Supplementary Information

Table S1. IR spectra of parent compounds and complex **1**.

	Components		$\{Mn^{II}(hfac)_2 \cdot (\mu_2\text{-TMI-NPS})\}_2$ (**1**)
	TMI-NPS	$Mn^{II}(hfac)_2$	
TMI-NPS	456w		459w
	551w		-
	589w		583w*
	687w		-
	734s		725w
	745s		749w*
	753s		756w
	808s		791w 796w sp
	820m		804w*
	862w		857w 867w
	936m		946w
	987s		954w 965w
	1014m		1020w
	1027m		1041w
	1085m		1089m 1096m sp*
	1108m		-
	1144w		1149vs*
	1156m		-
	1210w		1206s 1218m
	1238m		
	1250s		-
	1277m		1254s*
	1304m		1285m
	1340w		-
	1359m		1331m
	1379m		1362w
	1441w		1377w
	1461m		-
	1488s		1451m*
	1516w		1478m
	1590m		1504m 1511m
	1613m		1590m 1596m sp
	1640m		1616w
	2893w		1645s
	2925w		-
	2966m		-
	3045m		2963w*
	3063w		-
			3066w
$Mn^{II}(hfac)_2$		525w	-
		584m	583w*
		666s	664w 669w sp
		740w744w	749w*
		806s	804w*
		1090m	1089m 1096m sp*
		1134s	1149vs*
		1250m	1254s*
		1347w	-
		1460s	1451m*
		1538w	1527s
		1566w	1552m
		1612w	-
		1638m	1656m
		2971w	2963w*

*bands are coincided, sp. –split band, w- weak, m- middle, s- strong intensity.
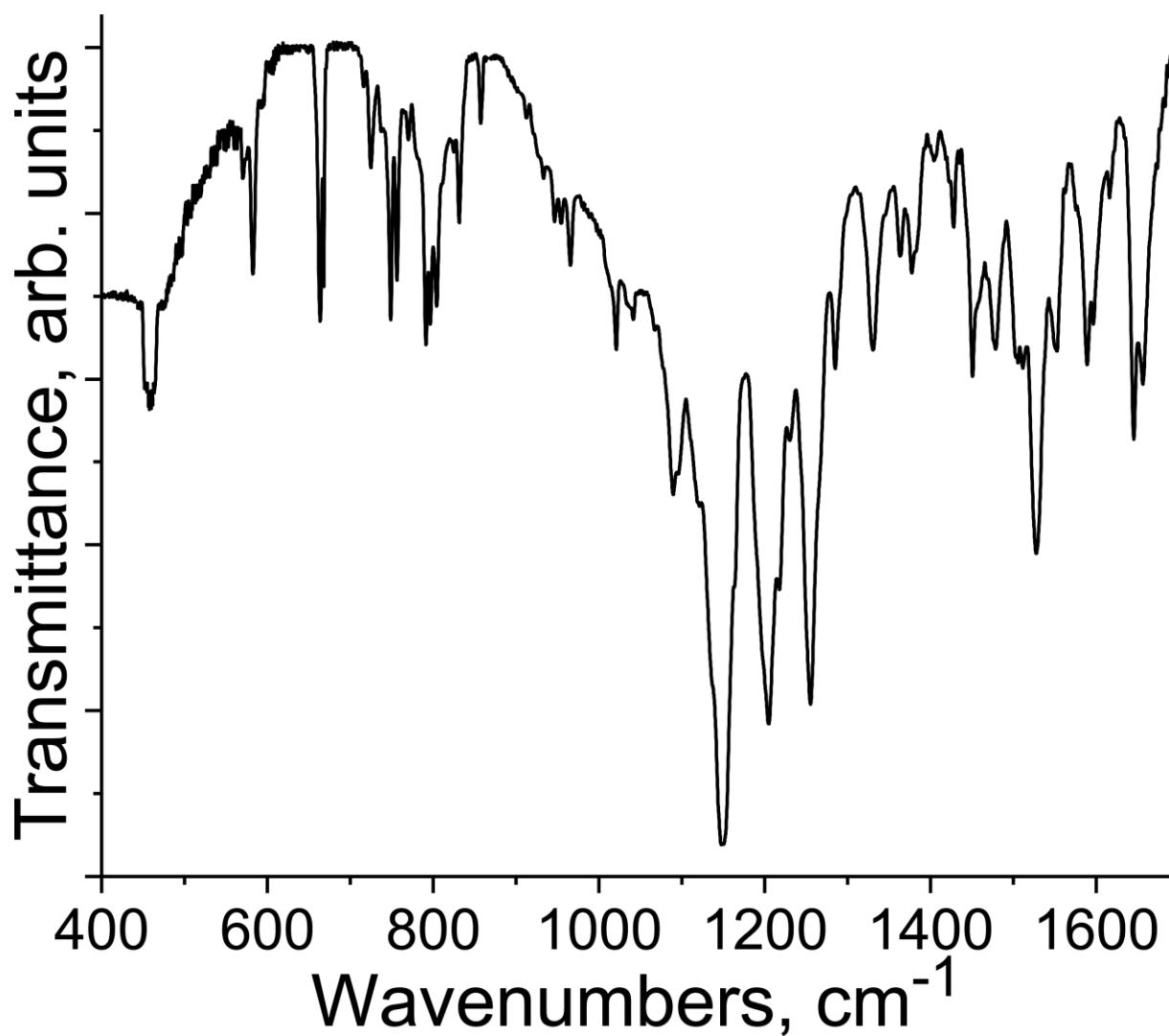
Fig. S1. IR-spectrum of {Mn^{II}(hfac)$_2$·(μ_2-TMI-NPS)}$_2$ (**1**) measured in KBr pellet prepared in anaerobic conditions.
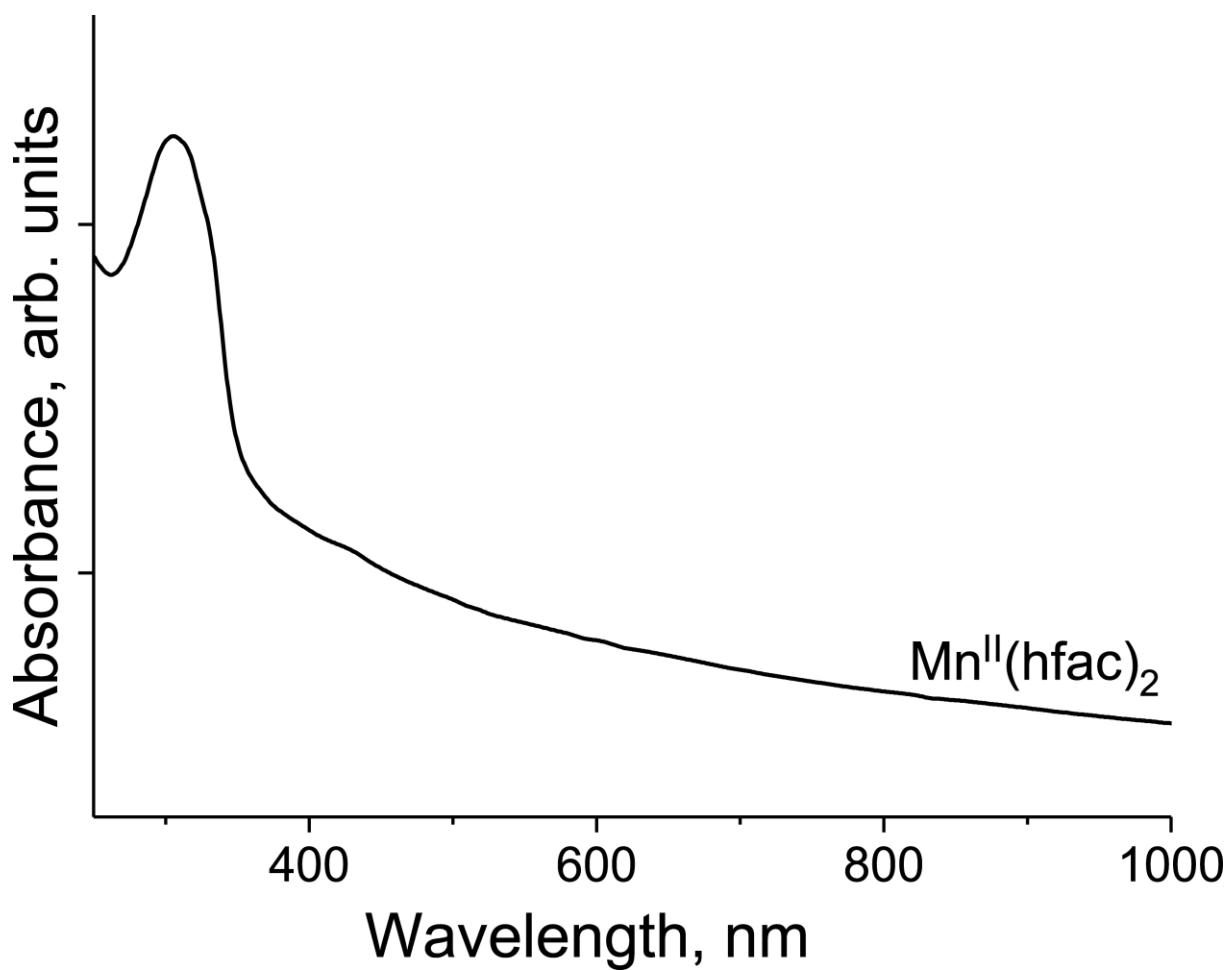
**Fig. S2.** UV-visible-NIR spectrum of starting $Mn^{II}(hfac)_2$ in KBr pellet in the 250-1000 nm range..

Crystal structure of 1.
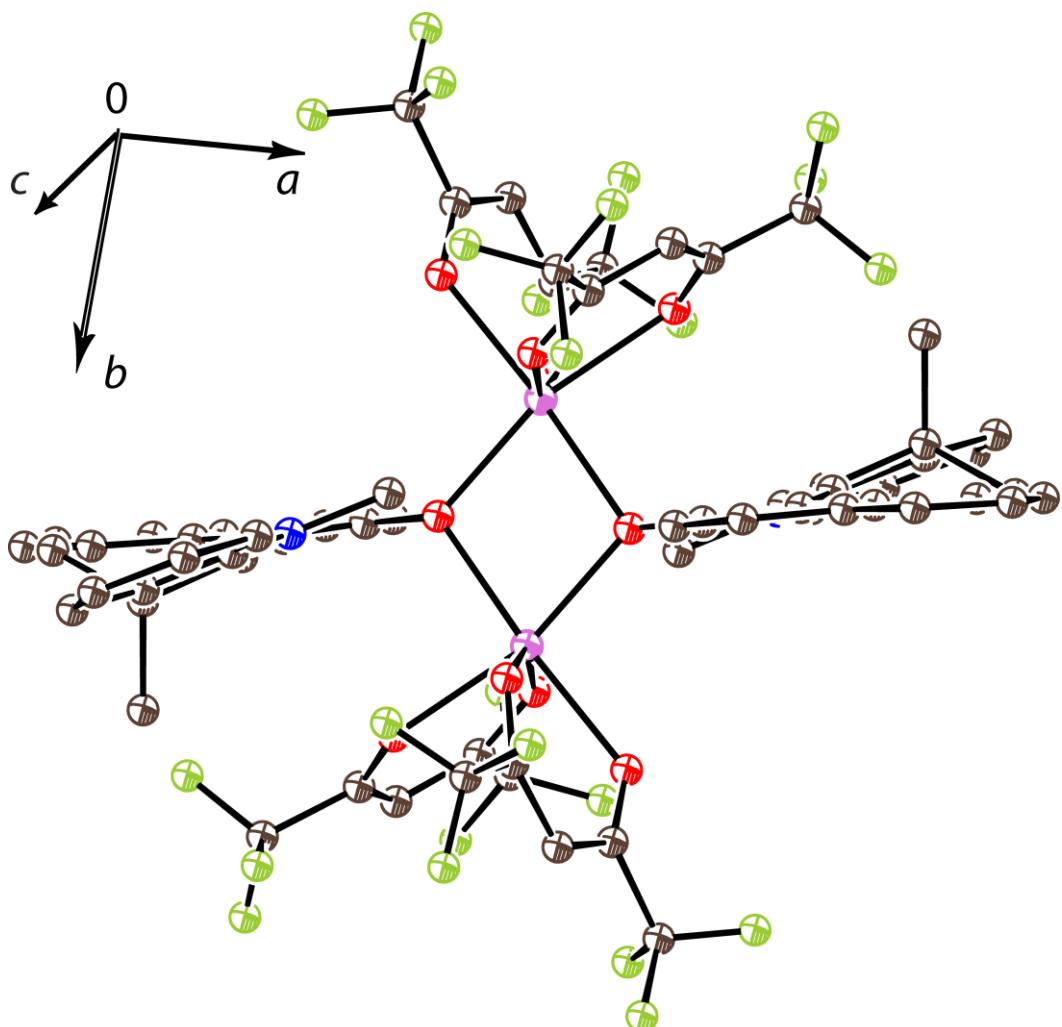
**Fig. S3.** View on the $\{Mn^{II}(hfac)_2 \cdot (\mu_2\text{-TMI-NPS})\}_2$ dimer in **1** approximately perpendicular to the Mn_2O_2 plane. Oxygen is red, nitrogen is blue, fluorine is green, carbon is brown and manganese is pink.
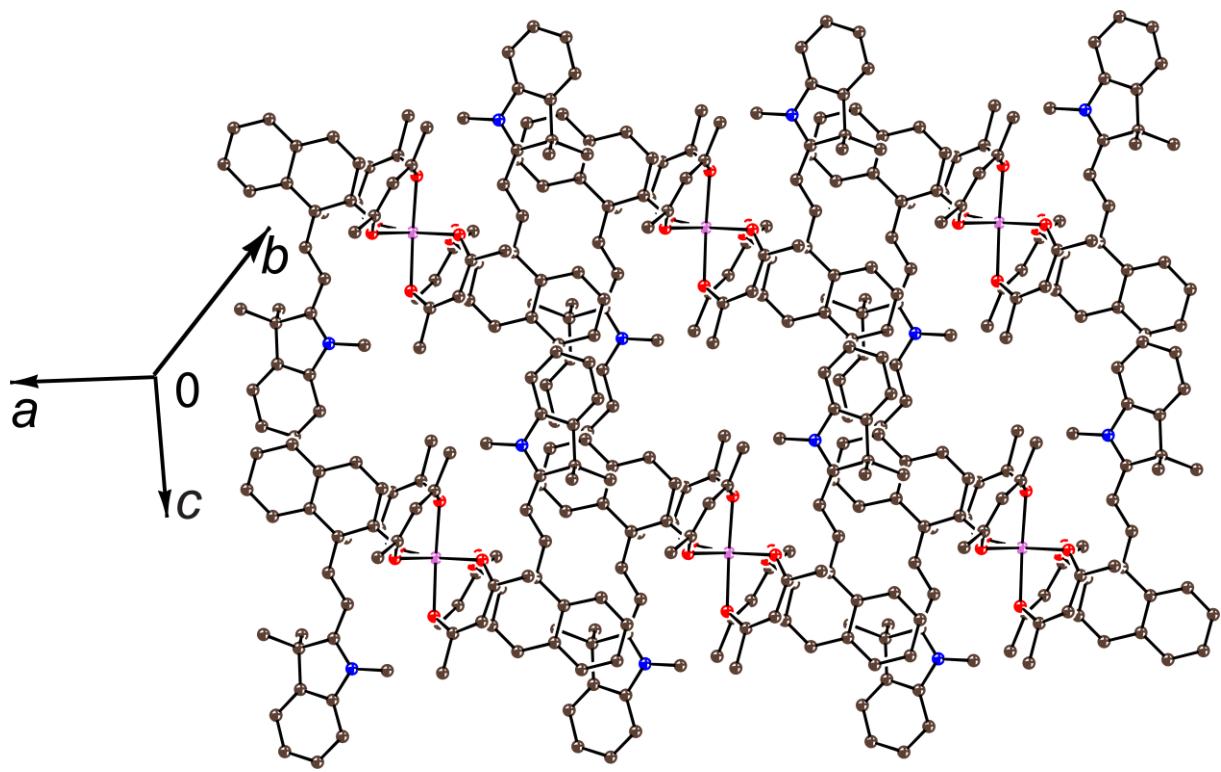
**Fig. S4.** View on the layers composed of the $\{Mn^{II}(hfac)_2 \cdot (\mu_2\text{-TMI-NPS})\}_2$ dimers in **1**. The formation of van der Waals contacts between the TMI-NPS ligands is observed in the chains and between the chains indicating layered packing of the components.

