

A Combined Experimental and Theoretical Study on a Single, Unsupported Oxo-Bridged Mn(III,III) Dimer Coordinated to Two Iminobenzosemiquinone π -Radical Anions

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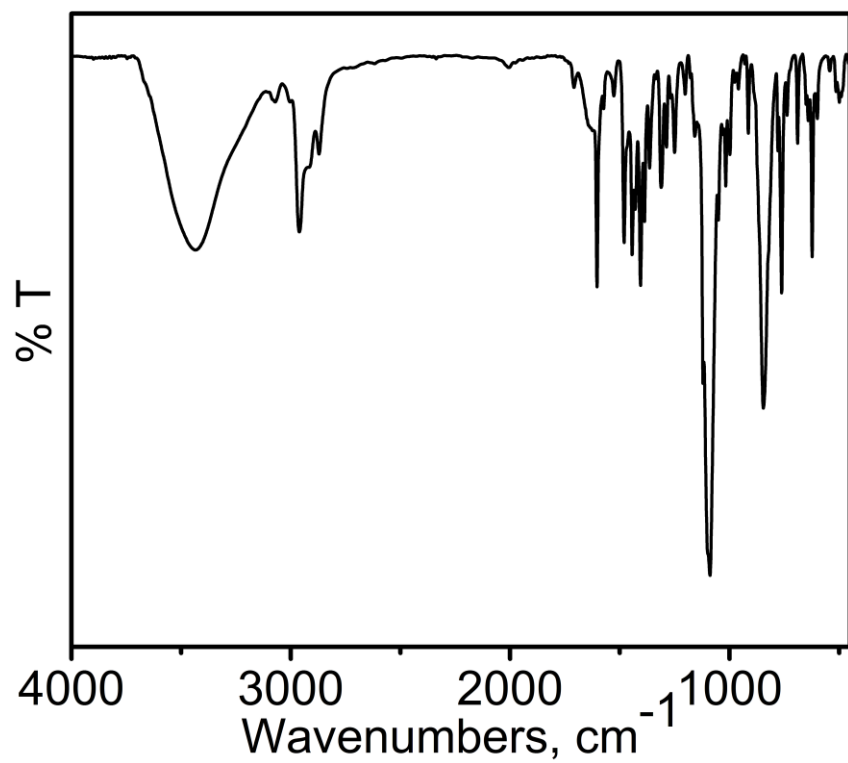


Figure S1. FT-IR spectrum of complex **1**.

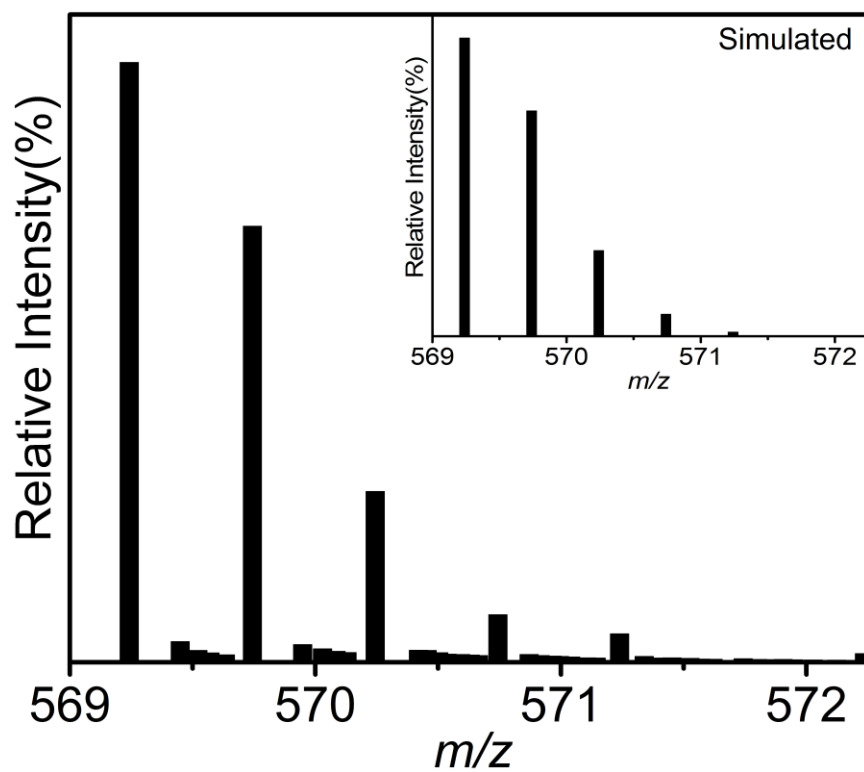


Figure S2. ESI (positive mode) Mass spectra of complex **1**²⁺ ($m/z = C_{66}H_{76}Mn_2N_8O_3$ where $z = 2$); experimental and simulated isotope distribution pattern (inset).

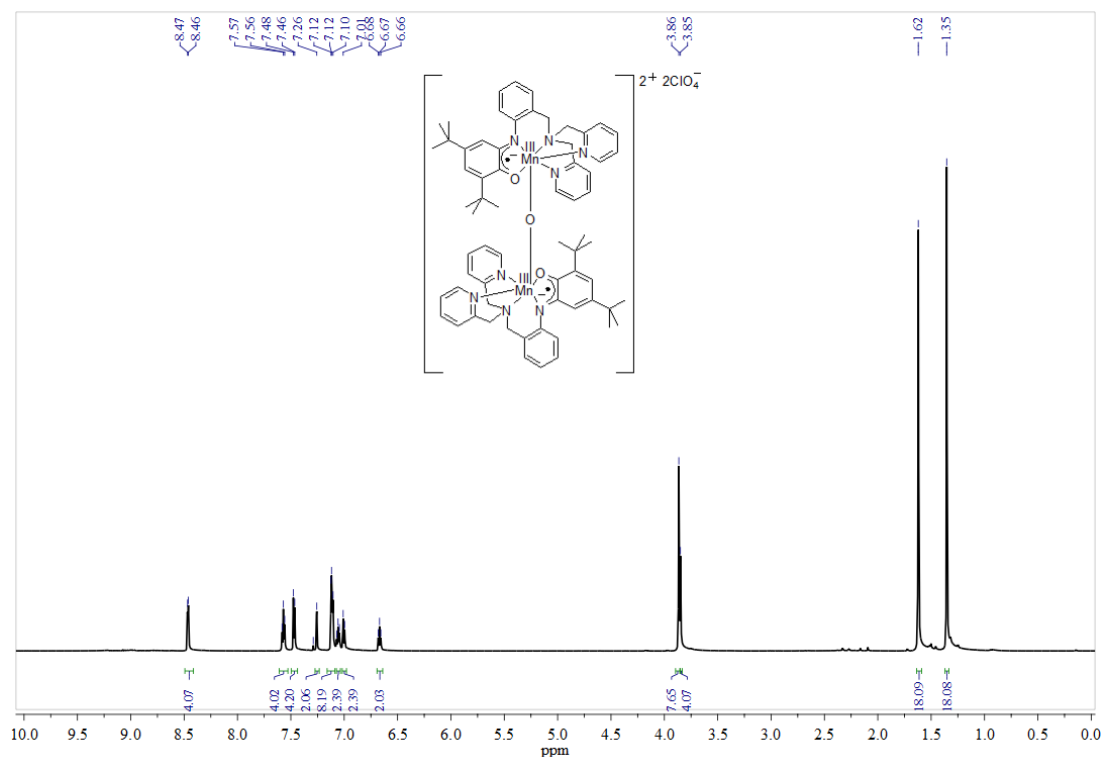


Figure S3. ^1H -NMR spectrum of complex **1** in CDCl_3 .

