

Supplementary Information for
Electronic Structure Contributions to O—O Bond Cleavage
Reactions for Mn^{III}-alkylperoxo complexes

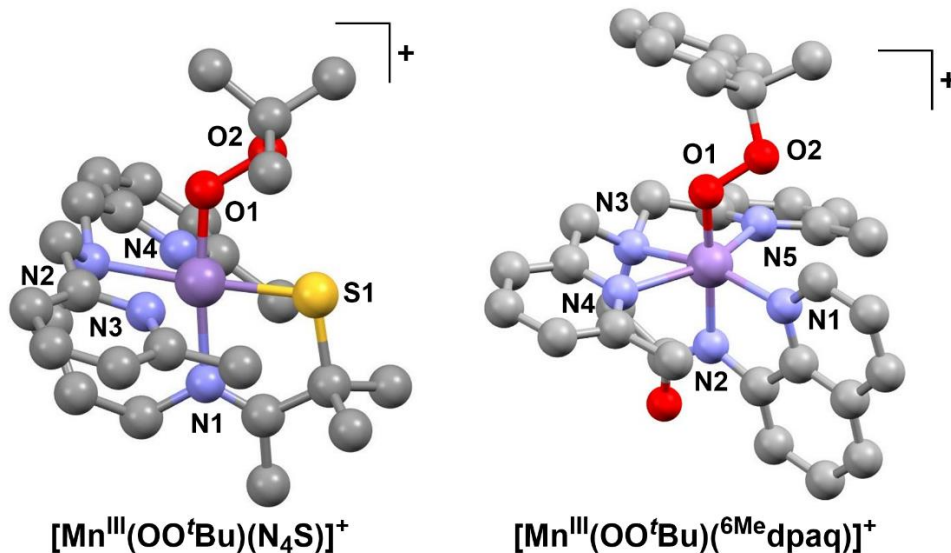
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Table S1. Metric Parameters for $[\text{Mn}^{\text{III}}(\text{OO}^t\text{Bu})(\text{N}_4\text{S})]^+$ and $[\text{Mn}^{\text{III}}(\text{OOCm})(^6\text{Me}\text{dpaq})]^+$ from X-ray Crystallography and DFT Geometry Optimizations using a Variety of Density Functionals.



Bond	$[\text{Mn}^{\text{III}}(\text{OOCm})(^6\text{Me}\text{dpaq})]^+$						
	XRD	TPSS	TPSS-D3	TPSSh-D3	B3LYP	B3LYP-D3	M06-L
Mn–O1	1.849(3)	1.840	1.838	1.836	1.840	1.840	1.858
Mn–N1	2.044(4)	2.044	2.040	2.047	2.063	2.058	2.068
Mn–N2	1.955(4)	1.958	1.958	1.955	1.963	1.959	1.980
Mn–N3	2.100(4)	2.150	2.155	2.146	2.169	2.169	2.187
Mn–N4	2.284(4)	2.409	2.345	2.403	2.434	2.362	2.335
Mn–N5	2.394(4)	2.415	2.351	2.404	2.440	2.363	2.346
Mn–N(py) _{avg}	2.339	2.412	2.348	2.404	2.437	2.362	2.340
O1–O2	1.466(4)	1.471	1.469	1.454	1.447	1.444	1.448
Mn–O1–O2	110.4(2)	115.4	111.8	114.5	115.4	111.6	107.0
$[\text{Mn}^{\text{III}}(\text{OO}^t\text{Bu})(\text{N}_4\text{S})]^+$							
Mn–O1	1.843(3)	1.843	1.840	1.838	1.849	1.845	1.860
Mn–S1	2.260(1)	2.252	2.247	2.253	2.268	2.266	2.273
Mn–N1	2.061(4)	2.108	2.089	2.091	2.131	2.109	2.115
Mn–N2	2.178(4)	2.238	2.229	2.224	2.271	2.255	2.253
Mn–N3	2.516(3)	2.585	2.504	2.501	2.648	2.532	2.514
Mn–N4	2.504(4)	2.476	2.419	2.430	2.535	2.464	2.450
Mn–N(py) _{avg}	2.510	2.531	2.460	2.466	2.591	2.498	2.482
O1–O2	1.431(5)	1.463	1.465	1.448	1.439	1.440	1.437
Mn–O1–O2	124.3(3)	114.07	110.84	110.04	113.94	110.68	108.57

Table S2. Relative Single-Point Energies of Different Spin States of $[\text{Mn}^{\text{III}}(\text{OO}'\text{Bu})(\text{N}_4\text{S})]^+$ and $[\text{Mn}^{\text{III}}(\text{OO}'\text{Bu})(^6\text{Me}^{\text{d}}\text{paq})]^+$ Optimized using Different Density Functionals.

	$[\text{Mn}^{\text{III}}(\text{OO}'\text{Bu})(^6\text{Me}^{\text{d}}\text{paq})]^+$			$[\text{Mn}^{\text{III}}(\text{OO}'\text{Bu})(\text{N}_4\text{S})]^+$		
	quintet	triplet	singlet	quintet	triplet	singlet
Optimization: TPSSh-D3						
Energy: TPSSh-D3	0.0	8.0	16.1	0.0	13.9	20.9
B3LYP-D3	0.0	17.4	28.1	0.0	20.9	31.1
Optimization: TPSS-D3						
Energy: TPSSh-D3	0.0	8.3	16.6	0.0	14.2	21.2
B3LYP-D3	0.0	17.7	28.4	0.0	21.5	31.5
Optimization: B3LYP-D3						
Energy: TPSSh-D3	0.0	8.4	17.1	0.0	13.7	20.8
B3LYP-D3	0.0	17.3	27.8	0.0	20.9	31.2

Table S3. Relative Single-Point Energies using Different Functionals for $[\text{Mn}^{\text{III}}(\text{OO}'\text{Bu})(\text{N}_4\text{S})]^+$ and $[\text{Mn}^{\text{III}}(\text{OO}'\text{Bu})(^6\text{Me}^{\text{d}}\text{paq})]^+$ in Various Spin States.^a

Functional	$[\text{Mn}^{\text{III}}(\text{OO}'\text{Bu})(\text{N}_4\text{S})]^+$			$[\text{Mn}^{\text{III}}(\text{OO}'\text{Bu})(^6\text{Me}^{\text{d}}\text{paq})]^+$		
	quintet	triplet	singlet	quintet	triplet	singlet
TPSS-D3	0.0	6.7	13.7	0.0	2.1	8.4
PBE	0.0	10.6	19.2	0.0	2.8	16.8
TPSSh-D3 (10%)	0.0	14.0	20.9	0.0	8.2	16.3
TPSS0 (25%)	0.0	24.6	31.6	0.0	14.0	23.8
B3LYP-D3	0.0	20.9	31.1	0.0	17.5	28.1
B3LYP (25%)	0.0	27.5	37.2	0.0	14.9	25.3
PBE0-D3	0.0	25.6	35.8	0.0	18.1	29.8
PBE0	0.0	27.4	37.6	0.0	16.9	28.4
M06L	0.0	25.2	38.9	0.0	16.9	30.0
M06 (27%)	0.0	37.7	^b	0.0	27.8	43.6
M062X	0.0	39.5	53.9	0.0	29.0	43.8
wB97X	0.0	25.1	36.1	0.0	15.1	43.6
<i>def2-QZVPP</i>						
TPSSh-D3	0.0	14.3	21.1	0.0	8.6	16.8
B3LYP-D3	0.0	21.1	31.2	0.0	17.7	28.3

^a Structures used for all calculations were determined using the TPSSh-D3 functional. ^b We were unable to converge the SCF cycle for this calculation.

Table S4. Comparison of TPSSh and B3LYP DFT-computed Energies for Reactants, Transition States (TS), and Product Complexes (PC) involved in the Homolytic and Heterolytic Cleavage of the O–O Bond of $[\text{Mn}^{\text{III}}(\text{OO}'\text{Bu})(\text{N4S})]^+$ and $[\text{Mn}^{\text{III}}(\text{OO}'\text{Bu})(^6\text{Me}^{\text{d}}\text{paq})]^+$.

	⁵ reactant	³ reactant	¹ reactant	⁵ TS	³ TS	¹ TS	⁵ PC	³ PC	¹ PC
$[\text{Mn}^{\text{III}}(\text{OO}'\text{Bu})(\text{N4S})]^+$									
<i>TPSSh</i> ^a									
<i>E</i>	0	13.9	20.9	24.9	21.8	32.8	19.1	19.0	30.6
ΔH	0	15.1	19.7	23.2	21.6	32.3	18.7	17.0	28.4
T ΔS	0	-1.3	-1.3	0.1	-1.8	-1.4	0.3	-0.1	0.4
ΔG	0	16.3	21.0	23.1	23.3	33.6	18.4	17.1	28.0
<i>B3LYP</i> ^b									
<i>E</i>	0	20.9	31.1	27.5	32.1	45.7	26.7	27.2	41.2
ΔH	0	22.1	29.9	25.8	31.9	45.2	26.3	25.3	38.9
T ΔS	0	-1.3	-1.3	0.1	-1.8	-1.4	0.3	-0.1	0.4
ΔG	0	23.3	31.2	25.7	33.7	46.6	25.9	25.4	38.5
$[\text{Mn}^{\text{III}}(\text{OO}'\text{Bu})(^6\text{Me}^{\text{d}}\text{paq})]^+$									
<i>TPSSh</i> ^a									
<i>E</i>	0	8.0	16.1	25.1	27.8	27.2	20.9	20.6	24.1
ΔH	0	8.6	16.6	23.4	26.7	26.3	20.6	20.8	24.8
T ΔS	0	-2.1	-1.9	0.4	-1.7	-2.0	0.4	0.3	0.1
ΔG	0	10.7	18.5	23.0	28.4	28.3	20.2	20.5	24.7
<i>B3LYP</i> ^b									
<i>E</i>	0	15.0	25.6	25.4	38.5	48.3	24.9	31.9	31.9
ΔH	0	15.6	26.2	23.6	37.6	47.6	24.5	32.4	32.5
T ΔS	0	-2.1	-1.9	0.4	-2.2	-2.4	0.4	-0.1	0.1
ΔG	0	17.7	28.1	23.2	39.7	50.1	24.1	32.5	32.4

^a Calculations used the TPSSh functional for geometry optimizations and single point energies. ^b Calculations used the TPSSh functional for geometry optimizations and the B3LYP functional for single point energies.

Table S5. Selected Structural Parameters, DFT-computed Energies, and Mulliken Spin Densities for Quintet and Triplet Reactants and Quintet-Triplet Minimum Energy Crossing Point (MECP) of $[\text{Mn}^{\text{III}}(\text{OO}^t\text{Bu})(\text{N4S})]^+$.

	$^5\text{reactant}$	$^3\text{reactant}$	MECP	
<i>structural parameters^a</i>				
Mn–O1	1.84	1.82	1.83	
O1–O2	1.45	1.46	1.46	
Mn–S1	2.25	2.22	2.21	
Mn–N1	2.09	2.12	2.1	
Mn–N2	2.22	2.16	2.12	
Mn–N3	2.5	2.22	2.14	
Mn–N4	2.43	2.19	2.13	
Mn–O1–O2	110.0	114.2	114	
N1–Mn–O1	174.8	173.3	172	
<i>energies^b</i>				
<i>E</i>	0	13.9	17.6	
ΔH	0	15.1	16.1	
$T\Delta S$	0	-1.3	-0.7	
ΔG	0	16.3	16.8	
<i>spin densities</i>				
			quintet	triplet
Mn	3.97	1.09	3.79	1.87
O1	0.01	0.12	0.03	0.12
O2	0.02	0.01	0.04	0.02
S1	-0.01	0.09	0.04	0.07

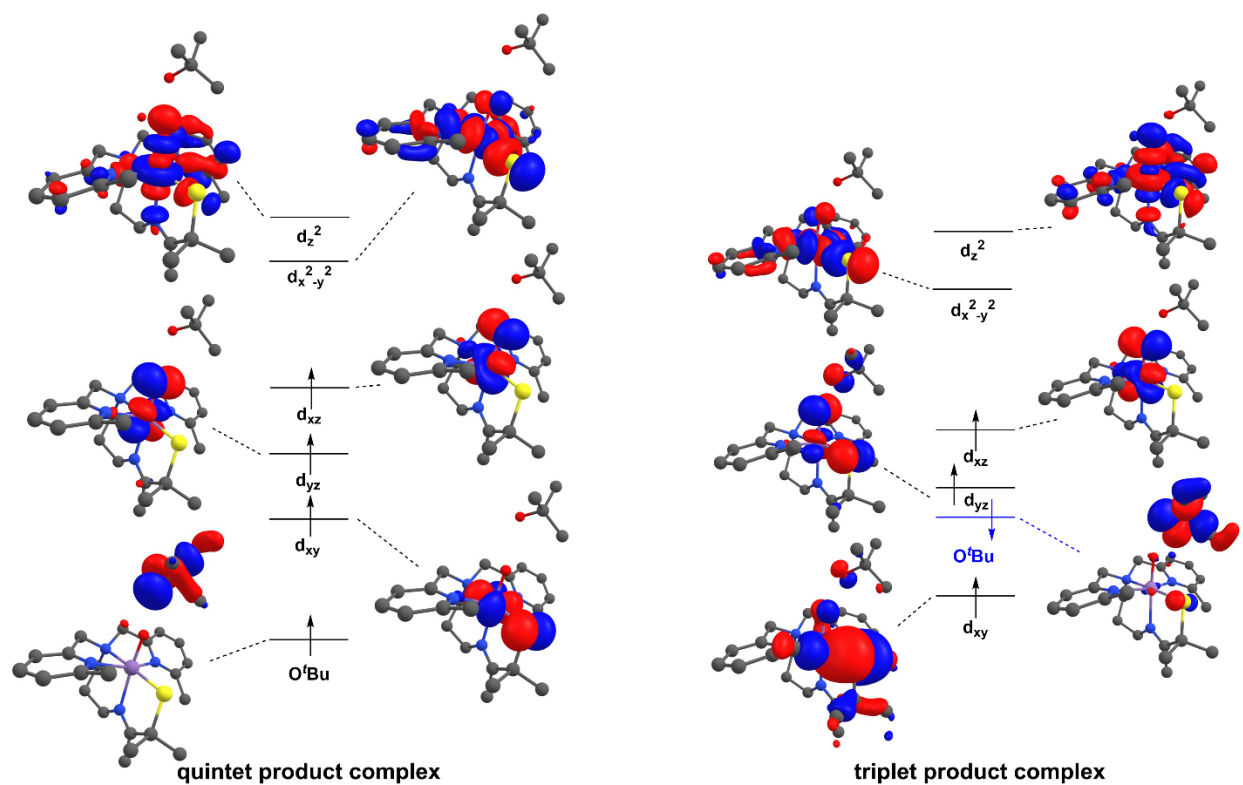


Figure S1. Surface contour plots (quasi-restricted MOs) and qualitative frontier MO splitting diagrams for the quintet (left) and triplet (right) product complexes of O–O bond homolysis of $[\text{Mn}^{\text{III}}(\text{OO}'\text{Bu})(\text{N4S})]^+$.

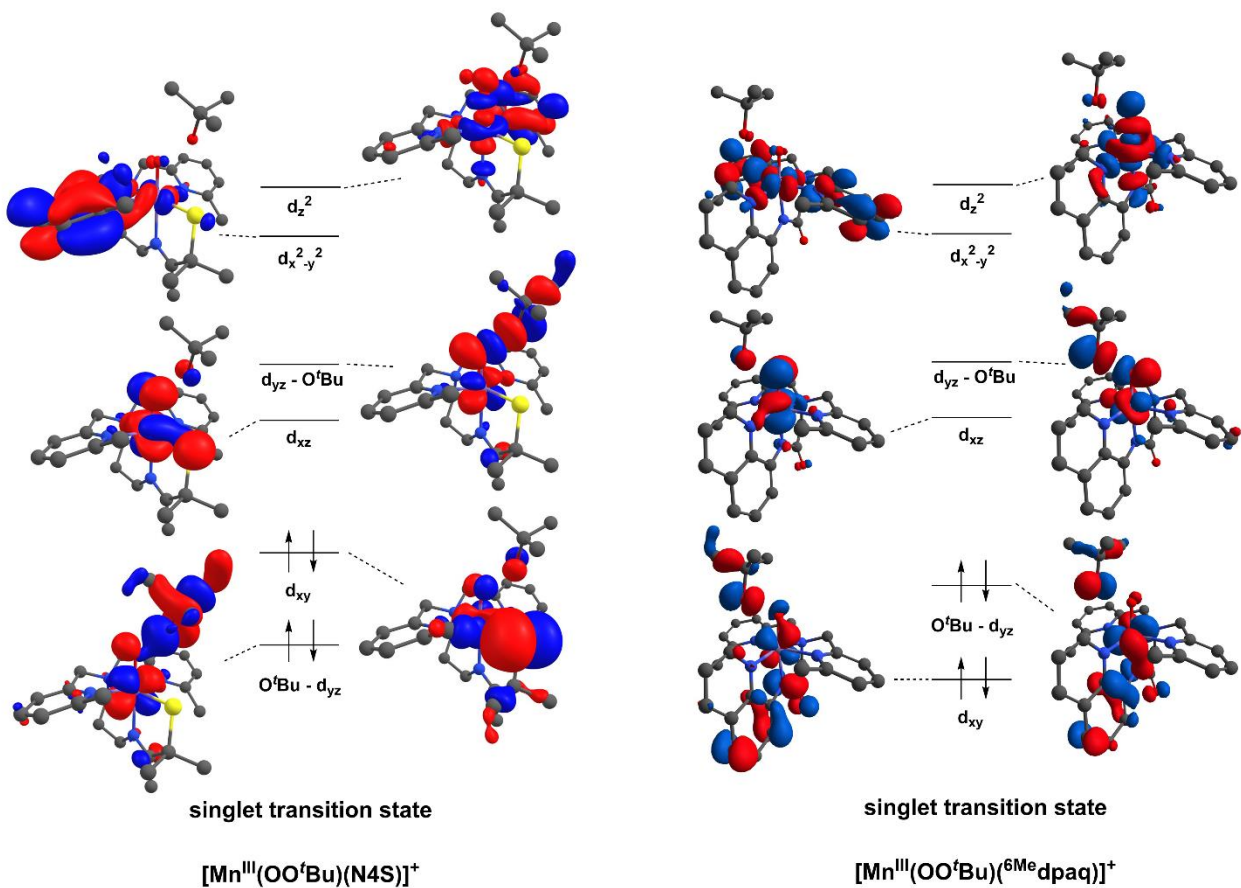


Figure S2. Surface contour plots (quasi-restricted MOs) and qualitative frontier MO splitting diagrams for the singlet transition states of $[\text{Mn}^{\text{III}}(\text{OO}'\text{Bu})(\text{N4S})]^+$ (left) and $[\text{Mn}^{\text{III}}(\text{OO}'\text{Bu})(^6\text{Me dpaq})]^+$ (right).