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Data of magnetic measurements.
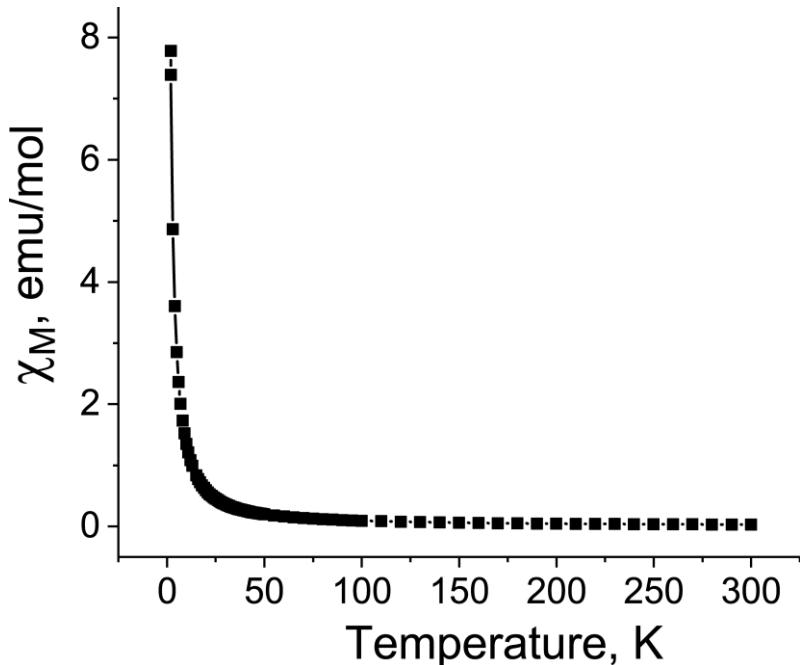
Fig. S5a. Data of SQUID measurement for polycrystalline **1**. Temperature dependence of molar

magnetic susceptibility is shown in the 1.9-300 K range after subtraction of temperature

independent contribution.
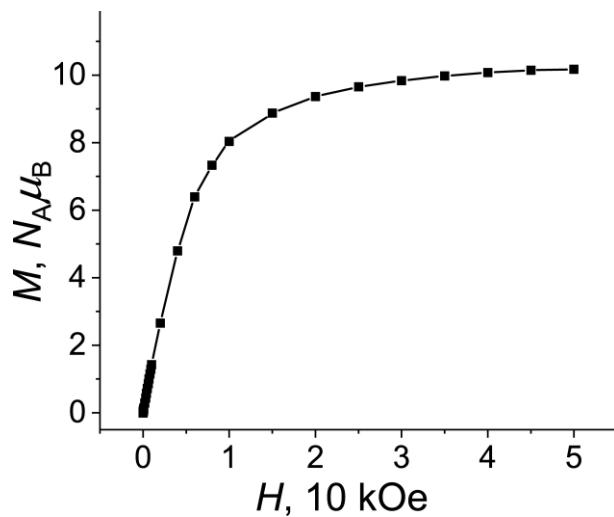
Fig. S5b. Magnetization of **1** in μ_B *vs* magnetic field up to 50 kOe (black line is a guide to the

eye);
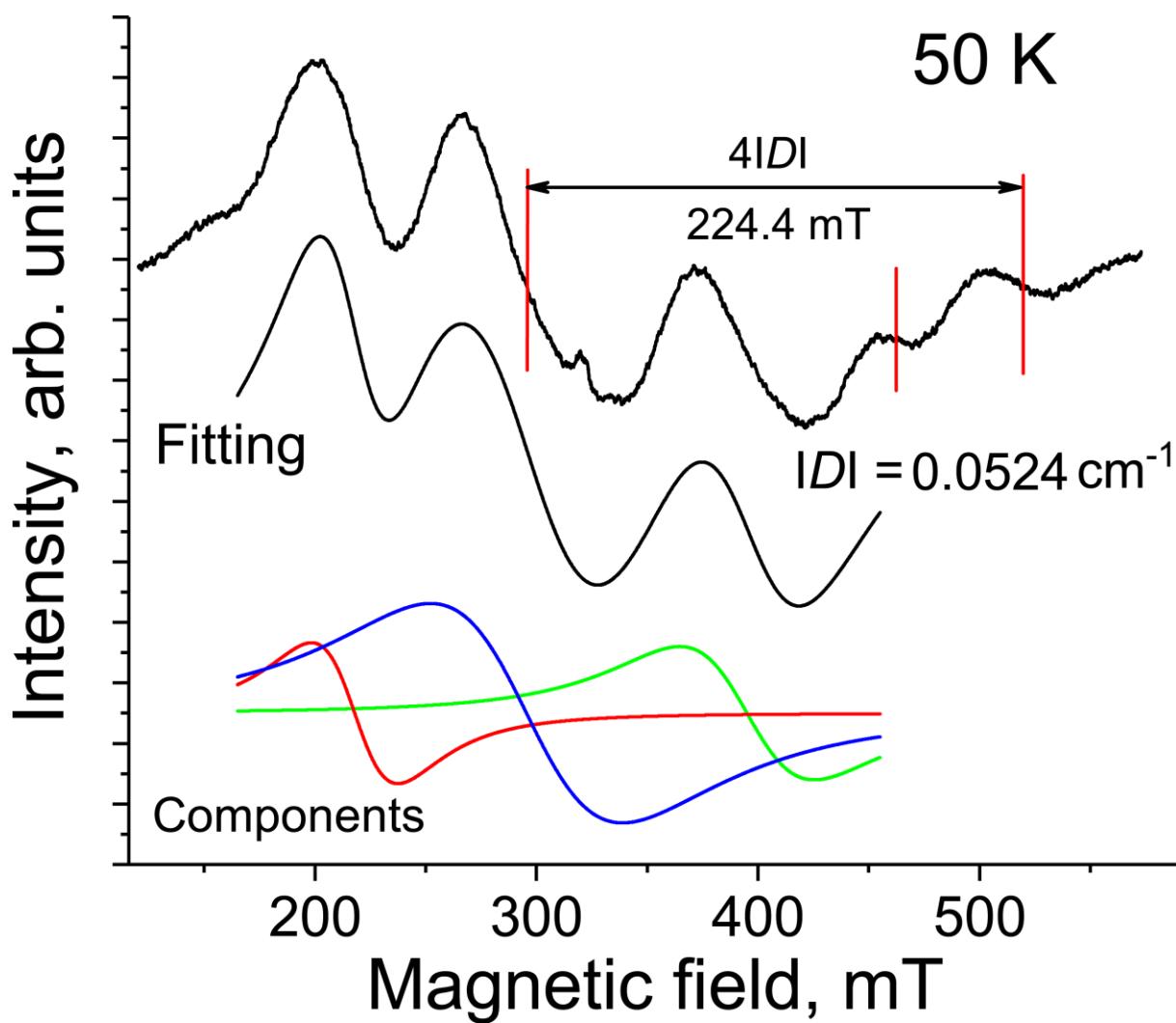
Fig. S6. EPR spectrum of polycrystalline **1** at 50 K. Determination of the g_1, g_2, and g_3 values together with zero-field splitting $|D|$ is shown. Determined values are given in the text.
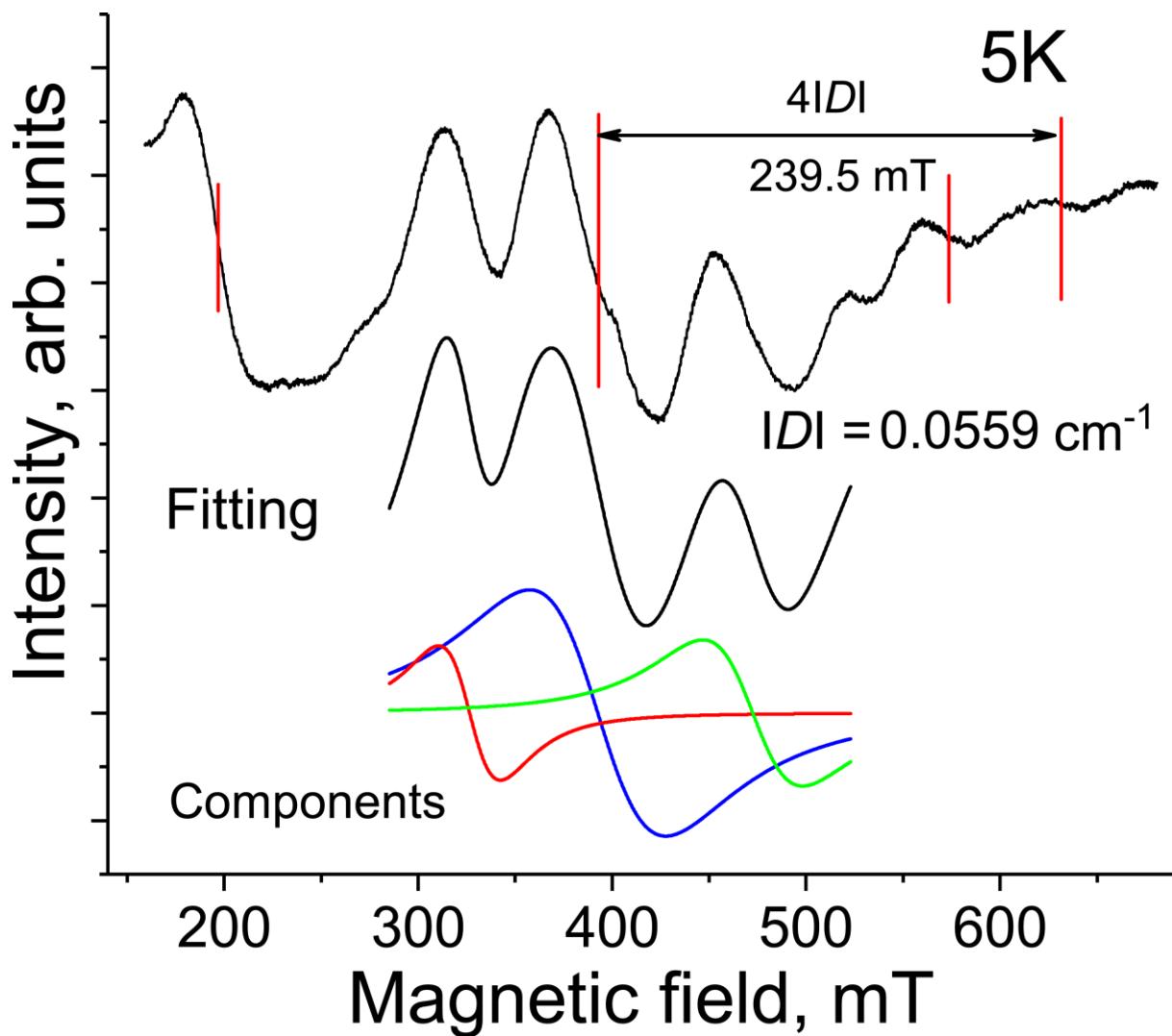
Fig. S7. EPR spectrum of polycrystalline **1** at 5 K. Determination of the g_1, g_2, and g_3 values together with zero-field splitting |D| is shown. Determined values are given in the text.

Theoretical calculations

Optimization of the molecular structures was performed using the PBE exchange-correlation functional[2] and with the extended basis set Mn: [9s9p8d/5s5p4d], O,N,C : [5s5p2d/3s3p2d], H :[5s1p/3s1p] for the valence electrons and the SBK pseudopotential[3] implemented in the **PRIRODA** package[4]. The Hirschfeld method[5] was used to calculate atomic charges. Electronic spectra are estimated using results of TDDFT calculations with Gaussian widening of lines with half width 20 nm. Energetic effects are given at $T = 0$ taking into account the contribution of zero point vibration energies. All calculations were performed at Joint Supercomputer Center of the Russian Academy of Sciences.

