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Supporting Information

Theoretical modeling of two-step spin-crossover transitions in Fe^{II} dinuclear systems

Jordi Cirera and Eliseo Ruiz

Departament de Química Inorgànica and Institut de Recerca de Química Teòrica i Computacional, Universitat de Barcelona, Diagonal 645, 08028 Barcelona, Spain

Email corresponding authors: eliseo.ruiz@qi.ub.es; jordi.cirera@qi.ub.es

S1. Cartesian atomic coordinates for the optimized geometries.

S1.1 $[Fe(bt)(NCS)_2]_2(\mu\text{-bpym})$ [LS-LS], S=0, E= -7293.89943730 au, ν_1= 13.2872 cm^{-1}

Fe	-1.573036843	0.267733278	-0.253814369
Fe	2.224393900	3.967130024	0.408441408
S	-6.288669676	0.269174568	-0.176496216
S	-0.318362283	0.182807786	4.269946298
S	0.969027797	4.051576705	-4.115025041
S	6.939863553	3.967553838	0.329105344
S	2.709059416	5.333911824	4.584472839
S	3.042992238	7.982025752	2.006019584
S	-2.392978229	-3.747582463	-1.849526400
S	-2.058976259	-1.100583701	-4.429171887
N	-1.385240957	0.118199216	1.666902071
N	-3.482821081	0.374725438	-0.182118123
N	-1.443424086	2.225225142	-0.061756653
N	0.242241400	3.868507606	0.425414213
N	0.409023579	0.366482922	-0.271206626
N	2.094724657	2.009745717	0.215750343
N	2.036551818	4.117461848	-1.512286836
N	4.134081422	3.860434320	0.336253434
N	2.321902228	4.042911509	2.386230488
N	2.388305267	5.908642154	0.627597205
N	-1.737390874	-1.673832954	-0.472159325
N	-1.670688025	0.191064345	-2.231557167
C	-0.943869193	0.154573783	2.762481733
C	-4.664082900	0.312175390	-0.174174063
C	-0.174726256	2.620947498	0.133622042
C	-2.404322506	3.160016277	0.061184111
C	-2.059023304	4.473614440	0.368267583
C	-0.720247939	4.804084138	0.543313557
C	1.371573943	-0.569002229	-0.389686682
C	0.826003372	1.613999087	0.020696687
C	3.055641149	1.075099047	0.092258280
C	2.710340969	-0.238442716	-0.215086554
C	5.315276374	3.923677271	0.327685066
C	1.594892065	4.080513858	-2.607729621
C	2.593212049	5.263382996	2.857568049
C	2.188521211	3.123966073	3.400442831
C	2.362868893	3.634571697	4.648802773
C	2.656385691	6.298235066	1.874972794
C	2.499553454	6.939611617	-0.273681800
C	2.832613588	8.133670577	0.286238442
C	-2.005552729	-2.063931773	-1.719332970
C	-1.849072548	-2.704275389	0.429626868
C	-2.182617238	-3.898499792	-0.129678762
C	-1.942399897	-1.029524650	-2.702395083
C	-1.537604329	1.109677743	-3.246139181
C	-1.712578752	0.598673055	-4.494236390
H	-3.420199474	2.818008589	-0.076803888
H	-2.826780307	5.228825556	0.468862115
H	-0.391399480	5.808472111	0.771105407
H	1.042676306	-1.573335292	-0.617609985
H	4.071534350	1.417073123	0.230050841
H	3.478153617	-0.993509354	-0.316189613
H	2.303600001	3.116401659	5.592246487
H	2.335064670	6.732071602	-1.319571492
H	2.982567475	9.083781498	-0.200717629
H	1.935978780	2.097984691	3.179318058
H	-1.684504196	-2.496302394	1.475419604

H	-2.332796590	-4.848357435	0.357703412
H	-1.284813831	2.135685825	-3.025385068
H	-1.653754710	1.116497758	-5.437892832

S1.2 $[Fe(bt)(NCS)_2]_2(\mu\text{-bpym})$ [HS-LS], S=2, E= -7293.89569541 au, ν_1= 13.9183 cm^{-1}

Fe	-1.819345453	0.220539679	-0.099059850
Fe	2.244216264	4.070822219	0.452080055
S	-6.516021490	0.681866288	-0.838429007
S	0.294460066	-0.098435968	4.163437702
S	0.952112887	3.921490237	-4.060787415
S	6.951988176	4.252942962	0.229868542
S	2.888671793	5.447420012	4.601657989
S	3.031898571	8.106854115	2.014749868
S	-2.724393220	-3.929408048	-1.939829171
S	-1.998843020	-1.516184706	-4.461609128
N	-1.309147185	-0.081473594	1.852524128
N	-3.765328999	0.507278046	-0.329508141
N	-1.459105883	2.346662680	0.114868248
N	0.280476043	3.938629706	0.541496193
N	0.493252626	0.447794325	-0.261165347
N	2.112997691	2.126599964	0.258214228
N	1.998169764	4.209064956	-1.464225183
N	4.156140274	4.002576150	0.313180162
N	2.419699234	4.151138807	2.421699669
N	2.375329273	6.015517633	0.663292588
N	-2.023258663	-1.952550135	-0.451320969
N	-1.612900662	-0.068562259	-2.366570076
C	-0.642701949	-0.086346759	2.833646187
C	-4.933501716	0.574935516	-0.546000637
C	-0.171987850	2.696769891	0.243566148
C	-2.383891259	3.308861726	0.292385122
C	-2.004084637	4.606028815	0.610719529
C	-0.648492771	4.893095176	0.729869787
C	1.479321208	-0.448618752	-0.404320525
C	0.846135402	1.695204207	0.065266047
C	3.102349111	1.227180273	0.109046449
C	2.810872401	-0.091308305	-0.220884522
C	5.332151433	4.126018198	0.272624244
C	1.565387202	4.078805307	-2.555979480
C	2.685196021	5.377310500	2.882366188
C	2.362887837	3.226501029	3.438219711
C	2.588837987	3.739031169	4.677544437
C	2.683567904	6.413029963	1.899224019
C	2.424500244	7.048040315	-0.241585945
C	2.749143545	8.250869278	0.304356080
C	-2.199899836	-2.284640031	-1.718502915
C	-2.295912362	-2.992140102	0.399545077
C	-2.682516995	-4.143168269	-0.217820423
C	-1.957115912	-1.290258830	-2.736189377
C	-1.354727938	0.738260381	-3.445737194
C	-1.509468733	0.134112496	-4.658023697
H	-3.414159501	2.999179876	0.178725220
H	-2.745638276	5.379509010	0.759015572
H	-0.280405904	5.882610085	0.961982526
H	1.179329383	-1.455997066	-0.664607745
H	4.105508795	1.606222200	0.245216572
H	3.605506716	-0.815548645	-0.338771498
H	2.597056310	3.217694302	5.621116836
H	2.224409298	6.833841574	-1.279994382

H	2.856399860	9.203759040	-0.188434833
H	2.129363338	2.193920036	3.223918023
H	-2.193917175	-2.829893791	1.462191376
H	-2.953470232	-5.088310410	0.225243497
H	-1.034225208	1.760564255	-3.297585322
H	-1.366183090	0.557719147	-5.639345526

S1.3 $[Fe(bt)(NCS)_2]_2$(μ-bpym) [HS-HS], S=4, E= -7293.88820254 au, ν_1= 13.2675 cm^{-1}

Fe	-1.80193258	0.10090662	-0.17320032
Fe	2.45501689	4.13297493	0.32797711
S	-6.52330815	0.40768550	-0.85996289
S	0.22099729	0.10439916	4.15155294
S	0.43538800	4.12941289	-3.99816188
S	7.17602444	3.82931896	1.01721067
S	2.84813319	5.88030261	4.67587869
S	3.36986588	8.30413205	2.11252534
S	-2.72625973	-4.06827413	-1.95649091
S	-2.20230611	-1.64538872	-4.52026155
N	-1.26529404	-0.17514134	1.77963915
N	-3.76347517	0.34852904	-0.37024854
N	-1.47260374	2.22448463	0.06621593
N	0.20318312	3.84647567	0.56016205
N	0.44988911	0.38825051	-0.40746620
N	2.12553658	2.01024184	0.08675605
N	1.92071527	4.41014139	-1.62574008
N	4.41636305	3.88744718	0.52639434
N	2.33967065	4.42933244	2.60905997
N	2.62733122	6.30843875	0.66840128
N	-1.97908269	-2.07390299	-0.51294505
N	-1.68884218	-0.19549875	-2.45388690
C	-0.64597880	-0.05603260	2.78426354
C	-4.93474031	0.36761520	-0.57814851
C	-0.19017891	2.61241056	0.20478600
C	-2.42678547	3.14566042	0.28785959
C	-2.09894178	4.44262879	0.65747729
C	-0.75007970	4.75783271	0.78995548
C	1.40315400	-0.52303031	-0.63743613
C	0.84310793	1.62227261	-0.05195910
C	3.07979792	1.08910630	-0.13504566
C	2.75202670	-0.20775709	-0.50497641
C	5.58758363	3.86874752	0.73476859
C	1.30172092	4.29034508	-2.63051027
C	2.69277635	5.65483616	2.95598044
C	2.16578895	3.61791124	3.70127801
C	2.39387785	4.22295189	4.90165784
C	2.86415415	6.64893571	1.92412686
C	2.83607257	7.34967155	-0.19848184
C	3.23341555	8.50993907	0.39420825
C	-2.21749055	-2.41397108	-1.76851705
C	-2.18891936	-3.11477259	0.35407499
C	-2.58879093	-4.27432164	-0.23829417
C	-2.04480974	-1.42028136	-2.80049651
C	-1.51423842	0.61552992	-3.54623248
C	-1.74470341	0.01102648	-4.74642653
H	-3.44570368	2.80145604	0.16689361
H	-2.86829787	5.18150413	0.83706041
H	-0.40982157	5.74672786	1.07151919
H	1.06295965	-1.51191633	-0.91907383

H	4.09870034	1.43332926	-0.01389357
H	3.52145378	-0.94650568	-0.68477271
H	2.32809402	3.79672281	5.89011261
H	2.68364482	7.17991221	-1.25394611
H	3.46534304	9.45741881	-0.06569740
H	1.85705894	2.58975144	3.56699981
H	-2.03530389	-2.94533782	1.40940701
H	-2.82208934	-5.22137367	0.22179459
H	-1.20335659	1.64307199	-3.41223136
H	-1.67882032	0.43714207	-5.73492394