[Mn^{III}(OO^tBu)(⁶Me dpaq)]⁺ - quintet reactant (TPSSh)

Mn	5.00991100984683	1.09032551870600	2.94741555693639
O	5.11387500492476	1.57127322545113	4.71479784592105
O	5.34721161656063	3.00886668008999	4.77885516765633
O	5.54661231019340	-1.06252935221355	-0.46611360343429
N	3.28130440110176	2.07410545656571	2.48995035556188
N	4.75093363015761	0.43067680629312	1.12573730934715
N	6.69501072641384	-0.25801314506156	2.88084864271184
N	4.03807612894754	-0.99658920015940	3.61233148067851
N	6.81681364590229	2.37984305408677	2.41469053399371
C	2.62196045997100	2.92638503031385	3.26494891098443
C	1.38902728597141	3.47974946076245	2.86992331526009
C	0.84486761951525	3.12422400165960	1.64755143474912
C	1.52963842133758	2.21546224910854	0.79986706840323
C	1.05960936905940	1.77802933763264	-0.46719216520087
C	1.81979017008654	0.88449256743715	-1.19925792820789
C	3.06107064126903	0.38460565391835	-0.73364127845288
C	3.55497297120064	0.79194358378023	0.50475441727427
C	2.77582933218986	1.70932974727696	1.27001374597646
C	5.64476898871441	-0.45864269976253	0.59322544882433
C	6.90804957782780	-0.59265107036493	1.44226587379316
C	6.38632503791810	-1.46771537436652	3.67873726705448
C	4.97999431722747	-1.94232090066594	3.42985280260200
C	4.67379198778679	-3.26122739218412	3.11350898753038
C	3.32504500641747	-3.61823637351238	3.00706247247691
C	2.35437989698286	-2.65499855762520	3.25948074057525
C	2.73899112816282	-1.33893855554027	3.56958071064120
C	7.84967718766304	0.46290672503808	3.45713317258728
C	7.96342784428252	1.83860381690497	2.85343767399643
C	9.18136775062390	2.51487485540901	2.79274792749908
C	9.19432556659998	3.80668255597144	2.26539822844826
C	8.00041849050982	4.36000934655923	1.80442379446912
C	6.81433717094009	3.61936365890468	1.88607260841621
C	1.71243046096509	-0.29199172048885	3.89501081748889
C	5.50587617948525	4.17142100243612	1.40742536329837
C	5.76206391540533	3.36838791800464	6.12817596962551
C	7.05899057234423	2.64385854800198	6.48793677133655
C	5.98748002984978	4.87408738752899	5.98005894062776
C	4.63837895070567	3.05163166095122	7.11434606509472
H	3.09665123835458	3.17042512986900	4.21590112277643
H	0.87885327190866	4.17727784318887	3.53503135403380
H	-0.11357587747556	3.53715120929490	1.32486422508365
H	0.10698631765122	2.15200004551192	-0.84611029445321
H	1.46095115194081	0.54585283082490	-2.17333060504105
H	3.63621694138678	-0.31683238231398	-1.33323915166191
H	7.31919765251645	-1.60632211832691	1.33205199655136
H	7.64175362574946	0.11363854156854	1.02753366859626
H	6.46780499521885	-1.18383066948159	4.73801477862110
H	7.11994879257719	-2.26320764201930	3.47230142151008
H	5.46872560795998	-3.99266370306220	2.96090904111017
H	3.04029434017871	-4.64024114444976	2.75009084018558
H	1.29368163828482	-2.90909631518557	3.22621361520452
H	8.78464913544272	-0.10519419649614	3.31674636598553
H	7.66500846913262	0.56198234674253	4.53675843424565
H	10.09525157310909	2.03662008691616	3.14877907407135
H	10.12691408082356	4.37080376828013	2.20282578784363
H	7.97901074581167	5.36110154814044	1.37195012475702
H	2.14927466996124	0.48109274627718	4.53795163144517
H	0.85456617517945	-0.74693207960386	4.40944580767626
H	1.33084812716969	0.18522936803397	2.97862855259933
H	4.99666649946174	3.44860242667080	0.75417981799433
H	5.65093199243919	5.10831772856117	0.85526142416944
H	4.84945440091614	4.37104848280674	2.26761356517866
H	7.42496455666032	2.98486646813546	7.46781248337093
H	7.83569593868534	2.85316948578926	5.73660022259192
H	6.89042037327718	1.55897684498306	6.54526432588155
H	5.06196449687597	5.37693506261767	5.66252601469866
H	6.77375006861457	5.07725576369088	5.23778925533756
H	6.29847894015915	5.29999469817984	6.94536068274577

H	4.92480840315590	3.35428064831986	8.13281285198817
H	4.42457567740538	1.97356631940404	7.11806202160643
H	3.72041017440445	3.59393835028405	6.84009809675089

[Mn^{III}(OO^tBu)(⁶Me²dpaq)]⁺ - triplet reactant (TPSSh)

Mn	5.14075903555799	1.01556131226635	2.83498299479633
O	5.28178449546600	1.44451333469604	4.61474959211128
O	5.67304034928825	2.82512541046400	4.84849740198820
O	5.70301439600802	-1.10111765199745	-0.56748572867423
N	3.50326428521013	2.05146762255439	2.40881378819481
N	4.85519026202856	0.35987618703788	1.03260400390191
N	6.77790826935678	-0.18835533544393	2.77417872579333
N	4.15102208025007	-0.74478293082366	3.48804688316247
N	6.59399717963443	2.39238269403808	2.27194344237939
C	2.92966987381796	2.98823484096542	3.15351812090127
C	1.70757162768719	3.58599319602940	2.78315029951055
C	1.07779426059936	3.19345384094092	1.61544200246180
C	1.67876673192455	2.20615095431123	0.78923483867889
C	1.14145428501479	1.73392377174251	-0.43907924164159
C	1.83698352770365	0.78703331890395	-1.17034276309300
C	3.08444183566633	0.26701941732026	-0.74496886948379
C	3.63692488612705	0.70314358927614	0.45710388988187
C	2.91788301849566	1.66367167755953	1.23020641812292
C	5.77633170901534	-0.48238497998602	0.48611767885421
C	7.04693308172078	-0.52369792585394	1.34040010173633
C	6.47430196820307	-1.39621347487117	3.56849937023562
C	5.02840072122032	-1.77884369522775	3.42654300670415
C	4.62686819045242	-3.10720181890994	3.36990816451914
C	3.26039352825614	-3.39379345146150	3.42690982054958
C	2.37296437019993	-2.34133835591568	3.61122469398495
C	2.83827082643743	-1.01639267711727	3.65773801530292
C	7.84419057222418	0.63515879839126	3.38618111575195
C	7.79128239453458	2.00957937819001	2.78219740557880
C	8.92075833385463	2.82089762651041	2.75068061808230
C	8.82089519257073	4.08280683260919	2.16740061928275
C	7.61155952717449	4.44615222494303	1.58428488706594
C	6.50956989570637	3.58044677862636	1.62565198374445
C	1.87733976578164	0.09073248939650	3.97279288339576
C	5.25033114983881	3.96620473121546	0.91191504585390
C	5.76526288433484	3.04134444619234	6.28541553705633
C	6.85102066793082	2.14001252585565	6.87506550095869
C	6.16676495056500	4.51586920905846	6.34770194880301
C	4.40638157545017	2.79568644104986	6.94204955640462
H	3.46030179411020	3.26078228092224	4.06608710358415
H	1.27279572890245	4.34924324397619	3.42974869554752
H	0.12636628299255	3.63854398157358	1.31659862247106
H	0.18878421533266	2.12992514735178	-0.79512089353949
H	1.42217084490777	0.42861504979935	-2.11472651256303
H	3.62086322589229	-0.46276138336231	-1.34799623366892
H	7.53347123096570	-1.50533621364470	1.25425539017909
H	7.73382632954605	0.23221519677148	0.93357753876828
H	6.64169060856110	-1.14223352068992	4.62579638839566
H	7.14262928353432	-2.22948361625332	3.30339771411737
H	5.37240229527379	-3.89960475094755	3.29434696139954
H	2.90238559707800	-4.42309302584958	3.36576272743434
H	1.30461951304555	-2.52601104226168	3.73126257105154
H	8.84143063538825	0.18394897026486	3.25172127815002
H	7.62357668731621	0.70058194488231	4.46048032694206
H	9.85999363732731	2.45943850651529	3.17156122207446
H	9.68019070809919	4.75521877478713	2.13610454237770
H	7.50618094393667	5.40213554676282	1.07028783604629
H	2.37425960798926	0.86749416482446	4.56401184210400
H	1.03370327774303	-0.31418153231108	4.54756005301469
H	1.46616094813424	0.54800788727691	3.06112408815473
H	4.83472260692034	3.11249246921413	0.36369603241713
H	5.46262258128469	4.77374518628671	0.19990331567691
H	4.48625177988464	4.32652528411066	1.61453712975635
H	6.97555405334907	2.34134983778672	7.94952682026454
H	7.81532996919374	2.32582589006530	6.37701285993500

H	6.57930207680296	1.08141377380950	6.75449577142673
H	5.39491864888752	5.14900314566440	5.88566509936580
H	7.11866842384632	4.68075004940420	5.82141398224967
H	6.28809587308894	4.82524798893000	7.39627303665238
H	4.46307820991079	2.99304971672972	8.02304673732958
H	4.09153044407775	1.75314587769062	6.79442910036398
H	3.64259923136724	3.46277781738317	6.51294609966242

[Mn^{III}(OO^tBu)(⁶Me₂dpaq)]⁺ - singlet reactant (TPSSh)

Mn	5.13198044086733	1.03958537667641	2.84931909295934
O	5.23939897443504	1.51059036168379	4.59411057990898
O	5.75639120972548	2.83319079062451	4.87967871098565
O	5.71569872626664	-1.13764527957201	-0.53279177430475
N	3.49330720692576	2.05670332392069	2.37272148383797
N	4.84998701030644	0.33860660934777	1.04559736372785
N	6.77487252350836	-0.15073481887075	2.79173706020276
N	4.15468716807135	-0.71986164324869	3.51402748667136
N	6.57824708474539	2.42369506055206	2.25722423868730
C	2.91450284444666	3.00639790068366	3.09687392259593
C	1.69108457618989	3.59154162140584	2.71208388672294
C	1.06747165718233	3.17383100007186	1.54958121921811
C	1.67353772842089	2.17202640076878	0.74547015829428
C	1.14240389827398	1.67307385461419	-0.47440613513430
C	1.84379294969537	0.71162216105421	-1.18161278509439
C	3.08926316650753	0.20193226994000	-0.73969836830758
C	3.63718125914180	0.66442904644531	0.45569126786117
C	2.91240406596069	1.64111805950581	1.20285692967789
C	5.77866111386312	-0.50077970571002	0.51160168625504
C	7.05027697641745	-0.50962329557256	1.36487775132457
C	6.48061422695531	-1.34961571430741	3.60572250750450
C	5.03927725480140	-1.74813202104043	3.46680795730216
C	4.64894936869539	-3.08018161994713	3.42300792199072
C	3.28446182576632	-3.37691296882622	3.47706748567069
C	2.38794405037803	-2.32913713785776	3.64304563104012
C	2.84311257371901	-1.00021955669222	3.67666167717218
C	7.83707879469986	0.68802974847689	3.39214793260918
C	7.78045302501405	2.05130141610678	2.76348195640209
C	8.91159321123158	2.85856397795914	2.70551299211164
C	8.80929436916512	4.10892338837009	2.09815804417231
C	7.59545737523000	4.46143842721167	1.51820661431605
C	6.49267889965982	3.59784990841929	1.58594132905440
C	1.87064811869473	0.10426216086654	3.96605329056353
C	5.23012147781035	3.97156110291466	0.87108244170168
C	5.78926934648584	3.02063629596496	6.32624133581411
C	6.73800019624132	2.00087743355400	6.95703119108509
C	6.33860634306695	4.44329372757149	6.43829126496410
C	4.37609274622904	2.91187905989703	6.89911599949713
H	3.43745175343601	3.29985413446705	4.00714685231843
H	1.25102254108288	4.36543276774122	3.34220466842786
H	0.11584813234428	3.61024262874184	1.23867390440462
H	0.19036655356917	2.05891472895521	-0.84295983140254
H	1.43373246388185	0.33215227769576	-2.11987710759649
H	3.62872375626113	-0.54055533990477	-1.32419771986561
H	7.55140018411252	-1.48544444417444	1.29961146550754
H	7.72621741504894	0.24871110325830	0.94457854108316
H	6.64462024444609	-1.07680693382688	4.65893864771177
H	7.15847994017911	-2.17924580021239	3.35415651701681
H	5.40097474265451	-3.86745366280141	3.35886291048421
H	2.93481312029082	-4.40962959269412	3.42645519817579
H	1.32019020457871	-2.52070154961923	3.75758084681852
H	8.83578039985402	0.23762228617812	3.26739076590166
H	7.61627931657550	0.76889146319328	4.46546379852084
H	9.85393868728008	2.50298269973135	3.12450542674081
H	9.66930808614605	4.77905428373586	2.04564239604200
H	7.48700460779865	5.40669341262445	0.98528533728786
H	2.35602699830696	0.89733335303781	4.54514595954324
H	1.02680844700109	-0.29643624883567	4.54350437735387
H	1.46125162553346	0.54055381358083	3.04327750172342
H	4.81296932831839	3.10882600655460	0.33832061086283

H	5.43937822682084	4.76731212937627	0.14503746974898
H	4.46779305974944	4.34323569906193	1.56969852988224
H	6.81145323763307	2.16635800267870	8.04220684218602
H	7.74741366068745	2.09754708523643	6.52781668210522
H	6.36972968153235	0.97821305850097	6.79060878506898
H	5.66701704489336	5.15940891708029	5.94241258510422
H	7.33305694491629	4.51296647639376	5.97319177799663
H	6.42746933384064	4.72549506064519	7.49773965620438
H	4.39014224790047	3.09268430637773	7.98434975381622
H	3.96327902721964	1.90917237214625	6.71967315021528
H	3.71302420130431	3.65959178211177	6.43709335154525

[Mn^{III}(OO'Bu)^{(6Me)dpq}]⁺ - quintet transition state (TPSSh)

Mn	0.13800165832112	-0.39764204314679	0.00587152778875
O	0.16431550017976	-0.10284960346657	1.65580961070460
O	0.47094389885746	2.23831921450157	1.73701771222103
O	0.64275803428513	-2.40177146778595	-3.50867747857203
N	-1.57542185943849	0.60207743203149	-0.38517976809631
N	-0.12293038351223	-0.95141490897776	-1.85957918000667
N	1.76292395877617	-1.78333320404351	-0.10030715675956
N	-0.92181540400070	-2.59014990637464	0.41308450202073
N	1.87185932467779	0.85706284350266	-0.53601398296703
C	-2.22237769818932	1.39584718736731	0.45823834684295
C	-3.43994542998894	2.00399500762310	0.10102095640761
C	-3.98128911741162	1.75761004985539	-1.14923689627107
C	-3.30810507197846	0.90625629701055	-2.06442222317032
C	-3.78317507322170	0.56445053233030	-3.35902392420944
C	-3.03779569719129	-0.28962700835218	-4.15214686634304
C	-1.80369783905009	-0.83956380827197	-3.72498656832299
C	-1.30503475772560	-0.52719089144190	-2.46112566243416
C	-2.07344323675169	0.34649087621710	-1.63318009599012
C	0.74030198444727	-1.85673056271993	-2.41819334427869
C	1.97368429567765	-2.10355967452618	-1.54446192671740
C	1.43258685736558	-2.99170098222991	0.69120965830678
C	0.05842168963531	-3.50955064553721	0.35337914188331
C	-0.18286706969098	-4.85167890965197	0.07343408944561
C	-1.50570843410988	-5.25635763657819	-0.13312862405302
C	-2.51984069868486	-4.31105589216804	-0.02670154360801
C	-2.20028179146295	-2.97160314965489	0.25430579733188
C	2.91288875724059	-1.06433593304620	0.49104203201876
C	3.02407110030153	0.31298584609261	-0.11163491965165
C	4.23902957219387	0.98891047037266	-0.19846132004167
C	4.24109150996147	2.27834713141136	-0.73285634225095
C	3.04069354646405	2.82874558407714	-1.17795955054223
C	1.85485696947370	2.09172291349848	-1.07627287621648
C	-3.28654731895792	-1.94548640771133	0.40560739819427
C	0.54924937679163	2.64605128730294	-1.55855514910326
C	0.92242669233538	2.41951296727668	3.03761248492575
C	2.24318003339912	1.67257162066022	3.26221841765087
C	1.16457263939016	3.96037523038261	3.07852346042516
C	-0.15925232483030	2.01887195563877	4.05004300498007
H	-1.74332987021451	1.54693094145178	1.42555305435957
H	-3.94039140238691	2.65403642471982	0.81929633589687
H	-4.93169476430037	2.21028504275567	-1.43992442461612
H	-4.73053772329838	0.97714361019017	-3.70945523822512
H	-3.40498568879038	-0.55582417977698	-5.14526170295126
H	-1.23978760673516	-1.50790761839560	-4.37192835536249
H	2.30560388894837	-3.14418008427219	-1.66922122003429
H	2.77080723535285	-1.45226664786702	-1.93196354225714
H	1.44105653598071	-2.69215601629537	1.74954327907962
H	2.19681997643673	-3.77109894930809	0.53973008604447
H	0.64160778813968	-5.56483946492308	0.02810211852140
H	-1.73976005332641	-6.29850750244004	-0.35813555842976
H	-3.56584330095889	-4.59559348250671	-0.15137552074965
H	3.85101955682667	-1.62849804426546	0.35920807860959
H	2.71419742827219	-0.97048198007984	1.56912418804910
H	5.15896853585777	0.51210628665195	0.14328312177552
H	5.17153843667498	2.84245528902110	-0.81626267388506
H	3.01025149565674	3.82638301345581	-1.61757051413456

H	-2.96318482703239	-1.13812038427448	1.07174860265056
H	-4.19533619774800	-2.40683998274543	0.81488381636536
H	-3.54925923325256	-1.50945964130452	-0.57100992174203
H	0.04436125134514	1.93050568945415	-2.22228489361728
H	0.70487713263735	3.58389785140549	-2.10587365256937
H	-0.11172326087342	2.84558183423476	-0.70302830463108
H	2.65490749410158	1.88217799731830	4.26019236537501
H	2.98010303728361	1.97021656321836	2.50147741348980
H	2.05691480049992	0.59194104321474	3.17701797695009
H	0.23134480898126	4.50606704142731	2.88424335506189
H	1.92198519842407	4.25213706843632	2.33800225568935
H	1.52734552640096	4.21339783994033	4.08653580806531
H	0.17675537110357	2.20353019483725	5.08114839648527
H	-0.38230307960887	0.94838773322370	3.93485204786363
H	-1.08065668397562	2.59399070202999	3.87304048133071

[Mn^{III}(OO'Bu)(⁶Me dpaq)]⁺ - triplet transition state (TPSSh)

Mn	5.10721573368899	0.91898372451310	2.92306871348550
O	5.24242316635697	1.25750573844782	4.53690309311769
O	5.56749404059772	3.33881929384643	4.86085444199523
O	5.71476371907042	-1.06831693626959	-0.59282753977577
N	3.46923393979590	1.95789087091368	2.48666162848988
N	4.85149941628881	0.33136941930802	1.05759733732508
N	6.72419073174626	-0.31731545083826	2.80925537539435
N	4.05687960280737	-0.90314044923500	3.37465268001123
N	6.59793822953013	2.26946005350257	2.39939652039309
C	2.87900571787716	2.85569526523091	3.26614380758561
C	1.66404170664332	3.46805508983922	2.89584943447897
C	1.06139450586908	3.13146312450308	1.69699394265623
C	1.67978667328579	2.18298244279531	0.83905073441042
C	1.16374902372827	1.76221476555794	-0.41694067668398
C	1.86982057532037	0.84382484753427	-1.17411057946290
C	3.10865331007766	0.30581851666154	-0.74785539161656
C	3.64314541874481	0.69396053666516	0.47920547432074
C	2.91143406569098	1.62215939558300	1.27971066676790
C	5.76999387777714	-0.49832767656177	0.48940489966234
C	7.01816823737510	-0.60048407482905	1.36933189510162
C	6.37736262502035	-1.54905535371269	3.54513151185834
C	4.94420784462017	-1.92689836444680	3.29753809744741
C	4.55593830733548	-3.24940234696043	3.12820415265283
C	3.19042443651538	-3.54323285572539	3.08147853082011
C	2.28729424542687	-2.50856335564703	3.28528612545255
C	2.73981656760324	-1.18801601209612	3.45263448693953
C	7.80103043431518	0.45597391806215	3.46643434786723
C	7.78379137434723	1.84808470218508	2.90358989403819
C	8.92777622000472	2.63805067919405	2.89903470569513
C	8.85237901835464	3.91986399293751	2.35559049672175
C	7.64992426781003	4.32713802051010	1.78986803875014
C	6.53079698019950	3.48229832055671	1.80338987911561
C	1.75394834661898	-0.11353436824857	3.80497602951008
C	5.27314764408852	3.92439006181356	1.12268763220646
C	5.83939324591253	3.46130622628085	6.22630977449450
C	7.10000387544434	2.67666174039965	6.61460257050829
C	6.10491497504963	4.98917921727723	6.34816892279878
C	4.62718692216746	3.05776680483244	7.07558571248631
H	3.39993890060348	3.08963736447322	4.19577201172796
H	1.21362960460994	4.19934968752510	3.56804735078860
H	0.11610415680861	3.58991717596604	1.39831798338227
H	0.21706012208902	2.17341946027741	-0.77179896983317
H	1.47045571049075	0.52395814465973	-2.13880635764277
H	3.65540203505536	-0.40060114425079	-1.36916080990377
H	7.48637046598288	-1.58837349821507	1.25699277638132
H	7.73048044630739	0.15527014566975	1.00894576037593
H	6.48043303863951	-1.32766531012861	4.61794832757208
H	7.06246757109104	-2.37251846275860	3.29190015280679
H	5.31022042830153	-4.03285356013048	3.04626121515493
H	2.84376758617630	-4.56674675437595	2.92837377814634
H	1.21503990864151	-2.70386680371166	3.33141248325380
H	8.78660505642406	-0.01791048871931	3.32707365492157

H	7.56802123728572	0.49478940441968	4.53899956670167
H	9.85920848860304	2.24572005996561	3.30941665608796
H	9.72500210839511	4.57549003734718	2.34490613733740
H	7.56062169180038	5.30362682235340	1.31278664807265
H	2.21869875246938	0.63003559731449	4.46108711525652
H	0.89983372185434	-0.56595476140640	4.32657636915516
H	1.36186085714498	0.39617376290423	2.91318009751216
H	4.85004003423276	3.11188787149437	0.52008949011024
H	5.48769866471872	4.77688737558715	0.46624909169339
H	4.51871728556611	4.23989199059641	1.85603317514333
H	7.39624909136414	2.89232400594130	7.65243550961132
H	7.93229280851781	2.94513123785981	5.94655339431656
H	6.90283443912800	1.59820637286164	6.52692633637794
H	5.22088660506193	5.56168097394611	6.03464875433447
H	6.96476836159673	5.28285338368005	5.72996951640571
H	6.32403039282551	5.21848220306291	7.40239544231312
H	4.83202173583835	3.19955670005630	8.14788248892486
H	4.39088903496056	1.99877529724276	6.89723249829805
H	3.74994963430571	3.66588918411073	6.80655598819406

[Mn^{III}(OO'Bu)(⁶Me dpaq)]⁺ - singlet transition state (TPSSh)

