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Supporting Information on Hemihelices in Molecular Scale: Extended Metal Atom Chains with Helical Perversions in Ligands

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Supporting Information Available

DFT Functional Comparison on the Full Geometry Optimization Calculations

In order to check our calculation results, besides the BP86 functional we used in the whole paper, we also do full geometry optimizations of $Mo_2MMo_2(tpda)_4(NCS)_2$ (M=Ni, Fe, Mn) with B3LYP and OPBE functionals. The results are shown in Table S1. Compared to the experimental crystal data listed in Table 1, the BP86 functional gives the closest metal-metal bond lengths, and the OPBE mostly under estimates these bond distances. However, all of these calculations give similar results. Except for a little longer Mo−Mo bond in M=Mn with B3LYP functional, dimolybdenum bonds are roughly the same in two conformations, while the Mo−M bonds are longer in *meso*-conformations. Changing the central from Ni to Fe and Mn, the Mo−M lengths gradually grow, and the *meso*-conformations become more and more relatively stable at the same time, which is also consist with our previous assumption.

Table S1: DFT Funtional Comparison on the $Mo_2MMo_2(tpda)_4(NCS)_2$ Calculations

Central metal M (*meso*/helical)	Functional	Mo−Mo (Å)	Mo−M (Å)	$E_m - E_h$ (eV)
Ni (S=1)	BP86	2.10/2.10	2.54/2.45	-0.011
	B3LYP	2.07/2.07	2.56/2.47	-0.0030
	OPBE	2.05/2.05	2.54/2.43	0.0012
Fe (S=2)	BP86	2.11/2.10	2.55/2.46	-0.17
	B3LYP	2.07/2.07	2.58/2.49	-0.0075
	OPBE	2.06/2.06	2.55/2.46	-0.0053
Mn (S=5/2)	BP86	2.10/2.09	2.58/2.50	-0.34
	B3LYP	2.06/2.12	2.60/2.47	-0.058
	OPBE	2.05/2.04	2.60/2.51	-0.013

Atomic coordinates from EMACs Full Optimizations

All DFT optimizations are calculated with ORCA 3.0.3 and the BP86 exchange-correlation functional. The def2-SVP basis set and def2-SVP/J auxiliary basis set are used for H and C atoms. For NOS atom, def2-TZVP(-f) basis set and def2-TZVP/J auxiliary basis set are used. And as for transition metal atoms, def2-TZVPP basis set and def2-TZVPP/J auxiliary basis set is chosen. Additional ZORA approximation was applied on the 4d transition metal Mo.

Table S2: Atomic coordinates of $Mo_2NiMo_2(tpda)_4(NCS)_2$ (*meso* conformation)

atom	x	y	z	atom	x	y	z
Ni	0.0000	0.0000	0.0000	H	1.6216	-1.6754	-6.7163
Mo	0.0000	0.0000	4.6450	H	3.3740	-3.4726	-6.7965
Mo	0.0000	0.0000	2.5415	H	4.1684	-4.4757	-4.5811
Mo	0.0000	0.0000	-4.6450	H	3.0821	-3.7134	-2.4625
Mo	0.0000	0.0000	-2.5415	H	0.8066	-4.5436	-2.1707
N	0.0000	0.0000	6.8992	N	1.9177	0.9139	0.0000
C	0.0000	0.0000	8.1014	C	4.7161	0.7697	0.0000
S	0.0000	0.0000	9.7134	H	5.8079	0.6250	0.0001
N	0.0000	0.0000	-6.8992	N	1.7483	1.3636	4.6571
C	0.0000	0.0000	-8.1014	N	1.8517	1.0652	2.3464
S	0.0000	0.0000	-9.7133	C	2.1809	1.9595	5.8021
N	-0.9139	1.9176	0.0000	C	3.1705	2.9361	5.8355
C	-0.7701	4.7161	0.0000	C	3.7302	3.3585	4.6111
H	-0.6259	5.8080	0.0001	C	3.3146	2.7522	3.4302
N	-1.3636	1.7483	4.6571	C	2.3396	1.7136	3.4595
N	-1.0652	1.8517	2.3464	C	2.6079	0.9699	1.1829
C	-1.9592	2.1811	5.8021	C	4.0207	0.8598	1.2079
C	-2.9356	3.1709	5.8356	H	1.6750	1.6220	6.7163
C	-3.3582	3.7305	4.6111	H	3.4720	3.3746	6.7964
C	-2.7520	3.3148	3.4302	H	4.4748	4.1693	4.5810
C	-1.7136	2.3396	3.4595	H	3.7129	3.0826	2.4625
C	-0.9700	2.6079	1.1829	H	4.5435	0.8060	2.1708
C	-0.8602	4.0207	1.2079	N	1.7484	1.3634	-4.6571
H	-1.6214	1.6756	6.7164	N	1.8518	1.0651	-2.3464

