

Supporting Information

The Electronic Structure of a β -Diketiminate Manganese Hydride Dimer

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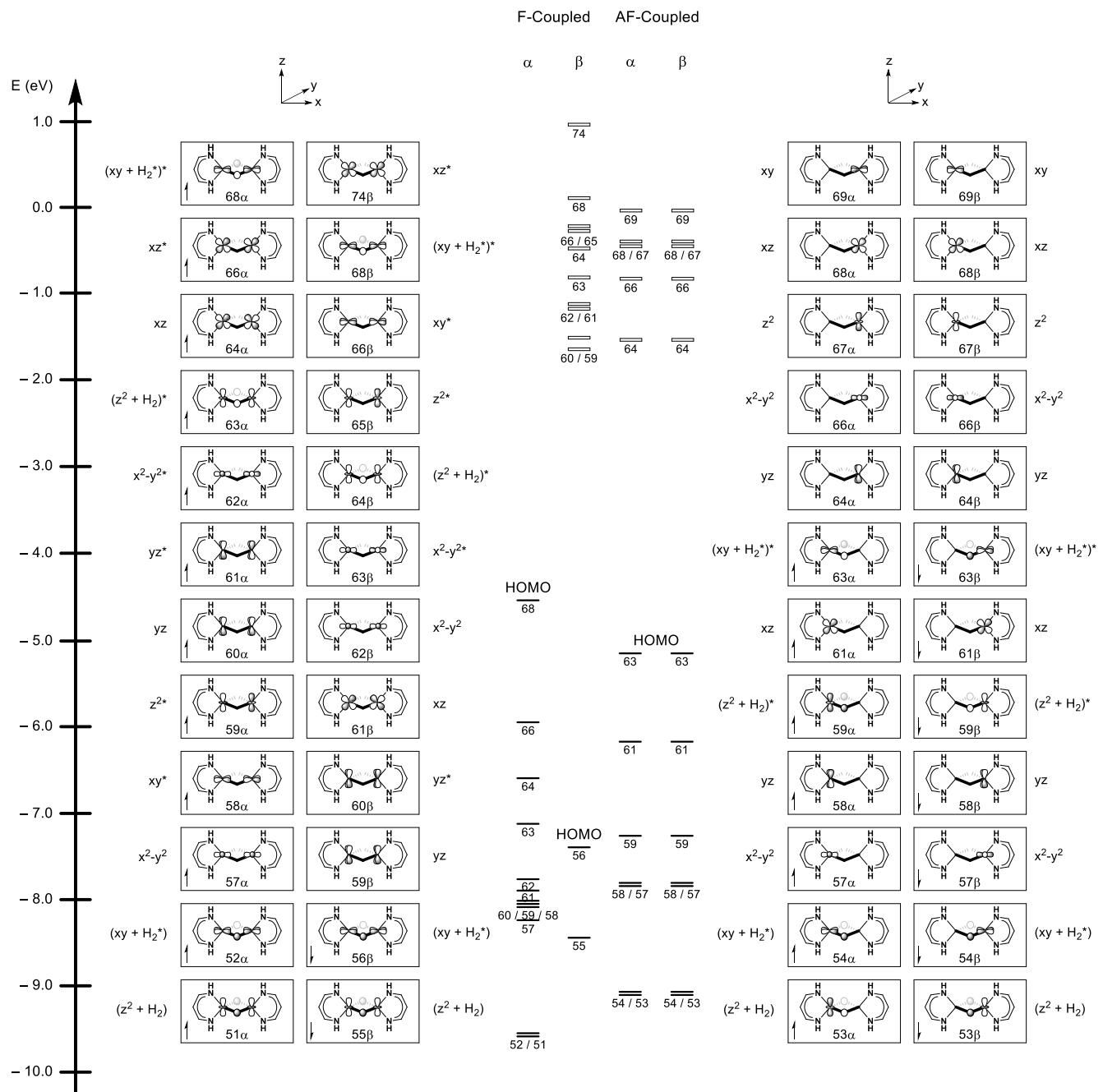


Fig. S1 The MO-diagrams of ferro (**2-F**)- and antiferromagnetically (**2-AF**) coupled manganese centers of the model compound.

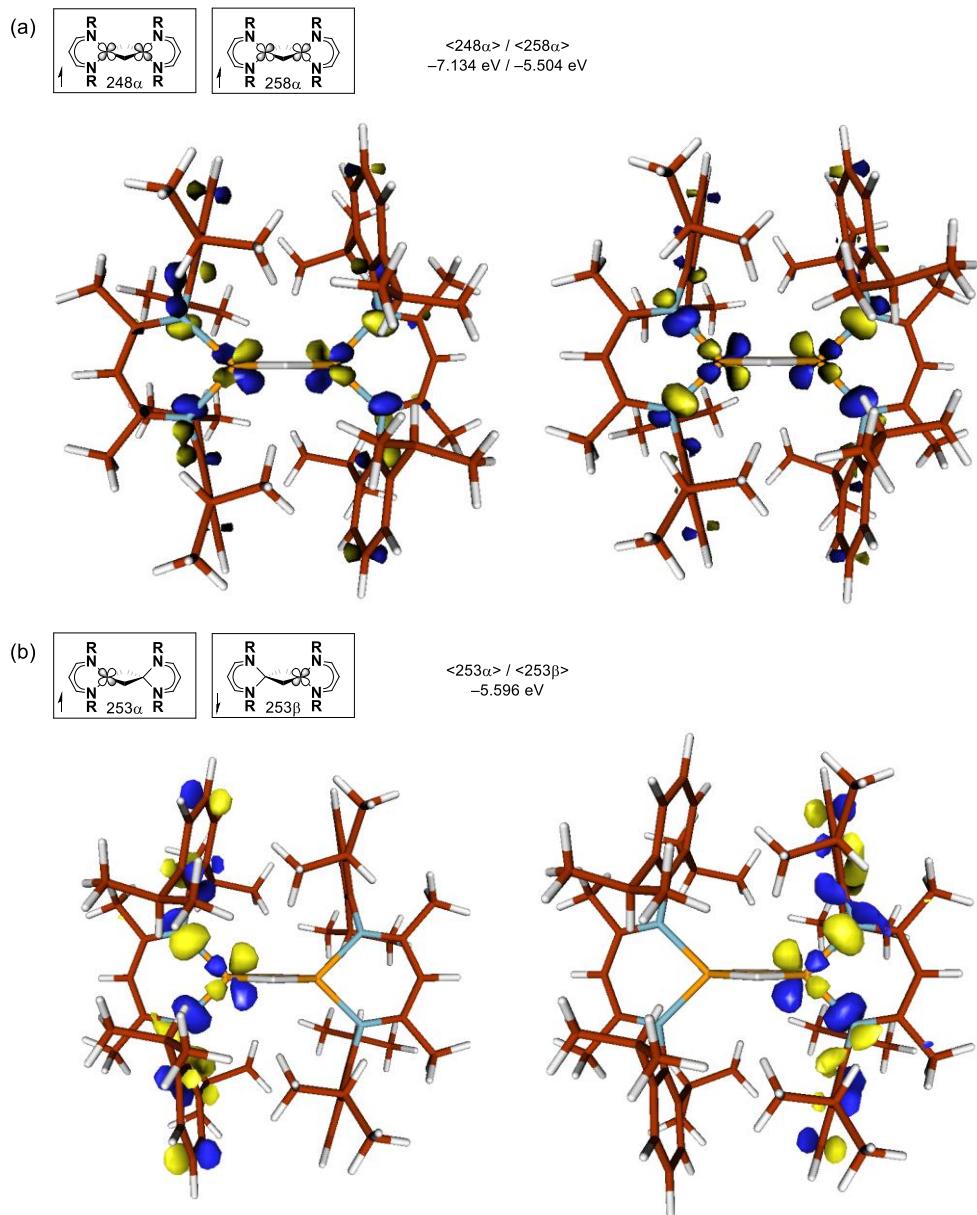


Fig. S2 Isosurface plots (isodensity = 0.05 au) of the metal d_{xz} -based MOs of **1**: (a) metal–metal in-phase, and out-of-phase α -spin, **1-F** (b) α -spin and β -spin, **1-AF**.

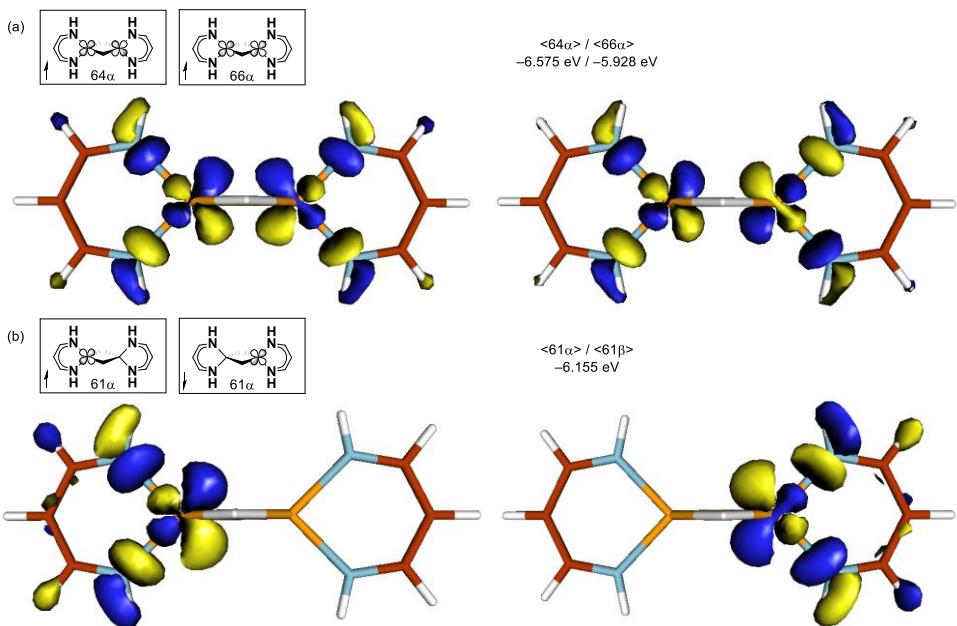


Fig. S3 Isosurface plots (isodensity = 0.05 au) of the metal d_{xz} -based MOs of **2**: metal–metal in-phase, and out-of-phase α -spin, **2-F** (b) α -spin and β -spin, **2-AF**.

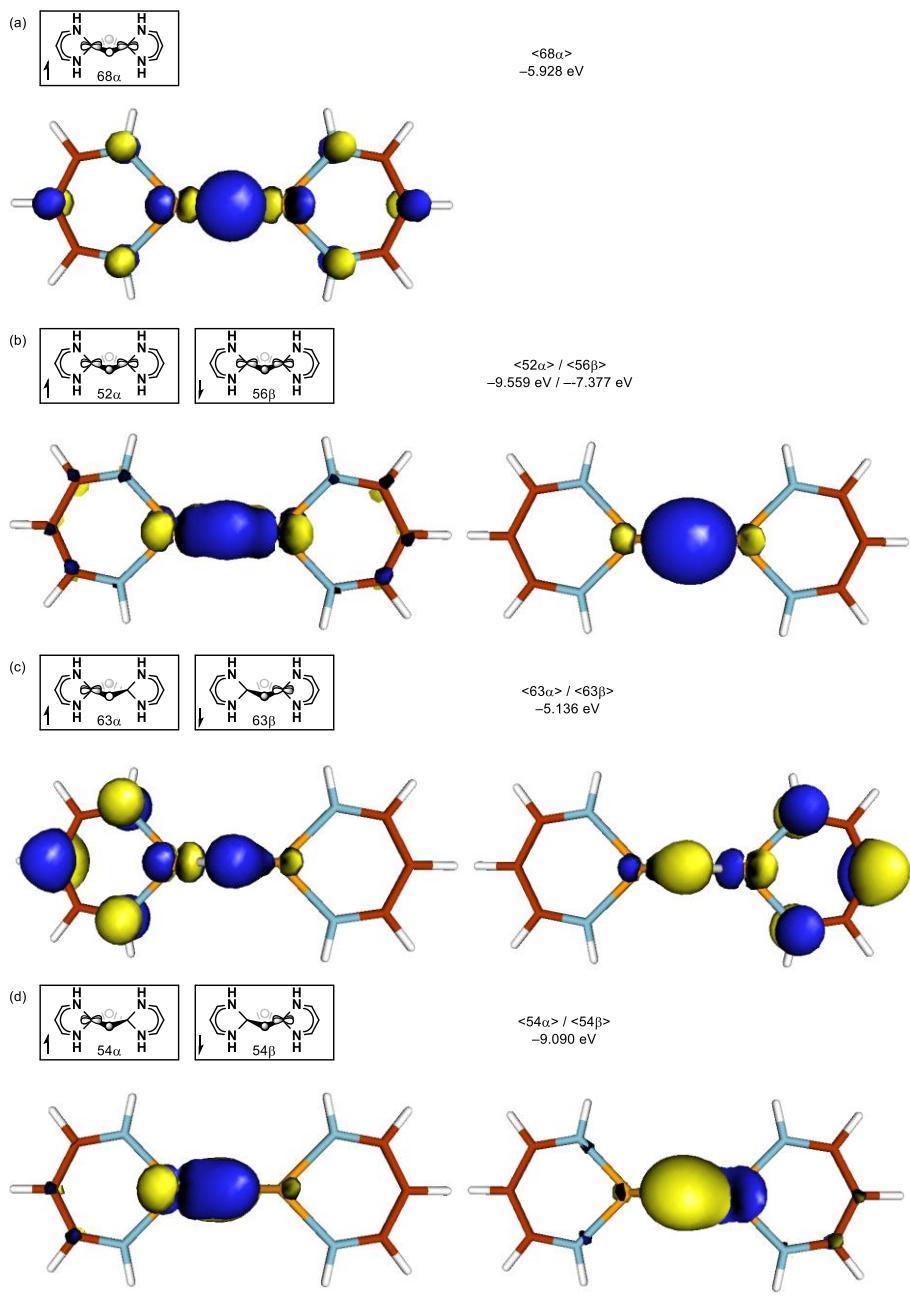


Fig. S4 Isosurface plots (isodensity = 0.05 au) of the metal d_{xy} -based MOs of **2**: (a) **2-F**, $<68\alpha>$, (b) **2-F**, $<52\alpha>$ and $<56\beta>$, (c) **2-AF**, $<63\alpha>$ and $<63\beta>$, and (d) **2-AF**, $<54\alpha>$ and $<54\beta>$.