Mn	0.24383367329457	-0.43717688209331	-0.10720799643308
O	0.42979770777674	-0.06808887251364	1.47807222025509
O	0.64949804066336	1.77766037835390	1.84162490848343
O	0.73242510748146	-2.61088396267457	-3.54540154364574
N	-1.36481962028082	0.61704890006720	-0.58261567785794
N	-0.05948183035666	-1.10145436820224	-1.95673802955332
N	1.86116064555417	-1.66959915382330	-0.22883402068746
N	-0.76630528080210	-2.22848772128270	0.42728766696962
N	1.71730122824501	0.92564445712039	-0.72557970916641
C	-1.91606601673790	1.55297648260869	0.18181444469577
C	-3.11190618116440	2.19630957243448	-0.19727030443926
C	-3.73330608069672	1.85180627356086	-1.38460944925026
C	-3.15394580991800	0.86419896299278	-2.22530280884528
C	-3.68532390484380	0.43783433241851	-3.47232150547629
C	-3.01014818892467	-0.51882883640804	-4.21123696573544
C	-1.79144987116427	-1.09316377054451	-3.77494371815894
C	-1.24378250911739	-0.70191204726011	-2.55399200587222
C	-1.94137061635344	0.26897414146350	-1.77637803425740
C	0.82451739278828	-1.98222882325430	-2.49827986837432
C	2.10472487251815	-2.03619708656511	-1.65934260333355
C	1.54955861521203	-2.86070942114253	0.58836873933863
C	0.11596113647673	-3.25857074350110	0.39895985022183
C	-0.27737074238646	-4.58772713495270	0.32328892474264
C	-1.64392393368848	-4.87958883642838	0.32190338012920
C	-2.54053639310734	-3.82993978350061	0.47066038432004
C	-2.08385934276262	-2.50233586039572	0.54115415458864
C	2.95819514513353	-0.86236453703784	0.35325884197759
C	2.91866181142831	0.51067540555676	-0.25408977102900
C	4.06848703670592	1.29019690805141	-0.31754660068970
C	3.98450684343749	2.55892039914008	-0.88763974080233
C	2.76623501216361	2.95886559113262	-1.42386651337998
C	1.64255274408088	2.12282388058218	-1.35523555636376
C	-3.06698739370633	-1.40459650472689	0.82313566225491
C	0.37610972999448	2.56127059591004	-2.02306041201195
C	0.82860169249472	1.90824292363628	3.23871675929446
C	2.07548848589472	1.14314838425092	3.70444907519393
C	1.04074622978349	3.42807498354237	3.40999757560244
C	-0.42441026900799	1.44955147534089	3.99706108269247
H	-1.37005550136622	1.79602505709077	1.09639119219984
H	-3.53140240816866	2.96020326959894	0.45842088163782
H	-4.66381648659386	2.33639436760445	-1.68862821480965
H	-4.61712980597879	0.87464121907177	-3.83558842420835
H	-3.42053079289286	-0.84257523629752	-5.17002619490242
H	-1.27188892265873	-1.83212845227177	-4.38159678725945
H	2.57418997364887	-3.02719718225642	-1.72834932038956
H	2.7987749564673	-1.29907733988275	-2.08787259157253
H	1.67909154732575	-2.57430780901823	1.64264629901486
H	2.23836947601923	-3.68889106772745	0.36320653581269

H	0.47419281406939	-5.37666434198281	0.27802836417770
H	-1.99601202692300	-5.90964099748493	0.24393540049934
H	-3.61239649428210	-4.01773810095054	0.54592100708458
H	3.93919255410628	-1.33846743803277	0.19260100494828
H	2.77039814249415	-0.78715377878420	1.43375091799542
H	5.00996557549294	0.89944968536962	0.07087678228994
H	4.85994000423092	3.20843754645804	-0.94261828264285
H	2.66741855153924	3.92346028229792	-1.92272582606934
H	-2.61100119886757	-0.63236153725696	1.45238973214220
H	-3.93444706949929	-1.82469112906847	1.34909636041569
H	-3.43660092087646	-0.93535434167959	-0.09989960888688
H	-0.05781345804881	1.74549616692261	-2.61348187051208
H	0.58699465704780	3.40466792608197	-2.69216364015276
H	-0.36872774208968	2.89062001184257	-1.28638579428146
H	2.28070193411761	1.33084806322494	4.76963335692506
H	2.95325122149917	1.45958289641412	3.11993851136784
H	1.92677214332271	0.06114546665466	3.57089268650964
H	0.16020498966001	3.98244407477667	3.05383971261769
H	1.92136406473402	3.75894075807182	2.84042773204486
H	1.19788320099505	3.66201284467706	4.47473869323177
H	-0.30987071658157	1.60156683035234	5.08151302814505
H	-0.60549332694007	0.38042579701745	3.81147206349885
H	-1.30489064029050	2.01951678731039	3.66135545773117

[Mn^{III}(OO'Bu)(⁶Me dpaq)]⁺ - quintet product complex (TPSSh)

Mn	5.08291308583106	0.91085699507267	3.09702561566434
O	5.08132526284417	1.01492116344160	4.73664463960812
O	5.34269807904718	4.14693158174536	4.71194165129267
O	5.54001207519987	-1.00503827525094	-0.49452097239812
N	3.39414565491959	1.92585920558463	2.75463918417928
N	4.80899911001597	0.44463182781994	1.17303707223577
N	6.60565507003256	-0.49304015703594	2.96451179590528
N	3.92328484309826	-1.32918500302252	3.27309495498794
N	6.66815409526975	2.12904669592254	2.60558380562121
C	2.75065498308136	2.66885106171218	3.64912254573517
C	1.53939880121406	3.31076205172162	3.33009507665677
C	0.99358179235184	3.14924589845497	2.06802436735393
C	1.65281868863740	2.34477973253475	1.10238857366788
C	1.16376108089070	2.08402263625547	-0.20575330189430
C	1.88974853561269	1.26375773749842	-1.05238355082507
C	3.11870146659084	0.67557641383800	-0.66709323834355
C	3.63475227535936	0.91388545152591	0.60715562790716
C	2.88431648365237	1.74719389831568	1.49278145951671
C	5.63008362889815	-0.48106243729680	0.60888641207838
C	6.83110141271264	-0.80665660119201	1.51202133962323
C	6.25180003435877	-1.70175963524426	3.74916002712597
C	4.91312098893846	-2.24046048519276	3.33250167541119
C	4.71156855836006	-3.59794555041669	3.09768722456164
C	3.41490421537595	-4.03496648795208	2.81404831211726
C	2.38610544267146	-3.10056927081524	2.80318216310595
C	2.66566312081313	-1.74229137171194	3.03838758140514
C	7.75117520965676	0.20814370624621	3.58879155107536
C	7.84583659531948	1.58320454929487	2.99933067187448
C	9.05493643563185	2.25430585354083	2.86825238443348
C	9.05041718701032	3.53929391557202	2.32416729999029
C	7.84155033640418	4.07877149028733	1.89999902962679
C	6.64727833568124	3.35614383132886	2.03363851850642
C	1.54881852211884	-0.73862183526418	3.04702831517661
C	5.36448919954833	3.92807956679100	1.52442257064380
C	5.84149629220117	4.17408209514992	6.00411128569661
C	7.15502428236812	3.38194410194999	6.09744802578409
C	6.11589033730983	5.69685226262459	6.21468476894826
C	4.79411205937732	3.67504442938926	7.01132172450354
H	3.22033497746300	2.74955896197327	4.62771273398375
H	1.04570034901149	3.92033794865398	4.08734691551367
H	0.04895054818198	3.63129903770298	1.80606200778197
H	0.22126166788129	2.53130438630897	-0.52589260790863
H	1.51090082067482	1.05961449558184	-2.05599064264482
H	3.66943741503755	0.03385914657734	-1.35197795600775

H	7.09928808399106	-1.86497957831113	1.39085367370987
H	7.67847900759702	-0.20320964295072	1.15539170250463
H	6.19574103164970	-1.38703688107287	4.80122633030245
H	7.04046952835401	-2.46303477684042	3.64017627364513
H	5.54847071059489	-4.29631544672236	3.14520315467290
H	3.21253671411576	-5.08979969693213	2.61936506399603
H	1.35586961474576	-3.40739970651682	2.61580328790028
H	8.69018655035296	-0.35289504525813	3.45695007953939
H	7.52930289948217	0.28764847296210	4.66378819446664
H	9.97904622164672	1.77075064312284	3.18676139212987
H	9.97963758869730	4.10123422665831	2.21427082059728
H	7.80083247377274	5.06837512498278	1.44464190680557
H	1.78361004234521	0.09933809710979	3.71281742650205
H	0.61622990019302	-1.21166438932630	3.38375098174663
H	1.37221544186586	-0.34552129614197	2.03387832482750
H	4.87434118344205	3.22565754380731	0.83750379344835
H	5.56016490941852	4.86397665597261	0.98757105479711
H	4.68629654337352	4.14062449708146	2.36081702090446
H	7.59834429513326	3.47417112614854	7.10059862000541
H	7.87717666241921	3.75146704713353	5.35451384333638
H	6.94295579205408	2.32069125469549	5.90162483357471
H	5.18637447087064	6.27349000248846	6.11583749691770
H	6.85227539734769	6.05996142074231	5.48482277394970
H	6.51688147063368	5.82639625049591	7.23141223310800
H	5.16960343059299	3.76164498909818	8.04243247908198
H	4.56881461685909	2.61752613990326	6.80855554183028
H	3.86974506179202	4.26543094764730	6.92486605641930

[Mn^{III}(OO^tBu)(⁶Me₂dpaq)]⁺ - triplet product complex (TPSSh)

Mn	5.06763735486044	0.88033591321520	3.06753978901170
O	5.17142756333878	0.98096336001409	4.66612777458249
O	5.31120917427620	4.25292228935040	4.78750436456013
O	5.60059014725278	-1.02843177215159	-0.53618565820489
N	3.41542900511773	1.92561872058195	2.65352791393867
N	4.81618995430789	0.36895040037629	1.15463539097930
N	6.64157591724085	-0.51079080053259	2.91061411778254
N	3.91413171624958	-1.27785716637574	3.32649402340369
N	6.66124661970765	2.13509298277423	2.62473149871845
C	2.77735801869371	2.72736553810811	3.50097396824325
C	1.55489356440764	3.33878748014080	3.16140351539637
C	0.99384995844176	3.10559145702662	1.91883603924292
C	1.65122216714967	2.25044652787011	0.99685195334701
C	1.15702367911227	1.91753035362743	-0.29366996657094
C	1.87900078675774	1.05535075711181	-1.09960979022853
C	3.11023848707530	0.48832030857813	-0.68864947286223
C	3.62930314828098	0.79577347290249	0.56818281285370
C	2.88473332494884	1.67523853957136	1.41192822705531
C	5.68062521546665	-0.51302668076827	0.57097071404814
C	6.89748848626019	-0.78403576125728	1.46154970514478
C	2.6555521448516	-1.74125907164553	3.64759982499677
C	4.88631386335049	-2.21163185096441	3.26794516028409
C	4.62630871573996	-3.54423644129197	2.96251011877994
C	3.30102361249966	-3.92851447735549	2.73587537302081
C	2.29897411071863	-2.97372561771024	2.85911928961728
C	2.63146440052428	-1.64116582311412	3.16292882705156
C	7.77329105778860	0.18845319685915	3.56003738243245
C	7.84333396770952	1.58599572976248	3.01110753218078
C	9.05095287543543	2.26502349211571	2.90475959616197
C	9.04907362864952	3.56102835101750	2.38815490975025
C	7.84264938596016	4.10222117989433	1.96113199408132
C	6.65021784810177	3.37173923590956	2.07206898257345
C	1.55325672064059	-0.61212600155616	3.34079708540859
C	5.37412245652274	3.95327377041428	1.55470965070142
C	5.83592867448928	4.20116906924984	6.06807336773483
C	7.18172959187386	3.45809142548870	6.07310674740415
C	6.05865705024107	5.71306075462310	6.39127842499263
C	4.83051516987503	3.58567802264205	7.05350964298677
H	3.25806730081411	2.89585948171986	4.46307134040116
H	1.07051444125191	3.99004482820918	3.88955059036557

H	0.04566280511521	3.56955824968487	1.63855429712347
H	0.21091653066852	2.34403824055735	-0.63133645046673
H	1.49548261833497	0.79802277161697	-2.08905480382110
H	3.65904175985859	-0.18608235606610	-1.34237587670695
H	7.23731980318121	-1.81915024393159	1.31715726380775
H	7.70175409344281	-0.11653195860029	1.11921390600845
H	6.25951902323899	-1.48101701178098	4.71604258166056
H	7.01265375710928	-2.53270961374717	3.47828129619091
H	5.44231275202907	-4.26660010444891	2.91243305780692
H	3.05729996833820	-4.96275737172484	2.48594480503337
H	1.24994908688315	-3.24394944960372	2.72818020886170
H	8.72568890991883	-0.34526496073841	3.40955445479722
H	7.55444973584142	0.22791063111590	4.63716585436253
H	9.97427281161351	1.77695758188541	3.21903759174294
H	9.97757193070565	4.12788292735549	2.29896046591907
H	7.80221478779478	5.09915201260958	1.52196308765173
H	1.88540462827424	0.17992635986808	4.02116161555123
H	0.64739142077959	-1.08002565270614	3.75011954132163
H	1.28253139407377	-0.15683170712180	2.37590326573370
H	4.86653040055227	3.24480799077089	0.88755964792139
H	5.58348890775570	4.87378359256446	0.99639454975881
H	4.70392525001695	4.19777962516969	2.38849561552210
H	7.64401714224958	3.49385735924422	7.07126678490884
H	7.87032131199728	3.91037694307275	5.34467496366197
H	7.01170252042547	2.40572557608458	5.80291408413766
H	5.10650123309659	6.25913361341888	6.35505481475464
H	6.76510332235420	6.15881812854819	5.67804815930730
H	6.47623654365663	5.77796994614781	7.40754436540636
H	5.22593824505069	3.60420966251952	8.08065483042641
H	4.63554042122513	2.53914627167697	6.77502168184585
H	3.88390150879473	4.14583077212578	7.03243257839971

[Mn^{III}(OO'Bu)(⁶Me dpaq)]⁺ - singlet product complex (TPSSh)

Mn	5.06654509321845	0.89442630394061	3.06660071725540
O	5.17142477276574	0.99555079000180	4.66503140064437
O	5.32492587495750	4.17259432012569	4.78864629476333
O	5.60436003570758	-1.02520414812324	-0.53195587930179
N	3.41170969383173	1.93449095646048	2.64734856292942
N	4.81773550343053	0.37607470527433	1.15455535009506
N	6.64040447795024	-0.49784828808334	2.91451068082502
N	3.91154664353654	-1.26175528238250	3.33176885679984
N	6.66143749058268	2.14596025177591	2.61945542931778
C	2.77024584105992	2.73616957664575	3.49225829858516
C	1.54520999964538	3.34121217997714	3.15045405781382
C	0.98617806679899	3.10310852324502	1.90793167897651
C	1.64772287251016	2.24869226032153	0.98833855382567
C	1.15588227299951	1.91129933181679	-0.30188123053239
C	1.88155603290392	1.04966963430827	-1.10499080077073
C	3.11401022531145	0.48733977733324	-0.69120307216482
C	3.63075103007639	0.79912746181490	0.56555661454873
C	2.88290274210843	1.67867971603412	1.40607663894840
C	5.68281367308434	-0.50718252549687	0.57417193965245
C	6.89805115513418	-0.77656486175519	1.46698897922670
C	6.26269065566642	-1.72519009118814	3.65560977378034
C	4.88351020167934	-2.19597715748067	3.27633568018641
C	4.62352018154316	-3.52950417286704	2.97491694741851
C	3.29827580468807	-3.91450891968661	2.74936376478440
C	2.29629099829656	-2.95936776167979	2.87032958526463
C	2.62880781638077	-1.62593514581331	3.17019766339508
C	7.77195611209287	0.20290005990624	3.56225386712231
C	7.84316086395002	1.59778558862441	3.00716740251616
C	9.05123544966449	2.27555532438849	2.89688089105209
C	9.04981953857578	3.56904745798743	2.37420532603175
C	7.84319087589264	4.10955780344137	1.94660528054771
C	6.65038534791507	3.38074054621207	2.06305717006478
C	1.55019207242370	-0.59707254999005	3.34683688568171
C	5.37281988668366	3.96236622935025	1.54957058726913
C	5.84495859870223	4.15638806172582	6.07222273041557
C	7.20299146873700	3.43663244390185	6.09812170855382

C	6.04187705938770	5.67812414476060	6.36390030389403
C	4.84563426397905	3.545327711479441	7.06622003742052
H	3.25190246153743	2.91072978336581	4.45288274927216
H	1.05748117101374	3.99215391396466	3.87668215620869
H	0.03644567920201	3.56273461828651	1.62570031416583
H	0.20871730787262	2.33391808807558	-0.64146522966219
H	1.50012100632186	0.78875797618729	-2.09430490105905
H	3.66539715184830	-0.18699554259092	-1.34278229718594
H	7.23670220571324	-1.81264679343729	1.32682638430456
H	7.70368151296174	-0.11141197441328	1.12331549650852
H	6.25567319758879	-1.46090901724772	4.72304942914212
H	7.00932541325240	-2.51786082077613	3.49003663777063
H	5.43949776359269	-4.25205744409121	2.92724723492400
H	3.05451351041865	-4.94945834500217	2.50242767838397
H	1.24719775889743	-3.22999737434191	2.74079535994765
H	8.72401930190768	-0.33229345693515	3.41508202324988
H	7.55188509714327	0.24721229126213	4.63891295595217
H	9.97443502263669	1.78832866056723	3.21280058096391
H	9.97868719282806	4.13468323857222	2.28117429482447
H	7.880298169443379	5.10473826662592	1.50342420405246
H	1.80101878068806	0.19456661669199	4.02833121335679
H	0.64370974411958	-1.06538636559543	3.75425210125464
H	1.28103800382614	-0.14109118144769	2.38186960661368
H	4.86372831628391	3.25470222396346	0.88264596530934
H	5.57980463837724	4.88397976081187	0.99218435668412
H	4.70462889775681	4.20382296592847	2.38590256088977
H	7.66172779170737	3.50354550641202	7.09628523701130
H	7.88594041764593	3.88335622286992	5.36101155115293
H	7.05177238903421	2.37553617346451	5.85214901045552
H	5.08152995711380	6.20824607662117	6.31011974255942
H	6.74572275726310	6.11958223569393	5.64541582939048
H	6.45170136464111	5.77210714347039	7.38103986489247
H	5.23872450259421	3.58540349078661	8.09365117675197
H	4.66297299108939	2.49269912060629	6.80319415368555
H	3.89235330481205	4.09368668202790	7.03474488138839

[Mn^{III}(OO^tBu)(⁶Me₂dpaq)]⁺ - quintet reactant (B3LYP)

Mn	4.95923693400343	1.08168915913440	2.97712268092399
O	5.04927035176162	1.54088594946862	4.75619797133078
O	5.24700741550111	2.97521910686549	4.84205928237914
O	5.53601027259262	-1.00653278959191	-0.46787294188458
N	3.24122743737976	2.10265808762567	2.50230916582731
N	4.72951420228965	0.46166058278511	1.13285240213975
N	6.65931511643398	-0.26533183490065	2.92496583533902
N	4.00543611652665	-1.06086244100415	3.60482363743448
N	6.76967392244016	2.41434950801725	2.41833214349466
C	2.56522182148047	2.92803285376262	3.28479770721180
C	1.36513328782224	3.53014304680371	2.85969913394849
C	0.87826501776747	3.25085357606678	1.59584481208059
C	1.58337512162860	2.36652803129708	0.73966350116101
C	1.16499775607208	2.00469706782296	-0.56848427059296
C	1.93369721892784	1.12560862791196	-1.30532028156644
C	3.13451181253185	0.56551145460174	-0.80193940549271
C	3.57848676120272	0.89771553992559	0.47490399598119
C	2.78998675889432	1.80477947945926	1.24535164421218
C	5.60796090993138	-0.44363694212690	0.61256943939000
C	6.82965169291943	-0.68347051871915	1.50329254353172
C	6.37450536703387	-1.41488753984954	3.80977508418772
C	4.99400796531822	-1.96984168153772	3.58057767530043
C	4.75915762345051	-3.33241744430565	3.42834924368204
C	3.43512443918648	-3.76727067253079	3.32258211543250
C	2.41374710782111	-2.82692165663405	3.39487859758934
C	2.72780555188127	-1.46515708597364	3.53780698637712
C	7.82742488188136	0.48635151713935	3.42326461620205
C	7.92756439081375	1.83941082903642	2.76795850724467
C	9.15812854684558	2.46862348315761	2.58761574618761
C	9.17179329445544	3.75028634870631	2.03759221413111
C	7.96245301924393	4.34225884759340	1.67993601911815
C	6.76338509362618	3.64543563007637	1.87715804744041

C	1.64174431152064	-0.43293068027679	3.63277652108299
C	5.44107254556082	4.24495514449039	1.50522888747545
C	5.75806436740507	3.32764407129681	6.15588528246436
C	7.11036670576431	2.65692471174452	6.39611463602995
C	5.91054098017937	4.84405418974789	6.02917157002185
C	4.73830251342936	2.94788732692242	7.22834589667763
H	2.99765041453074	3.12085413180471	4.26745865644134
H	0.83789770676599	4.20695308639303	3.53355639407283
H	-0.05181711025554	3.70529556070453	1.24493866561824
H	0.24231656969898	2.42524436203263	-0.97331322370047
H	1.61498983730392	0.84404632964104	-2.31158096282628
H	3.71632291569799	-0.12672512378803	-1.40556443594103
H	7.11115216776922	-1.74427586271340	1.43793644103998
H	7.65033536376694	-0.10332910500614	1.05753042461128
H	6.42587404726792	-1.04761205938869	4.84553420332471
H	7.14073518151809	-2.19757023496036	3.68551849898485
H	5.59212378220002	-4.03701835597055	3.40097419162249
H	3.20676137681003	-4.82802656093986	3.19777395943447
H	1.36758790265198	-3.13340059131990	3.34370348679176
H	8.75829154700875	-0.08727570631756	3.27675028490180
H	7.68790402694492	0.63260672425014	4.50353659478778
H	10.08214394030774	1.96217912614591	2.87251880947724
H	10.11547602455183	4.27775182196714	1.88165260884796
H	7.93767730140350	5.34016208830726	1.23957060073874
H	1.93177613187447	0.36961373670062	4.32189561190043
H	0.70447686635621	-0.88588854910494	3.98337529411931
H	1.44445366687390	0.01689028047181	2.64749328740021
H	4.89524186147050	3.58550794062304	0.81526491558729
H	5.57016303738810	5.22276344468521	1.02415740267502
H	4.82214339160727	4.37426850066416	2.40469051789927
H	7.54541769210394	3.00832838671030	7.34366584183006
H	7.81135783350913	2.90256888349830	5.58364875479571
H	6.99765336996103	1.56531187973803	6.46131907238244
H	4.94257561942414	5.31698312496746	5.80512729219105
H	6.62015716484445	5.09818316659453	5.22712202961189
H	6.28766309735474	5.26353114428813	6.97372374501793
H	5.08960607188503	3.26544990238911	8.22197406770753
H	4.58028398178623	1.86046851607381	7.24725904781126
H	3.77220758409198	3.43835012684929	7.03266227734727