atom	x	y	z	atom	x	y	z
H	-3.3742	3.4723	6.7964	C	2.1811	1.9592	-5.8021
H	-4.1686	4.4755	4.5811	C	3.1708	2.9357	-5.8355
H	-3.0826	3.7129	2.4625	C	3.7306	3.3581	-4.6111
H	-0.8070	4.5436	2.1708	C	3.3149	2.7519	-3.4302
N	-1.3634	1.7484	-4.6571	C	2.3397	1.7134	-3.4595
N	-1.0651	1.8517	-2.3464	C	2.6080	0.9698	-1.1829
C	-1.9590	2.1814	-5.8021	C	4.0207	0.8597	-1.2078
C	-2.9352	3.1713	-5.8356	H	1.6751	1.6219	-6.7163
C	-3.3578	3.7309	-4.6112	H	3.4724	3.3742	-6.7964
C	-2.7516	3.3152	-3.4302	H	4.4753	4.1688	-4.5810
C	-1.7134	2.3398	-3.4595	H	3.7133	3.0822	-2.4626
C	-0.9699	2.6079	-1.1829	H	4.5436	0.8059	-2.1707
C	-0.8601	4.0207	-1.2078	N	-1.9177	-0.9139	0.0000
H	-1.6213	1.6757	-6.7164	C	-4.7161	-0.7699	0.0000
H	-3.3738	3.4727	-6.7965	H	-5.8079	-0.6253	0.0001
H	-4.1680	4.4760	-4.5812	N	-1.7483	-1.3637	4.6571
H	-3.0822	3.7133	-2.4626	N	-1.8517	-1.0652	2.3464
H	-0.8069	4.5436	-2.1707	C	-2.1810	-1.9595	5.8021
N	0.9139	-1.9177	0.0000	C	-3.1706	-2.9360	5.8355
C	0.7698	-4.7161	0.0000	C	-3.7303	-3.3585	4.6111
H	0.6255	-5.8080	0.0001	C	-3.3146	-2.7522	3.4302
N	1.3637	-1.7483	4.6570	C	-2.3396	-1.7136	3.4595
N	1.0652	-1.8517	2.3464	C	-2.6079	-0.9699	1.1829
C	1.9594	-2.1810	5.8021	C	-4.0207	-0.8600	1.2079
C	2.9359	-3.1707	5.8355	H	-1.6751	-1.6220	6.7163
C	3.3584	-3.7304	4.6111	H	-3.4720	-3.3746	6.7964
C	2.7521	-3.3148	3.4302	H	-4.4749	-4.1692	4.5810
C	1.7136	-2.3396	3.4595	H	-3.7130	-3.0826	2.4625
C	0.9699	-2.6080	1.1829	H	-4.5435	-0.8063	2.1708
C	0.8600	-4.0208	1.2079	N	-1.7484	-1.3635	-4.6571
H	1.6218	-1.6753	6.7163	N	-1.8518	-1.0651	-2.3464
H	3.3745	-3.4721	6.7964	C	-2.1812	-1.9592	-5.8021
H	4.1689	-4.4752	4.5810	C	-3.1709	-2.9357	-5.8355
H	3.0825	-3.7130	2.4625	C	-3.7306	-3.3581	-4.6111
H	0.8066	-4.5436	2.1708	C	-3.3149	-2.7519	-3.4302
N	1.3634	-1.7484	-4.6571	C	-2.3398	-1.7134	-3.4595
N	1.0651	-1.8518	-2.3464	C	-2.6080	-0.9699	-1.1829
C	1.9591	-2.1812	-5.8021	C	-4.0208	-0.8599	-1.2078
C	2.9355	-3.1711	-5.8355	H	-1.6752	-1.6218	-6.7163
C	3.3579	-3.7308	-4.6112	H	-3.4724	-3.3742	-6.7964
C	2.7517	-3.3151	-3.4302	H	-4.4754	-4.1687	-4.5810
C	1.7134	-2.3398	-3.4595	H	-3.7133	-3.0822	-2.4625
C	0.9698	-2.6080	-1.1829	H	-4.5436	-0.8062	-2.1707
C	0.8599	-4.0208	-1.2078				

Table S3: Atomic coordinates of $Mo_2NiMo_2(tpda)_4(NCS)_2$ (helical conformation)