S1.4 $[Fe(bt)(NCSe)_2]_2(\mu\text{-bpym})$ [LS-LS], S=0, E= -15306.9381055 au, ν_1= 7.6319cm^{-1}

Fe	-1.5659759	0.2577178	-0.2496104
Fe	2.2165144	3.9769652	0.4042474
Se	-6.4196886	0.5638493	-0.2247083
Se	-0.2549634	0.0533147	4.4067212
Se	0.9050571	4.1822053	-4.2520397
Se	7.0702800	3.6717982	0.3771480
S	2.6883573	5.3485377	4.5791927
S	2.9990512	7.9991644	2.0035461
S	-2.3470328	-3.7645679	-1.8494536
S	-2.0360900	-1.1137753	-4.4248333
N	-1.3798418	0.1111474	1.6687994
N	-3.4730521	0.3542687	-0.1804926
N	-1.4455300	2.2195500	-0.0612897
N	0.2358284	3.8694920	0.4186365
N	0.4147876	0.3652158	-0.2638696
N	2.0961396	2.0151936	0.2159250
N	2.0299715	4.1235153	-1.5141548
N	4.1235709	3.8805903	0.3341223
N	2.3130249	4.0536793	2.3820294
N	2.3661622	5.9216964	0.6217761
N	-1.7153889	-1.6869802	-0.4672950
N	-1.6618424	0.1811140	-2.2275011
C	-0.9453541	0.0985081	2.7634248
C	-4.6498291	0.4189117	-0.1929614
C	-0.1769106	2.6191760	0.1318195
C	-2.4080124	3.1536512	0.0563279
C	-2.0660792	4.4697767	0.3569140
C	-0.7284970	4.8037067	0.5312827
C	1.3790832	-0.5691039	-0.3759300
C	0.8275279	1.6155922	0.0226106
C	3.0585878	1.0809964	0.0988909
C	2.7166461	-0.2352080	-0.2013502
C	5.3003697	3.8162611	0.3461364
C	1.5954893	4.1364937	-2.6087767
C	2.5731808	5.2768288	2.8528927
C	2.1884716	3.1337683	3.3962718
C	2.3576106	3.6467945	4.6444669
C	2.6285765	6.3123225	1.8700565
C	2.4681781	6.9552031	-0.2780597
C	2.7893612	8.1514925	0.2841310
C	-1.9770535	-2.0776338	-1.7157324
C	-1.8175421	-2.7205457	0.4324426
C	-2.1381443	-3.9169038	-0.1299416
C	-1.9215807	-1.0420754	-2.6984861
C	-1.5371487	1.1010721	-3.2416682
C	-1.7056922	0.5880404	-4.4899467

H	-3.4249441	2.8148298	-0.0812540
H	-2.8361069	5.2232401	0.4520483
H	-0.4019585	5.8098192	0.7544231
H	1.0525350	-1.5752817	-0.5987599
H	4.0755056	1.4198085	0.2366097
H	3.4866390	-0.9887691	-0.2959894
H	2.3016565	3.1279464	5.5877576
H	2.3049266	6.7505375	-1.3247316
H	2.9297361	9.1038041	-0.2013987
H	1.9461200	2.1047285	3.1773943
H	-1.6548808	-2.5158735	1.4792060
H	-2.2784123	-4.8692955	0.3554610
H	-1.2951285	2.1301729	-3.0227103
H	-1.6495752	1.1069413	-5.4331980

S1.5 $[Fe(bt)(NCSe)_2]_2(\mu\text{-bpym})$ [HS-LS], S=2, E= -15306.9322542 au, ν_1= 9.5665 cm^{-1}

Fe	-1.8152040	0.2175678	-0.1106329
Fe	2.2262001	4.0787449	0.4497429
Se	-6.6572013	0.7895566	-0.8276775
Se	0.4271006	-0.2333042	4.2401461
Se	0.8468167	4.0723656	-4.1957320
Se	7.0904195	4.0474913	0.2877549
S	2.8881216	5.4681779	4.5912331
S	3.0538720	8.1136707	1.9952020
S	-2.6607507	-3.9436690	-1.9495119
S	-1.9680101	-1.5180190	-4.4688084
N	-1.3207459	-0.0897566	1.8562728
N	-3.7704772	0.4894016	-0.3175133
N	-1.4685001	2.3430614	0.1096301
N	0.2639608	3.9426447	0.5361273
N	0.4861733	0.4477921	-0.2448777
N	2.1046054	2.1305941	0.2675068
N	1.9802238	4.2081665	-1.4638673
N	4.1359101	4.0139134	0.3128772
N	2.4027370	4.1662945	2.4191391
N	2.3698981	6.0263895	0.6520206
N	-1.9874630	-1.9590398	-0.4594069
N	-1.6182148	-0.0638763	-2.3724399
C	-0.6394745	-0.1433363	2.8202521
C	-4.9331612	0.6020975	-0.5223614
C	-0.1826950	2.6985280	0.2404205
C	-2.3967830	3.3034047	0.2834185
C	-2.0221064	4.6029546	0.5977981
C	-0.6680083	4.8953149	0.7186058
C	1.4723371	-0.4522749	-0.3686572
C	0.8383106	1.6980580	0.0719553
C	3.0936440	1.2279711	0.1356927
C	2.8023346	-0.0943256	-0.1792343
C	5.3143171	4.0456329	0.2981715
C	1.5418036	4.1447405	-2.5549376
C	2.6798251	5.3922537	2.8734703
C	2.3405425	3.2464866	3.4396994
C	2.5736126	3.7633919	4.6760268
C	2.6853147	6.4242975	1.8859325
C	2.4274414	7.0560766	-0.2559000
C	2.7675892	8.2565471	0.2858793
C	-2.1593917	-2.2926856	-1.7270801
C	-2.2465947	-3.0030479	0.3907708

C	-2.6169916	-4.1586022	-0.2280048
C	-1.9346749	-1.2928937	-2.7439443
C	-1.3769400	0.7494754	-3.4506354
C	-1.5160445	0.1425751	-4.6634550
H	-3.4265522	2.9928032	0.1687719
H	-2.7670223	5.3741191	0.7407588
H	-0.3033215	5.8867840	0.9477643
H	1.1731545	-1.4624475	-0.6183415
H	4.0980100	1.6021217	0.2747050
H	3.5969580	-0.8209704	-0.2803298
H	2.5792721	3.2458287	5.6217158
H	2.2203420	6.8445471	-1.2934627
H	2.8831139	9.2068930	-0.2099421
H	2.0975246	2.2138740	3.2338071
H	-2.1468752	-2.8418042	1.4537700
H	-2.8738879	-5.1081379	0.2140167
H	-1.0787126	1.7788578	-3.3037883
H	-1.3789914	0.5701496	-5.6439438

S1.6 $[Fe(bt)(NCSe)_2]_2(\mu\text{-bpym})$ [HS-HS], S=4, E= -15306.9228353 au, ν_1= 8.8772 cm^{-1}

Fe	-1.7982350	0.1056283	-0.1837441
Fe	2.4497577	4.1283115	0.3392838
Se	-6.6671343	0.4928060	-0.8716499
Se	0.3437955	-0.0123279	4.2533464
Se	0.3037310	4.2500084	-4.0954095
Se	7.3203315	3.7443059	1.0175377
S	2.8227647	5.8860237	4.6784590
S	3.3469991	8.3058189	2.1128266
S	-2.6966562	-4.0710565	-1.9591962
S	-2.1737607	-1.6498289	-4.5235906
N	-1.2810236	-0.1718698	1.7848028
N	-3.7672003	0.3439736	-0.3646843
N	-1.4729134	2.2261478	0.0540189
N	0.2023177	3.8508221	0.5426711
N	0.4492096	0.3833637	-0.3875085
N	2.1243591	2.0080141	0.1014809
N	1.9334130	4.4053433	-1.6297572
N	4.4187803	3.8907979	0.5193411
N	2.3406280	4.4257320	2.6125301
N	2.6088011	6.3080514	0.6706225
N	-1.9590888	-2.0737772	-0.5159567
N	-1.6891421	-0.1910369	-2.4571687
C	-0.6451736	-0.1062589	2.7786708
C	-4.9343235	0.3962656	-0.5670243
C	-0.1909128	2.6140322	0.1973929
C	-2.4269978	3.1521354	0.2594945
C	-2.0988791	4.4529761	0.6142673
C	-0.7509406	4.7678056	0.7527295
C	1.4024944	-0.5334578	-0.5980625
C	0.8423742	1.6200720	-0.0419054
C	3.0785033	1.0821660	-0.1044116
C	2.7504426	-0.2185617	-0.4596519
C	5.5864474	3.8387798	0.7185993
C	1.2955694	4.3415175	-2.6224662
C	2.6780625	5.6560061	2.9591913
C	2.1716179	3.6139223	3.7053938
C	2.3875210	4.2242693	4.9053802
C	2.8437345	6.6505604	1.9262088
C	2.8181599	7.3483900	-0.1975931

C	3.2131497	8.5097496	0.3945037
C	-2.1938062	-2.4157657	-1.7717316
C	-2.1682714	-3.1145970	0.3517282
C	-2.5629406	-4.2757686	-0.2409414
C	-2.0277662	-1.4208540	-2.8042865
C	-1.5202724	0.6212577	-3.5497009
C	-1.7373785	0.0117201	-4.7498840
H	-3.4465440	2.8112178	0.1359450
H	-2.8682886	5.1954397	0.7777480
H	-0.4110358	5.7596252	1.0237982
H	1.0626330	-1.5251722	-0.8695752
H	4.0980463	1.4231381	0.0189903
H	3.5198931	-0.9609023	-0.6235138
H	2.3211447	3.7990348	5.8942262
H	2.6673608	7.1786753	-1.2532784
H	3.4433855	9.4573345	-0.0660200
H	1.8734469	2.5817298	3.5745447
H	-2.0176209	-2.9453563	1.4075113
H	-2.7930891	-5.2236084	0.2190989
H	-1.2214031	1.6532143	-3.4185146
H	-1.6713861	0.4374420	-5.7385471

S1.7 $[Fe(bt)(NCBH_3)_2]_2$(μ-bpym) [LS-LS], S=0, E= -5807.62771667 au, ν_1= 19.5714 cm^{-1}

