Supporting Information

Iron(II) Spin Crossover Complex with the 1,2,3-Triazole-containing Linear Pentadentate Schiff-base Ligand and the MeCN monodentate Ligand

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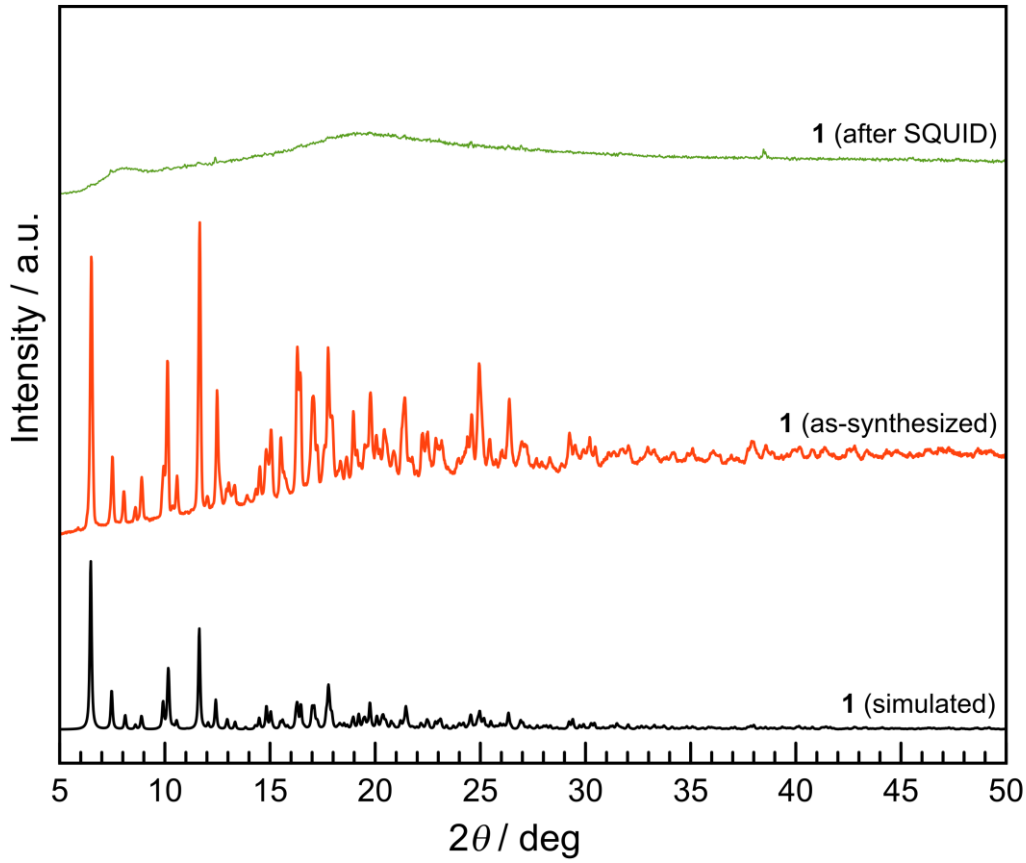


Figure S1. PXRD patterns of **1** at RT in different states: simulated from the single crystal X-ray data at 296 K (black); as-synthesized (red); after SQUID measurements (green).