The value of the exchange parameter J is determined by the set of matrix elements between magnetic orbitals localized at centers a and b:

$$\left\langle a_i(1)b_j(2)\left|h(1)+h(2)+\frac{1}{r_{12}}\right|b_j(1)a_i(2)\right\rangle = 2\langle a_i|b_j\rangle\langle a_i|h|b_j\rangle + \left\langle a_i(1)b_j(2)\left|\frac{1}{r_{12}}\right|b_j(1)a_i(2)\right\rangle$$
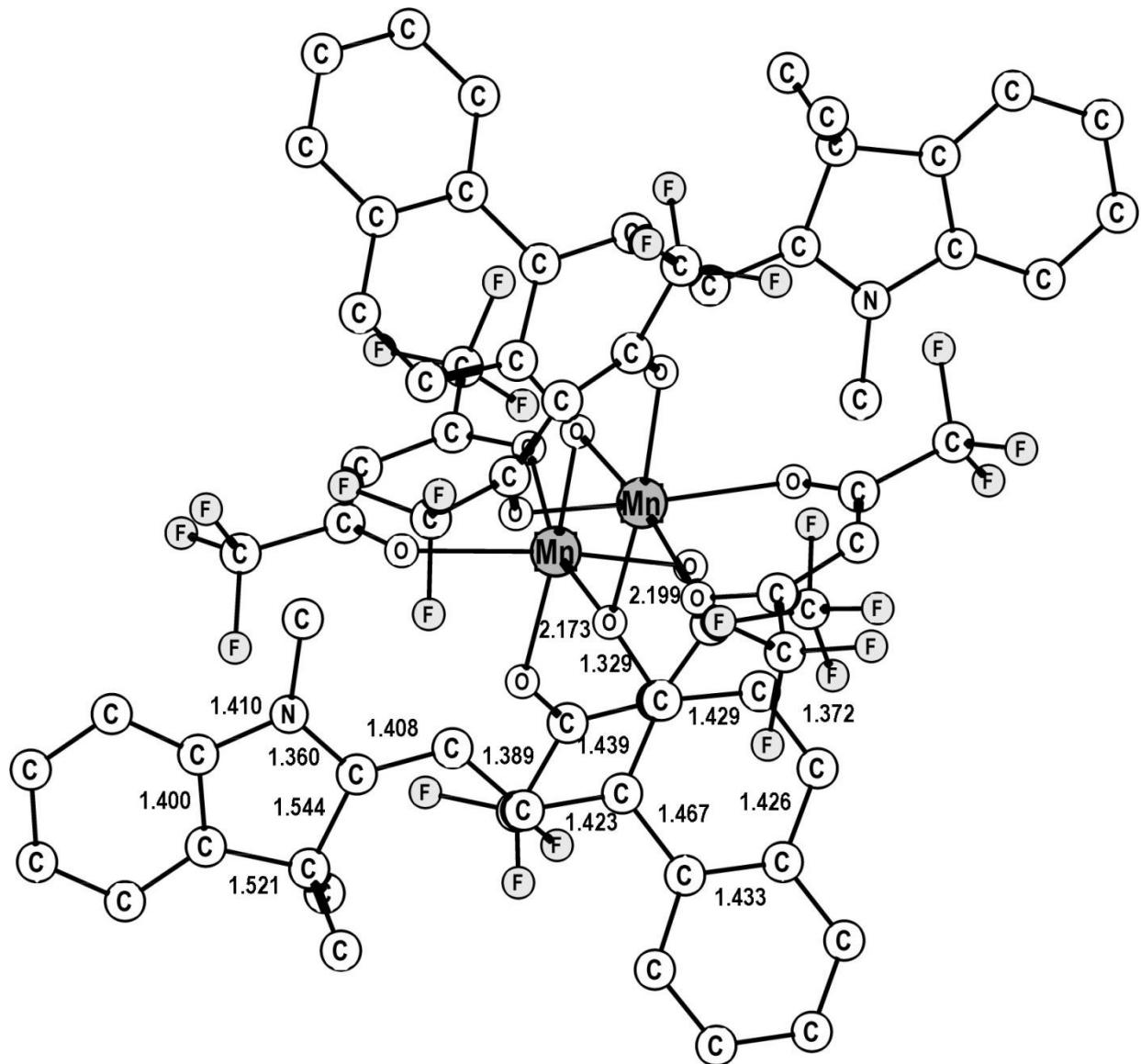
Fig S9. Optimized structure of the {Mn^{II}(hfac)$_2$·(μ_2-TMI-NPS)}$_2$ dimer.
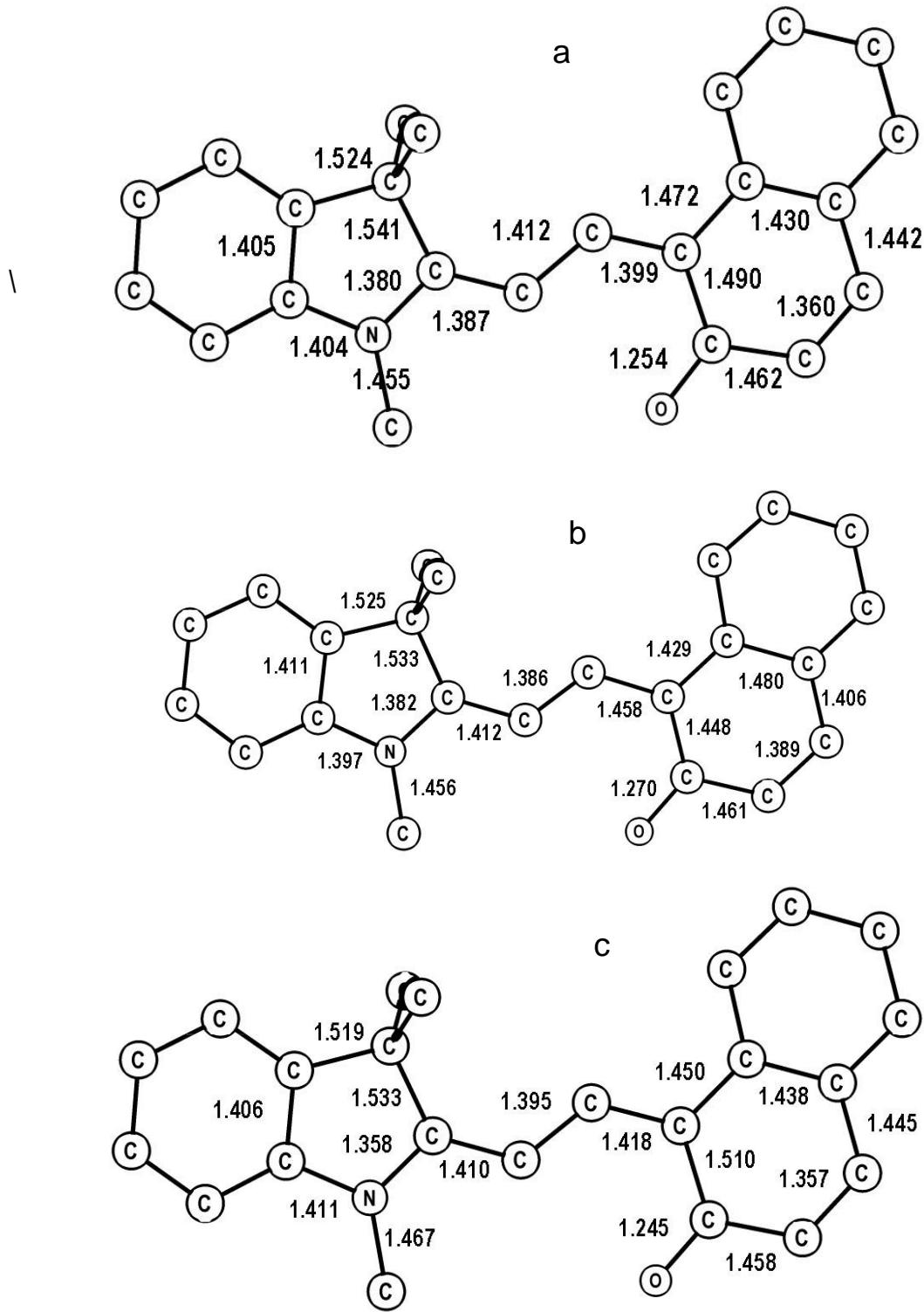
Fig. S10. Optimized structure of: (a) free TMI-NPS ligand in the open form; (b) the excited free TMI-NPS ligand in the open form. Excitation corresponds to intense transition for this ligand observed in visible range; (c) free ligand in the open form in the radical cation TMI-NPS$^{\bullet+}$ state.

References.

[1] Sheldrick, G. M., *Acta Crystallogr., Sect. A: Fundam. Crystallogr*. 2008, **64**, 112-122.

[2] J. P. Perdew, K. Burke, M. Ernzerhof, *Phys. Rev. Lett.***1996**, *77*, 3865-3868.

[3] Stevens, W. J.; Basch, H., Krauss, M. J. Chem. Phys., 1984, 81, 6026

[4] D. N. Laikov, *Chem. Phys. Lett.,***1997**, *281*, 151 - 156.

[5] F. L. Hirshfeld, *Theor. Chim.Acta* **1977**, *44*, 129-138.

Cartesian coordinates of the calculated structures

TMI-NPS open form

8	2.53449485	-2.23310386	1.26015346
7	1.22980962	0.02400531	-2.54086225
6	1.79233919	-2.01304483	2.24613454
6	2.14908831	-2.57459515	3.54773815
1	3.07360874	-3.15343465	3.57558022
6	1.37873052	-2.39578309	4.65389162
1	1.67703620	-2.83490802	5.61061148
6	0.14833284	-1.64477035	4.61585700
6	-0.63072724	-1.51030507	5.78621095
1	-0.27108950	-1.97625263	6.70692442
6	-1.83059306	-0.80792860	5.77856567
1	-2.42438091	-0.71196528	6.68853818
6	-2.26955571	-0.23135093	4.57466256
1	-3.21489418	0.31385758	4.54352208
6	-1.51238639	-0.35291851	3.41150525
1	-1.90834958	0.10007574	2.50252579
6	-0.27857904	-1.04898226	3.38743838
6	0.55286189	-1.18901582	2.18054600
6	0.19060303	-0.52515050	1.00408625
1	-0.70073648	0.10072054	1.06048633
6	0.86325640	-0.56231410	-0.23729286
1	1.74949645	-1.19630108	-0.26425044
6	0.48937781	0.12665558	-1.38129469
6	-0.70058473	1.06952589	-1.64688282
6	-0.47558871	1.43861038	-3.10847448
6	-1.20554513	2.26413110	-3.95695418
1	-2.10385247	2.77524837	-3.60360989
6	-0.77264841	2.43581110	-5.28414683
1	-1.33587487	3.08034918	-5.95983994
6	0.37847524	1.78185059	-5.74142734
1	0.70576097	1.92098581	-6.77291711
6	1.12498623	0.94600852	-4.89717392
1	2.01758688	0.44418168	-5.27123421
6	0.67812234	0.78957748	-3.58075554
6	2.43197085	-0.78719222	-2.65305553
1	3.18018725	-0.47275459	-1.91084464

1	2.85469366	-0.67321455	-3.65613858
1	2.20276528	-1.84878641	-2.47763525
6	-0.63669217	2.33635441	-0.75787102
1	-0.76282166	2.08922974	0.30446125
1	-1.43690886	3.03389158	-1.04623908
1	0.32592084	2.85220259	-0.87619568
6	-2.05644611	0.33939043	-1.48159072
1	-2.10210617	-0.55526868	-2.11734306
1	-2.87838099	1.00963652	-1.77347916
1	-2.22076301	0.02704110	-0.44193035

TMI-NPS open form, excited state $S = 0$

8	2.54692236	-2.16913119	1.26831189
7	1.23381980	0.06618501	-2.52637335
6	1.76596962	-1.98824838	2.25297627
6	2.08779467	-2.65522952	3.51253686
1	2.99140178	-3.26833075	3.49861976
6	1.31902490	-2.53736591	4.66307078
1	1.60581769	-3.05802211	5.58036261
6	0.15877505	-1.74339414	4.65827671
6	-0.63456920	-1.61667606	5.83250268
1	-0.31277795	-2.15337616	6.72782967
6	-1.77386009	-0.84337131	5.84687266
1	-2.37975420	-0.74844943	6.74807141
6	-2.15444611	-0.15978445	4.65039019
1	-3.05659940	0.45572571	4.65652508
6	-1.41545549	-0.25380523	3.48909740
1	-1.76475724	0.29479841	2.61718315
6	-0.21927832	-1.04388721	3.40945002
6	0.57311009	-1.16741313	2.22664757
6	0.16925039	-0.46620193	1.01324169
1	-0.74328959	0.12519233	1.07725103
6	0.83977934	-0.49039754	-0.19963704
1	1.74703896	-1.09940067	-0.20680915
6	0.46297657	0.17900341	-1.38462632
6	-0.73625516	1.08435503	-1.68766615
6	-0.48890009	1.42857922	-3.15205409
6	-1.21725594	2.21962381	-4.03315664

1	-2.13438967	2.71700887	-3.70906474
6	-0.76144760	2.37580000	-5.35544745
1	-1.32472202	2.99382432	-6.05540596
6	0.41635828	1.73820160	-5.77648776
1	0.76126413	1.86511148	-6.80395955
6	1.16337020	0.93758772	-4.90303762
1	2.07489467	0.45017930	-5.24999078
6	0.69354418	0.79428789	-3.58922471
6	2.45528247	-0.72177508	-2.60263402
1	3.19015512	-0.36892123	-1.86497231
1	2.88321747	-0.62873726	-3.60565812
1	2.24748957	-1.78198870	-2.39720444
6	-0.72598839	2.37037107	-0.81810681
1	-0.85205092	2.13422067	0.24699038
1	-1.54807597	3.03500758	-1.12353306
1	0.21943838	2.91672233	-0.93728667
6	-2.08531904	0.33356261	-1.52600511
1	-2.10722532	-0.57164659	-2.14780562
1	-2.91569383	0.98501837	-1.83729725
1	-2.25458415	0.03518723	-0.48276311

TMI-NPS open form, excited state $S = 1$

8	2.76374563	-1.66639706	1.40640945
7	1.14642376	-0.04987976	-2.54700552
6	1.94121088	-1.67237600	2.36878713
6	2.31362499	-2.29805440	3.62329980
1	3.30870674	-2.74492238	3.65020064
6	1.49572513	-2.29026971	4.71939732
1	1.81564884	-2.74201825	5.66146632
6	0.19064918	-1.70232897	4.65185459
6	-0.66241519	-1.72016731	5.77620498
1	-0.29478510	-2.17048876	6.70122402
6	-1.94678333	-1.18871359	5.72171426
1	-2.58941647	-1.21414808	6.60329004
6	-2.41935842	-0.62947190	4.51446345
1	-3.43407614	-0.23242383	4.45747460
6	-1.59996561	-0.59154125	3.39700058
1	-2.00033014	-0.17294297	2.47456573