atom	x	y	z	atom	x	y	z
Mo	0.0000	0.0000	2.4452	H	-3.9875	-2.6367	2.2707
Mo	0.0000	0.0000	4.5434	C	-2.5319	-1.4012	3.3179
Mo	0.0000	0.0000	-2.4453	C	-2.7869	-0.3735	1.1312
Mo	0.0000	0.0000	-4.5434	C	-4.2036	-0.3095	1.1697
Ni	0.0000	0.0000	0.0000	H	-4.7369	-0.4912	2.1101
N	-0.0001	2.1045	0.0000	N	-1.1582	-1.8998	-4.5221
C	0.0000	4.9001	-0.0001	N	-0.7137	-2.0157	-2.2356
H	0.0001	6.0018	0.0000	C	-1.7741	-2.3612	-5.6434
N	-1.1580	1.8999	4.5222	H	-1.5149	-1.8228	-6.5656
N	-0.7137	2.0157	2.2355	C	-2.6846	-3.4141	-5.6423
C	-1.7740	2.3613	5.6434	H	-3.1485	-3.7355	-6.5848
H	-1.5148	1.8229	6.5656	C	-3.0146	-4.0064	-4.4061
C	-2.6845	3.4141	5.6424	H	-3.7787	-4.7970	-4.3451
H	-3.1484	3.7356	6.5849	C	-2.3758	-3.5653	-3.2493
C	-3.0145	4.0065	4.4062	H	-2.6376	-3.9867	-2.2705
H	-3.7785	4.7971	4.3452	C	-1.4014	-2.5319	-3.3178
C	-2.3757	3.5654	3.2493	C	-0.3734	-2.7869	-1.1312
H	-2.6376	3.9868	2.2706	C	-0.3092	-4.2035	-1.1697
C	-1.4014	2.5319	3.3178	H	-0.4901	-4.7369	-2.1102
C	-0.3736	2.7870	1.1312	N	1.1582	1.8997	-4.5221
C	-0.3094	4.2036	1.1697	N	0.7136	2.0157	-2.2356
H	-0.4907	4.7369	2.1101	C	1.7743	2.3610	-5.6434
N	0.0000	-2.1044	0.0000	H	1.5153	1.8224	-6.5655
C	0.0001	-4.9000	0.0001	C	2.6846	3.4140	-5.6423
H	0.0005	-6.0018	0.0000	H	3.1486	3.7354	-6.5848
N	1.1581	-1.8998	4.5221	C	3.0142	4.0067	-4.4062
N	0.7137	-2.0156	2.2356	H	3.7780	4.7976	-4.3452
C	1.7742	-2.3610	5.6434	C	2.3753	3.5657	-3.2494
H	1.5151	-1.8225	6.5655	H	2.6368	3.9874	-2.2706
C	2.6845	-3.4141	5.6424	C	1.4014	2.5319	-3.3178
H	3.1484	-3.7355	6.5848	C	0.3735	2.7869	-1.1313
C	3.0139	-4.0069	4.4062	C	0.3094	4.2035	-1.1698
H	3.7777	-4.7978	4.3452	H	0.4911	4.7369	-2.1101
C	2.3752	-3.5659	3.2494	N	-1.8998	1.1581	-4.5222
H	2.6367	-3.9875	2.2707	N	-2.0157	0.7135	-2.2356

atom	x	y	z	atom	x	y	z
C	1.4014	-2.5318	3.3178	C	-2.3612	1.7741	-5.6435
C	0.3736	-2.7869	1.1312	H	-1.8227	1.5150	-6.5656
C	0.3097	-4.2035	1.1697	C	-3.4142	2.6844	-5.6424
H	0.4918	-4.7369	2.1100	H	-3.7356	3.1483	-6.5849
N	2.1044	0.0001	0.0000	C	-4.0067	3.0141	-4.4062
C	4.9001	0.0001	0.0000	H	-4.7975	3.7780	-4.3452
H	6.0018	0.0002	0.0000	C	-3.5657	2.3753	-3.2494
N	1.8999	1.1580	4.5222	H	-3.9872	2.6370	-2.2707
N	2.0157	0.7136	2.2356	C	-2.5320	1.4013	-3.3179
C	2.3613	1.7740	5.6435	C	-2.7870	0.3733	-1.1313
H	1.8228	1.5149	6.5656	C	-4.2036	0.3091	-1.1698
C	3.4143	2.6843	5.6424	H	-4.7369	0.4902	-2.1102
H	3.7358	3.1482	6.5849	N	1.8998	-1.1581	-4.5222
C	4.0070	3.0139	4.4062	N	2.0157	-0.7135	-2.2356
H	4.7978	3.7778	4.3452	C	2.3611	-1.7741	-5.6434
C	3.5658	2.3751	3.2494	H	1.8226	-1.5151	-6.5656
H	3.9874	2.6368	2.2707	C	3.4142	-2.6844	-5.6424
C	2.5319	1.4013	3.3179	H	3.7356	-3.1483	-6.5848
C	2.7869	0.3735	1.1312	C	4.0069	-3.0140	-4.4062
C	4.2035	0.3094	1.1697	H	4.7977	-3.7778	-4.3452
H	4.7369	0.4909	2.1101	C	3.5658	-2.3752	-3.2494
N	-2.1045	0.0000	0.0000	H	3.9874	-2.6368	-2.2706
C	-4.9001	-0.0002	0.0000	C	2.5319	-1.4013	-3.3179
H	-6.0018	-0.0004	-0.0001	C	2.7869	-0.3733	-1.1313
N	-1.8999	-1.1579	4.5222	C	4.2035	-0.3092	-1.1698
N	-2.0157	-0.7135	2.2356	H	4.7369	-0.4904	-2.1102
C	-2.3612	-1.7740	5.6435	N	0.0000	0.0000	-6.8035
H	-1.8227	-1.5149	6.5656	C	0.0000	0.0000	-8.0056
C	-3.4143	-2.6843	5.6424	S	-0.0001	0.0000	-9.6184
H	-3.7357	-3.1482	6.5849	N	0.0000	0.0000	6.8035
C	-4.0070	-3.0138	4.4063	C	0.0000	0.0000	8.0056
H	-4.7978	-3.7777	4.3453	S	0.0000	0.0001	9.6184
C	-3.5659	-2.3751	3.2494				