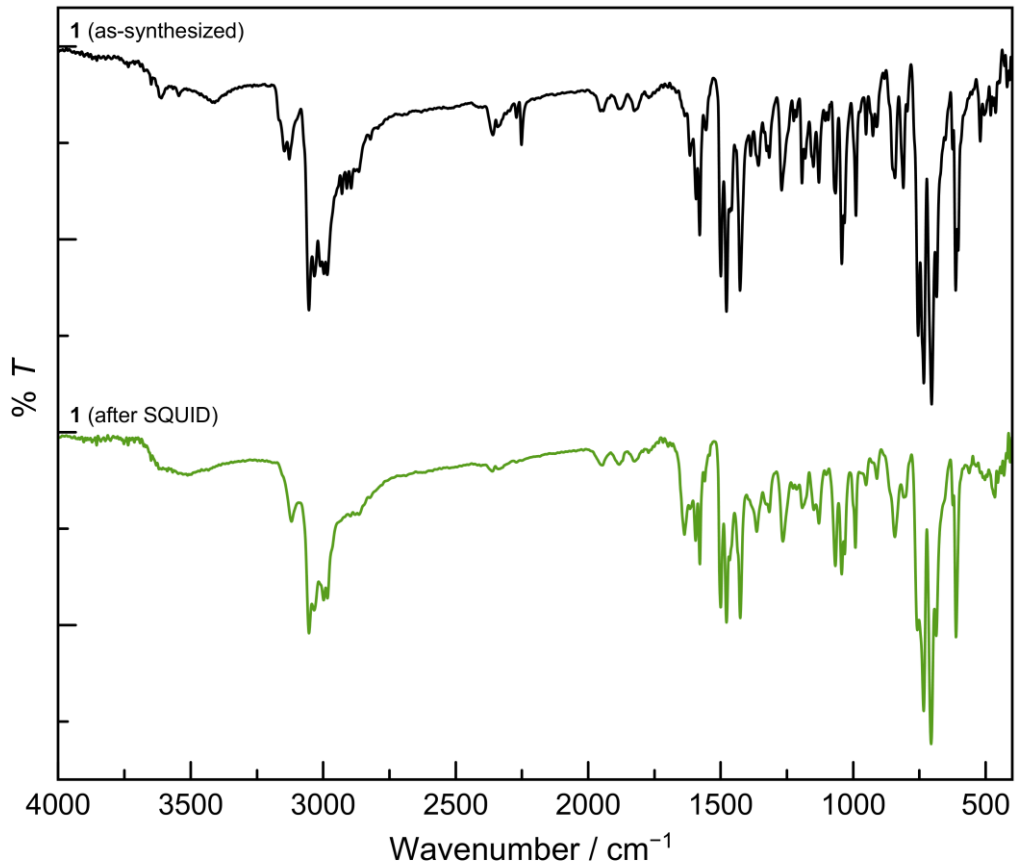


Figure S2. IR spectra (KBr) for **1** at RT in different states: as-synthesized (black); after SQUID measurements (green).

Table S1. HS–LS energy differences of **1** and **2** for Experimental geometry. DFT calculations for **2** were performed by using the reported crystal structure [1].

Complex	Experimental geometry (Single point DFT energy calculation)	
	ΔE [kJ mol^{-1}]	ΔE [cm^{-1}]
1 at 296 K	168.3	14073
Fe1 site of **2** at 296 K	45.5	3805
Fe2 site of **2** at 296 K	-13.3	−1109

Table S2. Relevant coordination bond lengths (Å) and structural parameters in DFT optimized structures for **1** and **2**. Σ [2] and Θ [3] are angular indices characteristic for spin state of the complex. S(Oh) is the continuous shape measures (CShMs) of the Fe^{II} centers relative to the ideal octahedron calculated by SHAPE 2.1 [4]. The octahedral volumes of the Fe^{II} centers were calculated by OLEX2 [5].

Complex	**1**		Complex	**2**	
Spin state	LS	HS	Spin state	LS	HS
Fe–N3(triazole)	1.992	2.202	Fe–N2(imidazole)	2.040	2.207
Fe–N4(imine)	2.015	2.163	Fe–N3(imine)	2.014	2.178
Fe–N5(amine)	2.115	2.214	Fe–N4(amine)	2.129	2.232
Fe–N6(imine)	1.966	2.153	Fe–N5(imine)	1.970	2.157
Fe–N7(triazole)	1.972	2.246	Fe–N6(imidazole)	2.042	2.241
Fe–N10(NCMe)	1.950	2.222	Fe–N8(NCMe)	1.939	2.261
Average Fe–N	2.002	2.200	Average Fe–N	2.022	2.213
Σ	63.3	96.5	Σ	63.9	100.4
Θ	96.7	186.0	Θ	98.2	186.3
S(Oh)	0.751	1.938	S(Oh)	0.743	1.940
Octahedral volume	10.497	13.552	Octahedral volume	10.825	13.784

Table S3. HS–LS energy differences of **1**, **2**, **1'** and **2'** for DFT optimized geometry (LS).