Fe	-1.5297048	0.2239374	-0.2652038
Fe	2.1811053	4.0111903	0.4191151
S	2.6150105	5.3574644	4.6067069
S	2.8681414	8.0370068	2.0556860
S	-2.2174485	-3.8020578	-1.9010942
S	-1.9668592	-1.1224911	-4.4523694
N	-1.3175420	0.0882542	1.6517493
N	-3.4395260	0.2906459	-0.1788160
N	-1.4481854	2.1884069	-0.0599901
N	0.1985132	3.8603518	0.4440029
N	0.4528840	0.3747778	-0.2902622
N	2.0995794	2.0466922	0.2138953
N	1.9688235	4.1467819	-1.4978466
N	4.0909413	3.9444325	0.3333293
N	2.2849650	4.0730269	2.3982460
N	2.2937020	5.9577647	0.6522975
N	-1.6422774	-1.7226828	-0.4982007
N	-1.6347596	0.1619149	-2.2441974
C	-0.9064600	0.1323889	2.7414643
C	-4.5938848	0.4516520	-0.1808570
C	-0.1893064	2.6098016	0.1397878
C	-2.4289428	3.1063424	0.0662797
C	-2.1114453	4.4222083	0.3861867
C	-0.7807057	4.7771298	0.5700614
C	1.4320982	-0.5420294	-0.4161710
C	0.8407071	1.6253235	0.0139624
C	3.0803275	1.1287330	0.0877391
C	2.7628247	-0.1871343	-0.2321747
C	5.2452429	3.7830190	0.3359013
C	1.5574106	4.1030141	-2.5874506
C	2.5074841	5.2985548	2.8806642
C	2.1847557	3.1399865	3.4032875
C	2.3344556	3.6472301	4.6565836
C	2.5388614	6.3438959	1.9055089
C	2.3753888	7.0023271	-0.2376059
C	2.6650010	8.2005288	0.3373639

C	-1.8882730	-2.1089091	-1.7512284
C	-1.7232437	-2.7672129	0.3917996
C	-2.0131172	-3.9654802	-0.1829076
C	-1.8576532	-1.0636182	-2.7264490
C	-1.5356053	1.0949962	-3.2493206
C	-1.6865493	0.5877824	-4.5024702
H	-3.4416810	2.7576190	-0.0795426
H	-2.8962654	5.1592736	0.4888478
H	-0.4714443	5.7849211	0.8090157
H	1.1228422	-1.5498190	-0.6551387
H	4.0930646	1.4774090	0.2336965
H	3.5476304	-0.9242393	-0.3346601
H	2.2872870	3.1181123	5.5947483
H	2.2216545	6.8054490	-1.2872163
H	2.7837067	9.1606771	-0.1385083
H	1.9757594	2.1057229	3.1766225
H	-1.5688546	-2.5702732	1.4413036
H	-2.1314021	-4.9256097	0.2931059
H	-1.3264052	2.1292570	-3.0228493
H	-1.6402736	1.1168933	-5.4406816
B	-6.1321024	0.7879436	-0.2099440
H	-6.6601738	0.2871264	0.7585244
H	-6.2032772	2.0064424	-0.1716786
H	-6.5900518	0.3582466	-1.2487946
B	-0.2358325	0.2161146	4.1686211
H	-0.6390487	-0.6927905	4.8583397
H	0.9680547	0.1119520	3.9761946
H	-0.5105928	1.2976373	4.6500295
B	0.8863449	4.0190781	-4.0143978
H	1.1604133	2.9371332	-4.4952850
H	-0.3174299	4.1240166	-3.8216871
H	1.2898723	4.9273428	-4.7047565
B	6.7833028	3.4460811	0.3659874
H	6.8538431	2.2274854	0.3288740
H	7.3120216	3.9456898	-0.6027446
H	7.2410609	3.8764525	1.4046290

S1.8 $[Fe(bt)(NCBH_3)_2]_2(\mu\text{-bpym})$ [HS-LS], S=2, E= -5807.61526526 au, ν_1= 10.0850 cm^{-1}

Fe	-1.7573417	0.0923596	-0.1878648
Fe	2.1480346	4.0793540	0.4603566
S	2.7880651	5.4993076	4.5952722
S	2.8526074	8.1427651	1.9959480
S	-2.3807273	-4.0391006	-2.1401801
S	-1.7565340	-1.5121591	-4.5829182
N	-1.2946010	-0.1970444	1.8177392
N	-3.7482449	0.3433884	-0.3508850
N	-1.4964855	2.2526198	0.0907180
N	0.1886882	3.8849360	0.5572777
N	0.5143691	0.4091722	-0.2598827
N	2.0806194	2.1264188	0.2822279
N	1.8833605	4.1741859	-1.4523366
N	4.0588370	4.0647439	0.3088641
N	2.3364151	4.1778303	2.4303599
N	2.2367285	6.0331655	0.6562118
N	-1.8170264	-2.0699578	-0.5882328
N	-1.5498175	-0.0993071	-2.4419116
C	-0.6511650	-0.1313274	2.7897905
C	-4.8516880	0.7249522	-0.4182199

C	-0.2237525	2.6385677	0.2356742
C	-2.4517442	3.1832255	0.2845851
C	-2.1119845	4.4843267	0.6332345
C	-0.7682572	4.8092135	0.7621984
C	1.5220419	-0.4701815	-0.3697071
C	0.8300420	1.6642602	0.0651576
C	3.0931649	1.2443235	0.1702024
C	2.8382918	-0.0822733	-0.1534727
C	5.2223477	3.9981013	0.2821124
C	1.4839099	4.0750465	-2.5426114
C	2.5721156	5.4132871	2.8805246
C	2.3127786	3.2571872	3.4519836
C	2.5349746	3.7858346	4.6857923
C	2.5395745	6.4430715	1.8892385
C	2.2588401	7.0640738	-0.2527576
C	2.5604774	8.2752816	0.2877721
C	-1.9589873	-2.3754260	-1.8677241
C	-2.0409168	-3.1474847	0.2304601
C	-2.3504024	-4.3005368	-0.4249674
C	-1.7770812	-1.3359139	-2.8540913
C	-1.3414460	0.7595738	-3.4911521
C	-1.4141780	0.1789321	-4.7227734
H	-3.4761390	2.8596901	0.1564347
H	-2.8796321	5.2295041	0.7923007
H	-0.4291296	5.8039620	1.0150248
H	1.2494590	-1.4855796	-0.6273804
H	4.0884390	1.6342007	0.3301113
H	3.6520643	-0.7894052	-0.2391502
H	2.5612754	3.2705919	5.6324695
H	2.0561173	6.8477543	-1.2901835
H	2.6424773	9.2287857	-0.2087475
H	2.1051990	2.2162454	3.2512710
H	-1.9630611	-3.0120633	1.2989204
H	-2.5679012	-5.2732526	-0.0132532
H	-1.1199952	1.8023031	-3.3126533
H	-1.2819725	0.6432922	-5.6871130
B	-6.2883088	1.3401893	-0.4992043
H	-6.6953935	1.1979894	-1.6324082
H	-6.9941723	0.7843572	0.3125966
H	-6.1510127	2.5228471	-0.2284962
B	0.3190635	0.0074532	4.0240553
H	0.2259572	-0.9677401	4.7335216
H	1.4439761	0.0841033	3.5446407
H	0.0304838	1.0262780	4.6205287
B	0.8441004	3.9061094	-3.9762665
H	1.1719088	4.8371745	-4.6765463
H	1.2286804	2.8477949	-4.4347981
H	-0.3666800	3.8998935	-3.8045211
B	6.7869740	3.8184531	0.2798593
H	7.2338802	4.3351705	-0.7211915
H	7.2196106	4.3398231	1.2880423
H	6.9907204	2.6162119	0.2866664

S1.9 $[Fe(bt)(NCBH_3)_2]_2(\mu\text{-bpym})$ [HS-HS], S=4, E= -5807.59930923 au, ν_1= 6.2486 cm^{-1}

Fe	-1.759797	0.058704	-0.232780
Fe	2.408642	4.148676	0.387274
S	2.633160	5.838843	4.746723
S	3.155310	8.314492	2.224095
S	-2.542698	-4.113868	-2.034793

S	-2.038301	-1.656683	-4.577453
N	-1.265249	-0.191081	1.772827
N	-3.759041	0.283813	-0.360747
N	-1.474912	2.197144	0.011740
N	0.172181	3.839769	0.521368
N	0.477968	0.373575	-0.383222
N	2.121248	2.018349	0.129810
N	1.932304	4.409592	-1.624314
N	4.409227	3.939340	0.513590
N	2.289182	4.394587	2.645049
N	2.479700	6.325167	0.744491
N	-1.849391	-2.117093	-0.573409
N	-1.650752	-0.202619	-2.490226
C	-0.673603	-0.037748	2.767751
C	-4.908197	0.478395	-0.459715
C	-0.202271	2.598570	0.179299
C	-2.442601	3.115346	0.191877
C	-2.133430	4.422784	0.541154
C	-0.793480	4.752098	0.702626
C	1.445701	-0.533782	-0.575790
C	0.849189	1.614152	-0.036448
C	3.091391	1.104873	-0.061574
C	2.785696	-0.200455	-0.420178
C	5.570853	3.843814	0.614709
C	1.347850	4.232604	-2.619581
C	2.548308	5.635454	3.022868
C	2.138841	3.552245	3.717611
C	2.291008	4.151671	4.933149
C	2.689743	6.654474	2.008700
C	2.683500	7.380606	-0.107323
C	3.046125	8.540757	0.507398
C	-2.070714	-2.453797	-1.833763
C	-2.048138	-3.166868	0.286660
C	-2.417855	-4.330154	-0.317732
C	-1.929527	-1.442899	-2.856203
C	-1.502268	0.630296	-3.570291
C	-1.674789	0.024233	-4.779792
H	-3.458418	2.770094	0.052416
H	-2.914115	5.158198	0.680620
H	-0.467586	5.749384	0.969890
H	1.122270	-1.530621	-0.847809
H	4.105623	1.455107	0.076760
H	3.568080	-0.931954	-0.570374
H	2.220394	3.703657	5.911609
H	2.553924	7.223195	-1.167723
H	3.262735	9.499892	0.064524
H	1.903695	2.507785	3.564354
H	-1.908391	-3.003468	1.344847
H	-2.632201	-5.286270	0.132717
H	-1.250381	1.672089	-3.425854
H	-1.609018	0.463874	-5.762373
B	-6.434080	0.798677	-0.596311
H	-6.771317	0.495668	-1.722420
H	-7.029885	0.155605	0.240966
H	-6.553611	1.995025	-0.406626
B	0.217253	0.190012	4.047569
H	0.158001	-0.784629	4.762063
H	1.356519	0.353780	3.631552
H	-0.185569	1.186051	4.617559
B	0.465582	3.963983	-3.897709

