572494000
C	4.361514000	0.349055000	-2.607824000
C	3.972560000	-0.993153000	-2.346676000
C	2.782686000	-1.483492000	-2.823475000

H	5.298953000	0.726065000	-2.215049000
H	1.349905000	-1.149757000	-4.414768000
H	3.883341000	2.187491000	-3.646521000
H	1.752341000	1.341924000	-4.577649000
H	4.616341000	-1.623683000	-1.742669000
H	2.478341000	-2.501895000	-2.597136000

⁴TS2-1_{is}

Mn	-0.319865000	0.045367000	0.042902000
O	-0.236239000	0.118646000	-1.862573000
C	-0.417271000	-0.099593000	2.170854000
C	0.079350000	0.120888000	4.402343000
H	0.557659000	0.556511000	5.262555000
C	-0.807323000	-0.901945000	4.286917000
H	-1.257833000	-1.542003000	5.025720000
C	-2.009351000	-2.062010000	2.435051000
H	-2.648627000	-2.376148000	3.265100000
H	-2.621982000	-1.658915000	1.636150000
H	-1.441525000	-2.917030000	2.062166000
C	1.254507000	1.685560000	2.856149000
H	1.376957000	2.254438000	3.782136000
H	2.217506000	1.277786000	2.540839000
H	0.866159000	2.336489000	2.080406000
N	0.304139000	0.600659000	3.111040000
N	-1.103506000	-1.021675000	2.928369000
N	-0.261512000	-1.938678000	-0.052785000
N	1.666013000	0.097099000	0.247332000
N	-0.366924000	2.052686000	0.022067000
N	-2.322713000	0.007228000	-0.120704000
C	-1.272494000	-2.756670000	-0.525543000
C	0.775422000	-2.750650000	0.378285000
C	2.456344000	-0.957354000	0.677800000
C	2.503119000	1.173877000	0.014912000
C	0.720507000	2.877975000	-0.214665000
C	-1.473718000	2.868883000	0.236052000
C	-3.180032000	1.084391000	0.025367000
C	-3.062687000	-1.042865000	-0.646403000
C	-0.858479000	-4.139637000	-0.374693000
H	-1.459416000	-4.993447000	-0.645842000
C	0.376198000	-4.136819000	0.216502000
H	0.970265000	-4.989491000	0.504587000
C	3.821124000	-0.513497000	0.773772000
H	4.652659000	-1.136214000	1.063217000
C	3.861146000	0.784199000	0.313399000

H	4.725921000	1.416606000	0.203870000
C	0.287921000	4.259621000	-0.117345000
H	0.936782000	5.113142000	-0.237244000
C	-1.041406000	4.252715000	0.208427000
H	-1.675313000	5.104191000	0.396524000
C	-4.505329000	0.691611000	-0.387953000
H	-5.366258000	1.341301000	-0.393003000
C	-4.424776000	-0.605212000	-0.834935000
H	-5.213465000	-1.200498000	-1.265855000
C	-2.566523000	-2.346270000	-0.880778000
C	2.024697000	-2.296207000	0.820523000
C	2.063899000	2.473260000	-0.310061000
C	-2.797612000	2.416294000	0.313506000
C	-3.482168000	-3.379353000	-1.439027000
C	-3.110013000	-4.094826000	-2.594795000
H	-2.164842000	-3.857427000	-3.071760000
C	-3.943091000	-5.086410000	-3.123190000
H	-3.641661000	-5.622559000	-4.018011000
C	-5.165400000	-5.382475000	-2.505556000
H	-5.813320000	-6.150674000	-2.916214000
C	-5.545094000	-4.682115000	-1.352832000
H	-6.485675000	-4.912793000	-0.861579000
C	-4.710282000	-3.692595000	-0.823345000
H	-4.998589000	-3.160299000	0.077003000
C	3.030329000	-3.279248000	1.311339000
C	3.483581000	-4.336374000	0.498209000
H	3.080501000	-4.438383000	-0.503927000
C	4.450129000	-5.234334000	0.965286000
H	4.790825000	-6.041024000	0.323185000
C	4.987301000	-5.086025000	2.250485000
H	5.738717000	-5.781315000	2.611740000
C	4.553338000	-4.030861000	3.064590000
H	4.966385000	-3.907948000	4.061358000
C	3.585455000	-3.135578000	2.597821000
H	3.247449000	-2.315290000	3.223085000
C	3.071544000	3.519684000	-0.643027000
C	3.010946000	4.170119000	-1.890941000
H	2.240673000	3.872926000	-2.594430000
C	3.933547000	5.167145000	-2.225087000
H	3.874095000	5.654138000	-3.193819000
C	4.934652000	5.533631000	-1.315403000
H	5.652342000	6.305825000	-1.574556000
C	5.000608000	4.900103000	-0.067724000
H	5.765725000	5.186223000	0.647784000
C	4.074619000	3.905266000	0.266192000

H	4.116762000	3.425072000	1.238203000
C	-3.897645000	3.391873000	0.558556000
C	-4.089684000	4.521490000	-0.260655000
H	-3.418469000	4.686159000	-1.096399000
C	-5.142532000	5.410527000	-0.017967000
H	-5.277930000	6.273005000	-0.663542000
C	-6.028333000	5.182211000	1.042972000
H	-6.846109000	5.871329000	1.229745000
C	-5.857201000	4.053968000	1.856229000
H	-6.541523000	3.866842000	2.678259000
C	-4.804006000	3.166387000	1.613739000
H	-4.670174000	2.289034000	2.238255000
H	-0.713907000	0.900604000	-2.204249000
H	0.870099000	-0.262537000	-2.726735000
C	2.434981000	0.697590000	-3.864382000
C	3.675404000	1.017384000	-3.354550000
C	1.764740000	-0.564398000	-3.509772000
C	4.381438000	0.089636000	-2.551060000
C	3.834467000	-1.196863000	-2.296917000
C	2.591662000	-1.534451000	-2.777504000
H	5.361731000	0.344322000	-2.164603000
H	1.159393000	-1.002649000	-4.317603000
H	4.120881000	1.984829000	-3.565831000
H	1.903513000	1.403868000	-4.497619000
H	4.396455000	-1.904696000	-1.696335000
H	2.162094000	-2.507757000	-2.556922000

²TS2-1_{is}

Mn	-0.298686000	0.010685000	0.051008000
O	-0.158309000	0.017963000	-1.830919000
C	-0.566196000	0.019749000	2.172218000
C	-0.514321000	0.608559000	4.392788000
H	-0.282583000	1.235652000	5.236231000
C	-1.145726000	-0.591200000	4.310185000
H	-1.571435000	-1.226493000	5.067513000
C	-1.782224000	-2.187758000	2.500731000
H	-2.362926000	-2.600844000	3.330236000
H	-2.441202000	-1.985836000	1.661559000
H	-1.016205000	-2.903376000	2.197883000
C	0.525205000	2.227420000	2.804300000
H	0.862092000	2.647672000	3.755913000
H	1.384825000	2.038088000	2.168479000
H	-0.144506000	2.932856000	2.310401000
N	-0.167210000	0.967368000	3.088916000

N	-1.172014000	-0.935742000	2.957629000
N	-0.068394000	-1.962066000	0.023535000
N	1.678190000	0.233492000	0.349393000
N	-0.502589000	1.999049000	-0.043694000
N	-2.288459000	-0.203515000	-0.150954000
C	-1.000498000	-2.877057000	-0.442662000
C	1.032416000	-2.678158000	0.464707000
C	2.550769000	-0.750357000	0.781096000
C	2.431174000	1.370161000	0.109375000
C	0.524113000	2.908814000	-0.246989000
C	-1.678649000	2.725638000	0.107839000
C	-3.230095000	0.801456000	-0.065361000
C	-2.930912000	-1.331961000	-0.638360000
C	-0.470087000	-4.214930000	-0.269365000
H	-0.993573000	-5.121695000	-0.528769000
C	0.758736000	-4.096153000	0.321023000
H	1.424894000	-4.888663000	0.622275000
C	3.880955000	-0.195648000	0.880689000
H	4.756505000	-0.747741000	1.182755000
C	3.816517000	1.095043000	0.422484000
H	4.628011000	1.793621000	0.303576000
C	-0.021936000	4.251071000	-0.199738000
H	0.560766000	5.152653000	-0.308298000
C	-1.359531000	4.141425000	0.066951000
H	-2.068802000	4.941322000	0.206224000
C	-4.516471000	0.284094000	-0.478247000
H	-5.425964000	0.862076000	-0.524872000
C	-4.323671000	-1.017884000	-0.864071000
H	-5.053360000	-1.695417000	-1.277555000
C	-2.321135000	-2.590012000	-0.821418000
C	2.238926000	-2.118264000	0.912112000
C	1.897859000	2.618673000	-0.265257000
C	-2.963972000	2.169944000	0.173858000
C	-3.138433000	-3.713737000	-1.359431000
C	-2.701542000	-4.415582000	-2.500163000
H	-1.778448000	-4.107174000	-2.979571000
C	-3.445987000	-5.483716000	-3.011536000
H	-3.097363000	-6.008731000	-3.895680000
C	-4.640587000	-5.871184000	-2.390148000
H	-5.219360000	-6.699278000	-2.787437000
C	-5.082406000	-5.185101000	-1.251187000
H	-6.001661000	-5.485850000	-0.757574000
C	-4.336667000	-4.118013000	-0.739264000
H	-4.672036000	-3.593455000	0.149203000
C	3.330826000	-3.019749000	1.377431000

C	3.871539000	-4.006478000	0.530113000
H	3.470023000	-4.115153000	-0.471993000
C	4.919648000	-4.825962000	0.963669000
H	5.327050000	-5.578671000	0.295432000
C	5.451263000	-4.667689000	2.250210000
H	6.265758000	-5.301912000	2.586239000
C	4.929610000	-3.681616000	3.098316000
H	5.337938000	-3.551130000	4.096040000
C	3.880098000	-2.864438000	2.664475000
H	3.475287000	-2.097221000	3.316793000
C	2.829807000	3.731288000	-0.603249000
C	2.757418000	4.332670000	-1.874849000
H	2.031800000	3.956081000	-2.587584000
C	3.613569000	5.384195000	-2.219038000
H	3.547275000	5.832679000	-3.205694000
C	4.556901000	5.854643000	-1.295812000
H	5.222779000	6.669548000	-1.562341000
C	4.632785000	5.270011000	-0.024925000
H	5.353099000	5.636729000	0.700198000
C	3.774108000	4.219977000	0.319101000
H	3.823452000	3.775973000	1.307829000
C	-4.142662000	3.062208000	0.363391000
C	-4.406295000	4.143588000	-0.499769000
H	-3.733292000	4.330468000	-1.329425000
C	-5.530030000	4.954778000	-0.307878000
H	-5.719800000	5.780544000	-0.986929000
C	-6.416253000	4.694827000	0.745534000
H	-7.288968000	5.323482000	0.892807000
C	-6.173517000	3.613020000	1.602473000
H	-6.857486000	3.401416000	2.418865000
C	-5.049253000	2.803580000	1.410784000
H	-4.859660000	1.962003000	2.069254000
H	-0.430405000	0.872535000	-2.219616000
H	0.982902000	-0.533581000	-2.710470000
C	2.327808000	0.551010000	-3.949609000
C	3.467842000	1.157892000	-3.470419000
C	1.891526000	-0.771128000	-3.445919000
C	4.322683000	0.475703000	-2.568371000
C	4.036248000	-0.863709000	-2.190316000
C	2.891892000	-1.485496000	-2.627123000
H	5.220571000	0.960496000	-2.201831000
H	1.407994000	-1.400909000	-4.208441000
H	3.728840000	2.163442000	-3.788078000
H	1.685383000	1.067321000	-4.658816000
H	4.719463000	-1.386964000	-1.529799000

H	2.660156000	-2.498243000	-2.308822000
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²TS2-1_s

Mn	-0.298201000	0.009206000	0.050304000
O	-0.169401000	0.013803000	-1.824996000
C	-0.577401000	0.021411000	2.173804000
C	-0.527989000	0.610210000	4.396704000
H	-0.290677000	1.233705000	5.241304000
C	-1.177313000	-0.579677000	4.311304000
H	-1.616425000	-1.208069000	5.066804000
C	-1.828043000	-2.167065000	2.499704000
H	-2.410951000	-2.576353000	3.329504000
H	-2.487439000	-1.955152000	1.663304000
H	-1.071857000	-2.891179000	2.192304000
C	0.543642000	2.212089000	2.813504000
H	0.885750000	2.625483000	3.766304000
H	1.401138000	2.010273000	2.178904000
H	-0.113244000	2.929602000	2.319704000
N	-0.169083000	0.962903000	3.094304000
N	-1.201719000	-0.924177000	2.958504000
N	-0.111339000	-1.965498000	0.018204000
N	1.677502000	0.196467000	0.359004000
N	-0.460862000	2.005609000	-0.041896000
N	-2.294505000	-0.163356000	-0.148396000
C	-1.061957000	-2.861480000	-0.446796000
C	0.975946000	-2.705219000	0.453204000
C	2.530283000	-0.808449000	0.781604000
C	2.455024000	1.319952000	0.128904000
C	0.582355000	2.896788000	-0.235896000
C	-1.623048000	2.754331000	0.104504000
C	-3.213885000	0.861662000	-0.067096000
C	-2.959726000	-1.276943000	-0.636396000
C	-0.558283000	-4.210589000	-0.278396000
H	-1.100900000	-5.106079000	-0.537496000
C	0.675119000	-4.117413000	0.306404000
H	1.327403000	-4.923326000	0.602504000
C	3.872893000	-0.281475000	0.884704000
H	4.736882000	-0.854492000	1.180904000
C	3.834618000	1.013325000	0.440204000
H	4.661132000	1.694309000	0.322704000
C	0.062781000	4.249699000	-0.188996000
H	0.663498000	5.140087000	-0.291196000
C	-1.278321000	4.164525000	0.068204000
H	-1.973405000	4.977038000	0.205204000

C	-4.511894000	0.371487000	-0.481596000
H	-5.408383000	0.969105000	-0.530796000
C	-4.346519000	-0.933616000	-0.865396000
H	-5.089132000	-1.596101000	-1.280196000
C	-2.377751000	-2.546754000	-0.821396000
C	2.194557000	-2.170143000	0.899004000
C	1.951249000	2.579562000	-0.244096000
C	-2.919758000	2.224056000	0.166704000
C	-3.220272000	-3.653138000	-1.356396000
C	-2.803586000	-4.363146000	-2.499596000
H	-1.877180000	-4.073164000	-2.983996000
C	-3.572106000	-5.416131000	-3.006796000
H	-3.239017000	-5.947837000	-3.892896000
C	-4.770513000	-5.780008000	-2.378596000
H	-5.367729000	-6.596496000	-2.772496000
C	-5.192400000	-5.085399000	-1.237296000
H	-6.114706000	-5.367882000	-0.738496000
C	-4.422880000	-4.033314000	-0.729596000
H	-4.742869000	-3.502308000	0.160804000
C	3.269239000	-3.095964000	1.358104000
C	3.791219000	-4.086574000	0.503904000
H	3.388318000	-4.180866000	-0.499096000
C	4.823503000	-4.928694000	0.932204000
H	5.217288000	-5.684001000	0.258704000
C	5.356806000	-4.789904000	2.220304000
H	6.158993000	-5.441820000	2.552104000
C	4.852825000	-3.800994000	3.075604000
H	5.262427000	-3.685802000	4.074704000
C	3.819341000	-2.960874000	2.646904000
H	3.428156000	-2.191267000	3.304704000
C	2.906970000	3.674543000	-0.572696000
C	2.848982000	4.285744000	-1.840396000
H	2.117375000	3.928759000	-2.556996000
C	3.726602000	5.322027000	-2.176096000
H	3.671111000	5.778229000	-3.159896000
C	4.677411000	5.767509000	-1.248096000
H	5.359726000	6.570796000	-1.507996000
C	4.739199000	5.172908000	0.018904000
H	5.465306000	5.520394000	0.747804000
C	3.859179000	4.138025000	0.354504000
H	3.897670000	3.686724000	1.340404000
C	-4.080240000	3.141979000	0.347404000
C	-4.318319000	4.221884000	-0.524996000
H	-3.638416000	4.388770000	-1.353296000
C	-5.425803000	5.057305000	-0.343496000

H	-5.596287000	5.881408000	-1.029596000
C	-6.320608000	4.823822000	0.708904000
H	-7.180795000	5.471239000	0.848204000
C	-6.102829000	3.744418000	1.575404000
H	-6.793532000	3.553532000	2.391304000
C	-4.994845000	2.910297000	1.394004000
H	-4.824561000	2.070493000	2.059804000
H	-0.321884000	0.900406000	-2.209996000
H	1.010687000	-0.577720000	-2.693296000
C	2.335609000	0.527654000	-3.938396000
C	3.482921000	1.141032000	-3.486296000
C	1.914683000	-0.797937000	-3.422196000
C	4.360908000	0.467215000	-2.600096000
C	4.088982000	-0.871980000	-2.210896000
C	2.939270000	-1.502357000	-2.619996000
H	5.262217000	0.959798000	-2.251996000
H	1.439471000	-1.434828000	-4.185096000
H	3.732840000	2.146027000	-3.814496000
H	1.676119000	1.038067000	-4.636196000
H	4.789772000	-1.389493000	-1.564196000
H	2.721450000	-2.515553000	-2.293496000

⁶INT2-1_{hs}

Mn	0.231869000	0.063773000	-0.376865000
O	0.126741000	0.127151000	2.045141000
C	0.385442000	0.134926000	-2.690249000
C	0.013708000	0.573907000	-4.918273000
H	-0.520421000	0.963740000	-5.768163000
C	1.196880000	-0.096812000	-4.830851000
H	1.893085000	-0.410744000	-5.590032000
C	2.569254000	-1.056978000	-2.930423000
H	3.302536000	-1.190990000	-3.730388000
H	3.004073000	-0.464844000	-2.125034000
H	2.276563000	-2.030670000	-2.529757000
C	-1.708216000	1.383634000	-3.247820000
H	-2.282912000	1.574147000	-4.158378000
H	-2.283968000	0.748629000	-2.574683000
H	-1.496602000	2.327948000	-2.739785000
N	-0.463037000	0.702351000	-3.609534000
N	1.404642000	-0.351876000	-3.471708000
N	1.270292000	-1.748945000	0.015669000
N	-1.603087000	-1.027726000	-0.277432000
N	-0.906104000	1.846604000	-0.037420000
N	2.018936000	1.145107000	-0.013647000

C	2.633970000	-1.858765000	0.184290000
C	0.752900000	-3.008856000	-0.200560000
C	-1.703321000	-2.403930000	-0.322775000
C	-2.876944000	-0.499388000	-0.218716000
C	-2.277503000	1.957503000	-0.134479000
C	-0.357969000	3.115079000	-0.123042000
C	2.084423000	2.507212000	0.167364000
C	3.220608000	0.596025000	0.381687000
C	3.006428000	-3.257682000	0.018961000
H	4.012894000	-3.643862000	0.060596000
C	1.855964000	-3.960800000	-0.228224000
H	1.763219000	-5.019528000	-0.413013000
C	-3.115340000	-2.764759000	-0.277425000
H	-3.500304000	-3.772618000	-0.272708000
C	-3.832753000	-1.600656000	-0.204434000
H	-4.903612000	-1.498248000	-0.125047000
C	-2.615771000	3.360978000	-0.319759000
H	-3.614176000	3.748299000	-0.452054000
C	-1.440672000	4.067788000	-0.325691000
H	-1.318093000	5.130028000	-0.467876000
C	3.411310000	2.846481000	0.671948000
H	3.739800000	3.840574000	0.932310000
C	4.103537000	1.675375000	0.811939000
H	5.098954000	1.544106000	1.206235000
C	3.535386000	-0.786170000	0.409967000
C	-0.623735000	-3.322222000	-0.344129000
C	-3.200066000	0.879547000	-0.159130000
C	1.018488000	3.431483000	0.002500000
C	4.951213000	-1.149460000	0.707609000
C	5.262797000	-2.052409000	1.743950000
H	4.453465000	-2.472337000	2.331349000
C	6.590316000	-2.394008000	2.021197000
H	6.810964000	-3.085665000	2.828595000
C	7.633382000	-1.838701000	1.267979000
H	8.663936000	-2.103168000	1.483923000
C	7.338112000	-0.938205000	0.235957000
H	8.139939000	-0.506024000	-0.355121000
C	6.010196000	-0.597485000	-0.041006000
H	5.778792000	0.098318000	-0.840690000
C	-0.979172000	-4.765271000	-0.493157000
C	-0.595890000	-5.711750000	0.477386000
H	-0.032857000	-5.376397000	1.342035000
C	-0.938169000	-7.060854000	0.336822000
H	-0.638703000	-7.774918000	1.098059000
C	-1.672574000	-7.488873000	-0.777070000

H	-1.938993000	-8.535640000	-0.886089000
C	-2.061860000	-6.557464000	-1.748737000
H	-2.627338000	-6.881586000	-2.617222000
C	-1.718343000	-5.208792000	-1.607574000
H	-2.014607000	-4.484952000	-2.359571000
C	-4.646518000	1.242573000	-0.129678000
C	-5.156403000	2.042286000	0.913345000
H	-4.476786000	2.386135000	1.686366000
C	-6.511221000	2.387858000	0.956498000
H	-6.885798000	2.999611000	1.771542000
C	-7.383633000	1.940845000	-0.044432000
H	-8.435346000	2.207587000	-0.011464000
C	-6.889706000	1.148324000	-1.089299000
H	-7.557682000	0.804536000	-1.873296000
C	-5.534653000	0.804388000	-1.131956000
H	-5.149937000	0.195479000	-1.943412000
C	1.390303000	4.875998000	0.033340000
C	0.779571000	5.772994000	0.932589000
H	0.026201000	5.397319000	1.616460000
C	1.145817000	7.122631000	0.957807000
H	0.669118000	7.796805000	1.662997000
C	2.132744000	7.601803000	0.086070000
H	2.417461000	8.649263000	0.106376000
C	2.752996000	6.719688000	-0.808607000
H	3.518053000	7.082708000	-1.488262000
C	2.386402000	5.370332000	-0.833000000
H	2.863983000	4.684115000	-1.524454000
H	-0.569465000	0.806700000	2.131135000
H	-0.234616000	-0.727333000	2.348207000
C	-1.126372000	-1.059823000	4.928911000
C	-1.634111000	0.245901000	4.941800000
C	-1.603848000	-1.988180000	3.990734000
C	-2.623998000	0.622093000	4.021698000
C	-3.104613000	-0.305883000	3.087686000
C	-2.590018000	-1.610328000	3.067404000
H	-3.019091000	1.633916000	4.033101000
H	-1.205747000	-2.998320000	3.974187000
H	-1.256532000	0.967416000	5.659547000
H	-0.356039000	-1.349434000	5.636634000
H	-3.862385000	-0.014993000	2.370161000
H	-2.945718000	-2.314114000	2.324012000

⁴INT2-1_{is}

Mn	-0.331087000	0.074836000	-0.124472000
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O	-0.174272000	0.097564000	2.204925000
C	-0.173547000	-0.087678000	-2.473626000
C	0.442941000	-1.045493000	-4.473007000
H	0.538020000	-1.837647000	-5.196560000
C	0.800034000	0.268007000	-4.528138000
H	1.272386000	0.842415000	-5.307148000
C	0.655552000	2.229768000	-2.947520000
H	0.443615000	2.869218000	-3.810620000
H	-0.005391000	2.490576000	-2.123065000
H	1.693656000	2.364484000	-2.629342000
C	-0.644431000	-2.537404000	-2.754877000
H	-1.078434000	-3.080016000	-3.600660000
H	0.171111000	-3.118800000	-2.313430000
H	-1.406380000	-2.369834000	-1.996885000
N	-0.152489000	-1.240421000	-3.222024000
N	0.412272000	0.832650000	-3.309469000
N	1.458470000	0.947319000	-0.164538000
N	0.557475000	-1.733257000	-0.053715000
N	-2.093296000	-0.804320000	0.048031000
N	-1.188917000	1.890366000	-0.017963000
C	1.746944000	2.292162000	0.074446000
C	2.637657000	0.347208000	-0.625339000
C	1.874524000	-1.993481000	-0.403862000
C	0.004116000	-2.928804000	0.397343000
C	-2.340706000	-2.146256000	0.350286000
C	-3.333755000	-0.204034000	-0.202609000
C	-2.551209000	2.140113000	-0.101668000
C	-0.575922000	3.084250000	0.368134000
C	3.132687000	2.541185000	-0.283002000
H	3.610392000	3.506426000	-0.223044000
C	3.657273000	1.373581000	-0.755782000
H	4.650564000	1.204361000	-1.139889000
C	2.163745000	-3.365930000	-0.139350000
H	3.123079000	-3.834184000	-0.295456000
C	1.015606000	-3.936852000	0.390907000
H	0.881670000	-4.955227000	0.718239000
C	-3.766829000	-2.398477000	0.211077000
H	-4.227540000	-3.363391000	0.351902000
C	-4.360465000	-1.233739000	-0.167227000
H	-5.402494000	-1.065922000	-0.386709000
C	-2.798835000	3.506107000	0.235248000
H	-3.774959000	3.963417000	0.271033000
C	-1.582140000	4.081193000	0.555792000
H	-1.402639000	5.091232000	0.886986000
C	0.829129000	3.280142000	0.425504000

C	2.830823000	-1.016126000	-0.797639000
C	-1.386762000	-3.125942000	0.612896000
C	-3.560978000	1.161253000	-0.316719000
C	1.363260000	4.623306000	0.780675000
C	2.323990000	4.746323000	1.804991000
H	2.640829000	3.850847000	2.330396000
C	2.860525000	5.992802000	2.142782000
H	3.596120000	6.066116000	2.938210000
C	2.444812000	7.144608000	1.462142000
H	2.857879000	8.113633000	1.724430000
C	1.493302000	7.036936000	0.438887000
H	1.173773000	7.923143000	-0.101155000
C	0.959945000	5.789201000	0.099870000
H	0.233125000	5.704994000	-0.700587000
C	4.148908000	-1.524839000	-1.267344000
C	5.341997000	-1.235320000	-0.577367000
H	5.297163000	-0.620875000	0.315885000
C	6.567505000	-1.744137000	-1.022619000
H	7.477114000	-1.514356000	-0.475924000
C	6.619665000	-2.558128000	-2.161196000
H	7.569763000	-2.954585000	-2.505675000
C	5.437239000	-2.862784000	-2.850041000
H	5.470236000	-3.493893000	-3.733117000
C	4.213630000	-2.353152000	-2.404988000
H	3.294736000	-2.582321000	-2.934874000
C	-1.867760000	-4.473152000	1.030372000
C	-2.658076000	-4.609374000	2.188908000
H	-2.889477000	-3.722151000	2.769459000
C	-3.136633000	-5.862012000	2.587855000
H	-3.740909000	-5.946984000	3.486011000
C	-2.833665000	-7.003822000	1.834747000
H	-3.203072000	-7.976623000	2.144274000
C	-2.054003000	-6.881565000	0.676807000
H	-1.825117000	-7.759757000	0.080434000
C	-1.578118000	-5.628345000	0.277528000
H	-0.985290000	-5.531959000	-0.625588000
C	-4.944952000	1.667468000	-0.538679000
C	-6.003840000	1.336202000	0.328813000
H	-5.803619000	0.695208000	1.180630000
C	-7.291590000	1.838562000	0.110676000
H	-8.094416000	1.575802000	0.793030000
C	-7.542381000	2.688693000	-0.974015000
H	-8.541152000	3.079675000	-1.142180000
C	-6.493894000	3.037705000	-1.836100000
H	-6.678664000	3.698670000	-2.677619000

C	-5.207548000	2.534677000	-1.617786000
H	-4.391820000	2.806490000	-2.279746000
H	0.254951000	-0.736143000	2.480757000
H	0.403517000	0.833990000	2.482173000
C	1.885531000	0.328501000	4.793817000
C	1.743376000	-1.061189000	4.666504000
C	2.574391000	1.055462000	3.810323000
C	2.295794000	-1.723826000	3.558759000
C	2.991961000	-0.996555000	2.582266000
C	3.126112000	0.393318000	2.703217000
H	2.177935000	-2.796811000	3.445830000
H	2.677584000	2.132608000	3.905452000
H	1.201594000	-1.622338000	5.421454000
H	1.455329000	0.841989000	5.647968000
H	3.399752000	-1.508559000	1.720469000
H	3.632608000	0.957415000	1.927959000

²INT2-1_h

Mn	-0.268307000	-0.000469000	0.188416000
O	0.043376000	0.017381000	-1.881964000
C	-0.561004000	-0.025470000	2.192031000
C	-1.039354000	0.621688000	4.344299000
H	-1.325553000	1.308664000	5.121863000
C	-0.724023000	-0.699218000	4.382246000
H	-0.674079000	-1.396649000	5.200513000
C	-0.025376000	-2.447093000	2.740302000
H	-0.265906000	-3.086945000	3.594138000
H	-0.570523000	-2.788330000	1.865735000
H	1.047249000	-2.488717000	2.539988000
C	-1.222426000	2.395561000	2.595166000
H	-1.214256000	3.026216000	3.488830000
H	-0.455439000	2.734879000	1.905249000
H	-2.199556000	2.456370000	2.110829000
N	-0.934562000	1.020292000	3.010916000
N	-0.435654000	-1.080370000	3.070900000
N	1.253655000	-1.309684000	0.260222000
N	1.027136000	1.478238000	0.303553000
N	-1.740640000	1.294663000	-0.149019000
N	-1.533313000	-1.487380000	-0.057462000
C	1.212273000	-2.641173000	-0.116152000
C	2.495803000	-1.079787000	0.834219000
C	2.339006000	1.385111000	0.767975000
C	0.856893000	2.776845000	-0.196526000
C	-1.596919000	2.632455000	-0.492119000

C	-3.095554000	1.065133000	0.053487000
C	-2.918309000	-1.395559000	0.012696000
C	-1.228204000	-2.784360000	-0.495899000
C	2.446804000	-3.272588000	0.252814000
H	2.674493000	-4.316178000	0.101474000
C	3.225210000	-2.317669000	0.879012000
H	4.207351000	-2.447002000	1.304556000
C	2.999285000	2.663252000	0.561356000
H	4.027797000	2.864910000	0.817049000
C	2.117323000	3.488878000	-0.071922000
H	2.291749000	4.495957000	-0.415585000
C	-2.885354000	3.264403000	-0.465164000
H	-3.063232000	4.309652000	-0.664394000
C	-3.805904000	2.307470000	-0.089853000
H	-4.867135000	2.438346000	0.047272000
C	-3.496257000	-2.674580000	-0.369864000
H	-4.555806000	-2.870468000	-0.421205000
C	-2.473166000	-3.498945000	-0.729103000
H	-2.542100000	-4.500959000	-1.120723000
C	0.053605000	-3.321549000	-0.578810000
C	3.000367000	0.210912000	1.133969000
C	-0.358219000	3.314887000	-0.623051000
C	-3.661031000	-0.224491000	0.194801000
C	0.248611000	-4.717228000	-1.059711000
C	1.160524000	-4.970391000	-2.104258000
H	1.690113000	-4.132294000	-2.545536000
C	1.379688000	-6.271453000	-2.566391000
H	2.080539000	-6.445351000	-3.377414000
C	0.694428000	-7.348583000	-1.987861000
H	0.863405000	-8.359399000	-2.345937000
C	-0.205489000	-7.112786000	-0.940725000
H	-0.730250000	-7.942943000	-0.477442000
C	-0.422774000	-5.810127000	-0.478198000
H	-1.106564000	-5.630334000	0.344354000
C	4.380698000	0.346589000	1.676539000
C	5.493934000	-0.215362000	1.019884000
H	5.338393000	-0.774399000	0.103542000
C	6.786362000	-0.043075000	1.526750000
H	7.632216000	-0.478405000	1.003146000
C	6.992032000	0.698452000	2.697709000
H	7.995192000	0.831529000	3.090761000
C	5.895013000	1.271227000	3.354751000
H	6.045227000	1.849385000	4.261581000
C	4.602968000	1.097645000	2.847570000
H	3.749685000	1.539579000	3.351954000

C	-0.413207000	4.719008000	-1.118242000
C	-1.003379000	4.998799000	-2.367227000
H	-1.403205000	4.176917000	-2.952420000
C	-1.080084000	6.309797000	-2.847772000
H	-1.533289000	6.503424000	-3.815329000
C	-0.572125000	7.370382000	-2.085479000
H	-0.630709000	8.388395000	-2.457913000
C	0.004309000	7.108565000	-0.835956000
H	0.386047000	7.925612000	-0.231071000
C	0.078074000	5.796602000	-0.355288000
H	0.506500000	5.597265000	0.621037000
C	-5.130626000	-0.365665000	0.388584000
C	-6.060499000	0.218044000	-0.494538000
H	-5.694781000	0.786880000	-1.342150000
C	-7.435468000	0.052014000	-0.298286000
H	-8.136509000	0.504503000	-0.993313000
C	-7.908613000	-0.706692000	0.780643000
H	-8.976017000	-0.835202000	0.931804000
C	-6.994682000	-1.303541000	1.658908000
H	-7.351695000	-1.896060000	2.496026000
C	-5.619857000	-1.135080000	1.463164000
H	-4.907613000	-1.595246000	2.140687000
H	-0.062330000	0.910095000	-2.256825000
H	0.922692000	-0.346220000	-2.105380000
C	2.056881000	-0.348331000	-4.531440000
C	2.221781000	1.013745000	-4.238193000
C	2.558235000	-1.319960000	-3.651570000
C	2.899377000	1.403662000	-3.073003000
C	3.412178000	0.432397000	-2.202514000
C	3.232330000	-0.930695000	-2.482841000
H	3.014644000	2.454574000	-2.829531000
H	2.410474000	-2.373676000	-3.866890000
H	1.824774000	1.765710000	-4.913574000
H	1.529044000	-0.651087000	-5.430228000
H	3.916185000	0.736060000	-1.294613000
H	3.580557000	-1.679119000	-1.778883000

⁶P-1_{hs}

Mn	-0.029968000	0.004997000	0.132615000
O	0.612190000	-0.024386000	-2.958163000
C	-0.008161000	-0.007177000	2.355709000
C	0.678983000	0.026901000	4.542744000
H	1.388366000	0.077846000	5.351120000
C	-0.681427000	-0.077313000	4.546187000

H	-1.385675000	-0.140783000	5.358151000
C	-2.465792000	-0.209653000	2.741698000
H	-3.136787000	-0.059172000	3.591316000
H	-2.653914000	0.550665000	1.982510000
H	-2.641315000	-1.193834000	2.299289000
C	2.450809000	0.192608000	2.728244000
H	3.128054000	0.055677000	3.575114000
H	2.644223000	-0.570435000	1.972952000
H	2.613576000	1.175789000	2.278831000
N	1.068097000	0.066323000	3.200948000
N	-1.079254000	-0.094293000	3.206578000
N	-1.707699000	-1.210805000	-0.394439000
N	1.198691000	-1.682627000	-0.371259000
N	1.669834000	1.214886000	-0.455097000
N	-1.241456000	1.697378000	-0.316523000
C	-3.019541000	-0.778671000	-0.431405000
C	-1.721104000	-2.589223000	-0.277133000
C	0.756878000	-2.994668000	-0.425379000
C	2.570215000	-1.693429000	-0.574001000
C	2.986204000	0.781050000	-0.442941000
C	1.680543000	2.593257000	-0.280468000
C	-0.796700000	3.000344000	-0.418684000
C	-2.603892000	1.698690000	-0.552325000
C	-3.896904000	-1.927305000	-0.269684000
H	-4.973798000	-1.885936000	-0.227330000
C	-3.100717000	-3.036483000	-0.165184000
H	-3.414782000	-4.058718000	-0.025881000
C	1.893054000	-3.861281000	-0.692921000
H	1.838148000	-4.930423000	-0.823979000
C	3.000928000	-3.064606000	-0.790870000
H	4.010264000	-3.368033000	-1.019324000
C	3.853163000	1.920752000	-0.211820000
H	4.927593000	1.875946000	-0.127141000
C	3.053218000	3.028874000	-0.102501000
H	3.362778000	4.044283000	0.088118000
C	-1.926638000	3.861623000	-0.733330000
H	-1.865035000	4.924415000	-0.906507000
C	-3.032779000	3.063079000	-0.822562000
H	-4.037794000	3.357035000	-1.080613000
C	-3.446797000	0.564024000	-0.548234000
C	-0.583090000	-3.427944000	-0.303909000
C	3.414968000	-0.561268000	-0.561522000
C	0.544688000	3.433834000	-0.302572000
C	-4.914110000	0.803350000	-0.674153000
C	-5.661279000	0.181846000	-1.694205000

H	-5.148973000	-0.465349000	-2.397940000
C	-7.037575000	0.403578000	-1.808039000
H	-7.596062000	-0.077474000	-2.605123000
C	-7.692398000	1.251310000	-0.904601000
H	-8.760401000	1.424014000	-0.994106000
C	-6.960370000	1.877300000	0.112866000
H	-7.460696000	2.533590000	0.818522000
C	-5.584102000	1.654956000	0.226358000
H	-5.014407000	2.137632000	1.013801000
C	-0.810585000	-4.902694000	-0.254041000
C	-1.628258000	-5.544878000	-1.204496000
H	-2.092519000	-4.950679000	-1.984241000
C	-1.829938000	-6.928247000	-1.155653000
H	-2.457683000	-7.407285000	-1.900773000
C	-1.215736000	-7.695214000	-0.156830000
H	-1.371659000	-8.768907000	-0.119736000
C	-0.395917000	-7.069086000	0.791369000
H	0.082551000	-7.656128000	1.569452000
C	-0.194566000	-5.685696000	0.741937000
H	0.439390000	-5.196667000	1.474308000
C	4.885041000	-0.796468000	-0.654603000
C	5.651140000	-0.163437000	-1.653380000
H	5.150498000	0.484613000	-2.364736000
C	7.031297000	-0.374444000	-1.736597000
H	7.604412000	0.115307000	-2.517821000
C	7.671393000	-1.222115000	-0.822637000
H	8.742429000	-1.386512000	-0.888277000
C	6.920897000	-1.858026000	0.175083000
H	7.409955000	-2.513203000	0.889629000
C	5.540819000	-1.646151000	0.258171000
H	4.957566000	-2.135057000	1.031714000
C	0.774243000	4.906614000	-0.246777000
C	1.630781000	5.545502000	-1.165298000
H	2.121623000	4.949143000	-1.926798000
C	1.834488000	6.928170000	-1.110141000
H	2.491731000	7.404529000	-1.831132000
C	1.184056000	7.698259000	-0.136847000
H	1.341698000	8.771534000	-0.094990000
C	0.325738000	7.075889000	0.779273000
H	-0.180676000	7.665352000	1.537567000
C	0.121921000	5.693349000	0.723484000
H	-0.541279000	5.207229000	1.431332000
H	0.973485000	0.605290000	-2.297279000
H	0.516762000	-0.879267000	-2.495812000

⁴P-1_{is}

Mn	-0.002302000	0.123093000	-0.250394000
C	0.037891000	-0.391708000	2.026906000
C	0.704679000	-1.492016000	3.933806000
H	1.409174000	-1.908024000	4.634206000
C	-0.655721000	-1.427400000	3.960406000
H	-1.368825000	-1.780991000	4.685706000
C	-2.434810000	-0.509279000	2.426406000
H	-3.001807000	-0.223072000	3.318106000
H	-2.460300000	0.298722000	1.698106000
H	-2.870420000	-1.407674000	1.979306000
C	2.505887000	-0.739037000	2.339406000
H	3.133089000	-0.614144000	3.227606000
H	2.813177000	-1.631440000	1.785206000
H	2.609898000	0.129862000	1.693406000
N	1.107486000	-0.852720000	2.756606000
N	-1.040413000	-0.752095000	2.798706000
N	-1.380819000	-1.307791000	-0.472894000
N	1.449481000	-1.262224000	-0.502494000
N	1.374014000	1.540876000	-0.237694000
N	-1.464886000	1.502810000	-0.255494000
C	-2.754717000	-1.138675000	-0.694994000
C	-1.178535000	-2.669494000	-0.192694000
C	1.288765000	-2.633023000	-0.330994000
C	2.784384000	-1.045940000	-0.846394000
C	2.742313000	1.400460000	-0.505394000
C	1.172630000	2.872379000	0.151606000
C	-1.291470000	2.858908000	-0.010394000
C	-2.790188000	1.331525000	-0.666394000
C	-3.416032000	-2.418167000	-0.516394000
H	-4.480234000	-2.568155000	-0.607594000
C	-2.468843000	-3.333678000	-0.165794000
H	-2.615055000	-4.375677000	0.069506000
C	2.529257000	-3.285137000	-0.598394000
H	2.681745000	-4.352639000	-0.568094000
C	3.445569000	-2.306048000	-0.950894000
H	4.475667000	-2.444760000	-1.236494000
C	3.407627000	2.657953000	-0.204994000
H	4.470929000	2.815640000	-0.292294000
C	2.464338000	3.534564000	0.232606000
H	2.610050000	4.549262000	0.565606000
C	-2.515562000	3.546022000	-0.274694000
H	-2.652750000	4.612024000	-0.187194000
C	-3.432373000	2.606633000	-0.707294000

H	-4.448871000	2.778745000	-1.021994000
C	-3.413003000	0.074833000	-0.874694000
C	0.056257000	-3.291008000	-0.067594000
C	3.400499000	0.231853000	-0.872094000
C	-0.059563000	3.492993000	0.302506000
C	-4.868204000	0.035450000	-1.192594000
C	-5.329312000	-0.674745000	-2.318494000
H	-4.604818000	-1.168853000	-2.957594000
C	-6.694813000	-0.742929000	-2.614694000
H	-7.029619000	-1.290525000	-3.490394000
C	-7.626705000	-0.100318000	-1.789394000
H	-8.686406000	-0.150205000	-2.019694000
C	-7.181997000	0.606777000	-0.664194000
H	-7.898291000	1.100085000	-0.014094000
C	-5.816896000	0.672161000	-0.367694000
H	-5.472790000	1.212057000	0.507706000
C	0.127040000	-4.743109000	0.257806000
C	-0.493871000	-5.717702000	-0.546194000
H	-1.037467000	-5.401495000	-1.430294000
C	-0.402087000	-7.076403000	-0.223194000
H	-0.884096000	-7.814597000	-0.857094000
C	0.319808000	-7.484911000	0.905406000
H	0.392996000	-8.539012000	1.154706000
C	0.951819000	-6.524919000	1.707906000
H	1.513516000	-6.834025000	2.584406000
C	0.857535000	-5.167617000	1.385506000
H	1.341344000	-4.419123000	2.004806000
C	4.852800000	0.321736000	-1.197994000
C	5.287109000	1.141330000	-2.257794000
H	4.546016000	1.683239000	-2.836394000
C	6.647611000	1.256314000	-2.563294000
H	6.963118000	1.889511000	-3.386894000
C	7.599403000	0.553303000	-1.813294000
H	8.655104000	0.640991000	-2.050394000
C	7.180593000	-0.261492000	-0.752994000
H	7.912787000	-0.801100000	-0.159794000
C	5.820192000	-0.374376000	-0.447394000
H	5.496284000	-0.996672000	0.380006000
C	-0.123646000	4.932694000	0.683206000
C	0.528866000	5.926886000	-0.071294000
H	1.090762000	5.633880000	-0.951494000
C	0.441782000	7.274787000	0.294306000
H	0.947890000	8.027981000	-0.301994000
C	-0.306714000	7.653996000	1.416006000
H	-0.375602000	8.699997000	1.698506000

C	-0.972425000	6.675504000	2.166706000
H	-1.557222000	6.961111000	3.036006000
C	-0.883841000	5.328503000	1.801506000
H	-1.400950000	4.568109000	2.377506000
O	-0.049703000	0.044593000	-2.748094000
H	0.608588000	-0.679215000	-2.765294000
H	-0.945408000	-0.346496000	-2.776194000

²P-1s

Mn	-0.000973000	0.005133000	-0.179786000
O	-0.035343000	0.034206000	-2.331548000
C	0.025018000	-0.029694000	1.842606000
C	-0.651818000	-0.071517000	4.041584000
H	-1.363393000	-0.088415000	4.848972000
C	0.706095000	-0.078443000	4.039079000
H	1.420450000	-0.095314000	4.843968000
C	2.518839000	-0.022610000	2.324396000
H	3.109472000	-0.287721000	3.206004000
H	2.700185000	-0.746473000	1.536082000
H	2.803952000	0.973213000	1.978692000
C	-2.469107000	-0.040939000	2.330192000
H	-3.054085000	0.228190000	3.214394000
H	-2.639169000	0.692560000	1.547676000
H	-2.772722000	-1.028621000	1.976340000
N	-1.054014000	-0.037884000	2.705473000
N	1.104841000	-0.053119000	2.701598000
N	1.637581000	1.159707000	-0.316804000
N	-1.124973000	1.626387000	-0.285308000
N	-1.625396000	-1.154528000	-0.346364000
N	1.124498000	-1.617376000	-0.281752000
C	2.914699000	0.742281000	-0.651419000
C	1.725640000	2.491792000	0.055398000
C	-0.703265000	2.934757000	-0.034053000
C	-2.461832000	1.704829000	-0.706040000
C	-2.914268000	-0.730585000	-0.662291000
C	-1.718349000	-2.494582000	0.023938000
C	0.708684000	-2.922179000	-0.050296000
C	2.454673000	-1.688178000	-0.721178000
C	3.835481000	1.829301000	-0.446102000
H	4.900761000	1.772809000	-0.605945000
C	3.109631000	2.896672000	0.032310000
H	3.478818000	3.870521000	0.310399000
C	-1.802415000	3.844780000	-0.303042000
H	-1.739693000	4.917643000	-0.210521000

C	-2.854003000	3.102805000	-0.753781000
H	-3.814323000	3.460361000	-1.088955000
C	-3.830646000	-1.816871000	-0.451142000
H	-4.898283000	-1.757091000	-0.593714000
C	-3.101369000	-2.891551000	0.008165000
H	-3.472681000	-3.864427000	0.287079000
C	1.804312000	-3.832746000	-0.341579000
H	1.737548000	-4.906875000	-0.269276000
C	2.849035000	-3.084692000	-0.794850000
H	3.802997000	-3.435194000	-1.154581000
C	3.290483000	-0.592823000	-0.933583000
C	0.605858000	3.337003000	0.244450000
C	-3.297312000	0.607604000	-0.927907000
C	-0.602582000	-3.334494000	0.221893000
C	4.698936000	-0.815365000	-1.368307000
C	5.186880000	-0.161228000	-2.516607000
H	4.515219000	0.481790000	-3.075507000
C	6.510395000	-0.337440000	-2.932672000
H	6.866754000	0.168936000	-3.824605000
C	7.373426000	-1.166961000	-2.204040000
H	8.401043000	-1.303857000	-2.526307000
C	6.903153000	-1.815068000	-1.054669000
H	7.568326000	-2.450541000	-0.477722000
C	5.578875000	-1.638133000	-0.639044000
H	5.217821000	-2.129609000	0.258134000
C	0.819922000	4.763185000	0.620022000
C	1.637251000	5.621033000	-0.141947000
H	2.129145000	5.230821000	-1.026207000
C	1.802941000	6.961515000	0.222369000
H	2.432377000	7.609060000	-0.380676000
C	1.150357000	7.472051000	1.352408000
H	1.279302000	8.512576000	1.634038000
C	0.326683000	6.632123000	2.113230000
H	-0.184438000	7.019230000	2.989644000
C	0.162971000	5.291482000	1.749120000
H	-0.473693000	4.636453000	2.335115000
C	-4.710509000	0.831445000	-1.347368000
C	-5.215515000	0.181759000	-2.491141000
H	-4.555333000	-0.466027000	-3.058788000
C	-6.543677000	0.360173000	-2.891176000
H	-6.911661000	-0.145001000	-3.779068000
C	-7.396266000	1.190118000	-2.151097000
H	-8.427304000	1.329837000	-2.460741000
C	-6.910646000	1.833618000	-1.005459000
H	-7.567778000	2.468013000	-0.418228000

C	-5.582220000	1.652472000	-0.605470000
H	-5.211083000	2.138512000	0.290452000
C	-0.811148000	-4.760703000	0.597304000
C	-1.633652000	-5.620150000	-0.157433000
H	-2.131425000	-5.231793000	-1.039190000
C	-1.794763000	-6.960708000	0.208670000
H	-2.427905000	-7.609363000	-0.389316000
C	-1.131909000	-7.470215000	1.333094000
H	-1.256902000	-8.510897000	1.615928000
C	-0.302062000	-6.629142000	2.086079000
H	0.217850000	-7.015689000	2.957563000
C	-0.143070000	-5.288550000	1.720289000
H	0.499037000	-4.632996000	2.299715000
H	-0.784236000	-0.551122000	-2.561918000
H	-0.232639000	0.958831000	-2.577220000

C-H bond activation of CHD by species 2

⁵RC-2_{hs}

Fe	0.168470000	0.020178000	-0.143155000
O	0.056176000	0.030406000	1.514133000
C	0.341988000	0.021535000	-2.335524000
C	0.030455000	0.487315000	-4.568688000
H	-0.413989000	0.984012000	-5.413782000
C	1.002019000	-0.456921000	-4.488739000
H	1.574606000	-0.957781000	-5.250103000
C	2.164401000	-1.719582000	-2.685366000
H	2.824220000	-1.942873000	-3.528481000
H	2.748436000	-1.307955000	-1.869047000
H	1.669659000	-2.634653000	-2.356053000
C	-1.399628000	1.762948000	-2.980484000
H	-1.903457000	1.995365000	-3.922845000
H	-2.118501000	1.352589000	-2.279006000
H	-0.963168000	2.673111000	-2.566212000
N	-0.361666000	0.767318000	-3.257798000
N	1.182163000	-0.728460000	-3.130861000
N	0.573804000	-1.989458000	-0.134068000
N	-1.851558000	-0.367008000	-0.415945000
N	-0.241886000	2.026616000	-0.197880000
N	2.204914000	0.403072000	-0.080919000
C	1.765566000	-2.557904000	0.258322000
C	-0.308245000	-2.997981000	-0.464797000
C	-2.398219000	-1.616895000	-0.603893000
C	-2.872097000	0.512561000	-0.109456000

C	-1.483307000	2.591034000	-0.003492000
C	0.681926000	3.037648000	-0.364383000
C	2.766263000	1.657923000	-0.137813000
C	3.151152000	-0.476873000	0.411568000
C	1.653109000	-3.999699000	0.111164000
H	2.444491000	-4.703689000	0.314793000
C	0.395927000	-4.267464000	-0.361271000
H	-0.022617000	-5.231135000	-0.602827000
C	-3.840920000	-1.517449000	-0.442029000
H	-4.526536000	-2.346799000	-0.515156000
C	-4.126634000	-0.220680000	-0.110724000
H	-5.090088000	0.198996000	0.130251000
C	-1.350349000	4.034089000	-0.113706000
H	-2.166334000	4.735289000	-0.036110000
C	-0.032816000	4.306632000	-0.368838000
H	0.417707000	5.272954000	-0.528566000
C	4.151609000	1.563055000	0.301042000
H	4.832211000	2.396812000	0.372737000
C	4.377528000	0.263472000	0.664075000
H	5.279130000	-0.154620000	1.082398000
C	2.953973000	-1.863382000	0.583408000
C	-1.684882000	-2.831102000	-0.730716000
C	-2.707293000	1.895980000	0.108629000
C	2.084615000	2.872736000	-0.384312000
C	4.094987000	-2.682034000	1.082927000
C	3.930230000	-3.502346000	2.216631000
H	2.970032000	-3.508817000	2.721544000
C	4.987463000	-4.285498000	2.690991000
H	4.845339000	-4.905649000	3.570684000
C	6.227818000	-4.264601000	2.039294000
H	7.048619000	-4.871760000	2.408198000
C	6.402482000	-3.456474000	0.908239000
H	7.357920000	-3.441369000	0.392613000
C	5.344766000	-2.673779000	0.433348000
H	5.475742000	-2.055154000	-0.448342000
C	-2.497961000	-4.042976000	-1.043928000
C	-2.561953000	-5.138054000	-0.160835000
H	-2.003881000	-5.097814000	0.768322000
C	-3.347822000	-6.254881000	-0.464885000
H	-3.390883000	-7.087711000	0.230296000
C	-4.087871000	-6.294035000	-1.653978000
H	-4.698323000	-7.160497000	-1.888581000
C	-4.041134000	-5.205606000	-2.534948000
H	-4.613769000	-5.226797000	-3.457211000
C	-3.255347000	-4.089132000	-2.230504000

H	-3.217938000	-3.242623000	-2.908588000
C	-3.914608000	2.707322000	0.430389000
C	-3.942969000	3.475207000	1.611178000
H	-3.085066000	3.440204000	2.273155000
C	-5.063418000	4.248071000	1.932344000
H	-5.072857000	4.826573000	2.850942000
C	-6.173587000	4.268851000	1.077533000
H	-7.043759000	4.867902000	1.327255000
C	-6.154913000	3.511833000	-0.101276000
H	-7.008381000	3.528686000	-0.772307000
C	-5.034108000	2.738524000	-0.422695000
H	-5.015306000	2.158118000	-1.339350000
C	2.939048000	4.088047000	-0.530297000
C	2.832692000	5.177100000	0.356599000
H	2.110146000	5.128904000	1.163908000
C	3.659084000	6.296922000	0.214633000
H	3.568136000	7.124515000	0.911477000
C	4.610833000	6.345363000	-0.812517000
H	5.252726000	7.214061000	-0.921201000
C	4.734740000	5.262922000	-1.693408000
H	5.472171000	5.291043000	-2.489840000
C	3.908198000	4.143394000	-1.550944000
H	4.002768000	3.301298000	-2.228956000
C	-2.001012000	1.233622000	3.871778000
C	-2.874181000	0.443007000	3.234989000
C	-0.703117000	0.724608000	4.457014000
C	-2.649842000	-1.040400000	3.045839000
C	-1.546255000	-1.575579000	3.929971000
C	-0.672250000	-0.783524000	4.563399000
H	0.129921000	1.048349000	3.810011000
H	-3.587575000	-1.590392000	3.228423000
H	-0.525855000	1.180230000	5.445131000
H	-2.390321000	-1.232610000	1.993962000
H	0.120830000	-1.217099000	5.170442000
H	-1.469756000	-2.658135000	4.020130000
H	-2.201465000	2.299489000	3.973900000
H	-3.781855000	0.863740000	2.808120000

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Fe	-0.170397000	0.000995000	-0.107098000
O	-0.018996000	-0.017799000	1.557802000
C	-0.408398000	0.016486000	-2.260898000
C	-0.428473000	-0.607315000	-4.477598000
H	-0.278846000	-1.272209000	-5.310798000
C	-0.897223000	0.665667000	-4.415698000