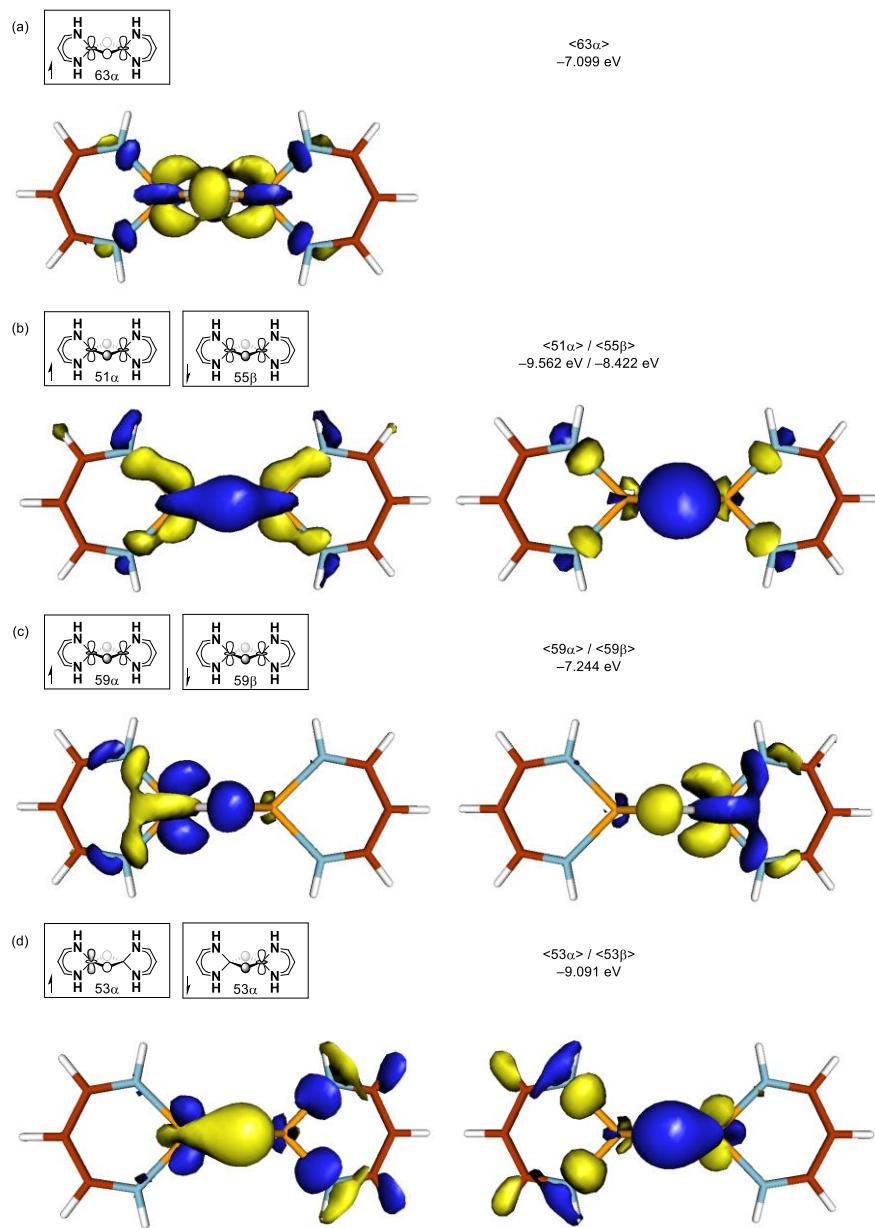


Fig. S5 Isosurface plots (isodensity = 0.05 au) of the metal d_{z^2} -based MOs of **2**: (a) **2-F**, $\langle 63\alpha \rangle$, (b) **2-F**, $\langle 51\alpha \rangle$ and $\langle 55\beta \rangle$, (c) **2-AF**, $\langle 59\alpha \rangle$ and $\langle 59\beta \rangle$, and (d) **2-AF**, $\langle 53\alpha \rangle$ and $\langle 53\beta \rangle$.

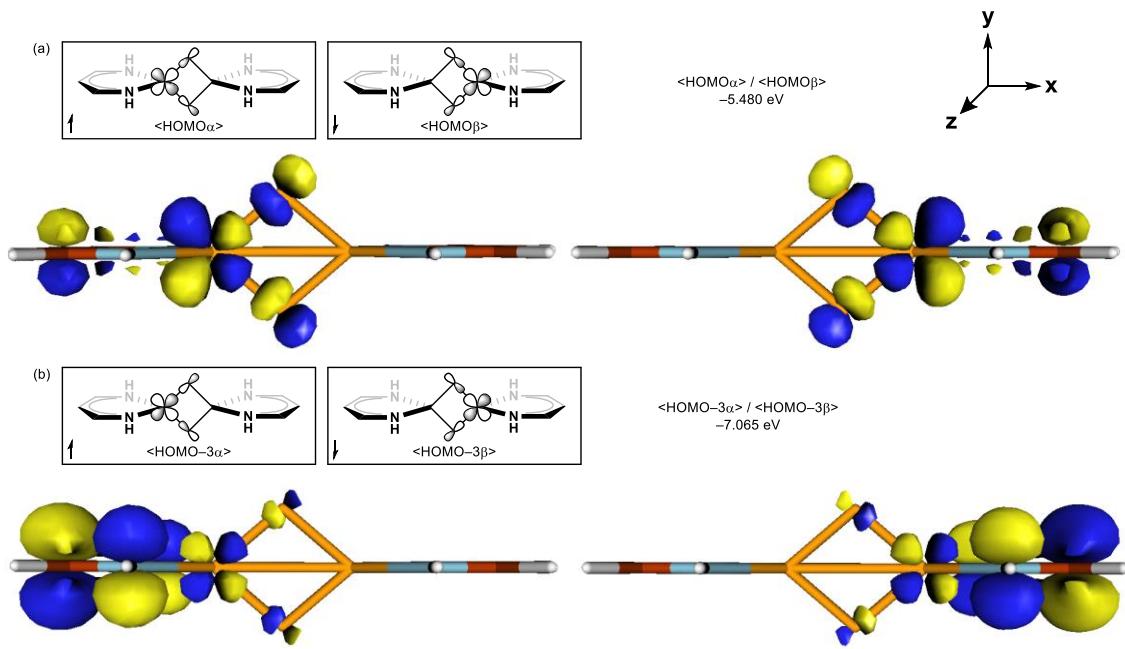


Fig. S6 Isosurface plots (isodensity = 0.05 au) of the metal d_{xy} -based MOs of **3**: (a) HOMO, (b) HOMO-3. To clearly visualize orbitals, the Cartesian coordinate system consistently adopted is rotated 90 degrees counter clockwise along the x-axis, as shown in the upper right corner.

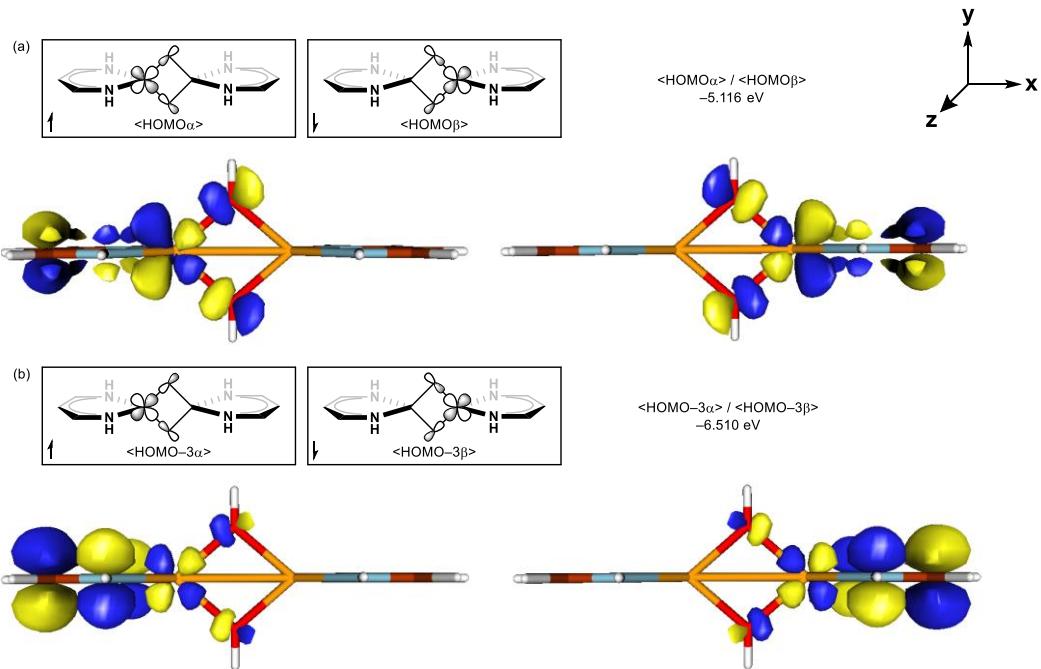


Fig. S7 Isosurface plots (isodensity = 0.05 au) of the metal d_{xy} -based MOs of **4**: (a) HOMO, (b) HOMO-3. To clearly visualize orbitals, the Cartesian coordinate system consistently adopted is rotated 90 degrees counter clockwise by the x-axis and shown at the upper right corner.

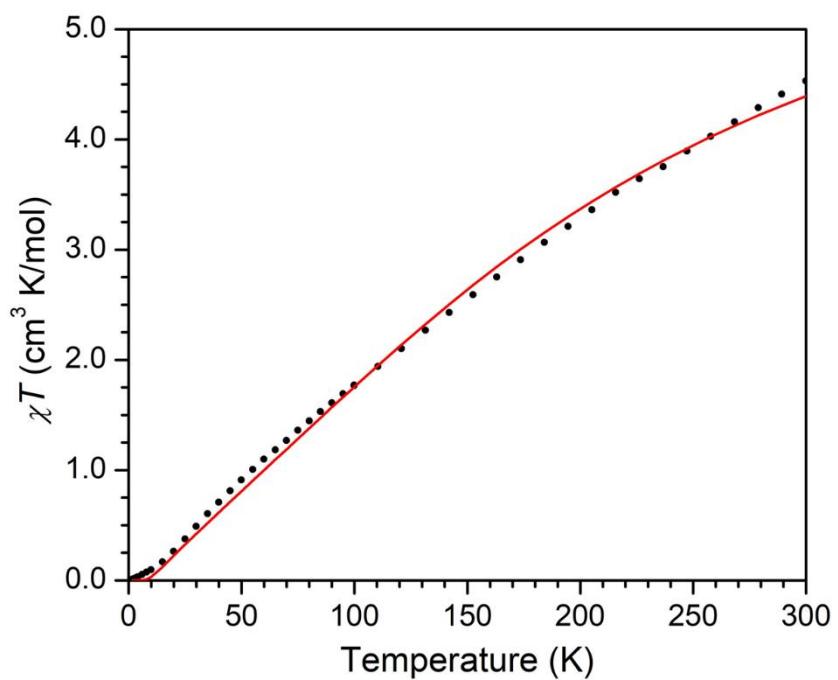


Fig. S8 Temperature-dependent χT vs. T data for **1** collected under an applied field of 0.1 T. The red line is the fit where g is 1.82 (± 0.25), as outlined in the main text.

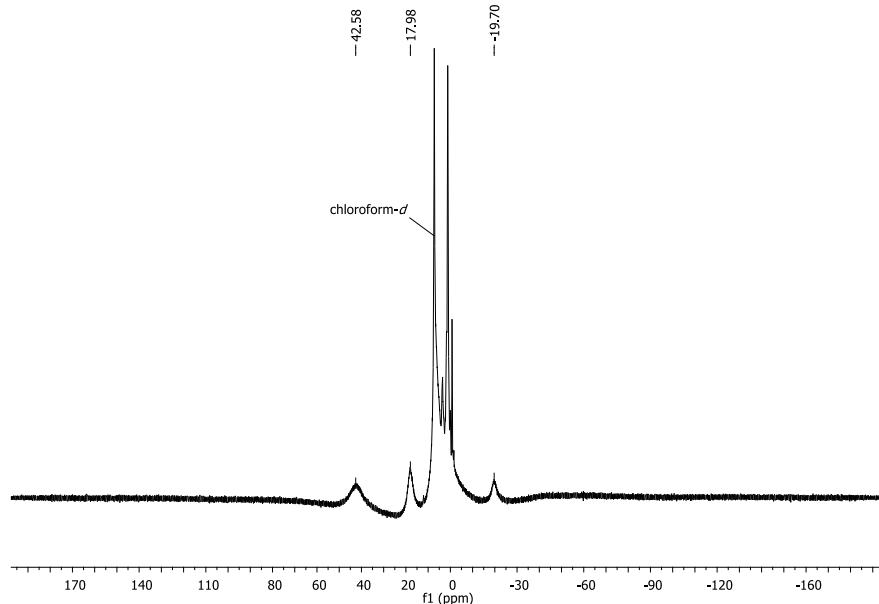


Fig. S9 ^1H NMR spectrum of **6** in chloroform-*d* at 25 °C.