H	-0.680647	3.838103	-3.488190
H	0.550110	4.900686	-4.658433
H	0.858184	2.934196	-4.414030
B	7.119241	3.672815	0.761076
H	7.307249	2.596249	1.292735
H	7.597926	3.710805	-0.353417
H	7.526777	4.584295	1.451003

S1.10 $[Fe(pypzH)(NCS)]_2(\mu\text{-pypz})$ [LS-LS], S=0, E= -5402.54358135 au, ν_1= 14.2344 cm^{-1}

Fe	-1.8972549	-0.1469736	0.6335976
Fe	1.8973532	0.1468967	-0.6335651
S	4.5708636	1.9798393	2.6108252
S	-4.5707458	-1.9797011	-2.6111123
N	-2.6860598	-0.5128557	-1.1153861
N	-0.7739526	1.3512024	0.0724789
N	-0.5440291	-1.5439189	0.3142651
N	-3.2225856	1.3483104	0.8720579
N	-3.1177758	-1.4157050	1.4214614
N	-4.1414649	-2.2168181	0.9550014
N	-1.3232293	-0.0588552	2.5326875
N	0.5441903	1.5438537	-0.3140849
N	2.6863577	0.5124873	1.1154037
N	0.7740837	-1.3512878	-0.0723978
N	3.2226026	-1.3484258	-0.8722718
N	3.1178062	1.4156834	-1.4214556
N	4.1416746	2.2166084	-0.9550502
N	1.3231011	0.0590030	-2.5326077
C	-3.4548940	-1.0920401	-1.7964921
C	-1.3625176	2.5743456	0.1395935
C	-0.4458414	3.5741758	-0.2000205
C	-0.7209046	-2.8817705	0.4718610
C	-2.7360922	2.5841409	0.5554422
C	-3.5408298	3.7243696	0.6393012
C	-4.8594670	3.6018197	1.0424295
C	-5.3561095	2.3364090	1.3524311
C	-4.5099999	1.2438698	1.2526784
C	-4.7283597	-2.8745409	1.9870718
C	-4.0910216	-2.5030781	3.1533440
C	-3.0902008	-1.5888010	2.7558665
C	-2.0462186	-0.8246638	3.4091127
C	-1.7453377	-0.8635420	4.7667928
C	-0.6704537	-0.1237746	5.2437683
C	0.0827673	0.6274422	4.3464746
C	-0.2709927	0.6372521	3.0042266
C	3.4549801	1.0918934	1.7965534
C	0.7210942	2.8817200	-0.4715336
C	0.4460457	-3.5742311	0.2004149
C	1.3626645	-2.5744270	-0.1394292
C	2.7361884	-2.5842341	-0.5554532
C	4.7285942	2.8742661	-1.9871449
C	4.0911449	2.5029072	-3.1533869
C	3.0901905	1.5888006	-2.7558614
C	2.0460758	0.8247961	-3.4090538
C	0.2707466	-0.6369726	-3.0040642
C	-0.0831641	-0.6270388	-4.3462733
C	0.6700279	0.1241694	-5.2435970
C	1.7450352	0.8638076	-4.7666949
C	4.5099429	-1.2439905	-1.2531438

C	5.3560607	-2.3365203	-1.3529399
C	4.8595042	-3.6019082	-1.0427082
C	3.5409431	-3.7244491	-0.6393281
H	-4.3468711	-2.2479333	-0.0467298
H	-0.5992007	4.6407765	-0.2383465
H	-1.6817409	-3.2679763	0.7626333
H	-3.1217739	4.6888796	0.3806276
H	-5.4961295	4.4768848	1.1087639
H	-6.3838545	2.1913952	1.6610517
H	-4.8598846	0.2477141	1.4786758
H	-5.5488152	-3.5505706	1.8087401
H	-4.3183975	-2.8487387	4.1480610
H	-2.3409972	-1.4775205	5.4317675
H	-0.4156494	-0.1459404	6.2970266
H	0.9472268	1.1947911	4.6674925
H	0.2991012	1.1864142	2.2707128
H	1.6819492	3.2679319	-0.7622364
H	4.3470803	2.2478235	0.0466679
H	5.5491112	3.5502293	-1.8088459
H	4.3185098	2.8485580	-4.1481103
H	2.3406664	1.4777867	-5.4316947
H	0.4150973	0.1464426	-6.2968225
H	-0.9477115	-1.1942805	-4.6672431
H	-0.2993296	-1.1861059	-2.2705101
H	3.1219585	-4.6889449	-0.3804848
H	5.4961745	-4.4769666	-1.1090620
H	6.3837439	-2.1915195	-1.6617719
H	4.8597615	-0.2478542	-1.4793292
H	0.5994391	-4.6408219	0.2388820

S1.11 $[Fe(pypzH)(NCS)]_2(\mu\text{-pypz})$ [HS-LS], S=2, E= -5402.52990960 au, ν_1= 14.9005 cm^{-1}

Fe	-1.8919323	-0.3556890	0.4314733
Fe	2.0372071	0.0713422	-0.6712235
S	4.9401364	1.7374897	2.4388394
S	-4.9119755	-2.6835509	-2.2419323
N	-2.8215447	-1.0515066	-1.2935387
N	-0.6482399	1.2856524	-0.0020551
N	-0.2824166	-1.7157930	0.3900660
N	-3.2606112	1.4033947	0.5601009
N	-3.3382016	-1.5968129	1.5338032
N	-4.4119046	-2.3958538	1.1878372
N	-1.4805203	-0.1222202	2.6542139
N	0.7276766	1.4604211	-0.1387969
N	2.9488444	0.3164152	1.0409972
N	0.9905568	-1.4870849	-0.1140247
N	3.3593250	-1.3910066	-1.0867280
N	3.1830061	1.4196148	-1.4484086
N	4.2449932	2.1870855	-1.0114736
N	1.3105489	0.1276054	-2.5125290
C	-3.6857894	-1.7231882	-1.7435893
C	-1.1874537	2.5103803	0.2442180
C	-0.1853193	3.4832628	0.2752616
C	-0.3602689	-3.0380981	0.6836021
C	-2.6211319	2.5941081	0.4405725
C	-3.3323451	3.7991452	0.4847161
C	-4.7091921	3.7687034	0.6400476
C	-5.3607991	2.5394841	0.7377284
C	-4.5946449	1.3837838	0.6943558

C	-5.0659102	-2.8337768	2.2880919
C	-4.4248731	-2.3163405	3.3942080
C	-3.3553913	-1.5503107	2.8784692
C	-2.2973800	-0.7789258	3.5147256
C	-2.0882287	-0.7406076	4.8938183
C	-1.0051950	-0.0274653	5.3904239
C	-0.1497801	0.6179867	4.5015408
C	-0.4230290	0.5467414	3.1413399
C	3.7636242	0.8713458	1.6874136
C	0.9856185	2.7763188	0.0328870
C	0.8254392	-3.6884222	0.3836936
C	1.6500088	-2.6714401	-0.1171787
C	2.9797621	-2.6321819	-0.6596913
C	4.7125975	2.9590574	-2.0248662
C	3.9563960	2.6996666	-3.1494765
C	3.0103758	1.7313912	-2.7459583
C	1.9219534	1.0055598	-3.3690286
C	0.2476464	-0.5694413	-2.9580589
C	-0.2303519	-0.4437698	-4.2549207
C	0.4047875	0.4282163	-5.1341492
C	1.4925757	1.1649320	-4.6825612
C	4.5780773	-1.2485497	-1.6405427
C	5.4618488	-2.3041796	-1.7973246
C	5.0803740	-3.5709865	-1.3582716
C	3.8295083	-3.7342755	-0.7874585
H	-4.6088736	-2.5810760	0.2008845
H	-0.2809068	4.5414804	0.4606571
H	-1.2793751	-3.4354899	1.0847732
H	-2.8042780	4.7395409	0.3851821
H	-5.2739733	4.6939577	0.6724718
H	-6.4364636	2.4761690	0.8467666
H	-5.0453650	0.4017385	0.7673794
H	-5.9293085	-3.4734962	2.1974513
H	-4.6956188	-2.4716931	4.4254692
H	-2.7558454	-1.2729456	5.5607658
H	-0.8214565	0.0106880	6.4582571
H	0.7200160	1.1630224	4.8462067
H	0.2195247	1.0166164	2.4087756
H	1.9975136	3.1411067	-0.0132033
H	4.5569043	2.1224740	-0.0375887
H	5.5430415	3.6273087	-1.8643393
H	4.0737770	3.1499716	-4.1211155
H	2.0018880	1.8664288	-5.3325181
H	0.0510836	0.5427045	-6.1522599
H	-1.0970351	-1.0190975	-4.5544452
H	-0.2252602	-1.2216156	-2.2398413
H	3.4972747	-4.7026257	-0.4344121
H	5.7511787	-4.4165675	-1.4603972
H	6.4306471	-2.1291024	-2.2482514
H	4.8402453	-0.2513322	-1.9617076
H	1.0522077	-4.7357934	0.5043806

S1.12 $[Fe(pypzH)(NCS)]_2(\mu\text{-pypz})$ [HS-HS], S=4, E= -5402.51512246 au, ν_1= 9.7914 cm^{-1}

Fe	-1.9809725	-0.2756311	0.5598471
Fe	2.0185117	0.2008941	-0.5126254
S	5.2657116	2.3320910	2.0267806
S	-4.0036490	-1.7486156	-3.6092159
N	-2.9903903	-0.8841971	-1.1321127