H	-1.233050000	1.339853000	-5.184798000
C	-1.303391000	2.364350000	-2.632998000
H	-1.851409000	2.830229000	-3.456998000
H	-1.954587000	2.276525000	-1.769298000
H	-0.439115000	2.979385000	-2.374898000
C	0.390195000	-2.319582000	-2.856898000
H	0.748113000	-2.766368000	-3.788798000
H	1.215892000	-2.230849000	-2.157998000
H	-0.387180000	-2.951913000	-2.423498000
N	-0.133958000	-0.986803000	-3.165398000
N	-0.880238000	1.030467000	-3.066998000
N	0.367127000	1.905517000	-0.163398000
N	1.718025000	-0.550030000	-0.391698000
N	-0.704521000	-1.904526000	-0.081198000
N	-2.072019000	0.551520000	0.034602000
C	-0.388515000	2.963287000	0.294602000
C	1.556907000	2.419864000	-0.642998000
C	2.756792000	0.270212000	-0.780798000
C	2.268973000	-1.763408000	-0.015598000
C	0.130921000	-2.964693000	0.197202000
C	-1.968001000	-2.416076000	-0.306198000
C	-3.167486000	-0.270224000	-0.114998000
C	-2.523367000	1.757102000	0.548202000
C	0.333736000	4.197315000	0.057502000
H	-0.038403000	5.180701000	0.297702000
C	1.509749000	3.867862000	-0.558998000
H	2.282923000	4.534193000	-0.905498000
C	4.004621000	-0.460539000	-0.671098000
H	4.975805000	-0.049000000	-0.895298000
C	3.708570000	-1.693350000	-0.159698000
H	4.394702000	-2.482923000	0.100702000
C	-0.624030000	-4.198323000	0.104002000
H	-0.208091000	-5.182706000	0.251702000
C	-1.901743000	-3.865973000	-0.255298000
H	-2.728217000	-4.531306000	-0.444998000
C	-4.359415000	0.449029000	0.294702000
H	-5.354698000	0.033489000	0.294002000
C	-3.957963000	1.676345000	0.743202000
H	-4.568594000	2.455221000	1.170302000
C	-1.725212000	2.896334000	0.726702000
C	2.673737000	1.654108000	-1.012098000
C	1.527418000	-2.900337000	0.332602000
C	-3.138431000	-1.647122000	-0.403498000
C	-2.320961000	4.133010000	1.302402000
C	-1.722485000	4.728334000	2.430602000

H	-0.849766000	4.255268000	2.868802000
C	-2.251731000	5.898713000	2.984102000
H	-1.783749000	6.340031000	3.858602000
C	-3.385055000	6.496668000	2.417002000
H	-3.796091000	7.404651000	2.847102000
C	-3.983332000	5.918144000	1.290002000
H	-4.855050000	6.381809000	0.838302000
C	-3.454186000	4.747565000	0.735702000
H	-3.908968000	4.307447000	-0.145498000
C	3.899110000	2.333457000	-1.519398000
C	4.558871000	3.326683000	-0.770298000
H	4.161260000	3.605068000	0.199602000
C	5.723447000	3.930530000	-1.256398000
H	6.223617000	4.689950000	-0.663198000
C	6.251962000	3.547251000	-2.496098000
H	7.156444000	4.015487000	-2.871698000
C	5.611402000	2.550925000	-3.244298000
H	6.017014000	2.245441000	-4.203998000
C	4.446626000	1.947579000	-2.758198000
H	3.947556000	1.173459000	-3.332298000
C	2.232467000	-4.127809000	0.790502000
C	1.912189000	-4.670322000	2.050602000
H	1.175568000	-4.161751000	2.662802000
C	2.549835000	-5.826896000	2.510902000
H	2.298751000	-6.227706000	3.488002000
C	3.514760000	-6.462058000	1.717802000
H	4.010596000	-7.359138000	2.075202000
C	3.836039000	-5.934345000	0.460202000
H	4.575758000	-6.427016000	-0.163498000
C	3.198493000	-4.777271000	-0.000698000
H	3.436577000	-4.374961000	-0.979898000
C	-4.444505000	-2.315274000	-0.664498000
C	-4.930564000	-3.348894000	0.159402000
H	-4.338751000	-3.666670000	1.010802000
C	-6.169740000	-3.944643000	-0.099298000
H	-6.532009000	-4.736057000	0.549702000
C	-6.947957000	-3.513074000	-1.181398000
H	-7.909739000	-3.975412000	-1.380798000
C	-6.481599000	-2.475655000	-1.999498000
H	-7.080612000	-2.132179000	-2.837498000
C	-5.242722000	-1.880306000	-1.740798000
H	-4.878254000	-1.074892000	-2.370398000
C	1.625661000	-1.451533000	4.006602000
C	2.650147000	-1.114692000	3.213002000
C	0.653921000	-0.440072000	4.571202000

C	2.941491000	0.314119000	2.812702000
C	2.190051000	1.317089000	3.658502000
C	1.162864000	0.978848000	4.448102000
H	-0.298276000	-0.519910000	4.019902000
H	4.025783000	0.507662000	2.861602000
H	0.427630000	-0.673681000	5.624602000
H	2.655885000	0.455508000	1.760402000
H	2.507309000	2.356602000	3.586902000
H	0.638134000	1.740928000	5.022502000
H	1.449802000	-2.497240000	4.255402000
H	3.302878000	-1.884067000	2.806702000

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Fe	0.320061000	-0.008114000	-0.000123000
O	0.264092000	-0.034018000	-1.697880000
C	0.736524000	-0.014385000	2.092474000
C	0.931107000	-0.665146000	4.293222000
H	0.844893000	-1.338983000	5.128179000
C	1.394745000	0.608478000	4.209702000
H	1.789528000	1.273726000	4.958208000
C	1.649671000	2.334746000	2.429128000
H	2.212722000	2.809981000	3.237293000
H	2.274527000	2.265622000	1.544817000
H	0.763961000	2.930500000	2.202372000
C	-0.034195000	-2.352311000	2.732979000
H	-0.345110000	-2.788685000	3.686609000
H	-0.898329000	-2.248529000	2.085144000
H	0.702061000	-3.002189000	2.256107000
N	0.532774000	-1.028982000	3.005206000
N	1.270253000	0.990933000	2.872302000
N	-0.159998000	1.908300000	0.043182000
N	-1.520082000	-0.508528000	0.386210000
N	0.819285000	-1.935871000	-0.088614000
N	2.247855000	0.507999000	-0.223038000
C	0.600077000	2.945667000	-0.456917000
C	-1.304507000	2.458893000	0.584020000
C	-2.516667000	0.333608000	0.849681000
C	-2.124268000	-1.719965000	0.063158000
C	-0.045004000	-2.971913000	-0.333796000
C	2.082990000	-2.474748000	0.060726000
C	3.322944000	-0.346479000	-0.131560000
C	2.704006000	1.697434000	-0.765216000
C	-0.081357000	4.199747000	-0.198640000
H	0.303323000	5.172207000	-0.462609000

C	-1.232807000	3.904267000	0.478564000
H	-1.970832000	4.592178000	0.858355000
C	-3.775173000	-0.380746000	0.850042000
H	-4.720470000	0.050954000	1.136230000
C	-3.543106000	-1.618281000	0.322478000
H	-4.264978000	-2.386307000	0.101263000
C	0.685911000	-4.225290000	-0.307884000
H	0.241285000	-5.198244000	-0.447863000
C	1.987451000	-3.924252000	-0.014358000
H	2.809151000	-4.609346000	0.117212000
C	4.513942000	0.341164000	-0.594403000
H	5.495646000	-0.102621000	-0.644107000
C	4.125126000	1.579929000	-1.023726000
H	4.735578000	2.341221000	-1.481614000
C	1.920715000	2.849868000	-0.928720000
C	-2.404526000	1.717876000	1.043389000
C	-1.447700000	-2.868755000	-0.361277000
C	3.269602000	-1.729979000	0.130194000
C	2.527668000	4.071872000	-1.523843000
C	1.909598000	4.687237000	-2.630320000
H	1.010117000	4.240659000	-3.040850000
C	2.450911000	5.845369000	-3.197653000
H	1.966523000	6.301645000	-4.055453000
C	3.616952000	6.411803000	-2.665790000
H	4.037621000	7.310264000	-3.106562000
C	4.235400000	5.813946000	-1.559987000
H	5.132807000	6.253349000	-1.135039000
C	3.694166000	4.655517000	-0.992498000
H	4.165327000	4.200754000	-0.127521000
C	-3.594294000	2.430054000	1.586358000
C	-4.269655000	3.408823000	0.831397000
H	-3.904356000	3.650300000	-0.160350000
C	-5.406885000	4.044325000	1.341042000
H	-5.918708000	4.792456000	0.743420000
C	-5.892940000	3.707547000	2.611431000
H	-6.776464000	4.199843000	3.005713000
C	-5.235946000	2.727456000	3.366853000
H	-5.607882000	2.459016000	4.351001000
C	-4.097798000	2.093191000	2.857162000
H	-3.587314000	1.331160000	3.437373000
C	-2.220101000	-4.072345000	-0.772551000
C	-2.005555000	-4.620205000	-2.052583000
H	-1.289041000	-4.141007000	-2.711425000
C	-2.711443000	-5.752538000	-2.471717000
H	-2.540215000	-6.157114000	-3.464512000

C	-3.640060000	-6.360076000	-1.616003000
H	-4.188905000	-7.238401000	-1.941235000
C	-3.852992000	-5.830698000	-0.336526000
H	-4.561515000	-6.303555000	0.336839000
C	-3.146599000	-4.698005000	0.082660000
H	-3.300758000	-4.296329000	1.078553000
C	4.570941000	-2.429005000	0.327358000
C	5.007148000	-3.452088000	-0.536493000
H	4.379473000	-3.738396000	-1.373193000
C	6.243291000	-4.076018000	-0.336079000
H	6.566957000	-4.858649000	-1.015415000
C	7.067876000	-3.683735000	0.726556000
H	8.027214000	-4.167956000	0.880418000
C	6.651194000	-2.656744000	1.583692000
H	7.286421000	-2.343137000	2.406543000
C	5.415487000	-2.032931000	1.383009000
H	5.089760000	-1.234859000	2.042570000
C	-2.960157000	-1.071091000	-3.172284000
C	-4.259414000	-1.236204000	-2.881033000
C	-2.218631000	0.217793000	-2.958183000
C	-5.127568000	-0.134789000	-2.317156000
C	-4.357526000	1.134435000	-2.031160000
C	-3.057587000	1.290327000	-2.324364000
H	-1.305008000	0.027353000	-2.329904000
H	-5.961314000	0.078553000	-3.011084000
H	-1.775467000	0.575263000	-3.903672000
H	-5.611695000	-0.485653000	-1.389835000
H	-2.549176000	2.220152000	-2.077333000
H	-2.384298000	-1.905114000	-3.567769000
H	-4.735351000	-2.201416000	-3.045671000
H	-4.908522000	1.939612000	-1.549014000

⁵TS1-2_{ss}

Fe	0.307742000	0.002041000	0.046132000
O	0.303653000	-0.064417000	-1.705550000
C	0.468121000	0.008202000	2.189488000
C	0.754752000	-0.653675000	4.374431000
H	0.942063000	-1.353826000	5.170107000
C	0.521227000	0.683307000	4.388295000
H	0.457734000	1.388288000	5.199054000
C	0.068227000	2.466134000	2.708743000
H	0.285419000	3.083365000	3.585073000
H	0.707221000	2.769687000	1.885979000
H	-0.978408000	2.589720000	2.426876000

C	0.948285000	-2.446166000	2.655341000
H	0.869479000	-3.058919000	3.557785000
H	0.191842000	-2.754537000	1.941310000
H	1.938814000	-2.569576000	2.214203000
N	0.719375000	-1.050411000	3.035872000
N	0.350358000	1.071942000	3.057836000
N	-1.153253000	1.418869000	0.114580000
N	-1.133459000	-1.488781000	0.223806000
N	1.743712000	-1.429842000	-0.075836000
N	1.743478000	1.512336000	0.001866000
C	-0.983516000	2.756081000	-0.175966000
C	-2.442386000	1.229633000	0.578529000
C	-2.461359000	-1.272812000	0.493340000
C	-0.979643000	-2.788622000	-0.216715000
C	1.522822000	-2.758525000	-0.362596000
C	3.100386000	-1.225881000	0.069705000
C	3.098109000	1.284650000	-0.022938000
C	1.507884000	2.797128000	-0.445557000
C	-2.213646000	3.454636000	0.155048000
H	-2.363357000	4.518401000	0.057229000
C	-3.089270000	2.529183000	0.657376000
H	-4.083030000	2.710156000	1.033166000
C	-3.191439000	-2.505155000	0.234279000
H	-4.258576000	-2.622916000	0.341022000
C	-2.288829000	-3.422678000	-0.233755000
H	-2.490146000	-4.426450000	-0.572897000
C	2.802353000	-3.449674000	-0.322471000
H	2.935418000	-4.509581000	-0.472373000
C	3.762986000	-2.520222000	-0.025392000
H	4.820191000	-2.688807000	0.101566000
C	3.763907000	2.504043000	-0.462564000
H	4.829786000	2.612105000	-0.589360000
C	2.788015000	3.419697000	-0.750165000
H	2.916525000	4.411671000	-1.153351000
C	0.230767000	3.392218000	-0.533550000
C	-3.052985000	-0.023865000	0.805710000
C	0.263733000	-3.389477000	-0.508544000
C	3.739811000	0.032809000	0.139909000
C	0.140851000	4.820090000	-0.947205000
C	-0.730471000	5.199975000	-1.987732000
H	-1.310250000	4.432571000	-2.489969000
C	-0.839873000	6.538213000	-2.378068000
H	-1.511135000	6.810239000	-3.186883000
C	-0.080607000	7.524047000	-1.733714000
H	-0.164519000	8.563069000	-2.036696000

C	0.786632000	7.160693000	-0.694963000
H	1.371634000	7.919586000	-0.184216000
C	0.894788000	5.822042000	-0.304336000
H	1.556682000	5.541768000	0.508157000
C	-4.451329000	-0.074008000	1.321093000
C	-5.512034000	0.632506000	0.719477000
H	-5.311901000	1.231474000	-0.159430000
C	-6.812513000	0.542533000	1.226901000
H	-7.616400000	1.089100000	0.743127000
C	-7.082184000	-0.259353000	2.343257000
H	-8.092102000	-0.329159000	2.735203000
C	-6.039844000	-0.975786000	2.945944000
H	-6.238128000	-1.601884000	3.810600000
C	-4.740142000	-0.885041000	2.438544000
H	-3.930666000	-1.438486000	2.902805000
C	0.273678000	-4.817413000	-0.935131000
C	0.913716000	-5.188253000	-2.134652000
H	1.381207000	-4.416484000	-2.736969000
C	0.938307000	-6.524014000	-2.548273000
H	1.429422000	-6.790382000	-3.479204000
C	0.325812000	-7.514589000	-1.769060000
H	0.344211000	-8.551344000	-2.090495000
C	-0.308735000	-7.159498000	-0.571458000
H	-0.777254000	-7.922401000	0.042976000
C	-0.332745000	-5.823404000	-0.157590000
H	-0.814323000	-5.548850000	0.774973000
C	5.228397000	0.070291000	0.239720000
C	6.053059000	-0.578229000	-0.700265000
H	5.591755000	-1.122129000	-1.517230000
C	7.446375000	-0.505671000	-0.597999000
H	8.066575000	-1.005783000	-1.335640000
C	8.040764000	0.221251000	0.442077000
H	9.122099000	0.277751000	0.519958000
C	7.231319000	0.881200000	1.375934000
H	7.683626000	1.449842000	2.182812000
C	5.838221000	0.808908000	1.272823000
H	5.207123000	1.321576000	1.991636000
C	-2.176797000	-0.995361000	-3.406157000
C	-3.418820000	-1.365916000	-3.037973000
C	-1.671516000	0.385491000	-3.237916000
C	-4.429501000	-0.396694000	-2.474346000
C	-3.933931000	1.030113000	-2.458243000
C	-2.679957000	1.375479000	-2.813291000
H	-0.768852000	0.268289000	-2.358167000
H	-5.375108000	-0.460881000	-3.043098000

H	-1.018271000	0.729033000	-4.050214000
H	-4.698404000	-0.706793000	-1.449522000
H	-1.480697000	-1.731960000	-3.798509000
H	-3.732174000	-2.402514000	-3.133474000
H	-4.638340000	1.798492000	-2.146739000
H	-2.374143000	2.417541000	-2.767379000

³TS1-2_{is}

Fe	0.310586000	0.006292000	-0.031049000
O	0.264026000	-0.015882000	-1.794270000
C	0.515861000	0.010890000	2.088317000
C	0.786665000	-0.655844000	4.275307000
H	0.929887000	-1.362663000	5.074396000
C	0.670025000	0.696602000	4.280686000
H	0.683023000	1.410617000	5.086063000
C	0.329300000	2.495051000	2.585017000
H	0.651799000	3.107313000	3.432073000
H	0.940286000	2.725455000	1.718639000
H	-0.717661000	2.706806000	2.359284000
C	0.802673000	-2.469996000	2.562706000
H	0.687430000	-3.072037000	3.468542000
H	0.017001000	-2.724305000	1.858314000
H	1.775422000	-2.673160000	2.110922000
N	0.690176000	-1.058824000	2.940468000
N	0.508229000	1.087432000	2.948819000
N	-1.027642000	1.456476000	0.082973000
N	-1.144996000	-1.318304000	0.147437000
N	1.637256000	-1.455146000	-0.157343000
N	1.769644000	1.346106000	-0.142605000
C	-0.821404000	2.763685000	-0.302634000
C	-2.291477000	1.380109000	0.638225000
C	-2.422948000	-1.075002000	0.601435000
C	-1.103812000	-2.630725000	-0.294963000
C	1.352857000	-2.759810000	-0.495174000
C	2.997368000	-1.367265000	0.065527000
C	3.118418000	1.092996000	-0.035570000
C	1.625009000	2.640833000	-0.615315000
C	-1.988836000	3.548379000	0.047499000
H	-2.088465000	4.608877000	-0.122411000
C	-2.870373000	2.708538000	0.672492000
H	-3.828904000	2.959543000	1.096249000
C	-3.216558000	-2.278563000	0.452986000
H	-4.260623000	-2.358683000	0.711258000
C	-2.421267000	-3.216650000	-0.144186000

H	-2.696094000	-4.210223000	-0.458552000
C	2.574355000	-3.540441000	-0.430955000
H	2.635265000	-4.600432000	-0.621387000
C	3.576719000	-2.695309000	-0.039720000
H	4.612114000	-2.937029000	0.137422000
C	3.857874000	2.278491000	-0.429298000
H	4.933873000	2.348333000	-0.454967000
C	2.942046000	3.212115000	-0.827136000
H	3.133105000	4.192324000	-1.233039000
C	0.399378000	3.313500000	-0.739164000
C	-2.939623000	0.180416000	0.970927000
C	0.068148000	-3.309507000	-0.663239000
C	3.707834000	-0.163438000	0.199428000
C	0.372356000	4.716990000	-1.234727000
C	-0.473422000	5.058324000	-2.308725000
H	-1.069506000	4.279085000	-2.772570000
C	-0.536385000	6.373528000	-2.779900000
H	-1.188081000	6.616432000	-3.613573000
C	0.242850000	7.373329000	-2.182726000
H	0.194901000	8.394357000	-2.548270000
C	1.081573000	7.048346000	-1.108544000
H	1.679499000	7.819713000	-0.632636000
C	1.143417000	5.732813000	-0.636874000
H	1.779360000	5.484579000	0.206124000
C	-4.279571000	0.201707000	1.618618000
C	-5.368759000	0.914419000	1.079621000
H	-5.231906000	1.460082000	0.154564000
C	-6.618093000	0.894600000	1.708858000
H	-7.447281000	1.444344000	1.273911000
C	-6.805337000	0.157489000	2.885205000
H	-7.775632000	0.142092000	3.371732000
C	-5.733665000	-0.565777000	3.425314000
H	-5.869686000	-1.142595000	4.335105000
C	-4.484775000	-0.544967000	2.796678000
H	-3.651838000	-1.103222000	3.211464000
C	-0.014925000	-4.715534000	-1.147655000
C	0.555379000	-5.050905000	-2.391767000
H	1.028909000	-4.269052000	-2.976309000
C	0.505698000	-6.364390000	-2.869741000
H	0.943303000	-6.603340000	-3.834169000
C	-0.110611000	-7.367615000	-2.110146000
H	-0.149968000	-8.387083000	-2.481118000
C	-0.671613000	-7.048537000	-0.866662000
H	-1.139271000	-7.822879000	-0.266046000
C	-0.621152000	-5.734741000	-0.388161000

H	-1.040866000	-5.491134000	0.582023000
C	5.178694000	-0.190767000	0.433787000
C	6.057781000	-0.881719000	-0.422803000
H	5.652751000	-1.407722000	-1.280255000
C	7.437107000	-0.871077000	-0.189148000
H	8.100811000	-1.403605000	-0.863502000
C	7.963160000	-0.164085000	0.900139000
H	9.033753000	-0.155684000	1.079720000
C	7.100163000	0.539038000	1.750913000
H	7.499863000	1.093371000	2.594671000
C	5.721175000	0.528269000	1.517106000
H	5.048712000	1.073813000	2.171391000
C	-2.474063000	-1.115769000	-3.226817000
C	-3.709023000	-1.384340000	-2.759757000
C	-1.869893000	0.233122000	-3.163398000
C	-4.609623000	-0.327985000	-2.165296000
C	-4.020234000	1.060634000	-2.244312000
C	-2.778373000	1.304736000	-2.707513000
H	-0.888301000	0.139938000	-2.369040000
H	-5.596601000	-0.348010000	-2.662639000
H	-1.275850000	0.499132000	-4.047748000
H	-4.822451000	-0.579895000	-1.111324000
H	-4.098062000	-2.399002000	-2.792440000
H	-1.862253000	-1.914844000	-3.638100000
H	-2.400610000	2.323934000	-2.727103000
H	-4.645686000	1.886599000	-1.912057000

¹TS1-2_s

Fe	0.310596000	0.006296000	-0.031001000
O	0.263996000	-0.015903000	-1.794301000
C	0.515896000	0.010892000	2.088299000
C	0.786685000	-0.655812000	4.275299000
H	0.929872000	-1.362715000	5.074399000
C	0.670008000	0.696590000	4.280699000
H	0.683021000	1.410590000	5.086099000
C	0.329340000	2.495096000	2.584999000
H	0.651851000	3.107290000	3.432099000
H	0.940344000	2.725485000	1.718599000
H	-0.717656000	2.706814000	2.359299000
C	0.802653000	-2.470013000	2.562699000
H	0.687342000	-3.072011000	3.468499000
H	0.016948000	-2.724299000	1.858299000
H	1.775349000	-2.673230000	2.110899000
N	0.690178000	-1.058811000	2.940499000

N	0.508215000	1.087393000	2.948799000
N	-1.027578000	1.456520000	0.082999000
N	-1.145027000	-1.318278000	0.147399000
N	1.637271000	-1.455127000	-0.157301000
N	1.769620000	1.346070000	-0.142601000
C	-0.821355000	2.763716000	-0.302601000
C	-2.291479000	1.380142000	0.638199000
C	-2.422923000	-1.074956000	0.601399000
C	-1.103850000	-2.630679000	-0.295001000
C	1.352848000	-2.759822000	-0.495201000
C	2.997372000	-1.367351000	0.065499000
C	3.118415000	1.092947000	-0.035601000
C	1.625043000	2.640773000	-0.615301000
C	-1.988741000	3.548437000	0.047499000
H	-2.088423000	4.608938000	-0.122401000
C	-2.870356000	2.708552000	0.672499000
H	-3.828852000	2.959569000	1.096199000
C	-3.216644000	-2.278542000	0.452999000
H	-4.260645000	-2.358623000	0.711299000
C	-2.421360000	-3.216656000	-0.144201000
H	-2.696178000	-4.210151000	-0.458601000
C	2.574334000	-3.540444000	-0.431001000
H	2.635215000	-4.600445000	-0.621401000
C	3.576649000	-2.695361000	-0.039701000
H	4.612044000	-2.937080000	0.137399000
C	3.857936000	2.278434000	-0.429301000
H	4.933938000	2.348215000	-0.455001000
C	2.942053000	3.212050000	-0.827101000
H	3.133170000	4.192246000	-1.233001000
C	0.399455000	3.313495000	-0.739201000
C	-2.939601000	0.180453000	0.970899000
C	0.068038000	-3.309500000	-0.663201000
C	3.707793000	-0.163464000	0.199399000
C	0.372479000	4.716995000	-1.234701000
C	-0.473315000	5.058310000	-2.308701000
H	-1.069428000	4.279120000	-2.772601000
C	-0.536291000	6.373511000	-2.779901000
H	-1.187987000	6.616422000	-3.613601000
C	0.243026000	7.373297000	-2.182701000
H	0.195044000	8.394398000	-2.548301000
C	1.081720000	7.048282000	-1.108501000
H	1.679634000	7.819672000	-0.632601000
C	1.143497000	5.732781000	-0.636901000
H	1.779493000	5.484570000	0.206099000
C	-4.279600000	0.201777000	1.618599000

C	-5.368788000	0.914496000	1.079599000
H	-5.231878000	1.460194000	0.154599000
C	-6.618088000	0.894718000	1.708899000
H	-7.447278000	1.444433000	1.273899000
C	-6.805301000	0.157621000	2.885199000
H	-7.775601000	0.142239000	3.371699000
C	-5.733714000	-0.565697000	3.425299000
H	-5.869724000	-1.142495000	4.335099000
C	-4.484813000	-0.544919000	2.796699000
H	-3.651823000	-1.103134000	3.211499000
C	-0.014987000	-4.715498000	-1.147701000
C	0.555307000	-5.050908000	-2.391801000
H	1.028821000	-4.269117000	-2.976301000
C	0.505584000	-6.364407000	-2.869701000
H	0.943180000	-6.603315000	-3.834201000
C	-0.110734000	-7.367596000	-2.110101000
H	-0.150152000	-8.387096000	-2.481101000
C	-0.671728000	-7.048487000	-0.866701000
H	-1.139442000	-7.822878000	-0.266001000
C	-0.621305000	-5.734687000	-0.388201000
H	-1.041001000	-5.491080000	0.581999000
C	5.178693000	-0.190890000	0.433799000
C	6.057781000	-0.881805000	-0.422801000
H	5.652771000	-1.407798000	-1.280301000
C	7.437081000	-0.871229000	-0.189101000
H	8.100771000	-1.403741000	-0.863501000
C	7.963193000	-0.164239000	0.900099000
H	9.033793000	-0.155858000	1.079699000
C	7.100206000	0.538876000	1.750899000
H	7.499915000	1.093269000	2.594699000
C	5.721206000	0.528201000	1.517099000
H	5.048715000	1.073713000	2.171399000
C	-2.474123000	-1.115755000	-3.226801000
C	-3.709028000	-1.384233000	-2.759801000
C	-1.869900000	0.233134000	-3.163401000
C	-4.609610000	-0.327917000	-2.165301000
C	-4.020185000	1.060672000	-2.244301000
C	-2.778381000	1.304751000	-2.707501000
H	-0.888301000	0.139917000	-2.369001000
H	-5.596610000	-0.347900000	-2.662601000
H	-1.275795000	0.499124000	-4.047701000
H	-4.822514000	-0.579813000	-1.111301000
H	-4.098146000	-2.398926000	-2.792401000
H	-1.862338000	-1.914766000	-3.638101000
H	-2.400563000	2.323944000	-2.727101000

H	-4.645671000	1.886683000	-1.912101000
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⁷INT1-2_{hs}

Fe	0.411714000	0.007418000	-0.133072000
O	0.076361000	-0.014956000	-1.991189000
C	0.807747000	0.062831000	2.281600000
C	1.434658000	-0.539970000	4.421027000
H	1.838887000	-1.189327000	5.178858000
C	0.930610000	0.720324000	4.491991000
H	0.800050000	1.389703000	5.325234000
C	-0.044141000	2.363213000	2.869276000
H	0.091727000	3.029843000	3.725751000
H	0.450705000	2.784610000	1.998092000
H	-1.109994000	2.252304000	2.658723000
C	1.819042000	-2.225808000	2.606293000
H	1.985308000	-2.868724000	3.475390000
H	1.061682000	-2.668978000	1.964923000
H	2.749891000	-2.122293000	2.044793000
N	1.350836000	-0.922562000	3.078526000
N	0.559061000	1.069579000	3.189702000
N	-1.286114000	1.146637000	0.233945000
N	-0.652864000	-1.738327000	0.253088000
N	2.121810000	-1.116238000	-0.321347000
N	1.515123000	1.771701000	-0.178745000
C	-1.401872000	2.508397000	0.051801000
C	-2.484945000	0.668606000	0.727582000
C	-1.993086000	-1.789983000	0.572141000
C	-0.256105000	-2.997422000	-0.159627000
C	2.171806000	-2.481435000	-0.499444000
C	3.414440000	-0.631006000	-0.278321000
C	2.884351000	1.826843000	-0.321575000
C	0.998748000	3.026501000	-0.450361000
C	-2.724091000	2.919142000	0.488641000
H	-3.087680000	3.934551000	0.486556000
C	-3.377084000	1.796832000	0.926832000
H	-4.373645000	1.734550000	1.333116000
C	-2.465895000	-3.148505000	0.358560000
H	-3.483603000	-3.474530000	0.501910000
C	-1.409597000	-3.881108000	-0.111227000
H	-1.411074000	-4.915895000	-0.414557000
C	3.565193000	-2.889304000	-0.523788000
H	3.909481000	-3.906907000	-0.621041000
C	4.325767000	-1.760771000	-0.359646000
H	5.400778000	-1.697631000	-0.306493000

C	3.255366000	3.184515000	-0.690530000
H	4.262575000	3.515054000	-0.889286000
C	2.100412000	3.911206000	-0.794645000
H	1.998627000	4.942730000	-1.091806000
C	-0.363965000	3.383832000	-0.349671000
C	-2.822813000	-0.692326000	0.894399000
C	1.063198000	-3.360021000	-0.508568000
C	3.780869000	0.733701000	-0.264082000
C	-0.746600000	4.800724000	-0.608262000
C	-1.762016000	5.100786000	-1.538402000
H	-2.242127000	4.285857000	-2.070317000
C	-2.142458000	6.424473000	-1.780688000
H	-2.921400000	6.636813000	-2.506513000
C	-1.516054000	7.473951000	-1.095352000
H	-1.810414000	8.501642000	-1.283853000
C	-0.509045000	7.188986000	-0.163892000
H	-0.025564000	7.995821000	0.378455000
C	-0.129635000	5.864759000	0.078806000
H	0.641699000	5.641896000	0.808306000
C	-4.218506000	-1.019325000	1.305007000
C	-5.317980000	-0.551960000	0.558861000
H	-5.140402000	0.058230000	-0.317927000
C	-6.623014000	-0.895512000	0.926991000
H	-7.458362000	-0.531724000	0.336060000
C	-6.851641000	-1.711577000	2.043266000
H	-7.865126000	-1.978049000	2.327265000
C	-5.764084000	-2.185508000	2.788890000
H	-5.932338000	-2.817599000	3.655592000
C	-4.458033000	-1.844357000	2.420504000
H	-3.612395000	-2.212810000	2.992324000
C	1.337230000	-4.785035000	-0.846564000
C	1.980454000	-5.112920000	-2.056839000
H	2.249740000	-4.313219000	-2.738590000
C	2.256641000	-6.445073000	-2.381045000
H	2.745601000	-6.679753000	-3.321521000
C	1.896934000	-7.474104000	-1.500553000
H	2.110645000	-8.508130000	-1.752692000
C	1.260943000	-7.160716000	-0.292109000
H	0.987153000	-7.951446000	0.399811000
C	0.985486000	-5.828348000	0.032550000
H	0.503215000	-5.583662000	0.973086000
C	5.234976000	1.068892000	-0.289645000
C	6.083488000	0.586236000	-1.305066000
H	5.665369000	-0.040705000	-2.085137000
C	7.441230000	0.922812000	-1.321051000

H	8.079226000	0.547290000	-2.115230000
C	7.974123000	1.751793000	-0.325063000
H	9.027645000	2.013323000	-0.338565000
C	7.138181000	2.246153000	0.684887000
H	7.542908000	2.889908000	1.459932000
C	5.780631000	1.909513000	0.700480000
H	5.129387000	2.290561000	1.480388000
H	-0.522853000	0.591131000	-2.465893000
C	-3.074062000	-0.663143000	-2.344718000
C	-4.079368000	-1.578677000	-2.526393000
C	-3.333741000	0.734479000	-2.404242000
C	-5.504543000	-1.167844000	-2.806218000
C	-5.694063000	0.328988000	-2.867544000
C	-4.651503000	1.200784000	-2.670134000
H	-5.857529000	-1.632913000	-3.748777000
H	-2.535816000	1.440760000	-2.204338000
H	-6.172376000	-1.597878000	-2.032075000
H	-2.060469000	-0.991149000	-2.135695000
H	-3.866695000	-2.641582000	-2.454210000
H	-6.694758000	0.702265000	-3.070849000
H	-4.833572000	2.272239000	-2.706734000

⁵INT1-2_{hs}

Fe	0.411668000	0.007628000	-0.133321000
O	0.076083000	-0.015487000	-1.991553000
C	0.807487000	0.063090000	2.281433000
C	1.432589000	-0.540166000	4.421244000
H	1.836427000	-1.189569000	5.179246000
C	0.927855000	0.719862000	4.492167000
H	0.796201000	1.388894000	5.325516000
C	-0.046061000	2.362847000	2.869018000
H	0.089526000	3.029603000	3.725441000
H	0.448833000	2.784256000	1.997867000
H	-1.111868000	2.251661000	2.658274000
C	1.819580000	-2.225179000	2.606249000
H	1.987977000	-2.867395000	3.475447000
H	1.061934000	-2.669783000	1.966155000
H	2.749477000	-2.120649000	2.043404000
N	1.350331000	-0.922306000	3.078524000
N	0.557440000	1.069397000	3.189637000
N	-1.286188000	1.146542000	0.233460000
N	-0.652444000	-1.738300000	0.252771000
N	2.122059000	-1.115800000	-0.321493000
N	1.514775000	1.772058000	-0.179388000

C	-1.402215000	2.508295000	0.051334000
C	-2.484841000	0.668361000	0.727429000
C	-1.992682000	-1.790163000	0.571775000
C	-0.255395000	-2.997378000	-0.159586000
C	2.172376000	-2.480995000	-0.499651000
C	3.414556000	-0.630276000	-0.278576000
C	2.884091000	1.827509000	-0.321472000
C	0.998322000	3.026921000	-0.450472000
C	-2.724386000	2.918825000	0.488573000
H	-3.088123000	3.934184000	0.486590000
C	-3.377055000	1.796443000	0.927045000
H	-4.373447000	1.734035000	1.333735000
C	-2.465169000	-3.148859000	0.358538000
H	-3.482812000	-3.475061000	0.501950000
C	-1.408685000	-3.881336000	-0.110993000
H	-1.409929000	-4.916196000	-0.414081000
C	3.565837000	-2.888537000	-0.524181000
H	3.910379000	-3.906045000	-0.621519000
C	4.326152000	-1.759813000	-0.360137000
H	5.401155000	-1.696425000	-0.307137000
C	3.255024000	3.185429000	-0.689580000
H	4.262263000	3.516254000	-0.887707000
C	2.099992000	3.911984000	-0.793822000
H	1.998190000	4.943641000	-1.090503000
C	-0.364499000	3.383985000	-0.350025000
C	-2.822493000	-0.692630000	0.894206000
C	1.063951000	-3.359790000	-0.508530000
C	3.780742000	0.734511000	-0.264069000
C	-0.747475000	4.800799000	-0.608534000
C	-1.762795000	5.100591000	-1.538870000
H	-2.242508000	4.285535000	-2.070952000
C	-2.143665000	6.424162000	-1.781117000
H	-2.922527000	6.636288000	-2.507092000
C	-1.517800000	7.473801000	-1.095540000
H	-1.812488000	8.501404000	-1.284010000
C	-0.510926000	7.189106000	-0.163853000
H	-0.027889000	7.996061000	0.378712000
C	-0.131094000	5.864992000	0.078817000
H	0.640085000	5.642349000	0.808544000
C	-4.218054000	-1.019801000	1.305067000
C	-5.317670000	-0.552504000	0.559106000
H	-5.140195000	0.057620000	-0.317749000
C	-6.622628000	-0.896116000	0.927437000
H	-7.458096000	-0.532397000	0.336632000
C	-6.851023000	-1.712159000	2.043772000

H	-7.864446000	-1.978677000	2.327953000
C	-5.763318000	-2.186015000	2.789241000
H	-5.931411000	-2.818080000	3.655992000
C	-4.457347000	-1.844813000	2.420639000
H	-3.611600000	-2.213192000	2.992347000
C	1.338233000	-4.784814000	-0.846323000
C	1.981253000	-5.112771000	-2.056683000
H	2.250186000	-4.313137000	-2.738653000
C	2.257689000	-6.444919000	-2.380693000
H	2.746492000	-6.679665000	-3.321234000
C	1.898433000	-7.473866000	-1.499915000
H	2.112339000	-8.507888000	-1.751903000
C	1.262643000	-7.160398000	-0.291388000
H	0.989200000	-7.951059000	0.400748000
C	0.986941000	-5.828029000	0.033075000
H	0.504827000	-5.583284000	0.973678000
C	5.234821000	1.069904000	-0.289254000
C	6.083533000	0.587846000	-1.304784000
H	5.665609000	-0.038771000	-2.085222000
C	7.441244000	0.924578000	-1.320398000
H	8.079400000	0.549524000	-2.114668000
C	7.973897000	1.753111000	-0.323910000
H	9.027393000	2.014763000	-0.337125000
C	7.137755000	2.246851000	0.686177000
H	7.542297000	2.890243000	1.461622000
C	5.780240000	1.910048000	0.701405000
H	5.128836000	2.290604000	1.481419000
H	-0.520027000	0.593584000	-2.466330000
C	-3.073119000	-0.664982000	-2.346620000
C	-4.078681000	-1.580402000	-2.527275000
C	-3.332761000	0.732670000	-2.406001000
C	-5.503933000	-1.169458000	-2.806632000
C	-5.693565000	0.327390000	-2.866926000
C	-4.650825000	1.199111000	-2.670099000
H	-5.857021000	-1.633825000	-3.749543000
H	-2.534443000	1.438826000	-2.207244000
H	-6.171674000	-1.600141000	-2.032815000
H	-2.059231000	-0.992798000	-2.138578000
H	-3.866242000	-2.643323000	-2.454706000
H	-6.694419000	0.700777000	-3.069253000
H	-4.832940000	2.270580000	-2.706095000

⁵INT1-2_{is}

Fe	0.297576000	0.039242000	-0.152886000
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O	0.099488000	0.013029000	-2.050768000
N	-1.471692000	0.941121000	0.144061000
N	-0.575826000	-1.744704000	0.111849000
N	2.068605000	-0.867833000	-0.267715000
N	1.189467000	1.831688000	-0.152137000
C	-1.737461000	2.275698000	-0.077107000
C	-2.601236000	0.383414000	0.720796000
C	-1.870727000	-1.966358000	0.526941000
C	-0.073938000	-2.953778000	-0.344812000
C	2.268759000	-2.205384000	-0.536943000
C	3.310353000	-0.291092000	-0.079171000
C	2.548420000	2.059177000	-0.132690000
C	0.575741000	3.025849000	-0.498529000
C	-3.072420000	2.578311000	0.393212000
H	-3.527584000	3.555622000	0.359946000
C	-3.585408000	1.426695000	0.926735000
H	-4.541776000	1.292959000	1.405427000
C	-2.207315000	-3.359766000	0.308317000
H	-3.168369000	-3.798912000	0.525416000
C	-1.117894000	-3.955592000	-0.266540000
H	-1.022804000	-4.975814000	-0.601609000
C	3.686629000	-2.493344000	-0.472253000
H	4.121287000	-3.469981000	-0.615460000
C	4.324014000	-1.325391000	-0.150173000
H	5.378983000	-1.171566000	0.009130000
C	2.804304000	3.446455000	-0.471670000
H	3.785702000	3.886999000	-0.548725000
C	1.596354000	4.028487000	-0.735598000
H	1.407723000	5.037378000	-1.064865000
C	-0.808974000	3.246657000	-0.498390000
C	-2.787822000	-0.987451000	0.956807000
C	1.267311000	-3.182376000	-0.684394000
C	3.552676000	1.088189000	0.025860000
C	-1.345818000	4.588338000	-0.853510000
C	-2.338538000	4.693672000	-1.848288000
H	-2.670006000	3.789692000	-2.348463000
C	-2.876828000	5.937426000	-2.192399000
H	-3.634860000	6.001095000	-2.967074000
C	-2.435720000	7.098834000	-1.544122000
H	-2.852849000	8.064914000	-1.810775000
C	-1.455736000	7.006004000	-0.547029000
H	-1.117701000	7.900097000	-0.031987000
C	-0.917297000	5.761511000	-0.202800000
H	-0.170670000	5.687307000	0.580695000
C	-4.042464000	-1.470408000	1.598142000

C	-5.320054000	-1.124912000	1.115159000
H	-5.398245000	-0.490686000	0.241226000
C	-6.475676000	-1.611816000	1.734993000
H	-7.450973000	-1.339928000	1.342875000
C	-6.377356000	-2.457272000	2.847473000
H	-7.274682000	-2.835299000	3.327316000
C	-5.112969000	-2.816184000	3.333137000
H	-5.026625000	-3.471306000	4.194617000
C	-3.958154000	-2.329124000	2.713373000
H	-2.977056000	-2.602226000	3.087397000
C	1.692542000	-4.539204000	-1.126036000
C	2.378029000	-4.688516000	-2.348041000
H	2.564982000	-3.807012000	-2.952240000
C	2.799756000	-5.950103000	-2.779971000
H	3.319636000	-6.048645000	-3.727950000
C	2.547867000	-7.083855000	-1.995947000
H	2.874962000	-8.063135000	-2.331387000
C	1.875014000	-6.946520000	-0.774728000
H	1.687092000	-7.818780000	-0.156004000
C	1.453260000	-5.684642000	-0.342235000
H	0.945977000	-5.574900000	0.610391000
C	4.951172000	1.574596000	0.191315000
C	5.968055000	1.231387000	-0.720643000
H	5.723656000	0.598654000	-1.566908000
C	7.269674000	1.715983000	-0.552829000
H	8.040124000	1.447658000	-1.269196000
C	7.576288000	2.555509000	0.526337000
H	8.586512000	2.931431000	0.655262000
C	6.570332000	2.912755000	1.433823000
H	6.799256000	3.564711000	2.271359000
C	5.268915000	2.428739000	1.265657000
H	4.485606000	2.702680000	1.965104000
H	-0.807932000	0.035841000	-2.413183000
C	0.596634000	0.077491000	2.308093000
C	1.278893000	-0.456856000	4.448749000
H	1.731832000	-1.066485000	5.212414000
C	0.687105000	0.767229000	4.509943000
H	0.514740000	1.432970000	5.338847000
C	-0.421789000	2.305266000	2.847523000
H	-0.358129000	3.001911000	3.688409000
H	0.046821000	2.745363000	1.969372000
H	-1.470712000	2.097608000	2.622665000
C	1.768809000	-2.119568000	2.619588000
H	1.876728000	-2.807682000	3.463344000
H	1.090053000	-2.543965000	1.883533000

H	2.743255000	-1.957041000	2.150610000
N	1.210740000	-0.858732000	3.109407000
N	0.283076000	1.073552000	3.205084000
C	-2.389319000	-0.920487000	-3.945454000
C	-3.081901000	-1.801131000	-3.153878000
C	-2.682541000	0.474348000	-3.937679000
C	-4.204578000	-1.355556000	-2.252208000
C	-4.437523000	0.134127000	-2.279903000
C	-3.705039000	0.971421000	-3.082895000
H	-5.140229000	-1.890767000	-2.517502000
H	-2.109380000	1.153429000	-4.558872000
H	-3.996849000	-1.688151000	-1.220014000
H	-2.819857000	-2.855050000	-3.142057000
H	-1.577221000	-1.282226000	-4.568747000
H	-3.907664000	2.039281000	-3.066944000
H	-5.212697000	0.540486000	-1.636697000

³INT1-2_{is}

Fe	0.302476000	0.038140000	-0.157305000
O	0.116722000	0.025124000	-2.054239000
N	-1.390866000	1.078328000	0.126942000
N	-0.713091000	-1.670656000	0.104051000
N	1.997535000	-1.005694000	-0.252158000
N	1.332486000	1.755450000	-0.160889000
C	-1.552470000	2.426956000	-0.109529000
C	-2.567106000	0.612362000	0.690781000
C	-2.023302000	-1.788758000	0.513528000
C	-0.302155000	-2.919123000	-0.336933000
C	2.094444000	-2.357636000	-0.507063000
C	3.279208000	-0.525710000	-0.058792000
C	2.704828000	1.876610000	-0.136213000
C	0.815293000	2.992555000	-0.514119000
C	-2.867302000	2.833457000	0.339394000
H	-3.246495000	3.842103000	0.292616000
C	-3.472542000	1.728580000	0.874939000
H	-4.442633000	1.671324000	1.341093000
C	-2.463993000	-3.154455000	0.306468000
H	-3.456572000	-3.517657000	0.522206000
C	-1.420129000	-3.837322000	-0.256100000
H	-1.401756000	-4.865134000	-0.580786000
C	3.485380000	-2.754730000	-0.426319000
H	3.844263000	-3.763495000	-0.556159000
C	4.209323000	-1.636911000	-0.110678000

H	5.271900000	-1.564183000	0.055800000
C	3.069500000	3.238186000	-0.479734000
H	4.082575000	3.600398000	-0.554261000
C	1.911607000	3.911870000	-0.749697000
H	1.802778000	4.931270000	-1.082615000
C	-0.547801000	3.321362000	-0.523934000
C	-2.863486000	-0.738462000	0.930655000
C	1.021470000	-3.254756000	-0.657740000
C	3.628977000	0.831074000	0.034756000
C	-0.973083000	4.702271000	-0.881289000
C	-1.940709000	4.890369000	-1.888264000
H	-2.336478000	4.018297000	-2.398311000
C	-2.373852000	6.174268000	-2.233399000
H	-3.113901000	6.300975000	-3.017630000
C	-1.850269000	7.294308000	-1.573885000
H	-2.185461000	8.291534000	-1.841438000
C	-0.894316000	7.119875000	-0.564491000
H	-0.492947000	7.982198000	-0.040831000
C	-0.461603000	5.835103000	-0.219142000
H	0.266350000	5.698331000	0.573457000
C	-4.155735000	-1.117571000	1.567588000
C	-5.400808000	-0.682227000	1.072439000
H	-5.426246000	-0.054208000	0.191007000
C	-6.593562000	-1.074054000	1.689384000
H	-7.543190000	-0.733637000	1.287864000
C	-6.566090000	-1.912818000	2.810851000
H	-7.492286000	-2.217164000	3.288212000
C	-5.335314000	-2.360815000	3.308692000
H	-5.303689000	-3.011815000	4.177016000
C	-4.143391000	-1.968369000	2.691974000
H	-3.187927000	-2.310759000	3.075305000
C	1.345944000	-4.646883000	-1.074918000
C	2.037185000	-4.868362000	-2.282593000
H	2.300898000	-4.013778000	-2.896755000
C	2.369304000	-6.165276000	-2.687398000
H	2.895605000	-6.318570000	-3.624508000
C	2.020028000	-7.263529000	-1.890223000
H	2.277809000	-8.270149000	-2.204485000
C	1.339847000	-7.055169000	-0.683298000
H	1.076689000	-7.900108000	-0.054155000
C	1.008185000	-5.757941000	-0.277881000
H	0.496231000	-5.594616000	0.664509000
C	5.060947000	1.207410000	0.201266000
C	6.050117000	0.774991000	-0.703310000
H	5.758688000	0.154832000	-1.543940000

C	7.385618000	1.156264000	-0.535334000
H	8.134580000	0.820157000	-1.245869000
C	7.754520000	1.980236000	0.536263000
H	8.790994000	2.276223000	0.665243000
C	6.777405000	2.425938000	1.436147000
H	7.054954000	3.066577000	2.267685000
C	5.442165000	2.044955000	1.267998000
H	4.680830000	2.387364000	1.961471000
H	-0.785392000	0.021810000	-2.431854000
C	0.567562000	0.050328000	2.307929000
C	1.101590000	-0.559983000	4.470329000
H	1.467984000	-1.211856000	5.245445000
C	0.609640000	0.707897000	4.521204000
H	0.454130000	1.377499000	5.350330000
C	-0.287347000	2.349428000	2.831119000
H	-0.145154000	3.050648000	3.658644000
H	0.215423000	2.723541000	1.941838000
H	-1.354468000	2.244892000	2.618160000
C	1.544286000	-2.237676000	2.642616000
H	1.616471000	-2.922371000	3.492778000
H	0.838842000	-2.630211000	1.913578000
H	2.524039000	-2.136795000	2.168343000
N	1.065435000	-0.941269000	3.123720000
N	0.295454000	1.059843000	3.203193000
C	-2.454093000	-1.031958000	-3.949018000
C	-3.299382000	-1.766069000	-3.157376000
C	-2.491556000	0.393139000	-3.954740000
C	-4.327394000	-1.117273000	-2.265774000
C	-4.287562000	0.389857000	-2.306257000
C	-3.412404000	1.074220000	-3.110332000
H	-5.343208000	-1.477206000	-2.531626000
H	-1.802113000	0.952541000	-4.576609000
H	-4.187135000	-1.471181000	-1.229206000
H	-3.234920000	-2.850110000	-3.139294000
H	-1.718803000	-1.538645000	-4.567078000
H	-3.415349000	2.160970000	-3.100647000
H	-4.976469000	0.935337000	-1.667959000

³INT1-2_{is}

Fe	0.436058000	0.003046000	0.029357000
O	0.115132000	-0.089343000	-1.792052000
C	0.822225000	0.022140000	2.094071000
C	1.421893000	-0.604296000	4.224685000
H	1.778451000	-1.276832000	4.985607000

C	1.029727000	0.694573000	4.284225000
H	0.968380000	1.383601000	5.108841000
C	0.169088000	2.406431000	2.691874000
H	0.404468000	3.048913000	3.545027000
H	0.658361000	2.790969000	1.803111000
H	-0.910612000	2.387704000	2.535013000
C	1.643643000	-2.356611000	2.467856000
H	1.721136000	-2.980763000	3.362649000
H	0.866534000	-2.748039000	1.819555000
H	2.597565000	-2.358291000	1.937656000
N	1.289540000	-1.000139000	2.893140000
N	0.670561000	1.062224000	2.986708000
N	-1.145364000	1.179643000	0.265549000
N	-0.689093000	-1.619888000	0.268531000
N	2.005451000	-1.167736000	-0.270660000
N	1.560898000	1.626404000	-0.192409000
C	-1.243488000	2.518580000	-0.057529000
C	-2.348355000	0.809589000	0.843070000
C	-1.992868000	-1.630691000	0.715692000
C	-0.422077000	-2.879511000	-0.244709000
C	1.981044000	-2.501911000	-0.610756000
C	3.331435000	-0.795498000	-0.160046000
C	2.940530000	1.641387000	-0.209745000
C	1.133212000	2.888723000	-0.584785000
C	-2.528815000	3.022480000	0.379216000
H	-2.855496000	4.044695000	0.273079000
C	-3.190550000	1.982243000	0.970492000
H	-4.169744000	1.993678000	1.420625000
C	-2.561074000	-2.947926000	0.501544000
H	-3.576060000	-3.221240000	0.740892000
C	-1.609052000	-3.702286000	-0.124180000
H	-1.696695000	-4.715658000	-0.480938000
C	3.339483000	-3.007121000	-0.661326000
H	3.605792000	-4.029955000	-0.875840000
C	4.168796000	-1.969081000	-0.337858000
H	5.243162000	-1.984260000	-0.251990000
C	3.398425000	2.956706000	-0.612710000
H	4.434134000	3.235118000	-0.726813000
C	2.289113000	3.707577000	-0.886344000
H	2.251178000	4.718472000	-1.258596000
C	-0.202793000	3.318056000	-0.564230000
C	-2.745744000	-0.509230000	1.105115000
C	0.832817000	-3.306287000	-0.699943000
C	3.787756000	0.528234000	-0.061781000
C	-0.548246000	4.700844000	-0.993021000

C	-1.546719000	4.897774000	-1.968188000
H	-2.031031000	4.030134000	-2.404871000
C	-1.905341000	6.186601000	-2.375268000
H	-2.671393000	6.318474000	-3.133160000
C	-1.274165000	7.303730000	-1.812259000
H	-1.551167000	8.304501000	-2.128589000
C	-0.285941000	7.121775000	-0.835995000
H	0.199279000	7.982712000	-0.386254000
C	0.071687000	5.832329000	-0.427940000
H	0.824680000	5.692342000	0.340205000
C	-4.118246000	-0.764889000	1.623569000
C	-5.250165000	-0.299344000	0.926404000
H	-5.112984000	0.260332000	0.008671000
C	-6.537253000	-0.587023000	1.392764000
H	-7.399346000	-0.227128000	0.839135000
C	-6.714426000	-1.345206000	2.558165000
H	-7.714145000	-1.568477000	2.918076000
C	-5.594086000	-1.820438000	3.252752000
H	-5.723110000	-2.411127000	4.154709000
C	-4.305929000	-1.535508000	2.786071000
H	-3.434628000	-1.907476000	3.315953000
C	1.002376000	-4.696327000	-1.204318000
C	1.565957000	-4.911297000	-2.477679000
H	1.843499000	-4.050920000	-3.077419000
C	1.752252000	-6.208797000	-2.965578000
H	2.179888000	-6.356516000	-3.952469000
C	1.382808000	-7.314183000	-2.187597000
H	1.526788000	-8.321219000	-2.566644000
C	0.829098000	-7.112888000	-0.916442000
H	0.550807000	-7.964576000	-0.303071000
C	0.643067000	-5.815284000	-0.428072000
H	0.228499000	-5.658791000	0.562169000
C	5.249342000	0.799513000	0.047359000
C	6.167983000	0.321919000	-0.907408000
H	5.801087000	-0.258755000	-1.746591000
C	7.532100000	0.610167000	-0.791635000
H	8.225611000	0.239331000	-1.540180000
C	8.001106000	1.386591000	0.276183000
H	9.059650000	1.610597000	0.364482000
C	7.095027000	1.879375000	1.224503000
H	7.449753000	2.485575000	2.052551000
C	5.731248000	1.590649000	1.108641000
H	5.024520000	1.971781000	1.838875000
H	-0.239136000	0.765265000	-2.118887000
C	-3.062576000	-0.509884000	-2.198019000

C	-4.063244000	-1.447947000	-2.244197000
C	-3.357028000	0.877803000	-2.301076000
C	-5.516005000	-1.074071000	-2.416166000
C	-5.742265000	0.415767000	-2.516636000
C	-4.702985000	1.311718000	-2.456649000
H	-5.937299000	-1.581222000	-3.308189000
H	-2.554058000	1.601405000	-2.221985000
H	-6.107706000	-1.486472000	-1.573539000
H	-2.024666000	-0.803649000	-2.061084000
H	-3.824669000	-2.501967000	-2.136728000
H	-6.765266000	0.763600000	-2.639003000
H	-4.909338000	2.377678000	-2.521903000

¹INT1-2_{is}

Fe	0.438033000	0.001941000	0.030329000
O	0.117514000	-0.089535000	-1.791224000
C	0.823588000	0.020774000	2.094901000
C	1.422495000	-0.606264000	4.225561000
H	1.778761000	-1.279018000	4.986428000
C	1.030270000	0.692575000	4.285315000
H	0.968547000	1.381347000	5.110117000
C	0.169763000	2.404797000	2.693328000
H	0.404981000	3.047054000	3.546701000
H	0.658904000	2.789718000	1.804672000
H	-0.909925000	2.385790000	2.536469000
C	1.644488000	-2.358099000	2.468227000
H	1.721925000	-2.982512000	3.362841000
H	0.867247000	-2.749240000	1.819876000
H	2.598357000	-2.359794000	1.937948000
N	1.290605000	-1.001708000	2.893857000
N	0.671569000	1.060610000	2.987772000
N	-1.145403000	1.178518000	0.267028000
N	-0.689524000	-1.619730000	0.267619000
N	2.006518000	-1.167241000	-0.269846000
N	1.559194000	1.627824000	-0.191408000
C	-1.244655000	2.517614000	-0.055582000
C	-2.348337000	0.807988000	0.844688000
C	-1.993246000	-1.631669000	0.714304000
C	-0.421319000	-2.879073000	-0.245991000
C	1.982479000	-2.501244000	-0.610182000
C	3.332093000	-0.793835000	-0.159859000
C	2.938963000	1.643175000	-0.209575000
C	1.130994000	2.889713000	-0.584075000
C	-2.529912000	3.020891000	0.382000000