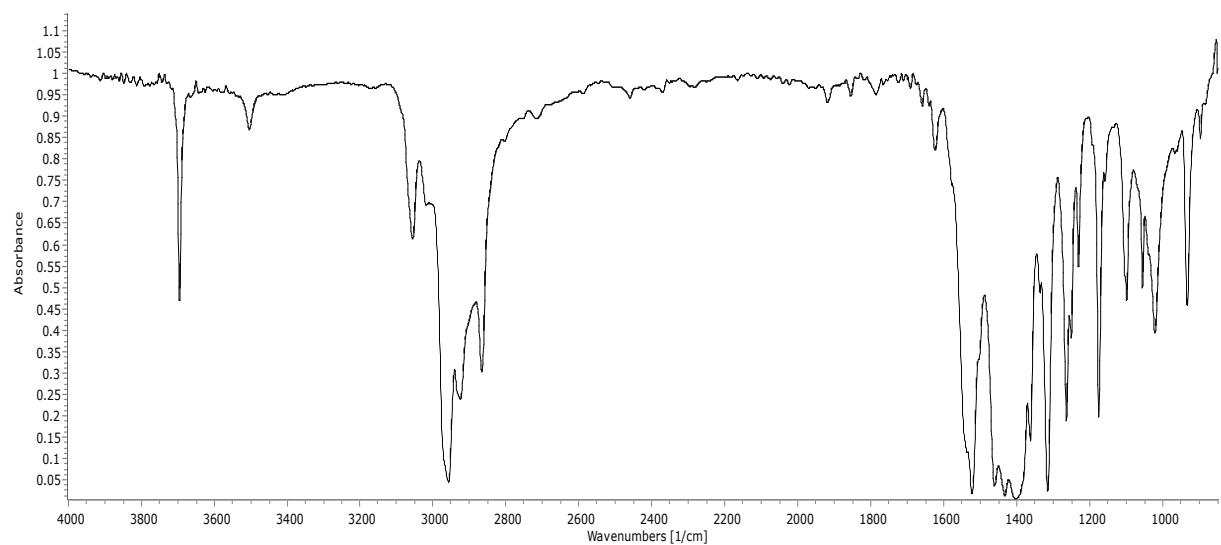


Fig. S10 Solid-state infrared spectrum of **6** in KBr.

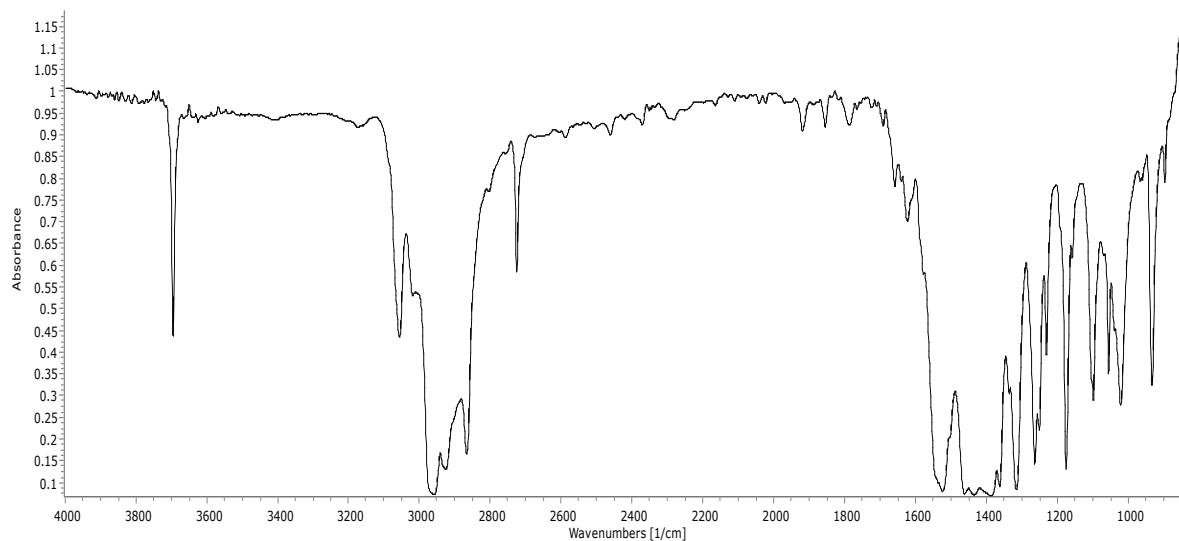
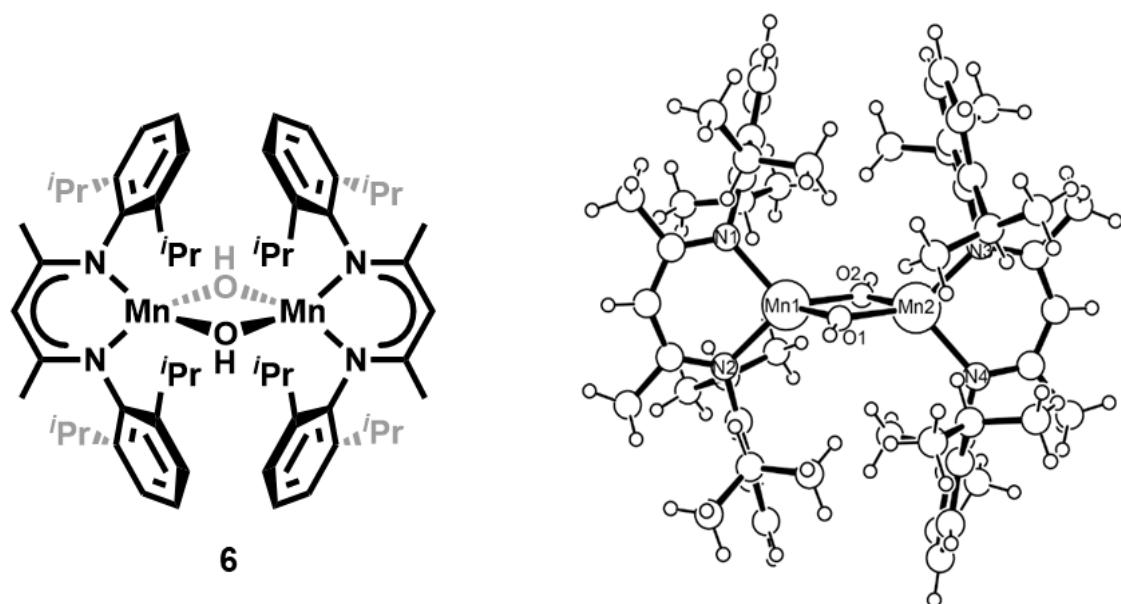


Fig. S11 Solid-state infrared spectrum of **6-d₂** in KBr.

Table S1 Structural comparison between **1** and **6**



	6 exp.	6 calc.	1-CS exp.	1-AF calc.	1-F calc.
Spin-Coupling	–	AF	–	AF	F
Mn1–O1/H1 (Å)	2.038(2)	2.056	1.79(2)	1.834	1.897
Mn1–O2/H2 (Å)	2.054(2)	2.071	1.79(2)	1.923	1.919
Mn1–N1 (Å)	2.108(2)	2.107	2.086(2)	2.103	2.099
Mn1–N2 (Å)	2.106(2)	2.119	2.098(2)	2.110	2.116
Mn1–Mn2 (Å)	3.1426(9)	3.189	2.8138(10)	2.871	2.871
$\angle \text{O1/H1–Mn1–N2}$ (°)	126.96(9)	125.0	121.1(8)	120.5	116.9
$\angle \text{N2–Mn1–N1}$ (°)	91.34(9)	89.2	91.48(8)	90.5	90.1
$\angle \text{N1–Mn1–O2/H2}$ (°)	120.53(9)	124.5	122.8(8)	119.8	121.9
$\angle \text{O2–Mn1–O1}$ (°)	79.64(10)	78.9	–	–	–
$\angle \text{Mn1–O1–Mn2}$ (°)	100.37(10)	101.2	–	–	–
$\tau_4 \text{ Mn1}$	0.80	0.78	0.85	0.85	0.86
Spin-Densities ^a Mn1	–	4.80	–	4.75	4.91
Spin-Densities ^a Mn2	–	–4.80	–	–4.75	4.91

^aMulliken spin-density.

CRYSTALLOGRAPHIC DATA

Table S2 Crystallographic data for **6**

	6
chemical formula	C ₅₈ H ₈₄ Mn ₂ N ₄ O ₂
formula weight	979.17
crystal dimensions	0.193 x 0.134 x 0.073
crystal system	monoclinic
space group	C 1 2/c 1
<i>a</i> (Å)	22.969(3)
<i>b</i> (Å)	14.6534(17)
<i>c</i> (Å)	16.1143(19)
α (deg)	90
β (deg)	91.558(2)
γ (deg)	90
<i>V</i> (Å ³)	5421.6(11)
<i>Z</i>	4
T (°C)	123.00(10)
ρ_{calcd} (g cm ⁻³)	1.200
μ (mm ⁻¹)	0.509
reflections collected	22387
data/restraints/parameters	4978/0/312
R ₁ [<i>I</i> > 2σ(<i>I</i>)]	0.0560
wR ₂ (all data)	0.01464
Goodness-of-fit	1.028
Largest peak, hole (eÅ ⁻³)	0.800, -0.294

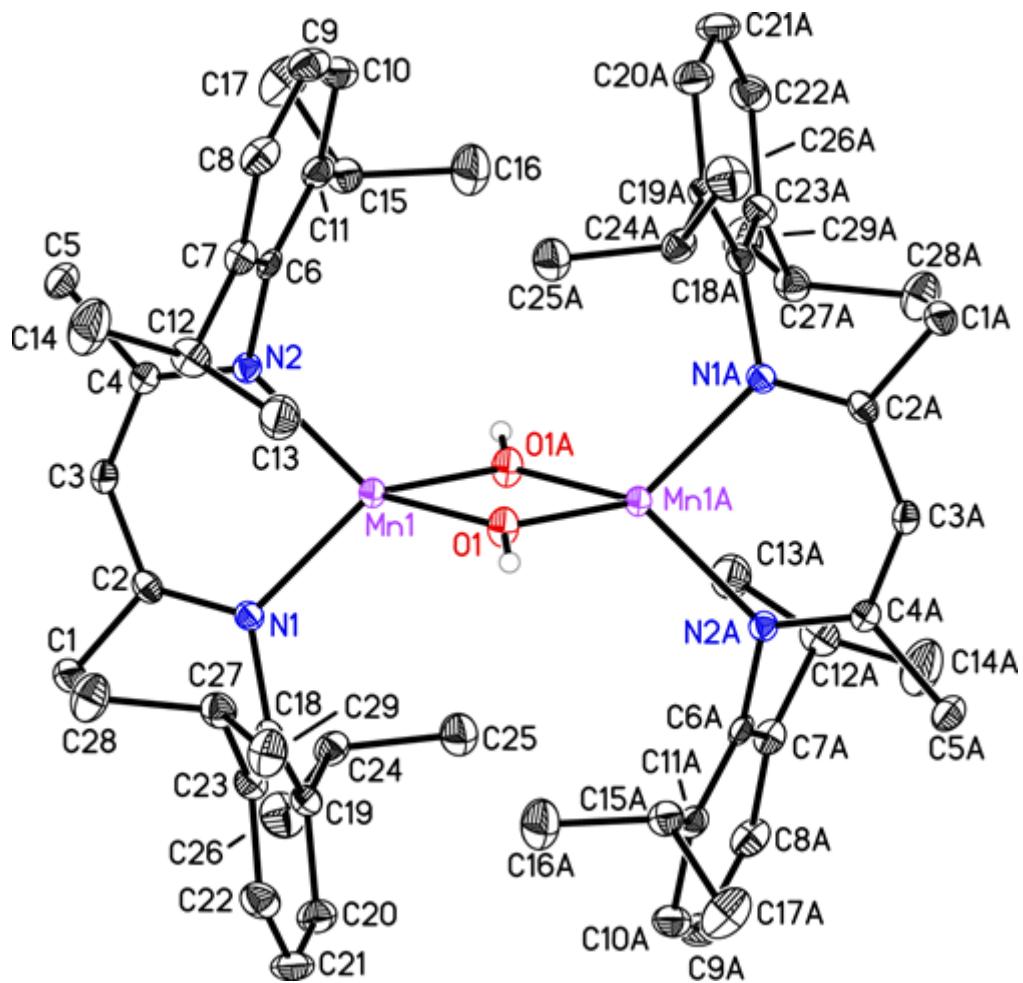


Fig. S12 The molecular structure of **6** shown at 30% probability ellipsoids. Hydrogen atoms other than the hydroxyl hydrogens are omitted for clarity.