N	-0.8224645	1.4426215	0.1866651
N	-0.4287562	-1.7319039	0.3588416
N	-3.4087330	1.4691693	0.8371430
N	-3.3120037	-1.5752182	1.6262032
N	-4.3546386	-2.3680215	1.2040265
N	-1.4865386	-0.1760854	2.7998873
N	0.5101218	1.6733475	-0.1594077
N	3.1067587	0.7305687	1.1824717
N	0.8765792	-1.5095155	-0.0811744
N	3.4275857	-1.5326785	-0.8581048
N	3.3439961	1.5590952	-1.6293547
N	4.4335533	2.3540295	-1.3245891
N	1.3879531	0.1596369	-2.6756261
C	-3.4148627	-1.2414611	-2.1810116
C	-1.4341578	2.6527007	0.2719925
C	-0.5225563	3.6766043	-0.0063239
C	-0.5542325	-3.0601265	0.5685644
C	-2.8448746	2.6800656	0.6038524
C	-3.6057382	3.8535569	0.6765596
C	-4.9551102	3.7696045	0.9802428
C	-5.5299741	2.5192994	1.2051980
C	-4.7155902	1.3988051	1.1237733
C	-4.9750746	-2.9579506	2.2565948
C	-4.3320195	-2.5421803	3.4038722
C	-3.3000204	-1.6786772	2.9642553
C	-2.2503655	-0.9252537	3.6357883
C	-2.0003333	-0.9758897	5.0069525
C	-0.9311754	-0.2532925	5.5209066
C	-0.1337585	0.4927926	4.6568769
C	-0.4466570	0.5060831	3.3027814
C	4.0042975	1.3839030	1.5906549
C	0.6672794	3.0090329	-0.2713350
C	0.6288919	-3.7276162	0.2767198
C	1.5036404	-2.7117647	-0.1251848
C	2.8921079	-2.7390425	-0.5455667
C	4.9229046	2.9514116	-2.4354135
C	4.1525629	2.5486218	-3.5064443
C	3.1806722	1.6811418	-2.9589445
C	2.0692953	0.9460212	-3.5461025
C	0.3091194	-0.5111764	-3.1110889
C	-0.1342005	-0.4419933	-4.4260672
C	0.5772305	0.3461758	-5.3263795
C	1.6904981	1.0498977	-4.8844605
C	4.7117200	-1.4624990	-1.2345128
C	5.5291364	-2.5799715	-1.3303229
C	4.9830552	-3.8252104	-1.0237599
C	3.6569756	-3.9083099	-0.6286662
H	-4.5225868	-2.4207488	0.2077935
H	-0.6925793	4.7417057	-0.0182907
H	-1.4949355	-3.4589378	0.9148543
H	-3.1371213	4.8116811	0.4887778
H	-5.5576486	4.6696099	1.0358090
H	-6.5827675	2.4137725	1.4368208
H	-5.1073492	0.4025404	1.2886741
H	-5.8145381	-3.6185831	2.1095078
H	-4.5782467	-2.8259393	4.4138609
H	-2.6260729	-1.5794329	5.6538746
H	-0.7153267	-0.2817183	6.5830123
H	0.7199623	1.0530489	5.0169713
H	0.1435983	1.0619386	2.5857488

H	1.6337874	3.4113277	-0.5316466
H	4.7523580	2.4275810	-0.3535046
H	5.7743332	3.6106357	-2.3764472
H	4.2789160	2.8414372	-4.5356495
H	2.2520827	1.6832288	-5.5609354
H	0.2604272	0.4220647	-6.3605088
H	-1.0239896	-0.9854497	-4.7189805
H	-0.2060855	-1.1057602	-2.3692201
H	3.2103356	-4.8630475	-0.3797412
H	5.5889518	-4.7223415	-1.0887015
H	6.5631293	-2.4745603	-1.6348936
H	5.0814558	-0.4699349	-1.4597887
H	0.8185993	-4.7870073	0.3489467

S1.13 $[Fe(pypzH)(NCSe)]_2(\mu\text{-pypz})$ [LS-LS], S=0, E= -9409.06570046 au, ν_1= 11.4281 cm^{-1}

Fe	-1.8963418	-0.1406043	0.6359783
Fe	1.8971986	0.1396329	-0.6363810
Se	4.6340043	2.0214164	2.7455795
Se	-4.6307544	-2.0261949	-2.7458038
N	-2.6838780	-0.5113059	-1.1041176
N	-0.7701289	1.3534822	0.0711601
N	-0.5462545	-1.5426107	0.3206556
N	-3.2187105	1.3575437	0.8707205
N	-3.1178420	-1.4074754	1.4250005
N	-4.1397574	-2.2097659	0.9580720
N	-1.3244743	-0.0482134	2.5366697
N	0.5478608	1.5418418	-0.3186887
N	2.6860017	0.5084479	1.1034677
N	0.7711559	-1.3544087	-0.0711348
N	3.2189256	-1.3587517	-0.8731871
N	3.1182159	1.4069608	-1.4251587
N	4.1407984	2.2083951	-0.9582204
N	1.3237159	0.0492137	-2.5365861
C	-3.4287074	-1.0659650	-1.8247793
C	-1.3553192	2.5782852	0.1377149
C	-0.4367192	3.5749919	-0.2051292
C	-0.7253585	-2.8796430	0.4830355
C	-2.7289838	2.5919950	0.5540678
C	-3.5308734	3.7341196	0.6373663
C	-4.8500601	3.6145877	1.0397809
C	-5.3500078	2.3504863	1.3495764
C	-4.5065541	1.2558673	1.2506901
C	-4.7235383	-2.8714818	1.9891133
C	-4.0852344	-2.5013215	3.1554449
C	-3.0872726	-1.5837256	2.7587776
C	-2.0439510	-0.8181971	3.4120650
C	-1.7417951	-0.8579770	4.7693999
C	-0.6698801	-0.1141377	5.2468944
C	0.0781321	0.6439725	4.3511497
C	-0.2772595	0.6543426	3.0093049
C	3.4312821	1.0622238	1.8243435
C	0.7278528	2.8791115	-0.4780272
C	0.4392681	-3.5754814	0.2102839
C	1.3569364	-2.5790248	-0.1357659
C	2.7300258	-2.5928793	-0.5539841
C	4.7232515	2.8718095	-1.9889337
C	4.0834287	2.5035977	-3.1550388
C	3.0859396	1.5853740	-2.7586154

C	2.0420172	0.8205506	-3.4117717
C	0.2765213	-0.6534683	-3.0090683
C	-0.0801230	-0.6417570	-4.3505634
C	0.6665703	0.1178927	-5.2461087
C	1.7385306	0.8617675	-4.7687642
C	4.5058985	-1.2573957	-1.2561761
C	5.3493539	-2.3519880	-1.3553084
C	4.8503496	-3.6157222	-1.0424943
C	3.5320048	-3.7349494	-0.6372624
H	-4.3448866	-2.2415160	-0.0437692
H	-0.5870919	4.6419309	-0.2444838
H	-1.6860470	-3.2635624	0.7770481
H	-3.1094904	4.6976099	0.3788084
H	-5.4846938	4.4911123	1.1055590
H	-6.3783554	2.2080096	1.6571873
H	-4.8588672	0.2604723	1.4762396
H	-5.5422966	-3.5492488	1.8098427
H	-4.3102520	-2.8501682	4.1495625
H	-2.3341379	-1.4757286	5.4337867
H	-0.4137952	-0.1376574	6.2997704
H	0.9391783	1.2162307	4.6726213
H	0.2868353	1.2113646	2.2772368
H	1.6890429	3.2631416	-0.7702541
H	4.3469330	2.2387869	0.0434495
H	5.5423287	3.5491817	-1.8096352
H	4.3072573	2.8540205	-4.1488721
H	2.3299247	1.4805990	-5.4329930
H	0.4094673	0.1424959	-6.2987116
H	-0.9410898	-1.2141985	-4.6719245
H	-0.2865070	-1.2116650	-2.2770789
H	3.1113215	-4.6981672	-0.3765601
H	5.4850388	-4.4922069	-1.1082684
H	6.3769873	-2.2097708	-1.6654159
H	4.8575064	-0.2622678	-1.4840194
H	0.5902281	-4.6422624	0.2516304

S1.14 $[Fe(pypzH)(NCSe)]_2(\mu\text{-pypz})$ [HS-LS], S=2, E= -9409.05056616 au, ν_1= 11.7402 cm^{-1}

Fe	-1.8893044	-0.3464529	0.4484211
Fe	2.0332192	0.0701511	-0.6744497
Se	5.0012173	1.7802385	2.5792736
Se	-5.0176713	-2.7268423	-2.3603653
N	-2.8347187	-1.0419506	-1.2783670
N	-0.6489194	1.2894104	-0.0001984
N	-0.2888130	-1.7152747	0.3864218
N	-3.2598676	1.4094232	0.5679825
N	-3.3298434	-1.5911868	1.5445358
N	-4.3998640	-2.3943809	1.1993101
N	-1.4725054	-0.1148548	2.6636841
N	0.7268730	1.4629870	-0.1407970
N	2.9437771	0.3167943	1.0292362
N	0.9839863	-1.4877452	-0.1191049
N	3.3530694	-1.3939274	-1.0925918
N	3.1792819	1.4180008	-1.4506841
N	4.2394497	2.1858389	-1.0115758
N	1.3068775	0.1274423	-2.5169113
C	-3.6858347	-1.6937373	-1.7704320
C	-1.1873529	2.5152089	0.2429331
C	-0.1848068	3.4875628	0.2683164

C	-0.3703045	-3.0389475	0.6725817
C	-2.6208127	2.5997908	0.4424598
C	-3.3318156	3.8048364	0.4834149
C	-4.7084151	3.7748385	0.6416339
C	-5.3596669	2.5460125	0.7453943
C	-4.5937347	1.3901069	0.7051747
C	-5.0431213	-2.8463749	2.2998966
C	-4.3976390	-2.3342585	3.4060845
C	-3.3371418	-1.5565547	2.8896961
C	-2.2796962	-0.7831087	3.5247010
C	-2.0623974	-0.7522747	4.9025958
C	-0.9814198	-0.0347849	5.3975894
C	-0.1366791	0.6239325	4.5082797
C	-0.4180162	0.5600746	3.1494520
C	3.7341741	0.8446678	1.7203961
C	0.9854033	2.7794359	0.0257283
C	0.8126780	-3.6912858	0.3663627
C	1.6395585	-2.6742769	-0.1301280
C	2.9695285	-2.6362092	-0.6727544
C	4.7059016	2.9614726	-2.0224770
C	3.9503485	2.7036064	-3.1480311
C	3.0059879	1.7326978	-2.7473101
C	1.9176183	1.0073297	-3.3715885
C	0.2464854	-0.5719181	-2.9641738
C	-0.2313034	-0.4456732	-4.2611219
C	0.4021931	0.4296465	-5.1381281
C	1.4884868	1.1677430	-4.6850522
C	4.5733617	-1.2514400	-1.6431587
C	5.4543588	-2.3086808	-1.8042006
C	5.0684391	-3.5768594	-1.3732711
C	3.8162068	-3.7399626	-0.8053600
H	-4.6041583	-2.5726104	0.2128030
H	-0.2793230	4.5463701	0.4506335
H	-1.2897378	-3.4362250	1.0730172
H	-2.8040376	4.7448644	0.3791602
H	-5.2732429	4.7001171	0.6714879
H	-6.4351172	2.4830065	0.8563711
H	-5.0444713	0.4084301	0.7826206
H	-5.9026427	-3.4912134	2.2091008
H	-4.6599821	-2.5005460	4.4377971
H	-2.7222531	-1.2936532	5.5699494
H	-0.7912509	-0.0029553	6.4644684
H	0.7309508	1.1734913	4.8512221
H	0.2152727	1.0419696	2.4167186
H	1.9970399	3.1444978	-0.0232989
H	4.5496855	2.1218266	-0.0371995
H	5.5350176	3.6307373	-1.8595112
H	4.0671976	3.1566895	-4.1184318
H	1.9968146	1.8709066	-5.3339305
H	0.0487293	0.5450415	-6.1561928
H	-1.0957842	-1.0233001	-4.5626647
H	-0.2233264	-1.2279038	-2.2473840
H	3.4808412	-4.7093037	-0.4581202
H	5.7370863	-4.4236690	-1.4789724
H	6.4246573	-2.1337158	-2.2518522
H	4.8390662	-0.2530945	-1.9577268
H	1.0361518	-4.7400453	0.4806123