Table S4: Atomic coordinates of $Mo_2MnMo_2(tpda)_4(NCS)_2$ (*meso* conformation)

atom	x	y	z	atom	x	y	z
Mn	-0.0001	0.0000	0.0000	H	1.5894	-1.6950	-6.7375
Mo	0.0000	0.0000	4.6782	H	3.3381	-3.4964	-6.8335
Mo	0.0000	0.0000	2.5819	H	4.1609	-4.4894	-4.6235
Mo	0.0000	0.0000	-4.6782	H	3.1066	-3.7136	-2.4950
Mo	0.0000	0.0000	-2.5819	H	0.8184	-4.5616	-2.1720
N	0.0000	0.0000	6.9642	N	1.9440	1.0212	0.0000
C	0.0000	0.0000	8.1667	C	4.7245	0.7999	0.0000
S	0.0000	0.0000	9.7794	H	5.8143	0.6400	-0.0001
N	0.0000	0.0000	-6.9643	N	1.7570	1.3608	4.6746
C	0.0000	0.0000	-8.1667	N	1.8557	1.0917	2.3540
S	0.0000	0.0000	-9.7794	C	2.1976	1.9393	5.8258
N	-1.0212	1.9441	0.0000	C	3.1897	2.9129	5.8682
C	-0.7996	4.7246	0.0000	C	3.7434	3.3511	4.6467
H	-0.6394	5.8144	-0.0001	C	3.3198	2.7624	3.4598
N	-1.3607	1.7571	4.6746	C	2.3429	1.7246	3.4786
N	-1.0917	1.8558	2.3540	C	2.6248	1.0274	1.1895
C	-1.9393	2.1975	5.8257	C	4.0344	0.8919	1.2125
C	-2.9131	3.1895	5.8682	H	1.6953	1.5890	6.7376
C	-3.3511	3.7433	4.6467	H	3.4970	3.3374	6.8335
C	-2.7625	3.3197	3.4598	H	4.4899	4.1603	4.6236
C	-1.7246	2.3429	3.4786	H	3.7140	3.1062	2.4950
C	-1.0273	2.6249	1.1895	H	4.5616	0.8186	2.1720
C	-0.8917	4.0344	1.2125	N	1.7569	1.3610	-4.6746
H	-1.5894	1.6950	6.7375	N	1.8556	1.0918	-2.3540
H	-3.3375	3.4969	6.8336	C	2.1973	1.9396	-5.8257
H	-4.1605	4.4897	4.6236	C	3.1893	2.9133	-5.8682
H	-3.1062	3.7141	2.4951	C	3.7429	3.3515	-4.6466
H	-0.8179	4.5617	2.1720	C	3.3194	2.7628	-3.4597
N	-1.3610	1.7570	-4.6746	C	2.3427	1.7248	-3.4786
N	-1.0918	1.8557	-2.3540	C	2.6248	1.0274	-1.1895
C	-1.9396	2.1973	-5.8257	C	4.0343	0.8920	-1.2126
C	-2.9134	3.1892	-5.8682	H	1.6952	1.5892	-6.7376
C	-3.3516	3.7429	-4.6467	H	3.4965	3.3379	-6.8335
C	-2.7628	3.3194	-3.4597	H	4.4894	4.1608	-4.6235
C	-1.7248	2.3428	-3.4786	H	3.7135	3.1067	-2.4950

atom	x	y	z	atom	x	y	z
C	-1.0274	2.6249	-1.1895	H	4.5616	0.8187	-2.1720
C	-0.8918	4.0344	-1.2126	N	-1.9441	-1.0212	0.0000
H	-1.5895	1.6949	-6.7375	C	-4.7246	-0.7998	0.0000
H	-3.3380	3.4965	-6.8335	H	-5.8144	-0.6399	-0.0001
H	-4.1611	4.4892	-4.6235	N	-1.7571	-1.3607	4.6746
H	-3.1067	3.7137	-2.4950	N	-1.8558	-1.0916	2.3540
H	-0.8181	4.5616	-2.1720	C	-2.1976	-1.9393	5.8257
N	1.0212	-1.9441	0.0000	C	-3.1896	-2.9129	5.8682
C	0.7999	-4.7246	0.0000	C	-3.7433	-3.3511	4.6467
H	0.6399	-5.8144	-0.0001	C	-3.3197	-2.7625	3.4597
N	1.3608	-1.7570	4.6746	C	-2.3429	-1.7246	3.4786
N	1.0917	-1.8557	2.3540	C	-2.6249	-1.0274	1.1895
C	1.9393	-2.1975	5.8257	C	-4.0344	-0.8919	1.2126
C	2.9130	-3.1895	5.8682	H	-1.6953	-1.5890	6.7376
C	3.3511	-3.7433	4.6467	H	-3.4969	-3.3374	6.8335
C	2.7624	-3.3198	3.4597	H	-4.4898	-4.1604	4.6236
C	1.7246	-2.3429	3.4785	H	-3.7139	-3.1063	2.4950
C	1.0273	-2.6249	1.1895	H	-4.5617	-0.8185	2.1720
C	0.8919	-4.0344	1.2126	N	-1.7569	-1.3610	-4.6746
H	1.5892	-1.6951	6.7375	N	-1.8557	-1.0917	-2.3540
H	3.3375	-3.4968	6.8335	C	-2.1974	-1.9396	-5.8257
H	4.1604	-4.4898	4.6236	C	-3.1893	-2.9133	-5.8681
H	3.1062	-3.7140	2.4950	C	-3.7429	-3.3516	-4.6466
H	0.8182	-4.5617	2.1720	C	-3.3194	-2.7628	-3.4597
N	1.3610	-1.7569	-4.6746	C	-2.3427	-1.7248	-3.4786
N	1.0918	-1.8557	-2.3540	C	-2.6248	-1.0274	-1.1895
C	1.9397	-2.1972	-5.8257	C	-4.0344	-0.8920	-1.2126
C	2.9134	-3.1892	-5.8681	H	-1.6952	-1.5892	-6.7376
C	3.3516	-3.7429	-4.6466	H	-3.4965	-3.3380	-6.8335
C	2.7628	-3.3194	-3.4597	H	-4.4894	-4.1609	-4.6235
C	1.7248	-2.3427	-3.4785	H	-3.7135	-3.1067	-2.4950
C	1.0274	-2.6248	-1.1895	H	-4.5617	-0.8186	-2.1720
C	0.8919	-4.0344	-1.2126				