Table S3 Bond distances (\AA) and angles ($^\circ$) for **6**

Mn1-O1	2.038(2)	C3-C4	1.404(4)	C15-C17	1.529(4)
Mn1-O1A	2.054(2)	C4-C5	1.514(4)	C18-C19	1.401(4)
Mn1-N2	2.106(2)	C6-C11	1.401(4)	C18-C23	1.403(4)
Mn1-N1	2.108(2)	C6-C7	1.411(4)	C19-C20	1.391(4)
Mn1-Mn1A	3.1426(9)	C7-C8	1.382(4)	C19-C24	1.511(4)
O1-Mn1A	2.054(2)	C7-C12	1.516(4)	C20-C21	1.382(5)
O1-H1	0.71(4)	C8-C9	1.382(5)	C21-C22	1.381(5)
N1-C2	1.338(4)	C9-C10	1.374(5)	C22-C23	1.396(4)
N1-C18	1.442(4)	C10-C11	1.404(4)	C23-C27	1.526(4)
N2-C4	1.333(4)	C11-C15	1.509(4)	C24-C25	1.523(4)
N2-C6	1.444(3)	C12-C13	1.497(5)	C24-C26	1.527(4)
C1-C2	1.509(4)	C12-C14	1.526(5)	C27-C29	1.520(4)
C2-C3	1.398(4)	C15-C16	1.510(5)	C27-C28	1.528(4)

O1-Mn1-O1A	79.64(10)	C2-C3-C4	130.5(3)	C16-C15-C17	109.8(3)
O1-Mn1-N2	126.96(9)	N2-C4-C3	124.5(3)	C19-C18-C23	121.8(3)
O1A-Mn1-N2	120.82(9)	N2-C4-C5	120.2(2)	C19-C18-N1	120.5(3)
O1-Mn1-N1	121.34(9)	C3-C4-C5	115.2(2)	C23-C18-N1	117.7(3)
N2-Mn1-N1	91.34(9)	C11-C6-C7	121.0(3)	C20-C19-C18	117.6(3)
O1-Mn1-Mn1A	40.01(6)	C11-C6-N2	120.0(3)	C20-C19-C24	120.4(3)
O1A-Mn1-Mn1A	39.63(6)	C7-C6-N2	119.0(2)	C18-C19-C24	122.0(3)
N2-Mn1-Mn1A	136.44(7)	C8-C7-C6	118.3(3)	C21-C20-C19	121.6(3)
N1-Mn1-Mn1A	132.01(7)	C8-C7-C12	120.7(3)	C22-C21-C20	120.1(3)
Mn1-O1-Mn1A	100.37(10)	C6-C7-C12	121.0(3)	C21-C22-C23	120.6(3)
Mn1-O1-H1	134.(3)	C9-C8-C7	121.7(3)	C22-C23-C18	118.2(3)
Mn1A-O1-H1	120.(3)	C10-C9-C8	119.7(3)	C22-C23-C27	120.4(3)
C2-N1-C18	116.5(2)	C9-C10-C11	121.3(3)	C18-C23-C27	121.4(3)
C2-N1-Mn1	121.27(18)	C6-C11-C10	118.1(3)	C19-C24-C25	111.1(3)
C18-N1-Mn1	122.24(17)	C6-C11-C15	122.0(3)	C19-C24-C26	113.4(3)
C4-N2-C6	116.5(2)	C10-C11-C15	119.8(3)	C25-C24-C26	109.3(3)
C4-N2-Mn1	121.75(19)	C13-C12-C7	110.7(3)	C29-C27-C23	113.3(3)
C6-N2-Mn1	121.69(17)	C13-C12-C14	111.2(3)	C29-C27-C28	110.2(3)
N1-C2-C3	124.5(3)	C7-C12-C14	113.3(3)	C23-C27-C28	111.4(3)
N1-C2-C1	120.1(3)	C11-C15-C16	112.1(3)		
C3-C2-C1	115.4(3)	C11-C15-C17	111.6(3)		

Table S4 Electronic energies of the compounds

	E(SCF)/(eV)	ZPE/(kcal/mol)	S(gas)/(cal·mol ⁻¹ ·K ⁻¹)	G(solv)/(kcal/mol)
	cc-pVTZ(-f)/LACV3P**	6-31G**/LACVP**	6-31G**/LACVP**	6-31G**/LACVP**
1-F	-73166.711	811.50	377.68	-6.03
1-AF	-73166.750	811.47	372.94	-5.77
2-F	-18041.625	111.694	134.112	-15.55
2-AF	-18041.809	111.936	129.239	-14.53
3-AF	-23449.240	106.94	140.88	-9.86
3-MONO	-11723.712	53.26	92.46	-10.84
4-AF	-22140.984	120.70	145.93	-11.50
4-MONO	-11069.408	59.83	94.95	-11.36
5-AF	-78574.570	807.78	378.45	-3.99
5-MONO	-39286.137	402.09	226.10	-4.39
6-F	-77266.281	823.51	374.17	-4.33
6-AF	-77266.297	821.00	387.27	-4.33
6-MONO	-38631.848	408.64	230.41	-4.95

Table S5 Cartesian coordinates for the optimized geometries

	C	1.853051424	-0.426140249	7.215332985
	H	2.748556376	-0.068588853	6.695405483
	H	1.010511756	0.207723603	6.917748928
	H	1.641325593	-1.438813448	6.854476452
=====				
1-F				
=====				
Mn	2.671803474	0.852670729	12.490572929	
N	3.818702459	0.752598703	10.735632896	
N	3.467709541	2.769609213	12.901445389	
C	4.910710812	1.681708217	8.726149559	
H	5.720894337	0.947361887	8.743853569	
H	5.304716110	2.631563902	8.361642838	
H	4.172456264	1.310466051	8.008293152	
C	4.285784721	1.835643530	10.103071213	
C	4.285179138	3.132756710	10.639356613	
H	4.679800034	3.900930882	9.987278938	
C	4.027441502	3.541218281	11.961607933	
C	4.475242138	4.956397533	12.304807663	
H	3.628104925	5.582898140	12.600613594	
H	4.972789764	5.423869610	11.453719139	
H	5.166706085	4.947731495	13.151801109	
C	4.140941143	-0.523024678	10.166646957	
C	5.330584049	-1.164894581	10.578188896	
C	5.654015064	-2.397552013	10.000674248	
H	6.573797226	-2.897888660	10.293680191	
C	4.810429096	-2.998595715	9.068494797	
H	5.068974972	-3.964457273	8.642462730	
C	3.629978657	-2.362248659	8.689413071	
H	2.973408699	-2.839536667	7.967588902	
C	3.286135912	-1.109664559	9.208888054	
C	2.027221203	-0.390689790	8.743893623	
H	2.110193729	0.658124089	9.043516159	
	C	0.793345571	-0.970080972	9.447222710
	H	0.688210070	-2.035237312	9.229771614
	H	-0.115008712	-0.457725883	9.110843658
	H	0.859580755	-0.853029728	10.533177376
	C	6.277973175	-0.514968455	11.582695007
	H	5.825974941	0.428055555	11.900961876
	C	7.640460968	-0.184587017	10.941470146
	H	8.157869339	-1.093238115	10.612242699
	H	8.290218353	0.326662451	11.661228180
	H	7.525976658	0.468788147	10.069944382
	C	6.452149391	-1.380911231	12.844446182
	H	5.503914356	-1.479093790	13.383210182
	H	7.182960987	-0.926739872	13.522748947
	H	6.809565544	-2.387342691	12.599396706
	C	3.523333788	3.278803110	14.242914200
	C	4.601836205	2.892033577	15.071432114
	C	4.751220703	3.539504051	16.303815842
	H	5.589219093	3.284565687	16.945384979
	C	3.835867643	4.499703884	16.727920532
	H	3.969275236	4.991714001	17.688098907
	C	2.732208729	4.808269978	15.933427811
	H	2.010015011	5.536923885	16.287418365
	C	2.559464931	4.215018749	14.678866386
	C	1.362334847	4.544312477	13.795164108
	H	1.688283920	4.487686634	12.751071930
	C	0.267997593	3.483949900	13.989418030
	H	0.630473971	2.479186058	13.751456261

H	-0.591633022	3.686851025	13.341468811	H	-1.476902127	-5.061697483	13.381791115
H	-0.077847376	3.477636576	15.024568558	C	-0.736009181	0.600672007	16.162553787
C	0.796555817	5.955436707	14.019454002	C	-1.883837461	1.242033243	15.646853447
H	0.036744885	6.177681923	13.262604713	C	-2.263738632	2.471304178	16.196428299
H	1.578108072	6.720655918	13.952299118	H	-3.152323961	2.971508026	15.819621086
H	0.313947380	6.050115585	14.999222755	C	-1.515659451	3.065657377	17.210014343
C	5.595108986	1.820183158	14.624698639	H	-1.818929911	4.025234699	17.620775223
H	5.084404469	1.190010309	13.886574745	C	-0.365286022	2.436151743	17.684257507
C	6.813735008	2.446966410	13.916029930	H	0.221536726	2.914273262	18.463090897
H	7.338432312	3.143229961	14.583712578	C	0.036967251	1.192207456	17.185176849
H	6.512851238	2.995301962	13.016328812	C	1.280205846	0.496707708	17.724319458
H	7.523511410	1.669037580	13.610248566	H	1.212778091	-0.564095318	17.466312408
C	6.045417309	0.899006605	15.773317337	C	1.411077380	0.593820274	19.253839493
H	6.707091331	0.117602140	15.388413429	H	0.500905991	0.258173347	19.762702942
H	5.188005924	0.411756456	16.248107910	H	2.242953539	-0.029780760	19.599021912
H	6.604663372	1.441962004	16.546426773	H	1.618118048	1.618657827	19.581098557
H	2.683315277	-0.404635459	13.911099434	C	2.530660391	1.054210305	17.030046463
Mn	0.805982828	-0.810366452	13.903335571	H	2.605964899	2.134234190	17.177345276
N	-0.378743798	-0.683536828	15.634849548	H	3.437582493	0.591615558	17.436269760
N	0.057366755	-2.757213116	13.541716576	H	2.508802176	0.862937927	15.952391624
C	-1.566665173	-1.570334554	17.611032486	C	-2.720525980	0.600898802	14.544276237
H	-2.419714451	-0.895732582	17.488563538	H	-2.271984339	-0.368488997	14.312418938
H	-1.927594304	-2.524074793	17.998777390	C	-4.166992188	0.342251450	15.004279137
H	-0.913980842	-1.112457037	18.359687805	H	-4.684883595	1.276411295	15.249761581
C	-0.841849327	-1.754872084	16.287576675	H	-4.739534855	-0.155971676	14.213606834
C	-0.763022125	-3.073596239	15.809884071	H	-4.192633152	-0.296929091	15.893575668
H	-1.141019702	-3.830943108	16.484001160	C	-2.674927235	1.437691450	13.251806259
C	-0.453390241	-3.523976088	14.514476776	H	-1.651842594	1.498376369	12.865639687
C	-0.795325458	-4.981770039	14.232871056	H	-3.303877115	0.986403108	12.476373672
H	0.098182477	-5.557085991	13.972415924	H	-3.036721945	2.458283901	13.421918869
H	-1.266093493	-5.446041107	15.100775719	C	0.051804427	-3.334108591	12.226818085

C	-1.054256558	-3.078983068	11.380638123				
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C	-1.121762395	-3.762099743	10.161383629	Mn	2.723259926	0.824722528	12.543914795
H	-1.968234301	-3.600421190	9.501749039	N	3.887879372	0.666488707	10.799892426
C	-0.108445838	-4.633192539	9.766963959	N	3.460014582	2.772720098	12.880367279
H	-0.177289844	-5.150106907	8.813285828	C	5.064144135	1.534524441	8.808556557
C	1.001994967	-4.826228142	10.585482597	H	5.911763668	0.850557327	8.911772728
H	1.794547796	-5.491831303	10.258756638	H	5.429588795	2.483291388	8.412200928
C	1.097348452	-4.196300983	11.830956459	H	4.389215946	1.084841847	8.074536324
C	2.299563169	-4.419299126	12.741021156	C	4.365243435	1.730086923	10.144470215
H	1.966029882	-4.293903828	13.775897026	C	4.293539047	3.053894281	10.611359596
C	3.368593216	-3.350142717	12.472782135	H	4.670341015	3.803340435	9.927321434
H	2.980901241	-2.340833902	12.638648033	C	3.985392094	3.521960497	11.901403427
H	4.229299068	-3.486568451	13.136781693	C	4.345005989	4.978389263	12.168677330
H	3.718240261	-3.409909248	11.440908432	H	3.459956884	5.568307400	12.425725937
C	2.899464130	-5.829868793	12.626521111	H	4.819912910	5.428940773	11.295402527
H	3.659247398	-5.977481842	13.401626587	H	5.030352592	5.057542801	13.016942024
H	2.134154081	-6.604590416	12.746504784	C	4.234164238	-0.623694599	10.276488304
H	3.389828682	-5.987958908	11.659235954	C	5.392911911	-1.267320633	10.766880035
C	-2.148167372	-2.093954802	11.792525291	C	5.752461433	-2.502396107	10.216547966
H	-1.668890238	-1.323177934	12.407609940	H	6.651829720	-3.001324415	10.569527626
C	-3.230115414	-2.765833378	12.663347244	C	4.970459461	-3.105708122	9.234244347
H	-3.686181545	-3.607966185	12.128779411	H	5.256266117	-4.071871758	8.826091766
H	-2.821552753	-3.136826515	13.606157303	C	3.812052727	-2.472949505	8.784880638
H	-4.024293423	-2.050643206	12.906935692	H	3.198408365	-2.956530094	8.030085564
C	-2.812569618	-1.388134241	10.599057198	C	3.433377981	-1.219584703	9.279064178
H	-3.490684509	-0.607726276	10.958464622	C	2.197012186	-0.508449376	8.744483948
H	-2.073226929	-0.919453859	9.945858955	H	2.264858484	0.545280099	9.030405998
H	-3.412110090	-2.080074787	9.995950699	C	2.087917089	-0.569703221	7.210132599
H	0.794907331	0.451902509	12.499654770	H	2.994596958	-0.197626114	6.719680786
	=====			H	1.245449901	0.043066509	6.869757652
1-AF				H	1.910429239	-1.590525389	6.854077816