[Mn^{III}(OO'Bu)(⁶Me dpaq)]⁺ - quintet reactant (TPSS)

Mn	5.01334267141312	1.09892956788575	2.95873734767984
O	5.12214887785560	1.57755715650692	4.72935343631594
O	5.38829459525237	3.02675640243169	4.81445411035007
O	5.53992853920919	-1.09183614385538	-0.44705330041878
N	3.28420600101587	2.07479693099360	2.50676323692723
N	4.74818716162286	0.42226368742084	1.14185109393047
N	6.69790948953778	-0.24940215987054	2.90536935572103
N	4.03735603586397	-0.99676871661406	3.63510558809282
N	6.80777991974558	2.38405964702443	2.38997375157277
C	2.62734638968311	2.93868200648048	3.28142319893870
C	1.40096599684626	3.50739367385752	2.87716058127452
C	0.85702147031514	3.15839242313353	1.64765067431274
C	1.53700330614473	2.23986693735484	0.80137007312727
C	1.06961144915760	1.80724237897643	-0.47187382908888
C	1.82593263616506	0.90225109270406	-1.20311817730181
C	3.06144200439698	0.38757879431703	-0.73058698174754
C	3.55425943953981	0.79133440624317	0.51515578360293
C	2.77882226921472	1.71719700388855	1.27978857376461
C	5.64249095493028	-0.47856025165361	0.61330162396309
C	6.90833402060608	-0.61292858559929	1.46711119295379
C	6.39043445944745	-1.44924721476544	3.73073855772778
C	4.99064443973103	-1.93958984256667	3.45971038117496
C	4.69620775103697	-3.25921807727445	3.11878596203708
C	3.34827836362830	-3.62050939256207	2.97280550987849
C	2.36486282514025	-2.66091876271413	3.21179066210993
C	2.73636476202222	-1.34457800971412	3.55287641000754
C	7.85415387800868	0.49192275740851	3.47081996474009
C	7.96619824738721	1.85102648489951	2.82370320946567

C	9.18794344212588	2.52162366729702	2.71124333044609
C	9.19372793502455	3.79819201062466	2.13808489399062
C	7.98860209641054	4.34240758702420	1.68420861382008
C	6.79793281006565	3.60895031268134	1.81656251714318
C	1.69798664358732	-0.30196452898554	3.87056989463091
C	5.47847817323925	4.14712635106504	1.34170830915219
C	5.76657085005779	3.36187349233045	6.19039238406409
C	7.05794843198108	2.62819657998088	6.56783124398810
C	5.99335072995440	4.87428982923542	6.06901507148338
C	4.61499925502369	3.02642684758437	7.14307202635416
H	3.10125797736970	3.17626543658046	4.23730790424703
H	0.89399536342179	4.21284699832005	3.54070800659449
H	-0.09647695372164	3.58482886218911	1.31911652284681
H	0.12161127684199	2.19370896465686	-0.85753533923291
H	1.46758671453615	0.56791537259243	-2.18186202075340
H	3.63498322243376	-0.32077295343458	-1.32827121374605
H	7.30812250058576	-1.63580306505512	1.37589913858571
H	7.65327404101056	0.07927789630691	1.04157385442661
H	6.45089032887074	-1.13572109893647	4.78568362407173
H	7.13841472972384	-2.24205932011307	3.55264357669084
H	5.49899194345509	-3.98827471631076	2.97699506376761
H	3.07372449075694	-4.64240084866815	2.69423705817000
H	1.30392137535849	-2.91936429980751	3.14589543775959
H	8.79274058141734	-0.08031723414583	3.35262759795836
H	7.65672643135675	0.62131638432117	4.54787711684963
H	10.11049145477378	2.05056789099287	3.06266761630598
H	10.12913158238986	4.35653791001915	2.03452916071084
H	7.96178840425229	5.33098365406287	1.21760513643735
H	2.13093678427302	0.48204409415603	4.50731038149229
H	0.84140064931819	-0.76066916016624	4.39013670648457
H	1.31087747133346	0.16677973477962	2.94865399343281
H	4.97260628371652	3.41411267847441	0.69210567889210
H	5.61177998253630	5.08531535747504	0.78356233061134
H	4.81911269033956	4.34109787493471	2.20423318676069
H	7.40108736533118	2.94714904013882	7.56642244747661
H	7.85470989849583	2.85332939334887	5.83826067034569
H	6.88724573944441	1.53951653564088	6.59696607873653
H	5.07021686033325	5.38213334769432	5.74353489634144
H	6.79356622794357	5.09000008420549	5.34148964881299
H	6.28881305146434	5.28396114640872	7.04931021731288
H	4.87613864192929	3.31479850214530	8.17541236021018
H	4.40440815429746	1.94514537242855	7.12421088380536
H	3.70062541202097	3.57202682158969	6.85289700140843

[Mn^{III}(OO^tBu)(⁶Me₃dpaq)]⁺ - triplet reactant (B3LYP)

Mn	5.11240257371421	1.00776762748873	2.85834983535596
O	5.25467046838912	1.44260073991595	4.64347849482882
O	5.58775851105616	2.83600697417104	4.85815547530881
O	5.68694540633339	-1.08125323514901	-0.56498448039170
N	3.45809944729425	2.05992943939424	2.42071568283517
N	4.83658517301887	0.36638242511082	1.03751959968290
N	6.75989259233546	-0.21389702209042	2.80298211064494
N	4.12020391292656	-0.79702879631212	3.50682746189750
N	6.60109997203847	2.39933734731353	2.28356902209283
C	2.86827853253451	2.96953800727109	3.17612841698972
C	1.65949330392525	3.58464877276477	2.78887993163070
C	1.06868004681406	3.23073435482804	1.59080185162509
C	1.68838592652081	2.26366659197883	0.75588124109579
C	1.18133529965477	1.83115381292326	-0.49923854906150
C	1.88710349892325	0.89776889807390	-1.23408071180069
C	3.11572841272732	0.35292688625477	-0.78378206609193
C	3.64077097029327	0.74993206010552	0.44181944328446
C	2.91058674155308	1.70157437061231	1.21896621956327
C	5.74699691947166	-0.48602182653311	0.49980108185618
C	7.00082806451999	-0.59285727568768	1.37663207350951
C	6.45902035533731	-1.38998222448283	3.63896198637299
C	5.02297980430828	-1.80652092038264	3.48982263433100
C	4.65597391595092	-3.14482417632187	3.45879016952296
C	3.29680731741281	-3.46445725374023	3.49224343832958

C	2.37907103493959	-2.43087888270627	3.61712696178746
C	2.81220582022562	-1.09462569466996	3.63856678416641
C	7.84234694577712	0.61290203875439	3.37044630711928
C	7.80063466461295	1.98066434233627	2.74914028811742
C	8.95269034225820	2.75544293998397	2.67263105511317
C	8.87061986420046	4.01967049880721	2.09354845515178
C	7.64951824357908	4.42640532014128	1.56960434532695
C	6.52435330471318	3.59456954546215	1.65603761032239
C	1.81119107722047	-0.00383982999986	3.87646756151712
C	5.24581251443015	4.03394620905004	1.01076327038340
C	5.76472925708603	3.07041897532936	6.28017257189500
C	6.94178247921399	2.24435831481668	6.80156787712773
C	6.07959326682483	4.56647327292058	6.31692125707349
C	4.47300501388880	2.75207587760949	7.03348555690462
H	3.37315824593305	3.21731552080950	4.11074325400169
H	1.20700606749532	4.33050224891762	3.44418637299289
H	0.12948632774116	3.69044214673529	1.27315193175305
H	0.24221020217718	2.24683422730072	-0.87009549672265
H	1.49703294755089	0.56726888553431	-2.19958269693156
H	3.65946050878543	-0.36975132293783	-1.38872043216434
H	7.41625882123743	-1.60816773258104	1.30721245297440
H	7.74260853908774	0.09640815120737	0.94911756383919
H	6.60453317390262	-1.09408817833211	4.68831813452667
H	7.14468179960307	-2.22389875656429	3.42217665377446
H	5.42206352803855	-3.92069763325256	3.42047065763402
H	2.96599667555467	-4.50453495127264	3.45352715605745
H	1.31215955267209	-2.64000149922570	3.70858908551644
H	8.83132525824031	0.14618076111057	3.22618862164940
H	7.65522038065037	0.70590195168517	4.44863300673706
H	9.89639802685765	2.36427404390329	3.05646548471988
H	9.75036422931330	4.66322637959675	2.02490962290671
H	7.55288338788151	5.39038749962641	1.06858209861208
H	2.24897402352415	0.79132692230771	4.48894588503426
H	0.93619163089400	-0.41382552794606	4.39851364056039
H	1.45556343416539	0.43619417139983	2.93439824428528
H	4.81752235590097	3.22966230963346	0.40104578919718
H	5.43044278954991	4.90048828806202	0.36347861355359
H	4.49852070174605	4.32492750135194	1.76023199621122
H	7.14125035517582	2.48094560529172	7.85758957644951
H	7.85222899796009	2.46797520678556	6.22345879061942
H	6.72462018287236	1.16889767566800	6.73048175144883
H	5.24424726067167	5.15122859004960	5.90312474633119
H	6.98532237245528	4.79045849672378	5.73338801702880
H	6.24616011265313	4.88979819020633	7.35525866728649
H	4.58691045013137	2.98166259249815	8.10387256344860
H	4.21430118652985	1.68887538992618	6.93193156298985
H	3.63848447702221	3.35616734043839	6.64374741825921

[Mn^{III}(OO^tBu)(⁶Me dpaq)]⁺ - triplet reactant (TPSS)

Mn	5.14571450356200	1.01979119115509	2.84015811917486
O	5.30073061620971	1.44984964306487	4.62124790467575
O	5.69961081664671	2.84495994734267	4.86847196707153
O	5.69029362491634	-1.13088240385909	-0.55869332974811
N	3.51515749971643	2.04313909305328	2.42579095377570
N	4.85574107620031	0.35533342135270	1.03993405947901
N	6.78656259356300	-0.19017474429844	2.78153921630532
N	4.15351122387261	-0.74459699028200	3.48985519502241
N	6.59617979913420	2.39007637383332	2.26853900407241
C	2.93670217540706	2.98645704935508	3.17564885541236
C	1.71430145901697	3.58732061999632	2.80452660724174
C	1.07726938296631	3.20196285546875	1.63241050070075
C	1.67787981570048	2.21237865016878	0.80195972469852
C	1.13964261213707	1.74154347261065	-0.43056814163233
C	1.83217534012404	0.78958354845443	-1.16760891017639
C	3.07972751335951	0.26316373746470	-0.74309977121457
C	3.63385118231950	0.70033660187887	0.46359956776769
C	2.91936307569827	1.66291370346269	1.24110857394041
C	5.77502102440074	-0.50052912860939	0.49398206305366
C	7.05264813307075	-0.53780969214682	1.34430392745682

C	6.48029893146634	-1.39533470790277	3.58925190309908
C	5.03549766522633	-1.78273922810440	3.42664796399608
C	4.63374493767686	-3.11340906248830	3.34504924851855
C	3.26303745613457	-3.40252971045728	3.37612465160304
C	2.37046235143024	-2.35027407032733	3.56434848000292
C	2.83361168743086	-1.02136571837437	3.63904984781917
C	7.86015388670793	0.63945662117993	3.38831191629257
C	7.80659850129949	2.00758353564053	2.76559669807075
C	8.94219003353866	2.81490723060788	2.70136878694125
C	8.83958166636803	4.07224426241947	2.10033760270553
C	7.61827897774944	4.43501191688832	1.53325415585451
C	6.50812746806284	3.57550666310747	1.60462219680951
C	1.86465526663272	0.08032841640414	3.96341609189100
C	5.23739735072593	3.96129751110523	0.90593686986456
C	5.76337949522888	3.05761873974664	6.31789537757482
C	6.83849782405508	2.14981851493322	6.92594152655461
C	6.16712059290027	4.53581460282460	6.38380553067641
C	4.38709125515664	2.81390273633931	6.94673917036422
H	3.46946792796126	3.25913922933693	4.08934417059726
H	1.28204631086306	4.35200985736218	3.45580913682791
H	0.12532390594841	3.65273392250421	1.33498111529654
H	0.18606929747833	2.14295755043499	-0.78649315657216
H	1.41345089426121	0.43378965891773	-2.11431344159821
H	3.61548300123235	-0.47073912659495	-1.34614544699147
H	7.53990485794338	-1.52268959400343	1.26494769892546
H	7.74062144830630	0.21811261762390	0.93182404348166
H	6.63357407878109	-1.12364202931945	4.64701653450382
H	7.15855663565514	-2.22960337232590	3.34117094602336
H	5.38271832574145	-3.90612138430780	3.26920672711266
H	2.90571402147396	-4.43316797308183	3.29274343159269
H	1.29795758189415	-2.53758874954405	3.66657733674563
H	8.85853354188849	0.18233019111518	3.25937202353192
H	7.63607133724157	0.71435240551035	4.46426775151497
H	9.88884661354314	2.45252880866448	3.11149166567402
H	9.70392808423057	4.74058446083305	2.04396046673621
H	7.50752625031009	5.38737719656995	1.00805402001856
H	2.35869886472345	0.86306101387217	4.55375716674675
H	1.02613122323502	-0.33526484099045	4.54364927157516
H	1.44144994640223	0.53819213602287	3.05400818785576
H	4.82970513253459	3.11122279004875	0.34034639161331
H	5.43562642461048	4.78915691664493	0.20937751195413
H	4.46908870377567	4.29368512649041	1.62155588323908
H	6.94946519070662	2.35439648883757	8.00417324102692
H	7.81269773023634	2.32914336724628	6.43923879112467
H	6.56161327941431	1.08977345482325	6.80408186868631
H	5.40971434762358	5.16809422230891	5.89135623855619
H	7.13953341099334	4.69847000166922	5.88994262409895
H	6.25195524734580	4.84932995340708	7.43773111862261
H	4.42648387383359	2.99610079783864	8.03395617130040
H	4.06819202028662	1.77292021326745	6.77759300480103
H	3.63381067371018	3.49379248580825	6.51267439966100

[Mn^{III}(OO^tBu)(⁶Me dpaq)]⁺ - singlet reactant (B3LYP)

Mn	5.11659975889776	1.00433685863316	2.87080477054314
O	5.29099983398069	1.45190672346260	4.62539344471237
O	5.54972355978564	2.85243482656480	4.85883074924620
O	5.64541348161964	-1.15625484673130	-0.51746079384760
N	3.47263417275832	2.06949310445420	2.41483120223020
N	4.82837501112372	0.34188295523450	1.05809560488976
N	6.75790098080974	-0.22507781100233	2.81807512784093
N	4.12635736053001	-0.79733063343216	3.52919253966456
N	6.60733190156334	2.39366500460783	2.26985669068921
C	2.88669645607813	2.98867310736636	3.16206307736905
C	1.68905579451011	3.61841617726438	2.76337853549712
C	1.10456338363620	3.26998460807977	1.56086745032708
C	1.71851474398247	2.29185981620831	0.73487051238080
C	1.21602610930420	1.86218043674158	-0.52296983139232
C	1.91293866565617	0.91374298199548	-1.24700954035659
C	3.12731934715663	0.34987068354343	-0.78232261052206

C	3.64828039332591	0.74455782031109	0.44620072107525
C	2.92798254755555	1.71337671394750	1.211371347038840
C	5.72112644758433	-0.53770198608458	0.53320971464494
C	6.98343109927730	-0.63402455439092	1.39810877163946
C	6.46384666422944	-1.38479857371025	3.67840633472555
C	5.02882926705664	-1.80645786292708	3.53930359473767
C	4.66414418461180	-3.14587367771857	3.53738849975035
C	3.30557301668837	-3.46710395533373	3.57117930377055
C	2.38604366596426	-2.43165833521062	3.66368449656090
C	2.81762075787322	-1.09471039942105	3.65552768972591
C	7.85210828880829	0.60494490005873	3.35712676211956
C	7.80945613605926	1.96748443348379	2.72261294328833
C	8.96860879535744	2.72997682281575	2.62555646492289
C	8.89289800594875	3.99046745311947	2.03796858417015
C	7.66905503117211	4.40536481422082	1.52711435923351
C	6.53668436474689	3.58550509732082	1.63418501807768
C	1.81065580910515	-0.00063087233414	3.84983538599262
C	5.25658023801247	4.03580315334876	0.99950873344749
C	5.72369715032417	3.08049924783060	6.2842908887444
C	6.93819680238308	2.30063862811263	6.78981113688258
C	5.97365344124009	4.58806730170257	6.33326914064668
C	4.44962067892447	2.69748239033991	7.03707752107388
H	3.38691135818196	3.23599741538059	4.09906645809116
H	1.24108925133620	4.37184953663986	3.41308981694366
H	0.17472439111064	3.74159048337738	1.23330309453538
H	0.28679483143673	2.29076601668142	-0.90390145324747
H	1.52590367903611	0.58501205379423	-2.21433557132602
H	3.66246419242136	-0.38705540603689	-1.37750749859267
H	7.39678932038131	-1.65107536558795	1.34409328233446
H	7.72097250409633	0.04598446139022	0.94863988139806
H	6.61216151149712	-1.06888647399450	4.72163068375498
H	7.15115453662874	-2.22101950893414	3.47581768242253
H	5.43199334194569	-3.92077126114610	3.52022272069548
H	2.97618480764422	-4.50819596289258	3.55545192880137
H	1.31859789290375	-2.63977667146716	3.75059937593240
H	8.83643514240677	0.13188002479380	3.20203295914803
H	7.68512586516772	0.71045153787639	4.43760496030967
H	9.91294392485083	2.33144109505470	3.00021639501667
H	9.77823244372626	4.62427692726387	1.95282577770169
H	7.57550505941744	5.36659051857073	1.02025543654014
H	2.23116169134524	0.80579894630185	4.45972979107641
H	0.92175476377652	-0.40119972506826	4.35522127562893
H	1.48147976636409	0.42384847333081	2.89114260881640
H	4.81898376804810	3.23683820225013	0.38930882572435
H	5.44257690119127	4.90325453441269	0.35385842870322
H	4.51576386636741	4.32899813107940	1.75426091977164
H	7.13915482937282	2.54373646118535	7.84402579059280
H	7.83225291720531	2.56125601558101	6.20187421782286
H	6.76455907137927	1.21717949480442	6.71972799719341
H	5.11162885712358	5.14009764941837	5.92932712657271
H	6.86553494957530	4.85572184514584	5.74691609704210
H	6.13190944129142	4.90891720679956	7.37361713911915
H	4.55732514566796	2.91715891980641	8.11012622577598
H	4.23665685737815	1.62535302596891	6.92254915110175
H	3.58849877207616	3.27008184574577	6.65803513292387

[Mn^{III}(OO^tBu)(⁶Me⁺dpaq)]⁺ - singlet reactant (TPSS)

Mn	5.14452589550919	1.04453983531001	2.86266955650608
O	5.27049761152005	1.50596848536661	4.59405709111003
O	5.76533763033445	2.85542233915008	4.90801232254290
O	5.69061746966797	-1.18126965631090	-0.51895625942536
N	3.51756990471801	2.05279375228731	2.39110794121613
N	4.84948526549526	0.32606644661226	1.05876613662646
N	6.78734326120500	-0.15564274571336	2.79375864881450
N	4.16599716170172	-0.71393437858182	3.51800744481025
N	6.57846274272982	2.42001216779576	2.24613162357352
C	2.93990041657022	3.01318964339092	3.11976458505498
C	1.71879679863948	3.60788496965604	2.73423145252541
C	1.08585217228564	3.20056028946615	1.56748069098954

C	1.68568253075196	2.19272350192574	0.75931222695516
C	1.15141707897833	1.69881571125016	-0.46492980837994
C	1.84476443085495	0.72759569750764	-1.17726767402487
C	3.08613167358086	0.20320254844051	-0.73516703089203
C	3.63777832844235	0.66283001668765	0.46594120460222
C	2.92342623004754	1.64665545934816	1.21617763424587
C	5.77004460005343	-0.53109088825856	0.52361573744558
C	7.05375306582622	-0.53296530084764	1.36447291134436
C	6.49333419697801	-1.34926578590328	3.62585178910702
C	5.05184028934092	-1.74983049451599	3.47398158011569
C	4.65844612835977	-3.08405159713475	3.41511679746606
C	3.28950200363050	-3.38086345550642	3.44981673145022
C	2.39133984394257	-2.32953345235371	3.61541746403247
C	2.84681356170620	-0.99679933354858	3.66594386889669
C	7.86080128231521	0.69122908317555	3.37988283622711
C	7.79745365393804	2.04788180280365	2.73208031167730
C	8.93468308074964	2.84921695418878	2.63434043175043
C	8.82811738093319	4.09339655050275	2.00694539188323
C	7.60018897787724	4.44413912745415	1.44713516711443
C	6.48872791064845	3.58902255359771	1.55208673415514
C	1.86663825953140	0.10489620397219	3.95713433040274
C	5.21439395813849	3.96435795755604	0.85365595052907
C	5.76735417946202	3.02816510047160	6.36768209694041
C	6.72508897920805	2.01504250632349	7.00419326432153
C	6.28938445209368	4.46421091050072	6.49832050121656
C	4.34053417148615	2.88733603524750	6.90943588658646
H	3.46715150062139	3.30637169895579	4.02986524083797
H	1.28624529702662	4.38628942992615	3.36880390947971
H	0.13649414374123	3.64845770223750	1.25749698975415
H	0.20111479005964	2.09575804575297	-0.83421677518423
H	1.42919777268571	0.35344614461394	-2.11836025073100
H	3.62030614034271	-0.54725057437050	-1.31891358782073
H	7.55590061045808	-1.51185137976506	1.30833750589609
H	7.72769632186597	0.22412261919349	0.93169726058330
H	6.65009298854942	-1.05771537840664	4.67791426152709
H	7.17830663500937	-2.18115118594334	3.38891359183251
H	5.41234380082740	-3.87333702555988	3.35310833687092
H	2.93796781542458	-4.41478006492752	3.38509709345811
H	1.31934653066129	-2.52046627065574	3.71663749635665
H	8.85994573307193	0.23606600119197	3.25095812394311
H	7.64822113687635	0.78007106303915	4.45724235061610
H	9.88592511567915	2.49197988484481	3.03850722355891
H	9.69311211070026	4.75800912986469	1.92360054795188
H	7.48451447657157	5.38350561334830	0.89995736836522
H	2.34656466277390	0.90535333924603	4.53533329354227
H	1.02492924594434	-0.30356998541647	4.53779874275819
H	1.44967523298618	0.53977261526840	3.03359831436021
H	4.80486048482460	3.10699514104833	0.30036618781556
H	5.41005762185243	4.78227064168944	0.14468224272077
H	4.44738939358759	4.30694462599729	1.56587451426931
H	6.78567688133091	2.17856981752477	8.09329621414591
H	7.73935516728725	2.12519232330969	6.58335214966695
H	6.36973638489547	0.98605773450669	6.83044680557437
H	5.61718758243785	5.17094636474520	5.98418813285394
H	7.29863194942076	4.55547378560675	6.06373215639403
H	6.34013191614662	4.74271631273945	7.56425249151708
H	4.32892363071079	3.05198296701864	8.00003343839461
H	3.95022538437150	1.87730094839235	6.70506915188998
H	3.67251396199869	3.63165235366746	6.44318290728340