S1.15 $[Fe(pypzH)(NCSe)]_2(\mu\text{-pypz})$ [HS-HS], S=4, E= -9409.03651523au, ν_1= 5.9473 cm^{-1}

Fe	-1.9931478	-0.2263111	0.5222029
Fe	1.9927343	0.2265969	-0.5219641
Se	5.2484003	2.3915002	2.2864982
Se	-5.2490071	-2.3915386	-2.2856708
N	-3.0250212	-0.7492929	-1.2193238
N	-0.8352007	1.4847547	0.1446516
N	-0.4924907	-1.7138962	0.2210403
N	-3.4168878	1.5038137	0.8146976
N	-3.3690526	-1.5757794	1.5770057
N	-4.4464218	-2.3662433	1.2258146
N	-1.4496210	-0.1890937	2.7048286
N	0.4920939	1.7141299	-0.2212606
N	3.0244047	0.7495593	1.2197175
N	0.8348475	-1.4844414	-0.1445542
N	3.4165866	-1.5035187	-0.8146207
N	3.3687143	1.5761177	-1.5765849
N	4.4460523	2.3665546	-1.2251654
N	1.4499327	0.1889916	-2.7048177
C	-3.8953306	-1.3778178	-1.7068051
C	-1.4523597	2.6918582	0.2165056
C	-0.5489310	3.7148426	-0.0915141
C	-0.6416580	-3.0484602	0.3584145
C	-2.8597143	2.7156966	0.5670299
C	-3.6226301	3.8867948	0.6430003
C	-4.9685797	3.8005506	0.9625630
C	-5.5368387	2.5500516	1.2001180
C	-4.7207903	1.4308388	1.1165342
C	-4.9937517	-2.9521944	2.3153385
C	-4.2744545	-2.5455671	3.4199172
C	-3.2717057	-1.6880732	2.9141549
C	-2.1857280	-0.9551928	3.5488047
C	-1.8817839	-1.0414835	4.9076537
C	-0.7893272	-0.3393059	5.3994316
C	-0.0212687	0.4249811	4.5251274
C	-0.3863711	0.4755004	3.1859621
C	3.8946819	1.3779722	1.7073948
C	0.6410962	3.0486636	-0.3593018
C	0.5483641	-3.7146283	0.0904843
C	1.4519248	-2.6915954	-0.2169186
C	2.8593165	-2.7154156	-0.5672751
C	4.9939302	2.9520934	-2.3146380
C	4.2750376	2.5452666	-3.4193983
C	3.2719738	1.6880340	-2.9138154
C	2.1862532	0.9549948	-3.5486920
C	0.3868896	-0.4757833	-3.1861325
C	0.0222186	-0.4255959	-4.5254282
C	0.7904962	0.3385915	-5.3996379
C	1.8827111	1.0409890	-4.9076601
C	4.7205318	-1.4305398	-1.1162580
C	5.5365348	-2.5497794	-1.1999693
C	4.9681855	-3.8002934	-0.9627167
C	3.6221933	-3.8865377	-0.6433289
H	-4.7213665	-2.4443340	0.2419458
H	-0.7240480	4.7787575	-0.1199710
H	-1.6027538	-3.4516922	0.6367789
H	-3.1587654	4.8453457	0.4457306
H	-5.5730137	4.6991053	1.0204580
H	-6.5868472	2.4419381	1.4424144

H	-5.1081354	0.4346705	1.2899294
H	-5.8452180	-3.6068091	2.2187306
H	-4.4528303	-2.8303307	4.4436507
H	-2.4862729	-1.6578821	5.5622191
H	-0.5332304	-0.3972835	6.4513243
H	0.8496062	0.9712400	4.8649424
H	0.1789921	1.0481506	2.4629324
H	1.6021270	3.4518663	-0.6379243
H	4.7207414	2.4447983	-0.2412421
H	5.8454289	3.6066407	-2.2178410
H	4.4538497	2.8297167	-4.4431429
H	2.4873219	1.6573325	-5.5621681
H	0.5347376	0.3963282	-6.4516269
H	-0.8484678	-0.9720286	-4.8654426
H	-0.1786512	-1.0483232	-2.4631525
H	3.1582764	-4.8451005	-0.4462446
H	5.5725917	-4.6988630	-1.0206793
H	6.5865753	-2.4416752	-1.4421326
H	5.1079547	-0.4343519	-1.2893785
H	0.7233657	-4.7785757	0.1184500

S1.16 $[Fe(pypzH)(NCBH_3)]_2(\mu\text{-pypz})$ [LS-LS], S=0, E= -4659.41345093 au, ν_1= 14.8253 cm^{-1}

Fe	-1.9086598	-0.1053548	0.6120169
Fe	1.9086398	0.1054421	-0.6120177
N	-2.6945755	-0.3737163	-1.1384002
N	-0.7256443	1.3744402	0.1313789
N	-0.6007755	-1.5357086	0.2431642
N	-3.1807245	1.4237724	0.9086490
N	-3.1802053	-1.3695813	1.3225470
N	-4.2183870	-2.1155342	0.8018297
N	-1.3614195	-0.1236657	2.5252948
N	0.6007075	1.5358258	-0.2433971
N	2.6944497	0.3739806	1.1384052
N	0.7256793	-1.3743338	-0.1312053
N	3.1807498	-1.4236905	-0.9084684
N	3.1801573	1.3696452	-1.3226177
N	4.2184801	2.1154441	-0.8019759
N	1.3614469	0.1235773	-2.5253161
C	-3.4175829	-0.8222875	-1.9331124
C	-1.2692772	2.6141740	0.2534937
C	-0.3154170	3.5938569	-0.0375142
C	-0.8266353	-2.8721659	0.3377141
C	-2.6454679	2.6549724	0.6603477
C	-3.4079376	3.8186475	0.7968587
C	-4.7343679	3.7247026	1.1820208
C	-5.2809776	2.4646016	1.4211176
C	-4.4751761	1.3475624	1.2723162
C	-4.8331268	-2.8133096	1.7898549
C	-4.1992718	-2.5244319	2.9815889
C	-3.1708560	-1.6168403	2.6451270
C	-2.1148380	-0.9162918	3.3499261
C	-1.8349881	-1.0318404	4.7076648
C	-0.7522872	-0.3406775	5.2374484
C	0.0277728	0.4428613	4.3926808
C	-0.3060907	0.5284946	3.0478589
C	3.4174039	0.8225914	1.9331439
C	0.8264832	2.8722799	-0.3381300
C	0.3153254	-3.5937532	0.0373570

C	1.2693046	-2.6140783	-0.2532935
C	2.6455249	-2.6548788	-0.6600336
C	4.8332773	2.8131110	-1.7900437
C	4.1993344	2.5242777	-2.9817424
C	3.1707944	1.6168529	-2.6452076
C	2.1147833	0.9162539	-3.3499680
C	0.3062303	-0.5287728	-3.0478724
C	-0.0276127	-0.4432536	-4.3927052
C	0.7523435	0.3403744	-5.2374889
C	1.8349358	1.0317140	-4.7077166
C	4.4751789	-1.3474947	-1.2722196
C	5.2809992	-2.4645315	-1.4209353
C	4.7344373	-3.7246171	-1.1816430
C	3.4080273	-3.8185492	-0.7964111
H	-4.4148512	-2.0921423	-0.2027064
H	-0.4291995	4.6659575	-0.0272573
H	-1.8018354	-3.2371565	0.6069290
H	-2.9509777	4.7788923	0.5924029
H	-5.3388648	4.6183273	1.2883943
H	-6.3166505	2.3426633	1.7124521
H	-4.8638974	0.3546620	1.4422549
H	-5.6686316	-3.4563647	1.5655237
H	-4.4467621	-2.9187151	3.9531171
H	-2.4533566	-1.6658340	5.3317502
H	-0.5136272	-0.4233777	6.2914105
H	0.8964806	0.9775382	4.7555564
H	0.2806701	1.1091961	2.3529140
H	1.8016011	3.2372858	-0.6076247
H	4.4149661	2.0920728	0.2025564
H	5.6688773	3.4560610	-1.5657653
H	4.4468427	2.9184945	-3.9532927
H	2.4532261	1.6657678	-5.3318178
H	0.5136862	0.4229987	-6.2914574
H	-0.8962284	-0.9780810	-4.7555794
H	-0.2804753	-1.1095115	-2.3529088
H	2.9511031	-4.7787804	-0.5918111
H	5.3389561	-4.6182382	-1.2879227
H	6.3166495	-2.3426041	-1.7123544
H	4.8638749	-0.3546051	-1.4422829
H	0.4290701	-4.6658574	0.0270135
B	4.5021171	1.6050973	2.7783311
H	5.0668261	2.3234634	1.9423392
H	3.9602148	2.2992958	3.6104561
H	5.2987808	0.8343186	3.2624575
B	-4.5023381	-1.6047784	-2.7782742
H	-5.0663356	-2.3239107	-1.9424718
H	-5.2995063	-0.8340067	-3.2615888
H	-3.9605696	-2.2982260	-3.6111124

S1.17 $[Fe(pypzH)(NCBH_3)]_2(\mu\text{-pypz})$ [HS-LS], S=2, E= -4659.39607963 au, ν_1= 15.2562 cm^{-1}