H	-2.856994000	4.043028000	0.276360000
C	-3.190861000	1.980233000	0.973261000
H	-4.169828000	1.991022000	1.423895000
C	-2.560833000	-2.948945000	0.498687000
H	-3.575857000	-3.222816000	0.737260000
C	-1.608052000	-3.702462000	-0.126898000
H	-1.695031000	-4.715610000	-0.484459000
C	3.341261000	-3.005597000	-0.661060000
H	3.608231000	-4.028234000	-0.875692000
C	4.170092000	-1.966950000	-0.338056000
H	5.244514000	-1.981498000	-0.252744000
C	3.396158000	2.958637000	-0.612948000
H	4.431682000	3.237512000	-0.727571000
C	2.286413000	3.708981000	-0.886278000
H	2.247833000	4.719811000	-1.258657000
C	-0.205157000	3.318140000	-0.562856000
C	-2.746173000	-0.510927000	1.105163000
C	0.834218000	-3.305541000	-0.700056000
C	3.787023000	0.530469000	-0.061957000
C	-0.551879000	4.700602000	-0.991618000
C	-1.551239000	4.896731000	-1.966028000
H	-2.035405000	4.028725000	-2.402148000
C	-1.910903000	6.185266000	-2.373115000
H	-2.677634000	6.316542000	-3.130424000
C	-1.279889000	7.302874000	-1.810869000
H	-1.557714000	8.303415000	-2.127202000
C	-0.290770000	7.121696000	-0.835366000
H	0.194340000	7.983010000	-0.386227000
C	0.067902000	5.832544000	-0.427298000
H	0.821608000	5.693132000	0.340253000
C	-4.118822000	-0.767251000	1.622856000
C	-5.250528000	-0.301517000	0.925463000
H	-5.113026000	0.258884000	0.008208000
C	-6.537758000	-0.589966000	1.390945000
H	-7.399698000	-0.229920000	0.837176000
C	-6.715272000	-1.349134000	2.555656000
H	-7.715102000	-1.572995000	2.914893000
C	-5.595139000	-1.824606000	3.250411000
H	-5.724449000	-2.416092000	4.151806000
C	-4.306832000	-1.538918000	2.784602000
H	-3.435682000	-1.911089000	3.314592000
C	1.004344000	-4.695617000	-1.204265000
C	1.568710000	-4.910623000	-2.477268000
H	1.846392000	-4.050261000	-3.076964000
C	1.755630000	-6.208140000	-2.964884000

H	2.183893000	-6.355877000	-3.951501000
C	1.386000000	-7.313517000	-2.186978000
H	1.530457000	-8.320567000	-2.565806000
C	0.831441000	-7.112188000	-0.916198000
H	0.552948000	-7.963857000	-0.302893000
C	0.644792000	-5.814564000	-0.428114000
H	0.229498000	-5.658036000	0.561819000
C	5.248491000	0.802858000	0.046419000
C	6.166936000	0.325976000	-0.908884000
H	5.799976000	-0.254881000	-1.747914000
C	7.530921000	0.615149000	-0.793831000
H	8.224283000	0.244857000	-1.542782000
C	7.999970000	1.391802000	0.273801000
H	9.058406000	1.616533000	0.361545000
C	7.094067000	1.883882000	1.222656000
H	7.448824000	2.490254000	2.050566000
C	5.730425000	1.594234000	1.107511000
H	5.023822000	1.974817000	1.838151000
H	-0.236932000	0.765132000	-2.117655000
C	-3.060190000	-0.508613000	-2.199316000
C	-4.060277000	-1.447265000	-2.246657000
C	-3.355497000	0.878966000	-2.301274000
C	-5.513283000	-1.074094000	-2.418186000
C	-5.740438000	0.415685000	-2.517484000
C	-4.701701000	1.312197000	-2.456701000
H	-5.934307000	-1.580826000	-3.310569000
H	-2.553045000	1.603047000	-2.221340000
H	-6.104714000	-1.487480000	-1.575843000
H	-2.022145000	-0.801917000	-2.062193000
H	-3.821069000	-2.501269000	-2.140513000
H	-6.763643000	0.763002000	-2.639605000
H	-4.908663000	2.378094000	-2.521077000

⁷TS2-2_{hs}

Fe	-0.279259000	0.030796000	-0.071020000
O	-0.221009000	0.105343000	-2.046854000
C	-0.551933000	0.074814000	2.273306000
C	-0.376778000	0.609934000	4.506008000
H	-0.021801000	1.165152000	5.357367000
C	-1.238361000	-0.437835000	4.410617000
H	-1.781496000	-0.984310000	5.162586000
C	-2.169173000	-1.841869000	2.551029000
H	-2.834748000	-2.162600000	3.357312000
H	-2.758557000	-1.488841000	1.708924000

H	-1.550907000	-2.681910000	2.228441000
C	0.967713000	1.991424000	2.900342000
H	1.388261000	2.352827000	3.842886000
H	1.767230000	1.614760000	2.266499000
H	0.458206000	2.809685000	2.388547000
N	0.030944000	0.906650000	3.202158000
N	-1.334288000	-0.747828000	3.051149000
N	-0.525493000	-1.996542000	-0.077430000
N	1.735479000	-0.197260000	0.261841000
N	-0.034305000	2.084423000	-0.053363000
N	-2.341760000	0.277361000	-0.177172000
C	-1.682460000	-2.662037000	-0.448130000
C	0.409677000	-2.932696000	0.334498000
C	2.360268000	-1.381625000	0.625258000
C	2.709859000	0.777611000	0.121121000
C	1.174727000	2.741173000	-0.161053000
C	-1.039575000	3.031538000	0.101861000
C	-3.008455000	1.487966000	-0.133998000
C	-3.223312000	-0.687576000	-0.631369000
C	-1.466928000	-4.085885000	-0.247919000
H	-2.204642000	-4.851275000	-0.430831000
C	-0.204207000	-4.248633000	0.256465000
H	0.271401000	-5.171874000	0.547625000
C	3.771133000	-1.133935000	0.755892000
H	4.508633000	-1.878308000	1.010128000
C	3.994820000	0.181876000	0.408422000
H	4.941511000	0.693091000	0.361192000
C	0.929074000	4.169387000	-0.046950000
H	1.694970000	4.928813000	-0.072035000
C	-0.416041000	4.343269000	0.151069000
H	-0.937838000	5.273735000	0.308767000
C	-4.374584000	1.272981000	-0.555068000
H	-5.123602000	2.044585000	-0.640147000
C	-4.499670000	-0.057779000	-0.882993000
H	-5.372645000	-0.555037000	-1.274672000
C	-2.918155000	-2.069659000	-0.772827000
C	1.734298000	-2.654262000	0.711440000
C	2.454700000	2.142907000	-0.162623000
C	-2.420699000	2.760945000	0.101719000
C	-4.007294000	-2.984366000	-1.217314000
C	-3.807774000	-3.837564000	-2.321207000
H	-2.860114000	-3.795259000	-2.847811000
C	-4.812308000	-4.717090000	-2.738104000
H	-4.641751000	-5.362280000	-3.594615000
C	-6.037291000	-4.760348000	-2.059369000

H	-6.818029000	-5.441481000	-2.383504000
C	-6.247901000	-3.919228000	-0.958562000
H	-7.190894000	-3.952849000	-0.421115000
C	-5.242139000	-3.041817000	-0.540576000
H	-5.401122000	-2.398058000	0.318080000
C	2.606213000	-3.795884000	1.113627000
C	2.851445000	-4.867363000	0.232879000
H	2.386223000	-4.856979000	-0.747355000
C	3.687589000	-5.925158000	0.607685000
H	3.868308000	-6.740985000	-0.085741000
C	4.298613000	-5.926819000	1.868233000
H	4.948603000	-6.746300000	2.158952000
C	4.069068000	-4.862063000	2.750260000
H	4.538664000	-4.856371000	3.729349000
C	3.231783000	-3.806124000	2.375335000
H	3.053080000	-2.978716000	3.054344000
C	3.616662000	3.053773000	-0.369905000
C	3.714719000	3.795369000	-1.564223000
H	2.946100000	3.666410000	-2.318501000
C	4.785906000	4.668025000	-1.781875000
H	4.846038000	5.226874000	-2.710964000
C	5.781722000	4.816842000	-0.807023000
H	6.615308000	5.491526000	-0.975607000
C	5.691763000	4.092347000	0.388605000
H	6.452013000	4.211300000	1.154830000
C	4.617242000	3.222656000	0.606301000
H	4.540427000	2.673787000	1.538905000
C	-3.368409000	3.904423000	0.244279000
C	-3.326572000	5.014982000	-0.621177000
H	-2.585959000	5.035975000	-1.413215000
C	-4.235414000	6.069000000	-0.477127000
H	-4.191732000	6.914031000	-1.157549000
C	-5.207218000	6.029111000	0.531125000
H	-5.913071000	6.846471000	0.641733000
C	-5.267160000	4.924280000	1.391118000
H	-6.018861000	4.884137000	2.173627000
C	-4.358425000	3.871262000	1.246584000
H	-4.403604000	3.011926000	1.907555000
H	0.944523000	-0.315927000	-2.843369000
H	-0.620897000	0.915990000	-2.420740000
C	2.669089000	0.578114000	-3.792173000
C	3.914710000	0.728325000	-3.221124000
C	1.867980000	-0.637661000	-3.574933000
C	4.494232000	-0.327955000	-2.477145000
C	3.811078000	-1.566171000	-2.340712000

C	2.560959000	-1.735735000	-2.885456000
H	5.481477000	-0.207158000	-2.046294000
H	1.283435000	-0.957026000	-4.452026000
H	4.461073000	1.659338000	-3.335041000
H	2.234003000	1.383473000	-4.378834000
H	4.274624000	-2.371149000	-1.780389000
H	2.030097000	-2.675466000	-2.761099000

⁵TS2-2_{ss}

Fe	-0.317534000	0.016248000	-0.085765000
O	-0.164190000	0.049975000	-2.004622000
C	-0.648868000	0.112514000	2.313809000
C	-0.535587000	0.678689000	4.548826000
H	-0.212998000	1.253160000	5.400457000
C	-1.366926000	-0.392214000	4.448968000
H	-1.911090000	-0.943819000	5.196623000
C	-2.220852000	-1.841385000	2.588602000
H	-2.882284000	-2.181780000	3.390370000
H	-2.815495000	-1.510363000	1.740991000
H	-1.574838000	-2.663069000	2.272898000
C	0.805734000	2.072342000	2.952018000
H	1.192531000	2.463187000	3.897365000
H	1.630847000	1.704956000	2.346032000
H	0.290077000	2.868302000	2.411670000
N	-0.109402000	0.969377000	3.248744000
N	-1.425339000	-0.720324000	3.090805000
N	-0.574926000	-2.012230000	-0.047500000
N	1.698949000	-0.200490000	0.350038000
N	-0.062439000	2.080108000	-0.062266000
N	-2.386200000	0.264194000	-0.199473000
C	-1.730469000	-2.681795000	-0.404571000
C	0.371018000	-2.945061000	0.333117000
C	2.322698000	-1.395340000	0.649652000
C	2.671805000	0.774135000	0.229661000
C	1.149016000	2.738618000	-0.102860000
C	-1.071241000	3.022831000	0.034802000
C	-3.041159000	1.476509000	-0.211925000
C	-3.267736000	-0.710250000	-0.625274000
C	-1.509351000	-4.104139000	-0.216143000
H	-2.246671000	-4.871786000	-0.390541000
C	-0.232755000	-4.264304000	0.256194000
H	0.255887000	-5.186795000	0.526626000
C	3.750626000	-1.155103000	0.762911000
H	4.488704000	-1.913781000	0.967236000

C	3.967431000	0.164836000	0.479175000
H	4.914459000	0.673013000	0.408272000
C	0.898423000	4.166188000	-0.010288000
H	1.663657000	4.926452000	0.005157000
C	-0.456647000	4.338811000	0.105591000
H	-0.989548000	5.268403000	0.226190000
C	-4.413669000	1.254759000	-0.640493000
H	-5.154744000	2.028997000	-0.761509000
C	-4.545012000	-0.080204000	-0.915282000
H	-5.414925000	-0.588539000	-1.299605000
C	-2.969550000	-2.088366000	-0.733554000
C	1.707812000	-2.665988000	0.691807000
C	2.428804000	2.137672000	-0.040403000
C	-2.456701000	2.750840000	-0.008580000
C	-4.060800000	-3.007730000	-1.165869000
C	-3.868299000	-3.864898000	-2.267343000
H	-2.923755000	-3.826957000	-2.799636000
C	-4.878527000	-4.741912000	-2.675430000
H	-4.715476000	-5.390175000	-3.530939000
C	-6.099421000	-4.779011000	-1.988738000
H	-6.883899000	-5.459071000	-2.305897000
C	-6.301671000	-3.933906000	-0.889704000
H	-7.241794000	-3.962548000	-0.347150000
C	-5.290786000	-3.057614000	-0.481051000
H	-5.442490000	-2.409352000	0.375680000
C	2.587184000	-3.820368000	1.042945000
C	2.824054000	-4.856247000	0.119006000
H	2.348108000	-4.809739000	-0.854968000
C	3.667822000	-5.923952000	0.444063000
H	3.844446000	-6.711564000	-0.282137000
C	4.291895000	-5.971901000	1.697634000
H	4.947488000	-6.799714000	1.949488000
C	4.068200000	-4.943628000	2.622814000
H	4.547651000	-4.974155000	3.596566000
C	3.223758000	-3.876638000	2.297228000
H	3.048284000	-3.077300000	3.009935000
C	3.600569000	3.046746000	-0.195275000
C	3.746724000	3.800042000	-1.376543000
H	3.007661000	3.684845000	-2.161574000
C	4.832611000	4.665485000	-1.543410000
H	4.932849000	5.233502000	-2.463319000
C	5.791842000	4.795025000	-0.529957000
H	6.635933000	5.465242000	-0.659364000
C	5.653136000	4.057057000	0.652747000
H	6.386099000	4.159806000	1.447228000

C	4.565196000	3.192989000	0.819361000
H	4.450810000	2.629363000	1.739327000
C	-3.399883000	3.905196000	0.067637000
C	-3.324507000	4.980091000	-0.839423000
H	-2.562552000	4.963656000	-1.611189000
C	-4.226450000	6.046585000	-0.760647000
H	-4.157578000	6.863573000	-1.472422000
C	-5.223418000	6.055313000	0.223765000
H	-5.923810000	6.882536000	0.283967000
C	-5.314782000	4.987268000	1.126122000
H	-6.085083000	4.985759000	1.891322000
C	-4.412615000	3.921374000	1.046893000
H	-4.480033000	3.091518000	1.742785000
H	-0.196965000	0.929408000	-2.432750000
H	1.278457000	-0.582675000	-2.836444000
C	2.843732000	0.577469000	-3.730082000
C	4.109159000	0.873889000	-3.281951000
C	2.202315000	-0.750793000	-3.477864000
C	4.889080000	-0.098875000	-2.603026000
C	4.365515000	-1.404301000	-2.391362000
C	3.101253000	-1.737105000	-2.807666000
H	5.886605000	0.150065000	-2.256008000
H	1.766744000	-1.169723000	-4.405713000
H	4.525692000	1.864160000	-3.443393000
H	2.259289000	1.326969000	-4.259160000
H	4.973359000	-2.139708000	-1.872106000
H	2.706900000	-2.732417000	-2.619711000

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Fe	-0.336153000	0.125615000	-0.111369000
O	-0.298052000	0.237783000	-2.106432000
C	-0.402842000	-0.156741000	2.311234000
C	0.529788000	-0.535193000	4.386128000
H	1.216182000	-0.372802000	5.200217000
C	-0.514446000	-1.398436000	4.251055000
H	-0.912706000	-2.141625000	4.921187000
C	-2.216265000	-1.889073000	2.465468000
H	-2.935917000	-2.060437000	3.272705000
H	-2.677375000	-1.294672000	1.681421000
H	-1.893597000	-2.846823000	2.046862000
C	1.584182000	1.242093000	2.954027000
H	1.770867000	1.795295000	3.880143000
H	2.512380000	0.784695000	2.598977000
H	1.206877000	1.920794000	2.193415000

N	0.575113000	0.214453000	3.205781000
N	-1.071949000	-1.147465000	2.993443000
N	-0.613826000	-1.836691000	-0.184342000
N	1.618804000	-0.156673000	0.156972000
N	-0.052724000	2.090655000	0.004325000
N	-2.319604000	0.402092000	-0.161244000
C	-1.759369000	-2.474607000	-0.628553000
C	0.273089000	-2.814602000	0.238015000
C	2.218113000	-1.336753000	0.574039000
C	2.627200000	0.775042000	-0.014848000
C	1.156486000	2.743063000	-0.179688000
C	-1.012868000	3.063343000	0.271499000
C	-2.986734000	1.595032000	0.054330000
C	-3.246754000	-0.505087000	-0.654715000
C	-1.577330000	-3.905907000	-0.494296000
H	-2.319512000	-4.643546000	-0.755357000
C	-0.351381000	-4.111687000	0.078001000
H	0.098569000	-5.050565000	0.358777000
C	3.632114000	-1.125110000	0.711605000
H	4.339254000	-1.883577000	1.007121000
C	3.894695000	0.160415000	0.295143000
H	4.851315000	0.648860000	0.223245000
C	0.951709000	4.166840000	-0.009894000
H	1.733013000	4.907318000	-0.078947000
C	-0.364153000	4.356829000	0.312636000
H	-0.856169000	5.286847000	0.547224000
C	-4.377422000	1.427267000	-0.289894000
H	-5.121658000	2.205860000	-0.234632000
C	-4.529366000	0.145960000	-0.758767000
H	-5.425631000	-0.310508000	-1.146392000
C	-2.982421000	-1.861438000	-0.930786000
C	1.575340000	-2.584491000	0.690244000
C	2.418355000	2.138668000	-0.286470000
C	-2.389869000	2.835549000	0.362646000
C	-4.071897000	-2.725044000	-1.463464000
C	-3.865597000	-3.457086000	-2.649638000
H	-2.917810000	-3.354012000	-3.167692000
C	-4.865213000	-4.293980000	-3.156560000
H	-4.691019000	-4.845696000	-4.075321000
C	-6.089337000	-4.415496000	-2.485832000
H	-6.865939000	-5.063901000	-2.879511000
C	-6.304335000	-3.697226000	-1.302021000
H	-7.246094000	-3.794546000	-0.770306000
C	-5.303803000	-2.861947000	-0.794146000
H	-5.464040000	-2.316733000	0.129959000

C	2.386180000	-3.724020000	1.202186000
C	2.701055000	-4.827193000	0.386727000
H	2.336696000	-4.846128000	-0.635203000
C	3.483518000	-5.877991000	0.879422000
H	3.721117000	-6.720374000	0.236847000
C	3.969121000	-5.838149000	2.192852000
H	4.577818000	-6.652132000	2.574252000
C	3.668067000	-4.740372000	3.010749000
H	4.040349000	-4.704159000	4.030236000
C	2.884028000	-3.691507000	2.518971000
H	2.640166000	-2.841290000	3.148459000
C	3.585831000	3.025118000	-0.553251000
C	3.652095000	3.736162000	-1.767196000
H	2.859998000	3.595960000	-2.494695000
C	4.726461000	4.589410000	-2.039790000
H	4.763490000	5.125413000	-2.983342000
C	5.754969000	4.747967000	-1.101051000
H	6.590558000	5.407955000	-1.312430000
C	5.695773000	4.053371000	0.113878000
H	6.481951000	4.180810000	0.851994000
C	4.618075000	3.203117000	0.386833000
H	4.563726000	2.679817000	1.335639000
C	-3.306010000	3.970771000	0.669099000
C	-3.335903000	5.135417000	-0.121864000
H	-2.673761000	5.207975000	-0.977911000
C	-4.219325000	6.178830000	0.175930000
H	-4.232701000	7.067236000	-0.448131000
C	-5.093513000	6.073095000	1.265442000
H	-5.779687000	6.882293000	1.495319000
C	-5.081958000	4.913652000	2.052345000
H	-5.758058000	4.822463000	2.897015000
C	-4.198395000	3.871207000	1.754626000
H	-4.187461000	2.970245000	2.359374000
H	-0.624898000	1.099505000	-2.436952000
H	0.911939000	-0.235947000	-2.928803000
C	2.690894000	0.567684000	-3.859786000
C	3.952400000	0.645052000	-3.312593000
C	1.813240000	-0.599105000	-3.623608000
C	4.480560000	-0.436725000	-2.564855000
C	3.723281000	-1.629940000	-2.403509000
C	2.457352000	-1.730534000	-2.924669000
H	5.480936000	-0.371948000	-2.151292000
H	1.246274000	-0.908004000	-4.518321000
H	4.552214000	1.540111000	-3.447272000
H	2.296975000	1.394105000	-4.446664000

H	4.147717000	-2.455341000	-1.840536000
H	1.872562000	-2.634745000	-2.778469000

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Fe	0.249615000	0.059279000	-0.122808000
O	-0.053437000	0.147288000	-2.053345000
C	0.953118000	-0.311749000	2.233249000
C	1.640559000	-1.633216000	3.997389000
H	1.584075000	-2.456121000	4.690136000
C	2.544875000	-0.622553000	3.877149000
H	3.425785000	-0.386756000	4.450694000
C	2.823167000	1.360119000	2.355476000
H	3.144936000	1.945045000	3.223592000
H	3.693032000	1.075715000	1.754840000
H	2.148669000	1.952783000	1.743418000
C	-0.461010000	-2.310682000	2.792846000
H	-0.854727000	-2.624662000	3.765173000
H	-1.226418000	-1.764142000	2.247516000
H	-0.164328000	-3.189283000	2.212551000
N	0.681169000	-1.422441000	3.001609000
N	2.106544000	0.171229000	2.811373000
N	0.240943000	2.029774000	0.051337000
N	-1.677233000	-0.015020000	0.407519000
N	0.278866000	-1.938092000	-0.220255000
N	2.238671000	0.103117000	-0.390008000
C	1.234717000	2.884453000	-0.405993000
C	-0.763667000	2.818908000	0.586869000
C	-2.429470000	1.029641000	0.915402000
C	-2.544982000	-1.079067000	0.210374000
C	-0.827617000	-2.756831000	-0.346512000
C	1.394033000	-2.758798000	-0.132383000
C	3.094745000	-0.977929000	-0.323755000
C	2.976506000	1.189353000	-0.820070000
C	0.841953000	4.251034000	-0.131441000
H	1.440511000	5.117549000	-0.363497000
C	-0.366230000	4.209207000	0.506641000
H	-0.942464000	5.037013000	0.887201000
C	-3.795239000	0.592079000	1.094321000
H	-4.595229000	1.215300000	1.459343000
C	-3.875683000	-0.688496000	0.623467000
H	-4.752975000	-1.306617000	0.539050000
C	-0.394556000	-4.138332000	-0.351778000
H	-1.057139000	-4.986162000	-0.425719000
C	0.962904000	-4.140647000	-0.171264000

H	1.615672000	-4.994248000	-0.084382000
C	4.424063000	-0.553520000	-0.708204000
H	5.283521000	-1.203061000	-0.761774000
C	4.340996000	0.769670000	-1.054979000
H	5.126326000	1.402338000	-1.435876000
C	2.496855000	2.507363000	-0.886419000
C	-1.997365000	2.356520000	1.063453000
C	-2.169302000	-2.355265000	-0.232251000
C	2.723029000	-2.315790000	-0.100631000
C	3.393824000	3.585957000	-1.389275000
C	2.987478000	4.381122000	-2.478424000
H	2.030374000	4.175879000	-2.946472000
C	3.805423000	5.411448000	-2.953981000
H	3.480072000	6.010771000	-3.798750000
C	5.042174000	5.666487000	-2.346743000
H	5.677032000	6.465928000	-2.715941000
C	5.453708000	4.886226000	-1.258300000
H	6.405805000	5.084890000	-0.775561000
C	4.635139000	3.856373000	-0.782304000
H	4.946367000	3.261078000	0.069796000
C	-2.972747000	3.335721000	1.623357000
C	-3.469541000	4.394621000	0.839607000
H	-3.122361000	4.499273000	-0.183016000
C	-4.407454000	5.290803000	1.364057000
H	-4.784857000	6.099221000	0.745290000
C	-4.868075000	5.138888000	2.678516000
H	-5.596928000	5.833339000	3.084758000
C	-4.387080000	4.083101000	3.464176000
H	-4.740091000	3.958707000	4.483411000
C	-3.448331000	3.187950000	2.939723000
H	-3.073814000	2.367492000	3.543352000
C	-3.216059000	-3.384402000	-0.485760000
C	-3.296456000	-3.990992000	-1.754152000
H	-2.608656000	-3.670757000	-2.528949000
C	-4.258828000	-4.971153000	-2.017572000
H	-4.311318000	-5.423744000	-3.003096000
C	-5.156863000	-5.363432000	-1.015778000
H	-5.905307000	-6.122658000	-1.220309000
C	-5.081076000	-4.772562000	0.252084000
H	-5.766144000	-5.078675000	1.036875000
C	-4.115683000	-3.794424000	0.515777000
H	-4.046977000	-3.347301000	1.501851000
C	3.821437000	-3.307777000	0.074588000
C	4.014735000	-4.369208000	-0.829263000
H	3.347022000	-4.466621000	-1.678692000

C	5.063989000	-5.277159000	-0.648482000
H	5.203635000	-6.087136000	-1.357861000
C	5.939806000	-5.134905000	0.435718000
H	6.754839000	-5.838433000	0.574416000
C	5.761094000	-4.077242000	1.337451000
H	6.435770000	-3.961473000	2.180338000
C	4.711648000	-3.170014000	1.157269000
H	4.561243000	-2.353345000	1.856354000
H	0.204440000	-0.655550000	-2.550660000
H	-1.566260000	0.612849000	-2.786460000
C	-3.169484000	-0.539034000	-3.635735000
C	-4.362552000	-0.942718000	-3.083894000
C	-2.558813000	0.789951000	-3.322886000
C	-5.099584000	-0.081081000	-2.229924000
C	-4.611284000	1.226768000	-1.950327000
C	-3.419256000	1.662617000	-2.469575000
H	-6.041805000	-0.411850000	-1.805086000
H	-2.239244000	1.315385000	-4.243664000
H	-4.751205000	-1.934999000	-3.295609000
H	-2.618296000	-1.204590000	-4.296442000
H	-5.186206000	1.877399000	-1.297157000
H	-3.047737000	2.656308000	-2.231668000

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Fe	-0.312448000	0.005896000	0.038555000
O	-0.140342000	-0.007846000	-1.840307000
C	-0.565680000	-0.031269000	2.091978000
C	-0.545866000	0.552433000	4.312684000
H	-0.345195000	1.187352000	5.158164000
C	-1.119249000	-0.674766000	4.225169000
H	-1.516796000	-1.331802000	4.979172000
C	-1.677800000	-2.298756000	2.416521000
H	-2.272748000	-2.715408000	3.234170000
H	-2.314835000	-2.137267000	1.552810000
H	-0.878348000	-2.994065000	2.154624000
C	0.412363000	2.230539000	2.734819000
H	0.745981000	2.648822000	3.688488000
H	1.269165000	2.095715000	2.082166000
H	-0.299482000	2.912222000	2.266720000
N	-0.214284000	0.933288000	3.009944000
N	-1.126744000	-1.017845000	2.870825000
N	0.046465000	-1.934329000	0.004420000
N	1.614226000	0.326881000	0.317796000
N	-0.643938000	1.949635000	-0.078653000

N	-2.251384000	-0.314292000	-0.185855000
C	-0.800689000	-2.886433000	-0.523055000
C	1.153129000	-2.591897000	0.515113000
C	2.531313000	-0.579264000	0.832237000
C	2.306958000	1.488304000	0.026004000
C	0.319805000	2.906307000	-0.335881000
C	-1.846095000	2.616232000	0.144689000
C	-3.267187000	0.612542000	-0.028662000
C	-2.815046000	-1.462952000	-0.720396000
C	-0.207980000	-4.199186000	-0.329463000
H	-0.665313000	-5.127890000	-0.632430000
C	0.966876000	-4.021996000	0.347585000
H	1.653969000	-4.780127000	0.687771000
C	3.817865000	0.052687000	0.928457000
H	4.715915000	-0.432004000	1.276837000
C	3.696750000	1.308031000	0.379881000
H	4.469709000	2.044738000	0.241281000
C	-0.290568000	4.219579000	-0.259188000
H	0.240530000	5.148044000	-0.400702000
C	-1.603299000	4.043345000	0.089224000
H	-2.344132000	4.805898000	0.268375000
C	-4.513532000	0.020582000	-0.445929000
H	-5.464811000	0.529185000	-0.446494000
C	-4.229106000	-1.240919000	-0.909652000
H	-4.913295000	-1.947843000	-1.350104000
C	-2.122342000	-2.672305000	-0.947059000
C	2.295587000	-1.958125000	1.012791000
C	1.707631000	2.688929000	-0.401320000
C	-3.090646000	1.984792000	0.252598000
C	-2.840795000	-3.824466000	-1.556987000
C	-2.304577000	-4.451429000	-2.699888000
H	-1.386031000	-4.060811000	-3.125370000
C	-2.944496000	-5.550626000	-3.281519000
H	-2.518873000	-6.016052000	-4.165407000
C	-4.133764000	-6.046119000	-2.730759000
H	-4.632217000	-6.898114000	-3.182660000
C	-4.673839000	-5.436715000	-1.590485000
H	-5.588505000	-5.821871000	-1.149680000
C	-4.031780000	-4.339061000	-1.007474000
H	-4.441747000	-3.878588000	-0.114890000
C	3.407862000	-2.769807000	1.578783000
C	4.044483000	-3.772665000	0.821863000
H	3.706194000	-3.960161000	-0.191660000
C	5.108720000	-4.506094000	1.358480000
H	5.590352000	-5.272982000	0.759384000

C	5.560688000	-4.243563000	2.658184000
H	6.387289000	-4.811371000	3.073897000
C	4.944094000	-3.238531000	3.415788000
H	5.291054000	-3.026644000	4.422698000
C	3.879446000	-2.506993000	2.879416000
H	3.401612000	-1.724917000	3.460741000
C	2.565931000	3.842469000	-0.789368000
C	2.432374000	4.402449000	-2.075042000
H	1.719553000	3.959811000	-2.762579000
C	3.214641000	5.494199000	-2.466240000
H	3.101729000	5.908826000	-3.463453000
C	4.145551000	6.047908000	-1.576852000
H	4.755215000	6.893367000	-1.880295000
C	4.280963000	5.506518000	-0.292013000
H	4.990674000	5.937665000	0.407764000
C	3.494630000	4.416915000	0.099193000
H	3.587993000	4.008948000	1.100064000
C	-4.316341000	2.788045000	0.515995000
C	-4.681484000	3.882766000	-0.291614000
H	-4.055173000	4.145829000	-1.136845000
C	-5.847793000	4.608816000	-0.026546000
H	-6.116333000	5.446280000	-0.663330000
C	-6.674953000	4.248841000	1.045256000
H	-7.580271000	4.812104000	1.249329000
C	-6.331431000	3.151481000	1.846033000
H	-6.969737000	2.861984000	2.675350000
C	-5.165229000	2.426519000	1.581126000
H	-4.897294000	1.573613000	2.196404000
H	1.046196000	-0.303939000	-2.635352000
H	-0.682386000	0.709811000	-2.227997000
C	2.526437000	0.783242000	-3.770251000
C	3.705239000	1.275441000	-3.250893000
C	2.001076000	-0.531478000	-3.365130000
C	4.493497000	0.481601000	-2.383185000
C	4.094237000	-0.846145000	-2.069289000
C	2.914785000	-1.354682000	-2.557841000
H	5.425447000	0.871453000	-1.989278000
H	1.487419000	-1.082809000	-4.167809000
H	4.036868000	2.278295000	-3.503302000
H	1.933252000	1.387866000	-4.452027000
H	4.718742000	-1.449235000	-1.417878000
H	2.596464000	-2.359433000	-2.293308000

¹TS2-2_h

Fe	-0.304780000	-0.005097000	0.101112000
O	-0.025157000	0.080997000	-1.746939000
C	-0.603929000	-0.001069000	2.155340000
C	-0.921960000	0.670937000	4.331566000
H	-1.032852000	1.382087000	5.131872000
C	-0.950241000	-0.686062000	4.323341000
H	-1.082430000	-1.401844000	5.116211000
C	-0.706892000	-2.498029000	2.625702000
H	-1.144463000	-3.077157000	3.443918000
H	-1.283030000	-2.658564000	1.720422000
H	0.324572000	-2.816855000	2.462419000
C	-0.650846000	2.491133000	2.646141000
H	-0.486390000	3.068360000	3.560484000
H	0.173877000	2.656073000	1.960409000
H	-1.584644000	2.807323000	2.176744000
N	-0.709093000	1.073700000	3.010449000
N	-0.758671000	-1.081591000	2.996741000
N	0.891166000	-1.558216000	0.254805000
N	1.256910000	1.188593000	0.314380000
N	-1.499477000	1.551609000	-0.103053000
N	-1.852738000	-1.199790000	-0.174006000
C	0.605318000	-2.835495000	-0.177045000
C	2.134216000	-1.593385000	0.869111000
C	2.508549000	0.832987000	0.764732000
C	1.346698000	2.478389000	-0.179335000
C	-1.087438000	2.833497000	-0.407339000
C	-2.871161000	1.585858000	0.087017000
C	-3.188574000	-0.849246000	-0.100004000
C	-1.791967000	-2.498534000	-0.660843000
C	1.684382000	-3.719483000	0.217606000
H	1.708103000	-4.781026000	0.027636000
C	2.596766000	-2.965636000	0.908562000
H	3.511793000	-3.299847000	1.370489000
C	3.423322000	1.938148000	0.560439000
H	4.474382000	1.915956000	0.801003000
C	2.723205000	2.930003000	-0.067511000
H	3.094198000	3.877738000	-0.422020000
C	-2.233513000	3.718552000	-0.352475000
H	-2.194168000	4.782990000	-0.522855000
C	-3.320494000	2.960617000	-0.002236000
H	-4.333558000	3.295290000	0.152755000
C	-3.996599000	-1.964329000	-0.548706000
H	-5.073487000	-1.953903000	-0.612260000
C	-3.139031000	-2.958608000	-0.936754000
H	-3.391033000	-3.913655000	-1.368506000

C	-0.618688000	-3.270058000	-0.721520000
C	2.895557000	-0.457545000	1.172246000
C	0.245992000	3.261639000	-0.560193000
C	-3.684564000	0.442233000	0.159662000
C	-0.663016000	-4.650635000	-1.275850000
C	0.236244000	-5.011022000	-2.299783000
H	0.928474000	-4.262688000	-2.672619000
C	0.233982000	-6.304183000	-2.832040000
H	0.929132000	-6.561382000	-3.625412000
C	-0.665288000	-7.263476000	-2.347472000
H	-0.668356000	-8.267306000	-2.760744000
C	-1.557038000	-6.920808000	-1.322681000
H	-2.247469000	-7.662367000	-0.932142000
C	-1.553463000	-5.627517000	-0.789155000
H	-2.231220000	-5.368921000	0.017314000
C	4.256680000	-0.606829000	1.756096000
C	5.246031000	-1.395748000	1.136086000
H	5.007219000	-1.910416000	0.212209000
C	6.529570000	-1.492671000	1.684405000
H	7.281590000	-2.099278000	1.189187000
C	6.848988000	-0.798293000	2.858499000
H	7.845332000	-0.873137000	3.282951000
C	5.877966000	0.000977000	3.476325000
H	6.119356000	0.546513000	4.383565000
C	4.595152000	0.098489000	2.927332000
H	3.840774000	0.719574000	3.399447000
C	0.461330000	4.653426000	-1.043322000
C	-0.087203000	5.051894000	-2.278612000
H	-0.638124000	4.322819000	-2.863215000
C	0.083760000	6.357426000	-2.749906000
H	-0.339045000	6.643947000	-3.708012000
C	0.803573000	7.291012000	-1.992420000
H	0.937649000	8.304355000	-2.358108000
C	1.346400000	6.909853000	-0.758434000
H	1.895173000	7.630629000	-0.159730000
C	1.174065000	5.604068000	-0.286738000
H	1.580396000	5.314108000	0.676286000
C	-5.153517000	0.581904000	0.358074000
C	-5.949267000	1.385431000	-0.481858000
H	-5.479721000	1.916713000	-1.302274000
C	-7.330377000	1.480718000	-0.280177000
H	-7.928990000	2.099865000	-0.941399000
C	-7.942663000	0.768998000	0.759777000
H	-9.014581000	0.842946000	0.914728000
C	-7.164352000	-0.045248000	1.593044000

H	-7.631341000	-0.603742000	2.398637000
C	-5.783579000	-0.139737000	1.391575000
H	-5.176099000	-0.769937000	2.033106000
H	-0.891476000	0.033514000	-2.204346000
H	1.179838000	-0.720514000	-2.575584000
C	2.277461000	0.118409000	-4.174861000
C	3.199652000	1.126126000	-4.004426000
C	2.135050000	-0.980502000	-3.179722000
C	4.123707000	1.093761000	-2.928348000
C	4.142913000	-0.020451000	-2.046261000
C	3.237297000	-1.044313000	-2.183321000
H	4.836397000	1.901438000	-2.797811000
H	1.916781000	-1.957941000	-3.641747000
H	3.233406000	1.954972000	-4.707113000
H	1.576202000	0.150436000	-5.004796000
H	4.885873000	-0.057056000	-1.255203000
H	3.251851000	-1.891154000	-1.504481000

⁵INT2-2

Fe	0.265607000	0.072989000	0.334895000
O	0.028403000	-0.014199000	-1.997905000
C	0.491309000	0.113778000	2.566095000
C	1.201488000	-0.321157000	4.713895000
H	1.786963000	-0.807387000	5.475595000
C	0.253536000	0.652790000	4.793195000
H	-0.157838000	1.177610000	5.638695000
C	-1.191403000	1.883562000	3.129895000
H	-1.337369000	2.560469000	3.976695000
H	-0.859675000	2.447745000	2.260395000
H	-2.133728000	1.383809000	2.890595000
C	2.265322000	-1.636010000	2.840995000
H	2.600091000	-2.264927000	3.670895000
H	1.755992000	-2.246285000	2.097795000
H	3.126446000	-1.152953000	2.372095000
N	1.328772000	-0.637364000	3.357495000
N	-0.161451000	0.905910000	3.481895000
N	-1.809677000	0.392893000	0.281695000
N	-0.082396000	-1.993093000	0.189495000
N	2.264290000	-0.276910000	-0.107905000
N	0.528209000	2.125576000	0.047195000
C	-2.448016000	1.615124000	0.221295000
C	-2.740924000	-0.559961000	0.657695000
C	-1.313226000	-2.604932000	0.333795000
C	0.829956000	-2.960439000	-0.202605000

C	2.873629000	-1.499441000	-0.283505000
C	3.244738000	0.693141000	-0.055105000
C	1.757639000	2.725615000	-0.134705000
C	-0.449143000	3.071225000	-0.215705000
C	-3.827625000	1.439093000	0.628895000
H	-4.556485000	2.230329000	0.711495000
C	-4.001591000	0.107402000	0.920495000
H	-4.899815000	-0.373354000	1.274595000
C	-1.175997000	-4.018639000	0.001095000
H	-1.983032000	-4.734699000	-0.001805000
C	0.129693000	-4.232004000	-0.342305000
H	0.579347000	-5.154526000	-0.674505000
C	4.313539000	-1.305312000	-0.264405000
H	5.047899000	-2.091349000	-0.345005000
C	4.542005000	0.037476000	-0.104705000
H	5.496030000	0.535629000	-0.036805000
C	1.548109000	4.117125000	-0.525305000
H	2.335143000	4.816686000	-0.759405000
C	0.200619000	4.322892000	-0.594405000
H	-0.312136000	5.222718000	-0.895705000
C	-1.838754000	2.855294000	-0.104605000
C	-2.526994000	-1.960072000	0.657995000
C	2.211967000	-2.747908000	-0.395505000
C	3.018608000	2.091452000	-0.069605000
C	-2.749596000	4.017639000	-0.304605000
C	-3.830301000	3.931393000	-1.206005000
H	-3.981447000	3.006501000	-1.752305000
C	-4.694947000	5.013336000	-1.397905000
H	-5.517151000	4.927977000	-2.101905000
C	-4.497487000	6.206226000	-0.689805000
H	-5.167345000	7.047360000	-0.838605000
C	-3.430982000	6.305173000	0.213395000
H	-3.276337000	7.222366000	0.773695000
C	-2.567636000	5.221530000	0.405495000
H	-1.746533000	5.294789000	1.110395000
C	-3.701538000	-2.842213000	0.919895000
C	-4.886732000	-2.727254000	0.165495000
H	-4.942095000	-1.977351000	-0.616005000
C	-5.973575000	-3.575100000	0.404395000
H	-6.875170000	-3.475755000	-0.192405000
C	-5.895823000	-4.555804000	1.401795000
H	-6.739056000	-5.213862000	1.587495000
C	-4.721430000	-4.684762000	2.155395000
H	-4.653367000	-5.441566000	2.931095000
C	-3.634988000	-3.837617000	1.914995000

H	-2.723692000	-3.934362000	2.495695000
C	3.059508000	-3.934750000	-0.708505000
C	3.883507000	-3.943591000	-1.851705000
H	3.881050000	-3.076991000	-2.504205000
C	4.687152000	-5.049731000	-2.146605000
H	5.310853000	-5.040362000	-3.035305000
C	4.683196000	-6.168931000	-1.303405000
H	5.306954000	-7.027462000	-1.532205000
C	3.869896000	-6.172490000	-0.162605000
H	3.865953000	-7.032590000	0.500195000
C	3.067051000	-5.065450000	0.132095000
H	2.441351000	-5.063819000	1.018395000
C	4.211852000	2.987393000	-0.118805000
C	5.180846000	2.866044000	-1.134105000
H	5.052508000	2.101751000	-1.892905000
C	6.283989000	3.725389000	-1.176005000
H	7.017184000	3.621753000	-1.970105000
C	6.437039000	4.724382000	-0.205405000
H	7.292972000	5.391439000	-0.238805000
C	5.476446000	4.860230000	0.805395000
H	5.587284000	5.631724000	1.561495000
C	4.373403000	4.000985000	0.846295000
H	3.626008000	4.103522000	1.626395000
H	-0.287343000	-0.929183000	-2.134105000
H	-0.709967000	0.586738000	-2.215905000
C	-2.085680000	0.328306000	-4.628705000
C	-1.645446000	-0.994016000	-4.772205000
C	-2.890662000	0.684546000	-3.535705000
C	-2.010294000	-1.960497000	-3.823505000
C	-2.815076000	-1.604457000	-2.731405000
C	-3.254910000	-0.280835000	-2.586505000
H	-1.664545000	-2.984415000	-3.928205000
H	-3.223111000	1.711663000	-3.420405000
H	-1.014560000	-1.267947000	-5.611905000
H	-1.796443000	1.078892000	-5.357505000
H	-3.079113000	-2.347344000	-1.988005000
H	-3.851496000	0.002794000	-1.727005000

³INT2-2

Fe	0.187619000	0.026255000	-0.139292000
O	-0.307852000	0.118347000	2.165373000
N	-1.482099000	-1.077359000	-0.367308000
N	-0.888900000	1.701600000	-0.286250000
N	1.812641000	1.136854000	0.267351000

N	1.203740000	-1.644855000	0.229569000
C	-1.620729000	-2.441782000	-0.174764000
C	-2.662934000	-0.634390000	-0.944699000
C	-2.209787000	1.785739000	-0.701782000
C	-0.527065000	2.977532000	0.145468000
C	1.871025000	2.497817000	0.486173000
C	3.118054000	0.680092000	0.222080000
C	2.581988000	-1.734748000	0.314308000
C	0.703149000	-2.910031000	0.512202000
C	-2.902005000	-2.875988000	-0.689677000
H	-3.250329000	-3.896671000	-0.694248000
C	-3.528336000	-1.767488000	-1.194620000
H	-4.487030000	-1.718422000	-1.685700000
C	-2.695305000	3.137385000	-0.499339000
H	-3.698746000	3.468150000	-0.717139000
C	-1.674466000	3.860153000	0.049050000
H	-1.687896000	4.892321000	0.359949000
C	3.257014000	2.921535000	0.534804000
H	3.586838000	3.939394000	0.670326000
C	4.024033000	1.805895000	0.334891000
H	5.099422000	1.744988000	0.283276000
C	2.956570000	-3.088265000	0.680280000
H	3.970303000	-3.421775000	0.838151000
C	1.802100000	-3.799576000	0.843494000
H	1.696888000	-4.826575000	1.153499000
C	-0.633211000	-3.299322000	0.345492000
C	-3.015059000	0.713594000	-1.119735000
C	0.766205000	3.367201000	0.520051000
C	3.492355000	-0.672329000	0.194450000
C	-1.032080000	-4.707593000	0.626695000
C	-2.094416000	-4.972349000	1.513572000
H	-2.597367000	-4.136506000	1.989093000
C	-2.499343000	-6.284507000	1.777679000
H	-3.316328000	-6.468445000	2.468810000
C	-1.850520000	-7.359192000	1.155299000
H	-2.163324000	-8.378414000	1.359599000
C	-0.798987000	-7.109948000	0.263670000
H	-0.299618000	-7.936512000	-0.232711000
C	-0.396274000	-5.796465000	-0.000501000
H	0.408085000	-5.601416000	-0.701517000
C	-4.370553000	1.043785000	-1.644912000
C	-5.537663000	0.557400000	-1.022935000
H	-5.443185000	-0.078008000	-0.148995000
C	-6.803852000	0.899810000	-1.509636000
H	-7.691952000	0.520589000	-1.013299000

C	-6.926522000	1.737449000	-2.625700000
H	-7.908917000	2.003201000	-3.003509000
C	-5.773608000	2.234060000	-3.248695000
H	-5.860148000	2.883712000	-4.114355000
C	-4.508152000	1.892341000	-2.760959000
H	-3.612503000	2.274505000	-3.239446000
C	1.020184000	4.787421000	0.893757000
C	1.629346000	5.093408000	2.126902000
H	1.889623000	4.280504000	2.796770000
C	1.892906000	6.419511000	2.485374000
H	2.357783000	6.636590000	3.442300000
C	1.554296000	7.465013000	1.616001000
H	1.758362000	8.494395000	1.894052000
C	0.954397000	7.173561000	0.383904000
H	0.699047000	7.976997000	-0.300474000
C	0.692537000	5.846928000	0.025299000
H	0.239351000	5.619364000	-0.933750000
C	4.939862000	-1.022583000	0.127835000
C	5.853387000	-0.592269000	1.108515000
H	5.491826000	0.009430000	1.935437000
C	7.204400000	-0.947943000	1.029397000
H	7.895264000	-0.613538000	1.797409000
C	7.663319000	-1.742651000	-0.029361000
H	8.711470000	-2.019119000	-0.089475000
C	6.761579000	-2.182145000	-1.007796000
H	7.110347000	-2.797558000	-1.831705000
C	5.411066000	-1.826624000	-0.928157000
H	4.707097000	-2.156533000	-1.685465000
H	-1.010196000	0.797285000	2.203156000
C	0.986046000	-0.111671000	-2.341129000
C	2.542950000	0.359283000	-3.979939000
H	3.172847000	0.987604000	-4.587253000
C	2.361715000	-0.990386000	-3.974752000
H	2.796675000	-1.766619000	-4.582122000
C	0.944101000	-2.601776000	-2.659975000
H	0.805728000	-3.168690000	-3.586854000
H	1.664258000	-3.114037000	-2.013852000
H	-0.004476000	-2.520617000	-2.134905000
C	1.603158000	2.294937000	-2.671426000
H	1.526337000	2.874851000	-3.597776000
H	0.712690000	2.445210000	-2.065302000
H	2.481229000	2.616423000	-2.103477000
N	1.695589000	0.872768000	-2.993579000
N	1.410125000	-1.255397000	-2.983601000
H	-0.722350000	-0.742471000	2.364843000

C	-2.605524000	-0.597075000	4.516659000
C	-2.711017000	0.799030000	4.454052000
C	-3.010346000	-1.380143000	3.424931000
C	-3.224427000	1.411883000	3.300934000
C	-3.631949000	0.627851000	2.211531000
C	-3.522040000	-0.768921000	2.271201000
H	-3.299185000	2.493334000	3.244051000
H	-2.921438000	-2.461595000	3.472036000
H	-2.387691000	1.405911000	5.293838000
H	-2.202306000	-1.071376000	5.405928000
H	-4.010448000	1.103625000	1.315674000
H	-3.808411000	-1.372892000	1.417699000

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Fe	0.262486000	0.007746000	0.233574000
O	0.010772000	-0.007125000	-1.854379000
N	-1.350769000	1.176743000	0.300321000
N	-0.921177000	-1.589063000	0.268102000
N	1.828595000	-1.160989000	-0.068740000
N	1.398976000	1.609004000	-0.045772000
C	-1.422084000	2.516394000	-0.037223000
C	-2.590881000	0.825056000	0.812040000
C	-2.246825000	-1.613133000	0.660089000
C	-0.625054000	-2.856987000	-0.223900000
C	1.813054000	-2.499814000	-0.407039000
C	3.155597000	-0.803814000	0.097036000
C	2.779180000	1.631942000	-0.011629000
C	0.987606000	2.870655000	-0.465257000
C	-2.725161000	3.037465000	0.327049000
H	-3.034582000	4.063698000	0.205416000
C	-3.429052000	2.007352000	0.890735000
H	-4.425320000	2.037344000	1.302089000
C	-2.804403000	-2.928364000	0.403577000
H	-3.827200000	-3.210866000	0.598932000
C	-1.820413000	-3.678433000	-0.178702000
H	-1.890005000	-4.692493000	-0.538623000
C	3.169505000	-3.019944000	-0.383446000
H	3.438312000	-4.046410000	-0.577509000
C	3.991007000	-1.987722000	-0.027842000
H	5.059942000	-2.012456000	0.110144000
C	3.254186000	2.943388000	-0.416891000
H	4.293543000	3.220874000	-0.497672000
C	2.156571000	3.689623000	-0.737507000
H	2.133171000	4.696197000	-1.122964000

C	-0.348663000	3.302796000	-0.499102000
C	-3.009185000	-0.494018000	1.042705000
C	0.662744000	-3.290481000	-0.578922000
C	3.615558000	0.518593000	0.189232000
C	-0.662448000	4.691464000	-0.938361000
C	-1.618956000	4.907277000	-1.950646000
H	-2.100848000	4.047093000	-2.403495000
C	-1.947100000	6.201651000	-2.365741000
H	-2.682568000	6.346278000	-3.151378000
C	-1.325798000	7.308700000	-1.772834000
H	-1.578291000	8.314274000	-2.094510000
C	-0.380170000	7.109476000	-0.758440000
H	0.096201000	7.962252000	-0.284270000
C	-0.054457000	5.813977000	-0.342863000
H	0.666057000	5.660940000	0.453179000
C	-4.391531000	-0.753833000	1.534174000
C	-5.523574000	-0.260900000	0.855575000
H	-5.383191000	0.333912000	-0.040630000
C	-6.814084000	-0.546974000	1.314333000
H	-7.674669000	-0.163094000	0.774875000
C	-6.996611000	-1.335968000	2.457362000
H	-7.997859000	-1.558204000	2.813175000
C	-5.879021000	-1.842343000	3.134499000
H	-6.011983000	-2.457322000	4.019442000
C	-4.589446000	-1.556392000	2.674792000
H	-3.720595000	-1.948643000	3.193183000
C	0.856348000	-4.685045000	-1.067177000
C	1.511397000	-4.912758000	-2.293765000
H	1.851496000	-4.058345000	-2.869726000
C	1.720208000	-6.213610000	-2.763502000
H	2.222258000	-6.369281000	-3.713618000
C	1.280600000	-7.312463000	-2.013280000
H	1.442099000	-8.322398000	-2.377342000
C	0.636027000	-7.099840000	-0.787665000
H	0.303823000	-7.946067000	-0.193797000
C	0.428729000	-5.798470000	-0.317835000
H	-0.056149000	-5.633978000	0.638438000
C	5.072796000	0.785944000	0.352426000
C	6.029694000	0.278929000	-0.548096000
H	5.696182000	-0.323877000	-1.385613000
C	7.389342000	0.563158000	-0.380689000
H	8.112641000	0.168423000	-1.087874000
C	7.816440000	1.365163000	0.685759000
H	8.871639000	1.585715000	0.814602000
C	6.872778000	1.887081000	1.580384000

H	7.194786000	2.512740000	2.407410000
C	5.513581000	1.602380000	1.412621000
H	4.777913000	2.005725000	2.101049000
H	-0.724083000	-0.613058000	-2.076766000
C	0.512032000	0.022721000	2.207283000
C	0.979416000	-0.611083000	4.378158000
H	1.282813000	-1.288653000	5.157680000
C	0.602672000	0.691475000	4.415882000
H	0.502856000	1.381619000	5.235996000
C	-0.147443000	2.411933000	2.777796000
H	0.067664000	3.059590000	3.633103000
H	0.377338000	2.782510000	1.903595000
H	-1.222035000	2.409049000	2.583372000
C	1.285189000	-2.363090000	2.633986000
H	1.277522000	-2.997053000	3.525882000
H	0.559204000	-2.736876000	1.919681000
H	2.280282000	-2.379557000	2.183845000
N	0.918635000	-1.006491000	3.039320000
N	0.324264000	1.065513000	3.098550000
H	-0.227034000	0.890128000	-2.154491000
C	-1.878598000	0.356928000	-4.540499000
C	-2.017336000	-1.022058000	-4.326183000
C	-2.446221000	1.267220000	-3.636115000
C	-2.731518000	-1.489548000	-3.211680000
C	-3.307458000	-0.576844000	-2.315204000
C	-3.159294000	0.801606000	-2.521909000
H	-2.825920000	-2.554476000	-3.027202000
H	-2.328219000	2.334528000	-3.798606000
H	-1.564756000	-1.727066000	-5.016217000
H	-1.322622000	0.719133000	-5.399613000
H	-3.840703000	-0.941172000	-1.446784000
H	-3.566399000	1.503390000	-1.802063000

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Fe	0.004718000	0.032072000	0.067003000
O	-0.128933000	-0.741257000	-2.920510000
C	0.006038000	0.022262000	2.229731000
C	0.681984000	0.100581000	4.424228000
H	1.389081000	0.170427000	5.233158000
C	-0.675803000	-0.008094000	4.423633000
H	-1.385068000	-0.060476000	5.231984000
C	-2.454569000	-0.175049000	2.628541000
H	-3.120601000	0.018721000	3.473683000
H	-2.636564000	0.554744000	1.840273000