6	-0.26628114	-1.10167131	3.41943181
6	0.60248958	-1.03846586	2.27084656
6	0.18052446	-0.35377034	1.07433837
1	-0.65115673	0.34093184	1.18381611
6	0.76113853	-0.50298361	-0.18867186
1	1.57114286	-1.22981527	-0.24128901
6	0.43172102	0.17606403	-1.36998408
6	-0.65828509	1.21813950	-1.65087762
6	-0.44905785	1.47569320	-3.13899785
6	-1.12790516	2.31304621	-4.01641385
1	-1.96339434	2.92539520	-3.66982689
6	-0.72712655	2.36665744	-5.36447378
1	-1.25206584	3.02058549	-6.06163878
6	0.34319324	1.58025492	-5.81592653
1	0.64185288	1.62587159	-6.86442847
6	1.03868384	0.72994678	-4.94680954
1	1.86140672	0.11787982	-5.31694297
6	0.62906080	0.69411251	-3.60514363
6	2.26979324	-0.96520020	-2.66255133
1	2.94623363	-0.84699115	-1.80590479
1	2.82558014	-0.74126728	-3.57971577
1	1.92968154	-2.01248704	-2.69671086
6	-0.43103261	2.51976832	-0.83738680
1	-0.52202923	2.33646462	0.24154233
1	-1.17806465	3.27582780	-1.12227943
1	0.56787862	2.93383754	-1.03061416
6	-2.08077280	0.65900301	-1.39266251
1	-2.25618113	-0.25539399	-1.97557481
1	-2.83633573	1.40363730	-1.68453305
1	-2.22929703	0.42107314	-0.33096416

TMI-NPS$^{\bullet+}$ radical-cation, open form, charge = +1, S = 1/2

8	2.52588204	-2.18820250	1.26570536
7	1.18912889	0.00635034	-2.52190369
6	1.81503310	-1.98179435	2.26690167
6	2.21284310	-2.51475213	3.56488576
1	3.15481609	-3.06294097	3.58781963
6	1.44525962	-2.33935219	4.67052304

1	1.76082274	-2.74856964	5.63320892
6	0.18350825	-1.63623413	4.62019286
6	-0.59378665	-1.51657045	5.78472030
1	-0.21863830	-1.94604807	6.71537051
6	-1.82977920	-0.86723686	5.76298395
1	-2.42166181	-0.78543887	6.67521566
6	-2.31200436	-0.33045273	4.55582104
1	-3.28450621	0.16177999	4.52781822
6	-1.55665110	-0.43200967	3.39427858
1	-1.97781748	-0.02198331	2.47733966
6	-0.28410749	-1.07061413	3.38355270
6	0.53817050	-1.17917301	2.19359832
6	0.16173032	-0.50856911	1.00246824
1	-0.71757591	0.13056491	1.07040978
6	0.82129270	-0.56910914	-0.22508381
1	1.69267751	-1.22208873	-0.26565294
6	0.45408785	0.13795257	-1.38789066
6	-0.70777537	1.10273185	-1.65042960
6	-0.47407365	1.45938138	-3.10845212
6	-1.17883035	2.29750529	-3.96653752
1	-2.06525928	2.83766866	-3.63003990
6	-0.72557822	2.43896667	-5.28851464
1	-1.26541872	3.09187557	-5.97493812
6	0.41334740	1.75156863	-5.74143315
1	0.74447710	1.87704304	-6.77243658
6	1.13254466	0.90593917	-4.89095061
1	2.01273924	0.37732389	-5.25546343
6	0.66395448	0.78065149	-3.57800963
6	2.38268225	-0.83667749	-2.64651362
1	3.12657433	-0.55169284	-1.89205940
1	2.81352513	-0.70165716	-3.64170880
1	2.11618188	-1.89280207	-2.50880493
6	-0.60667369	2.37066057	-0.76081482
1	-0.74527143	2.13106276	0.30126866
1	-1.39019425	3.08275847	-1.05415376
1	0.36633525	2.86604408	-0.87900524
6	-2.08091156	0.39945631	-1.48191004
1	-2.15222981	-0.49673560	-2.11268035

1	-2.88144920	1.09088167	-1.77857619
1	-2.25742040	0.10253783	-0.44011933

TMI-NPS closed form, $S = 0$

8	0.44612266	0.53213173	0.41571522
7	0.58755429	-0.17981914	-1.86649764
6	0.06982245	-0.33733070	1.39060013
6	0.98236871	-0.49614102	2.46387167
1	1.92706157	0.04755487	2.42766928
6	0.66028571	-1.32089648	3.52052581
1	1.36047290	-1.44341009	4.34969357
6	-0.57561665	-2.02870524	3.55495540
6	-0.90383542	-2.88596278	4.63932085
1	-0.18526581	-2.99356840	5.45530377
6	-2.10434335	-3.57322284	4.66826791
1	-2.34494019	-4.22850688	5.50670729
6	-3.02025555	-3.42444874	3.60040517
1	-3.96606508	-3.96902038	3.61891234
6	-2.72846143	-2.59642445	2.52835708
1	-3.45177179	-2.51113467	1.71691989
6	-1.50679072	-1.87044793	2.46888622
6	-1.16699255	-0.99537192	1.37828127
6	-2.03593207	-0.71801371	0.25359969
1	-3.05585772	-1.10494021	0.25292739
6	-1.61915712	0.02051530	-0.80056404
1	-2.28153796	0.20415192	-1.64493255
6	-0.22548010	0.56031539	-0.90782801
6	-0.09004760	2.05945201	-1.42189646
6	1.27461654	2.00567165	-2.09578730
6	2.13071415	3.02162761	-2.50354905
1	1.89128221	4.06823175	-2.30134469
6	3.32086727	2.68823682	-3.17902834
1	4.00349845	3.47638116	-3.49918334
6	3.62998133	1.34785545	-3.43528507
1	4.55677024	1.09659207	-3.95447045
6	2.77512489	0.31080193	-3.02422202
1	3.03705004	-0.73052931	-3.21494482
6	1.59548587	0.65992140	-2.35700198

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6    0.80089907  -1.61003437  -1.72803566
1    1.61480102  -1.85149299  -1.02030329
1    1.05195206  -2.04568715  -2.70623713
1   -0.12711436  -2.08036703  -1.37914849
6   -0.20476951   3.09010021  -0.29073334
1   -1.17351848   3.00241813   0.22400312
1   -0.14483446   4.10515764  -0.71091975
1    0.59359631   2.97474973   0.45087489
6   -1.15396973   2.36238105  -2.50501146
1   -1.14855472   1.60811524  -3.30480703
1   -0.93120220   3.33643782  -2.96256689
1   -2.16401318   2.41667557  -2.07149915
```

{[Mn(hfac)$_2$](TMI-NPS)}$_2$ dimer, S = 5