C	0.933463693	-1.077190280	9.404288292	H	1.371374607	6.666098118	13.779226303
H	0.843040466	-2.149357796	9.214534760	H	0.100025460	5.975197315	14.803177834
H	0.038474958	-0.585174143	9.006937981	C	5.651125431	2.078735828	14.631503105
H	0.947939694	-0.926411450	10.487932205	H	5.161210537	1.330195785	13.997261047
C	6.275850773	-0.619523764	11.828928947	C	6.766755104	2.727599382	13.786391258
H	5.791349411	0.312518388	12.132932663	H	7.230671883	3.558458805	14.332783699
C	7.665275574	-0.259779751	11.268526077	H	6.384165287	3.111719608	12.836611748
H	8.211827278	-1.157352209	10.954485893	H	7.548455715	1.994514704	13.555451393
H	8.269366264	0.244941548	12.031515121	C	6.270657063	1.338413358	15.829651833
H	7.590364456	0.407842070	10.403627396	H	6.931971073	0.541727662	15.474370003
C	6.386680126	-1.498150110	13.088532448	H	5.504181385	0.885029554	16.463342667
H	5.399063587	-1.669793129	13.529095650	H	6.879261017	2.004920721	16.453489304
H	7.018249989	-1.013940454	13.841498375	H	2.666523218	-0.398741841	13.908930779
H	6.831005573	-2.474926472	12.863499641	Mn	0.792243481	-0.839476883	13.865617752
C	3.477206707	3.360208035	14.191028595	N	-0.352500141	-0.713256121	15.618695259
C	4.580194950	3.091203690	15.036626816	N	0.018167496	-2.764876604	13.475522995
C	4.660137177	3.775711298	16.254352570	C	-1.417024851	-1.634999633	17.647844315
H	5.506322384	3.603894234	16.912418365	H	-2.237399101	-0.911937118	17.634937286
C	3.655318022	4.654827118	16.652698517	H	-1.796644568	-2.586536884	18.024570465
H	3.729692459	5.168573856	17.608024597	H	-0.674796999	-1.250488162	18.353822708
C	2.547202110	4.863219738	15.834165573	C	-0.808314323	-1.794061065	16.263944626
H	1.763609886	5.538743973	16.162830353	C	-0.789680183	-3.099305391	15.746174812
C	2.444401264	4.238729000	14.586422920	H	-1.166612267	-3.863494873	16.413692474
C	1.244848251	4.478616714	13.675973892	C	-0.531620622	-3.526739597	14.429781914
H	1.592563748	4.406781197	12.640219688	C	-0.965319335	-4.952763557	14.112009048
C	0.187305465	3.383984327	13.881717682	H	-0.112021357	-5.577094078	13.829085350
H	0.590559185	2.384060383	13.698792458	H	-1.459100366	-5.409837246	14.971342087
H	-0.657394409	3.530301571	13.198658943	H	-1.656705499	-4.967281342	13.264945984
H	-0.192136094	3.408232450	14.905031204	C	-0.666819453	0.565637052	16.186496735
C	0.617593944	5.872742653	13.842415810	C	-1.850969315	1.216812849	15.770269394
H	-0.123525098	6.045802593	13.054263115	C	-2.174355984	2.446363926	16.354120255

H -3.092500448	2.950199366	16.061647415	H -0.465950519	-5.003281116	8.691364288
C -1.331068397	3.041102409	17.290906906	C 0.774359524	-4.803474426	10.441666603
H -1.587972641	4.005691528	17.721416473	H 1.509082556	-5.515166283	10.079120636
C -0.152305633	2.399810076	17.667505264	C 0.941680670	-4.216554165	11.700363159
H 0.506763875	2.873837709	18.389680862	C 2.141942024	-4.546646118	12.581286430
C 0.189200625	1.147271752	17.145105362	H 1.797381401	-4.556851864	13.620863914
C 1.442826271	0.422856539	17.616077423	C 3.214173794	-3.453293085	12.461477280
H 1.372075558	-0.618019998	17.286918640	H 2.829015732	-2.465684891	12.727757454
C 1.588037848	0.422477573	19.148714066	H 4.061096191	-3.667037964	13.123560905
H 0.696820319	0.022324594	19.644823074	H 3.586320162	-3.399039030	11.437404633
H 2.444503784	-0.193679824	19.445463181	C 2.754142761	-5.928000927	12.299305916
H 1.761980414	1.430787921	19.540189743	H 3.500983000	-6.167337894	13.064215660
C 2.687404394	1.023831844	16.951824188	H 1.994938731	-6.718652725	12.308190346
H 2.800291777	2.078541040	17.213314056	H 3.262361050	-5.957069397	11.328470230
H 3.587826967	0.491607636	17.278890610	C -2.138832092	-1.881517529	11.782865524
H 2.632238388	0.948400140	15.862202644	H -1.635170579	-1.249294758	12.524551392
C -2.796150208	0.574331522	14.758543015	C -3.345923185	-2.530765057	12.493032455
H -2.301861525	-0.323811442	14.376114845	H -3.848127604	-3.247920990	11.829577446
C -4.117366791	0.133612975	15.420475006	H -3.036736727	-3.062603951	13.399840355
H -4.667429924	0.997019410	15.816075325	H -4.076170444	-1.767771602	12.788366318
H -4.764116764	-0.367468774	14.690443039	C -2.612570286	-0.960233629	10.643782616
H -3.943960905	-0.563121796	16.247520447	H -3.279227495	-0.188231006	11.043437958
C -3.058948040	1.491202235	13.549945831	H -1.766740680	-0.459230095	10.159399986
H -2.125327110	1.722031355	13.025933266	H -3.174954891	-1.507267714	9.873669624
H -3.738167048	1.003698826	12.841667175	H 0.854536891	0.375603378	12.488962173
H -3.521736622	2.439509392	13.849021912	=====		
C -0.035238743	-3.295195580	12.141819954	2-F		
C -1.130793333	-2.934744596	11.323457718	=====		
C -1.277495742	-3.582622051	10.091491699	Mn -0.321517855	0.011642214	0.006508314
H -2.128217697	-3.346311092	9.458933830	N -1.776808619	1.482091904	0.019861802
C -0.339580476	-4.514632225	9.654276848			

N	-1.759084225	-1.476462483	0.007912308	H	5.989875793	0.008472881	-0.002815822
C	-3.081608295	1.243887782	0.033342633	C	4.277950287	0.004376190	1.252161145
C	-3.709584951	-0.009433459	0.034285914	Mn	-1.537081838	-0.002371454	0.004037745
H	-4.793556213	-0.015896661	0.045610305	N	-2.976122141	-0.000347435	1.500521302
C	-3.066557407	-1.255232453	0.021262357	N	-2.970732212	0.001017200	-1.498311281
H	1.072514415	0.015487185	-1.264904499	C	-4.279667854	0.003420433	1.253032446
Mn	2.480552435	-0.000146741	-0.009902298	C	-4.905416489	0.005662850	-0.002446291
N	3.923375607	-1.482787967	-0.016694520	H	-5.989673138	0.008590785	-0.004443366
N	3.928359509	1.476670742	-0.010384298	C	-4.275086880	0.004362116	-1.255763531
C	5.229835987	-1.254671335	-0.015669178	H	2.774727345	-0.000902191	-2.496736526
C	5.867259026	-0.005931515	-0.013270819	H	2.776460648	0.000534205	2.493336678
H	6.951242924	-0.007798287	-0.013577412	H	4.952751637	0.004815585	-2.118042469
C	5.234044552	1.244906425	-0.011087477	H	4.954297066	0.006510354	2.113108397
H	1.087765574	0.003412989	1.261625767	H	-4.949654579	0.006347666	-2.118106842
H	-1.574066758	2.477013826	0.022404615	H	-4.957302570	0.004796400	2.112959623
H	-1.542908669	-2.468556881	-0.000701239	H	-2.770867586	0.000758979	-2.493713379
H	-3.753349781	2.108015060	0.044237174	H	-2.780195236	-0.001358095	2.496700525
H	-3.727649689	-2.127635002	0.022633223	F	0.000245807	1.306462526	-0.000070002
H	5.901741505	2.112210512	-0.009822653	F	-0.000061872	-1.311558604	0.001761840
H	5.894956589	-2.123934031	-0.017124245	=====			
H	3.719981194	2.470474958	-0.008545796	3-MONO			
H	3.712369442	-2.475991011	-0.017730325	=====			

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3-AF

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Mn	1.536853433	-0.002816108	-0.001331776
N	2.972986221	0.000087639	-1.501008272
N	2.974089861	0.000694503	1.497483253
C	4.277062416	0.003426941	-1.256575942
C	4.905618191	0.005635753	-0.002449264

Mn	1.507197499	-0.003370051	-0.085591353
N	2.996810436	0.000157701	-1.529242516
N	2.918253422	0.001207822	1.430596828
C	4.297786236	0.003774119	-1.263846159
C	4.898715019	0.005701877	0.002641021
H	5.982365608	0.008601150	0.030895056
C	4.231933117	0.004367821	1.235117912
H	2.815907240	-0.000589643	-2.528762579

H	2.684020042	0.000723898	2.418947220	O	-0.000213242	1.335972667	0.003626881
H	4.987904549	0.005391237	-2.113263607	H	-0.003302211	2.296551228	-0.001357182
H	4.875191212	0.006218741	2.120393991	H	-0.001865991	-2.286303997	-0.001777300
F	-0.288707703	-0.008372472	-0.152356222				

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4-MONO

4-AF

Mn	1.550173759	0.005637465	-0.003861207	Mn	1.546733618	0.115695909	0.058089212
N	3.028614521	0.001033878	-1.496230245	N	2.914332628	0.010028411	-1.493124723
N	3.028241396	-0.000922114	1.490118265	N	3.064009428	-0.044520084	1.470407128
C	4.332232952	-0.006864399	-1.255720258	C	4.226371765	-0.119435579	-1.324185133
C	4.962634087	-0.011964817	-0.002629475	C	4.917951584	-0.201275960	-0.109383322
H	6.047181129	-0.018586395	-0.002487958	H	5.995775223	-0.303461105	-0.165871158
C	4.331793308	-0.008805839	1.250522971	C	4.350570202	-0.164141998	1.173425078
Mn	-1.550244927	0.004598741	0.005929548	H	2.667340040	0.043301772	-2.477492332
N	-3.031670332	0.001425642	1.495236874	H	2.904947996	-0.043748718	2.473585367
N	-3.025042534	-0.001666134	-1.491274357	H	4.848714352	-0.168287382	-2.223345041
C	-4.334794521	-0.006542944	1.252018332	H	5.059186459	-0.243141830	2.004181623
C	-4.962541103	-0.011686628	-0.002410997	O	-0.260846406	0.307220459	0.374086410
H	-6.047086239	-0.017930008	-0.004732670	H	-0.978728175	0.373132557	-0.262217581
C	-4.329101563	-0.008932894	-1.254224658				
H	2.830842972	0.003998750	-2.492306709	=====			
H	2.829401255	-0.000638854	2.486014843	5-AF			
H	5.008523941	-0.009872790	-2.117779255				
H	5.007816792	-0.013523866	2.112822533	Mn	2.719877005	1.042344928	12.477032661
H	-5.003360748	-0.013358828	-2.117872953	N	3.809989214	0.909979761	10.707489014
H	-5.012847424	-0.009492698	2.112704515	N	3.509817600	2.942745447	12.816307068
H	-2.824199200	-0.000880627	-2.486753702	C	5.105800152	1.690071583	8.764772415
H	-2.835917950	0.003556580	2.491733551	H	5.946949959	1.005831838	8.918498039
O	0.000469001	-1.325718284	0.001859942	H	5.487339497	2.620483637	8.340620995
			H	4.446351051	1.212521672	8.033736229	

C	4.386816502	1.935944915	10.079250336	H	8.200135231	-0.105280988	11.947765350
C	4.419280529	3.248795986	10.583409309	H	7.662677765	-0.119588174	10.258891106
H	4.876586437	3.986155987	9.936060905	C	5.932906628	-1.242541671	13.087256432
C	4.081319809	3.700364351	11.872106552	H	4.920454502	-1.121106744	13.481073380
C	4.449725628	5.140879154	12.191756248	H	6.635409832	-0.806318820	13.807605743
H	3.553193331	5.744490147	12.362701416	H	6.144157887	-2.315740585	13.019341469
H	5.019533157	5.590867043	11.376927376	C	3.384614706	3.491204262	14.133076668
H	5.043724537	5.196135044	13.108016014	C	4.367858410	3.162303448	15.098508835
C	4.019946098	-0.411122143	10.201565742	C	4.246834278	3.734517336	16.369754791
C	5.119856358	-1.153603077	10.687289238	H	4.987899780	3.515707731	17.131275177
C	5.300953388	-2.452569962	10.201221466	C	3.174794197	4.567175865	16.688453674
H	6.140710354	-3.043339014	10.558252335	H	3.097555399	4.991379738	17.686372757
C	4.409079552	-3.007998466	9.286142349	C	2.197888613	4.845026970	15.736586571
H	4.554579258	-4.026412487	8.935008049	H	1.356801271	5.477642059	16.003299713
C	3.325607538	-2.262741327	8.824928284	C	2.288068056	4.325366020	14.441611290
H	2.635404110	-2.709167719	8.115844727	C	1.222483397	4.630443096	13.393140793
C	3.124095917	-0.946342528	9.251395226	H	1.657528043	4.445333004	12.407305717
C	1.989888072	-0.092543110	8.695844650	C	0.028246114	3.674289703	13.542283058
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 Mn 2.603049040 0.942815065 12.338946342
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 N 3.359487295 2.887943506 12.707058907
 C 4.976667404 1.727796435 8.622960091
 H 5.806558132 1.019898415 8.710571289
 H 5.363132954 2.673485041 8.238656998
 H 4.285552979 1.306264520 7.886300087
 C 4.284576893 1.915648699 9.963006973
 C 4.259373665 3.225181341 10.475719452
 H 4.675431252 3.985405684 9.826502800
 C 3.909876108 3.662759304 11.768692017
 C 4.230837822 5.115890503 12.086330414
 H 3.310892820 5.695005417 12.213193893
 H 4.818562984 5.573534489 11.288429260
 H 4.786054611 5.199266434 13.024188042
 C 4.081522465 -0.447268963 10.072502136
 C 5.221220493 -1.113655329 10.579196930
 C 5.539498329 -2.373346090 10.063244820
 H 6.420091629 -2.893867016 10.431708336
 C 4.735375881 -2.977816343 9.098257065
 H 4.990498066 -3.962715149 8.715396881
 C 3.594442844 -2.324233055 8.636834145
 H 2.961350918 -2.810274363 7.899567604
 C 3.256265879 -1.046921134 9.097418785
 C 2.024513006 -0.324792802 8.566126823
 H 2.096049309 0.722564876 8.873980522
 C 1.934106350 -0.355337083 7.030529976
 H 1.099722624 0.266941905 6.688062191
 H 1.758530259 -1.369874835 6.655962944
 C 0.750193834 -0.907377243 9.196145058
 H 0.636406302 -1.962546825 8.938651085
 H -0.136425227 -0.374425918 8.830522537
 H 0.772294104 -0.832423985 10.286846161
 C 6.084763527 -0.477931798 11.665171623
 H 5.619643211 0.471751273 11.942790985
 C 7.503990650 -0.162871003 11.160227776
 H 8.031085968 -1.074548125 10.855902672
 H 8.095713615 0.319540590 11.946968079
 H 7.478697300 0.512246013 10.298612595
 C 6.127667427 -1.352651358 12.931069374
 H 5.115669250 -1.549479365 13.296227455
 H 6.692767143 -0.852700889 13.725954056
 H 6.604238987 -2.320941687 12.739538193
 C 3.229781389 3.420454025 14.029513359
 C 4.227919579 3.103712797 14.984202385
 C 4.117020607 3.666165829 16.260057449
 H 4.874425888 3.456922293 17.008386612
 C 3.029983044 4.468802929 16.603483200
 H 2.956318378 4.882493973 17.606155396
 C 2.032253504 4.726133823 15.668062210
 H 1.176100016 5.330393314 15.953009605
 C 2.119292021 4.225050449 14.364764214
 C 1.031711221 4.528085232 13.340091705
 H 1.436958313 4.314566135 12.347145081
 C -0.169911623 3.593289614 13.544952393
 H 0.128841370 2.544753551 13.464462280
 H -0.944009483 3.785529852 12.791718483