H	-2.642518000	-1.176685000	2.232723000
C	2.466722000	0.231897000	2.633702000
H	3.128885000	0.037716000	3.481860000
H	2.649114000	-0.500493000	1.848131000
H	2.659842000	1.231598000	2.235311000
N	1.078209000	0.112942000	3.083042000
N	-1.068019000	-0.050222000	3.082040000
N	-1.629720000	-1.221145000	-0.397827000
N	1.274251000	-1.627150000	-0.289813000
N	1.640407000	1.249402000	-0.366313000
N	-1.273822000	1.662838000	-0.275803000
C	-2.960872000	-0.830454000	-0.462970000
C	-1.610278000	-2.594805000	-0.164707000
C	0.866083000	-2.949815000	-0.303136000
C	2.633729000	-1.612284000	-0.568063000
C	2.965761000	0.864654000	-0.467837000
C	1.617907000	2.625608000	-0.184229000
C	-0.860242000	2.979308000	-0.317975000
C	-2.622812000	1.643638000	-0.585602000
C	-3.798720000	-1.984339000	-0.227016000
H	-4.876641000	-1.968349000	-0.193456000
C	-2.972038000	-3.060912000	-0.024412000
H	-3.260365000	-4.076343000	0.195684000
C	2.010275000	-3.797774000	-0.602313000
H	1.971204000	-4.870448000	-0.707436000
C	3.088394000	-2.978465000	-0.780383000
H	4.092023000	-3.260717000	-1.055916000
C	3.808907000	2.030094000	-0.290755000
H	4.887284000	2.019662000	-0.292010000
C	2.983500000	3.106324000	-0.096637000
H	3.271207000	4.129613000	0.083625000
C	-1.996510000	3.826479000	-0.658273000
H	-1.949860000	4.895978000	-0.789423000
C	-3.072354000	3.006738000	-0.837635000
H	-4.069024000	3.282882000	-1.142995000
C	-3.431132000	0.491903000	-0.632849000
C	-0.456656000	-3.409356000	-0.143199000
C	3.439035000	-0.458138000	-0.623980000
C	0.463607000	3.439255000	-0.166609000
C	-4.897019000	0.670604000	-0.835214000
C	-5.566788000	-0.020813000	-1.864286000
H	-4.994080000	-0.670801000	-2.517166000
C	-6.943815000	0.135480000	-2.052007000
H	-7.441498000	-0.398949000	-2.855312000
C	-7.677479000	0.985634000	-1.213851000

H	-8.746154000	1.107655000	-1.360372000
C	-7.023641000	1.678232000	-0.186304000
H	-7.585795000	2.334499000	0.471132000
C	-5.646562000	1.521131000	0.001549000
H	-5.139319000	2.052406000	0.800102000
C	-0.646314000	-4.883737000	-0.013724000
C	-1.462905000	-5.597489000	-0.912651000
H	-1.957828000	-5.058942000	-1.713625000
C	-1.622203000	-6.981610000	-0.788069000
H	-2.249374000	-7.516932000	-1.494308000
C	-0.965407000	-7.677425000	0.235547000
H	-1.088584000	-8.751756000	0.331173000
C	-0.144992000	-6.979771000	1.131872000
H	0.366855000	-7.511666000	1.928103000
C	0.014034000	-5.595755000	1.006857000
H	0.648109000	-5.051138000	1.698778000
C	4.904919000	-0.638973000	-0.830331000
C	5.565114000	0.018437000	-1.887250000
H	4.986564000	0.646967000	-2.555917000
C	6.941082000	-0.141605000	-2.080303000
H	7.431683000	0.366967000	-2.904491000
C	7.682804000	-0.961826000	-1.219807000
H	8.750568000	-1.086784000	-1.370372000
C	7.038329000	-1.620515000	-0.164454000
H	7.606873000	-2.253401000	0.510182000
C	5.662301000	-1.459502000	0.028649000
H	5.161960000	-1.964759000	0.848253000
C	0.649470000	4.916593000	-0.063097000
C	1.446594000	5.622732000	-0.984995000
H	1.932550000	5.075981000	-1.785827000
C	1.597522000	7.009693000	-0.883001000
H	2.209768000	7.539163000	-1.606570000
C	0.951321000	7.715783000	0.140331000
H	1.068113000	8.792259000	0.218424000
C	0.149113000	7.025708000	1.058701000
H	-0.355366000	7.565734000	1.854174000
C	-0.001961000	5.638939000	0.955900000
H	-0.622989000	5.099852000	1.663879000
H	0.736901000	-0.912155000	-2.503306000
H	-0.808171000	-0.957703000	-2.245313000

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Fe	-0.025495000	0.091094000	-0.136197000
N	1.163484000	1.708636000	-0.236397000

N	-1.635137000	1.277472000	-0.204397000
N	-1.217172000	-1.491048000	-0.460797000
N	1.580049000	-1.056385000	-0.449597000
C	2.533486000	1.747169000	-0.473597000
C	0.795847000	2.996354000	0.138603000
C	-1.646971000	2.643473000	0.053103000
C	-2.941954000	0.935836000	-0.558497000
C	-2.581372000	-1.499082000	-0.694497000
C	-0.842536000	-2.811467000	-0.260597000
C	1.595482000	-2.436285000	-0.334197000
C	2.875568000	-0.674448000	-0.779797000
C	3.036251000	3.075245000	-0.201397000
H	4.070265000	3.369494000	-0.284197000
C	1.974087000	3.833296000	0.205503000
H	1.981438000	4.865096000	0.517703000
C	-2.983145000	3.164138000	-0.146897000
H	-3.258095000	4.201151000	-0.037797000
C	-3.770096000	2.123576000	-0.550197000
H	-4.810295000	2.150927000	-0.831097000
C	-3.080038000	-2.856558000	-0.616297000
H	-4.112152000	-3.141107000	-0.744497000
C	-2.015377000	-3.658909000	-0.310697000
H	-2.016429000	-4.724909000	-0.148797000
C	2.929058000	-2.932450000	-0.608297000
H	3.205207000	-3.975164000	-0.610197000
C	3.706210000	-1.853488000	-0.923297000
H	4.741111000	-1.847439000	-1.224597000
C	3.336732000	0.647830000	-0.817397000
C	-0.522732000	3.441618000	0.314603000
C	-3.397717000	-0.363242000	-0.813297000
C	0.478542000	-3.260231000	-0.128997000
C	4.767845000	0.914160000	-1.142297000
C	5.099286000	1.760544000	-2.217797000
H	4.300008000	2.195083000	-2.809297000
C	6.436100000	2.034579000	-2.525297000
H	6.674031000	2.683467000	-3.362397000
C	7.464572000	1.469629000	-1.759697000
H	8.502083000	1.681678000	-1.998297000
C	7.146932000	0.631744000	-0.682797000
H	7.938310000	0.198206000	-0.078797000
C	5.809718000	0.358309000	-0.375697000
H	5.561387000	-0.281878000	0.464303000
C	-0.766262000	4.866030000	0.683903000
C	-0.287811000	5.925106000	-0.111297000
H	0.273478000	5.695879000	-1.010797000

C	-0.544946000	7.254419000	0.241103000
H	-0.174307000	8.058901000	-0.386697000
C	-1.288332000	7.547355000	1.392003000
H	-1.488181000	8.579065000	1.664403000
C	-1.776783000	6.501679000	2.186203000
H	-2.354372000	6.720407000	3.079203000
C	-1.519947000	5.172666000	1.833403000
H	-1.897287000	4.359185000	2.444503000
C	-4.835227000	-0.578272000	-1.144997000
C	-5.190260000	-1.243155000	-2.334797000
H	-4.403576000	-1.571693000	-3.005897000
C	-6.533671000	-1.470389000	-2.651497000
H	-6.790296000	-1.977777000	-3.576297000
C	-7.544950000	-1.039740000	-1.782497000
H	-8.587458000	-1.215689000	-2.028597000
C	-7.203418000	-0.382057000	-0.593497000
H	-7.981002000	-0.052819000	0.089003000
C	-5.859807000	-0.155122000	-0.276797000
H	-5.592782000	0.346265000	0.647703000
C	0.736172000	-4.702243000	0.148303000
C	0.302722000	-5.716822000	-0.725397000
H	-0.232564000	-5.441296000	-1.627897000
C	0.572257000	-7.061035000	-0.444697000
H	0.237019000	-7.832219000	-1.131497000
C	1.281940000	-7.411270000	0.711503000
H	1.491289000	-8.454280000	0.927803000
C	1.723489000	-6.408392000	1.584903000
H	2.273276000	-6.672818000	2.483203000
C	1.454654000	-5.064678000	1.303903000
H	1.785992000	-4.282595000	1.979803000
C	0.088078000	-0.464212000	2.054303000
C	-0.419684000	-1.733587000	3.909803000
H	-1.061909000	-2.253056000	4.601103000
C	0.932124000	-1.565353000	3.895103000
H	1.695908000	-1.901990000	4.576003000
C	2.574182000	-0.393433000	2.385903000
H	3.144694000	-0.142261000	3.285903000
H	3.070642000	-1.203857000	1.843003000
H	2.509224000	0.477270000	1.737603000
C	-2.328448000	-1.007494000	2.432203000
H	-2.928340000	-0.845665000	3.333903000
H	-2.474708000	-0.183687000	1.737103000
H	-2.629094000	-1.941180000	1.947703000
N	-0.912651000	-1.052063000	2.793903000
N	1.219662000	-0.787067000	2.769103000

O	-0.026052000	0.978294000	-3.044797000
H	-0.611532000	1.389322000	-2.378897000
H	0.813538000	0.772353000	-2.590597000

'P-2

Fe	-0.015220000	0.004255000	-0.155214000
O	-0.001606000	0.008161000	-2.297746000
N	1.643582000	1.105913000	-0.320712000
N	-1.099910000	1.657355000	-0.262791000
N	-1.656797000	-1.098697000	-0.290961000
N	1.083430000	-1.652876000	-0.293486000
C	2.917987000	0.658660000	-0.641283000
C	1.766051000	2.445636000	0.030320000
C	-0.648440000	2.944782000	-0.045329000
C	-2.415834000	1.763390000	-0.696382000
C	-2.923540000	-0.653485000	-0.620841000
C	-1.776941000	-2.438600000	0.046067000
C	0.635192000	-2.943377000	-0.060527000
C	2.406824000	-1.761363000	-0.719325000
C	3.868362000	1.734606000	-0.442815000
H	4.933155000	1.650209000	-0.593408000
C	3.167129000	2.817812000	0.013206000
H	3.557060000	3.783390000	0.292440000
C	-1.711021000	3.890491000	-0.341687000
H	-1.613235000	4.962796000	-0.276508000
C	-2.781908000	3.167029000	-0.781043000
H	-3.729154000	3.539381000	-1.136465000
C	-3.876925000	-1.731537000	-0.434774000
H	-4.940238000	-1.646675000	-0.595159000
C	-3.178777000	-2.816517000	0.018516000
H	-3.567470000	-3.785854000	0.285967000
C	1.699612000	-3.885667000	-0.347539000
H	1.606397000	-4.957624000	-0.270276000
C	2.771960000	-3.164297000	-0.791553000
H	3.721403000	-3.540351000	-1.137222000
C	3.273432000	-0.674479000	-0.922501000
C	0.682259000	3.315727000	0.223461000
C	-3.278466000	0.677674000	-0.904513000
C	-0.692053000	-3.311645000	0.223690000
C	4.680358000	-0.929327000	-1.345570000
C	5.200915000	-0.283111000	-2.484113000
H	4.556038000	0.383043000	-3.048140000
C	6.524819000	-0.490278000	-2.885075000
H	6.905398000	0.012897000	-3.768743000

C	7.356212000	-1.346750000	-2.151514000
H	8.383750000	-1.508945000	-2.461796000
C	6.854129000	-1.988959000	-1.012036000
H	7.495104000	-2.644883000	-0.430702000
C	5.530245000	-1.779688000	-0.611354000
H	5.145695000	-2.266344000	0.278501000
C	0.931026000	4.737673000	0.593287000
C	1.766037000	5.574823000	-0.172040000
H	2.243913000	5.173279000	-1.058977000
C	1.963586000	6.911774000	0.189905000
H	2.605950000	7.543951000	-0.415725000
C	1.324983000	7.438491000	1.320241000
H	1.477983000	8.476281000	1.599812000
C	0.482161000	6.619411000	2.083117000
H	-0.019459000	7.020098000	2.958821000
C	0.285470000	5.282945000	1.720894000
H	-0.367724000	4.644713000	2.307010000
C	-4.679770000	0.930065000	-1.345359000
C	-5.177450000	0.286838000	-2.495616000
H	-4.517121000	-0.369265000	-3.052928000
C	-6.495300000	0.491991000	-2.916912000
H	-6.859331000	-0.006938000	-3.809937000
C	-7.341992000	1.341522000	-2.192516000
H	-8.364976000	1.501408000	-2.518901000
C	-6.861351000	1.980931000	-1.042335000
H	-7.514127000	2.632511000	-0.469230000
C	-5.543133000	1.774967000	-0.621336000
H	-5.174088000	2.260357000	0.275885000
C	-0.938665000	-4.734734000	0.592423000
C	-1.770422000	-5.572264000	-0.175795000
H	-2.248519000	-5.169756000	-1.062182000
C	-1.966116000	-6.910034000	0.184321000
H	-2.606494000	-7.542593000	-0.422998000
C	-1.329037000	-7.436729000	1.315555000
H	-1.480901000	-8.475041000	1.593822000
C	-0.489928000	-6.616827000	2.081569000
H	0.009892000	-7.017356000	2.958389000
C	-0.295058000	-5.279474000	1.721210000
H	0.354758000	-4.640293000	2.310127000
H	0.728428000	0.628905000	-2.495232000
C	-0.002328000	-0.001075000	1.829490000
C	-0.669219000	0.026700000	4.039822000
H	-1.377968000	0.058499000	4.849389000
C	0.685161000	-0.046404000	4.033341000
H	1.401306000	-0.084172000	4.836120000

C	2.491291000	-0.115340000	2.319173000
H	3.064969000	-0.410973000	3.202658000
H	2.634440000	-0.850934000	1.534477000
H	2.836289000	0.860622000	1.971661000
C	-2.491089000	0.113450000	2.343092000
H	-3.054549000	0.414185000	3.231461000
H	-2.636522000	0.848531000	1.558534000
H	-2.845018000	-0.861094000	2.000277000
N	-1.074772000	0.056181000	2.703234000
N	1.078360000	-0.064943000	2.692666000
H	0.263663000	-0.904969000	-2.525044000

C-H bond activation of CHD by species 3

⁶RC-3_{hs}

Co	0.107374000	0.024145000	-0.255854000
O	-0.077284000	0.429648000	1.686840000
C	0.377745000	0.121032000	-2.482020000
C	0.028402000	0.581012000	-4.711678000
H	-0.503064000	0.973202000	-5.561916000
C	1.217236000	-0.073179000	-4.617337000
H	1.928242000	-0.370776000	-5.369071000
C	2.585092000	-1.056276000	-2.750198000
H	3.295955000	-1.183131000	-3.571343000
H	3.044094000	-0.474143000	-1.953996000
H	2.299494000	-2.034544000	-2.358283000
C	-1.743271000	1.334954000	-3.094981000
H	-2.299417000	1.472259000	-4.026616000
H	-2.314143000	0.700434000	-2.420058000
H	-1.577654000	2.303847000	-2.619380000
N	-0.468196000	0.686685000	-3.408748000
N	1.412424000	-0.343287000	-3.259354000
N	1.159053000	-1.735092000	0.011481000
N	-1.655111000	-1.005345000	-0.404901000
N	-0.907780000	1.806801000	-0.131039000
N	1.932829000	1.076697000	-0.028157000
C	2.502118000	-1.874832000	0.290284000
C	0.654131000	-2.987793000	-0.288139000
C	-1.771542000	-2.377562000	-0.511370000
C	-2.917167000	-0.487557000	-0.190059000
C	-2.282020000	1.933115000	-0.037390000
C	-0.361969000	3.076666000	-0.250486000
C	2.055759000	2.445719000	-0.037790000
C	3.137715000	0.548220000	0.393698000

C	2.870382000	-3.269796000	0.133385000
H	3.865398000	-3.665832000	0.261272000
C	1.742434000	-3.948585000	-0.247258000
H	1.655679000	-4.997748000	-0.480136000
C	-3.176099000	-2.738488000	-0.386855000
H	-3.558093000	-3.746819000	-0.407375000
C	-3.874232000	-1.583751000	-0.168282000
H	-4.931471000	-1.480262000	0.016816000
C	-2.621241000	3.337317000	-0.153463000
H	-3.625722000	3.730635000	-0.151451000
C	-1.450317000	4.034132000	-0.312292000
H	-1.336092000	5.096674000	-0.455697000
C	3.410815000	2.804247000	0.364280000
H	3.778467000	3.813398000	0.462956000
C	4.066918000	1.641427000	0.651985000
H	5.070571000	1.527769000	1.029350000
C	3.417645000	-0.825302000	0.543371000
C	-0.703618000	-3.297780000	-0.541533000
C	-3.218291000	0.877574000	-0.003309000
C	1.013223000	3.380773000	-0.242472000
C	4.799084000	-1.220212000	0.941197000
C	5.005166000	-2.055160000	2.057438000
H	4.144046000	-2.389554000	2.626173000
C	6.296000000	-2.439572000	2.434055000
H	6.436302000	-3.076522000	3.301996000
C	7.405098000	-1.998992000	1.699651000
H	8.407082000	-2.297066000	1.992242000
C	7.213267000	-1.172104000	0.585005000
H	8.066714000	-0.832703000	0.005892000
C	5.922085000	-0.787595000	0.208786000
H	5.771347000	-0.153095000	-0.658304000
C	-1.064905000	-4.727349000	-0.769580000
C	-0.738467000	-5.725541000	0.169165000
H	-0.210272000	-5.442878000	1.073366000
C	-1.100739000	-7.058633000	-0.050394000
H	-0.846850000	-7.813847000	0.687156000
C	-1.799415000	-7.417396000	-1.210849000
H	-2.081112000	-8.451982000	-1.380402000
C	-2.136512000	-6.432462000	-2.148589000
H	-2.677603000	-6.702150000	-3.050471000
C	-1.774223000	-5.099500000	-1.928463000
H	-2.033250000	-4.333413000	-2.652012000
C	-4.641033000	1.251863000	0.235646000
C	-4.989097000	1.960132000	1.402815000
H	-4.207031000	2.207031000	2.112575000

C	-6.317858000	2.320892000	1.648775000
H	-6.570498000	2.859504000	2.556956000
C	-7.321261000	1.980891000	0.731614000
H	-8.352806000	2.259968000	0.922611000
C	-6.986335000	1.277925000	-0.433392000
H	-7.757600000	1.016595000	-1.151624000
C	-5.657109000	0.917518000	-0.679603000
H	-5.394452000	0.378029000	-1.583789000
C	1.416176000	4.813805000	-0.349901000
C	0.938583000	5.782553000	0.554115000
H	0.264752000	5.474612000	1.346289000
C	1.339081000	7.118695000	0.446920000
H	0.966380000	7.850940000	1.156678000
C	2.228295000	7.509264000	-0.562961000
H	2.539671000	8.545997000	-0.645142000
C	2.718530000	6.552838000	-1.461994000
H	3.409505000	6.846975000	-2.246207000
C	2.317708000	5.217067000	-1.354373000
H	2.696529000	4.472372000	-2.046933000
C	-2.399768000	0.629397000	3.852633000
C	-2.819652000	-0.447769000	3.174943000
C	-1.063390000	0.709488000	4.552591000
C	-2.005105000	-1.712449000	3.036401000
C	-0.717945000	-1.670887000	3.825322000
C	-0.299679000	-0.593087000	4.504382000
H	-0.453249000	1.493763000	4.075386000
H	-2.610104000	-2.583395000	3.343510000
H	-1.202866000	1.028886000	5.600162000
H	-1.771443000	-1.879119000	1.976414000
H	-0.108952000	-2.573244000	3.810496000
H	0.648556000	-0.621409000	5.038349000
H	-3.032016000	1.514701000	3.908725000
H	-3.784930000	-0.431722000	2.674521000

⁴RC-3_{is}

Co	-0.152601000	0.042248000	-0.226122000
O	-0.055063000	-0.024087000	1.468282000
C	-0.323833000	0.106527000	-2.323329000
C	-0.342403000	-0.484653000	-4.545074000
H	-0.240258000	-1.152751000	-5.382549000
C	-0.666296000	0.831242000	-4.478198000
H	-0.900317000	1.548564000	-5.245601000
C	-0.960847000	2.544728000	-2.699779000
H	-1.393004000	3.072410000	-3.554544000

H	-1.682228000	2.516681000	-1.890085000
H	-0.057818000	3.061264000	-2.371783000
C	0.226595000	-2.303319000	-2.947937000
H	0.510512000	-2.775010000	-3.892825000
H	1.069739000	-2.326790000	-2.265866000
H	-0.615754000	-2.841480000	-2.510975000
N	-0.136192000	-0.912599000	-3.232190000
N	-0.652539000	1.177520000	-3.125776000
N	0.533907000	1.910816000	-0.166419000
N	1.803004000	-0.684996000	-0.494181000
N	-0.826358000	-1.828687000	-0.179940000
N	-2.120935000	0.778963000	-0.128581000
C	-0.189680000	3.020237000	0.230932000
C	1.808251000	2.327893000	-0.517561000
C	2.915790000	0.093829000	-0.687913000
C	2.223525000	-1.948589000	-0.140836000
C	-0.052968000	-2.953137000	0.040866000
C	-2.141774000	-2.231602000	-0.344256000
C	-3.249019000	0.001974000	-0.171226000
C	-2.470000000	2.012736000	0.377154000
C	0.647636000	4.193824000	0.071149000
H	0.331777000	5.204770000	0.273668000
C	1.854527000	3.776202000	-0.420066000
H	2.703169000	4.387186000	-0.681278000
C	4.104900000	-0.727447000	-0.501151000
H	5.120000000	-0.370272000	-0.577486000
C	3.678376000	-1.975059000	-0.134571000
H	4.284184000	-2.824185000	0.139209000
C	-0.909286000	-4.120511000	-0.041492000
H	-0.567994000	-5.138519000	0.060554000
C	-2.176691000	-3.684068000	-0.317788000
H	-3.057737000	-4.284752000	-0.474406000
C	-4.387021000	0.795853000	0.277133000
H	-5.399861000	0.432638000	0.356321000
C	-3.902435000	2.021483000	0.643703000
H	-4.450671000	2.843839000	1.075282000
C	-1.562566000	3.071842000	0.568322000
C	2.914238000	1.499709000	-0.806012000
C	1.354020000	-3.016228000	0.147390000
C	-3.275200000	-1.391939000	-0.393454000
C	-2.081414000	4.362206000	1.101560000
C	-1.485529000	4.947191000	2.236805000
H	-0.656812000	4.434676000	2.713946000
C	-1.960191000	6.159189000	2.748207000
H	-1.494142000	6.591312000	3.628438000

C	-3.038327000	6.809965000	2.133445000
H	-3.407528000	7.750042000	2.531467000
C	-3.636223000	6.240860000	1.001428000
H	-4.466266000	6.743156000	0.513840000
C	-3.160630000	5.029131000	0.489235000
H	-3.616851000	4.592716000	-0.393116000
C	4.227342000	2.137206000	-1.114838000
C	4.836566000	3.043625000	-0.225178000
H	4.331605000	3.288437000	0.702928000
C	6.082792000	3.605870000	-0.520681000
H	6.540549000	4.298044000	0.179431000
C	6.745990000	3.266532000	-1.707505000
H	7.713783000	3.702207000	-1.935641000
C	6.156632000	2.355588000	-2.593940000
H	6.665644000	2.084368000	-3.513873000
C	4.910009000	1.793981000	-2.298051000
H	4.450608000	1.085840000	-2.980176000
C	1.944414000	-4.320193000	0.556714000
C	1.555871000	-4.905475000	1.778290000
H	0.840457000	-4.379495000	2.400855000
C	2.099309000	-6.127042000	2.188547000
H	1.796130000	-6.559941000	3.136857000
C	3.039065000	-6.785464000	1.384113000
H	3.462131000	-7.733035000	1.702844000
C	3.430507000	-6.214249000	0.166048000
H	4.152575000	-6.722544000	-0.465828000
C	2.886806000	-4.992292000	-0.244857000
H	3.182397000	-4.552803000	-1.191901000
C	-4.625237000	-2.010900000	-0.538440000
C	-5.097124000	-2.987407000	0.360450000
H	-4.457593000	-3.303214000	1.177472000
C	-6.378693000	-3.529908000	0.218029000
H	-6.727920000	-4.277128000	0.924106000
C	-7.214946000	-3.101150000	-0.821288000
H	-8.209767000	-3.521778000	-0.930335000
C	-6.762494000	-2.120449000	-1.713620000
H	-7.405473000	-1.779345000	-2.519349000
C	-5.480896000	-1.578383000	-1.570644000
H	-5.128044000	-0.815900000	-2.257685000
C	1.083058000	-1.824908000	3.924506000
C	2.210297000	-1.636820000	3.226303000
C	0.249050000	-0.689665000	4.474131000
C	2.771382000	-0.267497000	2.920414000
C	2.088236000	0.830714000	3.701683000
C	0.959587000	0.642376000	4.397696000

H	-0.689658000	-0.623348000	3.898011000
H	3.857336000	-0.253276000	3.111964000
H	-0.045374000	-0.903572000	5.515384000
H	2.657081000	-0.065412000	1.846227000
H	2.548409000	1.817129000	3.664580000
H	0.497691000	1.474659000	4.926535000
H	0.716803000	-2.834650000	4.106834000
H	2.754717000	-2.490789000	2.829759000

²RC-3_{is}

Co	-0.000184000	0.000017000	-0.306800000
O	-0.000009000	-0.000018000	1.540150000
C	-0.000428000	0.000016000	-2.350179000
C	-0.123800000	-0.667943000	-4.544579000
H	-0.257082000	-1.368221000	-5.351117000
C	0.122376000	0.667952000	-4.544617000
H	0.255444000	1.368225000	-5.351195000
C	0.469789000	2.448590000	-2.822347000
H	0.288615000	3.082787000	-3.694762000
H	-0.194597000	2.741961000	-2.015378000
H	1.506179000	2.560283000	-2.496686000
C	-0.470870000	-2.448544000	-2.822206000
H	-0.289886000	-3.082763000	-3.694642000
H	0.193659000	-2.741916000	-2.015357000
H	-1.507201000	-2.560199000	-2.496337000
N	-0.193839000	-1.060924000	-3.205186000
N	0.192729000	1.060956000	-3.205247000
N	1.444534000	1.302834000	-0.221057000
N	1.318606000	-1.447667000	-0.276809000
N	-1.444878000	-1.302791000	-0.220730000
N	-1.318960000	1.447719000	-0.276545000
C	1.327030000	2.604053000	0.213290000
C	2.751617000	1.116285000	-0.634309000
C	2.656344000	-1.331587000	-0.575988000
C	1.124584000	-2.705155000	0.270704000
C	-1.327280000	-2.603999000	0.213643000
C	-2.752056000	-1.116247000	-0.633676000
C	-2.656768000	1.331630000	-0.575447000
C	-1.124823000	2.705221000	0.270876000
C	2.592868000	3.280461000	0.024965000
H	2.772696000	4.317337000	0.261693000
C	3.453370000	2.381894000	-0.547653000
H	4.473151000	2.548801000	-0.854206000
C	3.330240000	-2.571508000	-0.238755000

H	4.388249000	-2.743699000	-0.359084000
C	2.398106000	-3.394981000	0.329753000
H	2.550728000	-4.375130000	0.751529000
C	-2.593166000	-3.280398000	0.025653000
H	-2.772954000	-4.317261000	0.262475000
C	-3.453802000	-2.381857000	-0.546795000
H	-4.473662000	-2.548742000	-0.853097000
C	-3.330585000	2.571560000	-0.238119000
H	-4.388620000	2.743754000	-0.358224000
C	-2.398336000	3.395049000	0.330178000
H	-2.550873000	4.375209000	0.751959000
C	0.130147000	3.249245000	0.569826000
C	3.325404000	-0.136508000	-0.897690000
C	-0.130315000	-3.249165000	0.569948000
C	-3.325893000	0.136533000	-0.896966000
C	0.237865000	4.589977000	1.203255000
C	0.975827000	4.719215000	2.397204000
H	1.420485000	3.830213000	2.832422000
C	1.108998000	5.964146000	3.020097000
H	1.672226000	6.046015000	3.944595000
C	0.511959000	7.100638000	2.458036000
H	0.614870000	8.066966000	2.941892000
C	-0.216861000	6.984358000	1.267171000
H	-0.672401000	7.862902000	0.820361000
C	-0.351041000	5.739303000	0.642946000
H	-0.900197000	5.652008000	-0.288565000
C	4.740147000	-0.243725000	-1.345892000
C	5.800976000	0.349674000	-0.633910000
H	5.584120000	0.899491000	0.275079000
C	7.121814000	0.207254000	-1.072330000
H	7.927980000	0.664992000	-0.507235000
C	7.407201000	-0.536442000	-2.224998000
H	8.432810000	-0.646939000	-2.563105000
C	6.362237000	-1.145020000	-2.932553000
H	6.575096000	-1.728302000	-3.823264000
C	5.041749000	-1.002475000	-2.494439000
H	4.228646000	-1.473153000	-3.037834000
C	-0.237873000	-4.589861000	1.203475000
C	-0.975550000	-4.719035000	2.397613000
H	-1.420099000	-3.830002000	2.832881000
C	-1.108561000	-5.963924000	3.020611000
H	-1.671567000	-6.045745000	3.945248000
C	-0.511639000	-7.100447000	2.458477000
H	-0.614425000	-8.066746000	2.942418000
C	0.216904000	-6.984229000	1.267440000

H	0.672353000	-7.862796000	0.820582000
C	0.350923000	-5.739207000	0.643106000
H	0.899873000	-5.651972000	-0.288534000
C	-4.740742000	0.243736000	-1.344841000
C	-5.801391000	-0.349685000	-0.632619000
H	-5.584324000	-0.899512000	0.276313000
C	-7.122338000	-0.207285000	-1.070729000
H	-7.928358000	-0.665042000	-0.505443000
C	-7.408009000	0.536417000	-2.223327000
H	-8.433701000	0.646893000	-2.561186000
C	-6.363217000	1.145011000	-2.931119000
H	-6.576292000	1.728295000	-3.821779000
C	-5.042624000	1.002485000	-2.493320000
H	-4.229656000	1.473178000	-3.036901000
C	-1.357387000	-0.420250000	4.421096000
C	-0.406056000	-1.363380000	4.423693000
C	-1.053409000	1.047213000	4.209139000
C	1.057032000	-1.047697000	4.207562000
C	1.361281000	0.419726000	4.419404000
C	0.409949000	1.362851000	4.423436000
H	-1.315810000	1.312424000	3.171283000
H	1.318080000	-1.312709000	3.169316000
H	-1.680582000	1.667028000	4.869842000
H	1.685060000	-1.667635000	4.867331000
H	2.407018000	0.692759000	4.554176000
H	0.672869000	2.410649000	4.563629000
H	-2.402948000	-0.693306000	4.557183000
H	-0.668787000	-2.411213000	4.563983000

⁶TS1-3_{hs}

Co	0.293599000	0.011543000	-0.067865000
O	0.375907000	-0.133044000	-1.986845000
C	0.471927000	0.028795000	2.251219000
C	0.783855000	-0.625443000	4.442869000
H	0.974524000	-1.322046000	5.241539000
C	0.570090000	0.717218000	4.452126000
H	0.529722000	1.426493000	5.261293000
C	0.114061000	2.478281000	2.722250000
H	0.340511000	3.131704000	3.569839000
H	0.748608000	2.740704000	1.879726000
H	-0.932576000	2.601121000	2.435615000
C	0.923414000	-2.412504000	2.685662000
H	0.845252000	-3.055157000	3.567466000
H	0.157197000	-2.686791000	1.965207000

H	1.906533000	-2.537640000	2.226148000
N	0.718943000	-1.025126000	3.103849000
N	0.385474000	1.095900000	3.118228000
N	-1.141881000	1.479521000	0.012488000
N	-1.154134000	-1.429637000	0.101486000
N	1.720195000	-1.469298000	-0.180175000
N	1.746898000	1.471241000	-0.132360000
C	-0.941526000	2.820023000	-0.229789000
C	-2.421447000	1.311490000	0.501599000
C	-2.470035000	-1.192710000	0.425006000
C	-1.023760000	-2.759448000	-0.254933000
C	1.477608000	-2.806152000	-0.394868000
C	3.075943000	-1.288057000	-0.017057000
C	3.100815000	1.223647000	-0.118883000
C	1.548119000	2.786589000	-0.505521000
C	-2.150930000	3.540989000	0.132956000
H	-2.274939000	4.610734000	0.069302000
C	-3.041593000	2.621908000	0.621123000
H	-4.024129000	2.815077000	1.020217000
C	-3.215719000	-2.430617000	0.257239000
H	-4.277369000	-2.536953000	0.416732000
C	-2.337713000	-3.380142000	-0.190963000
H	-2.556657000	-4.401566000	-0.458349000
C	2.742274000	-3.521865000	-0.307842000
H	2.855548000	-4.590642000	-0.401232000
C	3.717714000	-2.596482000	-0.047265000
H	4.770039000	-2.777968000	0.102377000
C	3.797548000	2.450818000	-0.481257000
H	4.868209000	2.547064000	-0.569834000
C	2.847080000	3.398053000	-0.746430000
H	3.004426000	4.408329000	-1.088844000
C	0.291332000	3.428004000	-0.567551000
C	-3.041007000	0.064271000	0.738568000
C	0.203318000	-3.409447000	-0.511993000
C	3.726938000	-0.035807000	0.043962000
C	0.247568000	4.876812000	-0.911878000
C	-0.599514000	5.329548000	-1.943137000
H	-1.193364000	4.603146000	-2.488445000
C	-0.669976000	6.687758000	-2.268343000
H	-1.322734000	7.016514000	-3.071237000
C	0.103847000	7.620931000	-1.565683000
H	0.050249000	8.675414000	-1.817886000
C	0.945454000	7.185035000	-0.533752000
H	1.540397000	7.902869000	0.022782000
C	1.014901000	5.826365000	-0.208609000

H	1.656052000	5.489723000	0.599046000
C	-4.420520000	0.036808000	1.304725000
C	-5.491504000	0.752654000	0.733539000
H	-5.313156000	1.341443000	-0.156946000
C	-6.773811000	0.691197000	1.289491000
H	-7.586056000	1.245421000	0.828932000
C	-7.014039000	-0.090399000	2.426605000
H	-8.009509000	-0.138172000	2.856900000
C	-5.960639000	-0.813323000	3.001983000
H	-6.135734000	-1.421517000	3.884213000
C	-4.679371000	-0.750896000	2.445997000
H	-3.860876000	-1.307120000	2.890409000
C	0.180137000	-4.862911000	-0.844399000
C	0.802083000	-5.323080000	-2.021991000
H	1.276296000	-4.600904000	-2.678275000
C	0.804107000	-6.684026000	-2.344794000
H	1.282391000	-7.019686000	-3.259881000
C	0.187001000	-7.610860000	-1.494168000
H	0.188114000	-8.667160000	-1.744680000
C	-0.428346000	-7.166755000	-0.316485000
H	-0.898786000	-7.879838000	0.353785000
C	-0.429305000	-5.805582000	0.006527000
H	-0.893272000	-5.462797000	0.925243000
C	5.213621000	-0.021444000	0.173374000
C	6.041500000	-0.693315000	-0.746996000
H	5.583536000	-1.232012000	-1.569411000
C	7.433813000	-0.652956000	-0.616726000
H	8.057047000	-1.170788000	-1.339451000
C	8.023605000	0.063273000	0.433289000
H	9.104155000	0.094662000	0.533256000
C	7.210899000	0.743550000	1.349679000
H	7.659872000	1.302006000	2.165483000
C	5.818875000	0.703558000	1.218661000
H	5.185205000	1.229936000	1.925087000
C	-2.342903000	-1.128832000	-3.463134000
C	-3.579471000	-1.426669000	-3.021402000
C	-1.769447000	0.237123000	-3.375616000
C	-4.514992000	-0.394284000	-2.444832000
C	-3.950341000	1.004263000	-2.477703000
C	-2.703786000	1.284260000	-2.904858000
H	-0.829232000	0.143480000	-2.596363000
H	-5.482546000	-0.422352000	-2.977886000
H	-1.192451000	0.530066000	-4.263613000
H	-4.760670000	-0.667381000	-1.404678000
H	-1.703741000	-1.908728000	-3.868534000

H	-3.945428000	-2.449065000	-3.068834000
H	-4.597840000	1.810382000	-2.141010000
H	-2.342210000	2.309193000	-2.890268000

⁴TS1-3_{is}

Co	0.311507000	-0.002671000	0.057681000
C	0.478173000	0.006395000	2.174322000
C	0.788532000	-0.650627000	4.356570000
H	0.981943000	-1.349638000	5.151764000
C	0.562239000	0.687511000	4.369381000
H	0.512555000	1.395307000	5.178628000
C	0.097583000	2.468016000	2.691543000
H	0.317242000	3.084148000	3.568033000
H	0.736052000	2.769934000	1.867878000
H	-0.949275000	2.593557000	2.412091000
C	0.947309000	-2.449966000	2.642361000
H	0.873289000	-3.058286000	3.548227000
H	0.180422000	-2.754166000	1.937981000
H	1.932325000	-2.583407000	2.191970000
N	0.734032000	-1.051123000	3.019747000
N	0.376579000	1.073215000	3.040027000
N	-1.117810000	1.372274000	0.115880000
N	-1.150141000	-1.499564000	0.247785000
N	1.712104000	-1.381855000	-0.075727000
N	1.761417000	1.518378000	0.000596000
C	-0.952558000	2.712011000	-0.187042000
C	-2.408241000	1.196454000	0.597443000
C	-2.471976000	-1.292424000	0.526769000
C	-1.002000000	-2.790472000	-0.207423000
C	1.489371000	-2.714883000	-0.370729000
C	3.074304000	-1.191787000	0.081091000
C	3.113754000	1.303048000	-0.012888000
C	1.527401000	2.795603000	-0.459084000
C	-2.175250000	3.414155000	0.151908000
H	-2.320883000	4.477570000	0.046666000
C	-3.044721000	2.497655000	0.677372000
H	-4.030907000	2.684669000	1.069162000
C	-3.208721000	-2.522536000	0.266791000
H	-4.274675000	-2.641920000	0.385448000
C	-2.309440000	-3.432927000	-0.220248000
H	-2.510274000	-4.433630000	-0.569019000
C	2.763239000	-3.408599000	-0.325592000
H	2.889889000	-4.468628000	-0.478327000
C	3.725442000	-2.487684000	-0.011114000

H	4.779624000	-2.662948000	0.129239000
C	3.783485000	2.520545000	-0.456117000
H	4.850403000	2.630602000	-0.573922000
C	2.805551000	3.427710000	-0.760926000
H	2.930222000	4.416669000	-1.172990000
C	0.245321000	3.367622000	-0.562254000
C	-3.044606000	-0.039711000	0.841145000
C	0.242884000	-3.366973000	-0.524446000
C	3.741186000	0.050250000	0.158783000
C	0.130642000	4.786213000	-0.999734000
C	-0.744821000	5.135553000	-2.047375000
H	-1.311668000	4.351210000	-2.537793000
C	-0.873920000	6.465118000	-2.460620000
H	-1.548397000	6.713292000	-3.274449000
C	-0.130165000	7.473084000	-1.832566000
H	-0.229384000	8.505456000	-2.153176000
C	0.741338000	7.140352000	-0.787163000
H	1.314458000	7.916480000	-0.288966000
C	0.868926000	5.810315000	-0.373633000
H	1.533619000	5.553747000	0.444329000
C	-4.437796000	-0.069427000	1.369790000
C	-5.498247000	0.645527000	0.777711000
H	-5.300890000	1.243739000	-0.102075000
C	-6.795191000	0.565740000	1.295823000
H	-7.598567000	1.119343000	0.819190000
C	-7.062228000	-0.235016000	2.413568000
H	-8.069386000	-0.297012000	2.813853000
C	-6.020694000	-0.960681000	3.006574000
H	-6.216854000	-1.586351000	3.872035000
C	-4.724632000	-0.879962000	2.488452000
H	-3.915961000	-1.440923000	2.944990000
C	0.271278000	-4.783464000	-0.984642000
C	0.911976000	-5.117136000	-2.194899000
H	1.371156000	-4.325583000	-2.777671000
C	0.948170000	-6.441245000	-2.643371000
H	1.439807000	-6.678539000	-3.581888000
C	0.346607000	-7.457625000	-1.889188000
H	0.373953000	-8.485425000	-2.237633000
C	-0.288308000	-7.139811000	-0.681338000
H	-0.748090000	-7.922903000	-0.085965000
C	-0.323801000	-5.815299000	-0.232492000
H	-0.805381000	-5.569935000	0.708162000
C	5.228448000	0.068398000	0.271919000
C	6.056144000	-0.589578000	-0.658962000
H	5.597786000	-1.131482000	-1.478910000

C	7.449048000	-0.528448000	-0.544682000
H	8.071423000	-1.036030000	-1.275386000
C	8.040562000	0.196946000	0.498118000
H	9.121626000	0.244563000	0.585277000
C	7.228541000	0.867193000	1.422313000
H	7.678525000	1.435222000	2.230943000
C	5.835843000	0.806152000	1.307235000
H	5.202784000	1.326875000	2.018498000
O	0.298643000	-0.099116000	-1.702516000
C	-2.189658000	-0.974406000	-3.361143000
C	-3.425482000	-1.366873000	-2.999522000
C	-1.708529000	0.419327000	-3.189890000
C	-4.455255000	-0.418018000	-2.437512000
C	-3.987967000	1.017221000	-2.417373000
C	-2.740235000	1.389001000	-2.763087000
H	-0.822512000	0.320023000	-2.342820000
H	-4.718589000	-0.733769000	-1.412888000
H	-1.084100000	0.776619000	-4.020012000
H	-5.398019000	-0.499389000	-3.007866000
H	-1.476391000	-1.696806000	-3.748070000
H	-3.719150000	-2.408897000	-3.096889000
H	-4.710143000	1.770878000	-2.111036000
H	-2.455814000	2.436316000	-2.711580000

²TS1-3_{is}

Co	-0.325995000	-0.005813000	0.022423000
O	-0.266020000	0.012583000	-1.846241000
C	-0.530975000	-0.007613000	2.066014000
C	-0.791357000	0.666513000	4.247993000
H	-0.913739000	1.377010000	5.047255000
C	-0.726773000	-0.689799000	4.252118000
H	-0.772371000	-1.403575000	5.056487000
C	-0.443135000	-2.498976000	2.554530000
H	-0.809150000	-3.099887000	3.391879000
H	-1.043742000	-2.700105000	1.673658000
H	0.599118000	-2.752334000	2.350210000
C	-0.731459000	2.482807000	2.535961000
H	-0.590652000	3.080333000	3.441074000
H	0.059504000	2.707890000	1.827764000
H	-1.698317000	2.720284000	2.087966000
N	-0.669846000	1.068137000	2.914934000
N	-0.571383000	-1.085869000	2.921239000
N	0.964767000	-1.467543000	0.101797000
N	1.145840000	1.271487000	0.156688000

N	-1.590948000	1.464596000	-0.158850000
N	-1.785343000	-1.294068000	-0.156932000
C	0.751587000	-2.755482000	-0.334765000
C	2.210370000	-1.430689000	0.699921000
C	2.396147000	1.011639000	0.672482000
C	1.157784000	2.567470000	-0.326150000
C	-1.280255000	2.748649000	-0.547299000
C	-2.949110000	1.420851000	0.092452000
C	-3.126431000	-1.023886000	-0.012941000
C	-1.672944000	-2.571584000	-0.681586000
C	1.892030000	-3.571657000	0.028510000
H	1.978670000	-4.627190000	-0.175956000
C	2.764269000	-2.768842000	0.713246000
H	3.705754000	-3.047300000	1.157756000
C	3.223337000	2.193059000	0.531507000
H	4.256401000	2.254477000	0.834917000
C	2.480312000	3.128639000	-0.132385000
H	2.791657000	4.105039000	-0.465255000
C	-2.478716000	3.561788000	-0.488454000
H	-2.514005000	4.615501000	-0.716339000
C	-3.493965000	2.759035000	-0.043510000
H	-4.518849000	3.033857000	0.145717000
C	-3.893956000	-2.180767000	-0.434312000
H	-4.971452000	-2.229863000	-0.440392000
C	-3.002439000	-3.110892000	-0.891687000
H	-3.217336000	-4.070872000	-1.332226000
C	-0.464554000	-3.266751000	-0.821732000
C	2.872022000	-0.250041000	1.068268000
C	0.013265000	3.264029000	-0.737131000
C	-3.687201000	0.238577000	0.253199000
C	-0.450130000	-4.644023000	-1.383322000
C	0.413438000	-4.941355000	-2.456439000
H	1.028042000	-4.147231000	-2.867624000
C	0.467055000	-6.230921000	-2.994631000
H	1.132072000	-6.439923000	-3.826916000
C	-0.338793000	-7.248293000	-2.466360000
H	-0.298143000	-8.249423000	-2.884117000
C	-1.194367000	-6.967343000	-1.393087000
H	-1.812444000	-7.753484000	-0.970057000
C	-1.247338000	-5.677490000	-0.854090000
H	-1.895282000	-5.465293000	-0.010481000
C	4.187799000	-0.298839000	1.760171000
C	5.284328000	-1.019194000	1.247358000
H	5.171603000	-1.549036000	0.309953000
C	6.512377000	-1.022611000	1.917614000

H	7.348780000	-1.577238000	1.503204000
C	6.669914000	-0.301764000	3.108376000
H	7.623860000	-0.304656000	3.626451000
C	5.590725000	0.429876000	3.621671000
H	5.704632000	0.994996000	4.541783000
C	4.363044000	0.432740000	2.952130000
H	3.523761000	0.997458000	3.345168000
C	0.131507000	4.645009000	-1.278946000
C	-0.424812000	4.936017000	-2.540497000
H	-0.910280000	4.138236000	-3.092859000
C	-0.343989000	6.225611000	-3.075863000
H	-0.770497000	6.430580000	-4.052973000
C	0.289171000	7.248358000	-2.357276000
H	0.352621000	8.249190000	-2.772961000
C	0.835647000	6.973522000	-1.096881000
H	1.315633000	7.764033000	-0.527904000
C	0.754528000	5.683760000	-0.560770000
H	1.160804000	5.476037000	0.423322000
C	-5.149120000	0.293155000	0.528075000
C	-6.040595000	1.005102000	-0.298106000
H	-5.652788000	1.527227000	-1.165694000
C	-7.412394000	1.017044000	-0.023818000
H	-8.086038000	1.565432000	-0.675181000
C	-7.918862000	0.311609000	1.075695000
H	-8.983688000	0.320860000	1.286678000
C	-7.044160000	-0.413785000	1.895242000
H	-7.428984000	-0.968117000	2.745880000
C	-5.672691000	-0.425576000	1.621028000
H	-4.991179000	-0.988311000	2.250986000
C	2.584889000	1.105519000	-3.144595000
C	3.818630000	1.353229000	-2.669621000
C	1.948487000	-0.235974000	-3.085243000
C	4.693101000	0.287673000	-2.051111000
C	4.078401000	-1.090860000	-2.125190000
C	2.840194000	-1.318064000	-2.599801000
H	0.967848000	-0.141533000	-2.366408000
H	5.686678000	0.284788000	-2.534895000
H	1.421062000	-0.501896000	-4.012678000
H	4.894837000	0.545821000	-0.995740000
H	1.992013000	1.913224000	-3.566850000
H	4.227258000	2.360414000	-2.706841000
H	4.685954000	-1.924518000	-1.778064000
H	2.445763000	-2.331071000	-2.613091000

⁶INT1-3_{hs}

Co	-0.257739000	0.038131000	-0.038972000
O	0.035230000	0.042468000	1.789026000
C	-0.540084000	0.121734000	-2.391382000
C	-1.241425000	-0.368436000	-4.533975000
H	-1.776285000	-0.918416000	-5.289337000
C	-0.435728000	0.722287000	-4.616281000
H	-0.119749000	1.313354000	-5.458831000
C	0.874709000	2.122834000	-3.010975000
H	0.926376000	2.768618000	-3.892192000
H	0.478642000	2.685449000	-2.170486000
H	1.874326000	1.759976000	-2.765002000
C	-2.089036000	-1.853068000	-2.708340000
H	-2.389652000	-2.447426000	-3.575904000
H	-1.487306000	-2.462758000	-2.040481000
H	-2.977676000	-1.505379000	-2.178410000
N	-1.292797000	-0.720444000	-3.181899000
N	-0.021938000	1.006870000	-3.311416000
N	1.680837000	0.703580000	-0.350554000
N	0.359551000	-1.916648000	-0.328544000
N	-2.174999000	-0.612384000	0.147161000
N	-0.888244000	2.016872000	-0.048605000
C	2.124445000	1.995735000	-0.177098000
C	2.740443000	-0.061152000	-0.794216000
C	1.651042000	-2.312925000	-0.612878000
C	-0.342894000	-3.027004000	0.099771000
C	-2.565008000	-1.915513000	0.372698000
C	-3.312009000	0.171454000	0.074580000
C	-2.197745000	2.417257000	0.065918000
C	-0.081215000	3.106577000	0.230827000
C	3.519504000	2.064447000	-0.571614000
H	4.119768000	2.960616000	-0.568199000
C	3.889973000	0.807993000	-0.979345000
H	4.850336000	0.497008000	-1.358539000
C	1.765213000	-3.741585000	-0.362238000
H	2.669815000	-4.317591000	-0.477154000
C	0.551224000	-4.173625000	0.097177000
H	0.286660000	-5.167564000	0.421103000
C	-4.016086000	-1.968747000	0.392066000
H	-4.599580000	-2.866914000	0.519627000
C	-4.474594000	-0.695681000	0.178960000
H	-5.500684000	-0.372327000	0.108070000
C	-2.228326000	3.831795000	0.411829000
H	-3.125714000	4.405053000	0.583291000
C	-0.931856000	4.246656000	0.539649000

H	-0.580248000	5.222536000	0.834096000
C	1.327731000	3.108434000	0.184899000
C	2.738017000	-1.467669000	-0.924401000
C	-1.713611000	-3.040722000	0.433975000
C	-3.337052000	1.580481000	0.012874000
C	2.049475000	4.379067000	0.475241000
C	3.061106000	4.403316000	1.456275000
H	3.282503000	3.490272000	1.999036000
C	3.759959000	5.582060000	1.734405000
H	4.530818000	5.583804000	2.498957000
C	3.462048000	6.758979000	1.034573000
H	4.003678000	7.674590000	1.250591000
C	2.462093000	6.746867000	0.053191000
H	2.232027000	7.652393000	-0.499988000
C	1.763889000	5.567166000	-0.225425000
H	0.997433000	5.553454000	-0.993123000
C	4.022122000	-2.137695000	-1.280686000
C	5.181868000	-1.943104000	-0.504201000
H	5.132394000	-1.287428000	0.358624000
C	6.374756000	-2.598664000	-0.826600000
H	7.257207000	-2.443343000	-0.213500000
C	6.428077000	-3.462969000	-1.928209000
H	7.353678000	-3.972436000	-2.177533000
C	5.279040000	-3.670697000	-2.702788000
H	5.312728000	-4.339584000	-3.557383000
C	4.086011000	-3.015361000	-2.379910000
H	3.192711000	-3.174327000	-2.975112000
C	-2.336401000	-4.340000000	0.814869000
C	-3.037177000	-4.456975000	2.031729000
H	-3.095108000	-3.593482000	2.685928000
C	-3.638402000	-5.665900000	2.396721000
H	-4.168061000	-5.740011000	3.341550000
C	-3.552083000	-6.779669000	1.550812000
H	-4.018310000	-7.718162000	1.834274000
C	-2.861644000	-6.674839000	0.336082000
H	-2.797582000	-7.530739000	-0.329020000
C	-2.260674000	-5.465522000	-0.028896000
H	-1.734005000	-5.379846000	-0.973620000
C	-4.662515000	2.265598000	-0.001310000
C	-5.619892000	2.041591000	1.007236000
H	-5.383211000	1.354270000	1.812141000
C	-6.849724000	2.708039000	0.985221000
H	-7.573233000	2.528317000	1.774567000
C	-7.142615000	3.614314000	-0.042530000
H	-8.096771000	4.131869000	-0.058340000

C	-6.194294000	3.853670000	-1.045761000
H	-6.412529000	4.555836000	-1.844702000
C	-4.964694000	3.187348000	-1.023156000
H	-4.226119000	3.371475000	-1.796667000
C	2.147237000	-1.027245000	4.951604000
C	2.279000000	-1.870172000	3.876901000
C	2.520427000	0.343825000	4.869590000
C	2.785212000	-1.392803000	2.540273000
C	3.222550000	0.051814000	2.548410000
C	3.065216000	0.850369000	3.655083000
H	0.845358000	0.407690000	2.204320000
H	3.601551000	-2.043342000	2.172750000
H	2.399649000	0.996189000	5.727771000
H	1.983679000	-1.520613000	1.790767000
H	1.747570000	-1.408595000	5.887758000
H	1.976923000	-2.911155000	3.952353000
H	3.641257000	0.457346000	1.633991000
H	3.371355000	1.893312000	3.611649000

⁴INT1-3_{hs}

Co	-0.269923000	0.025122000	-0.052144000
O	0.054689000	0.030477000	1.770055000
C	-0.594514000	0.102561000	-2.398172000
C	-1.302643000	-0.414871000	-4.531904000
H	-1.802060000	-1.000556000	-5.284723000
C	-0.606027000	0.748805000	-4.612544000
H	-0.369639000	1.381584000	-5.450885000
C	0.608093000	2.238865000	-3.010342000
H	0.600208000	2.889882000	-3.889148000
H	0.165562000	2.760688000	-2.166303000
H	1.636210000	1.964846000	-2.767748000
C	-1.954062000	-2.006158000	-2.715252000
H	-2.190784000	-2.626810000	-3.584232000
H	-1.288554000	-2.549328000	-2.050757000
H	-2.873887000	-1.758189000	-2.181729000
N	-1.284115000	-0.793716000	-3.186207000
N	-0.186114000	1.048352000	-3.313004000
N	1.590884000	0.874201000	-0.378251000
N	0.526218000	-1.861913000	-0.368377000
N	-2.115054000	-0.808546000	0.148593000
N	-1.088384000	1.933284000	-0.035850000
C	1.910981000	2.200732000	-0.192868000
C	2.714446000	0.218237000	-0.838565000
C	1.848701000	-2.129352000	-0.661061000

C	-0.060607000	-3.036069000	0.064292000
C	-2.376010000	-2.144627000	0.367237000
C	-3.322463000	-0.137042000	0.094256000
C	-2.428669000	2.205022000	0.098168000
C	-0.385822000	3.091098000	0.251845000
C	3.289663000	2.406224000	-0.597332000
H	3.802266000	3.355316000	-0.588022000
C	3.774143000	1.195128000	-1.022910000
H	4.756448000	0.981434000	-1.412999000
C	2.104134000	-3.540245000	-0.414077000
H	3.060220000	-4.024198000	-0.535817000
C	0.941726000	-4.089468000	0.053297000
H	0.778877000	-5.104370000	0.379064000
C	-3.815163000	-2.336938000	0.400902000
H	-4.308944000	-3.287542000	0.527806000
C	-4.395627000	-1.112084000	0.202939000
H	-5.448514000	-0.887355000	0.145089000
C	-2.590113000	3.605412000	0.464537000
H	-3.536069000	4.087862000	0.653830000
C	-1.337688000	4.140302000	0.586129000
H	-1.077198000	5.140950000	0.891954000
C	1.015981000	3.227313000	0.193198000
C	2.846366000	-1.181395000	-0.976716000
C	-1.419867000	-3.183182000	0.414111000
C	-3.483059000	1.263566000	0.047816000
C	1.617024000	4.554925000	0.502185000
C	2.629007000	4.656422000	1.477969000
H	2.939638000	3.758303000	2.002063000
C	3.215251000	5.890592000	1.775171000
H	3.988067000	5.950967000	2.535346000
C	2.802137000	7.046978000	1.100055000
H	3.256315000	8.005550000	1.330772000
C	1.800361000	6.958759000	0.124426000
H	1.481270000	7.848770000	-0.409420000
C	1.214619000	5.723736000	-0.173057000
H	0.446734000	5.652352000	-0.936150000
C	4.188062000	-1.721855000	-1.341322000
C	5.326669000	-1.416502000	-0.569084000
H	5.217277000	-0.771258000	0.296148000
C	6.576969000	-1.949960000	-0.899051000
H	7.442610000	-1.710051000	-0.289245000
C	6.710288000	-2.801055000	-2.004122000
H	7.680520000	-3.215567000	-2.259610000
C	5.583600000	-3.118872000	-2.774224000
H	5.679040000	-3.778309000	-3.631496000