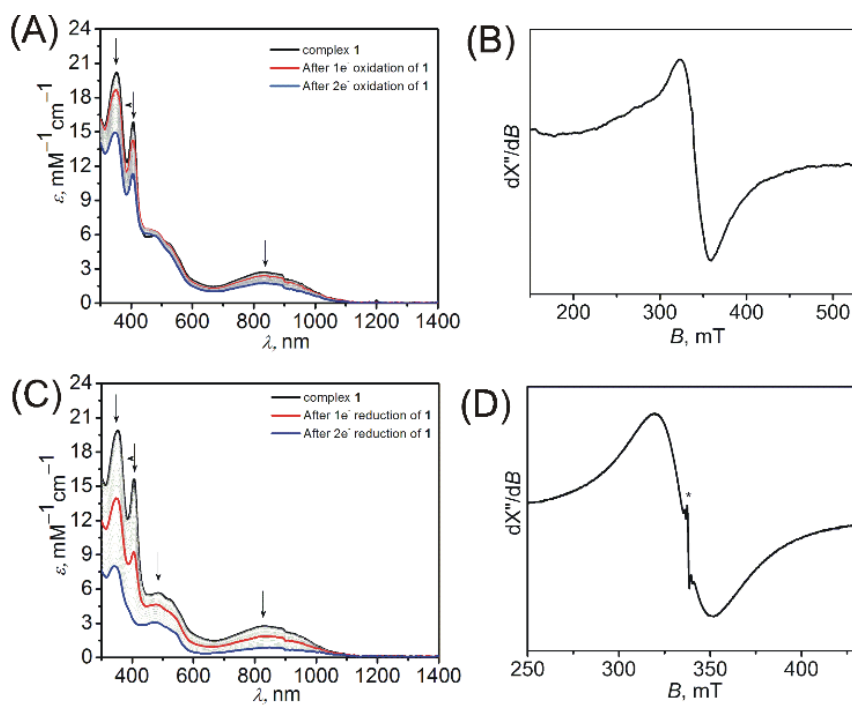


Figure S4. Change in UV-Vis-NIR spectrum of complex **1** during two one-electron fixed potential coulometric (A) oxidations and (C) reductions. (B) Experimental X-band (9.624 GHz) EPR spectrum of the one-electron oxidized solution. (D) Experimental X-band (9.448 GHz) EPR spectrum of the one-electron reduced solution. * A small quantity of organic radical impurity.

Table S1. Absorption data of complex **1** and its electrochemically generated oxidized and reduced species.

Complex	λ , nm($\epsilon = \text{M}^{-1}\text{cm}^{-1}$)
1	915(2200), 832(2700), 523(5100), 484(5700), 406(15700), 352(19950).
1¹⁺	836(2350), 523(5100), 456(6650), 406(14300), 352(18650).
1²⁺	836(1750), 526(4400), 456(1200), 406(11350), 352(15200).
1¹⁻	845(1850), 543(3450), 474(4650), 406(9200), 350(14000).
1²⁻	851(900), 549(2150), 477(3100), 387(14300), 342(8100).

Synthesis of Complex $\{[1]^{3+}[\text{SbF}_6][(\text{ClO}_4)_2]\}$; $\{[(\text{L}^{\text{ISQ}})\text{Mn}^{\text{IV}}\text{-O-Mn}^{\text{III}}(\text{L}^{\text{ISQ}})][\text{SbF}_6][(\text{ClO}_4)_2]\}$; $[\text{C}_{66}\text{H}_{76}\text{Mn}_2\text{Cl}_2\text{N}_8\text{O}_{11}\text{SbF}_6]$: To a stirred solution of complex **1** (0.035 g, 0.026 mmol) in CH_2Cl_2 (10 mL), solid AgSbF_6 (0.09 g, 0.026 mmol) was added. The colour of the solution was immediately changed from brown to reddish brown. After stirring for 10 min at room temperature, it was filtered through celite pad to remove Ag particles and the filtrate was evaporated to get black solid product. The solid was dissolved in CH_2Cl_2 (5 mL), filtered and hexane (2 mL) was added to the solution. Solid precipitate collected by filtration after 48h. Yield: 0.031 g, 76 %. FT-IR (KBr pellet, cm^{-1}): 3068, 2962, 2930, 2874, 1623, 1602, 1480, 1442, 1378, 1095, 1019, 899, 842, 764, 656.

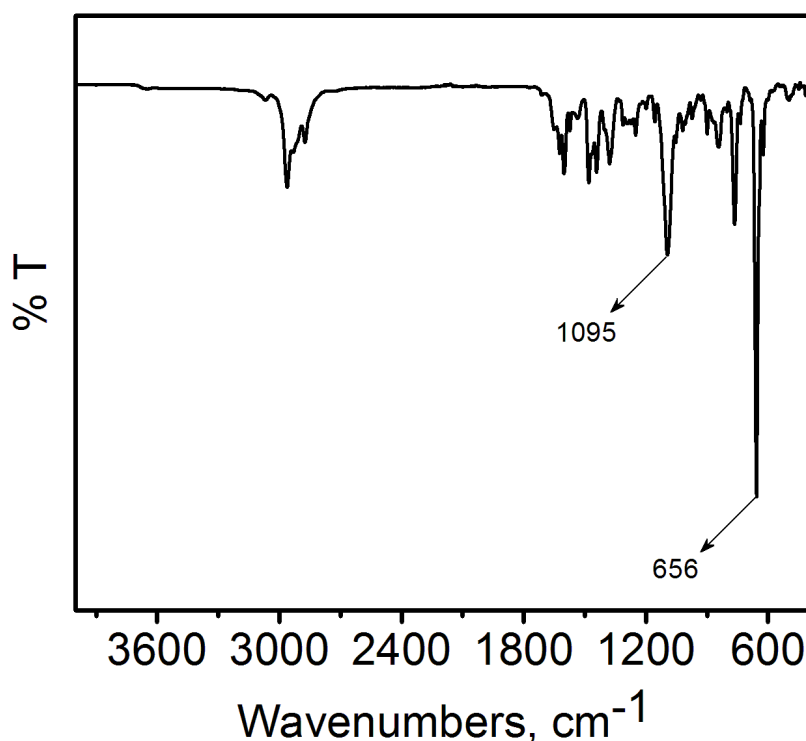


Figure S5. ATR-IR spectrum of $\{[1]^{3+}[\text{SbF}_6][(\text{ClO}_4)_2]\}$.