Table S5: Atomic coordinates of $Mo_2MnMo_2(tpda)_4(NCS)_2$ (helical conformation)

atom	x	y	z	atom	x	y	z
Mo	-0.0003	0.0000	2.5039	H	-4.0690	-2.5182	2.3153
Mo	-0.0003	-0.0001	4.5962	C	-2.5907	-1.3032	3.3553
Mo	-0.0004	-0.0001	-2.5040	C	-2.8510	-0.3172	1.1535
Mo	-0.0003	0.0000	-4.5963	C	-4.2668	-0.2355	1.1921
Mn	-0.0004	-0.0001	-0.0001	H	-4.8065	-0.3563	2.1387
N	-0.0003	2.1827	-0.0001	N	-1.0716	-1.9540	-4.5599
C	0.0022	4.9582	0.0005	N	-0.6281	-2.0655	-2.2646
H	0.0036	6.0601	0.0008	C	-1.6671	-2.4335	-5.6846
N	-1.0721	1.9537	4.5597	H	-1.4178	-1.8876	-6.6056
N	-0.6286	2.0652	2.2644	C	-2.5508	-3.5089	-5.6888
C	-1.6677	2.4332	5.6844	H	-2.9998	-3.8437	-6.6337
H	-1.4186	1.8872	6.6054	C	-2.8767	-4.1033	-4.4528
C	-2.5511	3.5088	5.6885	H	-3.6242	-4.9097	-4.3939
H	-3.0001	3.8436	6.6334	C	-2.2561	-3.6444	-3.2931
C	-2.8764	4.1037	4.4526	H	-2.5173	-4.0695	-2.3160
H	-3.6236	4.9104	4.3937	C	-1.3020	-2.5912	-3.3557
C	-2.2559	3.6446	3.2930	C	-0.3162	-2.8511	-1.1537
H	-2.5167	4.0700	2.3158	C	-0.2336	-4.2669	-1.1921
C	-1.3024	2.5909	3.3555	H	-0.3533	-4.8068	-2.1387
C	-0.3164	2.8509	1.1536	N	1.0713	1.9539	-4.5599
C	-0.2335	4.2666	1.1924	N	0.6280	2.0651	-2.2646
H	-0.3531	4.8062	2.1391	C	1.6674	2.4330	-5.6844
N	0.0004	-2.1828	-0.0002	H	1.4180	1.8874	-6.6056
C	0.0018	-4.9583	0.0000	C	2.5511	3.5085	-5.6884
H	0.0028	-6.0602	-0.0001	H	3.0003	3.8432	-6.6332
N	1.0718	-1.9537	4.5597	C	2.8762	4.1034	-4.4525
N	0.6285	-2.0650	2.2644	H	3.6236	4.9099	-4.3934
C	1.6677	-2.4329	5.6844	C	2.2555	3.6444	-3.2929
H	1.4183	-1.8872	6.6055	H	2.5163	4.0697	-2.3157
C	2.5514	-3.5083	5.6884	C	1.3021	2.5905	-3.3556
H	3.0005	-3.8431	6.6333	C	0.3169	2.8508	-1.1536
C	2.8768	-4.1031	4.4525	C	0.2368	4.2667	-1.1917
H	3.6240	-4.9098	4.3935	H	0.3587	4.8067	-2.1379
C	2.2561	-3.6441	3.2928	N	-1.9539	1.0722	-4.5596
H	2.5168	-4.0696	2.3157	N	-2.0654	0.6286	-2.2644