Fe	-1.8990837	-0.2600347	0.4086249
Fe	2.0544070	0.0675613	-0.6328740
N	-2.8557963	-0.8462307	-1.3794915
N	-0.5991684	1.3465852	0.0533520
N	-0.3527223	-1.6829111	0.2919604
N	-3.2161420	1.5302366	0.5765041
N	-3.4088899	-1.5147015	1.3880032
N	-4.4893022	-2.2673331	0.9709845

N	-1.5420120	-0.1538777	2.6345862
N	0.7837123	1.4806601	-0.0617305
N	2.9387322	0.2042947	1.0872705
N	0.9362923	-1.4770638	-0.1818999
N	3.3277361	-1.4214687	-1.1025005
N	3.2665085	1.4097326	-1.3096681
N	4.3410073	2.1124485	-0.8029076
N	1.3781343	0.2460975	-2.4898657
C	-3.6933376	-1.4159339	-1.9571009
C	-1.1028636	2.5794103	0.3339073
C	-0.0708125	3.5172774	0.4090257
C	-0.4890976	-3.0162682	0.5026598
C	-2.5361529	2.7029169	0.5148672
C	-3.2074606	3.9280933	0.6001944
C	-4.5867160	3.9374361	0.7364106
C	-5.2797413	2.7278971	0.7748229
C	-4.5521068	1.5497704	0.6934274
C	-5.1724597	-2.7613456	2.0279999
C	-4.5440709	-2.3289685	3.1776753
C	-3.4504619	-1.5538982	2.7323336
C	-2.3907431	-0.8449009	3.4359630
C	-2.2126718	-0.8922816	4.8188406
C	-1.1293074	-0.2302979	5.3814304
C	-0.2438041	0.4532783	4.5526639
C	-0.4868032	0.4682668	3.1851632
C	3.7040804	0.6088397	1.8655868
C	1.0800235	2.7813969	0.1565784
C	0.6729439	-3.6959750	0.1771000
C	1.5459923	-2.6860968	-0.2495070
C	2.8871628	-2.6699660	-0.7655015
C	4.8601289	2.9240758	-1.7581621
C	4.1250599	2.7562997	-2.9142557
C	3.1371900	1.8003998	-2.5903868
C	2.0406758	1.1484907	-3.2794523
C	0.3098156	-0.3937777	-3.0011895
C	-0.1287466	-0.1831261	-4.3012194
C	0.5554843	0.7170217	-5.1122051
C	1.6523824	1.3932211	-4.5925998
C	4.5647278	-1.2958716	-1.6194592
C	5.4068362	-2.3765034	-1.8262477
C	4.9620801	-3.6514387	-1.4805965
C	3.6923393	-3.7972543	-0.9478994
H	-4.6748107	-2.3924873	-0.0278769
H	-0.1345291	4.5713608	0.6280719
H	-1.4292415	-3.3994939	0.8669772
H	-2.6474011	4.8535705	0.5470468
H	-5.1210734	4.8789187	0.7998605
H	-6.3583239	2.6962274	0.8666399
H	-5.0363489	0.5814880	0.7192991
H	-6.0453585	-3.3767492	1.8790207
H	-4.8384770	-2.5446377	4.1914189
H	-2.9049963	-1.4503335	5.4377209
H	-0.9695211	-0.2598185	6.4532899
H	0.6257367	0.9624536	4.9488916
H	0.1773544	0.9740236	2.4971242
H	2.1027221	3.1165760	0.1329807
H	4.6280606	1.9852599	0.1729100
H	5.7079190	3.5525162	-1.5384834
H	4.2829416	3.2572840	-3.8548306
H	2.2004960	2.1120947	-5.1897390

H	0.2336183	0.8983980	-6.1311006
H	-1.0014677	-0.7160188	-4.6566200
H	-0.1974665	-1.0729843	-2.3330606
H	3.3117420	-4.7711286	-0.6662736
H	5.5991506	-4.5167538	-1.6241695
H	6.3928942	-2.2146121	-2.2432551
H	4.8766009	-0.2922221	-1.8676332
H	0.8545142	-4.7572592	0.2361680
B	4.8412947	1.3486078	2.6806752
H	5.3836192	2.0758518	1.8355883
H	4.3518441	2.0339375	3.5509372
H	5.6457510	0.5540286	3.1090449
B	-4.8885535	-2.2534656	-2.5580221
H	-5.3742973	-2.8599861	-1.5996280
H	-5.7111988	-1.5008716	-3.0280486
H	-4.4661737	-3.0479573	-3.3661401

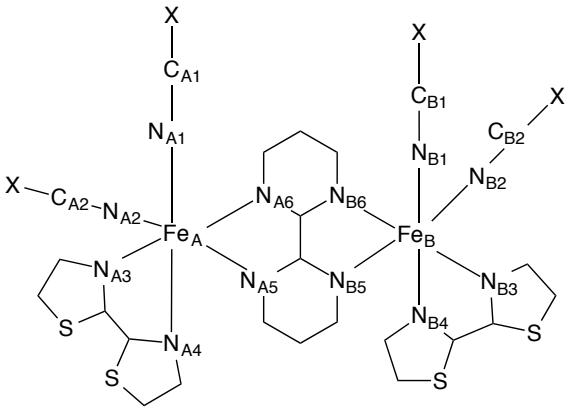
S1.18 $[Fe(pypzH)(NCBH_3)]_2(\mu\text{-pypz})$ [HS-HS], S=4, E= -4659.37995176 au, ν_1= 7.0743 cm^{-1}

Fe	-2.0087470	-0.1653714	0.4728888
Fe	2.0085281	0.1653109	-0.4730677
N	-3.0427214	-0.5710869	-1.3231078
N	-0.7749610	1.5085397	0.2059191
N	-0.5700435	-1.6996071	0.1165567
N	-3.3706026	1.6024364	0.8117719
N	-3.4716817	-1.5118837	1.3998051
N	-4.5638716	-2.2388402	0.9689936
N	-1.5408074	-0.2647954	2.6649457
N	0.5697184	1.6995875	-0.1172523
N	3.0422443	0.5706295	1.3231153
N	0.7746969	-1.5085496	-0.2062856
N	3.3704051	-1.6024807	-0.8119555
N	3.4716251	1.5120633	-1.3995327
N	4.5637030	2.2389957	-0.9684203
N	1.5411311	0.2649385	-2.6652554
C	-3.8955082	-1.1082993	-1.9090371
C	-1.3436599	2.7357069	0.3258420
C	-0.3913687	3.7333074	0.0921513
C	-0.7769419	-3.0318155	0.1819423
C	-2.7576438	2.8010586	0.6440247
C	-3.4728703	3.9978219	0.7658679
C	-4.8291418	3.9520998	1.0482166
C	-5.4545749	2.7161130	1.2035762
C	-4.6839442	1.5690553	1.0784270
C	-5.1683891	-2.8635080	2.0050010
C	-4.4730916	-2.5475939	3.1541217
C	-3.4233173	-1.7024553	2.7305300
C	-2.3335352	-1.0472106	3.4401194
C	-2.0811628	-1.2178534	4.8014061
C	-0.9830799	-0.5839786	5.3678936
C	-0.1586208	0.1985360	4.5639835
C	-0.4736238	0.3343522	3.2181389
C	3.8950713	1.1075366	1.9092644
C	0.7765676	3.0318024	-0.1827660
C	0.3910337	-3.7333226	-0.0928253
C	1.3433978	-2.7357290	-0.3262239
C	2.7574328	-2.8010915	-0.6441572
C	5.1684186	2.8638018	-2.0042307
C	4.4733831	2.5479727	-3.1535349

C	3.4235509	1.7027488	-2.7302547
C	2.3339488	1.0475289	-3.4401501
C	0.4740840	-0.3341892	-3.2187285
C	0.1593088	-0.1981716	-4.5646058
C	0.9838627	0.5845296	-5.3682393
C	2.0818060	1.2183804	-4.8014553
C	4.6837830	-1.5691105	-1.0784158
C	5.4544539	-2.7161718	-1.2033016
C	4.8290192	-3.9521462	-1.0478592
C	3.4727050	-3.9978571	-0.7657107
H	-4.8111405	-2.2572456	-0.0252051
H	-0.5214824	4.8037369	0.1147733
H	-1.7601753	-3.4079815	0.4173739
H	-2.9648058	4.9448525	0.6323196
H	-5.3972402	4.8711684	1.1406235
H	-6.5141078	2.6401570	1.4143676
H	-5.1166122	0.5824956	1.1875509
H	-6.0390085	-3.4788963	1.8431386
H	-4.6968196	-2.8824070	4.1534919
H	-2.7299568	-1.8457213	5.4002005
H	-0.7668700	-0.7081110	6.4229478
H	0.7171746	0.6943772	4.9632379
H	0.1354125	0.9257741	2.5474825
H	1.7597400	3.4079738	-0.4184412
H	4.8107184	2.2573565	0.0258471
H	6.0390070	3.4791701	-1.8421270
H	4.6973254	2.8828885	-4.1528231
H	2.7306643	1.8463891	-5.4000322
H	0.7678306	0.7088224	-6.4233111
H	-0.7163843	-0.6939987	-4.9641019
H	-0.1350184	-0.9257744	-2.5482713
H	2.9646488	-4.9448807	-0.6320821
H	5.3971503	-4.8712176	-1.1400386
H	6.5140157	-2.6402276	-1.4139510
H	5.1164473	-0.5825554	-1.1876075
H	0.5211063	-4.8037545	-0.1155773
B	5.1023899	1.9187512	2.5235761
H	5.5708406	2.5671832	1.5830103
H	4.6950006	2.6778152	3.3726743
H	5.9366210	1.1502990	2.9439138
B	-5.1027980	-1.9197673	-2.5230799
H	-5.5720446	-2.5669274	-1.5820630
H	-5.9364327	-1.1514880	-2.9449065
H	-4.6951645	-2.6799912	-3.3710405

S2. Selected bond lengths and angles for the systems

S2.1 $[Fe(bt)(NCX)_2]_2(\mu\text{-bpym})$ (X = S, Se or BH_3)