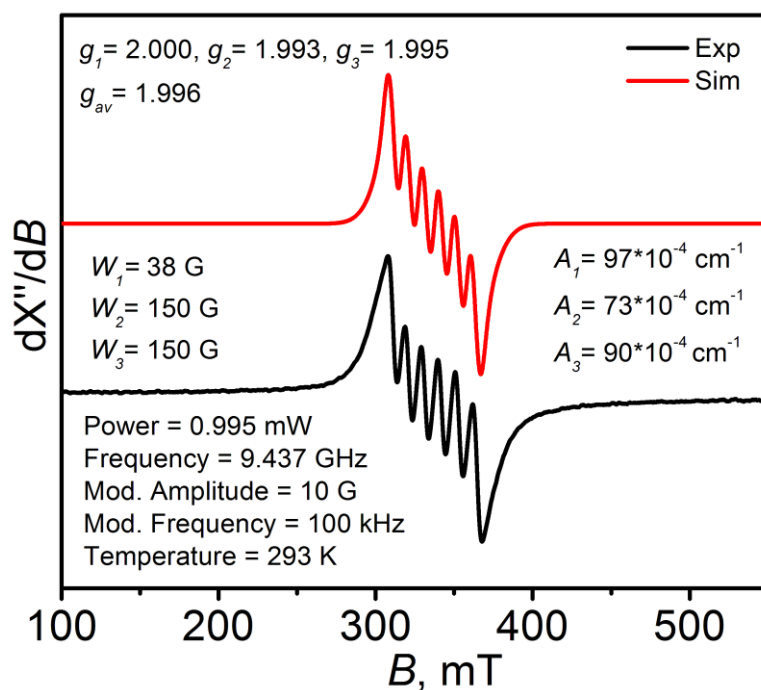


Figure S6. Experimental and simulated X-band ESR spectrum of isolated one-electron oxidized species $[1]^{3+}$ in MeOH.

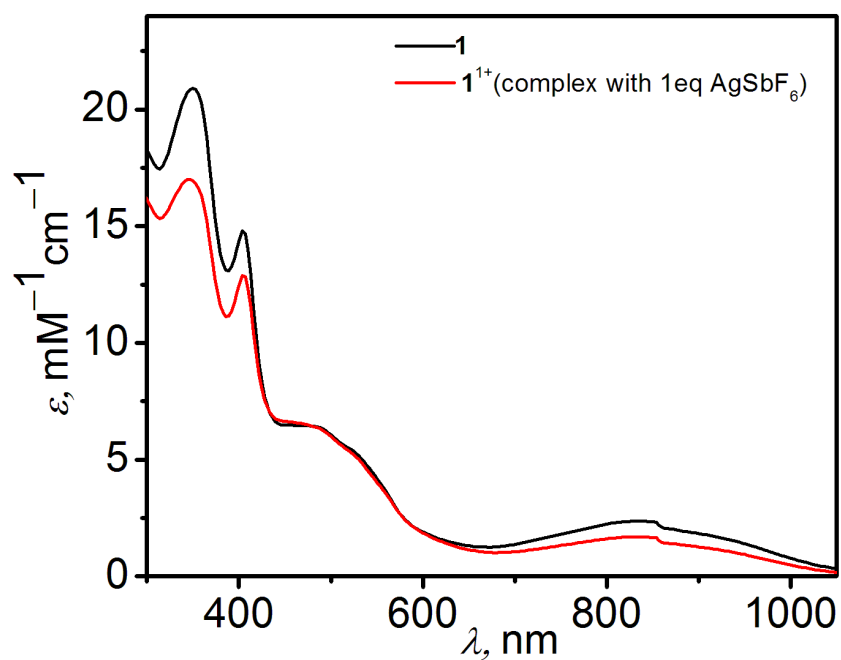


Figure S7. UV-VIS-NIR spectrum in dichloromethane of the chemically one-electron oxidized species; $[1]^{3+}$.

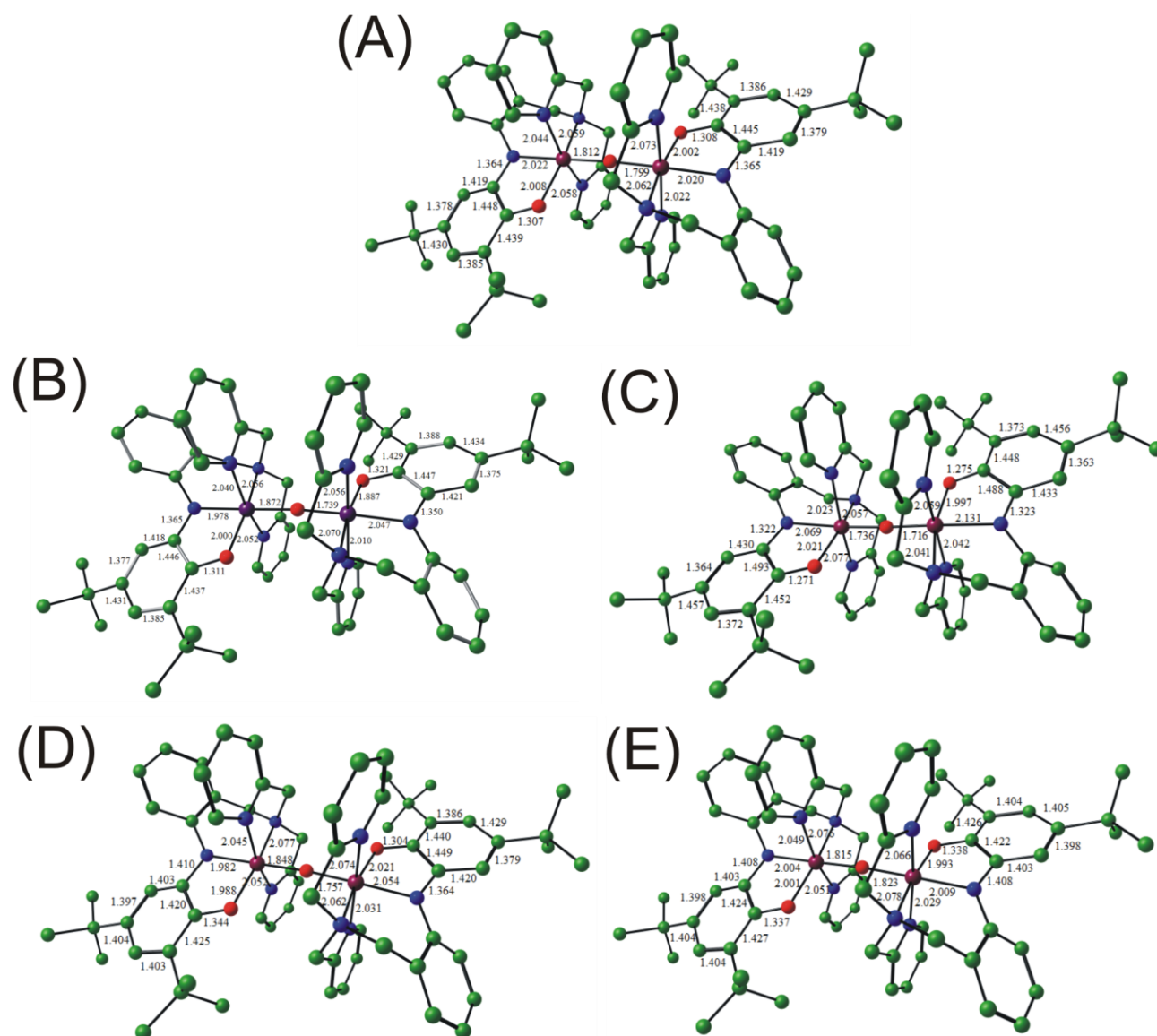


Figure S8. Optimized bond parameters of (A) complex **1**; (B) $[1^{3+}]$; (C) $[1^{4+}]$; (D) $[1^{4+}]$; (E) $[1^0]$.