[Mn^{III}(OO^tBu)(N4S)]⁺ - singlet reactant (TPSSh)

C	5.92681884798740	1.34698796855415	4.04494918068615
H	5.57558580708704	0.88834644241733	3.10737943452221
H	5.06621170048374	1.40976065499556	4.72611311871749
H	6.67397142364242	0.68516968102810	4.50211710012734
C	5.44461420073782	3.57084936617735	2.98016089254071
H	5.81727700352549	4.57868558309706	2.75572535227129
H	4.50119159551609	3.65457457763658	3.53764499391116

H	5.23782113954922	3.05570533048608	2.02750998325423
C	6.47174753572721	2.77174337693827	3.81893781677235
C	7.77088508546083	2.81426687519716	3.04846231796139
C	7.88885908322788	1.91879175632993	1.84141278472793
H	8.05085298828827	2.50616834172389	0.92380341353627
H	6.98747090718259	1.31363960503797	1.70374278552117
H	8.74765016909216	1.23574316895520	1.94322310824157
C	9.91933586849755	3.64021272068893	2.55962140146131
H	9.64050796935697	3.50441866937290	1.50586938343894
H	10.52464344900751	2.76122850444133	2.84519269715678
C	10.77999048463663	4.88987384518314	2.65228929265051
H	11.58765062381518	4.76963690568178	1.91342346953255
H	10.20803350536007	5.77541422450382	2.33584123843612
C	11.42596800530398	5.11149448213295	4.00894278285574
H	11.78389673829428	4.15254429756864	4.40962182787232
H	12.30041219549052	5.77972846523917	3.91903585247385
C	10.23126863583597	7.12152117043229	4.70302765136267
H	11.11278640448313	7.60026134221138	4.24737523689060
H	10.03018324552064	7.62817142811136	5.65823140535503
C	9.00260018607884	7.31570398131089	3.86205249264094
C	8.94671494266668	8.29492773029732	2.87606573129159
H	9.85167098378405	8.83296674201533	2.59020367016428
C	7.71181972790629	8.57531794867857	2.28473665830722
H	7.62838468301428	9.31237678130035	1.48387455120805
C	6.58469211010068	7.94232195359712	2.79218491867057
H	5.58842399538059	8.20083484629844	2.43043425370799
C	6.70221393243976	6.98502284982129	3.81694523868703
C	5.46911249073742	6.53669754367636	4.53797162946185
H	5.58869850307993	5.54888523420794	4.99790352683497
H	4.59142356576514	6.55564236591992	3.87825159985295
H	5.28997048013030	7.25966041636640	5.35239325019732
C	11.08386559463687	5.56537430190424	6.36546890478939
H	10.47505016974447	6.17311908938359	7.04866335982184
H	12.12444062413954	5.93206333380453	6.38295990934852
C	11.01606916882305	4.13206238095186	6.80296699388843
C	11.91683986342309	3.63873037154116	7.74350722148192
H	12.68719326575525	4.29410460441717	8.15252873677109
C	11.80722589615784	2.30827178418937	8.14026080166621
H	12.48411309309373	1.88737188164778	8.88610173340157
C	10.83388244995671	1.51970568921742	7.53563919138547
H	10.73643646872509	0.46286413109753	7.78649050368791
C	9.97000382563369	2.06754374385193	6.57706582414442
C	8.97270733533287	1.18610931728148	5.89885464172632
H	7.95281544089950	1.49064481933845	6.17775524742537
H	9.13871538503503	0.13619522258919	6.17159413995225
H	9.05300959000017	1.28660270288134	4.80729236753307
C	7.52854806212379	5.43318412457206	8.95817280930105
C	6.08103382793697	5.58191805905155	8.49162652086401
H	6.02269695566596	6.27133869592938	7.63828234501514
H	5.45806719745228	5.98009568272508	9.30694030896057
H	5.67661059869215	4.60788871743055	8.17998731072434
C	8.14828401089278	6.77822695998259	9.34079289486331
H	9.19224092836606	6.64310796855548	9.66472614333470
H	7.58674737523497	7.23821069695343	10.16834805028864
H	8.12672025747897	7.46810700811229	8.48453887104717
C	7.65206142826155	4.41241878767853	10.09033179869924
H	7.23027064983673	3.44413775229400	9.78357602480436
H	7.10469291967092	4.76860973807031	10.97560747979571
H	8.70684135555146	4.26633064146739	10.36690048639419
N	10.49780424150422	5.69954194482943	5.01019627126031
N	8.70576758903225	3.63946936661500	3.40027294129540
N	7.92467258618926	6.59263339145930	4.25069873279929
N	10.04214860694525	3.37864065475444	6.24483206332536
O	8.31283203030161	5.65021896583787	6.73576759253095
O	8.32740052262095	4.80667385808806	7.91620331397243
S	6.69969877411827	3.55497426669225	5.47769595026044
Mn	8.59371469657106	4.71746516717112	5.20716547013646

[Mn^{III}(OO'Bu)(N4S)]⁺ - triplet reactant (TPSSh)

C	5.88926213091932	1.39776101010479	3.98265970309290
H	5.54693934529748	0.94860768089202	3.03732984589603
H	5.01713679058332	1.47304337099447	4.64764919848215
H	6.61594332794045	0.72165953666511	4.45172203801074
C	5.46160566566467	3.64210621401267	2.93538313467706
H	5.85595989247077	4.64491503868868	2.72535177852333
H	4.51452827276932	3.73846052227696	3.48452196053359
H	5.25253587964621	3.14358736169468	1.97457241851595
C	6.46548476526402	2.81239256876884	3.77182142667214
C	7.77140133967169	2.82938169452569	3.01140142487090
C	7.87455100791362	1.95427048843364	1.78762979492855
H	8.06493024514750	2.55358193168087	0.88313550502841
H	6.95447085647893	1.38317698186348	1.62823228050900
H	8.70757606120237	1.23939525603231	1.88460189735521
C	9.95654433049456	3.59764547119867	2.58213292831593
H	9.70316988524057	3.44450125399237	1.52462389573011
H	10.55120826795887	2.72175322388150	2.89809571019735
C	10.81897816630764	4.84692546974700	2.67434246806129
H	11.63713765593869	4.71838399419835	1.94859545481286
H	10.25227354220574	5.73018537380939	2.34224238559943
C	11.44725471529370	5.08040056903383	4.03754057959463
H	11.79993500264032	4.12505255139474	4.45135836939073
H	12.32324229443915	5.74717003307034	3.95258898766311
C	10.24523334732391	7.09855230842043	4.69902422993664
H	11.12833306252970	7.56786846387360	4.23726280653453
H	10.04709088009463	7.61635298755644	5.64880310334648
C	9.01638653284584	7.28990827568736	3.85802447002976
C	8.96295032120660	8.26267639236157	2.86565245389802
H	9.87118010207032	8.79053952997252	2.57105428669248
C	7.72665040942319	8.55297808344225	2.28153608845908
H	7.64518809458238	9.28442887756758	1.47531972926838
C	6.59620893668041	7.93999246587190	2.80639901534767
H	5.59952609340968	8.21074958745797	2.45486118313919
C	6.71148729305245	6.98837857949632	3.83659133134249
C	5.48299267141434	6.56718619091406	4.58092475431556
H	5.58677925542529	5.57194650169527	5.02711613826167
H	4.59162096958189	6.61593699356010	3.94156951129188
H	5.34395944626703	7.28428209896777	5.40811394016460
C	11.06982333637461	5.54864085453412	6.38842956317057
H	10.44934517799076	6.15748369925744	7.05967322622506
H	12.11128374713606	5.91067891310321	6.42469959412743
C	10.98711979630303	4.11485029267197	6.81986401238720
C	11.88460928444429	3.60469590533840	7.75303238248240
H	12.66156548316416	4.25072880953555	8.16413445351692
C	11.76468560252063	2.27219524285821	8.14026952994839
H	12.43846630768492	1.83939082069465	8.88195225846679
C	10.78576261050547	1.49760386545908	7.52753219300333
H	10.68152788245757	0.43856727911714	7.76616306494442
C	9.92364136756102	2.05918358088873	6.57531650516897
C	8.92366878476235	1.18206139982841	5.89348791426683
H	7.90998930894607	1.41036314803422	6.25269131774212
H	9.15214400373919	0.12568696153995	6.08474407606160
H	8.93164139005673	1.36090938477723	4.81075874322244
C	7.56036853853544	5.44881229345816	8.97839415731027
C	6.09829603975934	5.29522252184682	8.55933337057732
H	5.90522614135928	5.85658421139399	7.63497442863500
H	5.43274675651330	5.67940965032269	9.34752478368074
H	5.85783742600927	4.23727957897246	8.38035189577206
C	7.92966588324784	6.91289340391545	9.22399239053270
H	8.99415117282147	7.00207829472880	9.49172863995105
H	7.33030454789194	7.32419534682969	10.05042636851679
H	7.73818097424054	7.51438574551095	8.32409811108180
C	7.89120365231829	4.57538794362150	10.19008063432689
H	7.66970139124243	3.51953570311769	9.97526027422996
H	7.28713860667760	4.89051271252535	11.05396883642588
H	8.95509884862411	4.66560045510655	10.45569079284708
N	10.50793456718265	5.67852059936607	5.02222527929224

N	8.72519714738966	3.61751591227947	3.39437481252476
N	7.93298518086120	6.57858102441816	4.25727752407234
N	10.00186289453285	3.37423263638883	6.25745825190547
O	8.276130181118564	5.64633607601486	6.73107012691167
O	8.43190974657753	4.88192738720009	7.96322197850044
S	6.69939513691926	3.56121874448515	5.43455822570649
Mn	8.59431722506552	4.68984766705271	5.21393905397386

[Mn^{III}(OO^tBu)(N4S)]⁺ - quintet reactant (TPSSh)

C	5.76818905917193	1.36985238895903	4.25219215301310
H	5.51634072167792	0.78040602090762	3.35681686953581
H	4.84690708016692	1.49133061866557	4.83904348224321
H	6.48416945557041	0.80448825667384	4.86176276292326
C	5.30125208729509	3.43941029494264	2.90627294263453
H	5.66681938207312	4.42004764896312	2.57662549223583
H	4.33394090988978	3.57539332070746	3.41012836174139
H	5.14242930997764	2.80514439125857	2.01913344871618
C	6.29688542410118	2.77249828797561	3.88888810482988
C	7.62963983597559	2.75700423103828	3.18136574336440
C	7.80346729318299	1.78265463762117	2.04481661856802
H	7.95361249324379	2.31207640910267	1.09041203238674
H	6.92879468670363	1.13326447038817	1.94042193644833
H	8.68898972996749	1.14907403154550	2.20937627909380
C	9.79676037039092	3.60462034481614	2.72287230357583
H	9.57197147684415	3.32918911223165	1.68436792409765
H	10.45646524852047	2.82003338590639	3.13335415868963
C	10.53451695858850	4.93768050798659	2.70395931687714
H	11.29354169298142	4.86601019277160	1.90921872233683
H	9.85207621709500	5.74628079282284	2.40368999407169
C	11.26786257588872	5.27255577753961	3.99468688308559
H	11.77494084473465	4.36755984088126	4.35803313315970
H	12.04600453079281	6.03338571071996	3.81114302699800
C	10.13720724807360	7.21526220501908	4.97069851635992
H	11.08000264032902	7.74648190789944	4.75984587185458
H	9.75953543638321	7.54952514415679	5.94752292399975
C	9.08367682478426	7.55446642828086	3.95509970102875
C	9.27697292958423	8.53107416916685	2.98095435237084
H	10.24946286352211	9.01286958976345	2.86720688584724
C	8.19270090519124	8.87648304139404	2.16756381977471
H	8.30488342571367	9.62234937834489	1.37799922616370
C	6.95991210894741	8.28042627897895	2.40997868807120
H	6.07821696988438	8.56670289342445	1.83404720106543
C	6.83416373093416	7.31925496220472	3.43038996403289
C	5.48460780314193	6.80916205255141	3.83616181842556
H	5.56529060554814	5.86256994045623	4.38493531747254
H	4.81314151675592	6.70140046375634	2.97266290149637
H	5.02815451942239	7.54738672875320	4.51760659601711
C	11.05449285447298	5.52229392664941	6.39722377033465
H	10.45135628725569	6.02642548696622	7.16568915586272
H	12.06693447988284	5.96152592166536	6.39795844945172
C	11.10661959424236	4.05786771664016	6.72956083593439
C	12.10313167130244	3.54618858507423	7.56138166928327
H	12.89633577943747	4.19701547113230	7.93293024791844
C	12.04822278026940	2.19760591024544	7.91087551982053
H	12.80354737729000	1.76137000035707	8.56753163976047
C	11.01307291709793	1.41574432888129	7.40228618488374
H	10.93696548684779	0.35652983372512	7.65191041311415
C	10.05870540342831	1.99345418321916	6.55421101613165
C	8.94279328234091	1.18039957156009	5.97522057919807
H	7.99391096747922	1.72549606789698	6.09059515693953
H	8.86972514444524	0.20029561255716	6.46376547395360
H	9.10890382933981	1.01125558758785	4.89880602494945
C	7.56690248692638	5.30376422249150	9.05653803371794
C	6.10706541695626	5.04061037800053	8.69585435076659
H	5.80435939250100	5.65597577936879	7.83720832735738
H	5.45917524674758	5.29155115813021	9.54943285911713
H	5.95553492225015	3.98221407974013	8.43994784327192
C	7.81618810210276	6.77169220512524	9.40240020884143

H	8.88003996714912	6.93720982431797	9.63281469692051
H	7.22193820185099	7.06392329029775	10.28136810057507
H	7.52995011872740	7.41798799093586	8.56045243344041
C	8.05402337361611	4.36729175395412	10.16341206865555
H	7.91512400570608	3.31683198982589	9.86828823099937
H	7.48007004005697	4.55137297488641	11.08356318870216
H	9.11982484322667	4.53698442788104	10.37729351603676
N	10.38802321648595	5.75812845486996	5.09360917414267
N	8.54979040599491	3.60658849100587	3.51094064477395
N	7.90892434250796	6.92097486864314	4.13781189615146
N	10.11408629864250	3.30226051814506	6.23210034201717
O	8.13420921308455	5.71878671760485	6.79262378587341
O	8.44369672311040	4.91446122375857	7.95651465929208
S	6.40920464853768	3.73787140069790	5.44883100361968
Mn	8.41622726563436	4.74392718758433	5.26027802358269

[Mn^{III}(OO^tBu)(N4S)]⁺ - singlet transition state (TPSSh)

C	5.87802259149797	1.45410483075095	3.93899803514393
H	5.50785685170169	1.01783421847915	2.99820715771052
H	5.02431676136104	1.52781572484284	4.62792681508749
H	6.61353531612605	0.76924140809904	4.38093882171072
C	5.45091380027450	3.69608424267486	2.89012310477075
H	5.84456115798717	4.69676819251926	2.67091811482975
H	4.50426076026107	3.79382928410844	3.43960241424592
H	5.24103024527805	3.19110774316573	1.93287833103474
C	6.45561633064180	2.86866196267690	3.72569236187864
C	7.76138094700051	2.88212431563899	2.96179417099734
C	7.85911172227242	1.98798576936521	1.75154078553324
H	8.05635295384157	2.57438675153417	0.84030252261242
H	6.93929538468581	1.41531188887995	1.59819835318815
H	8.69219948232488	1.27521791684706	1.86269495208262
C	9.93623824167959	3.63653760930739	2.49680548718822
H	9.66895567427264	3.53751558488877	1.43528849780059
H	10.49519258809529	2.72347089259249	2.77013331301239
C	10.85586973219969	4.83850658543755	2.63300401171997
H	11.69309128910098	4.67571646913191	1.93676464443515
H	10.34811884440888	5.75188622881805	2.28788003040005
C	11.44149014376594	5.03157902505690	4.02078917979656
H	11.71998479862918	4.05912746453880	4.44954720965394
H	12.35563032751881	5.64882932438049	3.97176710010981
C	10.26579759043869	7.09334350050337	4.57827972153523
H	11.15233691637479	7.52534601672890	4.08769358785799
H	10.08132277407601	7.66466226970172	5.50033265866993
C	9.03330642291096	7.26104956686588	3.73418903505730
C	8.96958045830691	8.22840194761321	2.73667589631314
H	9.87502633488994	8.75536987907025	2.43248274333018
C	7.72867314582631	8.51627747876222	2.16311042661920
H	7.64026962136237	9.24310138452206	1.35348082990162
C	6.60148316436848	7.91307137807555	2.70659127811681
H	5.60168006782614	8.18972268552141	2.36923916430715
C	6.72289339205115	6.96513655256713	3.73860512237061
C	5.50309834909114	6.56965145579705	4.51071086141794
H	5.58132298075594	5.56620203800707	4.94346543488467
H	4.59813385261178	6.66037178367499	3.89588224917166
H	5.41380323196121	7.27796213915173	5.35264072955152
C	11.05402081435677	5.59332539209233	6.34654146406951
H	10.44879663731028	6.23704532376428	6.99891980907586
H	12.10614411991771	5.92402237154621	6.37397445195340
C	10.92689003555753	4.17507460915626	6.82146076696183
C	11.78296807539295	3.68257267430139	7.80063712611361
H	12.55095285675881	4.33128820879235	8.22390088912808
C	11.62600184884317	2.36531102612209	8.22324297102572
H	12.26022724472744	1.94740378692302	9.00721314538089
C	10.66687491303270	1.58258568688801	7.59011441618239
H	10.54195506077022	0.53151494861176	7.85280104563205
C	9.85387121927684	2.12512979665185	6.58540298609949
C	8.89441677577808	1.23153521278277	5.86810789758420
H	7.85983586999006	1.49102236173900	6.13597939899095

H	9.09203972201778	0.18203360556571	6.12150739064087
H	8.99046292499185	1.35888460778420	4.78085700690699
C	7.66670381644486	5.32405619995033	9.17541607948449
C	6.22803250991419	5.06746190862417	8.70707561499740
H	6.04396085931003	5.59047445155235	7.75711692079396
H	5.49882073167366	5.42437910229303	9.45144958707040
H	6.06976952383766	3.99158921023873	8.54273033821822
C	7.93671647674904	6.82150665103450	9.37782660853412
H	8.97506707479878	6.97914524304049	9.70860986876306
H	7.26094183400779	7.24749177143116	10.13597176127142
H	7.78313660929641	7.36130721026483	8.43195102278354
C	7.94909534174410	4.54524180089437	10.48152138335100
H	7.77774655519790	3.46960445894023	10.33077390936457
H	7.27423963278721	4.90503511434932	11.27415823169816
H	8.98892774322335	4.69903954066578	10.80476296780317
N	10.50478609053135	5.68817846721460	4.97160027943523
N	8.71472622138416	3.67636406449077	3.32182843144018
N	7.95075266516505	6.54787324916969	4.13661721517892
N	9.95514441275152	3.43198828366547	6.24388505407264
O	8.31272417673807	5.68427199409979	6.57800955959127
O	8.59603918881989	4.75695648198324	8.28328040193923
S	6.70683092417586	3.59162805422289	5.40881857389876
Mn	8.57120824494624	4.81359661885386	5.21324527051445

[Mn^{III}(OO'Bu)(N4S)]⁺ - triplet transition state (TPSSh)