H	-0.612472057	3.738430738	14.533564568	C	-1.827988863	1.218945861	15.875704765
C	0.589440703	6.001297951	13.352100372	C	-1.963052630	2.509492636	16.397161484
H	-0.097383253	6.195263863	12.520754814	H	-2.818419933	3.114836216	16.107294083
H	1.441941023	6.682387829	13.256096840	C	-1.009313226	3.039001226	17.264019012
H	0.060511235	6.259592056	14.276079178	H	-1.119855762	4.051815987	17.643077850
C	5.380603313	2.163257837	14.622190475	C	0.085167579	2.266898870	17.646411896
H	4.948529243	1.361842752	14.008195877	H	0.826724648	2.686411619	18.320426941
C	6.473994732	2.846899986	13.774513245	C	0.243280604	0.957857013	17.180095673
H	6.874491692	3.722277641	14.299561501	C	1.400365472	0.093741037	17.665975571
H	6.103978634	3.166135788	12.799667358	H	1.220695019	-0.926679790	17.314956665
H	7.304523945	2.153088808	13.597403526	C	1.488890529	0.052216578	19.202859879
C	6.037341595	1.499253631	15.843165398	H	0.541693926	-0.256752312	19.657522202
H	6.740595818	0.727627277	15.511972427	H	2.264382362	-0.653988361	19.520669937
H	5.303013802	1.029188991	16.500419617	H	1.749634743	1.032884240	19.616184235
H	6.610371113	2.221567392	16.436384201	C	2.732456446	0.560781419	17.063869476
Mn	0.568059325	-0.954096913	13.898471832	H	2.977178097	1.573913574	17.393932343
N	-0.533041060	-0.850544989	15.699741364	H	3.544393063	-0.107489444	17.377216339
N	-0.285279751	-2.851070881	13.532521248	H	2.690371275	0.573522031	15.971749306
C	-1.762055516	-1.688834071	17.662942886	C	-2.877148867	0.657494009	14.918837547
H	-2.581225872	-0.966997087	17.584915161	H	-2.631855488	-0.391262084	14.731747627
H	-2.159984827	-2.625540018	18.057352066	C	-4.291967869	0.702082634	15.522982597
H	-1.052321076	-1.275815368	18.385805130	H	-4.631369114	1.731961370	15.680742264
C	-1.101901412	-1.892435074	16.310091019	H	-5.009407997	0.217069417	14.851099014
C	-1.166200161	-3.189508200	15.770253181	H	-4.332258224	0.187418953	16.488500595
H	-1.614387751	-3.938311815	16.411228180	C	-2.842632771	1.378222108	13.559217453
C	-0.856210887	-3.617513180	14.465742111	H	-1.861991286	1.267698526	13.088830948
C	-1.227374196	-5.053443432	14.129137993	H	-3.599677086	0.964053988	12.883426666
H	-0.325329483	-5.650373936	13.959782600	H	-3.039223909	2.450262070	13.671390533
H	-1.800577044	-5.513809204	14.935869217	C	-0.228113472	-3.363684893	12.198098183
H	-1.812860966	-5.102922440	13.207813263	C	-1.261231184	-3.001921415	11.300975800
C	-0.707988918	0.450315773	16.268743515	C	-1.261556149	-3.581438303	10.028652191

H	-2.056303024	-3.343147755	9.328618050	=====
C	-0.236403048	-4.438153744	9.628770828	6-MONO
H	-0.248761967	-4.870796680	8.631561279	=====
C	0.817871809	-4.713874340	10.495565414	Mn 0.005179527 -0.823412001 13.704684258
H	1.631773710	-5.351004601	10.161429405	N -0.629300654 -0.835652292 15.659189224
C	0.836304724	-4.197916985	11.796387672	N -0.303017169 -2.850777864 13.567411423
C	1.983975410	-4.513321400	12.748340607	C -1.569416523 -1.677923679 17.760585785
H	1.645307899	-4.288570881	13.763960838	H -2.393225193 -0.956118584 17.775888443
C	3.183234930	-3.596194506	12.453793526	H -1.908984065 -2.610122204 18.215118408
H	2.915504456	-2.541521549	12.564490318	H -0.772026002 -1.252243996 18.379161835
H	4.011919975	-3.809088945	13.140628815	C -1.083516002 -1.889251232 16.340402603
H	3.543662071	-3.743227482	11.433072090	C -1.150066018 -3.192414045 15.811742783
C	2.402631521	-5.992838383	12.715946198	H -1.538879037 -3.950246096 16.480497360
H	3.139748335	-6.193496704	13.501329422	C -0.802978039 -3.639234781 14.520083427
H	1.547962427	-6.659950733	12.872776985	C -1.023731589 -5.105853081 14.204523087
H	2.864958763	-6.263837814	11.760385513	H -0.080256715 -5.583872795 13.920087814
C	-2.337116480	-2.003795862	11.726387978	H -1.448214650 -5.642279625 15.054702759
H	-1.867684484	-1.318092823	12.442288399	H -1.695782781 -5.211623192 13.346236229
C	-3.511766434	-2.678057671	12.461580276	C -0.634922922 0.476173639 16.225339890
H	-3.986466646	-3.431838989	11.822127342	C -1.729110837 1.332426906 15.963718414
H	-3.186262846	-3.163800716	13.384059906	C -1.663848162 2.652240992 16.423036575
H	-4.272032738	-1.934089065	12.729351044	H -2.492640257 3.326478720 16.224290848
C	-2.859880924	-1.152761221	10.558224678	C -0.551745653 3.117869377 17.119800568
H	-3.506222010	-0.353839308	10.936095238	H -0.518253922 4.147068977 17.466762543
H	-2.038939953	-0.693572640	9.999393463	C 0.522706330 2.264063358 17.364208221
H	-3.456509352	-1.744072318	9.854543686	H 1.390476227 2.640217304 17.898170471
O	0.594823420	0.438339919	12.383190155	C 0.503912091 0.936411917 16.926111221
H	-0.101620466	0.700492680	11.774504662	C 1.708125710 0.022655040 17.128265381
O	2.584591866	-0.484357446	13.818829536	H 1.365266442 -1.009925961 17.014183044
H	3.296964407	-0.826352000	14.365790367	C 2.337988853 0.146607876 18.524517059
			H 1.590872765 -0.000300122 19.311428070	

H	3.123204470	-0.606012106	18.653755188	C	3.193334579	-5.213126659	13.126543045
H	2.799838066	1.127494097	18.680667877	H	3.846796036	-5.234976292	14.005429268
C	2.758300543	0.275382370	16.027992249	H	2.568394423	-6.112204552	13.143150330
H	3.141479492	1.300472736	16.085742950	H	3.837654114	-5.269437313	12.242552757
H	3.604218483	-0.414341390	16.124492645	C	-2.309530258	-2.605140686	11.483937263
H	2.331532478	0.144400269	15.026027679	H	-2.403704643	-2.436995983	12.561883926
C	-2.927198648	0.856110454	15.148281097	C	-3.472830057	-3.517903090	11.059995651
H	-2.812470675	-0.220620051	14.988870621	H	-3.470344305	-3.699387550	9.979516983
C	-4.260669231	1.073094964	15.883483887	H	-3.420285463	-4.490669727	11.561082840
H	-4.472363472	2.137619257	16.032661438	H	-4.433168411	-3.055640936	11.314092636
H	-5.088582993	0.651050985	15.303195000	C	-2.393916368	-1.227623582	10.794611931
H	-4.255949974	0.593382955	16.868124008	H	-3.349562645	-0.742385387	11.027252197
C	-2.940976381	1.524379015	13.758163452	H	-1.582504153	-0.565995693	11.118410110
H	-2.011673689	1.329220414	13.211338997	H	-2.327666759	-1.334724545	9.705533981
H	-3.773920774	1.143686533	13.155749321	O	0.258020401	0.485319227	12.404191017
H	-3.059303522	2.610313892	13.849712372	H	0.351406425	1.427744865	12.578169823
C	0.002730114	-3.372396231	12.270207405				
C	-0.949311614	-3.247611046	11.234997749				
C	-0.593428969	-3.678353071	9.952197075				
H	-1.310367703	-3.583087683	9.141192436				
C	0.665350139	-4.214112282	9.696271896				
H	0.924385488	-4.541289330	8.692951202				
C	1.599303842	-4.318158150	10.726044655				
H	2.584352493	-4.722275734	10.511997223				
C	1.290578127	-3.901795626	12.023982048				
C	2.335996628	-3.937807322	13.133926392				
H	1.808396459	-3.905486822	14.091876030				
C	3.225044727	-2.679469585	13.062407494				
H	2.627002239	-1.761019111	13.096560478				
H	3.936678171	-2.651237965	13.895579338				
H	3.790830135	-2.658128023	12.124204636				

Table S6 Vibrational frequencies (in cm⁻¹) of the optimized structures

1-F	12.40	19.74	28.80	31.49	41.60	44.53
	46.82	49.12	51.69	52.26	54.69	55.99
	57.14	60.13	62.91	65.96	68.71	78.40
	79.76	82.10	83.92	88.92	93.41	97.73
	99.24	101.36	102.55	105.48	115.60	125.35
	127.66	129.83	130.69	140.61	140.92	144.31
	146.88	148.70	154.20	156.32	158.47	160.99
	169.26	170.67	185.93	187.12	196.36	198.28
	202.66	203.98	210.63	225.74	232.71	238.97
	243.52	246.07	246.98	248.67	250.18	252.81
	256.78	259.27	263.07	266.33	267.22	269.48
	272.77	274.52	275.94	280.99	286.33	290.99
	292.64	293.81	294.74	295.99	298.13	299.83
	302.53	303.53	305.64	313.37	314.42	314.96
	319.50	322.83	330.67	334.33	341.55	342.31