Optimized coordinates of complex **1**; $[1]^{2+}$:

Mn	1.67937400	-0.68125800	-0.16288600
O	-0.01741400	-0.13235800	0.15702500
O	2.61450100	0.96857200	0.49598100
N	3.60687700	-1.26872300	-0.32450000
N	1.01426800	-2.43323100	-1.01704200
N	1.55598700	-0.03696800	-2.11305600

C	3.51464500	3.19689500	2.41525400
H	2.71793000	2.45720400	2.33348300
H	3.08826400	4.12895300	2.80275200
H	4.24357400	2.83306500	3.14776800
N	1.67071000	-1.78195600	1.55882800
C	3.89932300	0.99545200	0.25753800
C	4.48976100	-0.23265100	-0.23350800
C	4.75214200	2.13165600	0.48588400
C	4.02377800	-2.60200500	-0.18805300
C	0.31954800	-3.16212800	0.08341800
H	0.20626100	-4.22633000	-0.14865500
H	-0.67618000	-2.72319500	0.17637000
C	3.24222000	-3.62296500	-0.77668500
C	4.69960200	-5.31491200	0.18674000
H	4.95964400	-6.35973000	0.32146800
C	1.03585400	-2.96374800	1.40167900
C	6.67453100	0.80745900	-0.40571600
C	4.20334500	3.45371300	1.05280200
C	3.59459500	-4.96108400	-0.58900200
H	2.99611500	-5.73506500	-1.06149900
C	0.75476600	-0.83928300	-2.85190200
C	0.09622600	-1.97286100	-2.10132800
H	-0.82121200	-1.60729000	-1.63764200
H	-0.15496600	-2.79631700	-2.77911300
C	5.86463500	-0.29344400	-0.58026300
H	6.24789900	-1.21197200	-1.00395500
C	5.31375100	4.49650700	1.29360600
H	6.06583600	4.13880600	2.00444700
H	4.86677400	5.40285000	1.71399700
H	5.82149600	4.78325800	0.36712000
C	6.08802500	1.98724000	0.14911400
H	6.74302300	2.83484900	0.30088600
C	2.08952700	-3.26145400	-1.66539800
H	2.45017600	-2.67845100	-2.51749400
H	1.62245400	-4.16994400	-2.06286800
C	2.15002600	1.01906100	-2.69169900
H	2.77669600	1.62808600	-2.05243700
C	5.11790500	-2.97157000	0.62289700
H	5.68782200	-2.20451700	1.13319100
C	5.45307800	-4.31102000	0.79897400
H	6.29935200	-4.56927200	1.42818400
C	0.53893900	-0.60059500	-4.20730100
H	-0.09582600	-1.26977500	-4.77772400
C	1.97403800	1.32173000	-4.03860300
H	2.47359900	2.18284500	-4.46712000
C	8.16521000	0.82016800	-0.78010700
C	1.15534800	0.49674400	-4.80882400
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C	3.20687400	4.06511000	0.03926400
H	3.72578500	4.34736300	-0.88313800

H	2.74611700	4.96860000	0.45476100
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H	0.49414600	-4.85320700	2.27593900
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C	1.63273100	-3.61585600	3.63635900
H	1.62005700	-4.33749800	4.44658700
C	9.00767200	1.10646600	0.48734700
H	8.75978200	2.07246700	0.93728700
H	10.07283900	1.12322200	0.23280200
H	8.85152900	0.33110800	1.24469200
C	8.42574400	1.92697000	-1.83074300
H	7.85087700	1.74214800	-2.74438500
H	9.48789500	1.94924100	-2.09714300
H	8.15742600	2.91997200	-1.45813000
Mn	-1.68192800	0.50307300	0.40780100
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N	-3.56823500	1.22316800	0.48290400
N	-1.04017200	1.93678000	1.74393500
N	-1.86935700	-0.58166600	2.16431400
C	-3.52663800	-2.38733900	-3.29779800
H	-2.71734600	-1.72597600	-2.98587700
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C	-3.87080700	2.58650500	0.62468400
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H	-6.87667000	-2.29953000	-1.44776500
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H	-2.29414200	1.06441600	-2.58606300
C	-0.44105800	4.13164800	-1.24764600
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H	-1.88890900	3.01315000	-4.11537400
C	-0.86817100	4.14758600	-2.57443200
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C	-8.74700200	-1.74505800	0.65432800
H	-8.27556200	-1.83105600	1.63908500
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H	8.49426300	-1.34870700	-0.66275300
H	8.08560800	-0.77238300	-2.29133200
H	9.69060300	-0.47070700	-1.61979900

Optimized coordinates of [1]³⁺:

Mn	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.87173784
O	1.98618746	0.00000000	-0.23689856
N	0.10350896	-0.17110348	-1.96803746
N	-2.05033530	0.14365174	-0.06200102
N	-0.15367306	2.04574032	0.00365730
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H	5.72161537	-0.88910382	0.67503124
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C	2.37847952	0.16842610	-1.47633933
C	1.33644068	0.11487132	-2.47790468
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C	-0.86367569	-0.83883921	-2.74489068
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C	-2.84175270	-2.25586052	-4.15937674
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C	-1.66396099	-2.29355122	0.16559549
C	2.91612023	0.56811336	-4.25450838
C	4.90995059	0.38224288	-0.90177788
C	-3.20143160	-1.33548604	-3.17361603
H	-4.25066565	-1.15669836	-2.95616351
C	-1.39325580	2.45697058	0.36284692
C	-2.34948678	1.35644851	0.75789560
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H	-3.38988371	1.67181594	0.62939725
C	1.61999599	0.34241508	-3.84897213
H	0.79784971	0.35609654	-4.55132754
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H	4.95742746	0.69889870	-3.59784393
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H	1.75096795	2.57353690	-0.60332827
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H	-1.19398322	-3.22316871	-5.16158331
C	-1.73247602	3.80653974	0.38717264