```
25  -0.24528638  -1.65913021  -0.15586152
 9  -3.53624330  -4.94992419  -0.89919873
 9  -4.73780832  -3.62133167   0.36580453
 9  -3.94654381  -5.49380216   1.18332281
 9   0.00168280  -3.10285113   4.67958220
 9  -0.37850825  -5.17572798   4.08049648
 9   1.47449496  -4.18542616   3.46771447
 9   1.90401731  -5.93602729  -0.18653329
 9   3.44446898  -4.79254607  -1.24982813
 9   2.13549116  -6.16144744  -2.35221188
 9  -0.66683048  -3.91754159  -5.22767254
 9  -0.52267245  -1.73406988  -5.14447790
 9  -2.31687277  -2.74837713  -4.39328530
 8  -1.28701768   0.23162220   0.39529205
 8  -2.11926668  -2.69464375   0.01180524
 8   0.02120325  -2.39676448   1.91203525
 8   1.10017638  -3.32067557  -0.51466020
 8  -0.64728381  -1.89406518  -2.31265215
 7  -3.49433370   1.48714488  -3.72769341
 6   0.14176910  -3.99931563   3.65654252
 6  -2.17987899   0.32333017   1.37499073
 6  -1.74167299   0.06109946   2.71014453
 1  -0.69545332  -0.20313852   2.84430494
 6  -2.58432632   0.15120187   3.78835180
```

1	-2.20667739	-0.04980190	4.79384406
6	-3.96045693	0.49019836	3.62754565
6	-4.82835751	0.53590388	4.74721976
1	-4.41364694	0.32670576	5.73581230
6	-6.17423948	0.82784500	4.59582555
1	-6.83704393	0.85961404	5.46144182
6	-6.68114305	1.06194108	3.30203044
1	-7.74502902	1.26279765	3.16404461
6	-5.84559240	1.02420268	2.19177365
1	-6.29922455	1.16542577	1.21129499
6	-4.45548130	0.76585481	2.31221655
6	-3.54280008	0.73695495	1.16402198
6	-4.03147149	1.20758432	-0.08547417
1	-4.98098096	1.73624502	-0.02145958
6	-3.47232278	1.10928400	-1.35293456
1	-2.54958552	0.54806078	-1.47085877
6	-4.03987797	1.69065014	-2.50162288
6	-5.26100409	2.61753557	-2.64753144
6	-5.24268721	2.89974951	-4.14308320
6	-6.07787148	3.68493474	-4.93169568
1	-6.91186545	4.23586498	-4.49215371
6	-5.82788547	3.76381813	-6.31238226
1	-6.47111028	4.37775597	-6.94382721
6	-4.75656305	3.06386631	-6.88466185
1	-4.57335772	3.13888634	-7.95730745
6	-3.90869368	2.26784529	-6.10177285
1	-3.07336313	1.73565885	-6.55561976
6	-4.17848321	2.20261483	-4.73248711
6	-2.33066147	0.63865196	-3.96916964
1	-1.43791943	1.09614065	-3.52220100
1	-2.18589322	0.52222056	-5.04622981
1	-2.48785472	-0.34914562	-3.52024754
6	-5.08706966	3.92909615	-1.84281427
1	-5.07753922	3.74036510	-0.76175672
1	-5.92186771	4.60912667	-2.06621278
1	-4.14971051	4.43545863	-2.10654718
6	-6.58155110	1.89312709	-2.27596745
1	-6.68982646	0.95273863	-2.83303980

1	-7.43390651	2.54026117	-2.52745815
1	-6.63594309	1.66693758	-1.20356455
6	-3.66456976	-4.45142917	0.35684059
6	-2.37904801	-3.67368637	0.76255584
6	-1.65767940	-4.12365864	1.88522836
1	-2.00183459	-5.00899345	2.40998429
6	-0.52689259	-3.44180327	2.36629347
6	2.16801530	-5.26444600	-1.33317812
6	1.17760433	-4.07717523	-1.51899599
6	0.51383935	-3.95906089	-2.75353613
1	0.67546836	-4.71841753	-3.51162399
6	-0.33328195	-2.87495835	-3.04351099
6	-0.96355421	-2.83582032	-4.46725720
25	0.28038716	1.70080082	0.10985802
9	3.50846920	5.06858550	0.72128253
9	4.70422516	3.76833524	-0.57833140
9	3.83560286	5.61509478	-1.37533177
9	-0.18702882	3.10614930	-4.71876937
9	0.19105101	5.18906529	-4.15468068
9	-1.62330166	4.18274942	-3.45856784
9	-1.80270561	6.01199746	0.20179082
9	-3.34431336	4.86546014	1.25909889
9	-2.01935825	6.20929554	2.37249471
9	1.03428502	4.08341778	5.07023673
9	0.71534297	1.91674396	5.11746685
9	2.54445165	2.74216455	4.23072409
8	1.33118362	-0.19030220	-0.41027778
8	2.12583628	2.77051247	-0.13775485
8	-0.07755751	2.41809144	-1.95443748
8	-1.06775350	3.34879294	0.51544910
8	0.77022658	1.95100091	2.24815969
7	3.41427596	-1.52886053	3.75429142
6	-0.29712891	4.01055091	-3.69930443
6	2.24677301	-0.28663119	-1.36891066
6	1.85525111	0.03488991	-2.70539191
1	0.82653467	0.35370587	-2.85801758
6	2.72100436	-0.06430466	-3.76428693
1	2.37958667	0.18270585	-4.77247774

6	4.07406891	-0.47604762	-3.58058588
6	4.96376150	-0.53777159	-4.68232712
1	4.58235792	-0.28228672	-5.67343800
6	6.28897284	-0.90293573	-4.51046604
1	6.96882825	-0.94684988	-5.36219848
6	6.75283905	-1.19751532	-3.21296800
1	7.80098298	-1.45927245	-3.05769332
6	5.89559054	-1.14417284	-2.12010399
1	6.32005541	-1.33956934	-1.13604258
6	4.52394795	-0.80859193	-2.26195002
6	3.58689077	-0.75825129	-1.13341260
6	4.03168910	-1.25313707	0.12325098
1	4.96799720	-1.80623011	0.07868075
6	3.44781656	-1.14592212	1.37897701
1	2.53325765	-0.56779468	1.47740152
6	3.98126637	-1.73799472	2.53865292
6	5.18615328	-2.68261151	2.70827568
6	5.13259322	-2.96812210	4.20228489
6	5.93930871	-3.76731243	5.00634380
1	6.77553815	-4.32786201	4.58353425
6	5.65691948	-3.84819308	6.38067158
1	6.27763431	-4.47292116	7.02395301
6	4.58168343	-3.13704835	6.93141867
1	4.37263222	-3.21469152	7.99913926
6	3.76231110	-2.32689670	6.13279586
1	2.92243440	-1.78713600	6.56896068
6	4.06506319	-2.25909238	4.77054052
6	2.25658735	-0.66843441	3.97908485
1	1.35357615	-1.14654629	3.57597328
1	2.13766633	-0.49700199	5.05228584
1	2.40389297	0.29526374	3.47824019
6	5.01069393	-3.99129955	1.89936943
1	5.02722450	-3.80323373	0.81843104
1	5.83035266	-4.68340026	2.14095119
1	4.06053193	-4.48383757	2.14297931
6	6.52404334	-1.97620253	2.36562397
1	6.63522886	-1.03984158	2.92891227
1	7.36187468	-2.63680957	2.63061555

1	6.60258563	-1.74552584	1.29565983
6	3.60983331	4.56858773	-0.53676481
6	2.33303535	3.75492791	-0.89749632
6	1.56127055	4.18301473	-1.99509631
1	1.86462836	5.07477494	-2.53394646
6	0.43007135	3.47357306	-2.43243155
6	-2.06527908	5.32644672	1.34177994
6	-1.08077559	4.13106873	1.50285742
6	-0.34393159	4.03996561	2.69786874
1	-0.45392420	4.82072310	3.44336779
6	0.50924807	2.95566133	2.96805692
6	1.20881860	2.94322612	4.35956744

{[Mn(hfac)$_2$]$_2$(TMI-NPS)$_2$} complex, $Sz = 4$

25	-0.52989856	-1.78199727	-0.27958655
9	-3.70236703	-5.03448081	-0.88152824
9	-4.68960883	-3.83379622	0.66321165
9	-3.80167101	-5.76984870	1.18001101
9	0.50563859	-3.72029944	4.37331307
9	0.19759151	-5.70163004	3.49025067
9	1.88332652	-4.46535977	2.83903290
9	0.78185521	-6.10495454	-0.86033126
9	2.32686768	-5.09667551	-2.04217452
9	0.70338557	-6.16996340	-3.04948937
9	-2.95442952	-3.72485352	-4.68672919
9	-1.88758788	-1.91893691	-5.32292181
9	-3.56803435	-1.76685717	-3.92246455
8	-1.41207822	-0.07231999	0.32559533
8	-2.13730109	-2.89514093	-0.02393633
8	0.11703673	-2.61332491	1.74025605
8	0.46019452	-3.32311433	-0.96975688
8	-1.38288707	-1.61091673	-2.34532231
7	-2.61389794	2.17109543	-3.93734336
6	0.57653498	-4.43105857	3.20769537
6	-2.55909072	-0.11067339	1.06193660
6	-2.49777279	-0.74071203	2.33250290
1	-1.54508932	-1.17687710	2.63002302

6	-3.58415686	-0.77581716	3.17610072
1	-3.50434431	-1.26116837	4.15108756
6	-4.82164673	-0.18670782	2.79653392
6	-5.94956500	-0.25210207	3.65593196
1	-5.83862048	-0.75084641	4.62124143
6	-7.16597817	0.29008550	3.28024958
1	-8.02808837	0.23327878	3.94612306
6	-7.28533667	0.89915991	2.01306222
1	-8.24768140	1.30248177	1.69318544
6	-6.19496552	0.97723153	1.15728430
1	-6.35104933	1.41380452	0.17164819
6	-4.92073065	0.46612861	1.52242953
6	-3.75436262	0.54432657	0.64182211
6	-3.86523011	1.35811635	-0.53612320
1	-4.67748815	2.08080106	-0.48951137
6	-3.10873729	1.35385108	-1.69852507
1	-2.33195439	0.60026493	-1.80446782
6	-3.31789114	2.24649248	-2.77092787
6	-4.30244171	3.43145404	-2.87364114
6	-3.96492972	3.99018043	-4.24738297
6	-4.48007867	5.07765628	-4.94604669
1	-5.25863407	5.70853782	-4.51223502
6	-3.97636329	5.35783244	-6.22841256
1	-4.36744688	6.20856422	-6.78769406
6	-2.97473563	4.55662894	-6.79510038
1	-2.59428072	4.79103546	-7.79017965
6	-2.44833223	3.45711083	-6.10249830
1	-1.66486616	2.84026662	-6.54192912
6	-2.96631964	3.20066772	-4.82990618
6	-1.61322534	1.17795983	-4.30292679
1	-0.62652187	1.65278061	-4.38853429
1	-1.88513885	0.73293538	-5.26996550
1	-1.57493726	0.38663216	-3.55150733
6	-4.05260453	4.49807553	-1.78086335
1	-4.30847789	4.12314488	-0.78294226
1	-4.67457342	5.38179720	-1.98441825
1	-3.00089157	4.81210258	-1.76688858
6	-5.77785984	2.94919588	-2.87139380

1	-5.94931573	2.19156536	-3.64798780
1	-6.43881455	3.80376828	-3.07541659
1	-6.06760171	2.52269269	-1.90298453
6	-3.63693143	-4.65586441	0.42067813
6	-2.30520525	-3.92716973	0.71372547
6	-1.45428916	-4.43377622	1.69980418
1	-1.71082802	-5.37585715	2.17384543
6	-0.29081222	-3.75163012	2.11186660
6	0.99857601	-5.37726899	-1.98727813
6	0.17045797	-4.07460072	-1.96762311
6	-0.77517092	-3.85046971	-2.97260286
1	-0.95080868	-4.63232587	-3.70548938
6	-1.49800602	-2.64518637	-3.07137781
6	-2.49789818	-2.52535009	-4.25144496
25	0.05283351	1.44771615	0.59931354
9	3.76861318	3.82224836	2.30047261
9	4.84321314	2.23382241	1.23804003
9	4.75305609	4.25232915	0.39116664
9	1.21130059	3.18223274	-3.99239805
9	1.81599216	5.07548654	-3.07169606
9	-0.27769550	4.44212634	-2.99063016
9	-1.97034463	5.75279816	0.95179767
9	-3.70255351	4.60800006	1.66161396
9	-2.43931411	5.69125719	3.08809943
9	-1.19756729	2.25415987	5.95871172
9	-0.67046440	0.24976121	5.25679257
9	0.88680959	1.77591701	5.48440458
8	1.07581198	-0.64735313	-0.39343278
8	2.06295311	2.02128893	0.96729152
8	0.37143914	2.34509648	-1.34039519
8	-1.15584469	3.18625489	0.97246633
8	-0.02844420	1.23893542	2.77420071
7	3.40185593	-1.63044633	3.76094484
6	1.00324115	4.00235978	-2.91784110
6	1.98738473	-0.59683943	-1.36880538
6	1.54073121	-0.43828894	-2.71275124
1	0.46637591	-0.39238274	-2.87393551
6	2.41453424	-0.35232574	-3.76947331

1	2.03404547	-0.23336740	-4.78668223
6	3.82339120	-0.37488733	-3.56177100
6	4.72265315	-0.21904254	-4.64748179
1	4.31092793	-0.11281268	-5.65367531
6	6.09186103	-0.18830225	-4.44148215
1	6.77652866	-0.06599812	-5.28181545
6	6.59145375	-0.29197551	-3.12653713
1	7.66649480	-0.23241527	-2.94776600
6	5.72838925	-0.45108396	-2.04953712
1	6.15707833	-0.47490336	-1.04802509
6	4.32180174	-0.53041423	-2.22709509
6	3.39400196	-0.72831233	-1.11211747
6	3.94103364	-1.15208874	0.13607805
1	4.96470236	-1.51667293	0.06487113
6	3.35875696	-1.19069855	1.39475573
1	2.36141080	-0.77952800	1.51806456
6	3.98892349	-1.71839649	2.53623328
6	5.33114554	-2.45745815	2.67772820
6	5.32992349	-2.79141334	4.16309635
6	6.25817943	-3.47456865	4.94229352
1	7.16569409	-3.89044897	4.49965308
6	6.00876189	-3.62680505	6.31713663
1	6.72473311	-4.16342685	6.94069131
6	4.84625591	-3.09552352	6.89312916
1	4.66621329	-3.22219734	7.96152598
6	3.90383170	-2.40294407	6.12035272
1	3.00252874	-1.99752173	6.57893089
6	4.17113189	-2.26575574	4.75505365
6	2.14812845	-0.92530428	4.01122417
1	1.34288593	-1.35733306	3.40298195
1	1.88859253	-1.01502888	5.06889702
1	2.25628982	0.13573951	3.75192738
6	5.38042590	-3.74597337	1.82133092
1	5.35602117	-3.51554490	0.74819773
1	6.30987280	-4.29412192	2.03359313
1	4.53266854	-4.40562620	2.04658526
6	6.53195845	-1.52520464	2.36373516
1	6.48126316	-0.60012379	2.95349502

1	7.46962872	-2.04169018	2.61465320
1	6.56982329	-1.25418471	1.30100431
6	4.03947238	3.31743707	1.07041060
6	2.72207453	2.90693689	0.35220087
6	2.39794851	3.55039056	-0.85538279
1	3.05784035	4.32636136	-1.22956439
6	1.24596085	3.22099370	-1.59304259
6	-2.41191723	4.95454460	1.94801762
6	-1.54014862	3.66950697	2.07341062
6	-1.31925947	3.17709151	3.37146671
1	-1.72656336	3.72388101	4.21610490
6	-0.58857213	2.00034943	3.60994802
6	-0.40374808	1.57194089	5.09660209

{[Mn(acac)$_2$](TMI-NPS)}$_2$ dimer, $S = 5$

25	-0.24612247	-1.65454132	-0.15772066
1	-3.56141541	-4.85079995	-0.66286067
1	-4.53549557	-3.77386847	0.36224864
1	-3.89350247	-5.29004467	1.02354581
1	0.02824411	-3.27358843	4.47764191
1	-0.28162268	-4.95017817	3.99900772
1	1.21979172	-4.14538560	3.50182464
1	1.95283348	-5.80512863	-0.40405129
1	3.19699955	-4.87913656	-1.26779196
1	2.14083372	-5.98645425	-2.16048412
1	-0.72353199	-3.70929251	-5.08636510
1	-0.60944690	-1.94423842	-5.01433059
1	-2.06047189	-2.76040933	-4.40920492
8	-1.28785377	0.23621109	0.39343291
8	-2.12010277	-2.69005486	0.00994610
8	0.02036716	-2.39217559	1.91017611
8	1.09934029	-3.31608668	-0.51651934
8	-0.64811990	-1.88947629	-2.31451129
7	-3.49516979	1.49173377	-3.72955255
6	0.14093301	-3.99472674	3.65468338
6	-2.18071508	0.32791906	1.37313159
6	-1.74250908	0.06568835	2.70828539
1	-0.69628941	-0.19854963	2.84244580

6	-2.58516241	0.15579076	3.78649266
1	-2.20751348	-0.04521301	4.79198492
6	-3.96129302	0.49478725	3.62568651
6	-4.82919360	0.54049277	4.74536062
1	-4.41448303	0.33129465	5.73395316
6	-6.17507557	0.83243389	4.59396641
1	-6.83788002	0.86420293	5.45958268
6	-6.68197914	1.06652997	3.30017130
1	-7.74586511	1.26738654	3.16218547
6	-5.84642849	1.02879157	2.18991451
1	-6.30006064	1.17001466	1.20943585
6	-4.45631739	0.77044370	2.31035741
6	-3.54363617	0.74154384	1.16216284
6	-4.03230758	1.21217321	-0.08733331
1	-4.98181705	1.74083391	-0.02331872
6	-3.47315887	1.11387289	-1.35479370
1	-2.55042161	0.55264967	-1.47271791
6	-4.04071406	1.69523903	-2.50348202
6	-5.26184018	2.62212446	-2.64939058
6	-5.24352330	2.90433840	-4.14494234
6	-6.07870757	3.68952363	-4.93355482
1	-6.91270154	4.24045387	-4.49401285
6	-5.82872156	3.76840702	-6.31424140
1	-6.47194637	4.38234486	-6.94568635
6	-4.75739914	3.06845520	-6.88652099
1	-4.57419381	3.14347523	-7.95916659
6	-3.90952977	2.27243418	-6.10363199
1	-3.07419922	1.74024774	-6.55747890
6	-4.17931930	2.20720372	-4.73434625
6	-2.33149756	0.64324085	-3.97102878
1	-1.43875552	1.10072954	-3.52406014
1	-2.18672931	0.52680945	-5.04808895
1	-2.48869081	-0.34455673	-3.52210668
6	-5.08790575	3.93368504	-1.84467341
1	-5.07837531	3.74495399	-0.76361586
1	-5.92270380	4.61371556	-2.06807192
1	-4.15054660	4.44004752	-2.10840632
6	-6.58238719	1.89771598	-2.27782659

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1   -6.69066255   0.95732752  -2.83489894
1   -7.43474260   2.54485006  -2.52931729
1   -6.63677918   1.67152647  -1.20542369
6   -3.66540585  -4.44684028   0.35498145
6   -2.37988410  -3.66909748   0.76069670
6   -1.65851549  -4.11906975   1.88336922
1   -2.00267068  -5.00440456   2.40812515
6   -0.52772868  -3.43721438   2.36443433
6    2.16717921  -5.25985711  -1.33503726
6    1.17676824  -4.07258634  -1.52085513
6    0.51300326  -3.95447200  -2.75539527
1    0.67463227  -4.71382864  -3.51348313
6   -0.33411804  -2.87036946  -3.04537013
6   -0.96439030  -2.83123143  -4.46911634
25   0.27955107   1.70538971   0.10799888
1    3.52686389   4.97831493   0.48074696
1    4.49651535   3.92419646  -0.57233318
1    3.79161761   5.41967485  -1.21692369
1   -0.20938567   3.28751746  -4.52135833
1    0.09849911   4.97224318  -4.07098694
1   -1.37155109   4.15454089  -3.50627836
1   -1.85309940   5.88719656   0.41509147
1   -3.09904519   4.95874935   1.27314875
1   -2.02891599   6.04620663   2.17487387
1    1.06627640   3.87355165   4.93471006
1    0.81120010   2.12246509   4.96710244
1    2.29081128   2.78480972   4.25325200
8    1.33034753  -0.18571331  -0.41213692
8    2.12500019   2.77510136  -0.13961399
8   -0.07839360   2.42268033  -1.95629662
8   -1.06858959   3.35338183   0.51358996
8    0.76939049   1.95558980   2.24630055
7    3.41343987  -1.52427164   3.75243228
6   -0.29796500   4.01513980  -3.70116357
6    2.24593692  -0.28204230  -1.37076980
6    1.85441502   0.03947880  -2.70725105
1    0.82569858   0.35829476  -2.85987672
6    2.72016827  -0.05971577  -3.76614607
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1	2.37875058	0.18729474	-4.77433688
6	4.07323282	-0.47145873	-3.58244502
6	4.96292541	-0.53318270	-4.68418626
1	4.58152183	-0.27769783	-5.67529714
6	6.28813675	-0.89834684	-4.51232518
1	6.96799216	-0.94226099	-5.36405762
6	6.75200296	-1.19292643	-3.21482714
1	7.80014689	-1.45468356	-3.05955246
6	5.89475445	-1.13958395	-2.12196313
1	6.31921932	-1.33498045	-1.13790172
6	4.52311186	-0.80400304	-2.26380916
6	3.58605468	-0.75366240	-1.13527174
6	4.03085301	-1.24854818	0.12139184
1	4.96716111	-1.80164122	0.07682161
6	3.44698047	-1.14133323	1.37711787
1	2.53242156	-0.56320579	1.47554238
6	3.98043028	-1.73340583	2.53679378
6	5.18531719	-2.67802262	2.70641654
6	5.13175713	-2.96353321	4.20042575
6	5.93847262	-3.76272354	5.00448466
1	6.77470206	-4.32327312	4.58167511
6	5.65608339	-3.84360419	6.37881244
1	6.27679822	-4.46833227	7.02209387
6	4.58084734	-3.13245946	6.92955953
1	4.37179613	-3.21010263	7.99728012
6	3.76147501	-2.32230781	6.13093672
1	2.92159831	-1.78254711	6.56710154
6	4.06422710	-2.25450349	4.76868138
6	2.25575126	-0.66384552	3.97722571
1	1.35274006	-1.14195740	3.57411414
1	2.13683024	-0.49241310	5.05042670
1	2.40305688	0.29985263	3.47638105
6	5.00985784	-3.98671066	1.89751029
1	5.02638841	-3.79864484	0.81657190
1	5.82951657	-4.67881137	2.13909205
1	4.05969584	-4.47924868	2.14112017
6	6.52320725	-1.97161364	2.36376483
1	6.63439277	-1.03525269	2.92705313

1	7.36103859	-2.63222068	2.62875641
1	6.60174954	-1.74093695	1.29380069
6	3.60899722	4.57317662	-0.53862395
6	2.33219926	3.75951680	-0.89935546
6	1.56043446	4.18760362	-1.99695545
1	1.86379227	5.07936383	-2.53580560
6	0.42923526	3.47816195	-2.43429069
6	-2.06611517	5.33103561	1.33992080
6	-1.08161168	4.13565762	1.50099828
6	-0.34476768	4.04455450	2.69600960
1	-0.45476029	4.82531199	3.44150865
6	0.50841198	2.96025022	2.96619778
6	1.20798251	2.94781501	4.35770830

{[Mn(acac)$_2$]$_2$(TMI-NPS)$_2$} complex, Sz = 4

25	-1.68775017	-2.87484364	0.04273997
1	-2.10356959	-7.48204982	-0.09705737
1	-3.65715023	-7.13297704	0.66978200
1	-2.30331161	-7.75822505	1.66373584
1	-0.93007083	-2.99809482	4.50380867
1	-0.42556324	-4.71671636	4.59046985
1	0.63303634	-3.49481217	3.82954657
1	2.06744850	-5.14076771	-0.88330136
1	2.68852187	-3.50296636	-1.14914148
1	2.34399492	-4.54911680	-2.55808116
1	-1.34522778	-2.96969644	-5.01777507
1	-2.16169261	-1.54154965	-4.30542594
1	-2.94709007	-3.12184203	-4.22483580
8	-3.22071717	-1.81737147	0.41821263
8	-2.39468037	-4.84667915	0.10370131
8	-1.17152342	-2.96113903	1.90300020
8	0.10544269	-3.48552574	-0.38838315
8	-2.01127920	-2.45847438	-1.82980953
7	-2.81446204	2.08638946	-2.16934128
6	-0.41203459	-3.81076715	3.97324367
6	-4.21465188	-1.77845063	1.27511327
6	-4.46594832	-2.89353422	2.13258692
1	-3.80483319	-3.75505529	2.05002237

6	-5.51823416	-2.90660173	3.01389132
1	-5.69373127	-3.78060512	3.64588610
6	-6.40230258	-1.79087066	3.12591981
6	-7.47178380	-1.81609859	4.05638865
1	-7.60162306	-2.71039386	4.67100074
6	-8.33424383	-0.74005735	4.19369802
1	-9.15352109	-0.77158729	4.91355773
6	-8.13014756	0.40113332	3.39289905
1	-8.79086587	1.26412940	3.49571137
6	-7.08895189	0.44569551	2.47265385
1	-6.97052828	1.36069975	1.89343012
6	-6.19453593	-0.64244545	2.29060322
6	-5.09237148	-0.62564922	1.31850371
6	-4.95151015	0.49182255	0.45508867
1	-5.74547774	1.23223344	0.52901761
6	-3.93513064	0.77099768	-0.47510791
1	-3.12471340	0.05129287	-0.55062136
6	-3.87769958	1.88757981	-1.30717110
6	-4.87202250	3.05118510	-1.48262043
6	-4.17309883	3.88725792	-2.54865723
6	-4.54991748	5.08092109	-3.15400018
1	-5.49144946	5.56846929	-2.89069493
6	-3.70038403	5.66036260	-4.11462792
1	-3.98320959	6.59732455	-4.59596823
6	-2.48718675	5.04214536	-4.44646649
1	-1.82647480	5.50705441	-5.18019233
6	-2.09235459	3.83909860	-3.84298198
1	-1.13278790	3.38676395	-4.09248641
6	-2.95802966	3.27144386	-2.89982643
6	-1.67859239	1.18321964	-2.28461452
1	-1.01013451	1.26108976	-1.41395495
1	-1.10750519	1.43688523	-3.18374886
1	-2.03246152	0.14557073	-2.36659075
6	-5.03630211	3.88290146	-0.18577265
1	-5.50195605	3.29595927	0.61682297
1	-5.67330322	4.75807718	-0.38322017
1	-4.06267084	4.24224272	0.17352743
6	-6.24540963	2.55348497	-1.99862338

1	-6.12968785	1.97832148	-2.92737020
1	-6.90106655	3.41242397	-2.20610990
1	-6.74263458	1.91064980	-1.25996858
6	-2.56812086	-7.10244471	0.82531658
6	-2.13684209	-5.66566331	1.04562166
6	-1.49725813	-5.31595312	2.26529796
1	-1.33949787	-6.10972239	2.99345181
6	-1.06211911	-4.03084738	2.62556465
6	2.00859140	-4.26967170	-1.55258296
6	0.60181176	-3.72712468	-1.55424255
6	-0.07586664	-3.50551713	-2.76654029
1	0.42277847	-3.77972050	-3.69355159
6	-1.32945021	-2.87896085	-2.84504204
6	-1.96904728	-2.61889567	-4.18757021
25	1.86549217	2.89550128	-0.74160943
1	4.51822716	4.23958762	2.91127869
1	4.86447696	2.50889998	2.83043111
1	6.08984384	3.68602252	2.25514060
1	5.63105830	3.30203441	-3.38761524
1	6.63072240	4.30738407	-2.28968330
1	5.23505574	5.01094396	-3.16866922
1	0.20410049	7.14655556	-0.96748078
1	-1.00447550	6.41543149	-2.03280186
1	-1.46362206	6.86543288	-0.36254878
1	-2.26341072	3.25323142	2.41809275
1	-1.87375659	1.60597428	1.82963936
1	-0.79293634	2.40969626	2.98357413
8	1.88006834	1.02264990	-1.55640644
8	3.12243710	3.08187674	0.93191320
8	3.45297049	3.50791900	-1.89185184
8	0.77638440	4.58692094	-1.19594595
8	0.27629178	2.35524447	0.50201332
7	2.56580835	-0.80193894	2.72067027
6	5.61190592	4.11723495	-2.64866322
6	2.67034143	0.49854339	-2.44184389
6	2.60567834	0.97383127	-3.79785842
1	1.90362110	1.78472469	-3.99786113
6	3.39874353	0.46014945	-4.78808191

1	3.32744483	0.84671843	-5.80804845
6	4.33868596	-0.58666296	-4.52089434
6	5.13298096	-1.11891156	-5.56557138
1	5.01688328	-0.70302969	-6.56940295
6	6.03695049	-2.14519093	-5.33223977
1	6.64369334	-2.54693507	-6.14495485
6	6.14929704	-2.67064774	-4.03071185
1	6.84076680	-3.49198227	-3.83297261
6	5.37705755	-2.16243569	-2.99095385
1	5.48125319	-2.62587350	-2.00990924
6	4.46217671	-1.09531546	-3.18602791
6	3.64297925	-0.52945633	-2.10788618
6	3.86372056	-0.95207402	-0.77409399
1	4.75771254	-1.55673179	-0.62330310
6	3.08583580	-0.68983291	0.36343155
1	2.15520094	-0.14931401	0.20996390
6	3.40743010	-1.07074576	1.66693353
6	4.65563434	-1.79492260	2.20800912
6	4.34955232	-1.85193826	3.69871961
6	5.08373319	-2.37692559	4.75674626
1	6.06036983	-2.83591522	4.58760306
6	4.55142227	-2.31027820	6.05707392
1	5.11684631	-2.71646688	6.89649698
6	3.29659276	-1.72707580	6.27806864
1	2.89104141	-1.68507508	7.29014724
6	2.54442696	-1.19477725	5.22054591
1	1.56619727	-0.75216758	5.40731353
6	3.09575738	-1.26379526	3.93577419
6	1.25781057	-0.16614860	2.59708236
1	0.51318949	-0.88170520	2.21533829
1	0.94101942	0.18392003	3.58552625
1	1.30491901	0.70018687	1.92393966
6	4.77062832	-3.23596367	1.64693651
1	4.97576819	-3.23613599	0.56841216
1	5.59379105	-3.76379770	2.15043432
1	3.84347095	-3.79957849	1.81866131
6	5.95202324	-0.98992019	1.94745085
1	5.87403406	0.02536152	2.35923200

1	6.80438120	-1.49085253	2.42984134
1	6.16452062	-0.90653302	0.87354156
6	5.01650178	3.46523109	2.30789782
6	4.35848298	3.40697787	0.93980328
6	5.13291931	3.72117880	-0.20040419
1	6.18059752	3.97123423	-0.04156323
6	4.65458547	3.75438814	-1.52925287
6	-0.65793596	6.46356769	-0.98899801
6	-0.21052036	5.08334881	-0.55108189
6	-0.89180513	4.44235190	0.50964697
1	-1.69440832	4.99400826	0.99626444
6	-0.62494145	3.13730985	0.97449400
6	-1.45155706	2.58013669	2.11737047

{[Mn(hfac)$_2$](TMI-NPS)$_2$} complex, $S = 5/2$

8	-1.88123572	-0.82879742	-0.20978579
7	-3.31569442	1.47872307	-4.04551999
6	-2.83478868	-0.87813183	0.65759661
6	-2.75244099	-1.84074443	1.72743543
1	-1.89966725	-2.51968461	1.70469883
6	-3.67753285	-1.88368999	2.73315206
1	-3.58295309	-2.61993215	3.53577897
6	-4.77062004	-0.95809605	2.79054981
6	-5.67520657	-0.98883353	3.87880659
1	-5.52581679	-1.73951717	4.65846886
6	-6.72398823	-0.08475372	3.96628035
1	-7.41330138	-0.11293719	4.81114492
6	-6.87772313	0.87921925	2.95211922
1	-7.68527740	1.61091310	3.01510113
6	-6.00642864	0.91768586	1.86813387
1	-6.15929125	1.69921415	1.12427568
6	-4.93209786	0.00127217	1.73937062
6	-3.99995428	-0.00227599	0.60472337
6	-4.27686186	0.80057555	-0.52207859
1	-5.15334201	1.44142498	-0.43803581
6	-3.61422295	0.80914909	-1.75503238
1	-2.76794923	0.13493776	-1.86410473
6	-3.95734063	1.61212806	-2.84428350

6	-4.99078766	2.74749314	-2.95982917
6	-4.78376762	3.19631010	-4.40024403
6	-5.40754341	4.19708437	-5.13811748
1	-6.18282895	4.82285949	-4.69091188
6	-5.02292680	4.39704269	-6.47549871
1	-5.50125966	5.17959158	-7.06555155
6	-4.02810141	3.59806704	-7.05465409
1	-3.73805051	3.76395872	-8.09315313
6	-3.39150654	2.58518476	-6.32273228
1	-2.61661128	1.97446934	-6.78547835
6	-3.78778067	2.40522745	-4.99424183
6	-2.29289351	0.47349651	-4.31108848
1	-1.49312790	0.54128791	-3.56071524
1	-1.86313015	0.65044091	-5.30118069
1	-2.73299226	-0.53489634	-4.28262409
6	-4.67223485	3.89929049	-1.97516370
1	-4.77019876	3.57236910	-0.93165894
1	-5.36720424	4.73495890	-2.14378112
1	-3.64788384	4.26800097	-2.11758943
6	-6.44212760	2.23271976	-2.77829348
1	-6.65483808	1.39952731	-3.46199049
1	-7.14980038	3.04468622	-2.99991639
1	-6.62994793	1.89124061	-1.75231853
25	0.01119695	0.02179457	0.00530392
9	3.49909859	2.88669758	1.68727593
9	4.70522764	1.50377568	0.48705417
9	4.31106762	3.53225742	-0.24150845
9	0.69427127	1.93614364	-4.57176789
9	1.44139469	3.84139065	-3.79381384
9	-0.65759166	3.29322926	-3.50366917
9	-0.90114394	4.61516262	1.14311330
9	-2.88367268	3.74758740	1.49610131
9	-1.60142729	4.28049173	3.19101990
9	0.15457350	0.76066058	5.52814660
9	-0.44306807	-1.22763141	4.83333990
9	1.61696046	-0.53409069	4.54077718
8	1.03233766	-1.64255891	-0.72840425
8	1.92817895	0.98785457	0.38456918

8	0.13359217	1.12743458	-1.91538592
8	-0.93278913	1.86629607	0.68698039
8	0.11966300	-0.41495806	2.17827863
7	2.65490651	-3.37317480	3.32824043
6	0.61256059	2.80413682	-3.51976359
6	1.95837113	-1.67693129	-1.62584484
6	1.58736663	-1.54855208	-3.01283554
1	0.52003229	-1.48459954	-3.22583447
6	2.52287643	-1.48175552	-4.00751480
1	2.21025167	-1.37558478	-5.04972720
6	3.92748352	-1.51512860	-3.72341761
6	4.87035464	-1.38245089	-4.77076714
1	4.50036576	-1.26840624	-5.79244247
6	6.23380353	-1.38680884	-4.51412567
1	6.95297086	-1.27925516	-5.32712619
6	6.67531007	-1.52061097	-3.18425418
1	7.74389637	-1.50681157	-2.96193890
6	5.76447767	-1.66455774	-2.14249020
1	6.16215933	-1.74293512	-1.13098092
6	4.36477151	-1.67703863	-2.36912250
6	3.37077640	-1.84149289	-1.30077948
6	3.79923522	-2.19628670	-0.00397027
1	4.87783809	-2.25071285	0.13608215
6	3.00925474	-2.56419909	1.09135693
1	1.93178469	-2.56302555	0.94403763
6	3.49869480	-2.92833402	2.34713479
6	4.93179078	-2.88975976	2.90840242
6	4.70808777	-3.37096076	4.33580943
6	5.60578658	-3.55990044	5.38153562
1	6.66904275	-3.34618610	5.25317060
6	5.12386281	-4.02938876	6.61596799
1	5.81538620	-4.17973549	7.44575022
6	3.76054420	-4.30416141	6.78724368
1	3.39910788	-4.66714876	7.75043225
6	2.84462309	-4.11888368	5.74146988
1	1.78659062	-4.33295513	5.89084049
6	3.34505249	-3.64923651	4.52357236
6	1.22152652	-3.56464873	3.13912450

1	1.03683490	-4.38154439	2.42506160
1	0.76206292	-3.81577724	4.09942385
1	0.76449313	-2.64043009	2.75935317
6	5.87414615	-3.87434361	2.16895571
1	6.05570237	-3.56626300	1.13129911
1	6.84389982	-3.91053691	2.68621729
1	5.45559359	-4.89003018	2.15741645
6	5.49934144	-1.44904899	2.89785704
1	4.83473661	-0.75940454	3.43469694
1	6.48333323	-1.43389075	3.38908596
1	5.61765261	-1.07320487	1.87310035
6	3.75782419	2.48095777	0.41975897
6	2.46603424	1.92802219	-0.25380804
6	2.05740923	2.51343299	-1.46903582
1	2.63519883	3.34065045	-1.86812941
6	0.93363670	2.06728065	-2.18543568
6	-1.59355075	3.75991483	1.93504691
6	-0.98806948	2.32616833	1.85575092
6	-0.58965040	1.71517056	3.06181190
1	-0.68878689	2.27514443	3.98594432
6	-0.07119651	0.41009269	3.11591519
6	0.31581942	-0.13467605	4.52300453

{[Mn(hfac)$_2$](TMI-NPS)} complex, $S = 5/2$

25	1.84241487	-2.36815752	0.18325708
9	-1.71562494	-3.33178734	-3.04266316
9	-2.33297501	-1.56703008	-1.89839708
9	-3.25042690	-3.51573215	-1.49219912
9	-0.60073258	-4.20500064	3.73234975
9	-2.03272027	-5.38491679	2.56514421
9	0.03395475	-6.07680912	2.78307999
9	6.08867801	-4.21669170	1.69610576
9	5.79783056	-2.28922109	2.70004734
9	7.22852178	-2.46211634	1.04833688
9	5.91224668	-0.39339581	-2.89213282
9	3.99810968	0.66002570	-2.71565123
9	4.14409132	-1.15549108	-3.93551421
8	1.32511984	-0.60913671	1.04476914

8	0.16118523	-2.64049981	-1.09859573
8	0.91951756	-3.82543200	1.38285367
8	3.72391025	-2.95152553	0.90749317
8	2.91265879	-1.66006028	-1.49896330
7	-0.69045786	1.29945103	-2.66613170
6	-0.73721543	-4.97600329	2.62260238
6	0.85938481	-0.16586327	2.16633324
6	1.25663645	-0.79871042	3.39464704
1	1.93137672	-1.65337710	3.32043882
6	0.80780346	-0.34943096	4.60675858
1	1.12450297	-0.85063192	5.52486319
6	-0.06114135	0.78396027	4.71621034
6	-0.47095080	1.24782655	5.98944463
1	-0.12381598	0.71148758	6.87545548
6	-1.28837603	2.36126630	6.11740791
1	-1.59778852	2.71289029	7.10232599
6	-1.70001168	3.04225226	4.95605150
1	-2.32444660	3.93342674	5.04129686
6	-1.31008614	2.60072408	3.69558699
1	-1.62943263	3.18404851	2.83192268
6	-0.49750087	1.45149620	3.52655989
6	-0.07986312	0.94327738	2.21588856
6	-0.66211125	1.48138997	1.04303903
1	-1.47076049	2.19179074	1.21457846
6	-0.36192294	1.18444105	-0.29005400
1	0.46409912	0.50330765	-0.47031150
6	-1.05757315	1.66743674	-1.40544530
6	-2.27431911	2.60479147	-1.49447677
6	-2.49579705	2.66626607	-2.99907548
6	-3.44816685	3.34694286	-3.75099744
1	-4.20674439	3.96686704	-3.26859468
6	-3.42254495	3.22354814	-5.15083962
1	-4.16298708	3.74994201	-5.75406927
6	-2.45409772	2.42737699	-5.77719072
1	-2.44766625	2.33880154	-6.86433676
6	-1.48828630	1.73648822	-5.03146511
1	-0.74385192	1.11784561	-5.53188862
6	-1.53119655	1.87488646	-3.64136686