C	5.86853006402741	1.45580204049027	3.97804958779295
H	5.52801863541711	0.98769461849573	3.04144996361643
H	4.99077307265315	1.56325528226380	4.63141993259982
H	6.57917542108297	0.78093944350324	4.47179090266375
C	5.48334104805336	3.66603588600163	2.85010303159331
H	5.88726775220236	4.65973439476673	2.61663517534418
H	4.52471590856617	3.78246981652305	3.37486887746737
H	5.29245797726749	3.13710763820470	1.90196469338859
C	6.46524112667234	2.85589744261146	3.73081560082837
C	7.78389918096053	2.84353791851045	2.98906944588203
C	7.89696313113691	1.92725903919692	1.79673485617524
H	8.09392601780054	2.49843051079337	0.87568486475946
H	6.98217988151764	1.34500242631516	1.64850936067087
H	8.73449168466946	1.22315305529362	1.92648878994697
C	9.96921194226060	3.60421049975459	2.54960541517428
H	9.72589782091116	3.44722344009121	1.48955579957822
H	10.55450326877074	2.72556037621255	2.87564738389147
C	10.83794119992118	4.84865820870381	2.64847352307145
H	11.67156398735252	4.70848133656596	1.94293192697897
H	10.28432457778664	5.73129818710312	2.29397474462772
C	11.43838982068564	5.09492534453135	4.02273531378204
H	11.77079291590420	4.14227829255954	4.45865934526843
H	12.32428953872814	5.74908666439502	3.94431570521509
C	10.23510540154826	7.13164546942401	4.62525133168893
H	11.12567847899813	7.59635745655515	4.17316745913711
H	10.00946661835480	7.66945592708106	5.55801450257150
C	9.02543757395208	7.29265955618678	3.75110505410157
C	8.98597423115048	8.25292961727481	2.745568837331262
H	9.89784970814260	8.78131430356733	2.46378760926284
C	7.76088332133137	8.53061722983342	2.13462950076907
H	7.69123419508462	9.25024806710090	1.31680840934472
C	6.62305916546869	7.92538997084337	2.65252797416311
H	5.63136613960309	8.19396532510557	2.28590322572833
C	6.71988741815501	6.98764064826412	3.69711709437210
C	5.47619487275124	6.60201181913776	4.43548261198116
H	5.52584030514641	5.59392102342706	4.85917403168992
H	4.58880235992137	6.71561868957905	3.79913620682274
H	5.37805491928218	7.29977735169674	5.28504874559790
C	11.03952440546751	5.61293118472832	6.35956187531624
H	10.41175109920218	6.22543025004822	7.02089261315792
H	12.08432401913604	5.96353794658651	6.40150309279628
C	10.92988631664292	4.18614172269677	6.80127067096748
C	11.81623909880605	3.66721556649611	7.73780218651267

H	12.60432482775151	4.30342349168920	8.14228385911472
C	11.66592000974751	2.34406562495825	8.14370591184086
H	12.32869965170662	1.90617081460684	8.89222729079650
C	10.66842831052561	1.58565335635624	7.54329449172252
H	10.53601680804048	0.53394842386936	7.79919523694641
C	9.81667555819906	2.15237382579523	6.585066641867283
C	8.78893141893863	1.28244621279983	5.93860844151711
H	7.79287202248735	1.50707281272137	6.34638172889379
H	9.02571364035633	0.22512164795248	6.11466088329778
H	8.74903460220553	1.46706316344219	4.85834441051051
C	7.67855673410244	5.29862484492159	9.16209021603873
C	6.23246415630546	5.04849911819867	8.71493969672889
H	6.03210138147102	5.58287502437285	7.77503321649067
H	5.51655075057511	5.39576358710990	9.47671093756237
H	6.07084965666003	3.97424774261694	8.54152551732583
C	7.95099236704073	6.79407905110870	9.37382534116144
H	8.99395725226990	6.94876746158192	9.69198961348695
H	7.28627554193709	7.21334776207410	10.14552601508590
H	7.78461995341593	7.34154778943985	8.43473200271239
C	7.98207949809571	4.50841804096450	10.45398623399182
H	7.80726756353937	3.43403560063900	10.29641374638257
H	7.32348397533347	4.85904916835027	11.26432527109587
H	9.02809789934589	4.65705217334814	10.76009604984769
N	10.49443206446440	5.72329582827141	4.98528871591131
N	8.73330371491495	3.64193342470455	3.35044500926208
N	7.93727566743078	6.57771048291852	4.13446438528085
N	9.93007742944566	3.45864915202454	6.24384789669191
O	8.29345637012583	5.66441490389337	6.60948950459047
O	8.59630500042845	4.74139491543255	8.24633191564405
S	6.66617189768586	3.65765532116635	5.38841099517265
Mn	8.57319165295699	4.77370124414932	5.21600723660929

[Mn^{III}(OO^tBu)(N4S)]⁺ - quintet transition state (TPSSh)

C	5.86853006402741	1.45580204049027	3.97804958779295
H	5.52801863541711	0.98769461849573	3.04144996361643
H	4.99077307265315	1.56325528226380	4.631411993259982
H	6.57917542108297	0.78093944350324	4.47179090266375
C	5.48334104805336	3.66603588600163	2.85010303159331
H	5.88726775220236	4.65973439476673	2.61663517534418
H	4.52471590856617	3.78246981652305	3.37486887746737
H	5.29245797726749	3.13710763820470	1.90196469338859
C	6.46524112667234	2.85589744261146	3.73081560082837
C	7.78389918096053	2.84353791851045	2.98906944588203
C	7.89696313113691	1.92725903919692	1.79673485617524
H	8.09392601780054	2.49843051079337	0.87568486475946
H	6.98217988151764	1.34500242631516	1.64850936067087
H	8.73449168466946	1.22315305529362	1.92648878994697
C	9.96921194226060	3.60421049975459	2.54960541517428
H	9.72589782091116	3.44722344009121	1.48955579957822
H	10.55450326877074	2.72556037621255	2.87564738389147
C	10.83794119992118	4.84865820870381	2.64847352307145
H	11.67156398735252	4.70848133656596	1.94293192697897
H	10.28432457778664	5.73129818710312	2.29397474462772
C	11.43838982068564	5.09492534453135	4.02273531378204
H	11.77079291590420	4.14227829255954	4.45865934526843
H	12.32428953872814	5.74908666439502	3.94431570521509
C	10.23510540154826	7.13164546942401	4.62525133168893
H	11.12567847899813	7.59635745655515	4.17316745913711
H	10.00946661835480	7.66945592708106	5.55801450257150
C	9.02543757395208	7.29265955618678	3.75110505410157
C	8.98597423115048	8.25292961727481	2.74556837331262
H	9.89784970814260	8.78131430356733	2.46378760926284
C	7.76088332133137	8.53061722983342	2.13462950076907
H	7.69123419508462	9.25024806710090	1.31680840934472
C	6.62305916546869	7.92538997084337	2.65252797416311
H	5.63136613960309	8.19396532510557	2.28590322572833
C	6.71988741815501	6.98764064826412	3.69711709437210
C	5.47619487275124	6.60201181913776	4.43548261198116

H	5.52584030514641	5.59392102342706	4.85917403168992
H	4.58880235992137	6.71561868957905	3.79913620682274
H	5.37805491928218	7.29977735169674	5.28504874559790
C	11.03952440546751	5.61293118472832	6.35956187531624
H	10.41175109920218	6.22543025004822	7.02089261315792
H	12.08432401913604	5.96353794658651	6.40150309279628
C	10.92988631664292	4.18614172269677	6.80127067096748
C	11.81623909880605	3.66721556649611	7.73780218651267
H	12.60432482775151	4.30342349168920	8.14228385911472
C	11.66592000974751	2.34406562495825	8.14370591184086
H	12.32869965170662	1.90617081460684	8.89222729079650
C	10.66842831052561	1.58565335635624	7.54329449172252
H	10.53601680804048	0.53394842386936	7.79919523694641
C	9.81667555819906	2.15237382579523	6.58506641867283
C	8.78893141893863	1.28244621279983	5.93860844151711
H	7.79287202248735	1.50707281272137	6.34638172889379
H	9.02571364035633	0.22512164795248	6.11466088329778
H	8.74903460220553	1.46706316344219	4.85834441051051
C	7.67855673410244	5.29862484492159	9.16209021603873
C	6.23246415630546	5.04849911819867	8.71493969672889
H	6.03210138147102	5.58287502437285	7.77503321649067
H	5.51655075057511	5.39576358710990	9.47671093756237
H	6.07084965666003	3.974242774261694	8.54152551732583
C	7.95099236704073	6.79407905110870	9.37382534116144
H	8.99395725226990	6.94876746158192	9.69198961348695
H	7.28627554193709	7.21334776207410	10.14552601508590
H	7.78461995341593	7.34154778943985	8.43473200271239
C	7.98207949809571	4.50841804096450	10.45398623399182
H	7.80726756353937	3.43403560063900	10.29641374638257
H	7.32348397533347	4.85904916835027	11.26432527109587
H	9.02809789934589	4.65705217334814	10.76009604984769
N	10.49443206446440	5.72329582827141	4.98528871591131
N	8.73330371491495	3.64193342470455	3.35044500926208
N	7.93727566743078	6.57771048291852	4.13446438528085
N	9.93007742944566	3.45864915202454	6.24384789669191
O	8.29345637012583	5.66441490389337	6.60948950459047
O	8.59630500042845	4.74139491543255	8.24633191564405
S	6.66617189768586	3.65765532116635	5.38841099517265
Mn	8.57319165295699	4.77370124414932	5.21600723660929

[Mn^{III}(OO^tBu)(N4S)]⁺ - singlet product complex (TPSSh)

C	5.63790956293384	1.64455418308344	3.69786319157941
H	5.32157541596143	1.19488153608841	2.74379142019162
H	4.73612803639442	1.78974124397835	4.30988828172976
H	6.29358046009297	0.93708332559296	4.22198056415253
C	5.42461298986082	3.86388462401230	2.54389464278976
H	5.88475484720962	4.83725077307190	2.33052731958761
H	4.43977184558139	4.02514773187723	3.00399268692027
H	5.27417255581441	3.33735300607243	1.58709282740926
C	6.30976126775428	3.01773556183230	3.48999153566987
C	7.67151170337990	2.93784025478306	2.83545479278417
C	7.81494006156313	1.99488297796267	1.66720013206477
H	8.11877610329424	2.53281035498780	0.75550543506964
H	6.87902784159297	1.46759390832374	1.45870270812568
H	8.59356359961678	1.24243438281220	1.87227698267888
C	9.90993388572330	3.56958392441006	2.51638428526861
H	9.71974433533803	3.42971748116155	1.44305770693025
H	10.40858840620126	2.65072831839689	2.87405905015395
C	10.86194232022605	4.74316594007604	2.67098422728818
H	11.73495600859149	4.53108345806774	2.03452794994769
H	10.40847932834568	5.66180452983038	2.26872510045004
C	11.36440103948764	4.95614697246547	4.08689092414966
H	11.59137349004306	3.98689945485409	4.55220078517755
H	12.29668630447888	5.54736662198199	4.08333125162549
C	10.24522299494751	7.07093282397989	4.55246221971102
H	11.18568567809656	7.46361483953085	4.13484800849489
H	10.00934198573679	7.65254044400288	5.45631601573161
C	9.09418187259511	7.28084471415348	3.61075050517338

C	9.15554337659399	8.23222680410772	2.59820235727796
H	10.10623041585962	8.71162904635595	2.36109518547266
C	7.97908487139496	8.56554395751712	1.92283537406293
H	7.98916183852221	9.28085323458471	1.09830690453941
C	6.78545521586198	8.02459535616131	2.38338532486994
H	5.82962046652969	8.34076645130273	1.96368363813059
C	6.77833224367284	7.09223522531881	3.43674178596752
C	5.48357513960925	6.77320910686479	4.11414690806288
H	5.46161848960507	5.76345569562260	4.53982589223760
H	4.63458908853091	6.93350702748825	3.43693105739765
H	5.38430932415359	7.47615670821563	4.95940592562568
C	10.85046528085300	5.55481514078143	6.37424249987173
H	10.24275568288613	6.22974294556005	6.99177242615485
H	11.91284634823948	5.83845098898937	6.46150478395499
C	10.64003675073040	4.14478845995820	6.84234542868628
C	11.45527374673950	3.60162018929338	7.83200754005096
H	12.23075583284100	4.21758668834711	8.28790293658271
C	11.25231049093035	2.27917312618627	8.21466475286335
H	11.86093401921532	1.82071222045188	8.99630828673869
C	10.27357744460865	1.54585996215653	7.55090529418902
H	10.10602570795659	0.49461461944415	7.78802012753169
C	9.49229454298863	2.14266423347845	6.55169075666011
C	8.49948455606148	1.30620997319256	5.81108911962838
H	7.47757232643483	1.65970654578528	6.01014850783347
H	8.59530490231890	0.25297546209929	6.10422121766301
H	8.66309009275998	1.38781385247440	4.72722880157841
C	8.18090890823403	5.39543825150641	9.72553012575877
C	7.77264732403796	3.97842353885161	9.29152370966987
H	7.46049598890043	3.99337677754886	8.23755574933269
H	6.93346237270179	3.60934898825349	9.90111503829726
H	8.62077465872785	3.28683805501725	9.40154335448964
C	7.03225851079732	6.40188397030583	9.55408959025548
H	7.34879823806931	7.40347822041852	9.88006312233465
H	6.15542581314442	6.09538255351193	10.14549657561421
H	6.74621202823800	6.44794429664463	8.49343089990177
C	8.66939322880798	5.38180571578327	11.20736998612632
H	9.50147025465031	4.67502089797858	11.33289391702849
H	7.82557106113835	5.06303449744562	11.83807151457245
H	8.99308618236729	6.38524357786851	11.51547203275423
N	10.39129562774510	5.65926778408727	4.96633614503472
N	8.63403788840375	3.69679859597766	3.24392098064435
N	7.95048191805456	6.62437976593466	3.93625656465079
N	9.65231228941489	3.45128496692013	6.23251613211939
O	8.10938103845186	5.74665575953568	6.43521347619041
O	9.31510573425601	5.81822631169532	9.04928940584725
S	6.46165474088528	3.78518215807461	5.16308215046657
Mn	8.40693705620683	4.92170190750852	5.08040114441842

[Mn^{III}(OO'Bu)(N4S)]⁺ -triplet product complex (TPSSh)

C	5.63154447730487	1.68715617936922	3.86787305423600
H	5.30750753445426	1.20165400116877	2.93442861817550
H	4.73240542789434	1.87163570885581	4.47322613166486
H	6.27616635111340	0.99205090982728	4.42019928846948
C	5.43291803029083	3.86058246877033	2.62986250083106
H	5.89917900200457	4.82220535179127	2.37864757876891
H	4.45470732677891	4.04709734264574	3.09496997217590
H	5.26610348247334	3.30108989777862	1.69492125188008
C	6.32177509843187	3.03922345838838	3.59567912850874
C	7.67305090359386	2.92001742341800	2.92399676014815
C	7.78684372776557	1.94916811016911	1.77546767737374
H	8.07488665381151	2.46497341030157	0.84600876634850
H	6.84359150641199	1.42332340576794	1.59743250396495
H	8.56495166282773	1.19702850291521	1.98296347093956
C	9.91934961750453	3.53829634196123	2.56962714447961
H	9.72393022855525	3.33970232954505	1.50654566714361
H	10.44423579444697	2.65156989234473	2.96869781528467
C	10.83614931594518	4.74851501379996	2.65953202272827
H	11.68932449503322	4.55270755243137	1.99171274621153

H	10.33116050011390	5.63965595727101	2.25689412061726
C	11.39238105549435	5.01638889998258	4.04822999978378
H	11.66621386012790	4.06528263524152	4.52640584249896
H	12.30923803292744	5.62803309820319	3.98514024568441
C	10.27943087725641	7.12755324794312	4.56210378032836
H	11.21588976914522	7.53931127145040	4.15348995826543
H	10.02783651443231	7.69110740357613	5.47291790947243
C	9.13046982963461	7.33085395704302	3.61918485293455
C	9.19662056994777	8.27181333045582	2.59692082042704
H	10.14943837005577	8.74662455919447	2.35905089798862
C	8.02395815546155	8.59939536447247	1.91323721219230
H	8.03672120228425	9.30473826691771	1.08023210930258
C	6.82940117015893	8.06452431715323	2.37772833233725
H	5.87480868425774	8.37714748999732	1.95249780924736
C	6.81764011879674	7.14547193101041	3.44316335842146
C	5.51416295867628	6.84958078252769	4.11551653841525
H	5.46565941683168	5.84108462100434	4.53754083852688
H	4.67244384857144	7.03170855568679	3.43477878716518
H	5.42645461928545	7.54875614441815	4.96497022264947
C	10.92319148124134	5.60415946068143	6.35332783129164
H	10.29886637964000	6.25129447828540	6.98489083653323
H	11.98108133063447	5.90438303025116	6.43540902754954
C	10.72945379090125	4.18982765372466	6.80225759114078
C	11.59470382645318	3.61732773534901	7.72955491431516
H	12.41293740630909	4.21265552172842	8.13527626503907
C	11.38359763741480	2.30032788193590	8.12303040376072
H	12.03115616738717	1.82162705886035	8.85982382557033
C	10.33812198140397	1.60081996934115	7.53026811723050
H	10.15109846791052	0.55646175431924	7.78216171116934
C	9.50936899751632	2.21825614996723	6.58349970608457
C	8.43067975850025	1.40638721129172	5.94380822161771
H	7.44201603485313	1.74465942072849	6.28452081618947
H	8.56064548998525	0.34534024612151	6.19237104913219
H	8.45418727546640	1.52098264950300	4.85272335495554
C	8.08835675407907	5.22658546807277	9.58249995928414
C	7.52075281570004	3.87100671617636	9.13376926764884
H	7.22722758457610	3.93215138397274	8.07586250585071
H	6.63634399452662	3.59573003214391	9.72929970060194
H	8.28087638740080	3.08339691817076	9.24732517764238
C	7.05208623019850	6.35302654453971	9.44737181020005
H	7.48644748368499	7.31004765218463	9.77192534256546
H	6.16343094294249	6.13941964620250	10.06194508065293
H	6.74817920710863	6.44208515027575	8.39480531279036
C	8.59427776128818	5.13510037083875	11.05241914982403
H	9.34972627197960	4.34290304714923	11.15339608016361
H	7.73472544298748	4.89618621942784	11.69730369690458
H	9.02797646944675	6.09294647692912	11.37122606287118
N	10.44344042499317	5.71593991577202	4.95615256985682
N	8.65001674826421	3.67471268630862	3.30284146071910
N	7.98653597632289	6.67958559539869	3.95339205807763
N	9.69247833063227	3.51916235233605	6.24286674681448
O	8.17706004954595	5.78007793495847	6.48922576065765
O	9.25053859930641	5.53354408434587	8.88570166525949
S	6.48516860466451	3.90339333828288	5.22592260380331
Mn	8.45728070462214	4.91071210962071	5.11251358063396

[Mn^{III}(OO'Bu)(N4S)]⁺ -quintet product complex (TPSSh)

C	5.67368117006068	1.53887921666035	3.34151626766788
H	5.42377870590511	1.13225134403581	2.34941575156864
H	4.73520660382157	1.63095537927701	3.90707497659406
H	6.31742234977617	0.82009627005130	3.86475502809801
C	5.45033616307593	3.82001958569258	2.31290832725685
H	5.89900054171084	4.81242727063749	2.17381600406961
H	4.44902379493921	3.93800430707160	2.75026171826327
H	5.33874899815123	3.34898739582592	1.32272983059903
C	6.32128467674578	2.93481071620670	3.23621055087016
C	7.70820962962941	2.91454059768118	2.63210402598859
C	7.90508246613000	2.07123571264841	1.39647510466018

H	8.25636460921641	2.68231372016639	0.55058180454600
H	6.97830309225837	1.57269355753919	1.09550399373443
H	8.66739861834916	1.29587094866719	1.57549695245989
C	9.96377355296111	3.57621146805743	2.48852409331685
H	9.84318891677265	3.45888700817200	1.40277633679988
H	10.47568978483882	2.66738639980085	2.85307521455528
C	10.85369681544405	4.78411999955944	2.73398948496903
H	11.75662417715498	4.64390354564981	2.11964745024718
H	10.36865765615751	5.69814693412429	2.35880571588100
C	11.30019743055234	4.95389097375134	4.17608521692121
H	11.54889268701823	3.97300506071654	4.60522947960159
H	12.21185173910068	5.57475762204573	4.22686329476508
C	10.09913499488152	7.00589288008299	4.72084476915216
H	11.04122114189558	7.45608711845973	4.36981685291884
H	9.80019014002840	7.52145275009408	5.64566671704353
C	8.98239638454289	7.23245870408560	7.74390156135902
C	9.06199926271310	8.22751831920618	2.77542517155869
H	10.01127431950891	8.73421597221114	2.59615767542597
C	7.90542838909151	8.56786598643393	2.07031368170566
H	7.93125604620675	9.31624647127120	1.27602099307252
C	6.70698227441758	7.98873081267297	2.46710622561901
H	5.76025777887029	8.30738236857626	2.02890974667714
C	6.67951990403073	7.01334474077875	3.48093317944957
C	5.36349094140724	6.65994033242733	4.09927413853914
H	5.32842136987525	5.63529116498279	4.48256474683677
H	4.53877571588438	6.84482283975905	3.39864033920061
H	5.23121791650737	7.32770975010147	4.96803857433325
C	10.67444722842577	5.40561356552352	6.47062615815783
H	10.02481262205785	6.03482843281077	7.09266989413399
H	11.72383216259967	5.70518630861926	6.62878808934886
C	10.46484942428063	3.97227750515397	6.85247334916349
C	11.22184028930730	3.39224928105608	7.86522922826634
H	11.96102570958987	3.99540297699615	8.39173181499447
C	11.00073664398404	2.05606665602945	8.18761728293422
H	11.56341582542750	1.57121228549631	8.98745646653805
C	10.06473778373373	1.34636065351087	7.44368049290196
H	9.88561705288516	0.28752703982912	7.63368848997935
C	9.33998045450457	1.97583479347463	6.42179639390837
C	8.38610878169903	1.16186202902186	5.60733133416124
H	7.34716197278652	1.41934553462923	5.85819063946574
H	8.55230386704969	0.09246894554451	5.79078153768040
H	8.52221584243873	1.36606243650860	4.53751136879016
C	8.52093224599238	5.67495635108378	9.95107090931891
C	8.02714504828945	4.25193459159154	9.64001625118226
H	7.80129505968634	4.17396013826317	8.56598718684259
H	7.11089490451380	4.02729914560366	10.20768152375420
H	8.79666628217084	3.51173162169844	9.90501920143366
C	7.46952471802173	6.73971940814981	9.59993361759449
H	7.85108278895288	7.74451487156290	9.83413634993485
H	6.54187883179578	6.57075448991909	10.16845088776759
H	7.24046528830179	6.68064948003364	8.52568480688550
C	8.92488185693743	5.78867240562875	11.45610784594441
H	9.69202602130716	5.04322869152447	11.70691506997860
H	8.02292037103775	5.59913185297285	12.05772283452309
H	9.30505112991239	6.79491665059292	11.67825341867247
N	10.27702154751721	5.58011334997694	5.05498522332862
N	8.64769040571888	3.63671785665248	3.14518322062645
N	7.84171511962926	6.54078175042240	4.00038401980755
N	9.51670663922394	3.29431742908580	6.15910657099322
O	7.92847383858384	5.45027740841589	6.47237326417618
O	9.72207646880086	5.93527824567161	9.31114865428643
S	6.37121837650582	3.63684701434365	4.94795109533384
Mn	8.30184963668952	4.71879655741540	5.03733951085967