H	-2.73776562	4.10519897	0.66292491
C	0.50810231	4.32181700	-0.32124445
H	1.28505420	5.02411598	-0.59968060
C	3.30136098	0.84399644	-5.71575514
C	-0.76740442	4.75301079	0.04006690
H	-1.01216077	5.80993640	0.04475728
C	4.75917325	1.61695987	0.01847127
H	4.87064251	2.53886630	-0.56176466
H	5.53378079	1.61235914	0.79335415
H	3.78262066	1.64610824	0.50434140
C	0.51238631	-2.99622164	-0.29865826
H	1.54333481	-2.69776236	-0.45281293
C	-2.14047235	-3.59879237	0.05648595
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H	0.83482081	-5.08847532	-0.64924097
C	-1.24261143	-4.62539177	-0.23154399
H	-1.59423408	-5.64737130	-0.32638000
C	4.27611935	-0.25728894	-6.20138347
H	5.19374121	-0.28790825	-5.60655671
H	4.56203225	-0.06850315	-7.24141849
H	3.80734555	-1.24558252	-6.15202146
C	3.99405194	2.22514256	-5.81496771
H	3.32165893	3.02487908	-5.48716390
H	4.27885493	2.42583564	-6.85305142
H	4.90257506	2.27647545	-5.20770086
Mn	0.11072777	0.07913651	3.60577773
O	-1.69555793	0.51588095	3.93454928
N	0.17738439	0.40238962	5.62581791
N	2.07133685	-0.58522207	3.62141668
N	-0.16862709	-1.94951450	3.78787482
C	-4.32504325	2.31639941	3.83101798
H	-3.37161364	2.27164570	3.30346569
H	-5.11632337	2.48876337	3.09392063
H	-4.29953514	3.17909527	4.50465396
N	0.97951390	1.88799165	3.49706035
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C	-1.05298631	0.46462955	6.17857541
C	-3.45719564	0.76558571	5.60835778
C	1.32734561	0.79503455	6.32722467
C	2.87676593	0.48567986	2.95925994
H	3.92847246	0.41473697	3.25002579
H	2.80224179	0.32732437	1.88025981
C	2.56348553	0.20629714	5.97816034
C	3.69439379	1.64389056	7.57543925
H	4.61101282	1.96336086	8.05962245
C	2.30952692	1.84644687	3.26654955
C	-2.66121594	0.53394159	7.97949575
C	-4.61269655	1.01710682	4.62146567
C	3.72916516	0.62944115	6.61569632

H	4.67324967	0.15603196	6.36431621
C	0.88036802	-2.67318674	3.32908159
C	2.04100804	-1.85471409	2.83353645
H	1.89113732	-1.59193482	1.78615939
H	2.98836165	-2.39434910	2.93121440
C	-1.35443555	0.42410057	7.56709553
H	-0.54806896	0.26669505	8.26958010
C	-5.96294782	1.20329920	5.34222460
H	-5.95259191	2.05809058	6.02570904
H	-6.73862783	1.39237220	4.59430180
H	-6.25884174	0.31047476	5.90231963
C	-3.67011016	0.73210091	6.97949223
H	-4.68549421	0.85199545	7.33072763
C	2.60195911	-0.92328878	4.99510081
H	2.00712732	-1.76274565	5.36296551
H	3.63011487	-1.27586695	4.86650711
C	-1.26015854	-2.58063908	4.25587452
H	-2.07032654	-1.96033596	4.61648351
C	1.30397642	1.84313303	7.27132035
H	0.37248802	2.35167736	7.48862033
C	2.47900788	2.25548821	7.89127838
H	2.44526029	3.06510496	8.61271522
C	0.85594602	-4.06294875	3.32450872
H	1.71600445	-4.61407957	2.96236664
C	-1.35169773	-3.96787085	4.27532749
H	-2.24791483	-4.43930274	4.66081684
C	-3.08205464	0.45525082	9.45342867
C	-0.27889135	-4.72080173	3.79972993
H	-0.31894678	-5.80466947	3.80872899
C	-4.76212844	-0.18463862	3.66167768
H	-5.01228804	-1.09526392	4.21574915
H	-5.56891465	0.00605125	2.94662741
H	-3.84619750	-0.36729382	3.10085920
C	0.35497643	3.06298911	3.69339831
H	-0.71146692	3.01711730	3.87741728
C	3.06554690	3.01602635	3.24147212
H	4.13503082	2.96192007	3.07465569
C	1.04861969	4.26544534	3.66035528
H	0.51750818	5.19649076	3.81782818
C	2.42671328	4.23917809	3.43787889
H	2.99874733	5.16074174	3.42324158
C	-3.77789540	1.78044739	9.85317370
H	-4.67452561	1.97700707	9.25793823
H	-4.08381807	1.73261661	10.90308069
H	-3.09916710	2.63143896	9.73565359
C	-4.06604316	-0.72574579	9.64147973
H	-3.59136649	-1.67656832	9.37795084
H	-4.37975430	-0.78194281	10.68866560
H	-4.96806983	-0.61655243	9.03233892
C	-1.87741240	0.23816731	10.38756581

H	-1.35957729	-0.70293179	10.17488033
H	-1.15326496	1.05630347	10.31706010
H	-2.22401611	0.19474359	11.42398389
C	2.07460504	0.84968284	-6.64647694
H	1.55594783	-0.11457504	-6.64388716
H	1.35667540	1.62867700	-6.36967436
H	2.39562552	1.04778630	-7.67347160

Optimized coordinates of [1]⁴⁺:

Mn	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.73640462
O	2.00820490	0.00000000	-0.22569761
N	0.24707865	-0.39453194	-2.01565018
N	-2.01790306	0.30634901	-0.25448080
N	-0.02565909	2.06600491	-0.20794112
C	5.01309941	-1.17384483	0.07090473
H	4.05361419	-1.36919508	0.55174116
H	5.78161612	-1.13075218	0.84899479
H	5.24249970	-2.02101541	-0.58285983
N	-0.56724137	-1.94187335	0.02498884
C	2.47367290	-0.00460407	-1.40870375
C	1.46089471	-0.17881383	-2.49216588
C	3.87550225	0.09804996	-1.77364346
C	-0.75546787	-0.97508673	-2.81677471
C	-2.71489980	-0.87541300	0.33369072
H	-3.72412917	-0.97780183	-0.07591761
H	-2.80372708	-0.70107814	1.40732901
C	-2.09975252	-0.58824410	-2.62112857
C	-2.78697762	-2.21799541	-4.28727897
H	-3.57881309	-2.69020915	-4.85869459
C	-1.90111426	-2.12614401	0.12266493
C	3.14622472	0.08858307	-4.19577881
C	5.00762064	0.14914870	-0.73303362
C	-3.09669771	-1.20305176	-3.37701561
H	-4.12748792	-0.88594187	-3.25384973
C	-1.24191742	2.58297400	0.09493030
C	-2.28860988	1.57266098	0.48820034
H	-2.21081273	1.35356986	1.55429385
H	-3.29850417	1.94368906	0.28526077
C	1.83526610	-0.09692154	-3.86981104
H	1.05969004	-0.12729527	-4.62134269
C	6.39163189	0.29601559	-1.39648734
H	6.63201920	-0.54987341	-2.04798492
H	7.15423991	0.33009775	-0.61373030
H	6.47663592	1.22079178	-1.97611300
C	4.12970118	0.13021472	-3.12107750
H	5.16153455	0.21857253	-3.43101838
C	-2.44053840	0.53340917	-1.68601278