352.42	353.75	373.84	376.02	439.83	440.85		3037.25	3040.76	3042.72	3044.26	3049.55	3049.67
449.06	450.97	452.35	454.45	455.32	456.77		3051.53	3054.78	3062.95	3063.72	3063.82	3064.30
461.43	462.07	463.99	469.36	474.47	512.05		3065.10	3070.75	3077.14	3078.20	3085.82	3086.37
512.75	534.25	535.18	536.09	537.37	551.79		3092.22	3097.59	3099.95	3101.71	3103.12	3105.46
552.95	553.16	553.83	560.85	561.42	574.38		3105.93	3106.26	3107.03	3107.24	3108.04	3108.46
575.67	603.35	604.38	610.27	613.99	619.59		3108.55	3109.17	3109.42	3109.58	3110.76	3111.61
631.29	636.25	644.75	645.47	653.05	655.15		3113.39	3113.73	3114.27	3116.39	3117.83	3117.90
661.36	661.84	663.23	664.53	708.80	710.43		3120.70	3126.10	3126.24	3126.66	3128.52	3132.85
722.94	723.96	767.72	773.44	773.59	780.10		3140.74	3144.03	3145.61	3148.75	3150.48	3151.10
782.10	785.14	787.09	811.15	812.33	818.10		3152.09	3152.29	3160.79	3163.25	3168.34	3169.14
818.26	822.94	823.12	824.20	824.48	861.02		3173.29	3174.89	3182.39	3183.82	3195.22	3197.27
861.13	864.94	866.29	900.41	901.19	901.88		3198.07	3198.62	3204.66	3205.94	3216.44	3216.49
902.30	915.69	915.89	919.13	919.90	940.74		=====					
945.29	947.71	948.90	949.25	949.47	950.95		1-AF					
951.49	953.46	953.74	957.45	959.12	960.13		=====					
962.44	963.99	965.66	966.10	966.75	966.96		11.03	22.80	29.53	32.25	41.25	43.83
968.94	970.29	974.53	976.15	977.47	978.17		44.77	45.51	49.29	50.77	52.16	53.51
984.31	984.49	985.17	986.13	1040.29	1041.97		57.04	59.97	62.65	66.68	68.59	73.85
1053.62	1053.68	1055.86	1057.05	1066.41	1067.31		80.41	81.97	83.79	88.85	95.42	99.01
1067.73	1073.56	1074.65	1079.49	1079.75	1082.14		100.14	102.14	106.26	107.70	115.05	128.19
1090.35	1091.47	1095.08	1095.65	1125.88	1126.69		129.34	130.56	132.77	140.08	142.59	144.03
1132.83	1133.54	1134.41	1135.58	1136.70	1137.68		147.08	147.64	154.53	156.66	160.12	163.38
1140.82	1142.67	1146.09	1146.74	1178.27	1179.26		169.65	172.08	185.01	185.58	196.49	198.86
1183.21	1183.44	1198.27	1198.52	1199.61	1200.07		204.26	205.25	210.53	225.69	233.20	239.21
1208.55	1209.33	1214.86	1215.40	1218.45	1219.08		239.98	243.06	247.57	249.46	252.02	255.09
1229.10	1230.14	1263.88	1264.39	1276.55	1277.24		257.18	258.31	262.84	265.56	267.79	270.69
1284.39	1284.50	1285.34	1285.39	1295.70	1296.61		272.87	275.02	277.78	282.52	289.47	290.88
1301.81	1302.31	1306.03	1306.96	1308.06	1309.06		292.97	294.50	295.16	299.39	301.23	302.34
1335.75	1341.57	1350.67	1353.92	1358.34	1360.32		304.08	305.57	307.90	313.87	314.60	315.71
1365.12	1365.89	1370.27	1371.52	1377.15	1377.90		321.82	323.78	331.70	334.28	339.16	341.06
1391.46	1392.92	1395.72	1396.44	1412.24	1414.22		353.49	354.31	372.98	375.24	439.14	439.47
1415.09	1416.18	1418.65	1419.06	1420.13	1420.59		448.46	451.25	453.42	454.40	455.77	456.93
1422.47	1423.18	1423.40	1423.52	1432.58	1434.39		458.54	461.46	463.38	468.36	469.37	511.92
1438.16	1438.57	1440.44	1440.82	1441.89	1442.53		512.85	534.39	535.50	535.60	537.11	552.60
1444.55	1450.47	1477.53	1478.00	1484.00	1484.40		552.99	553.52	553.98	560.86	561.26	575.18
1493.27	1493.97	1494.48	1495.40	1495.87	1496.28		576.59	603.23	604.06	607.90	614.40	616.86
1496.66	1497.12	1497.77	1498.60	1499.20	1500.02		630.70	635.14	643.60	644.61	653.19	655.50
1500.18	1500.75	1500.83	1501.71	1503.28	1503.88		662.03	662.28	663.44	664.72	709.36	710.80
1504.23	1505.69	1506.26	1506.44	1507.16	1508.54		723.15	724.09	774.68	774.92	780.37	782.22
1510.08	1511.85	1513.55	1514.07	1515.75	1516.70		785.56	787.49	810.97	811.42	817.63	818.18
1519.25	1519.83	1520.80	1521.43	1522.86	1523.65		822.37	822.93	824.70	824.84	844.16	860.99
1524.22	1525.28	1526.16	1526.53	1527.10	1527.85		861.47	865.52	866.11	900.15	900.72	901.60
1529.93	1531.16	1577.07	1578.94	1583.98	1585.22		901.91	911.85	917.34	917.56	920.48	920.56
1629.77	1630.44	1631.43	1631.66	1642.12	1643.01		942.04	946.72	948.71	949.08	949.59	949.99
1643.50	1644.20	3023.29	3031.92	3032.22	3032.90		951.47	951.67	952.60	952.79	957.18	958.41
3034.31	3034.65	3034.82	3035.18	3035.72	3036.08		961.73	963.34	966.31	966.51	967.25	967.81

968.36	968.72	974.90	976.48	976.67	977.30		134.83	135.97	231.55	264.55	278.44	293.37
983.83	984.67	985.03	985.61	1041.15	1041.88		322.87	360.32	362.24	408.01	413.49	446.38
1053.89	1054.15	1055.70	1056.70	1067.73	1068.20		468.19	503.59	537.82	560.94	713.37	717.01
1073.75	1074.93	1079.63	1081.10	1090.91	1091.86		727.72	730.45	756.60	757.02	884.06	884.82
1095.35	1096.59	1114.21	1125.89	1126.21	1131.77		898.77	981.90	982.48	1006.98	1007.30	1009.37
1133.11	1133.81	1134.31	1135.79	1136.71	1140.00		1030.60	1030.73	1116.94	1146.62	1170.42	1170.72
1141.00	1145.73	1147.08	1154.01	1177.97	1178.96		1284.42	1286.03	1316.91	1317.92	1378.70	1383.85
1183.30	1183.87	1198.23	1198.57	1199.83	1200.27		1436.96	1439.58	1513.85	1515.09	1590.99	1591.81
1208.31	1209.06	1215.19	1215.41	1218.88	1219.49		1660.48	1663.42	3089.43	3089.82	3090.00	3090.17
1228.86	1229.71	1263.70	1264.46	1275.86	1276.77		3210.88	3211.47	3559.00	3559.03	3559.51	3559.58
1284.63	1284.72	1285.70	1285.73	1295.59	1296.30		=====	=====	=====	=====	=====	=====
1300.80	1301.49	1305.66	1306.23	1307.64	1307.85	2-AF	=====	=====	=====	=====	=====	=====
1335.04	1341.83	1346.45	1350.42	1360.25	1361.28		21.22	30.42	37.24	41.65	66.12	118.72
1365.28	1365.94	1369.56	1370.05	1375.86	1376.79		137.55	140.49	232.09	271.62	279.23	292.06
1391.58	1391.96	1395.85	1396.05	1412.89	1414.11		328.21	358.26	362.23	410.60	416.02	442.32
1415.26	1415.47	1418.57	1419.07	1420.44	1420.77		467.24	495.92	538.28	552.66	716.38	719.83
1423.11	1423.39	1423.85	1423.94	1433.34	1434.47		729.95	732.86	756.89	757.41	883.74	884.61
1438.04	1438.69	1440.38	1440.77	1442.23	1442.91		981.84	982.32	983.30	1007.16	1007.54	1019.99
1444.10	1450.51	1476.92	1477.08	1484.27	1484.35		1030.49	1030.72	1142.20	1170.27	1170.72	1193.57
1493.83	1494.42	1495.00	1495.46	1496.82	1497.13		1284.14	1285.86	1316.54	1317.74	1378.35	1383.60
1497.29	1497.66	1498.27	1498.88	1499.33	1499.57		1436.42	1438.86	1513.62	1515.09	1591.08	1592.36
1500.17	1500.50	1501.05	1501.90	1503.46	1503.93		1660.14	1663.08	3087.85	3088.24	3088.28	3088.92
1504.30	1505.40	1506.25	1506.64	1508.02	1509.39		3210.59	3211.10	3560.11	3560.25	3560.70	3560.86
1509.70	1511.25	1513.65	1514.08	1515.77	1516.79		=====	=====	=====	=====	=====	=====
1520.27	1520.44	1520.76	1521.36	1522.62	1522.93	3-AF	=====	=====	=====	=====	=====	=====
1523.44	1524.94	1526.60	1526.83	1527.28	1528.17		13.85	26.44	33.63	40.24	51.36	74.12
1529.93	1530.91	1576.35	1578.27	1582.60	1583.79		113.00	132.31	140.91	144.51	210.50	257.80
1629.22	1629.81	1631.10	1631.15	1642.22	1642.81		291.05	291.69	320.62	361.45	361.87	363.45
1643.63	1643.85	3020.03	3023.06	3027.29	3029.69		399.50	410.89	422.99	424.85	454.12	476.66
3031.43	3031.50	3031.59	3033.39	3033.60	3034.17		536.39	538.59	713.35	715.57	727.41	729.44
3035.40	3038.87	3042.86	3044.00	3047.16	3047.47		758.06	758.41	882.50	883.20	975.58	975.85
3050.25	3051.32	3061.15	3063.02	3063.23	3064.84		1006.45	1006.63	1030.58	1030.63	1171.57	1171.84
3065.03	3066.57	3076.64	3077.39	3077.79	3080.88		1284.90	1286.32	1316.67	1317.60	1380.21	1385.01
3087.80	3094.50	3094.65	3095.26	3098.67	3102.82		1434.18	1436.35	1514.59	1516.18	1591.28	1592.56
3103.04	3103.12	3103.74	3104.01	3104.82	3105.39		1659.09	1661.52	3086.03	3086.33	3086.35	3086.41
3106.51	3107.70	3108.52	3109.69	3110.15	3110.99		3207.84	3207.89	3559.54	3559.72	3559.94	3560.12
3112.59	3113.83	3115.91	3117.06	3118.38	3118.97		=====	=====	=====	=====	=====	=====
3120.23	3122.87	3124.81	3126.29	3128.81	3129.47	3-MONO	=====	=====	=====	=====	=====	=====
3130.26	3139.70	3147.41	3147.44	3147.66	3148.18		63.98	72.01	144.20	217.57	294.17	356.54
3148.68	3150.25	3159.70	3166.84	3167.08	3169.44		409.09	452.76	534.54	682.30	737.92	746.59
3172.09	3172.11	3180.30	3181.32	3192.50	3194.70		764.64	883.42	982.59	1010.78	1034.11	1170.37
3195.83	3195.87	3203.39	3204.58	3213.01	3213.81		1288.79	1319.61	1379.60	1437.22	1510.62	1592.64
=====	=====	=====	=====	=====	=====		1660.09	3093.10	3094.50	3212.46	3554.95	3555.27
20.23	31.72	38.01	38.45	64.90	120.93	S34						