[Mn^{III}(OO^tBu)(N4S)]⁺ -singlet reactant (B3LYP-D3)

C	5.90921229291036	1.36947024419331	3.99853405625767
H	5.53583946211265	0.93427977167233	3.05902572688941
H	5.05898427115422	1.42177291039758	4.69358802721232

H	6.65214235977306	0.68507863411146	4.42871381643244
C	5.45394463887371	3.61409392243361	2.97231206360039
H	5.83403724592911	4.62026883608794	2.75636438637711
H	4.50897333053044	3.70362523683561	3.52620296917555
H	5.23996419020895	3.11638963672433	2.01229202194539
C	6.47040187430542	2.79135309573897	3.79780093376397
C	7.77119110964282	2.82403554451036	3.02047666224555
C	7.87393423488767	1.93213576590686	1.80884039218660
H	8.06275515892415	2.51728235226199	0.89531333748321
H	6.96075576808417	1.35068465519276	1.65300844911281
H	8.71306911664411	1.22506689752966	1.91388537054867
C	9.93448975155043	3.62299225365868	2.55202676142236
H	9.67774158874247	3.48783606557914	1.49277389445212
H	10.53029324782559	2.73904721922409	2.84497304962162
C	10.80710746917565	4.86379867951951	2.65388958565627
H	11.62565679835150	4.73142885561870	1.92858706195140
H	10.25178102521476	5.75238267225671	2.31925978844080
C	11.43754105477757	5.08736133165070	4.01726323014913
H	11.79402796061992	4.12720486466329	4.41431106385927
H	12.31770634026047	5.74891742994103	3.93065765444881
C	10.24062675052352	7.09475483018722	4.69589866653711
H	11.11548053991782	7.57228482727448	4.22632365672148
H	10.05106599622722	7.61810326960963	5.64419474429376
C	9.00326647875045	7.28947809307828	3.86648527917364
C	8.94076815650683	8.28144909088999	2.89517041709045
H	9.84494406904004	8.82032803094975	2.60722431521230
C	7.70105708690202	8.57810844694633	2.32350392493102
H	7.61236032431144	9.32929307588966	1.53556180072701
C	6.57727430713829	7.94319596213754	2.83302634535220
H	5.57765953695319	8.21304569816613	2.48828975810100
C	6.70421961823508	6.96825739588637	3.83959771404700
C	5.47542088155181	6.51980284893366	4.56857609592071
H	5.60240802033194	5.54585008146293	5.04964853760116
H	4.59592923814588	6.51096482923914	3.91061463720135
H	5.28436059348570	7.25863731145325	5.36645778824001
C	11.08554339822253	5.54186165523183	6.37018980658735
H	10.49018094524945	6.16061679931814	7.05345024824444
H	12.13219880117658	5.89128240912836	6.39529554710733
C	10.99652976577298	4.11072700169557	6.81486110526204
C	11.88310189886656	3.61622966698757	7.76593427937735
H	12.64868271386582	4.27079717702848	8.18596556057864
C	11.76868821997297	2.28530646043523	8.15822627636402
H	12.43364070970666	1.86345710315801	8.91503251617982
C	10.81162850665324	1.49587495500019	7.53164577215631
H	10.71749371574980	0.43640895005177	7.77362772923941
C	9.96335813822229	2.04619289255878	6.56084174566176
C	8.99639653342758	1.15522207275731	5.84941249839602
H	7.96651786821942	1.39748317835883	6.14600489214535
H	9.20515653903686	0.10106369431087	6.07339614951260
H	9.06075474487955	1.30571486465710	4.76368221299607
C	7.53821034266609	5.47160947474747	8.97102484665835
C	6.07592517993593	5.48043168866509	8.52567198546947
H	5.94903327176115	6.10516482022649	7.63133938521518
H	5.43528684999581	5.88294614807365	9.32535645938527
H	5.73877194162557	4.46123929273513	8.28630544215935
C	8.04484251817230	6.88075475520362	9.28357996117328
H	9.10730282627976	6.85223217110324	9.57317950775561
H	7.47446917539898	7.31781282439855	10.11746611161553
H	7.93342065823445	7.53834476787008	8.40972281856706
C	7.75432903734476	4.52728553202367	10.15401707389375
H	7.42621130952681	3.50823048421725	9.90037501266071
H	7.17510507710940	4.87361481680106	11.02310002510099
H	8.81755280574756	4.49286406228612	10.43637144728682
N	10.51231603228336	5.68031395377304	5.01416250831625
N	8.71300976982373	3.63006382503202	3.37382322681534
N	7.92722517521516	6.56461066572600	4.24977096286526
N	10.03046672229745	3.35941036543214	6.24567531497607
O	8.28666537283140	5.65036034622914	6.73830231646601
O	8.36803367559737	4.86585392076072	7.94600302408152
S	6.72395132547874	3.52196358817329	5.47118443034083

Mn 8.59218954512999 4.70584594803038 5.21781281500477

[Mn^{III}(OO^tBu)(N4S)]⁺ -triplet reactant (B3LYP-D3)

C	5.88525119048906	1.39877384845536	3.98477486079605
H	5.51792489074506	0.96250507838599	3.04343105382802
H	5.02683809149862	1.46651190466703	4.66838209090214
H	6.61373628367592	0.70772832237024	4.42879911765612
C	5.47013232929642	3.64443509468338	2.94139281846464
H	5.86126129036512	4.64844054104534	2.73369101005230
H	4.51759511210216	3.74113709412728	3.48092111529211
H	5.26617113523493	3.15044615553071	1.97731821225846
C	6.46713310135553	2.81187825786955	3.78174377711426
C	7.77501716643959	2.82357220533006	3.01698305833752
C	7.87526009435864	1.92989403310108	1.80625380651355
H	8.07361820688371	2.51273325270247	0.89322433874303
H	6.95679241796410	1.35799538208871	1.64610037898165
H	8.70616098953285	1.21392843923307	1.91565974334304
C	9.95550431634355	3.59650952146679	2.57140191411816
H	9.71202590046295	3.43721439963260	1.51268962840785
H	10.55313882684116	2.72279937854717	2.89030727247706
C	10.81848377205386	4.84577446889530	2.65773380894705
H	11.63790181297462	4.71190785718231	1.93368292278625
H	10.24502210382178	5.72612400025635	2.31442471129012
C	11.44824227313968	5.08837521269043	4.01815000290236
H	11.81556201101372	4.13528066327773	4.42260808983521
H	12.32175588808921	5.75759996835641	3.92481325163889
C	10.24502210382178	7.09498535188527	4.69613287599495
H	11.12000532921154	7.57431904419531	4.22904975485922
H	10.05162098426486	7.61500774004267	5.64527904942895
C	9.00933918972011	7.28786154929172	3.86473576578051
C	8.95248732714720	8.26837116610788	2.88175746778030
H	9.85966941309080	8.79881516306380	2.58765989137814
C	7.71439826824033	8.56553485874376	2.30672380938489
H	7.62993654239380	9.30698723634091	1.50916321121824
C	6.58700358053976	7.94491789747930	2.82568148969629
H	5.58905706931317	8.21786254850970	2.47873100781684
C	6.70770399340850	6.98258733485740	3.84519042673592
C	5.47890182676629	6.55292075757634	4.58364275097200
H	5.57820116235715	5.55665672061749	5.02401157537558
H	4.58658310255514	6.60571483122254	3.94545436465807
H	5.33656147416675	7.26195607227499	5.41779455359037
C	11.08748955678482	5.53989904742734	6.37106943079473
H	10.49014358429553	6.15866242995537	7.05252903770082
H	12.13526752415045	5.88495722379460	6.39969761157066
C	10.98866186468948	4.10944371281047	6.81276427140885
C	11.87231140103553	3.60644704902958	7.76145223959010
H	12.64535702031409	4.25419344921137	8.17819468831404
C	11.74451348561456	2.27818462336972	8.15741756816831
H	12.40627609945624	1.85080049858500	8.91385794930912
C	10.77704234075317	1.49855495712346	7.53486730078595
H	10.67195971767270	0.44078194883165	7.77947861868198
C	9.93186490506540	2.05436520101949	6.56489277729315
C	8.95598738786835	1.16757750275255	5.86011943911193
H	7.92862177516103	1.41781005578963	6.15736163309507
H	9.15846528838576	0.11352285834817	6.08994188394102
H	9.01969005861334	1.31020894876403	4.77351770822823
C	7.55623499339941	5.46112235287157	8.97697467744637
C	6.09441763990153	5.33384780550736	8.54765924469542
H	5.90915836039348	5.91173507156076	7.63226673271926
H	5.42853484729472	5.71183117060720	9.33875440778307
H	5.83971170580301	4.28246250902527	8.34933115039174
C	7.94033977966697	6.91699566929681	9.24811765762128
H	9.00654203093547	6.99056004607441	9.51539350441886
H	7.34864049543679	7.32109403694891	10.08382720494495
H	7.75540770790967	7.54038415312530	8.36198639095014
C	7.85973271437492	4.57320047975574	10.18469429777680
H	7.62304609713077	3.52210535429291	9.96138178845171
H	7.25489911272735	4.89020427277128	11.04753629317837

H	8.92275878824874	4.64113092851935	10.46162597840348
N	10.51941061729722	5.68018047831095	5.01238871027747
N	8.72555431504566	3.61571209880995	3.37919770376748
N	7.92875217136493	6.57411765802092	4.25799718794419
N	10.01224729747977	3.36672645893145	6.24626474560691
O	8.29066110769660	5.66440624757172	6.74014036555569
O	8.42675158013762	4.90012657357160	7.96335602287139
S	6.70009310332789	3.55218252510710	5.45431661361209
Mn	8.59885730542245	4.69765425040174	5.21661718423219

[Mn^{III}(OO^tBu)(N4S)]⁺ -quintet reactant (B3LYP-D3)

C	5.76721181440121	1.35200912744455	4.28846644696253
H	5.51208112782595	0.74993558466526	3.40309145370491
H	4.84801947978220	1.46648359552803	4.88028385490648
H	6.48930726571259	0.79574375546675	4.89886394757028
C	5.28061053843309	3.39280629149597	2.91122708741097
H	5.62802247001124	4.37536709380459	2.56914537026051
H	4.30662438493659	3.52095283455350	3.40465363062047
H	5.13571003693743	2.74611763278900	2.03090969656516
C	6.28008906126577	2.75528276660435	3.90741987034420
C	7.61715823814073	2.74360965092616	3.19946929085937
C	7.80381447500337	1.74710406727901	2.08432413205207
H	7.93369272398123	2.25779364335016	1.11682765871013
H	6.94918560109420	1.07035762182225	1.99636566103553
H	8.70860761099930	1.14205368591106	2.25243540500578
C	9.76492289136036	3.62356064287020	2.70977569311406
H	5.53911068828723	3.35484381110720	1.66985246304019
H	10.43455622388511	2.83879240545280	3.10495974479086
C	10.49686122722935	4.96009997829632	2.68837899186813
H	11.24662338335028	4.89341161321953	1.88383323630177
H	9.80871110143163	5.76457049273942	2.39312810333437
C	11.24894878161123	5.30151444239870	3.96684581259629
H	11.78437473874541	4.40328652785708	4.30414291380024
H	12.01307594531559	6.07239663295420	3.76503224571664
C	10.13623318718545	7.22142492637799	5.00009695604598
H	11.07745913044849	7.76597684710580	4.81624281338797
H	9.74280843461671	7.53423074063697	5.97721526475727
C	9.09788239080468	7.58555309408233	3.97622087580681
C	9.31492045425603	8.58124676932611	3.02858895905562
H	10.29048288028101	9.06414835105819	2.94852435108945
C	8.25230678725503	8.94560962913788	2.19540935526545
H	8.38500962884116	9.71045034477168	1.42668451922040
C	7.01668061745448	8.34050161174842	2.38760301038614
H	6.15049429830433	8.63462697727924	1.79176609169332
C	6.86726623663109	7.35649174521025	3.38276723944856
C	5.50705011849509	6.82620083842436	3.72373967794438
H	5.57014431560181	5.89884166054842	4.30395552203811
H	4.88948059730030	6.67689610466550	2.82590300304481
H	4.98919763888879	7.57205748912572	4.35155448895063
C	11.08319603783972	5.50326526350077	6.37589712213702
H	10.51098524049851	6.00573323228405	7.16759882620904
H	12.10131526506849	5.92993187363923	6.36374776411468
C	11.12894431930483	4.03605994120251	6.70257109691188
C	12.15117114612568	3.51723185688495	7.49766102589041
H	12.96351339989910	4.16206141158829	7.83809184455003
C	12.09892212599370	2.17045788031028	7.85146379752866
H	12.87559486069197	1.72909723529562	8.48016252034477
C	11.03982979278503	1.39609312326000	7.38374146719785
H	10.96487177982019	0.33767924924509	7.63809784046985
C	10.06027351702157	1.98203332927846	6.57170883504448
C	8.91447580570986	1.17746675717876	6.03935269627412
H	7.96448472432483	1.67815792876746	6.27526436646027
H	8.90839389494991	0.16204231761246	6.45639608641687
H	8.97944731066339	1.09498451949481	4.94302709960913
C	7.55305398484983	5.30407109331915	9.07006063873553
C	6.10251069692316	5.00654362435393	8.69953434659115
H	5.78357114629317	5.62055774424631	7.84617342971939
H	5.44357412039019	5.23131362804279	9.55213513963278

H	5.97774870619916	3.94728362448604	8.43230194475446
C	7.75951671533479	6.77546288804946	9.42822431630191
H	8.81819175402798	6.97000454930857	9.66108171990511
H	7.15795582748568	7.04427364328926	10.30997388626607
H	7.45646961079022	7.42398886365308	8.59393409144019
C	8.04823401167970	4.37842604477061	10.18170779924986
H	7.93849325900842	3.32427363948614	9.88609104345439
H	7.46042577557598	4.54615355123413	11.09646579881695
H	9.10738867761108	4.57117066940979	10.40997594935453
N	10.39700276752963	5.76722384532681	5.09179596922898
N	8.52432746545940	3.60983118906255	3.50342106832951
N	7.91933687134309	6.95189437624843	4.11260291489207
N	10.11666002249702	3.28672002979245	6.24617232522026
O	8.13009769331695	5.73244788250155	6.81200953761663
O	8.44625248663231	4.94562388903840	7.97602057396583
S	6.36979406436373	3.74602154181539	5.46056180903540
Mn	8.39182159588385	4.75131973498624	5.27175346962282

[Mn^{III}(OO'Bu)(N4S)]⁺ -singlet reactant (TPSS-D3)

C	5.92759892470683	1.33720149643120	3.98565104121571
H	5.58551214267617	0.88495873384919	3.03836915930656
H	5.05697985321015	1.39605398605944	4.65865496931713
H	6.67089805462814	0.66917278593704	4.44580099810547
C	5.44969909039132	3.577311226014985	2.93911406157571
H	5.82564991257317	4.58852675597938	2.72307783411229
H	4.50174475917411	3.65607734329650	3.49506264339657
H	5.24565360040451	3.06949006226379	1.97889999188388
C	6.47930658360837	2.76514469516369	3.77037586170687
C	7.78574350754120	2.81157868685003	3.00810603862338
C	7.91687297845381	1.92492342531925	1.79161304726314
H	8.10205159340496	2.51965784843539	0.87929130372230
H	7.00813188877964	1.33077787841899	1.63134916416612
H	8.76684175261786	1.22681988873579	1.89902757676735
C	9.95191922450122	3.63848320620646	2.56199874641998
H	9.68790359359230	3.50063564689858	1.50168138882563
H	10.55424712852420	2.75771659994223	2.85884042404814
C	10.81205116790851	4.89263870844804	2.66586878387768
H	11.63122147482725	4.77357895134189	1.93530936346898
H	10.24080063941856	5.77969808707164	2.34306982871878
C	11.44321578729662	5.11674481166483	4.03323820661439
H	11.80240585474846	4.15793356697413	4.44048713356524
H	12.31599381002692	5.79327046286476	3.95415391362543
C	10.21581026331963	7.12460548817670	4.70994604687542
H	11.09745926196825	7.61149908883949	4.25666719777273
H	10.00376920409086	7.63203254706844	5.66565903027865
C	8.98770336486905	7.29859852371778	3.85970864010660
C	8.91912161224487	8.27823824775837	2.86997258274718
H	9.82066143324778	8.82859475545509	2.58624463269017
C	7.67946920990461	8.54431914950881	2.27269142883311
H	7.58882614752225	9.27781177017598	1.46595163506278
C	6.55572786099745	7.90359751685698	2.78925926698357
H	5.55352282423200	8.15604779034338	2.43146747606928
C	6.68088946101425	6.94814215077437	3.81951262967074
C	5.45136271583199	6.50929216016800	4.55836271668305
H	5.56408718182555	5.51285058814546	5.00725901187720
H	4.56131201096062	6.54634273878133	3.91175803918586
H	5.29574747009996	7.22554832713833	5.38710216935797
C	11.05581827727290	5.56555810475352	6.39680171799986
H	10.42209767656931	6.16506917495558	7.06917944505267
H	12.09449355479725	5.94325628450331	6.44128441302379
C	10.99068604943410	4.12483052903922	6.81813607073570
C	11.89853365193965	3.61608568906307	7.74882008463813
H	12.67134193470264	4.26953313584845	8.16334275704147
C	11.79500294280828	2.27630550109173	8.12901928880938
H	12.47757497020137	1.84581500313660	8.86779199534651
C	10.81967707524768	1.49254574829358	7.51301166243762
H	10.72650177196532	0.42864019251499	7.74691476345908
C	9.94677275755192	2.05142668217564	6.56332740401569

C	8.95196085702974	1.17120969455707	5.87338368688185
H	7.92753979111864	1.45111003933374	6.17105090532557
H	9.13536407683414	0.11518561980799	6.12110203082116
H	9.01845978901076	1.29946620915431	4.78152482985413
C	7.54012948480293	5.46821523744838	9.00163345488427
C	6.07734819187829	5.62910259551377	8.57369855518020
H	6.00832403051035	6.27900815586659	7.68718872353398
H	5.48805368596154	6.08280813997303	9.38896865405453
H	5.64058721631804	4.64820088189629	8.32373732481461
C	8.20136373316342	6.81512643605346	9.31814799742685
H	9.26180266725690	6.66833924633811	9.58774917690491
H	7.69306136997302	7.30333599607552	10.16722088613728
H	8.14347120999585	7.48866084351593	8.44748954269017
C	7.68291758149644	4.47972243804638	10.16612246359093
H	7.24479373257199	3.50368844998223	9.89980243617716
H	7.15603080359347	4.87112674559163	11.05263339764986
H	8.74486016648642	4.33316734085812	10.42545704108369
N	10.49374340151523	5.70004542130811	5.02493162223500
N	8.72066175440192	3.63672036479625	3.38685015902153
N	7.91365133861197	6.55385109910589	4.24658257566854
N	10.00840884357801	3.37435435363011	6.25125598511677
O	8.26335521230523	5.61860862720596	6.72889522480211
O	8.29303298866862	4.78501045552528	7.94982591304197
S	6.70852471510426	3.54165645514252	5.43166583604452
Mn	8.57872235017757	4.69654937668625	5.19733298997658

[Mn^{III}(OO'Bu)(N4S)]⁺ -triplet reactant (TPSS-D3)

C	5.88867060515853	1.39168816068430	3.96275028836858
H	5.54954314173175	0.94454553021130	3.01204616817038
H	5.01144156375335	1.46654980143011	4.62564716842870
H	6.61535658257226	0.71243418757636	4.43297171010974
C	5.45896640237020	3.64661269937207	2.92359743331603
H	5.85602109934266	4.65112037341191	2.71385964577925
H	4.51080572289845	3.74151507342672	3.47657506263784
H	5.24739319064755	3.14887096071762	1.95984778978857
C	6.46901666496936	2.80903222615225	3.75241955303230
C	7.77997513770277	2.82849389045421	2.99535711483243
C	7.88975885416648	1.95615949646879	1.76615211448071
H	8.09673925129128	2.55726441588781	0.86271206041734
H	6.96289122744481	1.39399298729760	1.59374875218551
H	8.71551556984522	1.22889806067473	1.86767184789515
C	9.97733027176526	3.59823433086728	2.58668740969762
H	9.72817496119011	3.43812523555977	1.52628312165500
H	10.57186747954255	2.72236806129882	2.91223425936864
C	10.83932495520457	4.85285612852867	2.67511670812416
H	11.65896415039277	4.72405863367731	1.94675991232608
H	10.26857716844159	5.73637629204306	2.34162696616985
C	11.47058222731135	5.09268633477918	4.03973620144493
H	11.82970638627784	4.13841660899276	4.45797635339411
H	12.34391710364575	5.76747033365465	3.95299446640634
C	10.24751289627429	7.11067345631908	4.70150694220053
H	11.12998433080654	7.59138829093908	4.24356166965691
H	10.03771662967617	7.62476752948615	5.65408711020832
C	9.01857697976602	7.28365701895214	3.85201535787382
C	8.95374139297543	8.25707839711511	2.85623995730703
H	9.85912787213289	8.79678246164670	2.56439161523476
C	7.71300347180393	8.53333952473100	2.26517800468036
H	7.62523891834469	9.26192755675688	1.45374129395785
C	6.58557046364836	7.91185174128266	2.79696894423374
H	5.58335830237881	8.17612087392144	2.44781202653885
C	6.70712531653577	6.96179383066715	3.83263169213679
C	5.48018689300440	6.54929237925884	4.59089058350108
H	5.57547442540725	5.54752387631196	5.03133059624221
H	4.58017711825608	6.61380741765260	3.96052921221060
H	5.35929682092357	7.26339190782381	5.42731986837014
C	11.07845161000000	5.55337604418962	6.40165381641421
H	10.44362893655359	6.15478093046634	7.07095299598450
H	12.11963001699625	5.92247984485359	6.45190205411598