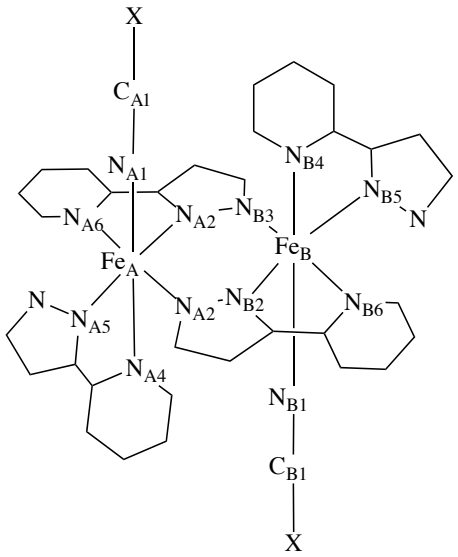


System	Fe_A-N_{A1}	Fe_A-N_{A2}	Fe_A-N_{A3}	Fe_A-N_{A4}	Fe_A-N_{A5}	Fe_A-N_{A6}
NCS[LS-LS]	1.9356	1.9141	1.9607	1.9816	1.9846	1.9712
NCS[HS-LS]	2.0397	1.9805	2.2109	2.2952	2.3294	2.1670
NCS[HS-HS]	2.0437	1.9869	2.2083	2.3027	2.2821	2.1623
NCSe[LS-LS]	1.9330	1.9108	1.9625	1.9817	1.9837	1.9745
NCSe[HS-LS]	2.0513	1.9849	2.2111	2.2877	2.3167	2.1648
NCSe[HS-HS]	2.0542	1.9916	2.2104	2.2953	2.2737	2.1585
$NCBH_3$[LS-LS]	1.9334	1.9129	1.9637	1.9828	1.9889	1.9768
$NCBH_3$[HS-LS]	2.0785	2.0133	2.1999	2.2717	2.2948	2.1937
$NCBH_3$[HS-HS]	2.0807	2.0159	2.2041	2.2751	2.2648	2.1711

System	Fe_B-N_{B1}	Fe_B-N_{B2}	Fe_B-N_{B3}	Fe_B-N_{B4}	Fe_B-N_{B5}	Fe_B-N_{B6}
NCS[LS-LS]	1.9357	1.9140	1.9607	1.9816	1.9847	1.9711
NCS[HS-LS]	1.9370	1.9182	1.9605	1.9791	1.9702	1.9583
NCS[HS-HS]	2.0443	1.9866	2.2087	2.3031	2.2818	2.1617
NCSe[LS-LS]	1.9330	1.9108	1.9626	1.9816	1.9837	1.9745
NCSe[HS-LS]	1.9337	1.9157	1.9634	1.9792	1.9689	1.9604
NCSe[HS-HS]	2.0544	1.9915	2.2105	2.2952	2.2736	2.1583
$NCBH_3$[LS-LS]	1.9334	1.9129	1.9637	1.9828	1.9885	1.9769
$NCBH_3$[HS-LS]	1.9333	1.9169	1.9656	1.9814	1.9714	1.9622
$NCBH_3$[HS-HS]	2.0836	2.0154	2.20675	2.2742	2.26167	2.1649

System	Fe_A-N_{A1}-C_{A1}	Fe_A-N_{A2}-C_{A2}	Fe_B-N_{B1}-C_{B1}	Fe_B-N_{B2}-C_{B2}
NCS[LS-LS]	162.5195	173.5207	162.4882	173.5002
NCS[HS-LS]	158.8505	173.7122	162.3175	171.6825
NCS[HS-HS]	158.8607	172.4129	158.7796	172.4563
NCSe[LS-LS]	163.4828	177.3097	163.4987	177.3024
NCSe[HS-LS]	158.1293	175.3892	163.8790	175.1453
NCSe[HS-HS]	159.0632	173.6948	158.9969	173.7922
$NCBH_3$[LS-LS]	164.3757	173.4818	164.3714	173.4614
$NCBH_3$[HS-LS]	156.6617	168.0643	165.5505	175.7106
$NCBH_3$[HS-HS]	157.8153	176.5985	156.6831	178.1363

S2.2 $[Fe(pypzH)(NCX)]_2(\mu\text{-pypz})$ (X = S, Se or BH_3)



System	Fe_A-N_{A1}	Fe_A-N_{A2}	Fe_A-N_{A3}	Fe_A-N_{A4}	Fe_A-N_{A5}	Fe_A-N_{A6}
NCS[LS-LS]	1.9532	1.9710	1.9548	1.9859	2.0123	1.9288
NCS[HS-LS]	2.0794	2.1076	2.1044	2.2725	2.2325	2.2016
NCS[HS-HS]	2.0620	2.1379	2.1057	2.2961	2.2715	2.1442
NCSe[LS-LS]	1.9456	1.9717	1.9544	1.9870	2.0120	1.9286
NCSe[HS-LS]	2.0879	2.1069	2.1014	2.2660	2.2306	2.1968
NCSe[HS-HS]	2.0542	1.9916	2.2104	2.2953	2.2737	2.1585
$NCBH_3$[LS-LS]	1.9374	1.9729	1.9546	1.9901	2.0111	1.9287
$NCBH_3$[HS-LS]	2.1109	2.1046	2.0969	2.2569	2.2288	2.1938
$NCBH_3$[HS-HS]	2.1117	2.1332	2.0965	2.2436	2.2571	2.1937

System	Fe_B-N_{B1}	Fe_B-N_{B2}	Fe_B-N_{B3}	Fe_B-N_{B4}	Fe_B-N_{B5}	Fe_B-N_{B6}
NCS[LS-LS]	1.9532	1.9709	1.9548	1.9859	2.0123	1.9288
NCS[HS-LS]	1.9552	1.9819	1.9582	1.9803	2.0147	1.9325
NCS[HS-HS]	2.0828	2.1373	2.1013	2.2534	2.2605	2.2019
NCSe[LS-LS]	1.9456	1.9718	1.9544	1.9869	2.0120	1.9285
NCSe[HS-LS]	1.9474	1.9827	1.9586	1.9813	2.0150	1.9320
NCSe[HS-HS]	2.0544	1.9915	2.2105	2.2952	2.2736	2.1583
$NCBH_3$[LS-LS]	1.9374	1.9729	1.9546	1.9901	2.0111	1.9287
$NCBH_3$[HS-LS]	1.9389	1.9844	1.9594	1.9843	2.0147	1.9309
$NCBH_3$[HS-HS]	2.1116	2.1333	2.0965	2.2437	2.2571	2.1938

System	Fe_A-N_{A1}-C_{A1}	Fe_B-N_{B1}-C_{B1}
NCS[LS-LS]	150.7549	150.7527
NCS[HS-LS]	146.2883	149.4822
NCS[HS-HS]	171.6049	144.8645
NCSe[LS-LS]	153.4673	153.4779
NCSe[HS-LS]	148.8486	152.3591
NCSe[HS-HS]	159.0632	173.6948
$NCBH_3$[LS-LS]	147.3581	147.3631
$NCBH_3$[HS-LS]	148.8486	152.3591
$NCBH_3$[HS-HS]	147.3581	147.3632

S3. Continuous Shape Measures (CShM) for the Fe^{II} coordination polyhedral

CShM can be calculated with the following expression,

$$S_P(R) = \frac{\sum_{k=1}^{N} q_k^2}{N} 100$$

where P is the coordination polyhedral, R the reference polyhedra, q_i the distance between the equivalent atomic positions in the two structures and N is a normalization factor that makes the CShM values size independent. The resulting value is zero if the problem structure P has exactly the desired shape R and will increase with the degree of distortion.

System	S_{Fe1}(OC6)	S_{Fe2}(OC6)
$[Fe(bt)(NCS)_2]_2$(μ-bpym) [LS-LS]	0.50	0.50
$[Fe(bt)(NCS)_2]_2$(μ-bpym) [HS-LS]	2.27	0.50
$[Fe(bt)(NCS)_2]_2$(μ-bpym) [HS-HS]	2.34	2.33
$[Fe(bt)(NCSe)_2]_2$(μ-bpym) [LS-LS]	0.49	0.49
$[Fe(bt)(NCSe)_2]_2$(μ-bpym) [HS-LS]	2.14	0.51
$[Fe(bt)(NCSe)_2]_2$(μ-bpym) [HS-HS]	2.21	2.21
$[Fe(bt)(NCBH_3)_2]_2$(μ-bpym) [LS-LS]	0.50	0.50
$[Fe(bt)(NCBH_3)_2]_2$(μ-bpym) [HS-LS]	1.91	0.51
$[Fe(bt)(NCBH_3)_2]_2$(μ-bpym) [HS-HS]	1.83	1.82
$[Fe(pypzH)(NCS)]_2$(μ-pypz) [LS-LS]	0.59	0.59
$[Fe(pypzH)(NCS)]_2$(μ-pypz) [HS-LS]	1.94	0.64
$[Fe(pypzH)(NCS)]_2$(μ-pypz) [HS-HS]	1.99	1.77
$[Fe(pypzH)(NCSe)]_2$(μ-pypz) [LS-LS]	0.59	0.59
$[Fe(pypzH)(NCSe)]_2$(μ-pypz) [HS-LS]	1.92	0.64
$[Fe(pypzH)(NCSe)]_2$(μ-pypz) [HS-HS]	1.76	1.76
$[Fe(pypzH)(NCBH_3)]_2$(μ-pypz) [LS-LS]	0.61	0.61
$[Fe(pypzH)(NCBH_3)]_2$(μ-pypz) [HS-LS]	1.95	0.66
$[Fe(pypzH)(NCBH_3)]_2$(μ-pypz) [HS-HS]	1.82	1.81

S4. Energy gap between the occupied and empty orbitals

System	Δ/cm^{-1}
(**1**) $[Fe(bt)(NCS)_2]_2(\mu\text{-bpym})$	27362
(**2**) $[Fe(bt)(NCSe)_2]_2(\mu\text{-bpym})$	28839
(**3**) $[Fe(bt)(NCBH_3)_2]_2(\mu\text{-bpym})$	33217
(**4**) $[Fe(pypzH)(NCS)]_2(\mu\text{-pypz})$	31953
(**5**) $[Fe(pypzH)(NCSe)]_2(\mu\text{-pypz})$	32239
(**6**) $[Fe(pypzH)(NCBH_3)]_2(\mu\text{-pypz})$	35012

Table 4: Energy gap between the non-bonding and andtibonding set of orbitals for the $[Fe(bt)(NCX)_2]_2(\mu\text{-bpym})$ and $[Fe(pypzH)(NCX)]_2(\mu\text{-pypz})$ (X = S, Se, BH_3) molecules in their [LS-LS] state. All energies in cm^{-1}.