atom	x	y	z	atom	x	y	z
C	1.3025	-2.5905	3.3555	C	-2.4332	1.6681	-5.6842
C	0.3171	-2.8508	1.1535	H	-1.8876	1.4186	-6.6053
C	0.2365	-4.2666	1.1920	C	-3.5080	2.5524	-5.6881
H	0.3579	-4.8064	2.1384	H	-3.8428	3.0017	-6.6329
N	2.1823	0.0003	-0.0001	C	-4.1023	2.8784	-4.4520
C	4.9578	-0.0003	0.0002	H	-4.9085	3.6261	-4.3929
H	6.0597	-0.0006	0.0003	C	-3.6436	2.2573	-3.2925
N	1.9530	1.0727	4.5594	H	-4.0687	2.5183	-2.3152
N	2.0646	0.6291	2.2642	C	-2.5908	1.3028	-3.3553
C	2.4324	1.6683	5.6841	C	-2.8512	0.3169	-1.1535
H	1.8868	1.4187	6.6053	C	-4.2670	0.2358	-1.1917
C	3.5072	2.5527	5.6881	H	-4.8070	0.3569	-2.1381
H	3.8420	3.0018	6.6330	N	1.9533	-1.0723	-4.5596
C	4.1013	2.8789	4.4520	N	2.0648	-0.6287	-2.2644
H	4.9077	3.6264	4.3931	C	2.4326	-1.6680	-5.6843
C	3.6426	2.2580	3.2924	H	1.8871	-1.4184	-6.6054
H	4.0678	2.5189	2.3152	C	3.5074	-2.5525	-5.6882
C	2.5901	1.3031	3.3553	H	3.8422	-3.0016	-6.6330
C	2.8504	0.3171	1.1535	C	4.1014	-2.8787	-4.4521
C	4.2662	0.2354	1.1921	H	4.9076	-3.6264	-4.3930
H	4.8059	0.3560	2.1386	C	3.6427	-2.2577	-3.2925
N	-2.1829	-0.0004	-0.0001	H	4.0677	-2.5188	-2.3153
C	-4.9584	0.0003	0.0003	C	2.5902	-1.3029	-3.3554
H	-6.0603	0.0006	0.0004	C	2.8505	-0.3169	-1.1535
N	-1.9537	-1.0727	4.5595	C	4.2663	-0.2358	-1.1918
N	-2.0652	-0.6292	2.2642	H	4.8063	-0.3568	-2.1382
C	-2.4330	-1.6686	5.6841	N	-0.0003	0.0001	-6.8880
H	-1.8873	-1.4191	6.6052	C	-0.0004	0.0001	-8.0904
C	-3.5080	-2.5527	5.6880	S	-0.0004	0.0001	-9.7038
H	-3.8429	-3.0018	6.6329	N	-0.0004	-0.0001	6.8879
C	-4.1025	-2.8784	4.4520	C	-0.0004	-0.0001	8.0903
H	-4.9090	-3.6258	4.3930	S	-0.0005	0.0000	9.7037
C	-3.6437	-2.2575	3.2924				

Table S6: Atomic coordinates of $Mo_2FeMo_2(tpda)_4(NCS)_2$ (*meso* conformation)

atom	x	y	z	atom	x	y	z
Fe	0.0000	0.0000	0.0000	H	1.6093	-1.6736	-6.7237
Mo	0.0000	0.0000	4.6547	H	3.3627	-3.4707	-6.8169
Mo	0.0000	0.0000	2.5479	H	4.1672	-4.4785	-4.6072
Mo	0.0000	0.0000	-4.6547	H	3.0923	-3.7205	-2.4824
Mo	0.0000	0.0000	-2.5479	H	0.8192	-4.5637	-2.1715
N	0.0000	0.0000	6.9335	N	1.9387	0.9737	0.0000
C	0.0000	0.0000	8.1358	C	4.7258	0.7832	0.0000
S	0.0000	0.0000	9.7487	H	5.8164	0.6286	0.0000
N	0.0000	0.0000	-6.9335	N	1.7513	1.3629	4.6639
C	0.0000	0.0000	-8.1358	N	1.8582	1.0788	2.3492
S	0.0000	0.0000	-9.7487	C	2.1858	1.9486	5.8136
N	-0.9630	1.9394	0.0000	C	3.1790	2.9213	5.8548
C	-0.7925	4.7295	0.0000	C	3.7403	3.3505	4.6337
H	-0.6444	5.8210	0.0000	C	3.3226	2.7547	3.4481
N	-1.3617	1.7522	4.6636	C	2.3440	1.7188	3.4689
N	-1.0747	1.8614	2.3493	C	2.6232	1.0008	1.1869
C	-1.9520	2.1821	5.8126	C	4.0341	0.8750	1.2110
C	-2.9284	3.1716	5.8533	H	1.6783	1.6052	6.7249
C	-3.3563	3.7338	4.6321	H	3.4814	3.3519	6.8189
C	-2.7559	3.3204	3.4473	H	4.4884	4.1583	4.6096
C	-1.7165	2.3456	3.4690	H	3.7224	3.0916	2.4833
C	-0.9977	2.6257	1.1875	H	4.5598	0.8084	2.1717
C	-0.8810	4.0373	1.2109	N	1.7512	1.3631	-4.6639
H	-1.6093	1.6736	6.7237	N	1.8582	1.0788	-2.3492
H	-3.3623	3.4710	6.8169	C	2.1856	1.9488	-5.8136
H	-4.1670	4.4788	4.6072	C	3.1788	2.9215	-5.8548
H	-3.0920	3.7209	2.4825	C	3.7400	3.3508	-4.6336
H	-0.8192	4.5638	2.1714	C	3.3224	2.7549	-3.4481
N	-1.3619	1.7521	-4.6636	C	2.3439	1.7189	-3.4689
N	-1.0748	1.8613	-2.3493	C	2.6232	1.0009	-1.1869
C	-1.9521	2.1819	-5.8126	C	4.0341	0.8750	-1.2110
C	-2.9287	3.1714	-5.8533	H	1.6782	1.6053	-6.7249
C	-3.3566	3.7335	-4.6321	H	3.4812	3.3522	-6.8189
C	-2.7561	3.3202	-3.4473	H	4.4881	4.1587	-4.6096
C	-1.7166	2.3455	-3.4690	H	3.7222	3.0919	-2.4833