4-AF	531.25 531.68 536.44 537.01 548.44 549.95 550.93 551.57 559.20 560.16 572.45 572.55 604.28 604.76 614.15 614.91 623.70 624.11 643.46 643.96 652.34 653.03 659.83 660.43 661.65 661.79 709.35 710.05 724.90 725.02 768.81 769.14 775.37 778.66 779.11 783.44 808.07 808.70 816.42 816.69 821.54 822.01 823.07 823.13 863.16 863.46 867.44 868.38 903.29 903.45 904.56 904.63 917.10 917.93 918.24 918.49 940.81 941.07 948.60 949.11 949.45 949.57 953.51 953.57 957.01 957.32 960.51 961.92 965.19 965.68 966.44 966.74 970.37 970.77 971.77 972.11 976.64 977.03 977.47 977.80 981.76 981.99 985.85 986.20 1042.38 1042.64 1053.00 1053.24 1057.99 1058.49 1067.08 1067.48 1076.04 1077.52 1079.41 1080.86 1092.53 1094.59 1095.02 1096.88 1125.34 1125.91 1132.67 1133.75 1135.10 1135.60 1139.09 1139.59 1140.46 1141.75 1145.31 1146.02 1175.17 1175.43 1182.14 1183.02 1198.48 1198.64 1200.77 1201.35 1209.98 1211.07 1216.27 1217.04 1219.26 1219.84 1233.06 1234.20 1262.56 1262.91 1277.07 1277.28 1284.49 1284.81 1285.39 1285.88 1300.08 1300.94 1306.38 1306.57 1307.95 1308.65 1309.38 1310.15 1326.28 1327.18 1355.69 1356.78 1358.68 1360.07 1363.78 1368.31 1370.79 1371.06 1373.51 1374.76 1391.59 1392.15 1396.61 1397.78 1413.32 1413.97 1417.68 1417.85 1420.78 1421.20 1422.27 1422.70 1423.23 1423.90 1424.35 1424.59 1435.30 1435.61 1441.22 1441.81 1444.96 1445.01 1445.53 1449.99 1450.41 1452.45 1476.78 1476.91 1483.70 1484.06 1491.40 1492.00 1495.55 1496.12 1496.71 1497.06 1499.14 1499.44 1500.56 1500.64 1502.68 1503.03 1503.50 1503.79 1505.88 1506.41 1507.02 1507.76 1508.13 1508.24 1509.02 1509.45 1510.41 1511.49 1513.23 1513.54 1515.19 1515.78 1518.84 1519.37 1521.38 1521.90 1523.84 1524.15 1525.16 1525.41 1527.40 1528.30 1533.33 1533.81 1535.86 1536.68 1537.20 1538.29 1575.51 1577.09 1590.90 1592.09 1630.25 1630.64 1632.23 1632.32 1643.22 1643.23 1644.71 1644.86 3031.88 3032.91 3032.96 3034.00 3034.52 3034.91 3035.54 3036.28 3036.46 3036.66 3036.88 3037.65 3038.31 3038.82 3044.64 3045.20 3045.90 3046.97 3057.54 3058.11 3064.76 3065.16 3076.52 3077.99 3078.76 3081.84 3081.95 3086.34 3094.02 3094.16 3097.97 3099.01 3103.79 3104.23
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3106.30	3107.04	3107.22	3107.81	3108.89	3109.06		3174.53	3187.88	3188.08	3201.26	3201.48	3213.55
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3109.50	3109.97	3110.34	3110.69	3111.98	3113.47	6-F						
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3117.33	3118.84	3119.64	3121.52	3126.46	3128.77		37.83	41.56	42.76	47.18	49.55	52.53
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3129.52	3129.68	3138.62	3142.32	3147.08	3148.53		71.56	72.98	75.67	78.55	80.72	82.88
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3148.67	3150.09	3150.26	3152.44	3156.25	3156.44		103.58	104.77	106.47	111.46	117.17	123.20
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3161.05	3161.47	3161.90	3163.03	3168.68	3169.39		152.21	154.14	156.03	158.25	162.66	166.39
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3173.16	3173.34	3184.94	3185.21	3196.34	3197.40		202.45	205.42	209.86	210.77	214.75	230.57
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3199.22	3201.30	3207.24	3207.34	3213.40	3214.32		255.17	255.80	256.90	259.53	261.45	266.59
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5-MONO							282.06	285.00	289.17	292.66	296.97	299.50
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20.75	27.25	48.75	49.44	53.99	56.59		315.84	317.76	323.83	326.49	332.05	334.81
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62.72	64.85	66.26	74.38	80.14	101.08		371.66	373.77	377.05	399.27	437.86	441.15
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105.59	113.11	119.07	121.61	129.55	136.98		461.15	463.59	464.35	466.69	468.39	474.14
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140.99	148.81	151.50	164.81	187.80	204.06		551.38	553.33	553.77	554.32	562.21	563.08
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207.94	222.20	234.79	242.76	250.00	253.81		629.44	633.69	644.90	646.88	653.35	654.63
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259.58	269.27	269.91	273.60	275.17	283.52		724.91	726.66	732.13	749.30	764.74	766.78
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289.95	295.22	304.47	312.98	314.05	317.90		819.03	821.11	824.28	824.52	824.80	825.62
<hr/>							863.01	863.86	866.65	867.75	903.87	905.37
330.62	335.79	337.88	369.48	437.18	438.78		905.99	906.83	918.33	919.99	922.16	922.46
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445.25	451.08	458.00	459.47	510.14	530.44		953.57	953.85	954.27	956.01	962.55	964.62
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533.71	543.79	547.26	555.06	568.86	605.65		971.19	972.45	978.16	979.56	980.03	980.75
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612.18	626.47	640.63	641.32	646.17	651.98		1053.79	1056.68	1058.93	1062.41	1068.10	1070.22
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660.30	711.40	728.43	766.31	774.32	778.82		1098.00	1099.33	1129.93	1131.88	1135.85	1136.88
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813.91	815.12	818.92	819.57	861.85	868.40		1144.28	1146.43	1178.42	1179.62	1183.01	1184.29
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897.27	898.26	919.04	919.15	937.46	938.49		1216.70	1217.24	1219.73	1220.86	1232.73	1233.04
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947.65	948.27	957.88	962.46	963.30	969.19							
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971.20	972.71	974.20	975.32	979.63	981.44							
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1043.12	1052.07	1056.03	1065.28	1074.68	1077.58							
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1090.75	1092.53	1125.70	1128.02	1132.28	1133.97							
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1136.83	1141.38	1177.07	1178.64	1199.38	1200.43							
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1205.06	1216.06	1216.49	1230.85	1262.70	1278.80							
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1284.98	1285.15	1303.58	1305.35	1306.81	1310.51							
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1353.44	1354.01	1366.03	1368.01	1370.25	1373.59							
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1393.48	1394.37	1412.28	1414.29	1418.86	1419.34							
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1423.70	1424.48	1434.10	1435.20	1444.07	1447.52							
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1450.43	1481.00	1482.77	1484.31	1491.70	1491.88							
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1492.56	1495.72	1500.73	1501.31	1502.17	1505.25							
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1505.61	1507.42	1507.89	1509.76	1511.21	1515.81							
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1518.14	1519.99	1522.58	1523.08	1525.54	1531.97							
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1540.68	1572.78	1596.76	1631.78	1631.94	1645.53							
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1645.77	3025.10	3028.38	3029.46	3031.69	3036.00							
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3036.39	3040.17	3040.36	3051.63	3052.17	3061.20							
<hr/>												
3062.16	3072.94	3075.41	3088.45	3092.38	3098.94							
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3100.86	3106.93	3107.43	3107.83	3108.33	3110.17							
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3110.54	3111.13	3111.58	3114.73	3115.36	3116.92							
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3117.76	3120.32	3122.86	3150.01	3150.43	3174.42							

1287.82	1288.82	1302.59	1303.13	1304.83	1306.25	263.57	264.48	267.44	268.57	270.26	273.62
1307.66	1309.02	1310.70	1312.76	1335.90	1345.76	275.43	278.41	282.44	286.58	290.80	293.70
1361.18	1362.16	1362.66	1363.60	1369.17	1369.46	296.80	298.18	303.80	305.64	307.02	308.22
1372.59	1373.62	1376.95	1380.84	1395.91	1397.16	310.62	311.48	319.45	321.45	328.13	329.79
1398.21	1398.55	1414.46	1414.74	1415.61	1416.32	333.93	337.05	341.95	345.50	356.26	360.43
1420.42	1420.94	1421.65	1422.68	1423.34	1423.80	365.07	368.64	370.73	391.08	433.97	437.65
1425.11	1425.93	1434.86	1435.18	1438.35	1438.68	441.20	446.20	448.23	452.47	454.16	455.72
1442.08	1443.91	1444.42	1445.66	1451.61	1458.61	457.81	460.01	460.76	462.78	464.67	470.93
1480.31	1482.44	1486.78	1486.84	1493.38	1496.35	511.52	511.94	531.11	531.68	534.55	535.18
1496.41	1496.85	1498.27	1499.47	1499.62	1500.67	549.05	550.37	550.71	551.02	559.07	560.09
1501.43	1501.72	1502.18	1502.61	1502.75	1503.61	571.85	572.36	605.63	605.95	614.08	615.14
1504.12	1505.59	1506.35	1506.73	1507.34	1508.87	626.78	631.07	641.88	643.75	649.92	651.36
1509.80	1509.99	1510.99	1511.80	1514.57	1514.71	657.50	657.92	660.17	661.21	708.00	709.26
1515.04	1515.32	1518.08	1518.76	1521.29	1521.96	722.94	724.06	726.86	747.94	764.15	766.25
1523.09	1523.84	1525.31	1526.60	1527.02	1528.93	776.15	778.71	781.04	784.15	808.90	809.70
1529.84	1531.95	1532.24	1533.85	1534.01	1538.43	816.11	817.48	821.80	822.15	822.58	822.83
1575.04	1577.60	1592.04	1594.56	1631.89	1633.17	860.91	861.31	864.13	864.99	901.46	902.91
1633.50	1634.61	1645.34	1646.94	1647.90	1648.37	903.28	904.90	915.52	917.86	918.97	919.08
3032.57	3034.11	3034.50	3035.30	3035.39	3035.89	940.37	940.84	947.24	947.57	949.58	949.74
3036.42	3036.96	3037.96	3038.86	3039.40	3039.57	950.67	952.01	952.69	953.89	960.13	961.78
3039.80	3041.58	3042.67	3045.25	3046.30	3053.92	962.74	964.22	964.37	964.95	966.03	968.75
3062.19	3064.28	3069.67	3078.01	3081.86	3084.45	970.19	970.41	975.40	976.52	976.82	977.04
3085.75	3089.21	3089.58	3090.44	3096.56	3096.87	981.33	982.80	983.03	984.17	1040.40	1041.14
3100.83	3103.02	3104.69	3106.91	3108.10	3108.61	1052.00	1052.48	1056.95	1057.37	1065.71	1065.79
3109.45	3109.73	3111.08	3112.03	3112.32	3112.45	1074.36	1075.84	1078.33	1079.92	1091.18	1092.25
3113.06	3113.23	3118.54	3118.92	3120.20	3120.99	1094.27	1095.67	1126.80	1129.23	1133.76	1134.08
3122.74	3125.27	3125.63	3126.03	3129.64	3131.84	1134.92	1135.87	1137.32	1138.06	1138.72	1140.51
3132.92	3136.24	3138.00	3146.69	3147.01	3148.82	1142.49	1144.71	1176.59	1177.55	1181.33	1182.19
3151.89	3152.45	3153.11	3153.48	3153.82	3154.32	1198.61	1198.91	1199.42	1200.18	1207.99	1208.83
3154.90	3165.94	3169.64	3170.50	3173.53	3173.91	1214.87	1215.26	1217.76	1218.79	1230.48	1230.94
3182.91	3183.35	3192.71	3194.79	3196.94	3198.40	1262.49	1263.57	1275.35	1276.88	1284.61	1284.89
3204.07	3206.03	3209.92	3210.38	3924.62	3928.69	1285.58	1285.96	1301.23	1302.13	1303.20	1304.84

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13.91	20.85	27.13	29.18	31.16	38.61	1358.93	1360.02	1360.38	1360.91	1365.14	1366.33
44.39	47.70	47.86	51.17	55.87	57.47	1369.29	1370.67	1374.52	1377.73	1390.22	1391.66
59.14	60.33	62.96	68.12	71.06	73.14	1395.14	1396.20	1412.43	1412.82	1413.90	1414.02
75.65	80.70	82.87	85.50	88.91	92.13	1418.84	1419.27	1420.19	1420.38	1421.58	1422.02
95.88	96.36	97.95	102.73	110.45	118.41	1422.15	1422.37	1432.98	1433.09	1436.19	1436.47
121.51	122.73	125.58	128.62	136.17	142.69	1439.83	1441.63	1442.27	1443.34	1449.85	1456.88
143.80	147.22	149.02	150.86	153.68	158.19	1477.51	1479.89	1484.18	1484.83	1492.26	1493.21
160.93	164.31	166.29	174.11	176.62	182.29	1495.02	1495.29	1496.71	1496.95	1498.50	1499.27
195.01	197.19	204.26	204.69	208.19	222.70	1500.31	1500.63	1501.05	1501.33	1501.65	1502.05
225.99	227.92	237.40	242.35	246.88	248.30	1502.97	1503.97	1504.37	1504.89	1505.51	1507.06
249.17	249.78	251.88	252.98	254.53	260.61	1507.87	1508.08	1509.14	1510.44	1513.03	1513.16
						1513.54	1513.75	1516.65	1517.50	1520.48	1520.90
						1521.91	1522.42	1523.63	1524.71	1525.61	1527.26

1528.42	1530.65	1531.00	1531.93	1532.69	1535.94	1502.30	1505.13	1505.87	1506.33	1507.26	1510.17
1574.08	1576.96	1590.70	1593.81	1630.52	1631.12	1510.46	1516.07	1518.61	1519.50	1522.09	1522.62
1631.20	1631.71	1643.67	1643.75	1644.86	1645.50	1523.08	1529.02	1535.12	1573.43	1598.73	1630.30
3030.89	3031.79	3032.30	3032.35	3033.30	3033.67	1632.32	1644.89	1645.86	3024.68	3027.08	3029.21
3034.15	3034.74	3036.16	3036.26	3037.23	3037.35	3029.56	3035.46	3036.83	3039.06	3039.56	3050.48
3037.45	3039.64	3040.04	3043.34	3044.82	3048.49	3051.89	3062.63	3069.77	3074.80	3075.92	3093.42
3060.50	3061.72	3062.92	3064.30	3076.00	3076.06	3096.39	3097.27	3100.71	3104.45	3105.56	3107.08
3076.70	3080.38	3083.37	3084.17	3094.23	3094.58	3108.76	3109.03	3109.72	3110.16	3110.97	3112.11
3099.45	3100.74	3102.96	3104.82	3105.79	3106.21	3112.51	3113.71	3113.93	3115.48	3116.18	3148.98
3106.44	3107.73	3108.71	3109.45	3109.61	3110.06	3149.67	3173.10	3173.29	3185.78	3186.48	3199.58
3110.22	3111.19	3115.24	3115.64	3116.21	3117.20	3199.82	3212.34	3880.1			
3117.69	3118.42	3122.81	3124.49	3127.47	3127.90						
3128.55	3129.32	3132.96	3142.48	3143.96	3147.44						
3148.03	3148.12	3148.35	3148.54	3150.17	3150.93						
3150.99	3159.29	3166.56	3166.77	3171.37	3171.47						
3180.15	3181.00	3190.61	3193.55	3194.60	3195.41						
3201.03	3204.50	3209.53	3210.31	3920.41	3925.06						

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6-MONO

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16.12	25.12	45.63	47.06	48.89	53.20
61.91	63.80	64.31	65.91	77.89	98.46
102.75	105.52	113.44	116.48	123.35	135.99
138.74	150.19	150.47	168.21	187.50	203.59
205.28	222.66	236.07	242.02	249.31	252.39
258.03	266.87	268.55	271.78	272.82	279.73
287.09	291.40	293.13	305.03	311.74	313.03
313.92	332.38	334.61	338.99	368.65	438.02
440.23	445.82	451.61	457.18	458.04	510.62
530.08	532.84	543.74	547.05	551.94	555.95
568.86	606.35	613.30	628.18	640.80	641.87
646.01	651.89	660.50	710.67	727.66	764.65
774.58	779.18	813.97	815.40	818.76	819.03
861.54	867.34	897.68	898.42	918.49	919.74
939.71	940.50	948.06	948.71	957.97	959.77
960.59	968.99	970.09	972.06	974.09	975.26
978.08	979.78	1043.07	1051.96	1056.42	1065.25
1074.22	1077.17	1090.59	1092.21	1126.17	1128.18
1131.83	1133.22	1135.81	1140.22	1177.55	1178.93
1198.65	1199.61	1205.26	1215.32	1215.91	1230.89
1262.40	1278.60	1283.97	1284.95	1303.35	1304.21
1306.85	1311.11	1355.27	1356.34	1366.08	1367.30
1368.80	1372.73	1393.84	1394.63	1414.07	1415.71
1418.39	1418.98	1422.75	1423.78	1434.90	1436.10
1442.64	1446.78	1448.38	1481.16	1483.47	1487.31
1492.05	1492.50	1494.32	1496.45	1500.47	1502.10