C	10.99762671302986	4.11198618361047	6.81549979223305
C	11.91745378264348	3.57905379185293	7.71845163659755
H	12.71181326215495	4.21644911096838	8.11663738962458
C	11.80021377193042	2.23861566501535	8.09321971487955
H	12.49361762047031	1.79028692958079	8.81081880150223
C	10.79562654493900	1.47885578896656	7.49600224444603
H	10.68835474965487	0.41488751793080	7.72354671311404
C	9.90726577459129	2.05837270952347	6.57328849148230
C	8.87674602154049	1.19257120432402	5.91709433014181
H	7.88236525218638	1.38380307599889	6.35293464737839
H	9.13404882740848	0.13044688359973	6.04699206903440
H	8.80821923295690	1.42285611946485	4.84440126239941
C	7.54892704947324	5.46234600492782	9.00640958819645
C	6.08392151474554	5.31094112858588	8.58107698150197
H	5.89842019854230	5.86338374438783	7.64652114319923
H	5.41470322468108	5.70930262307211	9.36298901792682
H	5.83858753071548	4.24945264004497	8.41316350091987
C	7.92996132314510	6.93114024745118	9.23019124028151
H	8.99647293525189	7.01698476049601	9.50179824801173
H	7.32831502646508	7.36113043815732	10.04914277786486
H	7.74586109749582	7.52059315306920	8.31749164269857
C	7.87005758968726	4.60280725177915	10.23662545383077
H	7.63889783763646	3.54287274589198	10.03904385807511
H	7.26323262300173	4.93978147906379	11.09396949213366
H	8.93609332558364	4.68910303713178	10.50581796080186
N	10.52418077709649	5.68820383517505	5.02648818924017
N	8.73578145689279	3.61957523677318	3.39419014673052
N	7.93845659377554	6.55157129095852	4.24901980070122
N	9.98470384269374	3.38262745104702	6.26649330705888
O	8.27121741795320	5.62965492866427	6.73277469953596
O	8.42450324045882	4.86543748984040	8.00107469770979
S	6.70956470169019	3.56006045791662	5.42419471962706
Mn	8.59903002635591	4.68229516918733	5.2176355922264

[Mn^{III}(OO^tBu)(N4S)]⁺ -quintet reactant (TPSS-D3)

C	5.76786861629230	1.37109172533206	4.22453598684325
H	5.51107187999740	0.78902938168730	3.32222381298963
H	4.84694201448999	1.49159301817289	4.81714571327527
H	6.48728523135086	0.79777058314978	4.82758425696083
C	5.30177737323614	3.46503781576585	2.89890306871696
H	5.67122942801021	4.45139012883982	2.58159593091010
H	4.33501508958109	3.59670937920298	3.41071553665510
H	5.13717049504654	2.84252781366788	2.00107912838198
C	6.30287248348578	2.77797379853811	3.86940351014982
C	7.63528501136507	2.76133095643518	3.15625399958160
C	7.80072521527055	1.79608418229588	2.00623386677751
H	7.96936599785202	2.33445405832222	1.05660977557654
H	6.91259192231839	1.16280479689989	1.88735211940997
H	8.67480118922578	1.14151380247663	2.16973356110171
C	9.81835268678717	3.59703866140019	2.70969277947379
H	9.59395820740378	3.31962372349449	1.66872923192772
H	10.47432138169758	2.80843975893474	3.12566057420759
C	10.56343309856417	4.93038968952757	2.69158560407855
H	11.32659462486230	4.85439124062490	1.89727048072259
H	9.88373403312350	5.74406933646352	2.38889316237559
C	11.29509300437864	5.26361785803114	3.98771312939147
H	11.79399929657233	4.35413576615186	4.35902741027738
H	12.08026425106025	6.02211509776328	3.80761176504377
C	10.15194309733307	7.22015686645514	4.94540834404805
H	11.09369496009595	7.75067293883577	4.71475204194560
H	9.78688311450337	7.56443181778241	5.92652851996617
C	9.08045141493391	7.54475534451609	3.93892101812286
C	9.25812929840594	8.50170762775733	2.93663495628440
H	10.23233586533676	8.97804497926864	2.79249272400643
C	8.15634010905634	8.83461284017006	2.13547653527652
H	8.25624431457338	9.56317130705752	1.32482064242483
C	6.92152688192385	8.25004263980716	2.41796523806713
H	6.02768932427091	8.53048224785014	1.85291126625456

C	6.81036420165530	7.31130188526713	3.46551888093741
C	5.46683564453321	6.81879059444831	3.92100883373141
H	5.55098957464461	5.84672396596832	4.42997428702360
H	4.74735231743427	6.76298443134913	3.08863883059959
H	5.06647406732412	7.53990874877393	4.65852331665469
C	11.07128877612512	5.53147782954919	6.39625062962614
H	10.46284413868039	6.04558750483118	7.15776945576926
H	12.08694307457892	5.97034878225130	6.39762669799136
C	11.11839472732817	4.06608861856585	6.73955751867733
C	12.10473060002909	3.55577441502616	7.59062031622412
H	12.89615554348677	4.20895548335708	7.96970086149621
C	12.04226121280648	2.20607517885153	7.94949058589411
H	12.78911496921954	1.77210839323148	8.62143720264834
C	11.01065189848024	1.41998792053398	7.42955452919517
H	10.93018250787006	0.35972845439793	7.68508267149110
C	10.06677872146482	1.99357087056418	6.56085650917003
C	8.95665242994461	1.17759485250315	5.96709028161558
H	8.00221112037861	1.72046456208560	6.07830616451171
H	8.88418340211965	0.19147394946683	6.44964183517809
H	9.12999061862764	1.01748809040027	4.88758362803378
C	7.55381961868660	5.30190872278289	9.07043755203228
C	6.09120349077975	5.05703411305626	8.69197674429860
H	5.81044329362917	5.67051842382311	7.82101815996826
H	5.43374941028600	5.32693094678607	9.53598584920632
H	5.92717159902418	3.99617726150775	8.44266381221324
C	7.82505852922210	6.77208520747732	9.40603907289881
H	8.89148808208595	6.92296610142839	9.64706565052159
H	7.22428655943960	7.08276118715464	10.27770692783826
H	7.55742811761855	7.41588586004746	8.55257017850338
C	10.1843213289470	4.36258686940394	10.19054833917467
H	7.86646205579681	3.30972666819477	9.90063397877958
H	7.43513824016090	4.56312888353367	11.10475538474571
H	9.08669531675772	4.51917019624432	10.41541471579629
N	10.40663227175349	5.75821129213398	5.08317456254652
N	8.56555806234460	3.60393653133959	3.49874371696998
N	7.90251642296735	6.91988098899813	4.16093178138062
N	10.12801167685785	3.30572406751425	6.23078310785932
O	8.15584359487711	5.69616169681570	6.79361743124985
O	8.44134570523508	4.88225583399651	7.97763980293747
S	6.43174859110409	3.73357635654060	5.44243735699325
Mn	8.43615976933905	4.73098007711846	5.25264214639031

[Mn^{III}(OO^tBu)(N₄S)]⁺ -quintet reactant (B3LYP)

C	5.86118340142653	1.22248242640905	4.28299628304147
H	5.63961615462670	0.59139231660175	3.40798812382315
H	4.94449574204704	1.27237770533595	4.88857001201014
H	6.63178624332186	0.72859599482650	4.88797083750526
C	5.17099552558446	3.22436547622211	2.93319353155430
H	5.42174838091947	4.23231113311031	2.57840629071699
H	4.21738345151229	3.28109711762129	3.47842184743926
H	5.01987181380119	2.57126354939596	2.05838330178048
C	6.26378453128411	2.65902347749531	3.87735778045812
C	7.58108827020417	2.71280957597315	3.12520763129910
C	7.73306886819759	1.78611809169403	1.94061242737419
H	7.83115301219207	2.35557539434206	1.00198484865679
H	6.87485147874691	1.11531389354572	1.83508620968006
H	8.64037072704915	1.16876061216220	2.03765451088046
C	9.72804512654879	3.61150561563190	2.63657579765992
H	9.47958583120708	3.38747808317893	1.59078051872744
H	10.41019412772232	2.81158711241039	2.97773499758813
C	10.46295942907977	4.95053727999026	2.64908041479476
H	11.20939356864279	4.89812682868858	1.83916390072416
H	9.77713747479556	5.76379178968313	2.37048175016231
C	11.22818107365809	5.27033488544523	3.92901896435862
H	11.78198378653757	4.37065913100114	4.23467570726398
H	11.98298338091634	6.05224724009745	3.73045010087222
C	10.13787046225033	7.16767868140262	5.05168882574890
H	11.08927559765064	7.70721767270144	4.90391460056538

H	9.74632881556720	7.43899238061931	6.04276400109080
C	9.11314383707232	7.62218403330959	4.04542203095641
C	9.35193758123804	8.72140962567916	3.22280344931018
H	10.33084759248488	9.20538095368924	3.21661894980092
C	8.30583186928100	9.19445811135092	2.42389949347568
H	8.45470911386313	10.04931882143785	1.75948924545849
C	7.06797531436866	8.57150057011805	2.51401906773528
H	6.21504302290528	8.93536861302330	1.93678497172077
C	6.90039244365456	7.46703483757276	3.37216326305946
C	5.53655172501109	6.86366578100904	3.55442071065660
H	5.57810432534270	5.95916113598696	4.17237484091583
H	5.06357168180511	6.63654667544845	2.58572894058697
H	4.88136402920629	7.59192298856882	4.06234779081227
C	11.11114993252162	5.41663455709051	6.35311551439685
H	10.54172218806225	5.88797125225023	7.16733880275413
H	12.11593586249129	5.87467399685368	6.33319613909041
C	11.21161625445119	3.94553728430955	6.65976470953827
C	12.31950558409846	3.44306233785434	7.34649822700985
H	13.15520483184194	4.09972124372045	7.59732285531914
C	12.32267882479329	2.09812531586259	7.71245027521556
H	13.16729706167846	1.66973708890963	8.25768536961992
C	11.22614110489288	1.31183404431588	7.36851555908433
H	11.18774331798151	0.25577272263897	7.64216094438281
C	10.15850250369949	1.88055921183952	6.65857770864978
C	8.97452019917310	1.04865698961233	6.26199036193280
H	8.03878105667830	1.55312835221353	6.54311058320838
H	9.00786458339120	0.05615178990937	6.73148911568082
H	8.95716494311075	0.90391912672905	5.16928681264362
C	7.45071253881806	5.40009463878861	9.08826048513495
C	5.99100037751730	5.13354192799974	8.71931743908167
H	5.69694813368373	5.70970919650445	7.83071038203432
H	5.33268460026051	5.42814598014883	9.55157850811094
H	5.82860025973333	4.06538762936658	8.51202194050300
C	7.70746314281031	6.88555358546139	9.35561334865220
H	8.76704548769545	7.05963349325586	9.60181924005029
H	7.09848632223471	7.23126792420217	10.20546143831698
H	7.44433662734328	7.49376316098227	8.47810007090171
C	7.89340976235495	4.53557790865333	10.27277809120330
H	7.74170062049744	3.46712327099623	10.05716059153020
H	7.30211517457480	4.79480488096077	11.16418964302166
H	8.95670089093741	4.69913165964788	10.50588902373014
N	10.39151959988139	5.70296689587770	5.08524288685209
N	8.50300341130419	3.55463052234867	3.46157663021033
N	7.92941768706461	6.98267340326065	4.08727124234338
N	10.16436366851634	3.18283878078155	6.31146090501226
O	8.09681515633579	5.65266634747327	6.81346289621620
O	8.34675956044925	4.92830833219086	8.03193534258154
S	6.34564415154422	3.67479795715909	5.42074901692570
Mn	8.38321876585154	4.66155457704923	5.27914692879365

[Mn^{III}(OO'Bu)(N4S)]⁺ -quintet reactant (M06-L)

C	5.73003531926176	1.38127773831097	4.25765685677120
H	5.45092038113439	0.79964311114747	3.36760328724619
H	4.81734437243783	1.49927561614038	4.85508580560213
H	6.43389712457225	0.78676777095456	4.85314463572139
C	5.31322678222378	3.45299274660650	2.92660912281495
H	5.69509918580214	4.42818747481443	2.59858628173629
H	4.33894108307849	3.61031808279549	3.40802112108432
H	5.14452639010577	2.83558029489467	2.03059021178381
C	6.27757447166335	2.76546353734412	3.90642281880892
C	7.60797012550374	2.73208638586338	3.20086603961097
C	7.78309665034022	1.73561552355923	2.10153966013859
H	7.89935180868207	2.23072075319808	1.12618297260630
H	6.93472647233174	1.05079130647954	2.02646876128175
H	8.69339761315845	1.13801718580514	2.25295377093414
C	9.75822641447447	3.59391180160424	2.71008995094896
H	9.53567951224518	3.31140878584856	1.67195191664875
H	10.41538289442663	2.79973620315886	3.11062807214304

C	10.50563260004687	4.91150335577183	2.68398786499151
H	11.25689731147503	4.82983058409065	1.88497775909947
H	9.83420412096174	5.72196755655390	2.36164827680782
C	11.24776217676254	5.26481061758231	3.95444936798075
H	11.76308348998339	4.36477913229734	4.32073916228944
H	12.03652366414835	6.01021038701201	3.75101593727312
C	10.15699673356742	7.22573174583659	4.92535065934689
H	11.09973452089589	7.75513036518678	4.70525590867420
H	9.80505512598529	7.57919445061495	5.90685867400031
C	9.09545556275964	7.57371570764200	3.93313287373274
C	9.28703418744674	8.55101045305954	2.96350914014961
H	10.26274465269989	9.02613276422500	2.84455030637553
C	8.20530747430188	8.90499570439127	2.15914132059400
H	8.32050657165921	9.65396501607121	1.37327996370843
C	6.97480722311869	8.31492678012031	2.40101145055208
H	6.09374775984015	8.60536463462777	1.82582496722856
C	6.84680021751109	7.35383283578299	3.41646345436211
C	5.50476719913940	6.84874157435785	3.81285578444378
H	5.56073844855442	5.88489274305076	4.33168201104628
H	4.81741739325864	6.78329165423600	2.96016294333710
H	5.05701841819050	7.56019426224818	4.52446721325050
C	11.08314344932853	5.54316518522917	6.34975319650844
H	10.53100389882035	6.09778179076099	7.12394826214043
H	12.10800858047197	5.95560314997909	6.32233445155027
C	11.10230524757779	4.09770208428848	6.73120127323934
C	12.03735941379144	3.62041637715946	7.64725149644220
H	12.79942078454780	4.28894591707491	8.05178785384744
C	11.96053593899711	2.29070937322473	8.03890458811897
H	12.66802862210488	1.88248131744617	8.76319635062463
C	10.97437800403380	1.48456719673101	7.48390622603315
H	10.89143342571864	0.43263430365425	7.76075002794578
C	10.08302485497433	2.02405763643372	6.55273562380361
C	9.02689430010916	1.18837397134950	5.92183691414096
H	8.04216024620704	1.66099465891866	6.05591282790637
H	8.99801971869336	0.17914209397041	6.34720633698911
H	9.19928380122086	1.08727398481071	4.83887178496316
C	7.57849958900507	5.24803707160449	9.05930286697732
C	6.12989855608618	5.00887218357083	8.68651285494590
H	5.83609306122801	5.62730943629701	7.82773748976987
H	5.47431392778581	5.27003490213573	9.52847100514674
H	5.95122727144928	3.95539211021749	8.43287271906479
C	7.83113478937996	6.69228179652086	9.44851365287308
H	8.89437481521976	6.86081280598436	9.67047265927983
H	7.25269941049427	6.96130348932881	10.34268518957372
H	7.53407020794649	7.37118988950429	8.63894997749134
C	8.05633056770565	4.28024491749326	10.12593750237193
H	7.91074705242722	3.23862261294826	9.80912554045250
H	7.49328829189432	4.43491939370160	11.05557119137597
H	9.12155351886570	4.42972872117913	10.34909224225836
N	10.39905797235273	5.77481251659822	5.06286927573433
N	8.51962893541814	3.60169694669131	3.49712763380041
N	7.91856971619825	6.94897885556740	4.12344863443116
N	10.15059063180592	3.32215739926968	6.19271446330725
O	8.16844268089743	5.74608941299186	6.82221391877596
O	8.45902789264006	4.89912136672767	7.94635662367562
S	6.38867201330726	3.71821186808817	5.47561585951885
Mn	8.39773035754395	4.75956961926223	5.26253015979393

[Mn^{III}(OO'Bu)(N4S)]⁺ -quintet reactant (TPSS)

C	5.86831295073649	1.24781373868942	4.22540776205873
H	5.63960307390858	0.64480684960737	3.32857639831189
H	4.95044316745788	1.30211959045639	4.83315895404055
H	6.63615246744464	0.72810165952632	4.81675085562419
C	5.19733463983285	3.30513749739999	2.93771407226822
H	5.47065463607160	4.31684159821467	2.60262343765378
H	4.25287155220203	3.36678141323857	3.50255090461933
H	5.02489928723779	2.67142277495808	2.04902167035269
C	6.29478821947231	2.69171279181824	3.85416082911978

C	7.60295200220416	2.74493522975795	3.09248912130200
C	7.73087057067332	1.85197814004122	1.87656779837530
H	7.88030544528562	2.44785760672054	0.95820405778357
H	6.83287139095661	1.23565083147657	1.73829466563034
H	8.60112474230549	1.17821666583890	1.97140593766497
C	9.77668194547182	3.60339763612686	2.62549276873241
H	9.51487739770089	3.39617440955187	1.57630409843763
H	10.43753159901615	2.78117426343652	2.96193440388315
C	10.54361555523962	4.92691180153091	2.65818469948364
H	11.30464029124061	4.86169582388544	1.85985695764907
H	9.87948951993977	5.76189576666667	2.37845237691281
C	11.28667643426088	5.21672919070685	3.96112654351042
H	11.77955626468112	4.29299011321384	4.30630330366852
H	12.08139755523287	5.96873968189874	3.79150195086880
C	10.17258923001571	7.17022837128698	4.98186948066406
H	11.12453862301385	7.69266796399150	4.77184511828617
H	9.81715110108234	7.48756046728969	5.97627048473171
C	9.10752065959577	7.57023070419148	3.99225280122749
C	9.30213637444076	8.61715685418930	3.08514311153445
H	10.28179911003793	9.09632370228488	2.99344655387294
C	8.21022934309787	9.04068274717396	2.31378088972085
H	8.32326436405447	9.84703937233015	1.58189767404247
C	6.97060988014453	8.43695248702728	2.52286006088851
H	6.08477214634054	8.77459221979416	1.97594102012901
C	6.84485708712491	7.39439343537661	3.46685091030609
C	5.49035982385733	6.84146984972824	3.81570974580772
H	5.57631866338236	5.86814480573187	4.32170985881457
H	4.84308614401527	6.76077650726941	2.92662029717958
H	4.99329267641500	7.53785482575796	4.51756954606183
C	11.10409795991476	5.45581023674718	6.38236670686468
H	10.49861158086843	5.94988552657514	7.16028866508903
H	12.11030460401449	5.91678890421812	6.37500661921468
C	11.19132720923005	3.98856818086221	6.71499493061071
C	12.25368776532802	3.48771451007795	7.47856925848482
H	13.07113119014501	4.14779623988682	7.78445477726023
C	12.23416700428155	2.13872366496983	7.84582640388059
H	13.04161610244477	1.71181635039303	8.44925485383405
C	11.16399829401370	1.34604503408715	7.42352095349820
H	11.11179455027945	0.28658827605568	7.69098379537664
C	10.14245458093753	1.91019053159466	6.63821194701103
C	8.99316987955457	1.07524107991650	6.15009066166320
H	8.03949270846043	1.59449163658685	6.34439974915203
H	8.98492230185645	0.08712927254813	6.63502821012227
H	9.07095434310421	0.91902439010171	5.05860250146231
C	7.46093019324111	5.39323011736682	9.07528434662222
C	5.99908284003584	5.15538026383079	8.68211389799088
H	5.74323971100797	5.72453051128982	7.77387306901328
H	5.33200763059286	5.48499300668952	9.49746162014851
H	5.81580111824383	4.08544745317381	8.49012499752449
C	7.75265620136517	6.87701318723410	9.33442348114881
H	8.81454016876510	7.02573028152864	9.59693098433641
H	7.13531476251573	7.24437235176309	10.17227785174746
H	7.51711221952162	7.48040917050940	8.44253365788193
C	7.87751412724069	4.51731665132837	10.26644635635641
H	7.70604756383881	3.45042466038622	10.04659829710131
H	7.27752099057859	4.79191125489316	11.15052775418426
H	8.94324266261799	4.66373707149889	10.51027062472313
N	10.41359677444994	5.69737284652478	5.07958054197033
N	8.54664944278782	3.56615730280197	3.45732926139211
N	7.92236203132637	6.93686864780544	4.14527658160970
N	10.16424092111815	3.22146939658604	6.29425826862621
O	8.14189915494548	5.63553100004846	6.79193479806664
O	8.36614813035455	4.88507144658930	8.02810193438754
S	6.42297815092546	3.66706612112216	5.41946344603489
Mn	8.43779219489925	4.66024703422152	5.25622207438830