```
6    0.43291166   0.41276003  -2.96728955
1    1.36430705   0.82950053  -2.56183564
1    0.53211936   0.31459285  -4.05185348
1    0.27239676  -0.58258887  -2.52986405
6   -1.94493758   4.01620447  -0.94565810
1   -1.74515270   3.99440895   0.13365598
1   -2.79746677   4.68785680  -1.12156386
1   -1.06522826   4.44086396  -1.44799059
6   -3.51651623   2.00192204  -0.79175941
1   -3.73972944   0.99683695  -1.17363274
1   -4.39124938   2.64135015  -0.97926300
1   -3.37029452   1.93144770   0.29407882
6   -2.08104816  -2.90752427  -1.80899611
6   -0.94552794  -3.17034818  -0.78088790
6   -1.25360277  -3.92388738   0.36389509
1   -2.26150166  -4.30577366   0.49070042
6   -0.29398086  -4.17997896   1.36237066
6    6.01493589  -2.87958729   1.49678830
6    4.85483092  -2.53893065   0.51940251
6    5.15746546  -1.81390245  -0.64892112
1    6.18686345  -1.53002433  -0.84298148
6    4.15674707  -1.42637094  -1.55551514
6    4.57320858  -0.57606195  -2.78736770
```

[Mn(hfac)$_2$] complex, $S = 5/2$