H	-1.96453714	1.45911957	-2.01801091
H	-3.52201592	0.70003858	-1.68358774
C	0.96495358	2.90464929	-0.56581376
H	1.92237469	2.46047694	-0.79917517
C	-0.45153922	-2.02381715	-3.70905595
H	0.56815216	-2.38090384	-3.79103726
C	-1.46379105	-2.63680441	-4.43930920
H	-1.21906964	-3.44818715	-5.11611795
C	-1.49151782	3.95018578	0.05192381
H	-2.48196751	4.32293517	0.28586187
C	0.78929422	4.28226291	-0.62486270
H	1.61891424	4.91558751	-0.91610424
C	3.63895349	0.26376371	-5.63180244
C	-0.45935457	4.81570237	-0.30901487
H	-0.63133938	5.88563474	-0.35418106
C	4.81288251	1.36389251	0.20223551
H	4.85012580	2.30020050	-0.36398127
H	5.61382753	1.38915504	0.94719712
H	3.86130001	1.32079378	0.73029641
C	0.24760611	-3.00398842	-0.10835079
H	1.30644389	-2.79259790	-0.19947123
C	-2.46108016	-3.40100237	0.08633640
H	-3.53689481	-3.51972246	0.14654417
C	-0.24090082	-4.30455964	-0.13274127
H	0.44654530	-5.13547396	-0.23703807
C	-1.61888974	-4.50508298	-0.03693642
H	-2.03317572	-5.50709626	-0.06805801
C	4.63169825	-0.88070082	-5.96431583
H	5.51020635	-0.87962013	-5.31260481
H	4.98634070	-0.76001553	-6.99231510
H	4.14684640	-1.85855410	-5.88423612
C	4.35970516	1.63090145	-5.75620752
H	3.67582974	2.45675297	-5.53695876
H	4.72481263	1.75407122	-6.78022046
H	5.22189750	1.71390988	-5.08839332
Mn	-0.08221491	-0.02420371	3.45071844
O	-2.03826244	-0.35120619	3.68639989
N	-0.38426943	0.17337265	5.55132132
N	1.92995406	0.11182978	3.76467161
N	0.39009840	-2.02709634	3.51152750
C	-5.10722347	0.13169524	3.22163963
H	-4.17205138	0.46906807	2.77406889
H	-5.82407867	-0.05830250	2.41676345
H	-5.50075719	0.94789532	3.83569131
N	-0.05151198	2.01472422	3.55780646
C	-2.50764017	-0.52857968	4.85802859
C	-1.56303176	-0.25330412	5.97445038
C	-3.87384588	-0.89459365	5.16668189
C	0.45948885	0.91537791	6.39331671
C	2.30875035	1.47228055	3.26551068

H	3.26085421	1.79779540	3.69396963
H	2.44099872	1.39194746	2.18534106
C	1.85449890	0.84113754	6.18504175
C	2.19116008	2.48683387	7.93698583
H	2.86751404	3.08695537	8.53612797
C	1.21737124	2.48466135	3.53808715
C	-3.23615820	-0.85266794	7.61144088
C	-4.92513458	-1.14786823	4.07281909
C	2.70433701	1.61274279	6.97361510
H	3.77785711	1.53519489	6.83220497
C	1.70211174	-2.25024788	3.25666326
C	2.49860542	-1.00787407	2.95058531
H	2.39786145	-0.74854611	1.89700861
H	3.56068836	-1.14921969	3.17083753
C	-1.96399311	-0.44755311	7.33599169
H	-1.22235009	-0.33395407	8.11343702
C	-6.30208779	-1.50327750	4.66851402
H	-6.70313363	-0.69676124	5.29013604
H	-7.00777169	-1.66568914	3.84905806
H	-6.27272926	-2.42331445	5.26081771
C	-4.16450113	-1.02014456	6.50259288
H	-5.17492473	-1.29941880	6.76854537
C	2.40784778	-0.11704768	5.17940037
H	2.13697790	-1.14203989	5.44047287
H	3.50041019	-0.05749722	5.17039991
C	-0.41022800	-3.07478251	3.77673051
H	-1.45345538	-2.86011860	3.96602600
C	-0.05411043	1.83260215	7.33667362
H	-1.12453808	1.96780697	7.43193337
C	0.80940178	2.60572833	8.10339375
H	0.40228038	3.31106291	8.81964778
C	2.24760953	-3.52956702	3.27588163
H	3.30623434	-3.66862632	3.08715424
C	0.06419463	-4.38261055	3.80583686
H	-0.61796628	-5.19490878	4.02713173
C	-3.73344279	-1.16026431	9.02526701
C	1.41515041	-4.61440308	3.55447875
H	1.81812998	-5.62105786	3.58136845
C	-4.47817372	-2.34615536	3.20167025
H	-4.45735500	-3.26445761	3.79683634
H	-5.18757675	-2.49362627	2.38113370
H	-3.48547233	-2.20443123	2.77139139
C	-1.07334330	2.86870584	3.75745191
H	-2.06643134	2.43710661	3.79830235
C	1.49112528	3.84070198	3.70470538
H	2.51774784	4.18898256	3.69838261
C	-0.87308757	4.23378625	3.91705064
H	-1.72308208	4.88785091	4.07171869
C	0.43225727	4.72767057	3.89013940
H	0.62388329	5.78679127	4.02509374

C	-4.91083580	-0.20844200	9.36025445
H	-5.75396328	-0.32775488	8.67425966
H	-5.27507248	-0.42719400	10.36861244
H	-4.59217793	0.83816332	9.33196739
C	-4.21948351	-2.63108363	9.08451095
H	-3.40342062	-3.32323432	8.85450216
H	-4.57959507	-2.85325275	10.09356321
H	-5.04230123	-2.83045057	8.39184979
C	-2.62926638	-0.96608542	10.07974253
H	-1.77881164	-1.63324431	9.90690997
H	-2.26447211	0.06569665	10.10452093
H	-3.03102615	-1.19546951	11.07029555
C	2.48378383	0.22293561	-6.64834554
H	1.95536235	-0.73555104	-6.62839338
H	1.75895116	1.02530830	-6.47632651
H	2.88597274	0.35466369	-7.65639177

Optimized coordinates of [1]¹⁺:

Mn	-1.70144700	-0.67492100	0.18800800
O	0.04334300	-0.14825200	-0.11519500
O	-2.56810400	0.95908800	-0.53986300
N	-3.58602300	-1.24446300	0.41353700
N	-1.02768500	-2.45040300	1.02905100
N	-1.54684500	-0.03677300	2.13161300
C	-3.43647800	3.17727300	-2.44356900
H	-2.67496500	2.40517800	-2.33342000
H	-2.96724800	4.08956700	-2.83217700
H	-4.16438300	2.83449500	-3.18821400
N	-1.67385400	-1.76103300	-1.54471800
C	-3.88593500	1.01645900	-0.28377600
C	-4.47400000	-0.16214600	0.24570500
C	-4.71112300	2.15716700	-0.50572000
C	-4.00780200	-2.54456100	0.16540100
C	-0.32457800	-3.15290900	-0.07983500
H	-0.19752700	-4.22043500	0.13411900
H	0.66394400	-2.69709100	-0.16904000
C	-3.24494800	-3.61714300	0.70055300
C	-4.69666600	-5.26086800	-0.35514800
H	-4.96230900	-6.29587100	-0.54645500
C	-1.05091500	-2.94921900	-1.39373800
C	-6.64469100	0.92953900	0.44374800
C	-4.14494300	3.46334700	-1.09779100
C	-3.59328800	-4.94440500	0.43715200
H	-2.99244600	-5.73962600	0.87363400
C	-0.77775700	-0.86201900	2.87717300
C	-0.12680600	-2.00628700	2.12961800
H	0.80387200	-1.65174300	1.68448700
H	0.10156500	-2.83354600	2.81271600