C	4.333062000	-2.585954000	-2.443558000
H	3.457283000	-2.830612000	-3.035728000
C	-1.908268000	-4.536068000	0.803565000
C	-2.583433000	-4.716139000	2.027302000
H	-2.722173000	-3.858970000	2.677582000
C	-3.055785000	-5.977462000	2.404061000
H	-3.566943000	-6.099196000	3.354128000
C	-2.863575000	-7.081976000	1.563478000
H	-3.229303000	-8.061256000	1.856342000
C	-2.197615000	-6.915225000	0.342059000
H	-2.052500000	-7.764460000	-0.318823000
C	-1.726036000	-5.653412000	-0.035112000
H	-1.218753000	-5.521050000	-0.985025000
C	-4.868228000	1.818242000	0.058478000
C	-5.784183000	1.494846000	1.078709000
H	-5.470479000	0.827235000	1.873827000
C	-7.072745000	2.039450000	1.080301000
H	-7.763624000	1.784823000	1.878225000
C	-7.467267000	2.920640000	0.064849000
H	-8.467192000	3.343371000	0.067259000
C	-6.561914000	3.258199000	-0.949808000
H	-6.859303000	3.941681000	-1.739336000
C	-5.273422000	2.713778000	-0.950843000
H	-4.568148000	2.973275000	-1.733759000
H	0.851022000	0.438667000	2.173758000
C	2.527909000	-1.007859000	4.954304000
C	2.627889000	-1.788052000	3.830105000
C	2.739858000	0.399075000	4.902532000
C	2.930061000	-1.206059000	2.474367000
C	3.199211000	0.278342000	2.507655000
C	3.083490000	1.011092000	3.664781000
H	3.771860000	-1.741510000	1.995755000
H	2.648360000	0.999052000	5.801650000
H	2.075897000	-1.400930000	1.799628000
H	2.280947000	-1.467842000	5.907700000
H	2.453863000	-2.859232000	3.885070000
H	3.473100000	0.762375000	1.577571000
H	3.267488000	2.083134000	3.640577000

⁴INT1-3_{is}

Co	0.443182000	-0.001878000	0.078988000
C	0.813608000	0.000829000	2.180425000
C	1.402957000	-0.634490000	4.309960000
H	1.764703000	-1.308070000	5.067413000

C	0.982255000	0.654459000	4.378282000
H	0.897702000	1.334436000	5.208254000
C	0.111173000	2.366746000	2.792203000
H	0.299788000	2.996122000	3.666373000
H	0.628963000	2.777191000	1.931476000
H	-0.960960000	2.330237000	2.593722000
C	1.670899000	-2.366556000	2.539669000
H	1.780087000	-2.988533000	3.432535000
H	0.888365000	-2.774031000	1.907600000
H	2.613930000	-2.346970000	1.991336000
N	1.294465000	-1.018871000	2.972151000
N	0.628489000	1.027443000	3.080116000
N	-1.124644000	1.170318000	0.284992000
N	-0.771981000	-1.701714000	0.370314000
N	1.985051000	-1.173971000	-0.216462000
N	1.662271000	1.708099000	-0.067720000
C	-1.173798000	2.530697000	0.011041000
C	-2.360119000	0.799021000	0.808575000
C	-2.098603000	-1.675179000	0.710034000
C	-0.489812000	-2.951727000	-0.134879000
C	1.931512000	-2.522510000	-0.515160000
C	3.318671000	-0.799260000	-0.163158000
C	3.026329000	1.676367000	-0.189516000
C	1.232771000	2.960191000	-0.450847000
C	-2.465877000	3.036553000	0.421737000
H	-2.768617000	4.068989000	0.352249000
C	-3.174122000	1.988604000	0.942315000
H	-4.168425000	2.009989000	1.357165000
C	-2.684405000	-2.982889000	0.449853000
H	-3.720884000	-3.235735000	0.607975000
C	-1.700369000	-3.759853000	-0.098701000
H	-1.784893000	-4.770773000	-0.464915000
C	3.287840000	-3.031878000	-0.588377000
H	3.545725000	-4.062715000	-0.771157000
C	4.134174000	-1.989133000	-0.332710000
H	5.210397000	-2.013772000	-0.281725000
C	3.495948000	2.983822000	-0.629599000
H	4.527048000	3.237298000	-0.821048000
C	2.388300000	3.763844000	-0.821966000
H	2.350590000	4.773784000	-1.198605000
C	-0.115618000	3.357865000	-0.432202000
C	-2.823032000	-0.512286000	1.034904000
C	0.786277000	-3.348065000	-0.570289000
C	3.822844000	0.516616000	-0.106680000
C	-0.461266000	4.750223000	-0.829114000

C	-1.453531000	4.981570000	-1.803387000
H	-1.945434000	4.129857000	-2.262102000
C	-1.794560000	6.283302000	-2.183050000
H	-2.555931000	6.441537000	-2.940672000
C	-1.150361000	7.380000000	-1.594831000
H	-1.413709000	8.390813000	-1.890256000
C	-0.165300000	7.164190000	-0.622220000
H	0.331836000	8.008823000	-0.154899000
C	0.174436000	5.861775000	-0.241484000
H	0.927656000	5.694036000	0.520900000
C	-4.236844000	-0.714870000	1.461127000
C	-5.306133000	-0.196794000	0.704308000
H	-5.092531000	0.374839000	-0.190369000
C	-6.629530000	-0.445245000	1.083116000
H	-7.441281000	-0.043550000	0.483912000
C	-6.907404000	-1.216878000	2.219765000
H	-7.935252000	-1.409537000	2.511746000
C	-5.850776000	-1.744197000	2.973780000
H	-6.057149000	-2.345174000	3.854302000
C	-4.526464000	-1.498313000	2.594426000
H	-3.704639000	-1.911417000	3.170647000
C	0.971566000	-4.743776000	-1.054655000
C	1.553811000	-4.982846000	-2.315596000
H	1.847346000	-4.134054000	-2.924064000
C	1.738790000	-6.288814000	-2.780483000
H	2.181798000	-6.454487000	-3.757723000
C	1.347016000	-7.379826000	-1.992973000
H	1.489955000	-8.393453000	-2.354440000
C	0.770939000	-7.155114000	-0.735743000
H	0.473285000	-7.995252000	-0.115556000
C	0.586760000	-5.848969000	-0.270274000
H	0.152192000	-5.673753000	0.708244000
C	5.299645000	0.729773000	-0.109345000
C	6.125092000	0.214152000	-1.127596000
H	5.674482000	-0.361743000	-1.928461000
C	7.502687000	0.457473000	-1.121747000
H	8.122775000	0.057610000	-1.918251000
C	8.079245000	1.226385000	-0.102035000
H	9.148222000	1.415608000	-0.099105000
C	7.266792000	1.756609000	0.908666000
H	7.704643000	2.357267000	1.700172000
C	5.889274000	1.513234000	0.902111000
H	5.255304000	1.925355000	1.680624000
O	0.183396000	-0.058176000	-1.741715000
H	-0.520615000	0.572817000	-2.002709000

C	-3.086648000	-0.521200000	-2.208688000
C	-4.131054000	-1.399123000	-2.352361000
C	-3.285665000	0.882157000	-2.327216000
C	-5.538137000	-0.939146000	-2.645375000
C	-5.664413000	0.560833000	-2.763019000
C	-4.584140000	1.393572000	-2.605611000
H	-6.220726000	-1.311138000	-1.854322000
H	-2.458943000	1.565052000	-2.166729000
H	-5.913512000	-1.424151000	-3.569119000
H	-2.091584000	-0.890831000	-1.980811000
H	-3.963108000	-2.465406000	-2.233930000
H	-6.649425000	0.968698000	-2.976091000
H	-4.719586000	2.469631000	-2.684742000

²INT1-3_k

Co	-0.455137000	0.005547000	0.055378000
C	-0.833650000	-0.007222000	2.064492000
C	-1.413590000	0.635538000	4.193317000
H	-1.747235000	1.319122000	4.954791000
C	-1.069230000	-0.676396000	4.250403000
H	-1.034382000	-1.369493000	5.073157000
C	-0.266265000	-2.414847000	2.650230000
H	-0.543699000	-3.056734000	3.491117000
H	-0.752617000	-2.770127000	1.747592000
H	0.816527000	-2.437763000	2.514094000
C	-1.569333000	2.398861000	2.434819000
H	-1.601121000	3.030418000	3.327211000
H	-0.790119000	2.753823000	1.768303000
H	-2.533237000	2.439634000	1.923634000
N	-1.264403000	1.030334000	2.861462000
N	-0.720867000	-1.054845000	2.951260000
N	1.092750000	-1.178121000	0.263735000
N	0.718997000	1.567076000	0.256666000
N	-1.974097000	1.182098000	-0.271518000
N	-1.609396000	-1.562958000	-0.193366000
C	1.164253000	-2.504068000	-0.115220000
C	2.287594000	-0.866223000	0.892455000
C	1.999576000	1.566096000	0.764605000
C	0.501780000	2.814689000	-0.306058000
C	-1.903840000	2.496873000	-0.670215000
C	-3.309575000	0.867869000	-0.113151000
C	-2.985127000	-1.561649000	-0.162313000
C	-1.211098000	-2.807288000	-0.654888000
C	2.422972000	-3.058347000	0.332815000

H	2.726349000	-4.082998000	0.187441000
C	3.092166000	-2.064899000	0.994301000
H	4.056292000	-2.123399000	1.472282000
C	2.604796000	2.863794000	0.538888000
H	3.613453000	3.122162000	0.818336000
C	1.701040000	3.615049000	-0.158551000
H	1.826954000	4.614067000	-0.543119000
C	-3.242204000	3.052104000	-0.712997000
H	-3.472611000	4.074151000	-0.968989000
C	-4.103478000	2.064940000	-0.318995000
H	-5.173681000	2.127115000	-0.207566000
C	-3.476611000	-2.855166000	-0.598859000
H	-4.520004000	-3.114328000	-0.685588000
C	-2.387679000	-3.601957000	-0.949828000
H	-2.373904000	-4.595102000	-1.368475000
C	0.114518000	-3.259648000	-0.666289000
C	2.711379000	0.434211000	1.194672000
C	-0.731260000	3.259416000	-0.796920000
C	-3.805793000	-0.436381000	0.025588000
C	0.442865000	-4.621057000	-1.167912000
C	1.437572000	-4.771791000	-2.155131000
H	1.924885000	-3.884675000	-2.546778000
C	1.784222000	-6.038905000	-2.634115000
H	2.546501000	-6.134831000	-3.401166000
C	1.145379000	-7.180251000	-2.131539000
H	1.413087000	-8.164258000	-2.503589000
C	0.161354000	-7.044490000	-1.143601000
H	-0.329568000	-7.925041000	-0.740425000
C	-0.184915000	-5.776709000	-0.663965000
H	-0.933601000	-5.674060000	0.114146000
C	4.063960000	0.656949000	1.772310000
C	5.215480000	0.154377000	1.135193000
H	5.107173000	-0.410339000	0.216470000
C	6.485964000	0.412853000	1.660324000
H	7.364005000	0.023744000	1.153439000
C	6.627497000	1.179987000	2.824754000
H	7.614447000	1.380589000	3.230242000
C	5.488424000	1.693706000	3.458768000
H	5.590029000	2.292085000	4.359123000
C	4.216945000	1.437162000	2.933822000
H	3.331483000	1.837526000	3.417487000
C	-0.856339000	4.623956000	-1.376286000
C	-1.402389000	4.778137000	-2.666141000
H	-1.696735000	3.891014000	-3.216932000
C	-1.548610000	6.049143000	-3.231168000

H	-1.962851000	6.149792000	-4.229604000
C	-1.156771000	7.188118000	-2.515080000
H	-1.269799000	8.174650000	-2.953865000
C	-0.621407000	7.047456000	-1.227998000
H	-0.327043000	7.926226000	-0.662157000
C	-0.475035000	5.776397000	-0.662213000
H	-0.076877000	5.668241000	0.341078000
C	-5.265529000	-0.674172000	0.194222000
C	-6.216344000	-0.168857000	-0.713973000
H	-5.876237000	0.407714000	-1.566937000
C	-7.579410000	-0.430184000	-0.538302000
H	-8.298130000	-0.038813000	-1.251779000
C	-8.015814000	-1.207271000	0.542779000
H	-9.073767000	-1.410150000	0.677139000
C	-7.078157000	-1.729303000	1.443528000
H	-7.407465000	-2.337522000	2.280529000
C	-5.715394000	-1.467692000	1.268077000
H	-4.984288000	-1.871110000	1.961418000
O	-0.163706000	0.075594000	-1.821538000
H	0.668696000	-0.414846000	-1.978278000
C	3.190639000	0.558973000	-2.135409000
C	4.276438000	1.396072000	-2.073182000
C	3.354780000	-0.846030000	-2.283437000
C	5.694678000	0.889356000	-2.171549000
C	5.783647000	-0.612390000	-2.300609000
C	4.662514000	-1.403111000	-2.352764000
H	6.271530000	1.226111000	-1.287061000
H	2.486952000	-1.496111000	-2.314027000
H	6.212699000	1.372604000	-3.025390000
H	2.184790000	0.960763000	-2.051406000
H	4.130154000	2.463045000	-1.936211000
H	6.774837000	-1.055714000	-2.357947000
H	4.770110000	-2.481481000	-2.442570000

⁶TS2-3_{hs}

Co	0.234367000	0.032157000	-0.048897000
O	0.391604000	0.217736000	-2.001290000
C	0.493460000	-0.036003000	2.234061000
C	0.907808000	-0.706891000	4.397879000
H	1.163104000	-1.405061000	5.176538000
C	0.606796000	0.617791000	4.439440000
H	0.541032000	1.308369000	5.262660000
C	-0.027123000	2.377830000	2.772932000
H	0.106333000	3.005943000	3.658153000

H	0.608326000	2.740076000	1.968926000
H	-1.070310000	2.413609000	2.454424000
C	1.091089000	-2.459480000	2.617368000
H	1.065134000	-3.110942000	3.495583000
H	0.318171000	-2.764057000	1.916525000
H	2.067258000	-2.533591000	2.134362000
N	0.830546000	-1.087632000	3.054974000
N	0.358466000	1.009123000	3.120551000
N	-1.224544000	1.423422000	0.039919000
N	-1.153095000	-1.449408000	0.055755000
N	1.755563000	-1.402677000	-0.232600000
N	1.697705000	1.539660000	-0.013918000
C	-1.048093000	2.784390000	-0.149503000
C	-2.527466000	1.218721000	0.472702000
C	-2.484868000	-1.282196000	0.356153000
C	-0.954423000	-2.792838000	-0.280076000
C	1.557619000	-2.747671000	-0.431267000
C	3.105912000	-1.191921000	-0.026730000
C	3.058090000	1.327949000	-0.069640000
C	1.451132000	2.837945000	-0.411628000
C	-2.274880000	3.461652000	0.199225000
H	-2.421287000	4.530197000	0.173536000
C	-3.172681000	2.504408000	0.612989000
H	-4.171996000	2.668879000	0.981497000
C	-3.167241000	-2.556672000	0.196157000
H	-4.226113000	-2.708046000	0.334678000
C	-2.242405000	-3.467927000	-0.228072000
H	-2.414084000	-4.499308000	-0.491583000
C	2.826051000	-3.429987000	-0.315421000
H	2.969686000	-4.496268000	-0.395857000
C	3.778845000	-2.473429000	-0.036897000
H	4.831157000	-2.632026000	0.136534000
C	3.707781000	2.566736000	-0.486063000
H	4.769646000	2.686331000	-0.634160000
C	2.720845000	3.481837000	-0.723619000
H	2.833329000	4.486279000	-1.099802000
C	0.173114000	3.433371000	-0.468458000
C	-3.119596000	-0.053993000	0.659445000
C	0.286059000	-3.390699000	-0.540648000
C	3.722838000	0.087409000	0.061726000
C	0.083318000	4.877331000	-0.817987000
C	-0.792808000	5.301337000	-1.837973000
H	-1.379891000	4.555614000	-2.363760000
C	-0.898001000	6.653904000	-2.174881000
H	-1.571142000	6.960389000	-2.969698000

C	-0.133224000	7.611086000	-1.494127000
H	-0.215127000	8.661670000	-1.754964000
C	0.736098000	7.204178000	-0.473534000
H	1.324498000	7.940454000	0.065608000
C	0.842668000	5.850445000	-0.138070000
H	1.507741000	5.535507000	0.658962000
C	-4.497805000	-0.133225000	1.223764000
C	-5.586820000	0.581925000	0.686465000
H	-5.430247000	1.199896000	-0.187938000
C	-6.861629000	0.481810000	1.252334000
H	-7.687438000	1.035356000	0.815698000
C	-7.078298000	-0.337212000	2.368456000
H	-8.068683000	-0.414680000	2.806103000
C	-6.007107000	-1.057137000	2.912177000
H	-6.162000000	-1.693490000	3.778248000
C	-4.732361000	-0.955421000	2.345975000
H	-3.900603000	-1.509101000	2.768544000
C	0.318756000	-4.847580000	-0.858241000
C	0.954728000	-5.296205000	-2.032793000
H	1.401215000	-4.564523000	-2.697759000
C	1.008344000	-6.659158000	-2.340966000
H	1.494595000	-6.986047000	-3.254977000
C	0.434460000	-7.600296000	-1.475585000
H	0.477180000	-8.658493000	-1.713969000
C	-0.190459000	-7.167947000	-0.298769000
H	-0.626984000	-7.891539000	0.382996000
C	-0.245881000	-5.804089000	0.007906000
H	-0.719608000	-5.468875000	0.924362000
C	5.206957000	0.145447000	0.176758000
C	6.050346000	-0.531786000	-0.727025000
H	5.605148000	-1.113141000	-1.526760000
C	7.441071000	-0.442482000	-0.610801000
H	8.074782000	-0.963589000	-1.321951000
C	8.016314000	0.325968000	0.410261000
H	9.096059000	0.393782000	0.500071000
C	7.189461000	1.011083000	1.310274000
H	7.626667000	1.610031000	2.103369000
C	5.798795000	0.924681000	1.191713000
H	5.154052000	1.455554000	1.884338000
H	1.166621000	-0.256838000	-2.365012000
C	-2.412198000	-1.199208000	-3.479723000
C	-3.598855000	-1.423102000	-2.822589000
C	-1.823525000	0.154604000	-3.577623000
C	-4.340397000	-0.343312000	-2.276534000
C	-3.879282000	0.989222000	-2.444609000

C	-2.692332000	1.246354000	-3.087982000
H	-0.851736000	0.168232000	-2.886978000
H	-5.273856000	-0.533945000	-1.760053000
H	-1.372961000	0.366634000	-4.562578000
H	-3.974865000	-2.434632000	-2.709072000
H	-1.851105000	-2.032419000	-3.894584000
H	-4.464513000	1.814257000	-2.049248000
H	-2.334359000	2.266734000	-3.193202000

⁴TS2-3_{hs}

Co	0.328435000	0.016762000	0.057868000
O	0.161994000	0.116971000	-1.806176000
C	0.528737000	-0.001007000	2.206907000
C	0.903820000	-0.689210000	4.368837000
H	1.158154000	-1.390518000	5.144759000
C	0.567432000	0.625773000	4.418656000
H	0.464079000	1.304715000	5.247457000
C	-0.045089000	2.403539000	2.776265000
H	0.136112000	3.023787000	3.658611000
H	0.559736000	2.762393000	1.949228000
H	-1.101248000	2.451557000	2.506613000
C	1.204912000	-2.414770000	2.588623000
H	1.213418000	-3.059549000	3.471848000
H	0.449565000	-2.763116000	1.891085000
H	2.184854000	-2.440097000	2.108810000
N	0.876059000	-1.055453000	3.021132000
N	0.344245000	1.029703000	3.100251000
N	-1.196041000	1.288417000	0.176650000
N	-0.997705000	-1.585244000	0.212561000
N	1.833662000	-1.254348000	-0.196319000
N	1.672825000	1.632648000	0.006379000
C	-1.132211000	2.638362000	-0.102122000
C	-2.467265000	1.004528000	0.647099000
C	-2.332217000	-1.477712000	0.505454000
C	-0.765490000	-2.859918000	-0.258522000
C	1.710484000	-2.611624000	-0.451061000
C	3.183253000	-0.970575000	-0.014991000
C	3.036961000	1.521086000	-0.048799000
C	1.332156000	2.902682000	-0.410125000
C	-2.404610000	3.242441000	0.251661000
H	-2.628834000	4.294205000	0.170040000
C	-3.203131000	2.252681000	0.755145000
H	-4.200480000	2.355709000	1.149234000
C	-2.981285000	-2.750868000	0.229290000

H	-4.036507000	-2.941751000	0.346269000
C	-2.024200000	-3.590883000	-0.272528000
H	-2.156604000	-4.597706000	-0.635825000
C	3.027978000	-3.211112000	-0.381424000
H	3.229680000	-4.262983000	-0.507790000
C	3.920931000	-2.217837000	-0.078715000
H	4.982760000	-2.317542000	0.077901000
C	3.602028000	2.794072000	-0.476054000
H	4.653909000	2.986736000	-0.620372000
C	2.550623000	3.633456000	-0.729330000
H	2.591396000	4.639098000	-1.116955000
C	0.010918000	3.384524000	-0.474347000
C	-3.000535000	-0.284649000	0.858778000
C	0.512117000	-3.353618000	-0.584844000
C	3.760018000	0.313908000	0.079092000
C	-0.213920000	4.794677000	-0.895191000
C	-1.131047000	5.081771000	-1.926461000
H	-1.649177000	4.257730000	-2.405898000
C	-1.362502000	6.399580000	-2.332153000
H	-2.067014000	6.600867000	-3.133380000
C	-0.682851000	7.456934000	-1.712385000
H	-0.861610000	8.480288000	-2.027477000
C	0.227164000	7.185767000	-0.682138000
H	0.750014000	8.000285000	-0.189962000
C	0.457970000	5.867255000	-0.276095000
H	1.152610000	5.657416000	0.530278000
C	-4.379573000	-0.435941000	1.404110000
C	-5.498707000	0.215853000	0.848826000
H	-5.360420000	0.841453000	-0.022385000
C	-6.775967000	0.030684000	1.387931000
H	-7.625991000	0.536746000	0.940044000
C	-6.963828000	-0.814194000	2.489740000
H	-7.956233000	-0.957686000	2.905842000
C	-5.862347000	-1.477021000	3.046030000
H	-5.996490000	-2.135487000	3.898946000
C	-4.585321000	-1.290734000	2.507147000
H	-3.729867000	-1.801869000	2.936350000
C	0.639893000	-4.776640000	-1.006485000
C	1.315196000	-5.104973000	-2.199247000
H	1.726090000	-4.303912000	-2.804752000
C	1.449946000	-6.437007000	-2.603229000
H	1.967317000	-6.669327000	-3.529060000
C	0.913598000	-7.468214000	-1.820696000
H	1.016951000	-8.502322000	-2.134313000
C	0.245026000	-7.156333000	-0.629554000

H	-0.164862000	-7.949843000	-0.012011000
C	0.1111604000	-5.823883000	-0.225514000
H	-0.395621000	-5.582629000	0.702503000
C	5.241765000	0.438665000	0.183324000
C	6.110993000	-0.171282000	-0.742868000
H	5.689757000	-0.754235000	-1.554557000
C	7.496629000	-0.013433000	-0.634833000
H	8.150114000	-0.485816000	-1.361970000
C	8.040136000	0.762858000	0.397306000
H	9.115596000	0.885475000	0.479994000
C	7.186476000	1.386234000	1.316923000
H	7.598664000	1.992681000	2.117720000
C	5.801118000	1.228075000	1.208247000
H	5.135915000	1.711118000	1.916584000
H	0.915877000	-0.341405000	-2.235874000
C	-2.645901000	-1.128822000	-3.406985000
C	-3.868671000	-1.410202000	-2.845830000
C	-2.107069000	0.259774000	-3.472456000
C	-4.706907000	-0.371010000	-2.362956000
C	-4.281883000	0.981068000	-2.460983000
C	-3.063454000	1.304032000	-3.010109000
H	-1.174586000	0.289261000	-2.798013000
H	-5.668020000	-0.609429000	-1.920833000
H	-1.688104000	0.496924000	-4.468356000
H	-4.203125000	-2.440500000	-2.766008000
H	-2.010692000	-1.934499000	-3.765521000
H	-4.934526000	1.771610000	-2.098253000
H	-2.750962000	2.342916000	-3.076344000

⁴TS2-3_{is}

Co	0.339034000	0.017791000	0.092411000
O	0.110349000	0.120458000	-1.767093000
C	0.578446000	-0.028150000	2.230359000
C	1.169398000	-0.675144000	4.355908000
H	1.621274000	-1.310852000	5.097746000
C	0.486615000	0.493776000	4.467108000
H	0.217469000	1.083691000	5.326227000
C	-0.620479000	2.101621000	2.910263000
H	-0.594350000	2.713761000	3.816217000
H	-0.155932000	2.643294000	2.091992000
H	-1.656058000	1.870169000	2.655828000
C	1.900235000	-2.175152000	2.497451000
H	2.094978000	-2.832546000	3.349401000
H	1.260779000	-2.684281000	1.783081000

H	2.844011000	-1.908945000	2.018192000
N	1.217271000	-0.979055000	2.993375000
N	0.135995000	0.874882000	3.169861000
N	-1.482566000	0.799041000	0.279619000
N	-0.476938000	-1.903240000	0.185231000
N	2.139413000	-0.764134000	-0.229307000
N	1.168633000	1.946619000	0.087236000
C	-1.807323000	2.121058000	0.063001000
C	-2.612410000	0.147961000	0.747623000
C	-1.789760000	-2.184527000	0.460088000
C	0.091596000	-3.025759000	-0.380095000
C	2.398791000	-2.087813000	-0.549896000
C	3.356069000	-0.118966000	-0.042802000
C	2.507738000	2.228157000	0.016983000
C	0.473474000	3.080619000	-0.278271000
C	-3.188006000	2.328503000	0.462612000
H	-3.702745000	3.275251000	0.425363000
C	-3.665492000	1.134208000	0.925936000
H	-4.643003000	0.936419000	1.333175000
C	-2.070794000	-3.558383000	0.070442000
H	-3.032864000	-4.039346000	0.156047000
C	-0.921760000	-4.065446000	-0.477227000
H	-0.776721000	-5.039188000	-0.917955000
C	3.832744000	-2.293887000	-0.513364000
H	4.320910000	-3.239222000	-0.690297000
C	4.414385000	-1.103233000	-0.165885000
H	5.464058000	-0.905131000	-0.021063000
C	2.680407000	3.622125000	-0.368887000
H	3.631676000	4.110192000	-0.515010000
C	1.429618000	4.136005000	-0.583674000
H	1.177134000	5.123308000	-0.936577000
C	-0.931761000	3.170792000	-0.304583000
C	-2.760740000	-1.247498000	0.883273000
C	1.453258000	-3.126007000	-0.726699000
C	3.545810000	1.273108000	0.097490000
C	-1.561719000	4.462812000	-0.690450000
C	-2.559471000	4.478950000	-1.687406000
H	-2.840538000	3.541253000	-2.155455000
C	-3.168552000	5.678823000	-2.067141000
H	-3.929643000	5.674548000	-2.841722000
C	-2.795856000	6.884065000	-1.456511000
H	-3.268679000	7.815586000	-1.752064000
C	-1.811845000	6.879302000	-0.459066000
H	-1.526257000	7.807038000	0.027635000
C	-1.201942000	5.679410000	-0.077895000

H	-0.450992000	5.673422000	0.704972000
C	-4.042987000	-1.813369000	1.389292000
C	-5.297974000	-1.456197000	0.856136000
H	-5.337452000	-0.746472000	0.040400000
C	-6.474419000	-2.030792000	1.348478000
H	-7.430463000	-1.747360000	0.918461000
C	-6.422626000	-2.978371000	2.378983000
H	-7.336810000	-3.424096000	2.758711000
C	-5.181404000	-3.351538000	2.910907000
H	-5.129466000	-4.086522000	3.708488000
C	-4.005395000	-2.776785000	2.419300000
H	-3.042698000	-3.063760000	2.829284000
C	1.963031000	-4.429321000	-1.236237000
C	2.696964000	-4.483580000	-2.438484000
H	2.871427000	-3.563476000	-2.986232000
C	3.186097000	-5.699808000	-2.925289000
H	3.742732000	-5.722147000	-3.857194000
C	2.952783000	-6.886755000	-2.218081000
H	3.331252000	-7.831339000	-2.596157000
C	2.229644000	-6.846509000	-1.018698000
H	2.052825000	-7.760155000	-0.459246000
C	1.741492000	-5.629578000	-0.531715000
H	1.191053000	-5.596327000	0.402390000
C	4.932352000	1.810542000	0.199863000
C	5.925480000	1.506925000	-0.752501000
H	5.675327000	0.858271000	-1.584815000
C	7.210501000	2.048743000	-0.643593000
H	7.960669000	1.808566000	-1.390911000
C	7.525956000	2.909771000	0.415925000
H	8.523336000	3.330238000	0.499264000
C	6.543929000	3.230854000	1.362176000
H	6.778464000	3.900139000	2.184372000
C	5.259265000	2.688945000	1.252624000
H	4.494844000	2.936680000	1.981948000
H	0.957676000	-0.071480000	-2.223215000
H	-1.220354000	0.103205000	-2.744527000
C	-2.848296000	-1.266478000	-2.842784000
C	-4.124163000	-1.167519000	-2.339931000
C	-2.137700000	-0.091968000	-3.419457000
C	-4.839908000	0.057815000	-2.396317000
C	-4.237762000	1.202276000	-2.984107000
C	-2.965630000	1.142478000	-3.504207000
H	-5.853761000	0.113712000	-2.011849000
H	-1.656491000	-0.332359000	-4.386140000
H	-2.301934000	-2.202409000	-2.767948000

H	-4.592612000	-2.033802000	-1.881701000
H	-4.800358000	2.131624000	-3.031134000
H	-2.520513000	2.021376000	-3.964265000

²TS2-3_{ts}

Co	-0.332257000	0.009894000	-0.016630000
O	-0.149325000	-0.093886000	-1.924633000
C	-0.559638000	0.044972000	1.971485000
C	-0.742054000	0.751557000	4.143866000
H	-0.773067000	1.473659000	4.941123000
C	-0.861652000	-0.600763000	4.149533000
H	-1.008948000	-1.300234000	4.953907000
C	-0.815833000	-2.442108000	2.467699000
H	-1.264778000	-2.974996000	3.310612000
H	-1.435795000	-2.571344000	1.586403000
H	0.183556000	-2.836064000	2.273665000
C	-0.427160000	2.545597000	2.439031000
H	-0.224572000	3.113742000	3.351098000
H	0.400182000	2.667485000	1.747473000
H	-1.347605000	2.908388000	1.978125000
N	-0.558046000	1.132992000	2.813019000
N	-0.751844000	-1.019544000	2.821891000
N	0.759157000	-1.596010000	0.091566000
N	1.293402000	1.082813000	0.134590000
N	-1.403327000	1.627473000	-0.247649000
N	-1.944616000	-1.065331000	-0.212144000
C	0.397381000	-2.839042000	-0.394392000
C	1.970258000	-1.740100000	0.743371000
C	2.474967000	0.679904000	0.703993000
C	1.500434000	2.360140000	-0.401473000
C	-0.918568000	2.866892000	-0.633286000
C	-2.745576000	1.788501000	0.076269000
C	-3.236002000	-0.637143000	-0.044939000
C	-1.993551000	-2.338294000	-0.795159000
C	1.379752000	-3.797708000	-0.000662000
H	1.331917000	-4.854127000	-0.214285000
C	2.336240000	-3.124720000	0.745165000
H	3.206401000	-3.547236000	1.218930000
C	3.461309000	1.724767000	0.549884000
H	4.484055000	1.650224000	0.881629000
C	2.879806000	2.728452000	-0.181794000
H	3.344886000	3.632207000	-0.538591000
C	-1.957427000	3.832631000	-0.510959000
H	-1.849085000	4.886215000	-0.716132000

C	-3.083094000	3.172216000	-0.029400000
H	-4.041454000	3.607522000	0.199554000
C	-4.141921000	-1.662915000	-0.513762000
H	-5.216907000	-1.573380000	-0.514967000
C	-3.376720000	-2.681860000	-1.023266000
H	-3.721601000	-3.583799000	-1.502214000
C	-0.876714000	-3.162022000	-0.944823000
C	2.750728000	-0.629068000	1.175883000
C	0.463109000	3.182798000	-0.846516000
C	-3.626705000	0.686838000	0.288080000
C	-1.007341000	-4.498175000	-1.575949000
C	-0.119795000	-4.856441000	-2.611772000
H	0.624676000	-4.135828000	-2.932817000
C	-0.206553000	-6.109827000	-3.223515000
H	0.475707000	-6.364502000	-4.028591000
C	-1.170488000	-7.035429000	-2.799931000
H	-1.235292000	-8.010628000	-3.272382000
C	-2.044598000	-6.698284000	-1.758594000
H	-2.782364000	-7.416306000	-1.413665000
C	-1.964432000	-5.440863000	-1.151120000
H	-2.627415000	-5.188211000	-0.331283000
C	3.974970000	-0.805628000	1.986101000
C	4.993010000	-1.726224000	1.660532000
H	4.896340000	-2.328034000	0.767401000
C	6.141481000	-1.833785000	2.451346000
H	6.917162000	-2.541902000	2.175585000
C	6.302046000	-1.024336000	3.583207000
H	7.193856000	-1.111420000	4.195986000
C	5.305875000	-0.094687000	3.912557000
H	5.421662000	0.541109000	4.785155000
C	4.160320000	0.015998000	3.120911000
H	3.388077000	0.736050000	3.371203000
C	0.753063000	4.515156000	-1.431395000
C	0.169029000	4.862295000	-2.667914000
H	-0.473129000	4.141281000	-3.162294000
C	0.413045000	6.109132000	-3.249785000
H	-0.035264000	6.353171000	-4.207946000
C	1.232356000	7.042209000	-2.599222000
H	1.419698000	8.012149000	-3.049216000
C	1.799200000	6.719090000	-1.359807000
H	2.418149000	7.443642000	-0.839369000
C	1.560937000	5.468595000	-0.779784000
H	1.979924000	5.231554000	0.191355000
C	-5.039792000	0.896401000	0.671334000
C	-5.883181000	1.817252000	0.013436000

H	-5.494295000	2.387092000	-0.821811000
C	-7.218686000	1.966204000	0.399631000
H	-7.853485000	2.672684000	-0.126651000
C	-7.743739000	1.198280000	1.447564000
H	-8.780235000	1.318183000	1.747142000
C	-6.923753000	0.266023000	2.098245000
H	-7.322890000	-0.339084000	2.906714000
C	-5.590250000	0.113153000	1.710427000
H	-4.952917000	-0.609798000	2.209226000
H	-0.777999000	0.538800000	-2.328594000
C	3.093329000	0.876511000	-3.141865000
C	4.275543000	0.934533000	-2.438298000
C	2.263359000	-0.348848000	-3.162901000
C	4.760978000	-0.197356000	-1.738727000
C	4.052550000	-1.427493000	-1.807846000
C	2.878215000	-1.525170000	-2.513623000
H	1.245994000	-0.146752000	-2.578685000
H	5.685013000	-0.135290000	-1.173321000
H	1.854250000	-0.576510000	-4.163300000
H	4.837289000	1.862845000	-2.398369000
H	2.728918000	1.753396000	-3.670316000
H	4.444391000	-2.302591000	-1.300198000
H	2.331038000	-2.463001000	-2.532533000

⁴INT2-3_{hs}

Co	0.259524000	0.034564000	0.302877000
O	0.041484000	0.053878000	-1.966315000
C	0.509826000	0.070226000	2.502157000
C	1.116991000	-0.501634000	4.649485000
H	1.582823000	-1.103210000	5.411441000
C	0.410046000	0.658599000	4.726347000
H	0.131449000	1.267695000	5.569382000
C	-0.734949000	2.173235000	3.068170000
H	-0.756087000	2.844303000	3.931621000
H	-0.267557000	2.673634000	2.222833000
H	-1.754063000	1.890556000	2.794378000
C	1.857191000	-2.028414000	2.784037000
H	2.094597000	-2.683909000	3.626780000
H	1.205950000	-2.550687000	2.085227000
H	2.777395000	-1.745082000	2.267504000
N	1.165420000	-0.843820000	3.294014000
N	0.052448000	0.990115000	3.415270000
N	-1.647537000	0.874050000	0.299365000
N	-0.600910000	-1.850597000	0.218663000

N	2.102997000	-0.798573000	-0.191428000
N	1.076764000	1.936636000	0.043417000
C	-1.947401000	2.208719000	0.156870000
C	-2.797616000	0.215532000	0.679731000
C	-1.937170000	-2.127902000	0.429784000
C	0.017922000	-3.023743000	-0.177042000
C	2.368155000	-2.146347000	-0.338428000
C	3.314644000	-0.134827000	-0.094110000
C	2.413363000	2.207223000	-0.128819000
C	0.372139000	3.090042000	-0.242848000
C	-3.342859000	2.416870000	0.515137000
H	-3.845022000	3.371683000	0.528061000
C	-3.858180000	1.195967000	0.865486000
H	-4.858266000	0.978461000	1.205756000
C	-2.177407000	-3.533851000	0.139423000
H	-3.137868000	-4.022297000	0.194076000
C	-0.984502000	-4.077774000	-0.251953000
H	-0.799788000	-5.090318000	-0.574292000
C	3.807096000	-2.348397000	-0.281587000
H	4.301643000	-3.305661000	-0.336034000
C	4.385747000	-1.118313000	-0.109266000
H	5.436029000	-0.898056000	-0.002026000
C	2.570153000	3.602690000	-0.523163000
H	3.510964000	4.079662000	-0.749289000
C	1.316511000	4.137271000	-0.616642000
H	1.048620000	5.132819000	-0.933144000
C	-1.030866000	3.235158000	-0.174680000
C	-2.943659000	-1.188169000	0.748294000
C	1.402935000	-3.180059000	-0.417762000
C	3.472035000	1.267768000	-0.069470000
C	-1.608159000	4.583315000	-0.441193000
C	-2.616552000	4.741826000	-1.413167000
H	-2.948946000	3.868676000	-1.965138000
C	-3.175102000	5.997998000	-1.668727000
H	-3.945997000	6.101382000	-2.426389000
C	-2.736697000	7.121599000	-0.955261000
H	-3.169210000	8.097399000	-1.153394000
C	-1.736940000	6.977835000	0.015848000
H	-1.396997000	7.842123000	0.578431000
C	-1.179348000	5.720593000	0.271158000
H	-0.410286000	5.606316000	1.027763000
C	-4.296352000	-1.737998000	1.053789000
C	-5.421128000	-1.385312000	0.281376000
H	-5.295647000	-0.696890000	-0.547265000
C	-6.680400000	-1.926783000	0.561212000

H	-7.533871000	-1.648119000	-0.049415000
C	-6.838460000	-2.833602000	1.617228000
H	-7.815564000	-3.253776000	1.834502000
C	-5.726695000	-3.198411000	2.388445000
H	-5.840619000	-3.900488000	3.208878000
C	-4.467826000	-2.657654000	2.107294000
H	-3.604137000	-2.938086000	2.701136000
C	1.909118000	-4.550234000	-0.719532000
C	2.692667000	-4.786557000	-1.866944000
H	2.910376000	-3.956609000	-2.531019000
C	3.181154000	-6.065704000	-2.152082000
H	3.777869000	-6.227769000	-3.044624000
C	2.896316000	-7.136124000	-1.293946000
H	3.274090000	-8.129479000	-1.515324000
C	2.122841000	-6.915129000	-0.146829000
H	1.905192000	-7.736624000	0.529090000
C	1.636644000	-5.635019000	0.138220000
H	1.045422000	-5.461685000	1.031121000
C	4.856152000	1.822519000	-0.075873000
C	5.800907000	1.440058000	-1.049099000
H	5.508866000	0.726907000	-1.812229000
C	7.090617000	1.981494000	-1.046708000
H	7.802629000	1.679716000	-1.808951000
C	7.459668000	2.919870000	-0.073873000
H	8.460542000	3.340456000	-0.072864000
C	6.527179000	3.316319000	0.893952000
H	6.804551000	4.043553000	1.651049000
C	5.237917000	2.774349000	0.891122000
H	4.512366000	3.078882000	1.638182000
H	0.773699000	-0.541380000	-2.213417000
H	-0.821550000	-0.339738000	-2.198024000
C	-1.871488000	-0.947930000	-4.687673000
C	-2.426339000	-1.722443000	-3.657678000
C	-2.022130000	0.445803000	-4.674879000
C	-3.134290000	-1.101211000	-2.617439000
C	-3.278900000	0.294523000	-2.602249000
C	-2.723037000	1.065528000	-3.631697000
H	-3.546490000	-1.698015000	-1.813528000
H	-1.580754000	1.046503000	-5.463839000
H	-2.302779000	-2.800914000	-3.655489000
H	-1.320510000	-1.427272000	-5.491234000
H	-3.790103000	0.779157000	-1.777821000
H	-2.815163000	2.146938000	-3.608434000

²INT2-3_h

Co	0.263141000	-0.006447000	0.161486000
O	-0.019443000	0.020643000	-1.850004000
C	0.538552000	-0.033510000	2.082262000
C	0.910466000	-0.740154000	4.222298000
H	1.094818000	-1.461331000	4.999125000
C	0.787594000	0.611193000	4.259332000
H	0.833193000	1.309776000	5.076316000
C	0.352089000	2.451553000	2.636486000
H	0.694702000	3.032448000	3.497162000
H	0.931130000	2.724176000	1.760785000
H	-0.705252000	2.651254000	2.454938000
C	0.860591000	-2.534104000	2.493968000
H	0.776890000	-3.137612000	3.401922000
H	0.053177000	-2.787542000	1.815159000
H	1.820435000	-2.726220000	2.011776000
N	0.754698000	-1.123977000	2.889527000
N	0.562501000	1.032404000	2.948120000
N	-1.090464000	1.396408000	0.254339000
N	-1.161522000	-1.338104000	0.298488000
N	1.572349000	-1.415581000	-0.168873000
N	1.664709000	1.323941000	-0.060884000
C	-0.929356000	2.706675000	-0.177214000
C	-2.318908000	1.318736000	0.902449000
C	-2.414644000	-1.132894000	0.855382000
C	-1.152080000	-2.620010000	-0.262859000
C	1.290295000	-2.718474000	-0.570471000
C	2.933426000	-1.351297000	0.106449000
C	3.023092000	1.100727000	0.076651000
C	1.496203000	2.610047000	-0.580786000
C	-2.065946000	3.468081000	0.221524000
H	-2.192697000	4.524025000	0.040565000
C	-2.910556000	2.617762000	0.926097000
H	-3.850049000	2.868311000	1.391062000
C	-3.215616000	-2.328182000	0.648737000
H	-4.240604000	-2.433988000	0.968484000
C	-2.470768000	-3.203337000	-0.087593000
H	-2.773096000	-4.165991000	-0.467742000
C	2.490074000	-3.487406000	-0.519590000
H	2.556528000	-4.538131000	-0.755041000
C	3.498853000	-2.654186000	-0.056953000
H	4.529271000	-2.914234000	0.121662000
C	3.736667000	2.298275000	-0.340059000
H	4.811501000	2.389749000	-0.349141000
C	2.812330000	3.188316000	-0.800382000

H	2.992806000	4.152625000	-1.247268000
C	0.274304000	3.258649000	-0.705951000
C	-2.929603000	0.090837000	1.284147000
C	-0.016984000	-3.260752000	-0.748873000
C	3.634753000	-0.131322000	0.317345000
C	0.190887000	4.631109000	-1.269206000
C	-0.741196000	4.902533000	-2.292527000
H	-1.366803000	4.091946000	-2.650245000
C	-0.857864000	6.183580000	-2.838284000
H	-1.575770000	6.368758000	-3.631793000
C	-0.048298000	7.226581000	-2.366701000
H	-0.137491000	8.222278000	-2.789991000
C	0.869691000	6.976423000	-1.339119000
H	1.488162000	7.782034000	-0.954689000
C	0.983506000	5.693656000	-0.791303000
H	1.676242000	5.509576000	0.022483000
C	-4.257269000	0.085178000	1.949975000
C	-5.365627000	0.780008000	1.422440000
H	-5.243917000	1.349556000	0.507837000
C	-6.614676000	0.718861000	2.048563000
H	-7.456785000	1.255221000	1.621354000
C	-6.786340000	-0.043404000	3.211995000
H	-7.756505000	-0.089918000	3.696935000
C	-5.697880000	-0.749844000	3.740291000
H	-5.821165000	-1.346359000	4.639397000
C	-4.448274000	-0.685562000	3.115443000
H	-3.601685000	-1.229473000	3.522179000
C	-0.104844000	-4.627885000	-1.327551000
C	0.477995000	-4.890449000	-2.584775000
H	0.976825000	-4.081135000	-3.108233000
C	0.423458000	-6.167622000	-3.150297000
H	0.872609000	-6.345978000	-4.122693000
C	-0.209916000	-7.214763000	-2.466747000
H	-0.252830000	-8.206926000	-2.905186000
C	-0.777123000	-6.973803000	-1.209132000
H	-1.252631000	-7.782961000	-0.662866000
C	-0.719214000	-5.695539000	-0.642690000
H	-1.134692000	-5.518862000	0.343331000
C	5.092552000	-0.136468000	0.601826000
C	6.017669000	-0.838749000	-0.198116000
H	5.656630000	-1.396558000	-1.054598000
C	7.386796000	-0.795643000	0.083546000
H	8.082752000	-1.337463000	-0.550103000
C	7.864050000	-0.043811000	1.165812000
H	8.927318000	-0.011502000	1.382832000

C	6.958816000	0.671820000	1.960164000
H	7.318192000	1.261574000	2.798353000
C	5.589321000	0.625494000	1.680108000
H	4.884551000	1.177174000	2.294246000
H	0.196620000	-0.847126000	-2.238163000
H	-0.935443000	0.289096000	-2.062956000
C	-2.367476000	-0.895207000	-4.157573000
C	-3.031595000	-1.141849000	-2.946704000
C	-2.071395000	0.422066000	-4.539402000
C	-3.396863000	-0.071918000	-2.117212000
C	-3.088694000	1.245997000	-2.489512000
C	-2.430530000	1.491294000	-3.705000000
H	-3.883846000	-0.266296000	-1.170506000
H	-1.553814000	0.613906000	-5.474070000
H	-3.243953000	-2.157808000	-2.632707000
H	-2.080808000	-1.723877000	-4.798114000
H	-3.325438000	2.065403000	-1.819150000
H	-2.181209000	2.507830000	-3.992014000

⁴P-3_{hs}

C	-0.041288000	-0.083729000	2.072522000
C	0.631064000	-0.151148000	4.279189000
H	1.339273000	-0.147051000	5.090313000
C	-0.727421000	-0.223373000	4.271578000
H	-1.440730000	-0.302346000	5.074356000
C	-2.512479000	-0.245858000	2.503497000
H	-3.151536000	-0.036597000	3.366402000
H	-2.683309000	0.499143000	1.730418000
H	-2.746810000	-1.235310000	2.104117000
C	2.428621000	0.049455000	2.536092000
H	3.061195000	-0.189448000	3.396007000
H	2.626765000	-0.650237000	1.728191000
H	2.645553000	1.062232000	2.189665000
N	1.028204000	-0.068473000	2.941500000
N	-1.115514000	-0.177800000	2.929719000
N	-1.578708000	-1.330139000	-0.384572000
N	1.360865000	-1.539116000	-0.384918000
N	1.588742000	1.341664000	-0.272918000
N	-1.382815000	1.559688000	-0.308137000
C	-2.921905000	-1.025319000	-0.503020000
C	-1.468179000	-2.690736000	-0.169290000
C	1.035772000	-2.880223000	-0.337758000
C	2.721987000	-1.441636000	-0.640141000
C	2.925531000	1.049987000	-0.420245000

C	1.466985000	2.699454000	-0.066981000
C	-1.042205000	2.892876000	-0.260450000
C	-2.726683000	1.472400000	-0.614308000
C	-3.696144000	-2.237696000	-0.289206000
H	-4.773493000	-2.293178000	-0.284065000
C	-2.806236000	-3.254113000	-0.062329000
H	-3.032193000	-4.286149000	0.154521000
C	2.233849000	-3.662586000	-0.603917000
H	2.270036000	-4.739477000	-0.658100000
C	3.261527000	-2.781914000	-0.809529000
H	4.284692000	-3.014680000	-1.058826000
C	3.698498000	2.268400000	-0.217105000
H	4.775207000	2.332830000	-0.235783000
C	2.804555000	3.276685000	0.021810000
H	3.024932000	4.311290000	0.231664000
C	-2.226637000	3.688942000	-0.560029000
H	-2.249637000	4.765870000	-0.618488000
C	-3.254579000	2.817925000	-0.795478000
H	-4.266631000	3.057396000	-1.081152000
C	-3.464219000	0.267978000	-0.688154000
C	-0.257940000	-3.420451000	-0.143522000
C	3.463736000	-0.237443000	-0.656494000
C	0.253575000	3.424849000	-0.050955000
C	-4.935954000	0.360272000	-0.908389000
C	-5.551018000	-0.364709000	-1.948620000
H	-4.932173000	-0.979050000	-2.594113000
C	-6.932805000	-0.293907000	-2.152894000
H	-7.386976000	-0.855146000	-2.963886000
C	-7.728221000	0.503396000	-1.319322000
H	-8.800713000	0.559357000	-1.477864000
C	-7.130599000	1.226786000	-0.278820000
H	-7.740439000	1.840548000	0.377271000
C	-5.748788000	1.154278000	-0.074634000
H	-5.285975000	1.707673000	0.735558000
C	-0.340100000	-4.900136000	0.039517000
C	-1.100747000	-5.707975000	-0.828287000
H	-1.636485000	-5.238919000	-1.646641000
C	-1.159438000	-7.094234000	-0.648845000
H	-1.746587000	-7.701263000	-1.331376000
C	-0.454945000	-7.699612000	0.400102000
H	-0.499884000	-8.775418000	0.538790000
C	0.310540000	-6.908277000	1.266740000
H	0.858270000	-7.368995000	2.083320000
C	0.367978000	-5.522386000	1.086776000
H	0.957941000	-4.905303000	1.756390000

C	4.936793000	-0.324235000	-0.878522000
C	5.546585000	0.409715000	-1.915183000
H	4.924708000	1.028167000	-2.554046000
C	6.928444000	0.345622000	-2.122365000
H	7.379008000	0.914535000	-2.929997000
C	7.728364000	-0.453710000	-1.295160000
H	8.800792000	-0.504345000	-1.455844000
C	7.135643000	-1.185263000	-0.257628000
H	7.749197000	-1.800126000	0.393957000
C	5.753755000	-1.119246000	-0.050523000
H	5.294645000	-1.678681000	0.757726000
C	0.334948000	4.906439000	0.124193000
C	1.085180000	5.710732000	-0.755487000
H	1.613115000	5.237745000	-1.576503000
C	1.140446000	7.098239000	-0.584592000
H	1.718889000	7.703341000	-1.276187000
C	0.443304000	7.707346000	0.467199000
H	0.485890000	8.784123000	0.599181000
C	-0.312739000	6.918987000	1.344668000
H	-0.855838000	7.382885000	2.162554000
C	-0.367840000	5.531880000	1.172681000
H	-0.952467000	4.917276000	1.849312000
Co	-0.019301000	0.015890000	-0.220201000
O	0.306063000	0.332389000	-2.368165000
H	1.158202000	-0.129601000	-2.499264000
H	-0.390631000	-0.098388000	-2.901828000

²P-3_s

Co	0.020517000	0.000473000	-0.146479000
O	-0.516567000	-0.041420000	-3.122144000
C	0.019623000	0.005456000	2.019240000
C	-0.653420000	-0.016363000	4.223932000
H	-1.361418000	-0.044891000	5.034833000
C	0.706505000	0.032037000	4.219522000
H	1.419630000	0.062105000	5.025847000
C	2.491380000	0.114111000	2.440367000
H	3.135352000	-0.148682000	3.284667000
H	2.646375000	-0.590331000	1.626371000
H	2.735964000	1.120437000	2.090479000
C	-2.448687000	-0.105636000	2.455304000
H	-3.088939000	0.153987000	3.303374000
H	-2.611188000	0.598887000	1.642715000
H	-2.691838000	-1.112492000	2.105885000
N	-1.051482000	-0.029158000	2.882360000

N	1.096280000	0.041986000	2.875656000
N	1.567362000	1.225604000	-0.345551000
N	-1.209080000	1.549840000	-0.336626000
N	-1.539065000	-1.227540000	-0.350074000
N	1.239958000	-1.549572000	-0.322695000
C	2.879200000	0.888420000	-0.625876000
C	1.570614000	2.571912000	-0.007007000
C	-0.865823000	2.876191000	-0.124692000
C	-2.549130000	1.549567000	-0.720556000
C	-2.859659000	-0.888294000	-0.605677000
C	-1.541157000	-2.573221000	0.003877000
C	0.895654000	-2.874000000	-0.118538000
C	2.569436000	-1.549049000	-0.730690000
C	3.733409000	2.039212000	-0.416206000
H	4.804327000	2.038986000	-0.542713000
C	2.933653000	3.064132000	0.005154000
H	3.228708000	4.064017000	0.278823000
C	-2.006720000	3.725075000	-0.397316000
H	-1.995878000	4.801741000	-0.335972000
C	-3.028308000	2.913783000	-0.801297000
H	-4.014165000	3.202438000	-1.127697000
C	-3.709334000	-2.035562000	-0.374925000
H	-4.782306000	-2.034651000	-0.483081000
C	-2.903714000	-3.059621000	0.040629000
H	-3.197337000	-4.056245000	0.327568000
C	2.030969000	-3.726072000	-0.412813000
H	2.017011000	-4.803149000	-0.360284000
C	3.046995000	-2.914475000	-0.826528000
H	4.026566000	-3.202350000	-1.171963000
C	3.354581000	-0.402973000	-0.901212000
C	0.422075000	3.357522000	0.155002000
C	-3.337203000	0.402881000	-0.876781000
C	-0.391611000	-3.357075000	0.164602000
C	4.784645000	-0.542796000	-1.295576000
C	5.267048000	0.136460000	-2.431267000
H	4.576335000	0.735948000	-3.014880000
C	6.610164000	0.033010000	-2.807641000
H	6.963648000	0.556355000	-3.690668000
C	7.495293000	-0.747655000	-2.052314000
H	8.537649000	-0.828266000	-2.344592000
C	7.028364000	-1.421947000	-0.916467000
H	7.710241000	-2.020891000	-0.320461000
C	5.684920000	-1.318567000	-0.540173000
H	5.324220000	-1.830761000	0.345604000
C	0.553794000	4.798931000	0.510722000