```
25  -0.00548853   0.01463543  -0.00324962
 9  -4.35934684   1.84699471   0.42480581
 9  -3.19566839   2.93902146   1.92941803
 9  -4.56864064   1.34752118   2.54795585
 9  -0.44580177  -2.70101806   3.85793831
 9  -2.63470722  -2.61700283   3.90551332
 9  -1.61860529  -3.77633087   2.34856047
 9   4.58099911   1.11114310   0.45362269
 9   3.68381842   2.99190200  -0.23050121
 9   4.83699858   1.75592520  -1.62465162
 9   2.39322186  -0.52538394  -4.80612108
 9   0.21920992  -0.26219102  -4.73344958
 9   1.11939563  -2.14847893  -4.06878714
```

8   -1.67617670   1.05281345   0.53261809
8   -0.47301880 -1.41210081   1.37768036
8   1.82577983   0.91113707   0.02869643
8   0.30861445 -0.51314090 -1.94794326
6   -1.55544414 -2.64336648   3.08567997
6   -3.68468959   1.72342885   1.59146956
6   -2.51702915   0.71108220   1.42261727
6   -2.49957496 -0.43736302   2.23257501
1   -3.30079456 -0.58236642   2.95044789
6   -1.48433812 -1.40567446   2.14754367
6   3.96488913   1.71712299 -0.58760415
6   2.65071055   0.96362704 -0.93695066
6   2.50184605   0.43449670 -2.23049071
1   3.30818993   0.56715866 -2.94500073
6   1.34786553 -0.25888829 -2.63421076
6   1.27778569 -0.80470400 -4.08818221

[Mn(hfac)$_2$]$^-$, complex charge= -1, $S = 2$
25   0.01375522 -0.03252022   0.00875487
 9   -4.32666974   1.87038868   0.38873241
 9   -3.16626504   2.95601580   1.89327624
 9   -4.53432598   1.35728762   2.51057235
 9   -0.46354860 -2.72466683   3.89425864
 9   -2.65230119 -2.59291047   3.90653498
 9   -1.63074684 -3.80360373   2.39036197
 9   4.60531226   1.13687921   0.45061686
 9   3.65823286   3.00148423 -0.19339266
 9   4.79194197   1.79592545 -1.63230685
 9   2.36513094 -0.47837594 -4.80142087
 9   0.18425889 -0.25963891 -4.72893439
 9   1.11416553 -2.14218222 -4.11261313
 8   -1.62466037   1.05595694   0.48555434
 8   -0.42770409 -1.45821544   1.37235160
 8   1.81774137   0.87893856   0.09126905
 8   0.27417934 -0.56779656 -1.92435332
 6   -1.55996718 -2.62720577   3.08355193
 6   -3.62576996   1.71447729   1.55212120
 6   -2.47775839   0.71313487   1.38913595

```
6   -2.46153575  -0.43483297   2.20260735
1   -3.26793839  -0.56628481   2.91808823
6   -1.46133267  -1.42245557   2.14251238
6    3.92054973   1.71677139  -0.58073228
6    2.63302361   0.95265107  -0.90476219
6    2.46431034   0.43168100  -2.20083940
1    3.25992987   0.58912952  -2.92312219
6    1.32198645  -0.27659664  -2.61688455
6    1.25600581  -0.78343555  -4.06093852
```

[Mn(acac)$_2$] complex, $S = 5/2$