Complex	**1** and **2**		**1'** and **2'** (Model complex)	
	ΔE [kJ mol^{-1}]	ΔE [cm^{-1}]	ΔE [kJ mol^{-1}]	ΔE [cm^{-1}]
1	149.7	12513	149.3	12486
2	121.2	10136	131.9	11024

Table S4. Relevant coordination bond lengths (Å) and structural parameters in DFT optimized structures for model complexes **1'** and **2'**. Σ [2] and Θ [3] are angular indices characteristic for spin state of the complex. S(Oh) is the continuous shape measures (CShMs) of the Fe^{II} centers relative to the ideal octahedron calculated by SHAPE 2.1 [4]. The octahedral volumes of the Fe^{II} centers were calculated by OLEX2 [5].

Complex	**1**'	Complex	**2**'
Spin state	LS	Spin state	LS
Fe–N3(triazole)	1.995	Fe–N2(imidazole)	2.024
Fe–N4(imine)	2.017	Fe–N3(imine)	2.014
Fe–N5(amine)	2.111	Fe–N4(amine)	2.123
Fe–N6(imine)	1.967	Fe–N5(imine)	1.967
Fe–N7(triazole)	1.971	Fe–N6(imidazole)	2.007
Fe–N10(NCMe)	1.954	Fe–N8(NCMe)	1.945
Average Fe–N	2.003	Average Fe–N	2.013
Σ	63.6	Σ	62.3
Θ	97.9	Θ	94.3
S(Oh)	0.751	S(Oh)	0.702
Octahedral volume	10.512	Octahedral volume	10.690

Table S5. Cartesian coordinates (Å) of DFT optimized geometry of **1** (LS, in gas-phase).

Atom	X	Y	Z	Atom	X	Y	Z
Fe	-1.453282	-0.527828	-0.04261	C	0.867403	4.805095	-0.725246
N	2.340566	-1.951885	-0.653974	C	-2.505239	-3.354416	-0.76811
N	1.313515	-1.788277	0.211198	C	-2.907764	-4.680345	-1.15424
N	0.359453	-1.23265	-0.473805	H	2.589258	-3.731896	1.294396
N	-1.379596	-0.137778	-2.0183	H	4.712908	-4.790022	2.034173
N	-3.389749	0.230831	0.340663	H	6.846011	-4.207944	0.911958
N	-1.318465	-0.781712	1.902642	H	6.86555	-2.54938	-0.93228
N	-0.484634	1.116429	0.452789	H	4.76731	-1.458668	-1.643099
N	-0.009571	2.13425	-0.204991	H	2.708429	-1.560278	-2.722593
N	0.755529	2.817258	0.67629	H	-0.091458	-0.218823	-3.659475
N	-2.190298	-2.288052	-0.44427	H	-3.000613	-0.501842	-3.252232
C	3.562322	-2.554851	-0.220603	H	-2.093605	0.945457	-3.675076
C	3.532048	-3.47742	0.82088	H	-4.226326	1.568262	-2.699043
C	4.722757	-4.064743	1.225739	H	-2.96768	2.078442	-1.612125
C	5.919308	-3.739433	0.593439	H	-5.124903	0.864757	-0.671783
C	5.931646	-2.813267	-0.444852	H	-4.399545	-0.61128	-1.290507
C	4.751516	-2.208576	-0.856207	H	-2.767036	1.466061	1.950883
C	2.028402	-1.488409	-1.887656	H	-4.35982	1.871672	1.285493
C	0.740931	-1.015137	-1.766307	H	-2.880069	2.290632	0.399416
C	-0.261161	-0.412375	-2.597997	H	-4.276347	-1.649672	0.617342
C	-2.482124	0.369816	-2.826618	H	-5.181092	-0.317158	1.312142
C	-3.462248	1.187652	-2.014085	H	-4.31797	-1.717581	3.059858
C	-4.163831	0.395032	-0.924964	H	-3.608131	-0.133986	3.200192
C	-3.346153	1.537512	1.031635	H	-1.897816	-1.819845	3.647425
C	-4.168006	-0.728504	1.194282	H	-2.216861	-2.642508	2.112021
C	-3.611885	-1.034688	2.575217	H	-0.453233	0.010344	3.635418
C	-2.221705	-1.6692	2.610824	H	1.298871	2.635456	2.735069
C	-0.577278	0.054033	2.551519	H	3.051831	3.731329	1.672052
C	-0.029285	1.108066	1.744988	H	4.16829	5.838279	1.030676
C	0.769133	2.21944	1.891887	H	3.199312	7.271995	-0.746529
C	1.422587	4.017793	0.279091	H	1.093078	6.601602	-1.870257
C	2.608771	4.373532	0.915038	H	-0.062822	4.50748	-1.198598
C	3.241575	5.551686	0.542387	H	-3.934185	-4.87971	-0.835983
C	2.699335	6.351775	-0.458539	H	-2.254866	-5.427448	-0.696159
C	1.518662	5.974776	-1.092039	H	-2.856662	-4.798179	-2.239372