C	1.313618000	5.690244000	-0.271034000
H	1.816524000	5.317060000	-1.156564000
C	1.405525000	7.042698000	0.075131000
H	1.990570000	7.717512000	-0.542194000
C	0.735040000	7.528463000	1.205382000
H	0.806212000	8.578146000	1.472844000
C	-0.033235000	6.653309000	1.984481000
H	-0.557922000	7.022358000	2.860472000
C	-0.125138000	5.301298000	1.638007000
H	-0.719798000	4.619288000	2.237047000
C	-4.772291000	0.542370000	-1.252668000
C	-5.267188000	-0.133368000	-2.384955000
H	-4.582616000	-0.728531000	-2.980210000
C	-6.615189000	-0.031305000	-2.744050000
H	-6.978556000	-0.551888000	-3.624670000
C	-7.492331000	0.744574000	-1.974664000
H	-8.538429000	0.824105000	-2.253532000
C	-7.012614000	1.415666000	-0.842198000
H	-7.688206000	2.010970000	-0.235490000
C	-5.664369000	1.313547000	-0.483125000
H	-5.293588000	1.823282000	0.399947000
C	-0.521596000	-4.798061000	0.521061000
C	-1.293347000	-5.687583000	-0.251227000
H	-1.806602000	-5.313161000	-1.130281000
C	-1.382938000	-7.040157000	0.094827000
H	-1.976909000	-7.713474000	-0.515571000
C	-0.698327000	-7.528079000	1.215647000
H	-0.767589000	-8.577920000	1.482980000
C	0.081905000	-6.654940000	1.985113000
H	0.617811000	-7.025778000	2.853516000
C	0.171624000	-5.302846000	1.638647000
H	0.775841000	-4.622468000	2.229888000
H	-0.732262000	-0.773981000	-2.511559000
H	-0.572907000	0.785401000	-2.604907000

OAT in SMe₂ by species 1

⁴RC-1_{hs}

Mn	0.211387000	0.028540000	-0.080055000
O	0.021961000	0.002836000	-1.759674000
C	0.483893000	0.062921000	2.163056000
C	0.261718000	0.570402000	4.400071000
H	-0.154291000	1.075617000	5.254876000

C	1.233406000	-0.373830000	4.298199000
H	1.841685000	-0.853808000	5.045594000
C	2.336317000	-1.641633000	2.446473000
H	2.669955000	-2.248733000	3.292830000
H	1.871781000	-2.281727000	1.702564000
H	3.194137000	-1.132485000	2.001693000
C	-1.251782000	1.784978000	2.822383000
H	-1.383159000	2.414877000	3.706737000
H	-0.972478000	2.403723000	1.974684000
H	-2.187559000	1.267416000	2.601251000
N	-0.180487000	0.825624000	3.099180000
N	1.355080000	-0.671934000	2.938199000
N	2.187971000	-0.179586000	-0.249583000
N	0.392033000	2.021102000	-0.058371000
N	-1.752323000	0.237114000	0.210567000
N	0.039159000	-1.962287000	0.041879000
C	2.848274000	-1.328313000	-0.631762000
C	3.138601000	0.792294000	0.005310000
C	1.581003000	2.715638000	0.017796000
C	-0.600739000	2.919771000	-0.422394000
C	-2.488255000	1.378293000	-0.026885000
C	-2.613132000	-0.722009000	0.715699000
C	-1.097840000	-2.652551000	0.407460000
C	0.926328000	-2.874860000	-0.511239000
C	4.275619000	-1.089383000	-0.563082000
H	5.030644000	-1.828303000	-0.779982000
C	4.454934000	0.197265000	-0.131420000
H	5.386761000	0.706490000	0.053518000
C	1.331186000	4.106892000	-0.305125000
H	2.091498000	4.870787000	-0.343349000
C	0.004502000	4.221970000	-0.617341000
H	-0.518485000	5.102741000	-0.952057000
C	-3.852688000	1.151619000	0.404178000
H	-4.640425000	1.885558000	0.352693000
C	-3.920029000	-0.120826000	0.898334000
H	-4.778249000	-0.621267000	1.316018000
C	-0.921853000	-4.053097000	0.077802000
H	-1.667128000	-4.815997000	0.236500000
C	0.301951000	-4.182093000	-0.518890000
H	0.745376000	-5.075142000	-0.928579000
C	2.255103000	-2.584838000	-0.856275000
C	2.863084000	2.158205000	0.183653000
C	-1.974274000	2.623941000	-0.434206000
C	-2.308355000	-2.085186000	0.847392000
C	3.129645000	-3.668951000	-1.382734000

C	3.813450000	-3.482615000	-2.600345000
H	3.668766000	-2.555303000	-3.144607000
C	4.654203000	-4.479380000	-3.106016000
H	5.166912000	-4.323247000	-4.050061000
C	4.829684000	-5.677543000	-2.401112000
H	5.481735000	-6.451441000	-2.793864000
C	4.161155000	-5.870672000	-1.185062000
H	4.300528000	-6.792035000	-0.627827000
C	3.319927000	-4.874056000	-0.679140000
H	2.812546000	-5.017272000	0.268983000
C	3.987695000	3.109632000	0.410818000
C	5.069691000	3.208526000	-0.485213000
H	5.084843000	2.575145000	-1.365419000
C	6.100302000	4.127249000	-0.259450000
H	6.923434000	4.195968000	-0.963993000
C	6.064627000	4.966122000	0.862201000
H	6.864571000	5.679085000	1.035792000
C	4.987139000	4.885157000	1.754081000
H	4.950207000	5.534180000	2.623658000
C	3.956293000	3.967262000	1.527810000
H	3.117875000	3.902662000	2.213895000
C	-2.959811000	3.680663000	-0.791048000
C	-3.950108000	3.400192000	-1.755096000
H	-3.967886000	2.416688000	-2.212455000
C	-4.895633000	4.368628000	-2.106448000
H	-5.646768000	4.137666000	-2.855357000
C	-4.874417000	5.630039000	-1.496476000
H	-5.608314000	6.381718000	-1.770137000
C	-3.906176000	5.913086000	-0.524188000
H	-3.894664000	6.881655000	-0.033518000
C	-2.959125000	4.945862000	-0.171557000
H	-2.224217000	5.159635000	0.597113000
C	-3.368095000	-3.027121000	1.306150000
C	-4.609155000	-3.112136000	0.645115000
H	-4.796994000	-2.469760000	-0.208439000
C	-5.580527000	-4.025061000	1.069455000
H	-6.529185000	-4.083047000	0.544934000
C	-5.326152000	-4.870638000	2.157258000
H	-6.080427000	-5.579088000	2.485192000
C	-4.090795000	-4.802449000	2.814996000
H	-3.885700000	-5.456496000	3.656987000
C	-3.118892000	-3.890558000	2.390240000
H	-2.159341000	-3.835504000	2.894278000
C	-2.572398000	-1.730461000	-2.647055000
H	-3.163366000	-2.294151000	-1.922554000

H	-2.325349000	-2.357691000	-3.506679000
H	-1.668239000	-1.326652000	-2.184474000
S	-3.639578000	-0.250310000	-3.225788000
C	-2.221065000	0.843023000	-3.905038000
H	-1.898451000	0.462536000	-4.876817000
H	-2.619457000	1.855391000	-4.008091000
H	-1.400885000	0.811926000	-3.181266000

³RC-1_s

Mn	0.218398000	0.021285000	-0.045899000
O	0.041798000	0.018894000	-1.757399000
C	0.475600000	0.049672000	2.164301000
C	0.241925000	0.545784000	4.401301000
H	-0.184950000	1.040506000	5.256701000
C	1.231678000	-0.378566000	4.297501000
H	1.848754000	-0.849298000	5.043401000
C	2.360415000	-1.625423000	2.455801000
H	2.706085000	-2.215341000	3.309401000
H	1.907881000	-2.283201000	1.720701000
H	3.207341000	-1.103766000	2.005801000
C	-1.292515000	1.740162000	2.838501000
H	-1.448484000	2.339370000	3.739901000
H	-1.014982000	2.390048000	2.014501000
H	-2.212942000	1.208808000	2.590501000
N	-0.204763000	0.796407000	3.102301000
N	1.360663000	-0.670673000	2.938101000
N	2.206089000	-0.155016000	-0.234299000
N	0.376600000	2.030077000	-0.022699000
N	-1.762793000	0.196785000	0.212101000
N	0.064696000	-1.984607000	0.046401000
C	2.887931000	-1.303950000	-0.581799000
C	3.144140000	0.839437000	-0.018499000
C	1.557236000	2.742817000	0.003201000
C	-0.637555000	2.918328000	-0.351299000
C	-2.508135000	1.342723000	0.020501000
C	-2.624643000	-0.788071000	0.665901000
C	-1.078440000	-2.696349000	0.349101000
C	0.985051000	-2.882554000	-0.474599000
C	4.311144000	-1.040822000	-0.525099000
H	5.079107000	-1.772461000	-0.719999000
C	4.469710000	0.263670000	-0.139899000
H	5.393737000	0.793123000	0.027301000
C	1.280706000	4.131131000	-0.311999000
H	2.029046000	4.904493000	-0.382799000

C	-0.058789000	4.229799000	-0.569399000
H	-0.604644000	5.102827000	-0.887599000
C	-3.873948000	1.089492000	0.429201000
H	-4.667811000	1.818233000	0.404101000
C	-3.936813000	-0.205604000	0.863501000
H	-4.794640000	-0.727361000	1.255101000
C	-0.872610000	-4.091360000	0.011901000
H	-1.614250000	-4.865822000	0.126101000
C	0.380484000	-4.198823000	-0.525299000
H	0.852140000	-5.081247000	-0.926699000
C	2.317367000	-2.573621000	-0.793899000
C	2.852009000	2.205552000	0.139401000
C	-2.008271000	2.605498000	-0.352899000
C	-2.309312000	-2.152887000	0.764401000
C	3.216612000	-3.652867000	-1.289299000
C	3.923221000	-3.477503000	-2.495599000
H	3.779567000	-2.560295000	-3.056799000
C	4.786270000	-4.471246000	-2.968699000
H	5.316678000	-4.322973000	-3.904299000
C	4.961210000	-5.656755000	-2.242499000
H	5.630471000	-6.428489000	-2.609999000
C	4.269401000	-5.839820000	-1.037999000
H	4.407355000	-6.751327000	-0.464399000
C	3.406552000	-4.845776000	-0.564599000
H	2.879645000	-4.981450000	0.373901000
C	3.969458000	3.174995000	0.322301000
C	5.031863000	3.265741000	-0.598099000
H	5.036129000	2.611441000	-1.463099000
C	6.056310000	4.200689000	-0.415599000
H	6.863713000	4.261948000	-1.138799000
C	6.034454000	5.065190000	0.686801000
H	6.829290000	5.791150000	0.826701000
C	4.976950000	4.992544000	1.603001000
H	4.950784000	5.660945000	2.458301000
C	3.952703000	4.057796000	1.420101000
H	3.130100000	3.999938000	2.125701000
C	-3.005717000	3.663448000	-0.672699000
C	-4.002130000	3.406799000	-1.636999000
H	-4.016979000	2.437800000	-2.124099000
C	-4.957081000	4.378747000	-1.951199000
H	-5.712992000	4.165386000	-2.700599000
C	-4.938618000	5.621646000	-1.304299000
H	-5.679580000	6.376284000	-1.549299000
C	-3.963205000	5.881997000	-0.332699000
H	-3.952557000	6.836096000	0.185601000

C	-3.007554000	4.910549000	-0.016999000
H	-2.264944000	5.106911000	0.749001000
C	-3.370561000	-3.115333000	1.174601000
C	-4.602464000	-3.184871000	0.494301000
H	-4.782530000	-2.515462000	-0.339899000
C	-5.576311000	-4.113821000	0.875701000
H	-6.517414000	-4.158074000	0.336201000
C	-5.334656000	-4.992434000	1.939901000
H	-6.090792000	-5.713295000	2.234701000
C	-4.109053000	-4.940096000	2.617101000
H	-3.913488000	-5.618906000	3.441701000
C	-3.135006000	-4.011745000	2.235301000
H	-2.183504000	-3.968793000	2.755401000
C	-2.617287000	-1.661071000	-2.689799000
H	-3.264020000	-2.317038000	-2.103899000
H	-2.229214000	-2.189491000	-3.563299000
H	-1.798868000	-1.285713000	-2.074899000
S	-3.681512000	-0.180817000	-3.259199000
C	-2.264056000	0.936111000	-3.894099000
H	-2.681405000	1.938332000	-4.017699000
H	-1.465756000	0.934470000	-3.147399000
H	-1.898675000	0.556992000	-4.851099000

⁴TS-1_{hs}

Mn	0.067045000	0.089693000	-0.109908000
O	0.247228000	0.178224000	-2.016467000
C	0.116776000	0.163287000	2.275203000
C	0.832269000	0.104780000	4.466936000
H	1.551542000	0.016081000	5.263492000
C	-0.511952000	0.314778000	4.489054000
H	-1.199248000	0.438301000	5.308854000
C	-2.323147000	0.529233000	2.753325000
H	-2.882459000	0.921622000	3.607635000
H	-2.370993000	1.236093000	1.927823000
H	-2.758921000	-0.421008000	2.434490000
C	2.573582000	-0.190076000	2.672202000
H	3.168764000	-0.528122000	3.525455000
H	2.588787000	-0.947018000	1.890828000
H	2.992250000	0.738588000	2.276544000
N	1.194387000	0.013781000	3.118595000
N	-0.926730000	0.349283000	3.153276000
N	-1.691688000	-0.861361000	-0.037453000
N	1.026983000	-1.689626000	-0.012662000
N	1.817895000	1.020258000	-0.129313000

N	-0.906319000	1.854056000	-0.099383000
C	-2.947385000	-0.290588000	-0.244656000
C	-1.903327000	-2.170308000	0.403921000
C	0.449466000	-2.917081000	0.239427000
C	2.324786000	-1.923734000	-0.458849000
C	3.050552000	0.439591000	-0.403414000
C	2.044770000	2.359813000	0.159656000
C	-0.312161000	3.094859000	0.020456000
C	-2.226439000	2.061870000	-0.485016000
C	-3.964882000	-1.262992000	0.091909000
H	-5.026213000	-1.075499000	0.046519000
C	-3.332190000	-2.394190000	0.526264000
H	-3.783531000	-3.303577000	0.888320000
C	1.397210000	-3.956848000	-0.069071000
H	1.198423000	-5.013653000	0.014192000
C	2.541535000	-3.343598000	-0.528852000
H	3.447320000	-3.816692000	-0.873317000
C	4.087149000	1.438057000	-0.213827000
H	5.143106000	1.248454000	-0.325997000
C	3.480427000	2.597832000	0.170632000
H	3.946359000	3.538017000	0.416965000
C	-1.279775000	4.115030000	-0.302546000
H	-1.075428000	5.173785000	-0.309445000
C	-2.446181000	3.476826000	-0.646051000
H	-3.368340000	3.927155000	-0.976996000
C	-3.204587000	1.050084000	-0.556013000
C	-0.909221000	-3.139183000	0.574270000
C	3.291076000	-0.914484000	-0.652316000
C	1.056323000	3.340704000	0.273934000
C	-4.609714000	1.423002000	-0.880917000
C	-5.290024000	0.764379000	-1.924637000
H	-4.766262000	0.001476000	-2.490588000
C	-6.614840000	1.088406000	-2.234579000
H	-7.119914000	0.573814000	-3.046447000
C	-7.286674000	2.077433000	-1.504544000
H	-8.314624000	2.330483000	-1.744708000
C	-6.623961000	2.735988000	-0.460208000
H	-7.140674000	3.496156000	0.117804000
C	-5.299490000	2.410559000	-0.150269000
H	-4.790121000	2.911841000	0.665555000
C	-1.282447000	-4.520154000	0.987912000
C	-2.243632000	-5.274624000	0.286409000
H	-2.728857000	-4.835034000	-0.578466000
C	-2.561650000	-6.577977000	0.683288000
H	-3.302353000	-7.144629000	0.126967000

C	-1.917530000	-7.156662000	1.784489000
H	-2.163151000	-8.168562000	2.091527000
C	-0.948946000	-6.422788000	2.482653000
H	-0.442550000	-6.864084000	3.335832000
C	-0.633757000	-5.119289000	2.086548000
H	0.116542000	-4.548065000	2.623381000
C	4.671485000	-1.306211000	-1.052426000
C	5.261593000	-0.723163000	-2.191305000
H	4.685458000	-0.007363000	-2.768233000
C	6.562079000	-1.064989000	-2.576618000
H	6.998636000	-0.610821000	-3.460913000
C	7.297381000	-1.993652000	-1.828214000
H	8.306677000	-2.259415000	-2.127057000
C	6.723714000	-2.575271000	-0.689796000
H	7.291145000	-3.287446000	-0.098246000
C	5.423118000	-2.233445000	-0.304559000
H	4.982611000	-2.674121000	0.583370000
C	1.450232000	4.754193000	0.536184000
C	2.353983000	5.437787000	-0.300200000
H	2.772382000	4.919186000	-1.155960000
C	2.694837000	6.770803000	-0.046112000
H	3.389241000	7.283690000	-0.704753000
C	2.132362000	7.446954000	1.044421000
H	2.396108000	8.481706000	1.240413000
C	1.221895000	6.781766000	1.876407000
H	0.779220000	7.299402000	2.722125000
C	0.882557000	5.448839000	1.622482000
H	0.175650000	4.930665000	2.262414000
C	-0.368146000	-2.569914000	-2.912041000
S	-0.339079000	-0.829969000	-3.670016000
C	-2.194685000	-0.435022000	-3.579253000
H	-2.590671000	-0.925895000	-2.690819000
H	-2.264127000	0.646625000	-3.455212000
H	-2.693748000	-0.768659000	-4.491850000
H	0.662640000	-2.818853000	-2.657062000
H	-0.964514000	-2.513847000	-2.003158000
H	-0.783042000	-3.277791000	-3.633140000

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Mn	-0.070790000	0.065994000	0.012740000
C	-0.119742000	0.138166000	2.119639000
C	-0.701142000	-0.233005000	4.314808000
H	-1.276513000	-0.658823000	5.118569000
C	0.356932000	0.617612000	4.318741000

H	0.893847000	1.083742000	5.126727000
C	1.824091000	1.701032000	2.618765000
H	2.106921000	2.275334000	3.505635000
H	2.671440000	1.103782000	2.277067000
H	1.523456000	2.381858000	1.828814000
C	-2.074905000	-1.416879000	2.603315000
H	-2.389830000	-1.953659000	3.502849000
H	-2.914208000	-0.850263000	2.195701000
H	-1.728609000	-2.129944000	1.861198000
N	-0.978621000	-0.518941000	2.976560000
N	0.699069000	0.835873000	2.982625000
N	-0.194589000	2.047848000	-0.067069000
N	-2.068357000	-0.080865000	-0.053962000
N	0.074117000	-1.917609000	-0.002186000
N	1.942854000	0.189720000	0.040666000
C	0.839501000	2.926305000	-0.377613000
C	-1.322395000	2.819094000	0.184353000
C	-2.958642000	0.962452000	0.114685000
C	-2.802153000	-1.185230000	-0.456638000
C	-0.950471000	-2.819798000	-0.294180000
C	1.181647000	-2.678684000	0.390585000
C	2.826980000	-0.831627000	0.320309000
C	2.689988000	1.276471000	-0.393892000
C	0.349825000	4.294014000	-0.257469000
H	0.951757000	5.175677000	-0.412414000
C	-0.955308000	4.229323000	0.125771000
H	-1.621086000	5.050548000	0.336997000
C	-4.293786000	0.498192000	-0.170340000
H	-5.180877000	1.110947000	-0.135869000
C	-4.191536000	-0.817820000	-0.558105000
H	-4.986375000	-1.468605000	-0.885735000
C	-0.477559000	-4.170265000	-0.047934000
H	-1.076912000	-5.059017000	-0.169346000
C	0.804286000	-4.081914000	0.411800000
H	1.444194000	-4.888687000	0.731353000
C	4.168807000	-0.385355000	0.053381000
H	5.055465000	-0.989959000	0.164500000
C	4.079928000	0.905797000	-0.423681000
H	4.888362000	1.539042000	-0.752674000
C	2.169317000	2.573498000	-0.621284000
C	-2.615528000	2.317717000	0.343644000
C	-2.273311000	-2.486696000	-0.609151000
C	2.465364000	-2.175108000	0.609225000
C	3.100006000	3.659254000	-1.042141000
C	2.825605000	4.406204000	-2.205101000

H	1.940452000	4.162062000	-2.783522000
C	3.672054000	5.444277000	-2.608274000
H	3.445199000	6.005712000	-3.509704000
C	4.810638000	5.757359000	-1.854186000
H	5.468780000	6.562442000	-2.166226000
C	5.091926000	5.027109000	-0.691920000
H	5.965670000	5.270797000	-0.094842000
C	4.243599000	3.990259000	-0.289015000
H	4.455023000	3.432877000	0.617164000
C	-3.739645000	3.253953000	0.631183000
C	-4.035689000	4.342932000	-0.211229000
H	-3.426171000	4.503849000	-1.093735000
C	-5.108704000	5.195509000	0.071403000
H	-5.324331000	6.027472000	-0.592381000
C	-5.911423000	4.969991000	1.197194000
H	-6.744848000	5.630789000	1.415159000
C	-5.635915000	3.881766000	2.035927000
H	-6.254869000	3.697539000	2.909017000
C	-4.562217000	3.031374000	1.753193000
H	-4.347823000	2.184816000	2.397502000
C	-3.178445000	-3.597267000	-1.017877000
C	-2.847918000	-4.395940000	-2.130779000
H	-1.942768000	-4.167847000	-2.684396000
C	-3.668491000	-5.459618000	-2.520275000
H	-3.399333000	-6.060350000	-3.383996000
C	-4.837137000	-5.746500000	-1.802634000
H	-5.475652000	-6.571005000	-2.104591000
C	-5.174845000	-4.963869000	-0.690516000
H	-6.073084000	-5.185954000	-0.122066000
C	-4.352169000	-3.901720000	-0.300757000
H	-4.607348000	-3.303467000	0.567285000
C	3.566168000	-3.089680000	1.022132000
C	3.892758000	-4.248114000	0.289721000
H	3.319877000	-4.487546000	-0.599893000
C	4.947496000	-5.076593000	0.688448000
H	5.184660000	-5.963187000	0.107895000
C	5.704309000	-4.757937000	1.823210000
H	6.523603000	-5.399857000	2.131896000
C	5.400018000	-3.601073000	2.553439000
H	5.982519000	-3.344512000	3.433292000
C	4.344136000	-2.775648000	2.154991000
H	4.107500000	-1.877609000	2.716185000
O	-0.041274000	0.270526000	-1.874274000
S	0.302905000	-1.148708000	-3.049192000
C	0.435320000	0.046204000	-4.514262000

H	-0.579076000	0.385951000	-4.723914000
H	1.048611000	0.878007000	-4.163342000
H	0.873297000	-0.469240000	-5.371679000
C	2.163857000	-1.447395000	-2.779103000
H	2.590312000	-1.827493000	-3.710734000
H	2.599591000	-0.494543000	-2.475776000
H	2.248452000	-2.171383000	-1.970692000

⁶INT-1_{ss}

Mn	-0.012251000	0.110783000	0.151054000
O	-0.218616000	0.443302000	-2.177673000
C	0.033356000	0.124536000	2.526327000
C	0.716024000	0.276511000	4.722757000
H	1.425736000	0.368154000	5.527541000
C	-0.642741000	0.180467000	4.729104000
H	-1.350319000	0.165267000	5.540800000
C	-2.426795000	-0.033863000	2.949493000
H	-3.084632000	0.152379000	3.803150000
H	-2.619404000	0.699093000	2.166812000
H	-2.615030000	-1.033162000	2.549357000
C	2.495439000	0.337306000	2.929207000
H	3.155516000	0.201339000	3.790652000
H	2.688971000	-0.439362000	2.190235000
H	2.682993000	1.310809000	2.469401000
N	1.106100000	0.238325000	3.379775000
N	-1.036129000	0.090932000	3.389888000
N	-1.686280000	-1.179179000	-0.057475000
N	1.261503000	-1.582807000	-0.024927000
N	1.681357000	1.348220000	-0.106237000
N	-1.301460000	1.782121000	0.037003000
C	-3.000513000	-0.766615000	-0.116128000
C	-1.662226000	-2.539175000	0.167550000
C	0.841297000	-2.898307000	0.002894000
C	2.629144000	-1.562337000	-0.221187000
C	2.991802000	0.942533000	-0.186411000
C	1.648985000	2.723321000	-0.007485000
C	-0.860586000	3.074553000	-0.125137000
C	-2.640862000	1.733564000	-0.286966000
C	-3.854654000	-1.923010000	0.122794000
H	-4.932115000	-1.901348000	0.175284000
C	-3.034380000	-3.005917000	0.312575000
H	-3.331028000	-4.019458000	0.532931000
C	1.999564000	-3.753582000	-0.226050000
H	1.975331000	-4.830476000	-0.288959000

C	3.090487000	-2.936576000	-0.371167000
H	4.106586000	-3.234609000	-0.576829000
C	3.847050000	2.119217000	-0.068501000
H	4.925835000	2.108883000	-0.062725000
C	3.025030000	3.208193000	0.052146000
H	3.319240000	4.238173000	0.178730000
C	-1.990237000	3.901113000	-0.539619000
H	-1.937357000	4.954924000	-0.764495000
C	-3.077473000	3.078522000	-0.648514000
H	-4.069390000	3.342813000	-0.980251000
C	-3.449741000	0.568960000	-0.294120000
C	-0.4955561000	-3.349079000	0.167281000
C	3.440344000	-0.400848000	-0.287985000
C	0.481904000	3.528122000	-0.026880000
C	-4.915517000	0.762829000	-0.487568000
C	-5.616718000	0.041897000	-1.475181000
H	-5.067968000	-0.650643000	-2.104480000
C	-6.992759000	0.217464000	-1.651694000
H	-7.512775000	-0.342845000	-2.422862000
C	-7.697323000	1.120150000	-0.844119000
H	-8.765354000	1.257837000	-0.981536000
C	-7.013572000	1.844909000	0.140935000
H	-7.551938000	2.542948000	0.774943000
C	-5.637686000	1.667103000	0.317462000
H	-5.107861000	2.224290000	1.082786000
C	-0.687635000	-4.823596000	0.301936000
C	-1.520935000	-5.534550000	-0.584570000
H	-2.029296000	-4.991816000	-1.374579000
C	-1.689519000	-6.917390000	-0.458091000
H	-2.332427000	-7.447883000	-1.154095000
C	-1.024162000	-7.618108000	0.556485000
H	-1.154080000	-8.691442000	0.654755000
C	-0.189186000	-6.924650000	1.442652000
H	0.327027000	-7.459096000	2.234440000
C	-0.022919000	-5.541605000	1.316107000
H	0.619482000	-5.000752000	2.002975000
C	4.910637000	-0.605157000	-0.444816000
C	5.609640000	0.001296000	-1.507716000
H	5.058943000	0.615805000	-2.212338000
C	6.988319000	-0.181570000	-1.657122000
H	7.507773000	0.290638000	-2.485527000
C	7.696523000	-0.976064000	-0.745798000
H	8.766431000	-1.118960000	-0.861630000
C	7.014951000	-1.583267000	0.317149000
H	7.557080000	-2.194186000	1.032707000

C	5.636578000	-1.397651000	0.466688000
H	5.108449000	-1.861548000	1.293179000
C	0.671086000	5.008914000	-0.037645000
C	1.480165000	5.638624000	-1.004168000
H	1.970713000	5.027994000	-1.754266000
C	1.637500000	7.028504000	-1.009956000
H	2.259453000	7.496733000	-1.766935000
C	0.985875000	7.815936000	-0.051461000
H	1.107807000	8.894756000	-0.056523000
C	0.171616000	7.203075000	0.910165000
H	-0.337173000	7.805802000	1.656458000
C	0.013944000	5.813297000	0.914731000
H	-0.616744000	5.334510000	1.656542000
S	-0.097182000	-0.593823000	-3.515673000
C	1.592744000	-1.491445000	-3.335307000
H	1.525697000	-2.201755000	-2.512997000
H	1.813914000	-1.977320000	-4.288634000
H	2.317190000	-0.711481000	-3.099300000
C	-1.202739000	-2.116960000	-3.132153000
H	-0.788227000	-2.632096000	-2.267013000
H	-2.192652000	-1.724296000	-2.898514000
H	-1.211290000	-2.744282000	-4.027116000

⁴INT-1_{ss}

Mn	0.064939000	0.087760000	-0.060122000
O	0.337649000	0.153184000	-2.306747000
C	0.091877000	0.164985000	2.303225000
C	0.803892000	0.137396000	4.491975000
H	1.518740000	0.045696000	5.292126000
C	-0.534285000	0.390090000	4.506998000
H	-1.217329000	0.554638000	5.323124000
C	-2.332606000	0.619168000	2.748590000
H	-2.892341000	1.042343000	3.587659000
H	-2.347487000	1.311723000	1.908715000
H	-2.790445000	-0.323768000	2.438512000
C	2.535324000	-0.248528000	2.696055000
H	3.120601000	-0.614150000	3.544748000
H	2.521075000	-0.998561000	1.907314000
H	2.984404000	0.667894000	2.304540000
N	1.164317000	0.001801000	3.147173000
N	-0.946783000	0.404847000	3.170437000
N	-1.704702000	-0.840239000	-0.067563000
N	0.994926000	-1.705735000	-0.030835000
N	1.824116000	0.993159000	-0.133089000

N	-0.881122000	1.864102000	-0.140899000
C	-2.959233000	-0.245571000	-0.262360000
C	-1.938853000	-2.149222000	0.389203000
C	0.403362000	-2.931318000	0.230725000
C	2.291616000	-1.958915000	-0.477681000
C	3.054408000	0.392978000	-0.398452000
C	2.070855000	2.335217000	0.161892000
C	-0.271572000	3.102121000	-0.029597000
C	-2.196346000	2.088580000	-0.549607000
C	-3.988198000	-1.200622000	0.099640000
H	-5.046312000	-0.992957000	0.068824000
C	-3.371883000	-2.336679000	0.535751000
H	-3.836144000	-3.231439000	0.918011000
C	1.328536000	-3.973533000	-0.078495000
H	1.119766000	-5.028416000	0.006534000
C	2.487992000	-3.371905000	-0.545813000
H	3.388636000	-3.859468000	-0.883076000
C	4.103676000	1.377594000	-0.187162000
H	5.157894000	1.171707000	-0.285771000
C	3.511284000	2.541727000	0.199652000
H	3.991354000	3.470265000	0.463513000
C	-1.209212000	4.121996000	-0.387838000
H	-0.990185000	5.177754000	-0.411098000
C	-2.389108000	3.493130000	-0.738489000
H	-3.299899000	3.955017000	-1.084429000
C	-3.198197000	1.086681000	-0.595362000
C	-0.968194000	-3.130463000	0.563057000
C	3.280962000	-0.955099000	-0.657885000
C	1.103732000	3.329662000	0.255595000
C	-4.599145000	1.479978000	-0.912242000
C	-5.309507000	0.806740000	-1.926546000
H	-4.809739000	0.016705000	-2.477477000
C	-6.633183000	1.145883000	-2.225285000
H	-7.160682000	0.617467000	-3.013831000
C	-7.274705000	2.168206000	-1.514422000
H	-8.301376000	2.434271000	-1.745989000
C	-6.582136000	2.843872000	-0.500470000
H	-7.074902000	3.630634000	0.062811000
C	-5.259382000	2.502369000	-0.201562000
H	-4.726587000	3.019173000	0.589082000
C	-1.360603000	-4.501643000	0.988776000
C	-2.348784000	-5.240086000	0.307595000
H	-2.839203000	-4.794773000	-0.551528000
C	-2.688090000	-6.534528000	0.716310000
H	-3.450144000	-7.087665000	0.175272000

C	-2.037744000	-7.121881000	1.808922000
H	-2.298970000	-8.127089000	2.125000000
C	-1.041644000	-6.405048000	2.486394000
H	-0.529829000	-6.853137000	3.332829000
C	-0.705513000	-5.110730000	2.078658000
H	0.067635000	-4.554296000	2.598029000
C	4.659676000	-1.365572000	-1.042728000
C	5.280675000	-0.774920000	-2.161640000
H	4.726306000	-0.040802000	-2.737125000
C	6.583754000	-1.127975000	-2.528128000
H	7.043390000	-0.664708000	-3.396030000
C	7.291709000	-2.079710000	-1.782661000
H	8.302561000	-2.355408000	-2.067072000
C	6.687438000	-2.671560000	-0.665232000
H	7.233289000	-3.401612000	-0.074973000
C	5.385370000	-2.316658000	-0.298002000
H	4.922862000	-2.765427000	0.574420000
C	1.506773000	4.736274000	0.533292000
C	2.458335000	5.408022000	-0.259028000
H	2.905138000	4.885632000	-1.097941000
C	2.810090000	6.734590000	0.014491000
H	3.542467000	7.236809000	-0.610540000
C	2.209684000	7.418421000	1.079425000
H	2.481333000	8.448254000	1.290204000
C	1.249740000	6.766841000	1.865828000
H	0.776441000	7.290349000	2.691220000
C	0.900246000	5.440785000	1.592961000
H	0.154043000	4.934475000	2.196642000
C	-0.353991000	-2.606484000	-2.848826000
S	-0.243487000	-0.835702000	-3.569445000
C	-2.124906000	-0.492439000	-3.622211000
H	-2.517471000	-0.696208000	-2.626600000
H	-2.238615000	0.563952000	-3.867687000
H	-2.565169000	-1.134378000	-4.389321000
H	0.650072000	-2.875896000	-2.518922000
H	-1.036699000	-2.581810000	-2.001005000
H	-0.706551000	-3.259887000	-3.650858000

²INT-1_s

Mn	0.060082000	0.091590000	0.011154000
O	0.298605000	0.233346000	-2.023588000
C	0.086126000	0.110375000	2.066573000
C	0.778446000	0.015433000	4.255614000
H	1.492055000	-0.085943000	5.054827000

C	-0.563646000	0.219932000	4.268561000
H	-1.261401000	0.326484000	5.081003000
C	-2.378941000	0.472472000	2.579820000
H	-2.900366000	0.851049000	3.463676000
H	-2.453667000	1.198892000	1.777039000
H	-2.829733000	-0.470407000	2.263975000
C	2.565427000	-0.233830000	2.538451000
H	3.107658000	-0.574911000	3.425084000
H	2.636900000	-0.985079000	1.759149000
H	2.996335000	0.704113000	2.182430000
N	1.161575000	-0.049152000	2.915189000
N	-0.971532000	0.278908000	2.935568000
N	-1.703299000	-0.851633000	-0.060962000
N	0.969266000	-1.658535000	0.006244000
N	1.837919000	1.014707000	-0.084617000
N	-0.860456000	1.831137000	-0.066511000
C	-2.936544000	-0.277591000	-0.347585000
C	-1.954163000	-2.148041000	0.399113000
C	0.404626000	-2.885368000	0.344240000
C	2.271501000	-1.914697000	-0.454183000
C	3.039820000	0.435921000	-0.439109000
C	2.094251000	2.331458000	0.249892000
C	-0.260876000	3.076357000	0.128705000
C	-2.167320000	2.067975000	-0.502336000
C	-3.973465000	-1.222978000	-0.066099000
H	-5.029470000	-1.031220000	-0.174395000
C	-3.369414000	-2.367728000	0.424438000
H	-3.854726000	-3.269389000	0.761944000
C	1.370512000	-3.936363000	0.078447000
H	1.181093000	-4.988135000	0.226671000
C	2.483027000	-3.352314000	-0.456224000
H	3.377005000	-3.841695000	-0.808564000
C	4.094235000	1.398158000	-0.268407000
H	5.140911000	1.204727000	-0.444087000
C	3.515349000	2.559442000	0.199598000
H	4.008449000	3.485519000	0.447464000
C	-1.224146000	4.115827000	-0.195481000
H	-1.014146000	5.173020000	-0.152836000
C	-2.363237000	3.505919000	-0.624690000
H	-3.262034000	3.975167000	-0.990956000
C	-3.148150000	1.091069000	-0.673963000
C	-0.942365000	-3.112083000	0.642363000
C	3.233603000	-0.941915000	-0.717699000
C	1.085505000	3.316817000	0.401948000
C	-4.531356000	1.486159000	-1.061226000

C	-5.182427000	0.839650000	-2.132086000
H	-4.653740000	0.062921000	-2.673256000
C	-6.487987000	1.182528000	-2.496495000
H	-6.966161000	0.674679000	-3.328921000
C	-7.177033000	2.179961000	-1.793793000
H	-8.190379000	2.448013000	-2.076155000
C	-6.549727000	2.822304000	-0.718665000
H	-7.079981000	3.585538000	-0.156873000
C	-5.244825000	2.474855000	-0.353409000
H	-4.769359000	2.960151000	0.491968000
C	-1.323674000	-4.477530000	1.096837000
C	-2.262403000	-5.264115000	0.399743000
H	-2.729326000	-4.859293000	-0.491517000
C	-2.582710000	-6.553807000	0.836173000
H	-3.304987000	-7.145879000	0.281945000
C	-1.965784000	-7.087255000	1.975719000
H	-2.214595000	-8.088462000	2.313801000
C	-1.022542000	-6.320768000	2.672580000
H	-0.537910000	-6.725728000	3.555982000
C	-0.705508000	-5.029995000	2.236775000
H	0.022992000	-4.431179000	2.773811000
C	4.585384000	-1.346629000	-1.195491000
C	5.108040000	-0.768454000	-2.369851000
H	4.503668000	-0.045034000	-2.907161000
C	6.380159000	-1.116579000	-2.834616000
H	6.763304000	-0.665167000	-3.744875000
C	7.158297000	-2.045527000	-2.130313000
H	8.146298000	-2.315534000	-2.490408000
C	6.656081000	-2.617403000	-0.954402000
H	7.258226000	-3.326466000	-0.394042000
C	5.383335000	-2.267710000	-0.489419000
H	5.002282000	-2.697128000	0.431035000
C	1.481255000	4.718830000	0.716035000
C	2.395739000	5.430502000	-0.085266000
H	2.824887000	4.941398000	-0.952586000
C	2.732615000	6.753941000	0.217507000
H	3.434251000	7.288720000	-0.415713000
C	2.157922000	7.393879000	1.323962000
H	2.419961000	8.421241000	1.557813000
C	1.238747000	6.701145000	2.122448000
H	0.786178000	7.189661000	2.980289000
C	0.903441000	5.377033000	1.819743000
H	0.191277000	4.836368000	2.434914000
C	-0.295048000	-2.582182000	-2.726233000
S	-0.232925000	-0.761853000	-3.314567000

C	-2.125131000	-0.495346000	-3.458545000
H	-2.623606000	-1.112454000	-2.712418000
H	-2.291802000	0.560453000	-3.242257000
H	-2.411174000	-0.752794000	-4.481072000
H	0.715637000	-2.865119000	-2.433358000
H	-0.974323000	-2.643327000	-1.879058000
H	-0.644987000	-3.163092000	-3.583959000

⁶P-1_{hs}

C	-0.000345000	-0.000821000	2.280707000
C	-0.678372000	-0.075794000	4.470814000
H	-1.383186000	-0.156182000	5.280825000
C	0.677664000	0.073124000	4.470859000
H	1.382475000	0.153035000	5.280921000
C	2.451303000	0.277420000	2.663906000
H	3.125477000	0.180234000	3.518763000
H	2.676161000	-0.493824000	1.925843000
H	2.584799000	1.255663000	2.194996000
C	-2.451997000	-0.279146000	2.663731000
H	-3.126115000	-0.183141000	3.518762000
H	-2.677074000	0.492937000	1.926585000
H	-2.585322000	-1.256847000	2.193673000
N	-1.070617000	-0.116861000	3.129807000
N	1.069932000	0.114814000	3.129881000
N	1.687826000	1.213997000	-0.484813000
N	-1.228977000	1.689061000	-0.406029000
N	-1.687758000	-1.213726000	-0.485154000
N	1.229088000	-1.688756000	-0.406287000
C	3.002287000	0.787396000	-0.505768000
C	1.694313000	2.592999000	-0.359203000
C	-0.786971000	2.995168000	-0.490080000
C	-2.596092000	1.692266000	-0.616244000
C	-3.002224000	-0.787119000	-0.506055000
C	-1.694219000	-2.592720000	-0.359647000
C	0.787098000	-2.994888000	-0.490328000
C	2.596224000	-1.691970000	-0.616332000
C	3.873280000	1.938989000	-0.331791000
H	4.949820000	1.902249000	-0.276164000
C	3.071408000	3.044697000	-0.232697000
H	3.380313000	4.067202000	-0.083670000
C	-1.923534000	3.859059000	-0.774548000
H	-1.867952000	4.925314000	-0.927839000
C	-3.030461000	3.060445000	-0.858360000
H	-4.040025000	3.358457000	-1.093491000

C	-3.873194000	-1.938740000	-0.332090000
H	-4.949729000	-1.902032000	-0.276349000
C	-3.071301000	-3.044446000	-0.233142000
H	-3.380174000	-4.066976000	-0.084212000
C	1.923726000	-3.858776000	-0.774578000
H	1.868217000	-4.925048000	-0.927781000
C	3.030652000	-3.060143000	-0.858283000
H	4.040259000	-3.358160000	-1.093217000
C	3.436291000	-0.554932000	-0.611407000
C	0.554469000	3.429594000	-0.382012000
C	-3.436195000	0.555240000	-0.611476000
C	-0.554340000	-3.429304000	-0.382435000
C	4.906338000	-0.789858000	-0.713457000
C	5.669318000	-0.166664000	-1.720926000
H	5.167315000	0.480408000	-2.432238000
C	7.048281000	-0.382653000	-1.811431000
H	7.618392000	0.101024000	-2.598759000
C	7.691315000	-1.227234000	-0.896684000
H	8.761414000	-1.395635000	-0.967810000
C	6.944335000	-1.854683000	0.108942000
H	7.435135000	-2.507958000	0.824093000
C	5.565576000	-1.637178000	0.199314000
H	4.985039000	-2.120397000	0.978371000
C	0.780340000	4.904702000	-0.340543000
C	1.605783000	5.542275000	-1.287721000
H	2.078130000	4.943046000	-2.058661000
C	1.805618000	6.926121000	-1.246609000
H	2.439869000	7.400795000	-1.989132000
C	1.181503000	7.699386000	-0.258789000
H	1.335996000	8.773521000	-0.227492000
C	0.353804000	7.078490000	0.686018000
H	-0.132409000	7.670114000	1.455847000
C	0.154589000	5.694585000	0.644243000
H	-0.485535000	5.209892000	1.374004000
C	-4.906230000	0.790223000	-0.713508000
C	-5.669254000	0.167123000	-1.721007000
H	-5.167285000	-0.479904000	-2.432383000
C	-7.048207000	0.383178000	-1.811491000
H	-7.618344000	-0.100417000	-2.598850000
C	-7.691200000	1.227722000	-0.896684000
H	-8.761292000	1.396177000	-0.967798000
C	-6.944185000	1.855081000	0.108975000
H	-7.434958000	2.508329000	0.824167000
C	-5.565436000	1.637519000	0.199324000
H	-4.984873000	2.120658000	0.978408000

C	-0.780237000	-4.904424000	-0.341058000
C	-1.605515000	-5.541906000	-1.288438000
H	-2.077724000	-4.942606000	-2.059410000
C	-1.805362000	-6.925757000	-1.247463000
H	-2.439472000	-7.400377000	-1.990138000
C	-1.181435000	-7.699097000	-0.259589000
H	-1.335939000	-8.773234000	-0.228398000
C	-0.353905000	-7.078286000	0.685418000
H	0.132147000	-7.669981000	1.455295000
C	-0.154667000	-5.694377000	0.643780000
H	0.485333000	-5.209742000	1.373690000
Mn	0.000032000	0.000095000	0.048112000

⁴P-1_s

C	-0.000058000	-0.000159000	2.009412000
C	0.677389000	0.072930000	4.201492000
H	1.383290000	0.154079000	5.010471000
C	-0.677374000	-0.074384000	4.201502000
H	-1.383225000	-0.155927000	5.010486000
C	-2.455939000	-0.288087000	2.414335000
H	-3.122289000	-0.094035000	3.259286000
H	-2.664015000	0.417386000	1.610938000
H	-2.614838000	-1.303818000	2.042335000
C	2.455803000	0.287867000	2.414298000
H	3.122251000	0.093733000	3.259154000
H	2.664024000	-0.417310000	1.610714000
H	2.614401000	1.303758000	2.042549000
N	1.070461000	0.112653000	2.860398000
N	-1.070533000	-0.113371000	2.860404000
N	-1.547565000	-1.276374000	-0.470350000
N	1.267273000	-1.521339000	-0.411775000
N	1.547583000	1.276467000	-0.470446000
N	-1.267261000	1.521441000	-0.411729000
C	-2.885771000	-0.959017000	-0.683866000
C	-1.509325000	-2.624084000	-0.107316000
C	0.939422000	-2.871384000	-0.237417000
C	2.623106000	-1.487559000	-0.787795000
C	2.885784000	0.959103000	-0.683858000
C	1.509343000	2.624193000	-0.107386000
C	-0.939408000	2.871470000	-0.237366000
C	-2.623111000	1.487651000	-0.787689000
C	-3.691547000	-2.108289000	-0.426476000
H	-4.767550000	-2.132482000	-0.494621000
C	-2.844385000	-3.129252000	-0.037274000

H	-3.113052000	-4.133574000	0.247053000
C	2.107605000	-3.684655000	-0.522953000
H	2.114964000	-4.762593000	-0.492992000
C	3.114225000	-2.849315000	-0.895657000
H	4.106336000	-3.114949000	-1.223025000
C	3.691571000	2.108352000	-0.426461000
H	4.767573000	2.132529000	-0.494640000
C	2.844412000	3.129323000	-0.037263000
H	3.113115000	4.133606000	0.247156000
C	-2.107601000	3.684742000	-0.522855000
H	-2.114960000	4.762679000	-0.492860000
C	-3.114254000	2.849406000	-0.895489000
H	-4.106362000	3.115055000	-1.222849000
C	-3.391411000	0.341323000	-0.933889000
C	-0.324766000	-3.388365000	0.023301000
C	3.391431000	-0.341228000	-0.933926000
C	0.324787000	3.388471000	0.023315000
C	-4.839371000	0.455466000	-1.265358000
C	-5.367761000	-0.251947000	-2.363463000
H	-4.699813000	-0.861830000	-2.962519000
C	-6.727305000	-0.170001000	-2.680225000
H	-7.114937000	-0.715806000	-3.535028000
C	-7.586524000	0.616918000	-1.901323000
H	-8.641979000	0.680652000	-2.147205000
C	-7.075713000	1.317179000	-0.800916000
H	-7.736283000	1.920115000	-0.185114000
C	-5.715449000	1.233933000	-0.484076000
H	-5.321258000	1.765954000	0.375387000
C	-0.431315000	-4.841695000	0.335353000
C	-1.200276000	-5.714632000	-0.459242000
H	-1.730570000	-5.314715000	-1.316622000
C	-1.270657000	-7.079098000	-0.159565000
H	-1.862946000	-7.738026000	-0.787286000
C	-0.570437000	-7.597794000	0.937997000
H	-0.625475000	-8.656974000	1.169755000
C	0.204431000	-6.741719000	1.731270000
H	0.750875000	-7.135062000	2.583217000
C	0.273311000	-5.376994000	1.431554000
H	0.871768000	-4.709474000	2.043109000
C	4.839408000	-0.455341000	-1.265370000
C	5.367828000	0.252237000	-2.363354000
H	4.699893000	0.862202000	-2.962343000
C	6.727384000	0.170340000	-2.680070000
H	7.115062000	0.716261000	-3.534780000
C	7.586572000	-0.616691000	-1.901237000

H	8.642035000	-0.680381000	-2.147086000
C	7.075731000	-1.317092000	-0.800942000
H	7.736282000	-1.920105000	-0.185192000
C	5.715445000	-1.233888000	-0.484142000
H	5.321222000	-1.766027000	0.375238000
C	0.431304000	4.841776000	0.335464000
C	1.200226000	5.714825000	-0.459034000
H	1.730490000	5.315040000	-1.316494000
C	1.270608000	7.079257000	-0.159195000
H	1.862880000	7.738265000	-0.786854000
C	0.570416000	7.597803000	0.938455000
H	0.625459000	8.656949000	1.170355000
C	-0.204427000	6.741621000	1.731634000
H	-0.750866000	7.134858000	2.583631000
C	-0.273306000	5.376935000	1.431756000
H	-0.871730000	4.709325000	2.043249000
Mn	0.000008000	0.000064000	-0.244168000

²P-1_s

C	0.000348000	-0.000093000	1.802783000
C	-0.657495000	-0.164481000	4.007460000
H	-1.347983000	-0.336772000	4.815018000
C	0.658879000	0.163653000	4.007305000
H	1.349539000	0.335910000	4.814721000
C	2.425271000	0.599342000	2.299108000
H	2.936610000	0.959848000	3.196296000
H	2.946715000	-0.276225000	1.905733000
H	2.424172000	1.383780000	1.547811000
C	-2.424286000	-0.599896000	2.299550000
H	-2.935397000	-0.960747000	3.196732000
H	-2.945954000	0.275664000	1.906513000
H	-2.423142000	-1.384083000	1.547977000
N	-1.048250000	-0.263252000	2.669509000
N	1.049243000	0.262835000	2.669251000
N	0.570211000	1.905025000	-0.342798000
N	-1.892972000	0.570350000	-0.387610000
N	-0.570361000	-1.904963000	-0.342951000
N	1.892815000	-0.570349000	-0.388102000
C	1.844879000	2.388882000	-0.625562000
C	-0.213649000	3.017221000	-0.039255000
C	-2.381411000	1.857463000	-0.186387000
C	-2.983435000	-0.207168000	-0.784692000
C	-1.845045000	-2.388822000	-0.625681000
C	0.213537000	-3.017133000	-0.039627000

C	2.381269000	-1.857408000	-0.186845000
C	2.983263000	0.207228000	-0.785145000
C	1.866943000	3.824517000	-0.438328000
H	2.739545000	4.444860000	-0.568166000
C	0.615481000	4.204762000	-0.044175000
H	0.273688000	5.197435000	0.200060000
C	-3.800652000	1.885414000	-0.471581000
H	-4.415670000	2.770094000	-0.423456000
C	-4.159637000	0.630741000	-0.876392000
H	-5.129044000	0.296726000	-1.209069000
C	-1.866997000	-3.824515000	-0.438813000
H	-2.739554000	-4.444882000	-0.568829000
C	-0.615513000	-4.204750000	-0.044718000
H	-0.273649000	-5.197453000	0.199288000
C	3.800539000	-1.885333000	-0.471997000
H	4.415528000	-2.770031000	-0.423908000
C	4.159510000	-0.630652000	-0.876777000
H	5.128903000	-0.296556000	-1.209441000
C	2.968834000	1.601236000	-0.917078000
C	-1.607384000	2.994506000	0.090861000
C	-2.969059000	-1.601177000	-0.916836000
C	1.607279000	-2.994460000	0.090430000
C	4.226435000	2.312016000	-1.290231000
C	4.248248000	3.156003000	-2.417183000
H	3.345242000	3.261146000	-3.009437000
C	5.412164000	3.846458000	-2.771174000
H	5.412836000	4.487924000	-3.647126000
C	6.574546000	3.707953000	-2.001273000
H	7.478195000	4.243361000	-2.275613000
C	6.563215000	2.876804000	-0.873566000
H	7.457079000	2.771622000	-0.266157000
C	5.398540000	2.186670000	-0.520379000
H	5.385865000	1.549283000	0.357406000
C	-2.337410000	4.256785000	0.405666000
C	-2.228020000	5.399070000	-0.409913000
H	-1.591944000	5.359560000	-1.287497000
C	-2.939144000	6.564845000	-0.104847000
H	-2.847249000	7.435119000	-0.747560000
C	-3.776333000	6.606824000	1.017748000
H	-4.328390000	7.511412000	1.253373000
C	-3.901349000	5.472903000	1.831087000
H	-4.549529000	5.496560000	2.701911000
C	-3.189570000	4.308138000	1.525534000
H	-3.284242000	3.426628000	2.151430000
C	-4.226651000	-2.311897000	-1.289988000

C	-4.248427000	-3.155968000	-2.416902000
H	-3.345378000	-3.261190000	-3.009073000
C	-5.412342000	-3.846368000	-2.770978000
H	-5.412930000	-4.487871000	-3.646905000
C	-6.574797000	-3.707758000	-2.001206000
H	-7.478463000	-4.243108000	-2.275593000
C	-6.563499000	-2.876561000	-0.873532000
H	-7.457411000	-2.771274000	-0.266211000
C	-5.398820000	-2.186489000	-0.520254000
H	-5.386205000	-1.549128000	0.357546000
C	2.337275000	-4.256714000	0.405357000
C	2.228053000	-5.399038000	-0.410157000
H	1.592149000	-5.359607000	-1.287871000
C	2.939109000	-6.564802000	-0.104868000
H	2.847305000	-7.435118000	-0.747543000
C	3.776074000	-6.606723000	1.017887000
H	4.328071000	-7.511298000	1.253693000
C	3.900933000	-5.472739000	1.831178000
H	4.548947000	-5.496337000	2.702126000
C	3.189217000	-4.308001000	1.525407000
H	3.283746000	-3.426450000	2.151277000
Mn	-0.000011000	0.000029000	-0.167867000

OAT in SMe₂ by species 2

⁵RC-2_{hs}

Fe	0.224614000	0.011795000	0.000569000
O	0.070857000	0.014347000	-1.656594000
C	0.458393000	0.013915000	2.184761000
C	0.205104000	0.486480000	4.422810000
H	-0.225904000	0.977113000	5.278298000
C	1.184149000	-0.447525000	4.319479000
H	1.787180000	-0.934788000	5.065982000
C	2.323220000	-1.693559000	2.493341000
H	2.650293000	-2.280843000	3.355965000
H	1.873388000	-2.352524000	1.758725000
H	3.181589000	-1.183484000	2.053073000
C	-1.296261000	1.725084000	2.873461000
H	-1.445252000	2.305496000	3.788214000
H	-1.003472000	2.390190000	2.067832000
H	-2.224023000	1.214494000	2.611392000
N	-0.224695000	0.758410000	3.122593000
N	1.326923000	-0.726206000	2.958727000

N	2.249937000	-0.228196000	-0.168250000
N	0.432984000	2.070352000	0.068365000
N	-1.798616000	0.244246000	0.249211000
N	0.018748000	-2.047643000	0.112963000
C	2.889200000	-1.397457000	-0.516412000
C	3.197139000	0.759507000	0.009421000
C	1.641630000	2.727888000	0.033504000
C	-0.563862000	2.966158000	-0.279066000
C	-2.497782000	1.416278000	0.064377000
C	-2.684514000	-0.736983000	0.649687000
C	-1.169311000	-2.707824000	0.334116000
C	0.925121000	-2.946778000	-0.421961000
C	4.322226000	-1.157780000	-0.485224000
H	5.076106000	-1.904157000	-0.680001000
C	4.512416000	0.152043000	-0.131327000
H	5.451374000	0.664359000	0.003356000
C	1.399037000	4.116382000	-0.326473000
H	2.168029000	4.863131000	-0.446702000
C	0.055476000	4.253047000	-0.550097000
H	-0.466531000	5.134853000	-0.884948000
C	-3.881875000	1.185392000	0.440605000
H	-4.658055000	1.933323000	0.423495000
C	-3.989559000	-0.121375000	0.830743000
H	-4.872617000	-0.628558000	1.183934000
C	-1.002410000	-4.098608000	-0.057633000
H	-1.777211000	-4.847517000	-0.011722000
C	0.269315000	-4.237844000	-0.544709000
H	0.718781000	-5.124209000	-0.963249000
C	2.273981000	-2.655144000	-0.716713000
C	2.924174000	2.138955000	0.140195000
C	-1.945625000	2.672876000	-0.278552000
C	-2.398812000	-2.117129000	0.710213000
C	3.146093000	-3.759938000	-1.206286000
C	3.880656000	-3.603823000	-2.398590000
H	3.781155000	-2.678629000	-2.956244000
C	4.714556000	-4.626060000	-2.862903000
H	5.267180000	-4.491740000	-3.787643000
C	4.831063000	-5.822308000	-2.142601000
H	5.477706000	-6.616064000	-2.503430000
C	4.109081000	-5.988050000	-0.953356000
H	4.200720000	-6.908666000	-0.385050000
C	3.275434000	-4.965470000	-0.488757000
H	2.723327000	-5.088478000	0.436991000
C	4.072679000	3.084687000	0.255346000
C	5.104339000	3.119724000	-0.703101000