```
25   0.00010254  -0.02011062   0.00502339
 1  -1.02655325   1.96097469  -4.03576770
 6  -1.93656250   1.61691081  -3.52158868
 1  -2.38618400   2.50028116  -3.04352474
 1  -2.63760722   1.20559672  -4.25748303
 1  -2.79609372  -0.90050623  -3.31090774
 6  -2.11003079  -0.68311745  -2.49412126
 6  -1.55339525   0.61513170  -2.45242118
 8  -0.72820369   1.04313594  -1.56720525
 8  -1.08083948  -1.64545570  -0.55466986
 6  -1.85759033  -1.72506140  -1.57384666
 6  -2.53841730  -3.06367424  -1.76835059
 1  -1.77151082  -3.84217026  -1.89960662
 1  -3.21618609  -3.07354028  -2.63018174
 1  -3.09985988  -3.31851662  -0.85714288
 8   2.00921684  -0.17992573   0.26000686
 8  -0.20802918   0.72908112   1.88304209
 1   4.56604832   0.52440657   0.37976367
 6   4.16677271  -0.05188633   1.22803617
 1   4.37163882  -1.11235975   1.01734281
 1   4.68726673   0.24436711   2.14644618
 6   2.66905504   0.15757102   1.30827493
 6   2.11050082   0.69147352   2.49118006
 1   2.79972278   0.92608949   3.30051955
 6   0.73940731   0.94356399   2.72223203
 6   0.30853101   1.50940574   4.05913292
```

1	-0.24756450	2.44434594	3.89435703
1	-0.38726387	0.80504268	4.54001695
1	1.15362894	1.69894638	4.73144328

[Mn(acac)$_2$]$^-$ complex charge=-1, complex $S = 2$

25	0.00114008	0.00099669	0.00153365
1	-4.21069054	1.83381326	0.63117945
1	-3.27830038	2.70663000	1.85543162
1	-4.37046871	1.37709903	2.35698457
1	-0.66293767	-2.68649224	3.72288028
1	-2.45187559	-2.57798728	3.72770321
1	-1.59420011	-3.56365081	2.50084541
1	4.46583470	1.22597896	0.25196728
1	3.73022376	2.74440609	-0.28023975
1	4.62828952	1.73588405	-1.45858593
1	2.19155473	-0.54448862	-4.63077124
1	0.40862338	-0.36413657	-4.60418889
1	1.14012963	-1.88653215	-4.07769624
8	-1.64475179	1.08105561	0.48728984
8	-0.42068256	-1.44239623	1.36179824
8	1.81180604	0.90934165	0.08964244
8	0.25724354	-0.54609787	-1.93424612
6	-1.56142008	-2.62679010	3.08403986
6	-3.66395210	1.70884602	1.58214801
6	-2.50901976	0.73878456	1.39401393
6	-2.45028260	-0.43051638	2.18788809
1	-3.25850101	-0.57289674	2.90819112
6	-1.45485472	-1.43475178	2.14709433
6	3.94776174	1.70875614	-0.59502711
6	2.65198397	0.97448838	-0.89835103
6	2.45023296	0.42956012	-2.18804586
1	3.25734199	0.57108096	-2.90976250
6	1.31297800	-0.27897125	-2.64153760
6	1.27679360	-0.79101350	-4.07217908

{[Mn(hfac)$_2$][Zn(hfac)$_2$](TMI-NPS)$_2$} complex $S = 5/2$

| 25 | -0.32929568 | -1.62807502 | -0.21819118 |
| 9 | -3.53935965 | -4.89127416 | -1.35530904 |

9	-4.77562423	-3.77726009	0.07287163
9	-3.91736012	-5.71139748	0.64124659
9	-0.03065138	-3.62289141	4.42255357
9	-0.38940292	-5.61670118	3.58993540
9	1.44419972	-4.53634144	3.08055920
9	1.44965383	-5.99853061	-0.55778636
9	3.08490026	-4.94129733	-1.56638961
9	1.65129191	-6.11496362	-2.73630362
9	-1.53209028	-3.76975214	-5.13448902
9	-0.79052487	-1.71624237	-5.31900198
9	-2.69400848	-2.11394706	-4.30277881
8	-1.39725516	0.20676230	0.32235477
8	-2.18220861	-2.73192743	-0.17154536
8	-0.06483533	-2.58688190	1.76824085
8	1.00461503	-3.23443035	-0.77982289
8	-0.78077758	-1.65721243	-2.39230665
7	-2.87731101	2.05724907	-3.93403667
6	0.11104936	-4.39117304	3.30148613
6	-2.44139008	0.20814104	1.14680969
6	-2.26886592	-0.33235956	2.45768060
1	-1.28561212	-0.72476154	2.70979387
6	-3.28597106	-0.34503306	3.37853118
1	-3.11312134	-0.75948548	4.37475621
6	-4.57889058	0.16718717	3.06513323
6	-5.62323565	0.12045401	4.02284459
1	-5.40658350	-0.29885934	5.00784443
6	-6.89199676	0.58526998	3.71892094
1	-7.69130555	0.54562564	4.45992980
6	-7.14183244	1.09360125	2.42840660
1	-8.14307465	1.44001591	2.16624460
6	-6.13194517	1.14741853	1.47527123
1	-6.39457676	1.51090454	0.48250262
6	-4.81120652	0.71273301	1.76070574
6	-3.71670777	0.76597748	0.78621811
6	-3.95297350	1.43356824	-0.44892921
1	-4.86129820	2.03234273	-0.46439390
6	-3.20653164	1.42585687	-1.61897533
1	-2.31514866	0.80621721	-1.65709048

6	-3.55117456	2.17506540	-2.76044556
6	-4.65612077	3.23979920	-2.93299392
6	-4.40657942	3.70515299	-4.35951854
6	-5.04339704	4.67119811	-5.13268880
1	-5.87063479	5.25969041	-4.73083702
6	-4.59795681	4.88416583	-6.44874773
1	-5.08296513	5.64097915	-7.06638512
6	-3.53446844	4.13732443	-6.97508436
1	-3.20032129	4.31957261	-7.99726957
6	-2.88665160	3.15889539	-6.20738599
1	-2.05429228	2.58640250	-6.61559042
6	-3.34917838	2.96683844	-4.90350980
6	-1.79567071	1.12568645	-4.23355915
1	-0.83639791	1.65867142	-4.27118372
1	-1.98869869	0.66442455	-5.21046562
1	-1.74880395	0.33470045	-3.48051101
6	-4.49267076	4.41457623	-1.93891150
1	-4.65320010	4.09449909	-0.90194748
1	-5.22869904	5.19696480	-2.17440264
1	-3.48956215	4.85456400	-2.00656654
6	-6.07288259	2.61043946	-2.84840687
1	-6.17432517	1.76496620	-3.54223294
1	-6.82158614	3.36813518	-3.12014452
1	-6.30564488	2.25502263	-1.83689380
6	-3.67580223	-4.56245620	-0.04505321
6	-2.41450586	-3.80007816	0.45569215
6	-1.68255532	-4.35547889	1.52299134
1	-1.99723929	-5.30835015	1.93596124
6	-0.57687473	-3.69861754	2.08897486
6	1.77275455	-5.28586255	-1.66736696
6	0.89104792	-4.00749104	-1.76890969
6	0.08860602	-3.84282230	-2.91286079
1	0.07619379	-4.62585528	-3.66420854
6	-0.66987893	-2.67828111	-3.12891798
6	-1.43718658	-2.58712241	-4.48077427
30	0.18221138	1.62298071	0.49623388
9	3.53240308	4.54482532	2.03506796
9	4.75912856	3.21004078	0.80141443

9	4.23669905	5.20831171	0.06984776
9	0.71169919	3.48124652	-4.10814801
9	1.06963512	5.45977783	-3.24053833
9	-0.89778124	4.52410418	-3.04427119
9	-1.80326217	5.90664744	0.92174795
9	-3.51686191	4.68553604	1.54022196
9	-2.33702486	5.76292316	3.04011032
9	-0.24851992	2.82401548	5.85094679
9	-0.13445069	0.70862238	5.30349753
9	1.63055698	1.99543823	5.09725645
8	1.27301833	-0.19897587	-0.20898818
8	2.04309913	2.52457906	0.78649781
8	0.17115202	2.53941212	-1.44566743
8	-1.12324672	3.24447802	0.87401690
8	0.29686891	1.41189252	2.64309119
7	3.29259919	-1.95812637	3.80207029
6	0.43805386	4.28093681	-3.03034573
6	2.19424760	-0.18147000	-1.16146294
6	1.79774085	0.18797748	-2.48569252
1	0.75165821	0.44336661	-2.63261989
6	2.67963133	0.20968123	-3.53561271
1	2.33316256	0.48884351	-4.53383326
6	4.05841726	-0.10853139	-3.35475493
6	4.96878012	-0.02958949	-4.43808061
1	4.58656287	0.25903187	-5.41982531
6	6.31609242	-0.29974138	-4.25923188
1	7.01178025	-0.23457455	-5.09674908
6	6.78096085	-0.63795292	-2.97253922
1	7.84470903	-0.82085558	-2.81045017
6	5.90302143	-0.72494741	-1.89822504
1	6.32131276	-0.94003720	-0.91526052
6	4.51168798	-0.49269323	-2.05208752
6	3.55666864	-0.59496616	-0.94487946
6	4.00086501	-1.20381771	0.26057317
1	4.95550695	-1.72015736	0.17237429
6	3.38525827	-1.26114446	1.50375112
1	2.45958564	-0.71050857	1.64985507
6	3.89735513	-1.99676795	2.58852308

6	5.10851386	-2.94488037	2.66461156
6	5.02301022	-3.41979085	4.10813559
6	5.82259600	-4.30546707	4.82383684
1	6.67490490	-4.79975485	4.35316869
6	5.51255763	-4.56075898	6.17052965
1	6.12751877	-5.25481897	6.74455172
6	4.41811656	-3.93339864	6.78192821
1	4.18916952	-4.14404066	7.82738778
6	3.60537123	-3.03803267	6.07262746
1	2.75355725	-2.56109818	6.55622984
6	3.93346740	-2.79916062	4.73572817
6	2.11976980	-1.13882670	4.09638609
1	1.27508055	-1.45855414	3.47223130
1	1.85742029	-1.24924614	5.15131237
1	2.33984855	-0.08499340	3.88804088
6	4.96519123	-4.13859490	1.68812315
1	5.00142055	-3.80933845	0.64165566
1	5.78786686	-4.84898407	1.85478017
1	4.01623044	-4.66753667	1.84407467
6	6.44660110	-2.19044453	2.44910505
1	6.53274363	-1.33153717	3.12827055
1	7.28522536	-2.87197227	2.65117315
1	6.55027882	-1.82702234	1.41891691
6	3.76784032	4.13689806	0.76292276
6	2.47908047	3.51855883	0.14485774
6	1.95852453	4.10524917	-1.02304195
1	2.44267314	4.99072028	-1.42171174
6	0.85974474	3.56361601	-1.71279304
6	-2.25049271	5.06146836	1.88098375
6	-1.33520126	3.80460333	1.98213318
6	-0.88353696	3.42612675	3.25818788
1	-1.15139759	4.04201535	4.11028625
6	-0.11862676	2.26642409	3.47397813
6	0.27853549	1.95891484	4.95022062

{[Mn(hfac)$_2$] [Zn(hfac)$_2$]((TMI-NPS)$_2$} complex $S = 3/2$

25	-0.38330251	-1.74457057	-0.30685854
9	-3.65856949	-4.85562852	-0.99398209

9	-4.61106289	-3.60390483	0.53093397
9	-3.81756259	-5.57497210	1.07007253
9	0.50893226	-3.57881197	4.32712996
9	0.10799297	-5.58180200	3.53374513
9	1.87001276	-4.46972213	2.85821631
9	0.78190921	-6.12357487	-0.96322891
9	2.35631289	-5.16521387	-2.14914131
9	0.68878200	-6.17155552	-3.15199749
9	-2.90051853	-3.61150790	-4.72907617
9	-1.76327256	-1.86311402	-5.40173429
9	-3.42480011	-1.61937872	-3.98993343
8	-1.38610029	-0.05536987	0.28048633
8	-1.99333116	-2.80294322	-0.14317535
8	0.22335297	-2.58189298	1.63810901
8	0.56828671	-3.32983631	-1.05497231
8	-1.21906366	-1.53508221	-2.43345473
7	-2.66608459	2.18117449	-3.95806290
6	0.55935365	-4.34815164	3.19712029
6	-2.51255996	-0.07865245	1.04929965
6	-2.44434691	-0.75182293	2.29600321
1	-1.49851256	-1.21950068	2.56320180
6	-3.50971768	-0.77225444	3.16609566
1	-3.42038006	-1.28321073	4.12704703
6	-4.73471507	-0.13115898	2.83639501
6	-5.83602797	-0.17585886	3.73141376
1	-5.71254976	-0.70444410	4.67913090
6	-7.04077403	0.42427710	3.41226053
1	-7.88264903	0.38353649	4.10462572
6	-7.17350051	1.07532278	2.16774209
1	-8.12643220	1.53045625	1.89229217
6	-6.10953237	1.13296214	1.27776545
1	-6.28286071	1.61386207	0.31636625
6	-4.84666221	0.55698214	1.58152942
6	-3.70229907	0.60789129	0.66647101
6	-3.83861213	1.39511614	-0.52557817
1	-4.67195916	2.09273900	-0.49321631
6	-3.09201119	1.39342792	-1.69439697
1	-2.27822262	0.67873851	-1.79029240

6	-3.35794471	2.24962267	-2.78404956
6	-4.40225482	3.38185758	-2.90089431
6	-4.11427633	3.91934618	-4.29447171
6	-4.69456914	4.96029445	-5.01256951
1	-5.49913720	5.56094407	-4.58341115
6	-4.22358981	5.23283020	-6.30899075
1	-4.66609321	6.04719077	-6.88386177
6	-3.18901908	4.47016939	-6.86955703
1	-2.83463748	4.69781274	-7.87577884
6	-2.59665648	3.41781995	-6.15711202
1	-1.78798030	2.83142208	-6.59253367
6	-3.08381634	3.16720697	-4.87110785
6	-1.61706992	1.23452201	-4.31291472
1	-0.65348896	1.75361352	-4.39834643
1	-1.86328438	0.77551686	-5.27994588
1	-1.54417473	0.44675917	-3.55968819
6	-4.18626513	4.49100211	-1.84297161
1	-4.38984422	4.13045478	-0.82772006
1	-4.86559333	5.33053908	-2.05070980
1	-3.15579467	4.86837226	-1.87029173
6	-5.85225319	2.82938829	-2.86036068
1	-5.99387167	2.03105664	-3.60128069
1	-6.55671455	3.64107447	-3.09219506
1	-6.11131491	2.43082664	-1.87166028
6	-3.59071022	-4.47380771	0.30803511
6	-2.23549294	-3.80983169	0.61918732
6	-1.43646919	-4.32283380	1.64368959
1	-1.75146534	-5.23307604	2.14418956
6	-0.25024525	-3.68482075	2.05625739
6	1.02053891	-5.39834352	-2.08590860
6	0.24056977	-4.06066599	-2.04787608
6	-0.70596887	-3.80260401	-3.04366739
1	-0.91892499	-4.57813738	-3.77328591
6	-1.38088133	-2.56804502	-3.14150619
6	-2.38969864	-2.42605262	-4.31809938
30	-0.10117378	1.49547617	0.67578651
9	3.55274103	3.74650228	2.46207904
9	4.62090506	2.12509102	1.44443401

9	4.58447699	4.13215290	0.56831174
9	1.21348975	3.14939115	-3.86607507
9	1.67566171	5.05202766	-2.88564072
9	-0.38912092	4.33087003	-2.94683247
9	-1.92723992	5.80734018	1.04426264
9	-3.71780779	4.67785097	1.61909332
9	-2.51068041	5.67928314	3.14950456
9	-1.24038382	2.24712622	5.98552658
9	-0.72242707	0.23769045	5.29077269
9	0.83550765	1.76834306	5.47421670
8	1.22656184	-0.70210472	-0.43139994
8	1.85810913	1.94062455	1.10748688
8	0.21526392	2.27871606	-1.24843780
8	-1.25249434	3.18967482	0.99208523
8	-0.17453806	1.17921620	2.79028686
7	3.44503924	-1.60032922	3.72458184
6	0.90136519	3.94401702	-2.79877229
6	2.12644188	-0.61757905	-1.40323555
6	1.68518672	-0.36648872	-2.73699393
1	0.61416822	-0.26021627	-2.89106914
6	2.56149012	-0.27201053	-3.78994934
1	2.18661568	-0.08397740	-4.79886990
6	3.96826099	-0.38197406	-3.59113164
6	4.86948940	-0.23368768	-4.67600570
1	4.45924714	-0.06398963	-5.67414635
6	6.23952359	-0.29046112	-4.47983092
1	6.92552673	-0.17489647	-5.32003712
6	6.73896410	-0.47639529	-3.17411604
1	7.81660000	-0.49012581	-3.00158154
6	5.87374044	-0.62587442	-2.09747673
1	6.30643182	-0.71730053	-1.10169809
6	4.46374765	-0.61688283	-2.26680398
6	3.53135328	-0.80213639	-1.15459544
6	4.05745277	-1.24929348	0.09386060
1	5.06350963	-1.66228484	0.03317176
6	3.46297810	-1.23069182	1.34795657
1	2.48734153	-0.76373336	1.44500047
6	4.04882455	-1.75329868	2.51351706

6	5.35370259	-2.54556583	2.70191702
6	5.31397325	-2.83004966	4.19707655
6	6.19853737	-3.52725187	5.01371009
1	7.09303319	-3.99761624	4.60000185
6	5.92189626	-3.62204159	6.38854017
1	6.60353194	-4.16861691	7.04125761
6	4.77595702	-3.02033797	6.92719033
1	4.57434822	-3.10256615	7.99610310
6	3.87722946	-2.31319223	6.11642070
1	2.98859602	-1.85236800	6.54652814
6	4.17047272	-2.23417306	4.75176600
6	2.21767845	-0.83535763	3.92911856
1	1.41124520	-1.24176792	3.30550759
1	1.92580774	-0.89691063	4.98038795
1	2.38025431	0.21587785	3.65708894
6	5.36100409	-3.86079456	1.88596538
1	5.36259710	-3.66179565	0.80621687
1	6.26311505	-4.44068816	2.12964073
1	4.48278104	-4.47703917	2.11665643
6	6.59832199	-1.67637088	2.37790457
1	6.57926968	-0.73134489	2.93719477
1	7.50921549	-2.22396003	2.65966465
1	6.66256327	-1.44242445	1.30754192
6	3.84251391	3.21908352	1.24527559
6	2.53016544	2.82744278	0.50569912
6	2.22709817	3.48535915	-0.69702988
1	2.89631420	4.26247266	-1.05147158
6	1.09644763	3.15718175	-1.46691457
6	-2.43876554	4.98404313	1.98626242
6	-1.60162489	3.67609446	2.10572937
6	-1.36867812	3.17906112	3.39766086
1	-1.73834485	3.74247037	4.24849355
6	-0.67655846	1.97606700	3.62788360
6	-0.46239790	1.55744384	5.11483229