atom	x	y	z	atom	x	y	z
C	-0.9977	2.6256	-1.1876	H	4.5597	0.8085	-2.1718
C	-0.8810	4.0373	-1.2109	N	-1.9387	-0.9737	0.0000
H	-1.6094	1.6736	-6.7237	C	-4.7258	-0.7833	0.0000
H	-3.3626	3.4708	-6.8169	H	-5.8164	-0.6287	0.0000
H	-4.1673	4.4785	-4.6072	N	-1.7513	-1.3629	4.6639
H	-3.0923	3.7206	-2.4824	N	-1.8582	-1.0788	2.3492
H	-0.8193	4.5637	-2.1715	C	-2.1857	-1.9486	5.8136
N	0.9629	-1.9394	0.0000	C	-3.1790	-2.9213	5.8548
C	0.7924	-4.7295	0.0000	C	-3.7403	-3.3506	4.6336
H	0.6444	-5.8210	0.0000	C	-3.3226	-2.7547	3.4481
N	1.3618	-1.7521	4.6636	C	-2.3440	-1.7188	3.4689
N	1.0747	-1.8614	2.3493	C	-2.6232	-1.0008	1.1869
C	1.9520	-2.1820	5.8126	C	-4.0341	-0.8750	1.2110
C	2.9284	-3.1716	5.8533	H	-1.6782	-1.6053	6.7249
C	3.3563	-3.7338	4.6321	H	-3.4814	-3.3519	6.8189
C	2.7559	-3.3204	3.4473	H	-4.4883	-4.1584	4.6096
C	1.7165	-2.3456	3.4690	H	-3.7224	-3.0916	2.4833
C	0.9976	-2.6257	1.1875	H	-4.5598	-0.8085	2.1717
C	0.8809	-4.0373	1.2109	N	-1.7512	-1.3631	-4.6639
H	1.6092	-1.6737	6.7237	N	-1.8582	-1.0788	-2.3492
H	3.3624	-3.4710	6.8169	C	-2.1856	-1.9488	-5.8135
H	4.1669	-4.4788	4.6072	C	-3.1788	-2.9215	-5.8547
H	3.0920	-3.7208	2.4824	C	-3.7400	-3.3509	-4.6336
H	0.8191	-4.5638	2.1714	C	-3.3224	-2.7549	-3.4481
N	1.3619	-1.7520	-4.6636	C	-2.3439	-1.7189	-3.4689
N	1.0748	-1.8613	-2.3493	C	-2.6232	-1.0009	-1.1869
C	1.9522	-2.1819	-5.8126	C	-4.0341	-0.8751	-1.2110
C	2.9287	-3.1714	-5.8532	H	-1.6782	-1.6053	-6.7249
C	3.3567	-3.7335	-4.6321	H	-3.4811	-3.3522	-6.8189
C	2.7561	-3.3202	-3.4472	H	-4.4881	-4.1587	-4.6095
C	1.7167	-2.3455	-3.4690	H	-3.7221	-3.0919	-2.4833
C	0.9977	-2.6256	-1.1876	H	-4.5597	-0.8085	-2.1718
C	0.8810	-4.0373	-1.2109				

Table S7: Atomic coordinates of $Mo_2FeMo_2(tpda)_4(NCS)_2$ (helical conformation)