C	-5.82150300	-0.18313800	0.63445800
H	-6.21114500	-1.09098800	1.07914300
C	-5.23350400	4.51939800	-1.38101600
H	-5.98767200	4.15082000	-2.08439100
H	-4.76899500	5.40575700	-1.82714400
H	-5.74562800	4.84413500	-0.46943200
C	-6.06227000	2.06787000	-0.13718600
H	-6.69400900	2.93178200	-0.30241800
C	-2.11762100	-3.29160800	1.62952500
H	-2.49920600	-2.71578100	2.47898400
H	-1.66230600	-4.21100200	2.02094400
C	-2.13956200	1.02104700	2.70443900
H	-2.74882500	1.63356900	2.05028800
C	-5.11703600	-2.88537200	-0.64873900
H	-5.71235200	-2.09464600	-1.08942000
C	-5.45117100	-4.21372900	-0.89536800
H	-6.30891700	-4.43307600	-1.52672900
C	-0.58567600	-0.63766700	4.23917800
H	0.02520800	-1.32179600	4.81848400
C	-1.98915500	1.30826500	4.05923500
H	-2.48713600	2.17086900	4.48733400
C	-8.13554300	0.94319700	0.83571000
C	-1.19809300	0.46451900	4.83776700
H	-1.06600700	0.65405500	5.89829400
C	-3.15791600	4.08345900	-0.08048500
H	-3.69429700	4.40670300	0.81878100
H	-2.65543400	4.96186100	-0.50506000
H	-2.40163800	3.35902900	0.22260900
C	-2.31630300	-1.48222700	-2.68953100
H	-2.81713700	-0.52039200	-2.71846900
C	-1.03909800	-3.89353100	-2.42088600
H	-0.54068700	-4.84579800	-2.27406700
C	-2.33930000	-2.37167300	-3.75817100
H	-2.86499600	-2.11091100	-4.66986200
C	-1.68733100	-3.59892300	-3.61892100
H	-1.69477400	-4.32214900	-4.42819400
C	-9.00204100	1.18350200	-0.42402300
H	-8.75968800	2.13529200	-0.90671900
H	-10.06690200	1.20271300	-0.16272000
H	-8.84812400	0.38690900	-1.16018300
C	-8.40167700	2.07623900	1.85544000
H	-7.81646600	1.92357800	2.76898000
H	-9.46204600	2.10480200	2.13333200
H	-8.13734600	3.05726200	1.44941200
Mn	1.66594400	0.47720100	-0.36362100
O	2.66306200	-0.88191700	0.75122000
N	3.57962100	1.21679500	-0.45991800
N	1.00171400	1.92295400	-1.67466000
N	1.85413700	-0.58310600	-2.13618500
C	3.56599100	-2.41907700	3.30235700

H	2.74830700	-1.76544000	2.99650600
H	3.14975800	-3.24777600	3.88670100
H	4.23405400	-1.84958300	3.95797800
N	1.35199200	1.90979100	1.04088900
C	3.96249100	-0.82087400	0.66129300
C	4.51689900	0.32187100	-0.03569500
C	4.86399600	-1.78450400	1.23822700
C	3.87342300	2.57759400	-0.60288900
C	0.13281000	2.81521800	-0.85659700
H	0.00450000	3.79217600	-1.33491600
H	-0.84584700	2.32898300	-0.78186300
C	3.08976900	3.35015000	-1.49362100
C	4.27674700	5.36429700	-0.81927300
H	4.43203900	6.43443200	-0.91079600
C	0.67369600	2.96761100	0.54779000
C	6.77695200	-0.52503600	0.24589000
C	4.34309600	-2.96526100	2.07952400
C	3.30790900	4.72566800	-1.59505600
H	2.71188900	5.30277700	-2.29684700
C	1.07833400	-0.05111600	-3.10877200
C	0.24922700	1.14534600	-2.70079200
H	-0.67848500	0.80500900	-2.23811300
H	0.00778300	1.76742500	-3.57108600
C	5.91619900	0.43182400	-0.24847800
H	6.28078800	1.26723800	-0.83131700
C	5.48358600	-3.85310700	2.61575600
H	6.17198100	-3.29618100	3.25977900
H	5.05429600	-4.66244500	3.21511800
H	6.06220700	-4.31408800	1.80839300
C	6.21696100	-1.59915100	1.00396600
H	6.90717000	-2.32497100	1.41411700
C	2.08893700	2.67573900	-2.38539900
H	2.59843900	1.94806600	-3.02360700
H	1.61396300	3.41604200	-3.04074700
C	2.61017100	-1.65818500	-2.40929100
H	3.21300100	-2.04026300	-1.59395400
C	4.83011400	3.23867300	0.19813800
H	5.39701000	2.67197700	0.92728300
C	5.03017400	4.61144700	0.08450900
H	5.77051200	5.09520400	0.71472500
C	1.04685500	-0.59362900	-4.39165300
H	0.42571800	-0.13814300	-5.15501100
C	2.62439800	-2.25695900	-3.66600900
H	3.25030600	-3.12397100	-3.84394900
C	8.29685900	-0.48130800	0.01724500
C	1.82744200	-1.71483600	-4.67353500
H	1.81963400	-2.15131100	-5.66702600
C	3.42404100	-3.86090500	1.21646600
H	3.98421200	-4.29540600	0.38093700
H	3.02501500	-4.68557000	1.81798000

H	2.58797300	-3.29158100	0.81127400
C	1.79827100	1.92750000	2.30637100
H	2.34221200	1.04588300	2.62647100
C	0.42812800	4.09411400	1.33423600
H	-0.10760500	4.93887700	0.91595500
C	1.57641900	3.00927200	3.15115700
H	1.94685800	2.98704000	4.16960000
C	0.88177800	4.11273300	2.65192100
H	0.70057400	4.97964500	3.27922500
C	9.01848300	-0.38921300	1.38410200
H	8.78895600	-1.24307700	2.02822400
H	10.10389400	-0.36735400	1.23689300
H	8.72981100	0.52258600	1.91763500
C	8.74811700	-1.76801900	-0.71553100
H	8.26111900	-1.85218600	-1.69290200
H	9.83152300	-1.75014900	-0.87717500
H	8.51384200	-2.67057200	-0.14339500
C	8.72234600	0.73050700	-0.83299600
H	8.26619300	0.71046200	-1.82837100
H	8.45761800	1.67849000	-0.35319800
H	9.80851200	0.72115000	-0.96722300
C	-8.58466800	-0.38509700	1.47448400
H	-8.45649200	-1.23016700	0.78992100
H	-8.02806800	-0.60422400	2.39193900
H	-9.64668600	-0.33007000	1.73692200

Optimized coordinates of [1]⁰:

Mn	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.81491586
O	1.98324369	0.00000000	-0.26281087
N	0.03606756	-0.12623725	-1.99977576
N	-2.07507754	0.05469974	-0.01178490
N	-0.23058133	2.03841004	-0.01865015
C	4.90496279	-0.84246904	-0.13723719
H	3.94985604	-1.02650770	0.35503660
H	5.69568343	-0.79604141	0.62209764
H	5.12322173	-1.69300936	-0.79392284
N	-0.29443138	-2.02736568	0.02587436
C	2.35333697	0.18884953	-1.53339715
C	1.32076742	0.13772090	-2.51200084
C	3.69265566	0.43078451	-1.96116982
C	-0.85866285	-0.90626173	-2.71395728
C	-2.48792645	-1.20561771	0.66181478
H	-3.53760524	-1.44968213	0.45782056
H	-2.36750476	-1.04177533	1.73508838
C	-2.23896947	-0.83763938	-2.37321218
C	-2.79819533	-2.54536313	-4.01785827
H	-3.53831215	-3.16296241	-4.51739610
C	-1.58142362	-2.35269664	0.26727543