H	5.061779000	2.439060000	-1.546244000
C	6.157583000	4.032845000	-0.585042000
H	6.940451000	4.051139000	-1.337043000
C	6.195636000	4.930868000	0.489870000
H	7.012719000	5.639886000	0.579849000
C	5.169176000	4.913754000	1.443297000
H	5.189371000	5.608564000	2.277371000
C	4.116021000	4.001052000	1.324629000
H	3.316905000	3.986675000	2.058719000
C	-2.910261000	3.763103000	-0.593297000
C	-3.921599000	3.544284000	-1.551911000
H	-3.976504000	2.577130000	-2.040462000
C	-4.841222000	4.551799000	-1.859445000
H	-5.609257000	4.367530000	-2.604293000
C	-4.771870000	5.793206000	-1.213031000
H	-5.485737000	6.575038000	-1.453253000
C	-3.779769000	6.017423000	-0.249381000
H	-3.728604000	6.971012000	0.267437000
C	-2.859147000	5.010793000	0.059694000
H	-2.101617000	5.180058000	0.817518000
C	-3.508659000	-3.057592000	1.038979000
C	-4.717977000	-3.050773000	0.315616000
H	-4.846433000	-2.336308000	-0.490168000
C	-5.735694000	-3.961526000	0.618111000
H	-6.657825000	-3.946541000	0.045399000
C	-5.561946000	-4.897730000	1.645924000
H	-6.351944000	-5.604658000	1.879505000
C	-4.360295000	-4.920585000	2.366311000
H	-4.217235000	-5.643877000	3.163358000
C	-3.342277000	-4.010811000	2.062942000
H	-2.408715000	-4.026941000	2.615974000
C	-2.636295000	-1.517108000	-2.739408000
H	-3.312574000	-2.163336000	-2.175952000
H	-2.270538000	-2.036695000	-3.628777000
H	-1.802510000	-1.196372000	-2.113530000
S	-3.626601000	0.018163000	-3.260255000
C	-2.165777000	1.113352000	-3.786701000
H	-1.769863000	0.768630000	-4.745341000
H	-2.549275000	2.132400000	-3.880223000
H	-1.395137000	1.058796000	-3.014081000

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Fe	-0.212453000	-0.008325000	-0.032877000
O	-0.014426000	0.000202000	-1.693994000

C	-0.490932000	-0.022286000	2.120337000
C	-0.834434000	-0.714968000	4.289355000
H	-0.992670000	-1.431873000	5.076512000
C	-0.727469000	0.638316000	4.313584000
H	-0.780278000	1.343375000	5.125222000
C	-0.373367000	2.460699000	2.648294000
H	-0.178216000	3.014988000	3.570626000
H	0.463046000	2.585871000	1.968221000
H	-1.283749000	2.840142000	2.180441000
C	-0.734633000	-2.513996000	2.565626000
H	-1.152456000	-3.081393000	3.402004000
H	-1.371243000	-2.633460000	1.694702000
H	0.266775000	-2.884130000	2.338529000
N	-0.690580000	-1.101864000	2.954513000
N	-0.517698000	1.044252000	2.993250000
N	-1.261550000	1.669384000	-0.129843000
N	-1.877434000	-1.078536000	-0.183771000
N	0.831534000	-1.684176000	0.121024000
N	1.439327000	1.060663000	0.251196000
C	-0.753818000	2.919961000	-0.411924000
C	-2.623585000	1.805821000	0.062853000
C	-3.163743000	-0.594669000	-0.086875000
C	-1.957807000	-2.378522000	-0.658371000
C	0.416039000	-2.929574000	-0.301646000
C	2.101732000	-1.825716000	0.648017000
C	2.661921000	0.573414000	0.663396000
C	1.633182000	2.370320000	-0.158563000
C	-1.828687000	3.890223000	-0.351692000
H	-1.705234000	4.950422000	-0.507025000
C	-2.968502000	3.213553000	-0.013369000
H	-3.953949000	3.619636000	0.146962000
C	-4.093139000	-1.632014000	-0.493175000
H	-5.164458000	-1.512935000	-0.528002000
C	-3.350668000	-2.710364000	-0.885650000
H	-3.704337000	-3.643029000	-1.294159000
C	1.444511000	-3.900765000	0.010287000
H	1.369009000	-4.957745000	-0.190072000
C	2.460763000	-3.230490000	0.635022000
H	3.377974000	-3.638256000	1.027652000
C	3.660369000	1.615215000	0.522685000
H	4.706488000	1.495262000	0.755176000
C	3.036797000	2.703794000	-0.020428000
H	3.479710000	3.643596000	-0.307268000
C	0.607191000	3.251468000	-0.527839000
C	-3.531876000	0.740452000	0.157656000

C	-0.869844000	-3.256178000	-0.767136000
C	2.958049000	-0.764369000	0.975023000
C	0.944716000	4.633495000	-0.965902000
C	0.480188000	5.097285000	-2.212372000
H	-0.101581000	4.426610000	-2.835906000
C	0.775559000	6.393850000	-2.645819000
H	0.418118000	6.732545000	-3.613267000
C	1.536004000	7.250301000	-1.838633000
H	1.766692000	8.255985000	-2.175810000
C	1.994887000	6.803067000	-0.592726000
H	2.574872000	7.464984000	0.043132000
C	1.699412000	5.506396000	-0.158865000
H	2.041910000	5.164561000	0.812124000
C	-4.980222000	1.019473000	0.369263000
C	-5.711631000	1.853042000	-0.498829000
H	-5.207244000	2.302894000	-1.346951000
C	-7.075932000	2.080027000	-0.287949000
H	-7.626522000	2.719907000	-0.970622000
C	-7.733908000	1.472692000	0.789670000
H	-8.792787000	1.648602000	0.951543000
C	-7.019738000	0.630392000	1.651922000
H	-7.523411000	0.152517000	2.486647000
C	-5.655675000	0.403659000	1.441082000
H	-5.098358000	-0.249442000	2.105023000
C	-1.079305000	-4.633412000	-1.292271000
C	-0.302771000	-5.086510000	-2.377041000
H	0.418189000	-4.409702000	-2.823485000
C	-0.467155000	-6.381223000	-2.879727000
H	0.132643000	-6.711441000	-3.722096000
C	-1.406668000	-7.246612000	-2.303735000
H	-1.534886000	-8.251186000	-2.694574000
C	-2.178019000	-6.809779000	-1.218775000
H	-2.899900000	-7.478622000	-0.760042000
C	-2.013941000	-5.514732000	-0.715568000
H	-2.599924000	-5.180760000	0.134258000
C	4.320490000	-1.052836000	1.504928000
C	5.232340000	-1.855469000	0.792392000
H	4.931968000	-2.272387000	-0.162495000
C	6.517910000	-2.088087000	1.292828000
H	7.211973000	-2.702469000	0.727730000
C	6.914921000	-1.517996000	2.509525000
H	7.913133000	-1.698165000	2.896128000
C	6.020217000	-0.706987000	3.220161000
H	6.322397000	-0.258051000	4.161407000
C	4.734989000	-0.473748000	2.719544000

H	4.038917000	0.156681000	3.263626000
C	3.090797000	-1.040829000	-2.442370000
H	3.732793000	-0.623331000	-1.663809000
H	2.046613000	-1.009340000	-2.125584000
H	3.393402000	-2.065186000	-2.674943000
S	3.269137000	-0.023075000	-4.033512000
C	2.391115000	1.540800000	-3.408060000
H	2.997527000	2.017718000	-2.634642000
H	2.275828000	2.208198000	-4.265851000
H	1.419227000	1.250842000	-3.001499000

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Fe	-0.182981000	0.003361000	-0.021872000
O	-0.137057000	-0.122350000	-1.701232000
C	-0.497124000	-0.069899000	2.100899000
C	-0.344912000	-0.632028000	4.328954000
H	0.034031000	-1.169220000	5.181266000
C	-1.277783000	0.349457000	4.226681000
H	-1.883539000	0.837386000	4.970722000
C	-2.278008000	1.722574000	2.406657000
H	-2.569468000	2.327761000	3.269955000
H	-1.775481000	2.351146000	1.679091000
H	-3.167277000	1.279106000	1.955077000
C	1.179809000	-1.855925000	2.786802000
H	1.294839000	-2.464420000	3.688127000
H	0.902103000	-2.492516000	1.953624000
H	2.123128000	-1.354218000	2.564611000
N	0.119927000	-0.876021000	3.035435000
N	-1.357329000	0.683193000	2.873651000
N	-2.149588000	0.291378000	-0.221954000
N	-0.454117000	-1.986043000	-0.007605000
N	1.744298000	-0.295747000	0.225348000
N	0.068751000	1.946224000	0.071233000
C	-2.755699000	1.449196000	-0.642043000
C	-3.143000000	-0.636746000	0.025378000
C	-1.672067000	-2.623165000	0.074003000
C	0.483640000	-2.924160000	-0.402355000
C	2.429910000	-1.465919000	-0.030626000
C	2.656785000	0.612649000	0.736868000
C	1.225630000	2.596354000	0.457152000
C	-0.776958000	2.903340000	-0.481458000
C	-4.194396000	1.272108000	-0.608802000
H	-4.912908000	2.035736000	-0.861707000
C	-4.434572000	0.004348000	-0.152753000

H	-5.389594000	-0.463950000	0.021378000
C	-1.495044000	-4.024075000	-0.260284000
H	-2.291803000	-4.750320000	-0.293193000
C	-0.181374000	-4.196888000	-0.599404000
H	0.294371000	-5.096390000	-0.954328000
C	3.807302000	-1.307433000	0.387893000
H	4.559549000	-2.076537000	0.319357000
C	3.936163000	-0.047510000	0.901636000
H	4.818202000	0.407134000	1.322361000
C	1.104521000	4.005093000	0.145638000
H	1.875117000	4.738088000	0.323538000
C	-0.104049000	4.184828000	-0.467718000
H	-0.507254000	5.096685000	-0.877108000
C	-2.104014000	2.675434000	-0.866760000
C	-2.928107000	-2.008208000	0.237061000
C	1.866472000	-2.683580000	-0.449897000
C	2.412345000	1.983459000	0.894972000
C	-2.914209000	3.787828000	-1.434553000
C	-3.561311000	3.611771000	-2.673677000
H	-3.434217000	2.671898000	-3.200579000
C	-4.344238000	4.633171000	-3.221238000
H	-4.828782000	4.484190000	-4.181229000
C	-4.498708000	5.846234000	-2.537152000
H	-5.106039000	6.639203000	-2.962270000
C	-3.867956000	6.029063000	-1.299544000
H	-3.992532000	6.961803000	-0.757901000
C	-3.084391000	5.007726000	-0.751798000
H	-2.608179000	5.143281000	0.213508000
C	-4.089681000	-2.908775000	0.484017000
C	-5.175552000	-2.988752000	-0.409186000
H	-5.167649000	-2.377305000	-1.304777000
C	-6.239506000	-3.862780000	-0.161410000
H	-7.065272000	-3.917497000	-0.864128000
C	-6.233937000	-4.675871000	0.979613000
H	-7.059751000	-5.354181000	1.170173000
C	-5.152527000	-4.614964000	1.868328000
H	-5.138117000	-5.245231000	2.752285000
C	-4.088265000	-3.742140000	1.619755000
H	-3.246152000	-3.694158000	2.302677000
C	2.803275000	-3.765605000	-0.854663000
C	3.784388000	-3.495221000	-1.831508000
H	3.830162000	-2.500589000	-2.263124000
C	4.685810000	-4.488021000	-2.227934000
H	5.430349000	-4.264471000	-2.985741000
C	4.629618000	-5.764309000	-1.651998000

H	5.329576000	-6.534584000	-1.960740000
C	3.670830000	-6.038202000	-0.667811000
H	3.633073000	-7.018720000	-0.202806000
C	2.767772000	-5.046858000	-0.269736000
H	2.041904000	-5.254304000	0.509070000
C	3.504155000	2.875305000	1.375671000
C	4.752489000	2.922686000	0.724561000
H	4.920777000	2.287163000	-0.138273000
C	5.755816000	3.789749000	1.170180000
H	6.709981000	3.818905000	0.653195000
C	5.526635000	4.627798000	2.269425000
H	6.305455000	5.301121000	2.613633000
C	4.284605000	4.597718000	2.917345000
H	4.098685000	5.246365000	3.767965000
C	3.281272000	3.730892000	2.471789000
H	2.316516000	3.705704000	2.968292000
C	2.435549000	1.525122000	-2.597713000
H	3.096644000	2.165962000	-2.010027000
H	1.975691000	2.095842000	-3.408153000
H	1.668160000	1.082913000	-1.959726000
S	3.490643000	0.123332000	-3.320151000
C	2.062767000	-0.969303000	-3.939575000
H	2.473905000	-1.965552000	-4.120473000
H	1.296209000	-0.997067000	-3.158810000
H	1.654642000	-0.554332000	-4.864719000

⁵TS-2_{hs}

Fe	0.061755000	0.075770000	-0.140796000
O	0.248013000	0.265251000	-1.959591000
C	0.129585000	0.162181000	2.325845000
C	0.857965000	0.199778000	4.521623000
H	1.586608000	0.177444000	5.314300000
C	-0.496271000	0.313541000	4.548283000
H	-1.187659000	0.403713000	5.369016000
C	-2.327978000	0.360258000	2.834346000
H	-2.910560000	0.660509000	3.710285000
H	-2.451309000	1.096264000	2.043754000
H	-2.679224000	-0.610286000	2.477325000
C	2.607742000	-0.027347000	2.739417000
H	3.215527000	-0.310513000	3.603976000
H	2.670658000	-0.802147000	1.979369000
H	2.977898000	0.912429000	2.323436000
N	1.217782000	0.106382000	3.172824000
N	-0.918198000	0.289976000	3.214648000

N	-1.738303000	-0.974205000	-0.028774000
N	1.118359000	-1.711192000	0.019994000
N	1.856961000	1.106920000	-0.093498000
N	-1.020848000	1.850822000	-0.018060000
C	-3.002376000	-0.426413000	-0.120348000
C	-1.869599000	-2.308810000	0.320056000
C	0.555693000	-2.961231000	0.149735000
C	2.446422000	-1.865563000	-0.335212000
C	3.101012000	0.560029000	-0.293864000
C	1.994578000	2.463990000	0.088146000
C	-0.442411000	3.100541000	-0.014901000
C	-2.359645000	1.991805000	-0.325246000
C	-3.977927000	-1.454566000	0.201892000
H	-5.045645000	-1.303891000	0.237620000
C	-3.284729000	-2.599307000	0.496289000
H	-3.690556000	-3.548752000	0.807652000
C	1.570456000	-3.959040000	-0.151526000
H	1.407636000	-5.025450000	-0.154959000
C	2.721975000	-3.287225000	-0.470352000
H	3.666008000	-3.711861000	-0.773437000
C	4.095329000	1.619461000	-0.161217000
H	5.162738000	1.479246000	-0.230289000
C	3.420627000	2.780779000	0.096876000
H	3.840006000	3.758886000	0.270193000
C	-1.468521000	4.085033000	-0.331120000
H	-1.299062000	5.146756000	-0.417529000
C	-2.636431000	3.404484000	-0.543707000
H	-3.590317000	3.814230000	-0.836035000
C	-3.300606000	0.936669000	-0.361243000
C	-0.811434000	-3.242888000	0.397584000
C	3.381699000	-0.813398000	-0.476478000
C	0.934221000	3.395664000	0.142984000
C	-4.730836000	1.275705000	-0.604300000
C	-5.454331000	0.610671000	-1.615033000
H	-4.946582000	-0.137091000	-2.215317000
C	-6.800263000	0.908961000	-1.849371000
H	-7.338220000	0.390158000	-2.637065000
C	-7.451372000	1.878750000	-1.075660000
H	-8.495925000	2.111792000	-1.257313000
C	-6.745933000	2.544401000	-0.064367000
H	-7.245389000	3.290324000	0.546444000
C	-5.400127000	2.244285000	0.170180000
H	-4.856283000	2.751188000	0.960015000
C	-1.154159000	-4.669232000	0.668308000
C	-2.089088000	-5.365101000	-0.123511000

H	-2.570123000	-4.846168000	-0.945681000
C	-2.387634000	-6.707396000	0.133028000
H	-3.106958000	-7.228142000	-0.491830000
C	-1.752654000	-7.382030000	1.184100000
H	-1.983643000	-8.423965000	1.382894000
C	-0.814691000	-6.704392000	1.974278000
H	-0.318545000	-7.219210000	2.791434000
C	-0.517694000	-5.362033000	1.717635000
H	0.206766000	-4.833623000	2.328398000
C	4.796204000	-1.174241000	-0.780740000
C	5.450165000	-0.604130000	-1.891154000
H	4.900288000	0.084279000	-2.524136000
C	6.781078000	-0.923956000	-2.178832000
H	7.266880000	-0.480100000	-3.042461000
C	7.483937000	-1.818445000	-1.360655000
H	8.516893000	-2.066773000	-1.584086000
C	6.846324000	-2.388934000	-0.251141000
H	7.386607000	-3.075811000	0.393365000
C	5.515478000	-2.068342000	0.036678000
H	5.023629000	-2.500911000	0.901533000
C	1.284879000	4.841344000	0.275083000
C	2.134761000	5.478614000	-0.649764000
H	2.539615000	4.901896000	-1.474268000
C	2.440829000	6.837510000	-0.519757000
H	3.092665000	7.314231000	-1.245576000
C	1.899568000	7.584496000	0.534861000
H	2.137179000	8.639089000	0.635069000
C	1.045488000	6.963909000	1.456107000
H	0.621074000	7.535839000	2.275738000
C	0.739184000	5.605268000	1.325227000
H	0.077071000	5.120371000	2.035146000
C	-0.348239000	-2.452757000	-2.984602000
S	-0.281374000	-0.713145000	-3.704872000
C	-2.104834000	-0.259790000	-3.578908000
H	-2.416124000	-0.471733000	-2.556760000
H	-2.165893000	0.813099000	-3.766549000
H	-2.685210000	-0.822012000	-4.315138000
H	0.672586000	-2.714226000	-2.702302000
H	-0.972944000	-2.413218000	-2.094105000
H	-0.742667000	-3.147872000	-3.729993000

³TS-2_{is}

Fe	0.068239000	0.080320000	-0.070220000
O	0.217307000	0.217340000	-1.980927000

C	0.114523000	0.145675000	2.256096000
C	0.816903000	0.035167000	4.453838000
H	1.524451000	-0.112503000	5.252189000
C	-0.502807000	0.362075000	4.471559000
H	-1.178839000	0.549424000	5.288673000
C	-2.286717000	0.722671000	2.738389000
H	-2.806667000	1.166408000	3.592683000
H	-2.277350000	1.426582000	1.910025000
H	-2.805115000	-0.187831000	2.427500000
C	2.531358000	-0.422618000	2.674825000
H	3.080642000	-0.822962000	3.532226000
H	2.485448000	-1.171208000	1.887642000
H	3.042943000	0.464717000	2.293914000
N	1.172495000	-0.094052000	3.106273000
N	-0.910003000	0.426140000	3.133992000
N	-1.771856000	-0.717491000	-0.034210000
N	0.848280000	-1.767950000	-0.010878000
N	1.898486000	0.856973000	-0.102467000
N	-0.727278000	1.915245000	-0.087316000
C	-2.958543000	-0.039585000	-0.245667000
C	-2.107848000	-1.998594000	0.387354000
C	0.171311000	-2.942103000	0.244925000
C	2.123101000	-2.115369000	-0.431616000
C	3.063167000	0.171854000	-0.375396000
C	2.248988000	2.164052000	0.174311000
C	-0.032311000	3.100102000	0.033930000
C	-2.021185000	2.239893000	-0.461983000
C	-4.073051000	-0.910579000	0.070046000
H	-5.111671000	-0.624204000	0.015958000
C	-3.550509000	-2.101424000	0.495580000
H	-4.086391000	-2.969593000	0.843784000
C	1.036465000	-4.069381000	-0.042256000
H	0.747847000	-5.104840000	0.047891000
C	2.223769000	-3.560864000	-0.496118000
H	3.088422000	-4.108177000	-0.836076000
C	4.196203000	1.064727000	-0.198322000
H	5.229053000	0.776557000	-0.315410000
C	3.699070000	2.279625000	0.178552000
H	4.249949000	3.174667000	0.418232000
C	-0.912069000	4.211012000	-0.282591000
H	-0.614712000	5.247667000	-0.287229000
C	-2.123265000	3.680167000	-0.622493000
H	-3.003734000	4.205909000	-0.955295000
C	-3.084647000	1.328668000	-0.554771000
C	-1.196841000	-3.053121000	0.558073000

C	3.175300000	-1.205852000	-0.629316000
C	1.345222000	3.231239000	0.282042000
C	-4.446240000	1.827849000	-0.896092000
C	-5.166449000	1.240969000	-1.955879000
H	-4.704059000	0.439149000	-2.521637000
C	-6.452813000	1.682847000	-2.281172000
H	-6.988842000	1.222229000	-3.105523000
C	-7.046644000	2.719877000	-1.549958000
H	-8.044879000	3.064138000	-1.801823000
C	-6.345209000	3.307197000	-0.488679000
H	-6.802491000	4.103501000	0.090782000
C	-5.059243000	2.863374000	-0.163230000
H	-4.521114000	3.308090000	0.666922000
C	-1.695045000	-4.397716000	0.961963000
C	-2.709078000	-5.061910000	0.244224000
H	-3.141325000	-4.578421000	-0.625236000
C	-3.145759000	-6.333083000	0.632185000
H	-3.925199000	-6.831389000	0.063635000
C	-2.571388000	-6.967878000	1.741298000
H	-2.909819000	-7.954704000	2.041548000
C	-1.553508000	-6.323344000	2.456668000
H	-1.101754000	-6.808505000	3.316612000
C	-1.118625000	-5.051891000	2.069037000
H	-0.330848000	-4.548869000	2.620175000
C	4.511844000	-1.720001000	-1.040615000
C	5.138459000	-1.196077000	-2.188862000
H	4.622300000	-0.433344000	-2.762428000
C	6.398761000	-1.653567000	-2.587188000
H	6.863464000	-1.243687000	-3.478768000
C	7.057945000	-2.640475000	-1.842213000
H	8.036143000	-2.995873000	-2.151142000
C	6.449236000	-3.162903000	-0.693537000
H	6.958859000	-3.918931000	-0.103765000
C	5.188812000	-2.704756000	-0.294995000
H	4.723644000	-3.097663000	0.602821000
C	1.863550000	4.605353000	0.539218000
C	2.823404000	5.202012000	-0.301148000
H	3.192569000	4.644732000	-1.155164000
C	3.281960000	6.500114000	-0.052246000
H	4.017732000	6.947108000	-0.713931000
C	2.785199000	7.226631000	1.037939000
H	3.141069000	8.234134000	1.230186000
C	1.821881000	6.647829000	1.874702000
H	1.430168000	7.204969000	2.720399000
C	1.363374000	5.350004000	1.625197000

H	0.615558000	4.897971000	2.268671000
C	-0.581287000	-2.500515000	-2.866090000
S	-0.279207000	-0.781398000	-3.581799000
C	-2.071027000	-0.204398000	-3.681182000
H	-2.509826000	-0.366349000	-2.697036000
H	-2.035826000	0.863997000	-3.897843000
H	-2.598882000	-0.751074000	-4.467223000
H	0.386072000	-2.879680000	-2.535294000
H	-1.243867000	-2.385125000	-2.009853000
H	-1.015508000	-3.141625000	-3.637652000

¹TS-2_{ts}

Fe	-0.129847000	0.016381000	-0.044571000
O	-0.110309000	-0.029559000	-1.721948000
C	-0.345338000	-0.002932000	2.110866000
C	-0.377608000	0.655310000	4.319227000
H	-0.258379000	1.341560000	5.139922000
C	-0.766403000	-0.644788000	4.283502000
H	-1.049780000	-1.325938000	5.067406000
C	-1.084916000	-2.397029000	2.538244000
H	-1.559182000	-2.891150000	3.390925000
H	-1.779767000	-2.369481000	1.705173000
H	-0.190697000	-2.951243000	2.248134000
C	0.314490000	2.389347000	2.666662000
H	0.657426000	2.867350000	3.588760000
H	1.134772000	2.344757000	1.957524000
H	-0.504943000	2.969732000	2.238468000
N	-0.123855000	1.031109000	2.997331000
N	-0.742138000	-1.030876000	2.940527000
N	0.486829000	-1.877247000	0.002099000
N	1.705949000	0.633557000	0.226363000
N	-0.758073000	1.895925000	-0.102483000
N	-2.019597000	-0.621927000	-0.083288000
C	-0.240611000	-2.968309000	-0.419172000
C	1.693208000	-2.345014000	0.481675000
C	2.784820000	-0.142501000	0.608414000
C	2.205143000	1.867346000	-0.174581000
C	0.025448000	2.986766000	-0.395173000
C	-2.032565000	2.359744000	0.157265000
C	-3.140699000	0.159699000	0.080846000
C	-2.435599000	-1.852505000	-0.575016000
C	0.530056000	-4.174521000	-0.181148000
H	0.188323000	-5.174328000	-0.397899000

C	1.702272000	-3.794674000	0.413531000
H	2.502883000	-4.428030000	0.759958000
C	3.997112000	0.637553000	0.473061000
H	4.987393000	0.268599000	0.687914000
C	3.645526000	1.851493000	-0.049589000
H	4.296927000	2.660071000	-0.337889000
C	-0.774392000	4.193828000	-0.291044000
H	-0.399710000	5.193213000	-0.447213000
C	-2.028843000	3.812509000	0.095583000
H	-2.876167000	4.444943000	0.304867000
C	-4.313298000	-0.613035000	-0.279777000
H	-5.323540000	-0.236404000	-0.256157000
C	-3.876872000	-1.830458000	-0.722968000
H	-4.468670000	-2.637116000	-1.123976000
C	-1.598777000	-2.958301000	-0.787776000
C	2.771930000	-1.526524000	0.848201000
C	1.424055000	2.974946000	-0.529434000
C	-3.161990000	1.545606000	0.325713000
C	-2.172934000	-4.226086000	-1.316373000
C	-1.597861000	-4.827208000	-2.453643000
H	-0.757246000	-4.337961000	-2.934459000
C	-2.106436000	-6.026605000	-2.962320000
H	-1.656266000	-6.471014000	-3.844643000
C	-3.196544000	-6.649667000	-2.340454000
H	-3.592320000	-7.579951000	-2.735855000
C	-3.770439000	-6.067104000	-1.202907000
H	-4.607342000	-6.550096000	-0.707668000
C	-3.261116000	-4.867859000	-0.693550000
H	-3.695935000	-4.425661000	0.196554000
C	4.031756000	-2.144412000	1.347246000
C	4.725076000	-3.115444000	0.598873000
H	4.328333000	-3.420473000	-0.363336000
C	5.920799000	-3.663348000	1.075718000
H	6.446351000	-4.405969000	0.483226000
C	6.446992000	-3.245523000	2.305177000
H	7.375431000	-3.670400000	2.673833000
C	5.772636000	-2.270697000	3.052313000
H	6.176268000	-1.939056000	4.004136000
C	4.577047000	-1.723116000	2.575529000
H	4.051353000	-0.966417000	3.149016000
C	2.082704000	4.236412000	-0.964088000
C	1.731070000	4.805061000	-2.203699000
H	1.006568000	4.291062000	-2.826057000
C	2.318446000	6.000037000	-2.631525000
H	2.043834000	6.420479000	-3.593999000

C	3.263297000	6.648913000	-1.825523000
H	3.720041000	7.575894000	-2.158099000
C	3.614273000	6.096410000	-0.586858000
H	4.337711000	6.599126000	0.047920000
C	3.026780000	4.901177000	-0.158463000
H	3.286774000	4.480514000	0.807278000
C	-4.485476000	2.163395000	0.618803000
C	-5.041124000	3.159606000	-0.207460000
H	-4.491396000	3.483640000	-1.084280000
C	-6.294730000	3.708934000	0.081961000
H	-6.710943000	4.471700000	-0.568969000
C	-7.018088000	3.267545000	1.197753000
H	-7.991112000	3.694008000	1.420928000
C	-6.482147000	2.266805000	2.018982000
H	-7.038113000	1.916097000	2.883170000
C	-5.228744000	1.717611000	1.729508000
H	-4.810123000	0.940507000	2.361011000
C	2.707811000	-1.124214000	-2.637376000
S	2.401635000	0.542809000	-3.480928000
C	0.979043000	-0.000899000	-4.603746000
H	0.170472000	-0.345178000	-3.956547000
H	0.666217000	0.878450000	-5.172200000
H	1.323191000	-0.784943000	-5.285124000
H	3.477789000	-0.957703000	-1.881889000
H	1.773363000	-1.426155000	-2.163183000
H	3.049277000	-1.854869000	-3.377213000

⁵INT-2_{ss}

Fe	0.056172000	0.085070000	0.098902000
O	0.388477000	0.412039000	-2.116758000
C	0.048846000	0.042406000	2.400126000
C	0.743042000	0.047111000	4.600966000
H	1.460105000	0.049971000	5.404362000
C	-0.617274000	0.053267000	4.609778000
H	-1.324091000	0.056170000	5.422190000
C	-2.420039000	0.036770000	2.851455000
H	-3.045210000	0.293827000	3.711603000
H	-2.563149000	0.771072000	2.061508000
H	-2.700786000	-0.950250000	2.475565000
C	2.526282000	0.055511000	2.825242000
H	3.157218000	-0.215394000	3.676955000
H	2.660063000	-0.667610000	2.024015000
H	2.806369000	1.045827000	2.458004000
N	1.128407000	0.039230000	3.256172000

N	-1.018904000	0.051746000	3.269850000
N	-1.654800000	-1.120376000	-0.090665000
N	1.255078000	-1.618504000	-0.008515000
N	1.760347000	1.256258000	-0.006506000
N	-1.176396000	1.757430000	-0.000199000
C	-2.963620000	-0.680123000	-0.162908000
C	-1.677039000	-2.476793000	0.207548000
C	0.798154000	-2.917541000	0.055990000
C	2.596996000	-1.647658000	-0.343293000
C	3.050361000	0.822501000	-0.208774000
C	1.780322000	2.626232000	0.139690000
C	-0.701197000	3.051790000	-0.017941000
C	-2.520534000	1.787409000	-0.322403000
C	-3.849112000	-1.797152000	0.122148000
H	-4.925758000	-1.738657000	0.164500000
C	-3.062873000	-2.890931000	0.371836000
H	-3.387901000	-3.882221000	0.645372000
C	1.894917000	-3.812858000	-0.272447000
H	1.821963000	-4.887793000	-0.328766000
C	2.991527000	-3.032819000	-0.538996000
H	3.972312000	-3.364025000	-0.842569000
C	3.948338000	1.966848000	-0.086228000
H	5.024121000	1.921577000	-0.154309000
C	3.173830000	3.068705000	0.148169000
H	3.505131000	4.083686000	0.299221000
C	-1.798063000	3.944359000	-0.365680000
H	-1.712858000	5.013939000	-0.476291000
C	-2.906582000	3.168598000	-0.571260000
H	-3.886998000	3.495374000	-0.880651000
C	-3.373999000	0.660069000	-0.366435000
C	-0.545529000	-3.322059000	0.264833000
C	3.446122000	-0.516116000	-0.421197000
C	0.644346000	3.464710000	0.154248000
C	-4.827961000	0.891160000	-0.594624000
C	-5.514582000	0.180740000	-1.600399000
H	-4.961784000	-0.526624000	-2.209749000
C	-6.881342000	0.381557000	-1.817500000
H	-7.389818000	-0.171972000	-2.601221000
C	-7.591657000	1.298996000	-1.032013000
H	-8.652454000	1.456608000	-1.200291000
C	-6.923522000	2.010086000	-0.026387000
H	-7.467719000	2.716278000	0.593429000
C	-5.557045000	1.806617000	0.191154000
H	-5.041685000	2.349474000	0.976140000
C	-0.770418000	-4.781241000	0.478828000

C	-1.641005000	-5.522851000	-0.344389000
H	-2.161228000	-5.015563000	-1.149917000
C	-1.829489000	-6.893628000	-0.138929000
H	-2.501195000	-7.448195000	-0.787365000
C	-1.145852000	-7.552320000	0.891470000
H	-1.291263000	-8.616309000	1.050704000
C	-0.270472000	-6.829134000	1.712551000
H	0.262852000	-7.330958000	2.514283000
C	-0.084382000	-5.458337000	1.507163000
H	0.591398000	-4.894727000	2.141694000
C	4.888733000	-0.754662000	-0.717193000
C	5.508221000	-0.108361000	-1.805385000
H	4.913377000	0.552887000	-2.426575000
C	6.862662000	-0.317263000	-2.085399000
H	7.321376000	0.185521000	-2.931473000
C	7.624261000	-1.176558000	-1.282269000
H	8.675451000	-1.339043000	-1.499657000
C	7.021007000	-1.823689000	-0.195825000
H	7.605702000	-2.484967000	0.436660000
C	5.666577000	-1.613581000	0.084204000
H	5.199985000	-2.108034000	0.929769000
C	0.870488000	4.938536000	0.249228000
C	1.667838000	5.620869000	-0.690095000
H	2.125472000	5.057766000	-1.496249000
C	1.857294000	7.003894000	-0.596802000
H	2.470924000	7.514136000	-1.333179000
C	1.248601000	7.730932000	0.434727000
H	1.395274000	8.804306000	0.506480000
C	0.445136000	7.065201000	1.369873000
H	-0.031118000	7.621218000	2.171868000
C	0.256426000	5.682214000	1.275855000
H	-0.366861000	5.162652000	1.996383000
C	-0.005477000	-2.290082000	-3.000138000
S	-0.108990000	-0.457232000	-3.491716000
C	-2.003371000	-0.303184000	-3.488387000
H	-2.359242000	-0.710495000	-2.543212000
H	-2.219010000	0.764251000	-3.547370000
H	-2.394154000	-0.841843000	-4.355384000
H	1.022990000	-2.466686000	-2.683453000
H	-0.688646000	-2.451231000	-2.168359000
H	-0.267072000	-2.885759000	-3.878287000

³INT-2_{is}

Fe	0.060317000	0.076084000	0.007647000
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O	0.467719000	0.193023000	-2.280409000
C	0.057134000	0.152468000	2.345311000
C	0.763299000	0.193762000	4.542711000
H	1.479650000	0.149988000	5.345790000
C	-0.585752000	0.376263000	4.551295000
H	-1.278996000	0.516102000	5.363630000
C	-2.387193000	0.486328000	2.790027000
H	-2.976207000	0.852437000	3.636150000
H	-2.443231000	1.196102000	1.966796000
H	-2.783508000	-0.475277000	2.454653000
C	2.515702000	-0.132806000	2.761418000
H	3.109320000	-0.475903000	3.614176000
H	2.537412000	-0.880548000	1.971536000
H	2.930641000	0.801576000	2.374658000
N	1.132817000	0.057689000	3.200069000
N	-0.993618000	0.349559000	3.213175000
N	-1.674458000	-0.917476000	-0.028652000
N	1.067325000	-1.671084000	-0.004167000
N	1.783645000	1.050334000	-0.068993000
N	-0.962313000	1.806580000	-0.119764000
C	-2.947105000	-0.387019000	-0.204572000
C	-1.852190000	-2.246841000	0.359083000
C	0.523761000	-2.923919000	0.202156000
C	2.382311000	-1.863095000	-0.401953000
C	3.036737000	0.514378000	-0.306019000
C	1.967910000	2.404688000	0.167083000
C	-0.407779000	3.067887000	-0.034803000
C	-2.291804000	1.977515000	-0.477980000
C	-3.941977000	-1.394087000	0.111189000
H	-5.008038000	-1.232962000	0.084727000
C	-3.270839000	-2.521571000	0.490037000
H	-3.690344000	-3.456400000	0.825782000
C	1.512922000	-3.934240000	-0.100288000
H	1.343573000	-4.998360000	-0.046511000
C	2.649012000	-3.281422000	-0.505497000
H	3.579843000	-3.716639000	-0.832203000
C	4.046582000	1.546396000	-0.131080000
H	5.109528000	1.386916000	-0.219348000
C	3.392827000	2.697545000	0.195862000
H	3.822095000	3.661347000	0.417736000
C	-1.406776000	4.059270000	-0.372220000
H	-1.230101000	5.122802000	-0.408593000
C	-2.559528000	3.386744000	-0.676448000
H	-3.499854000	3.801795000	-1.001938000
C	-3.246649000	0.947014000	-0.521512000

C	-0.829316000	-3.195822000	0.489796000
C	3.325410000	-0.833150000	-0.559328000
C	0.946956000	3.360583000	0.217588000
C	-4.665560000	1.281919000	-0.829501000
C	-5.345510000	0.603169000	-1.860441000
H	-4.813004000	-0.152576000	-2.428564000
C	-6.681833000	0.893803000	-2.153196000
H	-7.186117000	0.362981000	-2.955135000
C	-7.366779000	1.870415000	-1.418341000
H	-8.403738000	2.097887000	-1.645097000
C	-6.705066000	2.549147000	-0.386565000
H	-7.231119000	3.300107000	0.195123000
C	-5.369111000	2.255770000	-0.093638000
H	-4.859788000	2.773550000	0.711943000
C	-1.176258000	-4.603363000	0.836121000
C	-2.106068000	-5.345528000	0.081651000
H	-2.587062000	-4.875530000	-0.769482000
C	-2.399588000	-6.673082000	0.410910000
H	-3.115601000	-7.230363000	-0.185684000
C	-1.763359000	-7.286721000	1.497883000
H	-1.990158000	-8.317325000	1.752781000
C	-0.828653000	-6.563226000	2.250418000
H	-0.330175000	-7.031123000	3.093965000
C	-0.536915000	-5.235616000	1.921113000
H	0.186148000	-4.671477000	2.500832000
C	4.724317000	-1.182636000	-0.935158000
C	5.319203000	-0.580441000	-2.061617000
H	4.734677000	0.122186000	-2.646332000
C	6.635768000	-0.883942000	-2.423483000
H	7.076008000	-0.414101000	-3.297822000
C	7.383248000	-1.794145000	-1.664270000
H	8.405184000	-2.030044000	-1.944811000
C	6.805011000	-2.395319000	-0.538552000
H	7.380962000	-3.093543000	0.061439000
C	5.488494000	-2.090429000	-0.176332000
H	5.044096000	-2.546191000	0.702168000
C	1.299607000	4.793469000	0.435031000
C	2.190981000	5.472755000	-0.417726000
H	2.630123000	4.936698000	-1.252034000
C	2.493867000	6.822193000	-0.205748000
H	3.178960000	7.331906000	-0.876488000
C	1.906693000	7.517901000	0.859281000
H	2.141718000	8.565137000	1.023006000
C	1.009659000	6.855890000	1.707990000
H	0.548698000	7.388309000	2.534538000

C	0.706923000	5.506860000	1.495320000
H	0.011143000	4.990174000	2.148343000
C	-0.287307000	-2.490729000	-2.894601000
S	-0.150804000	-0.718201000	-3.572927000
C	-2.011311000	-0.324310000	-3.588834000
H	-2.398376000	-0.553415000	-2.596844000
H	-2.094986000	0.743904000	-3.792147000
H	-2.484253000	-0.921008000	-4.373092000
H	0.716979000	-2.779669000	-2.582699000
H	-0.955080000	-2.463633000	-2.035283000
H	-0.662563000	-3.130218000	-3.697478000

¹INT-2_h

Fe	0.093102000	0.035830000	0.097065000
O	0.159573000	0.262752000	-1.946062000
C	0.139636000	0.025472000	2.100160000
C	0.486623000	-0.587554000	4.300542000
H	0.825365000	-1.225931000	5.098423000
C	-0.118910000	0.626054000	4.316025000
H	-0.424317000	1.260393000	5.130392000
C	-0.979418000	2.248824000	2.635365000
H	-0.954161000	2.897330000	3.516567000
H	-0.443826000	2.725526000	1.821452000
H	-2.016468000	2.078314000	2.337943000
C	1.286094000	-2.196317000	2.576118000
H	1.323247000	-2.840424000	3.460003000
H	0.707694000	-2.684085000	1.798726000
H	2.300384000	-2.015418000	2.213928000
N	0.637104000	-0.942102000	2.957280000
N	-0.322017000	0.988734000	2.981977000
N	-1.683752000	0.917740000	0.048381000
N	-0.814302000	-1.729931000	0.018955000
N	1.850208000	-0.863184000	-0.055947000
N	0.980392000	1.802346000	-0.004979000
C	-1.936499000	2.228649000	-0.311494000
C	-2.891909000	0.368206000	0.447447000
C	-2.141673000	-1.979274000	0.330463000
C	-0.271136000	-2.936597000	-0.414014000
C	2.080679000	-2.177265000	-0.413059000
C	3.082674000	-0.303565000	0.235663000
C	2.325910000	2.044446000	0.170879000
C	0.411607000	2.990105000	-0.445175000
C	-3.340149000	2.524587000	-0.092720000
H	-3.800593000	3.485373000	-0.262231000

C	-3.918387000	1.393501000	0.417773000
H	-4.942762000	1.259420000	0.726320000
C	-2.445791000	-3.373226000	0.066137000
H	-3.416046000	-3.825648000	0.200327000
C	-1.308883000	-3.949945000	-0.429220000
H	-1.179832000	-4.964804000	-0.769679000
C	3.498015000	-2.472388000	-0.282717000
H	3.945567000	-3.436361000	-0.467480000
C	4.107668000	-1.333164000	0.160761000
H	5.150637000	-1.191471000	0.394227000
C	2.617334000	3.432140000	-0.151276000
H	3.599432000	3.877127000	-0.115670000
C	1.449237000	4.000925000	-0.569656000
H	1.298143000	5.004349000	-0.933944000
C	-0.962728000	3.193111000	-0.635539000
C	-3.104477000	-1.004821000	0.655430000
C	1.093192000	-3.145351000	-0.671476000
C	3.311270000	1.069404000	0.412700000
C	-1.450127000	4.524614000	-1.093616000
C	-2.288498000	4.615708000	-2.222423000
H	-2.550993000	3.705037000	-2.751214000
C	-2.775186000	5.851992000	-2.659078000
H	-3.415705000	5.901355000	-3.534641000
C	-2.434171000	7.024509000	-1.971967000
H	-2.810357000	7.985164000	-2.309912000
C	-1.607965000	6.948111000	-0.843122000
H	-1.348372000	7.850333000	-0.297462000
C	-1.124048000	5.710305000	-0.406415000
H	-0.496180000	5.649607000	0.475842000
C	-4.446868000	-1.492804000	1.081730000
C	-5.614980000	-1.200165000	0.351016000
H	-5.537129000	-0.594506000	-0.545474000
C	-6.858903000	-1.691786000	0.761591000
H	-7.747869000	-1.458835000	0.183004000
C	-6.957270000	-2.492644000	1.906814000
H	-7.922407000	-2.874810000	2.224769000
C	-5.801141000	-2.802178000	2.635491000
H	-5.867730000	-3.424598000	3.522764000
C	-4.558378000	-2.308870000	2.224876000
H	-3.659797000	-2.546484000	2.784889000
C	1.552373000	-4.486640000	-1.131685000
C	2.312370000	-4.599206000	-2.312738000
H	2.537552000	-3.698854000	-2.874975000
C	2.770636000	-5.844659000	-2.754631000
H	3.351526000	-5.911864000	-3.669650000

C	2.479791000	-7.002683000	-2.021313000
H	2.834992000	-7.969870000	-2.363456000
C	1.732955000	-6.903569000	-0.840117000
H	1.514581000	-7.794195000	-0.258450000
C	1.276816000	-5.656997000	-0.397990000
H	0.711804000	-5.578051000	0.524582000
C	4.686194000	1.557093000	0.718850000
C	5.787303000	1.249641000	-0.103803000
H	5.629889000	0.638596000	-0.985787000
C	7.063044000	1.739548000	0.196138000
H	7.899121000	1.496489000	-0.452817000
C	7.260629000	2.552311000	1.320086000
H	8.250706000	2.932866000	1.551794000
C	6.170795000	2.877170000	2.138581000
H	6.313686000	3.509894000	3.009475000
C	4.895757000	2.386604000	1.838217000
H	4.047865000	2.638262000	2.467025000
C	-2.547064000	-0.354996000	-2.735008000
S	-0.709217000	-0.779270000	-3.003803000
C	-0.462507000	0.258918000	-4.564706000
H	-0.770248000	1.273509000	-4.304452000
H	0.605408000	0.230167000	-4.781630000
H	-1.053522000	-0.162414000	-5.380991000
H	-2.886944000	-0.956032000	-1.894307000
H	-2.592773000	0.707865000	-2.490532000
H	-3.082003000	-0.604564000	-3.655100000

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C	-0.000015000	-0.000121000	2.155835000
C	-0.677237000	-0.072336000	4.350511000
H	-1.383662000	-0.151804000	5.159173000
C	0.677285000	0.071613000	4.350504000
H	1.383743000	0.150852000	5.159160000
C	2.454914000	0.265663000	2.557163000
H	3.122879000	0.103367000	3.407440000
H	2.660246000	-0.470383000	1.780387000
H	2.616175000	1.265489000	2.145539000
C	-2.454939000	-0.266005000	2.557200000
H	-3.122857000	-0.103815000	3.407532000
H	-2.660288000	0.470152000	1.780528000
H	-2.616226000	-1.265773000	2.145460000
N	-1.070689000	-0.109866000	3.008884000
N	1.070691000	0.109433000	3.008876000
N	1.619964000	1.250272000	-0.450107000

N	-1.290030000	1.633043000	-0.353137000
N	-1.619983000	-1.250196000	-0.450163000
N	1.289987000	-1.632998000	-0.353230000
C	2.950292000	0.877306000	-0.545606000
C	1.586639000	2.625414000	-0.254505000
C	-0.893937000	2.956701000	-0.375456000
C	-2.644154000	1.602584000	-0.641598000
C	-2.950319000	-0.877239000	-0.545580000
C	-1.586645000	-2.625334000	-0.254506000
C	0.893923000	-2.956672000	-0.375547000
C	2.644111000	-1.602517000	-0.641672000
C	3.782362000	2.048180000	-0.356386000
H	4.860829000	2.046681000	-0.350025000
C	2.947242000	3.116522000	-0.157982000
H	3.226175000	4.140499000	0.032205000
C	-2.045155000	3.794382000	-0.685939000
H	-2.014999000	4.866810000	-0.797349000
C	-3.113526000	2.963895000	-0.864356000
H	-4.118444000	3.233701000	-1.147876000
C	-3.782373000	-2.048101000	-0.356223000
H	-4.860839000	-2.046613000	-0.349753000
C	-2.947234000	-3.116434000	-0.157838000
H	-3.226149000	-4.140402000	0.032421000
C	2.045167000	-3.794335000	-0.685946000
H	2.015049000	-4.866771000	-0.797298000
C	3.113508000	-2.963814000	-0.864418000
H	4.118439000	-3.233604000	-1.147910000
C	3.437467000	-0.440975000	-0.699159000
C	0.425357000	3.429207000	-0.226723000
C	-3.437516000	0.441051000	-0.699115000
C	-0.425364000	-3.429150000	-0.226790000
C	4.905734000	-0.606680000	-0.901263000
C	5.565465000	0.064527000	-1.949931000
H	4.984182000	0.693678000	-2.615589000
C	6.943669000	-0.081280000	-2.138138000
H	7.433393000	0.438602000	-2.955890000
C	7.689228000	-0.901539000	-1.280958000
H	8.758820000	-1.015518000	-1.427551000
C	7.045773000	-1.574106000	-0.233780000
H	7.616902000	-2.207081000	0.438667000
C	5.667560000	-1.426734000	-0.045459000
H	5.168245000	-1.942810000	0.767918000
C	0.598407000	4.907140000	-0.108144000
C	1.391655000	5.629408000	-1.021065000
H	1.885101000	5.094292000	-1.825204000

C	1.532332000	7.016360000	-0.905030000
H	2.142635000	7.557430000	-1.621741000
C	0.878982000	7.707563000	0.123882000
H	0.987654000	8.784055000	0.213101000
C	0.080811000	7.001905000	1.033871000
H	-0.428817000	7.529881000	1.834194000
C	-0.059123000	5.615047000	0.917251000
H	-0.676621000	5.064477000	1.619345000
C	-4.905769000	0.606762000	-0.901231000
C	-5.565514000	-0.064510000	-1.949859000
H	-4.984235000	-0.693718000	-2.615466000
C	-6.943708000	0.081316000	-2.138096000
H	-7.433435000	-0.438619000	-2.955813000
C	-7.689262000	0.901662000	-1.280994000
H	-8.758848000	1.015660000	-1.427618000
C	-7.045803000	1.574299000	-0.233863000
H	-7.616924000	2.207339000	0.438527000
C	-5.667598000	1.426910000	-0.045510000
H	-5.168290000	1.943026000	0.767844000
C	-0.598409000	-4.907090000	-0.108248000
C	-1.391728000	-5.629313000	-1.021143000
H	-1.885269000	-5.094150000	-1.825194000
C	-1.532366000	-7.016274000	-0.905172000
H	-2.142723000	-7.557321000	-1.621853000
C	-0.878901000	-7.707523000	0.123634000
H	-0.987541000	-8.784024000	0.212797000
C	-0.080652000	-7.001910000	1.033585000
H	0.429061000	-7.529931000	1.833825000
C	0.059251000	-5.615041000	0.917031000
H	0.676816000	-5.064500000	1.619088000
Fe	0.000035000	0.000028000	-0.008243000

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C	-0.000031000	-0.000784000	2.009700000
C	0.679226000	0.050554000	4.209990000
H	1.387202000	0.109351000	5.019353000
C	-0.678934000	-0.054439000	4.210044000
H	-1.386771000	-0.114137000	5.019461000
C	-2.461411000	-0.205132000	2.425988000
H	-3.119953000	0.017040000	3.270608000
H	-2.641054000	0.503722000	1.620001000
H	-2.660869000	-1.214994000	2.057951000
C	2.461382000	0.203409000	2.425773000
H	3.120111000	-0.018602000	3.270287000

H	2.641307000	-0.505172000	1.619598000
H	2.660306000	1.213443000	2.057945000
N	1.071576000	0.077896000	2.867887000
N	-1.071503000	-0.080339000	2.867973000
N	-1.556746000	-1.259666000	-0.453542000
N	1.268234000	-1.537680000	-0.405719000
N	1.556644000	1.260002000	-0.453395000
N	-1.268315000	1.538055000	-0.405410000
C	-2.889458000	-0.936958000	-0.655968000
C	-1.521539000	-2.616389000	-0.155568000
C	0.932108000	-2.875170000	-0.262990000
C	2.617507000	-1.510387000	-0.753722000
C	2.889357000	0.937306000	-0.655781000
C	1.521450000	2.616699000	-0.155224000
C	-0.932192000	2.875530000	-0.262529000
C	-2.617619000	1.510778000	-0.753319000
C	-3.711608000	-2.107259000	-0.443508000
H	-4.787544000	-2.124733000	-0.512985000
C	-2.872111000	-3.132792000	-0.102572000
H	-3.138440000	-4.145582000	0.153456000
C	2.091023000	-3.702904000	-0.538372000
H	2.089902000	-4.781342000	-0.524888000
C	3.116744000	-2.867328000	-0.869800000
H	4.115584000	-3.133110000	-1.175573000
C	3.711516000	2.107563000	-0.443137000
H	4.787449000	2.125041000	-0.512630000
C	2.872024000	3.133058000	-0.102055000
H	3.138367000	4.145809000	0.154115000
C	-2.091132000	3.703283000	-0.537771000
H	-2.090010000	4.781718000	-0.524169000
C	-3.116879000	2.867739000	-0.869173000
H	-4.115744000	3.133542000	-1.174854000
C	-3.395112000	0.353784000	-0.883475000
C	-0.354048000	-3.385243000	-0.031110000
C	3.395021000	-0.353375000	-0.883607000
C	0.353988000	3.385571000	-0.030692000
C	-4.849144000	0.481802000	-1.187392000
C	-5.402229000	-0.196014000	-2.291334000
H	-4.749227000	-0.792427000	-2.919875000
C	-6.767922000	-0.100794000	-2.578281000
H	-7.175555000	-0.624700000	-3.437434000
C	-7.606554000	0.671931000	-1.764175000
H	-8.666434000	0.746455000	-1.986857000
C	-7.069570000	1.346192000	-0.659636000
H	-7.714115000	1.939820000	-0.018410000

C	-5.703707000	1.249909000	-0.372925000
H	-5.287805000	1.764519000	0.486897000
C	-0.470629000	-4.844168000	0.254773000
C	-1.221947000	-5.701648000	-0.572116000
H	-1.727672000	-5.287010000	-1.437430000
C	-1.304357000	-7.070412000	-0.294633000
H	-1.883060000	-7.717841000	-0.946425000
C	-0.633107000	-7.607157000	0.811958000
H	-0.696782000	-8.669470000	1.026398000
C	0.125329000	-6.765845000	1.636604000
H	0.649691000	-7.173948000	2.495362000
C	0.207498000	-5.397459000	1.358535000
H	0.794625000	-4.741814000	1.993261000
C	4.849050000	-0.481333000	-1.187512000
C	5.402172000	0.196720000	-2.291304000
H	4.749179000	0.793273000	-2.919722000
C	6.767864000	0.101551000	-2.578238000
H	7.175518000	0.625635000	-3.437274000
C	7.606479000	-0.671345000	-1.764267000
H	8.666362000	-0.745821000	-1.986937000
C	7.069467000	-1.345821000	-0.659881000
H	7.713987000	-1.939585000	-0.018752000
C	5.703591000	-1.249595000	-0.373185000
H	5.287679000	-1.764393000	0.486523000
C	0.470677000	4.844455000	0.255314000
C	1.222025000	5.701926000	-0.571546000
H	1.727639000	5.287318000	-1.436939000
C	1.304599000	7.070656000	-0.293944000
H	1.883326000	7.718080000	-0.945724000
C	0.633513000	7.607373000	0.812755000
H	0.697328000	8.669655000	1.027298000
C	-0.124921000	6.766060000	1.637404000
H	-0.649153000	7.174141000	2.496252000
C	-0.207253000	5.397708000	1.359221000
H	-0.794366000	4.742060000	1.993962000
Fe	-0.000054000	0.000205000	-0.227704000

'P-2

C	0.000093000	-0.000151000	1.784321000
C	0.657145000	0.167785000	3.987568000
H	1.347129000	0.344962000	4.794419000
C	-0.656581000	-0.168981000	3.987609000
H	-1.346445000	-0.346449000	4.794498000
C	-2.421033000	-0.616274000	2.283215000