atom	x	y	z	atom	x	y	z
Mo	0.0000	0.0000	2.4588	H	-4.0393	-2.5714	2.3022
Mo	0.0000	0.0000	4.5619	C	-2.5667	-1.3482	3.3415
Mo	0.0000	0.0000	-2.4587	C	-2.8285	-0.3426	1.1490
Mo	0.0000	0.0000	-4.5618	C	-4.2451	-0.2742	1.1839
Fe	0.0000	0.0000	0.0000	H	-4.7838	-0.4275	2.1263
N	-0.0032	2.1515	-0.0058	N	-1.1162	-1.9251	-4.5426
C	0.0011	4.9371	-0.0014	N	-0.6649	-2.0501	-2.2558
H	0.0029	6.0390	0.0003	C	-1.7284	-2.3865	-5.6659
N	-1.1198	1.9250	4.5332	H	-1.4765	-1.8391	-6.5851
N	-0.6705	2.0442	2.2436	C	-2.6271	-3.4494	-5.6703
C	-1.7274	2.3925	5.6563	H	-3.0884	-3.7709	-6.6140
H	-1.4733	1.8492	6.5773	C	-2.9487	-4.0513	-4.4367
C	-2.6259	3.4557	5.6582	H	-3.7046	-4.8500	-4.3785
H	-3.0842	3.7819	6.6017	C	-2.3130	-3.6101	-3.2784
C	-2.9525	4.0507	4.4226	H	-2.5709	-4.0398	-2.3023
H	-3.7091	4.8485	4.3628	C	-1.3482	-2.5666	-3.3414
C	-2.3205	3.6034	3.2644	C	-0.3428	-2.8285	-1.1490
H	-2.5809	4.0282	2.2867	C	-0.2747	-4.2451	-1.1839
C	-1.3553	2.5610	3.3298	H	-0.4285	-4.7837	-2.1262
C	-0.3462	2.8264	1.1385	N	1.1162	1.9251	-4.5426
C	-0.2742	4.2422	1.1792	N	0.6649	2.0501	-2.2558
H	-0.4266	4.7779	2.1235	C	1.7284	2.3865	-5.6659
N	0.0031	-2.1515	-0.0058	H	1.4764	1.8391	-6.5851
C	-0.0015	-4.9371	-0.0014	C	2.6272	3.4492	-5.6703
H	-0.0034	-6.0390	0.0003	H	3.0886	3.7707	-6.6140
N	1.1197	-1.9250	4.5332	C	2.9491	4.0510	-4.4367
N	0.6705	-2.0442	2.2436	H	3.7052	4.8495	-4.3785
C	1.7272	-2.3926	5.6563	C	2.3133	3.6099	-3.2783
H	1.4729	-1.8493	6.5774	H	2.5714	4.0394	-2.3022
C	2.6260	-3.4556	5.6582	C	1.3483	2.5666	-3.3414
H	3.0842	-3.7818	6.6018	C	0.3429	2.8285	-1.1489
C	2.9530	-4.0502	4.4226	C	0.2745	4.2451	-1.1838
H	3.7098	-4.8479	4.3629	H	0.4283	4.7838	-2.1261
C	2.3210	-3.6030	3.2643	N	-1.9250	1.1197	-4.5332
H	2.5816	-4.0276	2.2867	N	-2.0441	0.6706	-2.2435

atom	x	y	z	atom	x	y	z
C	1.3553	-2.5610	3.3298	C	-2.3927	1.7272	-5.6563
C	0.3463	-2.8265	1.1385	H	-1.8494	1.4729	-6.5774
C	0.2740	-4.2422	1.1792	C	-3.4559	2.6257	-5.6582
H	0.4263	-4.7780	2.1234	H	-3.7821	3.0839	-6.6018
N	2.1515	-0.0034	0.0059	C	-4.0507	2.9525	-4.4227
C	4.9371	0.0010	0.0014	H	-4.8486	3.7091	-4.3630
H	6.0390	0.0026	-0.0003	C	-3.6034	2.3206	-3.2644
N	1.9251	1.1162	4.5427	H	-4.0281	2.5811	-2.2868
N	2.0502	0.6647	2.2559	C	-2.5611	1.3553	-3.3298
C	2.3865	1.7282	5.6660	C	-2.8264	0.3465	-1.1384
H	1.8393	1.4762	6.5852	C	-4.2421	0.2744	-1.1792
C	3.4492	2.6272	5.6703	H	-4.7779	0.4270	-2.1234
H	3.7708	3.0885	6.6140	N	1.9249	-1.1196	-4.5332
C	4.0508	2.9492	4.4366	N	2.0441	-0.6706	-2.2436
H	4.8493	3.7053	4.3784	C	2.3926	-1.7270	-5.6564
C	3.6097	2.3134	3.2783	H	1.8494	-1.4727	-6.5774
H	4.0392	2.5714	2.3022	C	3.4558	-2.6256	-5.6583
C	2.5667	1.3481	3.3415	H	3.7821	-3.0837	-6.6020
C	2.8285	0.3425	1.1490	C	4.0505	-2.9525	-4.4228
C	4.2451	0.2741	1.1839	H	4.8483	-3.7092	-4.3631
H	4.7838	0.4273	2.1263	C	3.6032	-2.3207	-3.2645
N	-2.1515	0.0034	0.0059	H	4.0279	-2.5812	-2.2869
C	-4.9371	-0.0010	0.0014	C	2.5610	-1.3552	-3.3298
H	-6.0390	-0.0026	-0.0003	C	2.8264	-0.3464	-1.1384
N	-1.9252	-1.1162	4.5427	C	4.2421	-0.2743	-1.1792
N	-2.0502	-0.6647	2.2558	H	4.7779	-0.4268	-2.1234
C	-2.3865	-1.7283	5.6660	N	-0.0001	0.0000	-6.8442
H	-1.8392	-1.4764	6.5852	C	-0.0001	0.0000	-8.0465
C	-3.4492	-2.6273	5.6703	S	-0.0001	0.0000	-9.6601
H	-3.7708	-3.0886	6.6140	N	0.0000	0.0000	6.8442
C	-4.0509	-2.9492	4.4366	C	0.0000	0.0000	8.0465
H	-4.8494	-3.7053	4.3784	S	-0.0001	0.0001	9.6601
C	-3.6098	-2.3134	3.2783				