C	2.89749584	0.67749379	-4.29597551
C	4.86240121	0.46940128	-0.95707703
C	-3.17666417	-1.64586167	-3.02053510
H	-4.22472241	-1.55608737	-2.74120005
C	-1.48161767	2.40629617	0.33829292
C	-2.39996432	1.28293439	0.76754829
H	-2.22773491	1.07453306	1.82722286
H	-3.44996720	1.57191726	0.62997737
C	1.59540224	0.41489193	-3.85978140
H	0.76803445	0.41306470	-4.55963915
C	6.23790164	0.61963151	-1.63917801
H	6.44238608	-0.20220114	-2.33381368
H	7.02318804	0.61102010	-0.87503953
H	6.32846889	1.56209957	-2.18935280
C	3.91452050	0.66299836	-3.32746732
H	4.92970130	0.85042600	-3.65567656
C	-2.67752618	0.19199337	-1.37786562
H	-2.38213363	1.18602120	-1.73025665
H	-3.77131362	0.18313252	-1.27363719
C	0.66055101	2.97321245	-0.37920011
H	1.64075239	2.60586079	-0.65986701
C	-0.49286252	-1.83450247	-3.72341957
H	0.55080991	-1.92921065	-3.99885937
C	-1.44320654	-2.62911738	-4.35732014
H	-1.11837262	-3.33051773	-5.12260514
C	-1.86977084	3.74582197	0.33625527
H	-2.88324723	4.01435666	0.61512660
C	0.34446519	4.32986476	-0.39995582
H	1.09243850	5.05544552	-0.69966074
C	3.24345290	0.96770099	-5.77005224
C	-0.94337476	4.72103526	-0.03522935
H	-1.22714317	5.76880548	-0.04724410
C	4.67828348	1.68539527	-0.01849405
H	4.76248623	2.61969023	-0.58551355
H	5.44820070	1.69774639	0.76370145
H	3.69715176	1.66444132	0.45618078
C	0.58862096	-2.98699982	-0.28766162
H	1.59643351	-2.64075255	-0.49148741
C	-2.01454381	-3.67862453	0.21452958
H	-3.05677161	-3.91463723	0.40240750
C	0.23218263	-4.33023574	-0.34970730
H	0.97554983	-5.07848678	-0.60166094
C	-1.09540098	-4.67997345	-0.09348207
H	-1.41251829	-5.71695432	-0.14356304
C	4.21887538	-0.11170724	-6.29846445
H	5.14738517	-0.13631620	-5.71971249
H	4.48236574	0.08250989	-7.34536453
H	3.76470754	-1.10714726	-6.24239453
C	3.91489460	2.35661429	-5.89156777
H	3.23982661	3.14689345	-5.54502035

H	4.17881136	2.56981086	-6.93456780
H	4.83151125	2.41660837	-5.29711956
Mn	0.04260231	0.16315888	3.63019577
O	-1.84229313	0.75095778	3.89999939
N	0.08232958	0.39015681	5.62610379
N	2.02166150	-0.47101110	3.64215395
N	-0.29262277	-1.86875934	3.79451838
C	-4.40284359	2.48174426	3.85652613
H	-3.42477873	2.42749441	3.37686492
H	-5.16313316	2.67980191	3.09040237
H	-4.39904428	3.33051364	4.55032432
N	0.86995143	2.00748069	3.44945309
C	-2.23636355	0.71384212	5.17858165
C	-1.21820895	0.51362615	6.15067267
C	-3.58467587	0.86826965	5.61487858
C	1.16735485	0.93745796	6.28707972
C	2.75990395	0.58412701	2.89710130
H	3.83409892	0.55134951	3.11486838
H	2.61092743	0.39093196	1.82967864
C	2.46907612	0.47571958	5.94268081
C	3.50728372	2.05542527	7.47829267
H	4.39806807	2.47638585	7.93435471
C	2.19472451	1.95605120	3.19647359
C	-2.86271086	0.48427680	7.95451494
C	-4.71878087	1.16902291	4.61363415
C	3.60554067	1.03408764	6.53256904
H	4.58362307	0.64763501	6.25218479
C	0.80000492	-2.58431012	3.44547347
C	1.97668150	-1.77955333	2.93417277
H	1.82913143	-1.57211194	1.87318520
H	2.91307068	-2.33708755	3.06558656
C	-1.54250991	0.36980078	7.50780458
H	-0.73691387	0.17189196	8.20519594
C	-6.09075709	1.35084467	5.29333943
H	-6.08943379	2.17950357	6.00932024
H	-6.84460503	1.57430277	4.53009553
H	-6.41370230	0.44590226	5.81906333
C	-3.84843845	0.74653015	6.98844904
H	-4.87264897	0.85722222	7.32424949
C	2.58295944	-0.69405449	5.01496880
H	2.02288925	-1.53954840	5.42849680
H	3.63290714	-1.00008878	4.90976398
C	-1.38748969	-2.50158645	4.24052998
H	-2.22208931	-1.86589858	4.51446432
C	1.08826264	1.98001846	7.24664596
H	0.11482900	2.36470847	7.52782240
C	2.23321029	2.51941739	7.82542492
H	2.12839888	3.32080602	8.55343740
C	0.81390690	-3.97521066	3.53782479
H	1.70704224	-4.52604636	3.26254695

C	-1.44696611	-3.88903637	4.35487536
H	-2.35000766	-4.36368089	4.72232496
C	-3.25685577	0.34070826	9.43797461
C	-0.32652615	-4.63699705	3.99547800
H	-0.33448830	-5.71927256	4.07856001
C	-4.85112064	-0.00178883	3.61239553
H	-5.15650670	-0.91758563	4.13221166
H	-5.60985152	0.22024586	2.85133094
H	-3.89882241	-0.18804967	3.11672135
C	0.26960980	3.18856854	3.65685543
H	-0.79302656	3.13617466	3.86694821
C	2.96125096	3.12172462	3.14069307
H	4.02665119	3.05868108	2.94766528
C	0.96814382	4.39017122	3.60411717
H	0.44974177	5.32776452	3.77104722
C	2.33985599	4.35259395	3.34337977
H	2.91942425	5.26980422	3.30643832
C	-4.26381752	-0.82262792	9.60381071
H	-3.82001215	-1.77034592	9.27920094
H	-4.56307328	-0.93075814	10.65350319
H	-5.17059497	-0.65931777	9.01363772
C	-3.91395195	1.65148284	9.93345790
H	-4.80947929	1.89816109	9.35527299
H	-4.20894602	1.56403562	10.98625677
H	-3.21778749	2.49286142	9.84530448
C	-2.04282385	0.04955800	10.34133834
H	-1.54477063	-0.88571188	10.06467545
H	-1.30116445	0.85408824	10.29755034
H	-2.36922984	-0.04381087	11.38289274
C	1.99707517	0.96369769	-6.67588752
H	1.48955201	-0.00660019	-6.66564875
H	1.27278918	1.72791309	-6.37438131
H	2.28911494	1.17383381	-7.71064422