H	-2.928706000	-0.973607000	3.183776000
H	-2.947313000	0.253922000	1.885656000
H	-2.416395000	-1.405421000	1.537318000
C	2.421259000	0.615953000	2.283059000
H	2.928918000	0.973383000	3.183588000
H	2.947692000	-0.254135000	1.885454000
H	2.416405000	1.405109000	1.537177000
N	1.046815000	0.269333000	2.649197000
N	-1.046487000	-0.269941000	2.649262000
N	-0.588985000	-1.890474000	-0.342207000
N	1.877139000	-0.590100000	-0.386172000
N	0.588928000	1.890527000	-0.342134000
N	-1.877191000	0.590132000	-0.386086000
C	-1.864498000	-2.360830000	-0.626415000
C	0.175979000	-3.010588000	-0.033155000
C	2.352578000	-1.878496000	-0.184510000
C	2.974893000	0.169582000	-0.786687000
C	1.864422000	2.360891000	-0.626394000
C	-0.176013000	3.010648000	-0.033019000
C	-2.352614000	1.878549000	-0.184388000
C	-2.974956000	-0.169516000	-0.786585000
C	-1.909530000	-3.797271000	-0.436165000
H	-2.789700000	-4.406469000	-0.568168000
C	-0.665385000	-4.191100000	-0.034174000
H	-0.337232000	-5.186180000	0.219017000
C	3.771681000	-1.928940000	-0.473730000
H	4.375644000	-2.821228000	-0.424087000
C	4.143900000	-0.680687000	-0.884214000
H	5.114713000	-0.359350000	-1.225247000
C	1.909456000	3.797338000	-0.436192000
H	2.789615000	4.406541000	-0.568271000
C	0.665355000	4.191149000	-0.034056000
H	0.337215000	5.186224000	0.219177000
C	-3.771712000	1.929009000	-0.473617000
H	-4.375692000	2.821284000	-0.423940000
C	-4.143935000	0.680766000	-0.884150000
H	-5.114754000	0.359473000	-1.225198000
C	-2.978922000	-1.562659000	-0.926501000
C	1.568930000	-3.006013000	0.103251000
C	2.978831000	1.562713000	-0.926545000
C	-1.568960000	3.006050000	0.103416000
C	-4.240141000	-2.258649000	-1.312978000
C	-4.258338000	-3.103839000	-2.439368000
H	-3.349829000	-3.219184000	-3.021223000
C	-5.425532000	-3.781748000	-2.806344000

H	-5.423008000	-4.423969000	-3.681748000
C	-6.595227000	-3.629835000	-2.050128000
H	-7.501461000	-4.155554000	-2.334488000
C	-6.587741000	-2.797999000	-0.922901000
H	-7.487252000	-2.682803000	-0.325719000
C	-5.419792000	-2.120315000	-0.556717000
H	-5.410131000	-1.483443000	0.321484000
C	2.284949000	-4.271817000	0.433409000
C	2.162974000	-5.424003000	-0.366511000
H	1.527478000	-5.389683000	-1.244705000
C	2.862610000	-6.592668000	-0.046441000
H	2.761297000	-7.470441000	-0.677430000
C	3.700651000	-6.628084000	1.075732000
H	4.243691000	-7.535016000	1.322982000
C	3.838567000	-5.484477000	1.873284000
H	4.487779000	-5.502880000	2.743459000
C	3.138634000	-4.316664000	1.552610000
H	3.243267000	-3.427635000	2.166159000
C	4.240040000	2.258765000	-1.313035000
C	4.258174000	3.104026000	-2.439357000
H	3.349658000	3.219365000	-3.021205000
C	5.425333000	3.782034000	-2.806278000
H	5.422792000	4.424316000	-3.681637000
C	6.595030000	3.630137000	-2.050062000
H	7.501226000	4.155940000	-2.334389000
C	6.587600000	2.798221000	-0.922894000
H	7.487113000	2.683058000	-0.325711000
C	5.419687000	2.120442000	-0.556765000
H	5.410048000	1.483499000	0.321389000
C	-2.284957000	4.271865000	0.433623000
C	-2.162965000	5.424065000	-0.366285000
H	-1.527485000	5.389739000	-1.244490000
C	-2.862573000	6.592743000	-0.046193000
H	-2.761261000	7.470520000	-0.677176000
C	-3.700586000	6.628158000	1.076003000
H	-4.243599000	7.535099000	1.323279000
C	-3.838484000	5.484552000	1.873563000
H	-4.487658000	5.502963000	2.743766000
C	-3.138581000	4.316728000	1.552864000
H	-3.243213000	3.427698000	2.166409000
Fe	-0.000014000	0.000024000	-0.154686000

OAT in SMe₂ by species 3

⁶RC-3_{hs}

Co	0.203131000	0.036620000	0.076137000
O	-0.045770000	0.027069000	-1.821591000
C	0.498287000	0.047871000	2.327536000
C	0.123004000	0.328109000	4.580429000
H	-0.434934000	0.618459000	5.454158000
C	1.355186000	-0.231584000	4.444445000
H	2.090398000	-0.521912000	5.175333000
C	2.791197000	-0.975850000	2.522606000
H	3.367984000	-1.407236000	3.345279000
H	2.530255000	-1.754992000	1.810365000
H	3.386466000	-0.211806000	2.019124000
C	-1.706251000	1.056009000	3.021472000
H	-2.089561000	1.487837000	3.949933000
H	-1.623694000	1.831994000	2.264150000
H	-2.389256000	0.281053000	2.668089000
N	-0.381213000	0.492610000	3.287274000
N	1.564615000	-0.396477000	3.072642000
N	2.214468000	0.294718000	-0.310185000
N	-0.080936000	2.086686000	0.143955000
N	-1.800594000	-0.253795000	0.167075000
N	0.516636000	-2.033327000	0.078402000
C	3.139540000	-0.693468000	-0.573317000
C	2.897707000	1.486413000	-0.133503000
C	0.927157000	3.025193000	0.077132000
C	-1.278485000	2.734425000	-0.081458000
C	-2.771640000	0.736193000	0.076275000
C	-2.436005000	-1.446161000	0.493933000
C	-0.470163000	-2.973487000	0.256118000
C	1.642724000	-2.689355000	-0.392537000
C	4.464868000	-0.112765000	-0.532192000
H	5.384311000	-0.659118000	-0.671324000
C	4.318531000	1.219337000	-0.234041000
H	5.099982000	1.948355000	-0.091508000
C	0.333942000	4.334061000	-0.159054000
H	0.890496000	5.250380000	-0.276316000
C	-1.015301000	4.151890000	-0.278810000
H	-1.763213000	4.893308000	-0.509694000
C	-4.055234000	0.148558000	0.389053000
H	-4.987315000	0.689695000	0.421069000
C	-3.847087000	-1.177541000	0.673405000
H	-4.582815000	-1.905027000	0.976660000
C	0.056505000	-4.287870000	-0.084242000
H	-0.510621000	-5.204852000	-0.055004000
C	1.343793000	-4.110144000	-0.505268000

H	2.021565000	-4.858334000	-0.883908000
C	2.872724000	-2.079054000	-0.699480000
C	2.312390000	2.760827000	0.054666000
C	-2.547149000	2.116216000	-0.109363000
C	-1.826295000	-2.713263000	0.556363000
C	4.008698000	-2.946232000	-1.120726000
C	4.708287000	-2.668971000	-2.312253000
H	4.391697000	-1.828686000	-2.920988000
C	5.784350000	-3.467866000	-2.711806000
H	6.306082000	-3.244477000	-3.637268000
C	6.183203000	-4.557405000	-1.926105000
H	7.017986000	-5.177915000	-2.236685000
C	5.498900000	-4.840935000	-0.736841000
H	5.807119000	-5.678177000	-0.118042000
C	4.422928000	-4.041622000	-0.337196000
H	3.898361000	-4.254639000	0.588345000
C	3.217486000	3.943398000	0.135971000
C	4.163052000	4.216608000	-0.872343000
H	4.229415000	3.549709000	-1.725072000
C	4.992325000	5.339794000	-0.788738000
H	5.709792000	5.538899000	-1.578860000
C	4.889101000	6.212779000	0.302426000
H	5.532332000	7.084869000	0.366527000
C	3.946641000	5.957093000	1.307217000
H	3.859768000	6.629051000	2.155590000
C	3.117028000	4.834203000	1.223120000
H	2.385452000	4.632923000	1.998847000
C	-3.748216000	2.981259000	-0.283793000
C	-4.674216000	2.701993000	-1.308532000
H	-4.482356000	1.866962000	-1.975552000
C	-5.810210000	3.501832000	-1.472995000
H	-6.510044000	3.279363000	-2.272669000
C	-6.041205000	4.588091000	-0.618327000
H	-6.923431000	5.207472000	-0.748115000
C	-5.127232000	4.871553000	0.405546000
H	-5.302844000	5.707142000	1.076459000
C	-3.990421000	4.073865000	0.571895000
H	-3.284994000	4.286554000	1.368780000
C	-2.682015000	-3.897268000	0.860589000
C	-3.812952000	-4.210175000	0.081792000
H	-4.062301000	-3.577185000	-0.762687000
C	-4.592841000	-5.334162000	0.374228000
H	-5.457298000	-5.564063000	-0.241041000
C	-4.253146000	-6.167895000	1.447809000
H	-4.858580000	-7.040111000	1.673870000

C	-3.123954000	-5.873387000	2.223310000
H	-2.852620000	-6.515888000	3.055442000
C	-2.344375000	-4.749704000	1.930080000
H	-1.468123000	-4.518804000	2.527248000
C	-2.870727000	-1.557144000	-2.847904000
H	-3.600796000	-1.840679000	-2.088622000
H	-2.661957000	-2.391872000	-3.520251000
H	-1.956687000	-1.205545000	-2.366065000
S	-3.632986000	-0.105490000	-3.829624000
C	-2.010239000	0.656613000	-4.492964000
H	-1.589978000	0.007350000	-5.264268000
H	-2.269973000	1.629217000	-4.917091000
H	-1.312689000	0.765114000	-3.659145000

⁴RC-3_{is}

Co	0.221929000	0.017077000	0.089666000
O	0.061003000	-0.021202000	-1.608577000
C	0.445847000	0.058865000	2.182983000
C	0.757955000	0.775677000	4.344094000
H	0.920019000	1.500765000	5.122586000
C	0.611649000	-0.572523000	4.386598000
H	0.623894000	-1.266158000	5.209287000
C	0.233743000	-2.415846000	2.762262000
H	0.046466000	-2.939646000	3.703626000
H	-0.622664000	-2.535179000	2.107231000
H	1.123179000	-2.830488000	2.286080000
C	0.773624000	2.552561000	2.605558000
H	1.154130000	3.111373000	3.464970000
H	1.472997000	2.639615000	1.780669000
H	-0.196707000	2.954525000	2.311596000
N	0.656421000	1.146802000	3.002105000
N	0.422315000	-0.995690000	3.069738000
N	1.135709000	-1.741284000	-0.022902000
N	2.067136000	1.014482000	-0.043460000
N	-0.711276000	1.771043000	0.107460000
N	-1.610781000	-0.974472000	0.391960000
C	0.513866000	-2.957558000	-0.244920000
C	2.498309000	-1.965891000	0.100272000
C	3.290817000	0.398017000	-0.052268000
C	2.229674000	2.295655000	-0.525224000
C	-0.159022000	2.978609000	-0.283495000
C	-2.013519000	2.004372000	0.523610000
C	-2.807613000	-0.358532000	0.652745000
C	-1.870843000	-2.276556000	0.025697000

C	1.522194000	-3.998680000	-0.206132000
H	1.318696000	-5.051852000	-0.317763000
C	2.726326000	-3.399182000	0.046025000
H	3.684009000	-3.877942000	0.169027000
C	4.295852000	1.349145000	-0.511504000
H	5.345404000	1.129026000	-0.629568000
C	3.638246000	2.505351000	-0.831271000
H	4.055378000	3.404069000	-1.257059000
C	-1.140440000	4.022019000	-0.060380000
H	-0.973449000	5.070568000	-0.248545000
C	-2.258327000	3.433377000	0.466066000
H	-3.171565000	3.916409000	0.773303000
C	-3.883047000	-1.327503000	0.489526000
H	-4.932554000	-1.113057000	0.617751000
C	-3.309172000	-2.498828000	0.074190000
H	-3.807788000	-3.416073000	-0.195830000
C	-0.875141000	-3.211462000	-0.313441000
C	3.510710000	-0.983350000	0.136414000
C	1.181840000	3.225629000	-0.660709000
C	-2.986291000	1.029252000	0.826451000
C	-1.296463000	-4.580510000	-0.720703000
C	-0.861830000	-5.107885000	-1.953045000
H	-0.228658000	-4.497789000	-2.588440000
C	-1.251399000	-6.388238000	-2.358661000
H	-0.915208000	-6.775414000	-3.315527000
C	-2.079894000	-7.165504000	-1.538360000
H	-2.383816000	-8.158605000	-1.854086000
C	-2.513736000	-6.654240000	-0.308166000
H	-3.148828000	-7.253962000	0.336702000
C	-2.123993000	-5.373481000	0.097755000
H	-2.451502000	-4.980029000	1.054392000
C	4.935092000	-1.417590000	0.229362000
C	5.503720000	-2.307654000	-0.702676000
H	4.886254000	-2.693490000	-1.506434000
C	6.850631000	-2.673906000	-0.610253000
H	7.274055000	-3.355486000	-1.341617000
C	7.655015000	-2.152487000	0.411674000
H	8.700390000	-2.436476000	0.481942000
C	7.104474000	-1.255940000	1.336893000
H	7.721936000	-0.843793000	2.129189000
C	5.757815000	-0.889247000	1.243462000
H	5.328211000	-0.191275000	1.954914000
C	1.503996000	4.589710000	-1.165197000
C	0.800492000	5.120672000	-2.264585000
H	0.037005000	4.513474000	-2.739189000

C	1.088443000	6.402162000	-2.744823000
H	0.542566000	6.792208000	-3.598251000
C	2.083080000	7.177000000	-2.133150000
H	2.307208000	8.171283000	-2.506708000
C	2.786086000	6.661943000	-1.036191000
H	3.551913000	7.259746000	-0.551350000
C	2.497885000	5.380287000	-0.555562000
H	3.034023000	4.984479000	0.300607000
C	-4.359745000	1.475816000	1.200100000
C	-5.123917000	2.300320000	0.351503000
H	-4.697103000	2.622157000	-0.591997000
C	-6.423486000	2.678009000	0.705881000
H	-7.002069000	3.307441000	0.036822000
C	-6.983014000	2.233784000	1.911238000
H	-7.991946000	2.526399000	2.184750000
C	-6.236789000	1.402851000	2.757276000
H	-6.665103000	1.051265000	3.690986000
C	-4.937862000	1.024135000	2.402087000
H	-4.356920000	0.377566000	3.051962000
C	-3.058611000	0.943486000	-2.559484000
H	-3.743763000	0.557675000	-1.803424000
H	-2.037788000	0.954974000	-2.174299000
H	-3.361241000	1.945157000	-2.874222000
S	-3.118522000	-0.169828000	-4.108949000
C	-2.294142000	-1.708606000	-3.332410000
H	-2.952042000	-2.130484000	-2.570867000
H	-2.136749000	-2.426117000	-4.140968000
H	-1.345200000	-1.402245000	-2.888406000

²RC-3_{is}

Co	-0.151813000	0.007490000	-0.133591000
O	0.046693000	-0.013681000	1.715505000
C	-0.367994000	0.022180000	-2.163791000
C	0.067996000	0.111479000	-4.417470000
H	0.686430000	0.197649000	-5.294139000
C	-1.271695000	-0.055418000	-4.274435000
H	-2.061755000	-0.136951000	-5.000876000
C	-2.885577000	-0.263999000	-2.382136000
H	-3.522790000	-0.600175000	-3.204874000
H	-2.894262000	-1.007590000	-1.591426000
H	-3.260896000	0.684766000	-1.994171000
C	2.046017000	0.311663000	-2.909075000
H	2.492541000	0.668473000	-3.841360000
H	2.220456000	1.039386000	-2.123380000

H	2.498060000	-0.641907000	-2.629441000
N	0.604736000	0.158977000	-3.128446000
N	-1.523359000	-0.110281000	-2.901147000
N	-1.815075000	0.996690000	0.135306000
N	0.840272000	1.701247000	-0.198107000
N	1.530046000	-0.981306000	-0.241391000
N	-1.137711000	-1.684071000	-0.019976000
C	-2.986943000	0.487826000	0.655316000
C	-2.061257000	2.307167000	-0.237305000
C	0.297899000	2.948118000	-0.419315000
C	2.163762000	1.888337000	0.169989000
C	2.787415000	-0.480026000	0.024388000
C	1.688322000	-2.284197000	-0.681586000
C	-0.657935000	-2.924346000	-0.377059000
C	-2.349195000	-1.881738000	0.624237000
C	-4.019602000	1.498160000	0.568716000
H	-5.041291000	1.355699000	0.883428000
C	-3.464572000	2.598788000	-0.026902000
H	-3.948622000	3.528756000	-0.276510000
C	1.315537000	3.957881000	-0.203619000
H	1.149475000	5.020173000	-0.289323000
C	2.446679000	3.308950000	0.206079000
H	3.385556000	3.743203000	0.508174000
C	3.775277000	-1.488365000	-0.296419000
H	4.840269000	-1.351598000	-0.199036000
C	3.103737000	-2.578613000	-0.778704000
H	3.520790000	-3.504690000	-1.139204000
C	-1.607565000	-3.940999000	0.031062000
H	-1.465593000	-5.000694000	-0.111524000
C	-2.621600000	-3.303856000	0.689762000
H	-3.473764000	-3.747606000	1.178177000
C	-3.224556000	-0.854585000	0.997430000
C	-1.068113000	3.233830000	-0.585519000
C	3.098330000	0.856700000	0.325380000
C	0.641679000	-3.204166000	-0.833064000
C	-4.511930000	-1.175565000	1.670746000
C	-4.834765000	-0.537467000	2.884935000
H	-4.123011000	0.159993000	3.314020000
C	-6.043842000	-0.807439000	3.533851000
H	-6.272369000	-0.314038000	4.473443000
C	-6.954283000	-1.716012000	2.977976000
H	-7.892162000	-1.926669000	3.482185000
C	-6.649148000	-2.348515000	1.765684000
H	-7.355102000	-3.043972000	1.322002000
C	-5.439971000	-2.078240000	1.116069000

H	-5.212144000	-2.554543000	0.168476000
C	-1.437312000	4.621997000	-0.975337000
C	-2.235872000	5.442350000	-0.154646000
H	-2.588346000	5.054935000	0.794859000
C	-2.549168000	6.749520000	-0.541962000
H	-3.160314000	7.370383000	0.105932000
C	-2.064207000	7.262542000	-1.752270000
H	-2.307580000	8.277219000	-2.051384000
C	-1.255649000	6.461587000	-2.569460000
H	-0.871279000	6.853405000	-3.506266000
C	-0.942253000	5.154715000	-2.182042000
H	-0.315408000	4.530755000	-2.811039000
C	4.503910000	1.169503000	0.699555000
C	5.089492000	0.505433000	1.796635000
H	4.490855000	-0.199024000	2.365632000
C	6.413178000	0.771534000	2.162603000
H	6.843944000	0.261259000	3.018283000
C	7.175487000	1.695707000	1.435796000
H	8.202377000	1.901785000	1.721573000
C	6.606707000	2.350578000	0.335318000
H	7.195236000	3.057832000	-0.241286000
C	5.282619000	2.087775000	-0.031651000
H	4.848457000	2.582048000	-0.894334000
C	0.915266000	-4.583357000	-1.321548000
C	1.861237000	-5.422273000	-0.700744000
H	2.404722000	-5.055914000	0.163039000
C	2.078925000	-6.721468000	-1.171823000
H	2.806779000	-7.357503000	-0.677621000
C	1.350544000	-7.207041000	-2.265801000
H	1.520211000	-8.215637000	-2.629685000
C	0.395572000	-6.387223000	-2.881403000
H	-0.176814000	-6.758082000	-3.726186000
C	0.177785000	-5.088329000	-2.410524000
H	-0.561769000	-4.449292000	-2.882323000
C	0.976621000	-1.156762000	4.596935000
H	1.126175000	-2.221163000	4.793193000
H	0.393620000	-0.702822000	5.402269000
H	0.495892000	-0.996844000	3.627759000
S	2.712980000	-0.355677000	4.540317000
C	2.212974000	1.307644000	3.734920000
H	3.133238000	1.768302000	3.369506000
H	1.531648000	1.081459000	2.908734000
H	1.736076000	1.946690000	4.482271000

⁶TS-3_{hs}

Co	0.062498000	0.046206000	0.068903000
O	0.088194000	0.110608000	-1.899197000
C	0.145896000	0.075311000	2.247903000
C	-0.452604000	0.085077000	4.475803000
H	-1.134205000	0.106738000	5.309203000
C	0.904599000	0.022454000	4.425803000
H	1.645001000	-0.013804000	5.206803000
C	2.638402000	-0.022648000	2.609903000
H	3.273218000	-0.312212000	3.452503000
H	2.732244000	-0.755042000	1.812303000
H	2.949246000	0.955770000	2.236303000
C	-2.314609000	0.167071000	2.794703000
H	-2.877828000	0.506439000	3.669303000
H	-2.454349000	0.866763000	1.975403000
H	-2.670753000	-0.819449000	2.487803000
N	-0.895506000	0.119752000	3.149003000
N	1.249900000	0.015773000	3.070103000
N	1.688335000	1.152998000	-0.088097000
N	-1.063294000	1.670542000	0.041903000
N	-1.585738000	-1.074988000	0.082303000
N	1.169791000	-1.590231000	0.008503000
C	2.947060000	0.718770000	-0.441897000
C	1.800059000	2.487505000	0.257403000
C	-0.615367000	2.961168000	0.222503000
C	-2.384999000	1.755167000	-0.367597000
C	-2.868162000	-0.656560000	-0.201297000
C	-1.669363000	-2.398192000	0.476303000
C	0.738664000	-2.871856000	0.273003000
C	2.455697000	-1.693158000	-0.500497000
C	3.896798000	1.801824000	-0.264597000
H	4.958003000	1.722884000	-0.440897000
C	3.198437000	2.877584000	0.208003000
H	3.582982000	3.846906000	0.481103000
C	-1.686820000	3.893007000	-0.078297000
H	-1.594981000	4.966812000	-0.035497000
C	-2.760478000	3.153046000	-0.484097000
H	-3.715999000	3.512491000	-0.830397000
C	-3.799201000	-1.735713000	0.070703000
H	-4.870205000	-1.666374000	-0.037497000
C	-3.065541000	-2.792972000	0.532903000
H	-3.426986000	-3.754092000	0.861003000
C	1.784017000	-3.816596000	-0.076697000
H	1.695678000	-4.888001000	0.012303000
C	2.822576000	-3.094437000	-0.592797000

H	3.750798000	-3.467085000	-0.995097000
C	3.305635000	-0.605610000	-0.744197000
C	0.714110000	3.349843000	0.463903000
C	-3.248237000	0.658918000	-0.521197000
C	-0.567915000	-3.251330000	0.633003000
C	4.688149000	-0.844231000	-1.243297000
C	5.138510000	-0.171006000	-2.396497000
H	4.455272000	0.498556000	-2.908297000
C	6.438421000	-0.362232000	-2.875797000
H	6.765592000	0.160587000	-3.769497000
C	7.315070000	-1.227782000	-2.208197000
H	8.324279000	-1.376825000	-2.579597000
C	6.882808000	-1.895807000	-1.055097000
H	7.559946000	-2.558368000	-0.524297000
C	5.582697000	-1.703580000	-0.575497000
H	5.253126000	-2.208599000	0.326003000
C	0.954529000	4.778857000	0.808403000
C	1.767782000	5.611603000	0.015003000
H	2.233205000	5.199529000	-0.873597000
C	1.957406000	6.956114000	0.352003000
H	2.582770000	7.584749000	-0.274797000
C	1.332775000	7.494878000	1.484603000
H	1.480016000	8.538487000	1.744803000
C	0.511421000	6.680132000	2.275003000
H	0.020998000	7.090004000	3.152803000
C	0.322398000	5.335921000	1.937903000
H	-0.313566000	4.700885000	2.546103000
C	-4.657149000	0.877538000	-0.951097000
C	-5.170908000	0.151109000	-2.045097000
H	-4.521068000	-0.552954000	-2.554797000
C	-6.493118000	0.325834000	-2.466197000
H	-6.867986000	-0.239588000	-3.313997000
C	-7.330669000	1.228386000	-1.797897000
H	-8.356977000	1.365728000	-2.123797000
C	-6.837110000	1.947314000	-0.701097000
H	-7.484249000	2.637277000	-0.167997000
C	-5.514900000	1.771289000	-0.279797000
H	-5.139131000	2.315011000	0.579903000
C	-0.776134000	-4.666242000	1.049003000
C	-1.637585000	-5.532491000	0.347603000
H	-2.165406000	-5.157920000	-0.522597000
C	-1.796610000	-6.862800000	0.750703000
H	-2.460472000	-7.517837000	0.194503000
C	-1.092382000	-7.353660000	1.858003000
H	-1.215823000	-8.386267000	2.169503000

C	-0.222130000	-6.505810000	2.555903000
H	0.330291000	-6.878979000	3.413003000
C	-0.063705000	-5.175901000	2.152703000
H	0.609857000	-4.515063000	2.688503000
C	0.419759000	-1.024274000	-4.461297000
H	1.075504000	-1.818736000	-4.102097000
H	0.029672000	-1.249596000	-5.456997000
H	0.940804000	-0.066044000	-4.423097000
S	-0.990148000	-0.901354000	-3.198997000
C	-1.872435000	0.624996000	-3.901397000
H	-2.650049000	0.879352000	-3.180097000
H	-1.121880000	1.416939000	-3.930897000
H	-2.294923000	0.408272000	-4.885697000

⁴TS-3_{is}

Co	0.099481000	0.057984000	0.064261000
O	0.170381000	0.053069000	-1.747844000
C	0.196518000	0.089868000	2.279856000
C	-0.358154000	0.346412000	4.502855000
H	-1.001832000	0.586180000	5.331825000
C	0.928956000	-0.086320000	4.458887000
H	1.638072000	-0.295747000	5.241399000
C	2.569816000	-0.696447000	2.675783000
H	3.099964000	-1.083310000	3.550897000
H	2.453579000	-1.488285000	1.941035000
H	3.139540000	0.124462000	2.237084000
C	-2.145567000	0.872998000	2.838327000
H	-2.605179000	1.296225000	3.736198000
H	-2.102683000	1.628318000	2.059546000
H	-2.737486000	0.025397000	2.488607000
N	-0.786836000	0.448743000	3.177059000
N	1.248827000	-0.239014000	3.107560000
N	2.050325000	0.598043000	-0.082408000
N	-0.532440000	2.040478000	0.100147000
N	-1.886299000	-0.511315000	0.093518000
N	0.690189000	-1.947173000	0.101973000
C	3.120658000	-0.230597000	-0.332815000
C	2.525608000	1.880263000	0.103562000
C	0.330929000	3.108735000	0.088909000
C	-1.787433000	2.503571000	-0.242876000
C	-2.979269000	0.308181000	-0.099145000
C	-2.349657000	-1.781005000	0.383292000
C	-0.169449000	-3.015937000	0.203379000
C	1.915697000	-2.423902000	-0.319069000

C	4.344388000	0.551997000	-0.232951000
H	5.342138000	0.156571000	-0.340757000
C	3.982513000	1.837824000	0.061992000
H	4.634275000	2.679835000	0.231207000
C	-0.416719000	4.316058000	-0.243825000
H	0.011873000	5.301365000	-0.340399000
C	-1.711598000	3.940072000	-0.471494000
H	-2.532670000	4.564468000	-0.786739000
C	-4.189376000	-0.466341000	0.120205000
H	-5.193254000	-0.074515000	0.069061000
C	-3.803284000	-1.740025000	0.447440000
H	-4.440129000	-2.571765000	0.703249000
C	0.549479000	-4.233646000	-0.152221000
H	0.117172000	-5.221883000	-0.177863000
C	1.822073000	-3.866542000	-0.495408000
H	2.616576000	-4.503445000	-0.851192000
C	3.067085000	-1.630963000	-0.515264000
C	1.740088000	3.048878000	0.211130000
C	-2.944421000	1.702965000	-0.335043000
C	-1.559846000	-2.950103000	0.455145000
C	4.338152000	-2.315998000	-0.883963000
C	5.072014000	-1.899437000	-2.012870000
H	4.685943000	-1.082483000	-2.613252000
C	6.272852000	-2.527654000	-2.358567000
H	6.821037000	-2.196151000	-3.235292000
C	6.764667000	-3.584949000	-1.581453000
H	7.696661000	-4.072788000	-1.849775000
C	6.046595000	-4.007338000	-0.454957000
H	6.424567000	-4.820301000	0.157728000
C	4.846436000	-3.377811000	-0.109141000
H	4.294291000	-3.698003000	0.768136000
C	2.441468000	4.359910000	0.345398000
C	3.404606000	4.784485000	-0.590943000
H	3.643829000	4.136973000	-1.427494000
C	4.032182000	6.027716000	-0.457970000
H	4.767467000	6.340772000	-1.193114000
C	3.704627000	6.872609000	0.610796000
H	4.191173000	7.837782000	0.712782000
C	2.740624000	6.466870000	1.543017000
H	2.479152000	7.116160000	2.373167000
C	2.113654000	5.223671000	1.409314000
H	1.364056000	4.907002000	2.127161000
C	-4.239414000	2.368595000	-0.650748000
C	-5.028448000	1.915955000	-1.727006000
H	-4.664594000	1.090620000	-2.329806000

C	-6.251402000	2.525748000	-2.024337000
H	-6.842081000	2.168040000	-2.862300000
C	-6.709810000	3.600185000	-1.250302000
H	-7.658757000	4.074193000	-1.481406000
C	-5.935803000	4.058983000	-0.176365000
H	-6.286864000	4.886493000	0.432796000
C	-4.713331000	3.447799000	0.121177000
H	-4.116763000	3.796285000	0.957656000
C	-2.245557000	-4.254787000	0.691668000
C	-3.283351000	-4.709577000	-0.145429000
H	-3.596096000	-4.089933000	-0.978998000
C	-3.896136000	-5.946778000	0.080102000
H	-4.690840000	-6.282471000	-0.579357000
C	-3.478722000	-6.756290000	1.144740000
H	-3.953803000	-7.716677000	1.319487000
C	-2.440126000	-6.321079000	1.978488000
H	-2.108874000	-6.942817000	2.804773000
C	-1.828207000	-5.083914000	1.751659000
H	-1.022113000	-4.744112000	2.393617000
C	-1.934256000	-1.767350000	-2.837691000
H	-2.157722000	-2.277125000	-3.778415000
H	-1.113326000	-2.240386000	-2.296490000
H	-2.818216000	-1.705422000	-2.202987000
S	-1.395409000	0.013449000	-3.203140000
C	-0.062086000	-0.365887000	-4.498739000
H	-0.519697000	-0.804079000	-5.388696000
H	0.422751000	0.583058000	-4.730970000
H	0.648437000	-1.040165000	-4.018288000

²TS-3_{ts}

Co	0.062524000	0.046220000	0.068938000
O	0.088187000	0.110569000	-1.899181000
C	0.145883000	0.075324000	2.247902000
C	-0.452551000	0.085098000	4.475780000
H	-1.134191000	0.106772000	5.309163000
C	0.904559000	0.022385000	4.425757000
H	1.645004000	-0.013942000	5.206816000
C	2.638436000	-0.022756000	2.609897000
H	3.273212000	-0.312446000	3.452541000
H	2.732160000	-0.755167000	1.812252000
H	2.949282000	0.955602000	2.236275000
C	-2.314640000	0.167175000	2.794670000
H	-2.877790000	0.506587000	3.669254000

H	-2.454275000	0.866942000	1.975399000
H	-2.670815000	-0.819319000	2.487831000
N	-0.895540000	0.119791000	3.149024000
N	1.249867000	0.015694000	3.070090000
N	1.688425000	1.152906000	-0.088094000
N	-1.063249000	1.670592000	0.041923000
N	-1.585755000	-1.074903000	0.082287000
N	1.169669000	-1.590309000	0.008545000
C	2.947121000	0.718572000	-0.441892000
C	1.800195000	2.487428000	0.257379000
C	-0.615209000	2.961161000	0.222467000
C	-2.384859000	1.755337000	-0.367577000
C	-2.868230000	-0.656433000	-0.201296000
C	-1.669520000	-2.398059000	0.476274000
C	0.738472000	-2.871925000	0.272962000
C	2.455577000	-1.693285000	-0.500491000
C	3.896860000	1.801554000	-0.264553000
H	4.958060000	1.722613000	-0.440914000
C	3.198551000	2.877439000	0.208022000
H	3.583162000	3.846748000	0.481053000
C	-1.686602000	3.893058000	-0.078255000
H	-1.594684000	4.966920000	-0.035451000
C	-2.760296000	3.153202000	-0.484130000
H	-3.715767000	3.512719000	-0.830377000
C	-3.799345000	-1.735489000	0.070711000
H	-4.870340000	-1.666104000	-0.037496000
C	-3.065653000	-2.792774000	0.532893000
H	-3.427175000	-3.753938000	0.860961000
C	1.783772000	-3.816661000	-0.076692000
H	1.695386000	-4.888052000	0.012301000
C	2.822398000	-3.094578000	-0.592785000
H	3.750594000	-3.467266000	-0.995103000
C	3.305627000	-0.605788000	-0.744175000
C	0.714319000	3.349756000	0.463885000
C	-3.248205000	0.659143000	-0.521175000
C	-0.568147000	-3.251269000	0.632963000
C	4.688068000	-0.844536000	-1.243260000
C	5.138515000	-0.171284000	-2.396501000
H	4.455314000	0.498346000	-2.908347000
C	6.438404000	-0.362575000	-2.875844000
H	6.765623000	0.160198000	-3.769538000
C	7.315033000	-1.228152000	-2.208178000
H	8.324212000	-1.377255000	-2.579591000
C	6.882698000	-1.896226000	-1.055090000
H	7.559761000	-2.558808000	-0.524328000

C	5.582609000	-1.703881000	-0.575544000
H	5.252957000	-2.208914000	0.325991000
C	0.954831000	4.778833000	0.808424000
C	1.768077000	5.611501000	0.015002000
H	2.233529000	5.199413000	-0.873578000
C	1.957846000	6.955991000	0.351991000
H	2.583236000	7.584601000	-0.274768000
C	1.333171000	7.494788000	1.484577000
H	1.480479000	8.538448000	1.744822000
C	0.511813000	6.680096000	2.274966000
H	0.021369000	7.090004000	3.152759000
C	0.322679000	5.335905000	1.937873000
H	-0.313253000	4.700886000	2.546092000
C	-4.657123000	0.877830000	-0.951128000
C	-5.170851000	0.151418000	-2.045131000
H	-4.521107000	-0.552688000	-2.554828000
C	-6.493085000	0.326202000	-2.466196000
H	-6.868029000	-0.239164000	-3.313986000
C	-7.330553000	1.228760000	-1.797902000
H	-8.356860000	1.366237000	-2.123826000
C	-6.836989000	1.947652000	-0.701056000
H	-7.484081000	2.637660000	-0.167961000
C	-5.514837000	1.771588000	-0.279777000
H	-5.138961000	2.315342000	0.579950000
C	-0.776387000	-4.666245000	1.048988000
C	-1.637931000	-5.532367000	0.347627000
H	-2.165694000	-5.157845000	-0.522635000
C	-1.796981000	-6.862653000	0.750664000
H	-2.460887000	-7.517697000	0.194542000
C	-1.092766000	-7.353586000	1.857962000
H	-1.216330000	-8.386215000	2.169521000
C	-0.222491000	-6.505772000	2.555916000
H	0.329935000	-6.878991000	3.413009000
C	-0.063968000	-5.175917000	2.152736000
H	0.609637000	-4.515053000	2.688530000
C	0.419697000	-1.024257000	-4.461325000
H	1.075353000	-1.818833000	-4.102124000
H	0.029567000	-1.249593000	-5.456958000
H	0.940848000	-0.066054000	-4.423095000
S	-0.990179000	-0.901334000	-3.198970000
C	-1.872398000	0.625081000	-3.901367000
H	-2.649982000	0.879498000	-3.180107000
H	-1.121815000	1.416999000	-3.930917000
H	-2.294924000	0.408416000	-4.885722000

⁴INT-3_{ss}

Co	0.105183000	0.037162000	0.142036000
O	0.209893000	-0.081833000	-2.074535000
C	0.179762000	0.163664000	2.400525000
C	-0.405179000	0.431329000	4.615054000
H	-1.077003000	0.594252000	5.440690000
C	0.939775000	0.226736000	4.576682000
H	1.675625000	0.182734000	5.361612000
C	2.642249000	-0.174776000	2.769030000
H	3.249137000	-0.483486000	3.625325000
H	2.632010000	-0.964013000	2.020769000
H	3.063262000	0.730016000	2.324696000
C	-2.250661000	0.547187000	2.908511000
H	-2.816739000	0.865536000	3.788622000
H	-2.330223000	1.299589000	2.126613000
H	-2.652050000	-0.396164000	2.533127000
N	-0.847052000	0.390528000	3.289449000
N	1.274281000	0.063078000	3.229552000
N	1.953667000	0.930509000	-0.115866000
N	-0.854117000	1.879700000	-0.023396000
N	-1.776745000	-0.863927000	0.044533000
N	1.033143000	-1.820338000	0.065859000
C	3.163944000	0.298890000	-0.286944000
C	2.192216000	2.281604000	0.013099000
C	-0.193377000	3.087764000	-0.070303000
C	-2.191617000	2.120778000	-0.278830000
C	-3.004963000	-0.238808000	-0.054213000
C	-2.001833000	-2.202746000	0.313967000
C	0.369019000	-3.025702000	0.101208000
C	2.341549000	-2.069351000	-0.299001000
C	4.229706000	1.288497000	-0.191304000
H	5.285366000	1.074201000	-0.249875000
C	3.634778000	2.503214000	0.013740000
H	4.120600000	3.456520000	0.148818000
C	-1.155102000	4.140546000	-0.375861000
H	-0.911450000	5.183983000	-0.501239000
C	-2.377134000	3.545204000	-0.521045000
H	-3.310483000	4.016057000	-0.786744000
C	-4.050454000	-1.213911000	0.202476000
H	-5.107892000	-1.001004000	0.225687000
C	-3.433937000	-2.414222000	0.451378000
H	-3.905185000	-3.350112000	0.707313000
C	1.301988000	-4.090693000	-0.252085000
H	1.049138000	-5.136955000	-0.326531000

C	2.507303000	-3.501496000	-0.513244000
H	3.416025000	-3.980654000	-0.841874000
C	3.353879000	-1.093724000	-0.434630000
C	1.202765000	3.289890000	0.048206000
C	-3.210794000	1.143112000	-0.278063000
C	-1.015459000	-3.215629000	0.327221000
C	4.738705000	-1.564056000	-0.723933000
C	5.453703000	-1.050509000	-1.824503000
H	4.972347000	-0.316546000	-2.461908000
C	6.756168000	-1.481341000	-2.096732000
H	7.288858000	-1.078557000	-2.952989000
C	7.370126000	-2.434658000	-1.273349000
H	8.380999000	-2.769526000	-1.484825000
C	6.671174000	-2.952544000	-0.175026000
H	7.141674000	-3.686572000	0.472333000
C	5.369013000	-2.520226000	0.097203000
H	4.828354000	-2.915212000	0.950822000
C	1.658825000	4.709557000	0.131908000
C	2.543573000	5.255984000	-0.818334000
H	2.899146000	4.625582000	-1.626189000
C	2.950177000	6.591888000	-0.732968000
H	3.628212000	6.996911000	-1.478266000
C	2.476559000	7.408485000	0.302471000
H	2.791893000	8.445304000	0.368243000
C	1.590132000	6.879426000	1.249859000
H	1.218172000	7.504794000	2.055940000
C	1.184128000	5.543618000	1.163479000
H	0.496774000	5.130119000	1.894242000
C	-4.617583000	1.596347000	-0.471592000
C	-5.425001000	1.022628000	-1.473998000
H	-4.998234000	0.255446000	-2.111472000
C	-6.750109000	1.433005000	-1.651860000
H	-7.354105000	0.982451000	-2.433803000
C	-7.295688000	2.427374000	-0.829084000
H	-8.323941000	2.747187000	-0.966772000
C	-6.505381000	3.005538000	0.173057000
H	-6.922115000	3.771641000	0.819992000
C	-5.180862000	2.592635000	0.350742000
H	-4.569529000	3.034086000	1.130603000
C	-1.468518000	-4.627263000	0.503144000
C	-2.433874000	-5.202262000	-0.347023000
H	-2.858694000	-4.598178000	-1.141645000
C	-2.834577000	-6.532307000	-0.182039000
H	-3.575951000	-6.959076000	-0.851018000
C	-2.273945000	-7.315619000	0.835408000

H	-2.584265000	-8.348036000	0.963735000
C	-1.307326000	-6.759052000	1.683574000
H	-0.867985000	-7.358821000	2.474972000
C	-0.907453000	-5.429127000	1.516997000
H	-0.158228000	-4.994374000	2.170135000
C	-1.869841000	-1.915875000	-2.923755000
H	-2.223680000	-2.186629000	-3.921610000
H	-1.015152000	-2.517260000	-2.606255000
H	-2.666554000	-1.951753000	-2.182141000
S	-1.236537000	-0.099581000	-2.985273000
C	-0.500510000	-0.193196000	-4.746561000
H	-1.309905000	-0.341256000	-5.465282000
H	0.015295000	0.753062000	-4.911554000
H	0.209558000	-1.022390000	-4.743501000

²INT-3_s

Co	0.052999000	0.081783000	0.036172000
O	0.251351000	0.115633000	-2.264358000
C	0.063277000	0.173105000	2.287940000
C	-0.532331000	0.554854000	4.486493000
H	-1.190299000	0.834854000	5.291986000
C	0.760288000	0.129350000	4.489480000
H	1.455174000	-0.027323000	5.297353000
C	2.424978000	-0.554292000	2.724025000
H	2.931500000	-1.012666000	3.579043000
H	2.306631000	-1.287515000	1.929377000
H	3.020524000	0.282093000	2.347737000
C	-2.283986000	0.947254000	2.715092000
H	-2.790480000	1.450965000	3.543930000
H	-2.214713000	1.619842000	1.862868000
H	-2.852967000	0.061342000	2.420903000
N	-0.936086000	0.576069000	3.145982000
N	1.101409000	-0.100558000	3.151170000
N	1.928115000	0.696863000	-0.091275000
N	-0.581589000	1.948703000	-0.104476000
N	-1.831269000	-0.561213000	-0.037252000
N	0.673254000	-1.798349000	0.026563000
C	3.034520000	-0.074372000	-0.376664000
C	2.388924000	1.966107000	0.206221000
C	0.194988000	3.076703000	0.054402000
C	-1.828215000	2.379247000	-0.533566000
C	-2.953480000	0.194527000	-0.321803000
C	-2.283453000	-1.791594000	0.424247000
C	-0.088599000	-2.908173000	0.333164000

C	1.906698000	-2.265428000	-0.406193000
C	4.237817000	0.719202000	-0.197712000
H	5.243174000	0.349950000	-0.326179000
C	3.842190000	1.963773000	0.203611000
H	4.465251000	2.806730000	0.455161000
C	-0.581598000	4.256331000	-0.287643000
H	-0.202212000	5.265940000	-0.270975000
C	-1.812104000	3.824437000	-0.688579000
H	-2.634070000	4.417644000	-1.055646000
C	-4.144283000	-0.571196000	-0.013368000
H	-5.154102000	-0.207848000	-0.122696000
C	-3.732152000	-1.776641000	0.486161000
H	-4.346718000	-2.583164000	0.852600000
C	0.675163000	-4.110950000	0.062929000
H	0.304473000	-5.115785000	0.192422000
C	1.886964000	-3.716283000	-0.432872000
H	2.696325000	-4.342073000	-0.773291000
C	3.029790000	-1.455804000	-0.631229000
C	1.572446000	3.099025000	0.332189000
C	-2.956741000	1.558200000	-0.667400000
C	-1.459311000	-2.903906000	0.653850000
C	4.312643000	-2.078273000	-1.062253000
C	4.965966000	-1.597890000	-2.214926000
H	4.508196000	-0.787603000	-2.772799000
C	6.179762000	-2.152332000	-2.633869000
H	6.665900000	-1.772660000	-3.527526000
C	6.766133000	-3.195703000	-1.905126000
H	7.708403000	-3.626605000	-2.229354000
C	6.131920000	-3.675438000	-0.751627000
H	6.586588000	-4.474196000	-0.173321000
C	4.918166000	-3.119856000	-0.332463000
H	4.435586000	-3.479066000	0.570033000
C	2.186531000	4.421984000	0.637576000
C	3.211322000	4.968527000	-0.159227000
H	3.561668000	4.410197000	-1.020437000
C	3.758402000	6.220730000	0.140759000
H	4.544098000	6.629342000	-0.487600000
C	3.286772000	6.951932000	1.238931000
H	3.711717000	7.923701000	1.470946000
C	2.258959000	6.424527000	2.031822000
H	1.885670000	6.985817000	2.883127000
C	1.712070000	5.172655000	1.731338000
H	0.914580000	4.759780000	2.340538000
C	-4.258517000	2.154185000	-1.078218000
C	-4.966557000	1.604746000	-2.165499000

H	-4.532178000	0.765470000	-2.698703000
C	-6.201335000	2.132080000	-2.556965000
H	-6.729211000	1.699833000	-3.401751000
C	-6.753913000	3.218167000	-1.865373000
H	-7.712022000	3.628874000	-2.168628000
C	-6.063901000	3.768781000	-0.777285000
H	-6.490523000	4.603105000	-0.228654000
C	-4.829539000	3.239705000	-0.385549000
H	-4.300973000	3.655784000	0.465309000
C	-2.054712000	-4.187690000	1.117569000
C	-3.121570000	-4.807528000	0.437541000
H	-3.526108000	-4.334028000	-0.450507000
C	-3.646285000	-6.024476000	0.885897000
H	-4.465733000	-6.489023000	0.345625000
C	-3.109212000	-6.649327000	2.019025000
H	-3.516349000	-7.593908000	2.366279000
C	-2.039664000	-6.049955000	2.697350000
H	-1.616005000	-6.527985000	3.575412000
C	-1.516735000	-4.832762000	2.249303000
H	-0.688994000	-4.364178000	2.771336000
C	-0.877976000	-2.489519000	-2.798016000
H	-1.480597000	-2.625547000	-1.903271000
H	-1.280308000	-3.044495000	-3.649270000
H	0.166278000	-2.733506000	-2.592460000
S	-0.946943000	-0.622201000	-3.227475000
C	-0.034792000	-0.774095000	-4.905266000
H	0.105944000	0.242709000	-5.273187000
H	0.927475000	-1.243682000	-4.691439000
H	-0.642504000	-1.369622000	-5.590785000

⁴P-3_{hs}

C	0.000030000	-0.000093000	2.109996000
C	-0.678282000	-0.068632000	4.300827000
H	-1.384459000	-0.143922000	5.110096000
C	0.678500000	0.068173000	4.300787000
H	1.384736000	0.143363000	5.110014000
C	2.456048000	0.258803000	2.508688000
H	3.124294000	0.069156000	3.353050000
H	2.648579000	-0.458978000	1.712986000
H	2.623883000	1.266625000	2.120643000
C	-2.455967000	-0.259015000	2.508846000
H	-3.124143000	-0.069400000	3.353270000
H	-2.648532000	0.458826000	1.713208000
H	-2.623865000	-1.266807000	2.120748000

N	-1.070946000	-0.104998000	2.961092000
N	1.071065000	0.104712000	2.961028000
N	1.573539000	1.307556000	-0.445153000
N	-1.332486000	1.565179000	-0.380962000
N	-1.573559000	-1.307517000	-0.445186000
N	1.332459000	-1.565137000	-0.381030000
C	2.913215000	0.988651000	-0.575030000
C	1.496388000	2.675376000	-0.234026000
C	-0.991621000	2.903751000	-0.352324000
C	-2.684551000	1.493480000	-0.678732000
C	-2.913234000	-0.988609000	-0.575066000
C	-1.496409000	-2.675342000	-0.234098000
C	0.991597000	-2.903710000	-0.352419000
C	2.684524000	-1.493432000	-0.678796000
C	3.710231000	2.187884000	-0.388413000
H	4.787943000	2.225195000	-0.408615000
C	2.841437000	3.219851000	-0.157636000
H	3.084850000	4.251160000	0.041988000
C	-2.169280000	3.704375000	-0.647451000
H	-2.181317000	4.780471000	-0.720734000
C	-3.203589000	2.838322000	-0.866150000
H	-4.215502000	3.078713000	-1.150804000
C	-3.710251000	-2.187846000	-0.388481000
H	-4.787963000	-2.225156000	-0.408688000
C	-2.841458000	-3.219819000	-0.157725000
H	-3.084872000	-4.251134000	0.041871000
C	2.169253000	-3.704328000	-0.647577000
H	2.181290000	-4.780421000	-0.720889000
C	3.203562000	-2.838269000	-0.866258000
H	4.215474000	-3.078652000	-1.150921000
C	3.441126000	-0.307491000	-0.750541000
C	0.306407000	3.429188000	-0.179258000
C	-3.441147000	0.307539000	-0.750532000
C	-0.306428000	-3.429153000	-0.179353000
C	4.910842000	-0.422272000	-0.977515000
C	5.524012000	0.265802000	-2.043154000
H	4.906044000	0.866918000	-2.701701000
C	6.903204000	0.172556000	-2.256265000
H	7.356903000	0.704599000	-3.086880000
C	7.696221000	-0.610134000	-1.406668000
H	8.766605000	-0.683228000	-1.572345000
C	7.099335000	-1.297880000	-0.341896000
H	7.707454000	-1.901506000	0.325107000
C	5.719983000	-1.203412000	-0.129046000
H	5.256660000	-1.731442000	0.697866000

C	0.413678000	4.908396000	-0.010866000
C	1.167297000	5.697937000	-0.901281000
H	1.678778000	5.214575000	-1.726639000
C	1.246021000	7.084888000	-0.736078000
H	1.826468000	7.678283000	-1.436001000
C	0.569026000	7.708713000	0.320257000
H	0.629607000	8.785160000	0.447494000
C	-0.190626000	6.935593000	1.208080000
H	-0.718652000	7.411062000	2.029154000
C	-0.268804000	5.548923000	1.042123000
H	-0.856629000	4.946297000	1.726767000
C	-4.910862000	0.422328000	-0.977507000
C	-5.524028000	-0.265709000	-2.043173000
H	-4.906058000	-0.866802000	-2.701738000
C	-6.903219000	-0.172454000	-2.256286000
H	-7.356916000	-0.704468000	-3.086920000
C	-7.696239000	0.610207000	-1.406664000
H	-8.766623000	0.683307000	-1.572343000
C	-7.099356000	1.297916000	-0.341867000
H	-7.707477000	1.901520000	0.325154000
C	-5.720006000	1.203440000	-0.129015000
H	-5.256684000	1.731441000	0.697917000
C	-0.413694000	-4.908366000	-0.010995000
C	-1.167317000	-5.697888000	-0.901422000
H	-1.678805000	-5.214510000	-1.726766000
C	-1.246036000	-7.084843000	-0.736251000
H	-1.826486000	-7.678224000	-1.436183000
C	-0.569032000	-7.708691000	0.320065000
H	-0.629609000	-8.785141000	0.447278000
C	0.190624000	-6.935589000	1.207901000
H	0.718658000	-7.411076000	2.028960000
C	0.268797000	-5.548915000	1.041975000
H	0.856625000	-4.946303000	1.726629000
Co	-0.000012000	0.000028000	-0.038257000

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C	0.000089000	-0.000034000	1.942220000
C	0.679702000	0.035545000	4.145754000
H	1.389850000	0.076915000	4.954257000
C	-0.679088000	-0.036007000	4.145880000
H	-1.389075000	-0.077517000	4.954517000
C	-2.468369000	-0.151869000	2.374204000
H	-3.113084000	0.097868000	3.221982000
H	-2.640661000	0.550288000	1.561608000

H	-2.696061000	-1.162037000	2.024030000
C	2.468611000	0.151795000	2.373702000
H	3.113534000	-0.097870000	3.221343000
H	2.640802000	-0.550347000	1.561065000
H	2.696125000	1.161982000	2.023468000
N	1.073216000	0.053813000	2.802884000
N	-1.072876000	-0.054012000	2.803085000
N	-1.538762000	-1.247383000	-0.424267000
N	1.249834000	-1.532754000	-0.410890000
N	1.538702000	1.247414000	-0.424283000
N	-1.249898000	1.532783000	-0.410823000
C	-2.860981000	-0.929216000	-0.683443000
C	-1.518495000	-2.594608000	-0.087487000
C	0.922329000	-2.863111000	-0.214818000
C	2.585955000	-1.512466000	-0.798697000
C	2.860920000	0.929246000	-0.683466000
C	1.518442000	2.594632000	-0.087473000
C	-0.922386000	2.863138000	-0.214749000
C	-2.586024000	1.512500000	-0.798615000
C	-3.695092000	-2.092615000	-0.462467000
H	-4.767981000	-2.107926000	-0.570079000
C	-2.873906000	-3.106563000	-0.056618000
H	-3.150418000	-4.110880000	0.220363000
C	2.072263000	-3.698224000	-0.500131000
H	2.072979000	-4.775629000	-0.451671000
C	3.083086000	-2.870996000	-0.895437000
H	4.071692000	-3.144467000	-1.226750000
C	3.695035000	2.092639000	-0.462474000
H	4.767924000	2.107949000	-0.570092000
C	2.873855000	3.106583000	-0.056606000
H	3.150371000	4.110895000	0.220392000
C	-2.072327000	3.698254000	-0.500028000
H	-2.073042000	4.775659000	-0.451556000
C	-3.083157000	2.871032000	-0.895326000
H	-4.071768000	3.144507000	-1.226619000
C	-3.359494000	0.355187000	-0.951230000
C	-0.358301000	-3.364547000	0.063062000
C	3.359428000	-0.355152000	-0.951282000
C	0.358251000	3.364570000	0.063106000
C	-4.800327000	0.476455000	-1.312702000
C	-5.306027000	-0.217057000	-2.429682000
H	-4.625842000	-0.818249000	-3.023920000
C	-6.659259000	-0.130630000	-2.772736000
H	-7.029998000	-0.666347000	-3.641257000
C	-7.532862000	0.648141000	-2.002287000

H	-8.583118000	0.715822000	-2.268461000
C	-7.043582000	1.336493000	-0.884421000
H	-7.715916000	1.933693000	-0.275900000
C	-5.690120000	1.249231000	-0.541503000
H	-5.312391000	1.772576000	0.330449000
C	-0.469853000	-4.811108000	0.405174000
C	-1.224734000	-5.703330000	-0.380533000
H	-1.738876000	-5.326068000	-1.257839000
C	-1.298561000	-7.060468000	-0.048704000
H	-1.880426000	-7.735289000	-0.669144000
C	-0.614284000	-7.550760000	1.071288000
H	-0.671334000	-8.604065000	1.327859000
C	0.149372000	-6.674957000	1.854206000
H	0.684757000	-7.047242000	2.722376000
C	0.222893000	-5.318239000	1.521951000
H	0.814299000	-4.636070000	2.123923000
C	4.800259000	-0.476414000	-1.312764000
C	5.305955000	0.217122000	-2.429731000
H	4.625768000	0.818326000	-3.023954000
C	6.659186000	0.130703000	-2.772791000
H	7.029922000	0.666437000	-3.641302000
C	7.532793000	-0.648083000	-2.002361000
H	8.583047000	-0.715757000	-2.268539000
C	7.043517000	-1.336457000	-0.884507000
H	7.715854000	-1.933668000	-0.275999000
C	5.690056000	-1.249203000	-0.541582000
H	5.312331000	-1.772566000	0.330361000
C	0.469813000	4.811129000	0.405227000
C	1.224680000	5.703354000	-0.380491000
H	1.738803000	5.326095000	-1.257809000
C	1.298515000	7.060490000	-0.048657000
H	1.880368000	7.735314000	-0.669105000
C	0.614261000	7.550778000	1.071351000
H	0.671317000	8.604082000	1.327926000
C	-0.149382000	6.674972000	1.854279000
H	-0.684749000	7.047253000	2.722461000
C	-0.222911000	5.318256000	1.522019000
H	-0.814307000	4.636085000	2.123999000
Co	-0.000024000	0.000015000	-0.235483000