Table S6. Cartesian coordinates (Å) of DFT optimized geometry of **1** (HS, in gas-phase).

Atom	X	Y	Z	Atom	X	Y	Z
Fe	-1.772102	0.052239	0.022395	C	2.85318	-3.890019	0.997315
N	1.783979	2.437917	0.570808	C	-3.542954	2.918458	0.051437
N	0.890523	1.945497	-0.317058	C	-4.175946	4.208057	0.116681
N	-0.03426	1.356645	0.381178	H	1.933223	3.868601	-1.652283
N	-1.679146	0.192133	2.178498	H	3.918027	5.148927	-2.428134
N	-3.551263	-1.264851	-0.002853	H	5.992944	5.163117	-1.070569
N	-1.779741	-0.237798	-2.110572	H	6.098553	3.878844	1.048593
N	-0.100881	-1.393603	-0.377273	H	4.14593	2.56803	1.804326
N	0.848541	-1.96688	0.300084	H	1.988464	2.48044	2.697081
N	1.737193	-2.438071	-0.604327	H	-0.499218	0.942826	3.724766
N	-3.037377	1.878981	-0.007251	H	-3.399726	0.473746	3.291668
C	2.928657	3.166136	0.120219	H	-2.220207	-0.573815	4.069732
C	2.852616	3.874023	-1.075705	H	-4.076337	-1.911092	3.322425
C	3.96523	4.587374	-1.499614	H	-2.703024	-2.355346	2.359075
C	5.128675	4.596851	-0.735578	H	-5.083559	-1.988237	1.24822
C	5.188231	3.881307	0.45637	H	-4.74159	-0.272541	1.405328
C	4.08785	3.154839	0.891033	H	-2.566528	-2.661319	-1.254189
C	1.42178	2.147418	1.840901	H	-3.977893	-3.316928	-0.39606
C	0.245758	1.439202	1.71597	H	-2.451691	-3.015593	0.462581
C	-0.668889	0.832634	2.648109	H	-4.824255	0.219402	-0.748719
C	-2.677878	-0.33404	3.101652	H	-5.43715	-1.417973	-0.932945
C	-3.41	-1.537695	2.538388	H	-4.977551	-0.549711	-3.08128
C	-4.264931	-1.255813	1.309215	H	-3.859103	-1.851153	-2.803937
C	-3.116953	-2.639894	-0.314104	H	-2.761702	0.02192	-3.967357
C	-4.533417	-0.797118	-1.032281	H	-3.216274	1.144902	-2.673051
C	-4.098493	-0.828623	-2.489991	H	-0.763865	-1.135005	-3.69722
C	-2.953937	0.103501	-2.889725	H	1.905138	-2.47177	-2.733823
C	-0.819731	-0.916899	-2.624026	H	4.088318	-2.47892	-1.858489
C	0.160822	-1.466386	-1.718026	H	6.079354	-3.762145	-1.154025
C	1.346086	-2.152226	-1.867434	H	6.022446	-5.10449	0.930854
C	2.90228	-3.149487	-0.179868	H	3.959839	-5.176381	2.30496
C	4.053646	-3.090369	-0.960204	H	1.938209	-3.924277	1.580007
C	5.174831	-3.801353	-0.554255	H	-3.642306	4.923498	-0.513411
C	5.142561	-4.549394	0.618594	H	-4.178331	4.584001	1.142307
C	3.98609	-4.588008	1.392382	H	-5.209449	4.145577	-0.232052

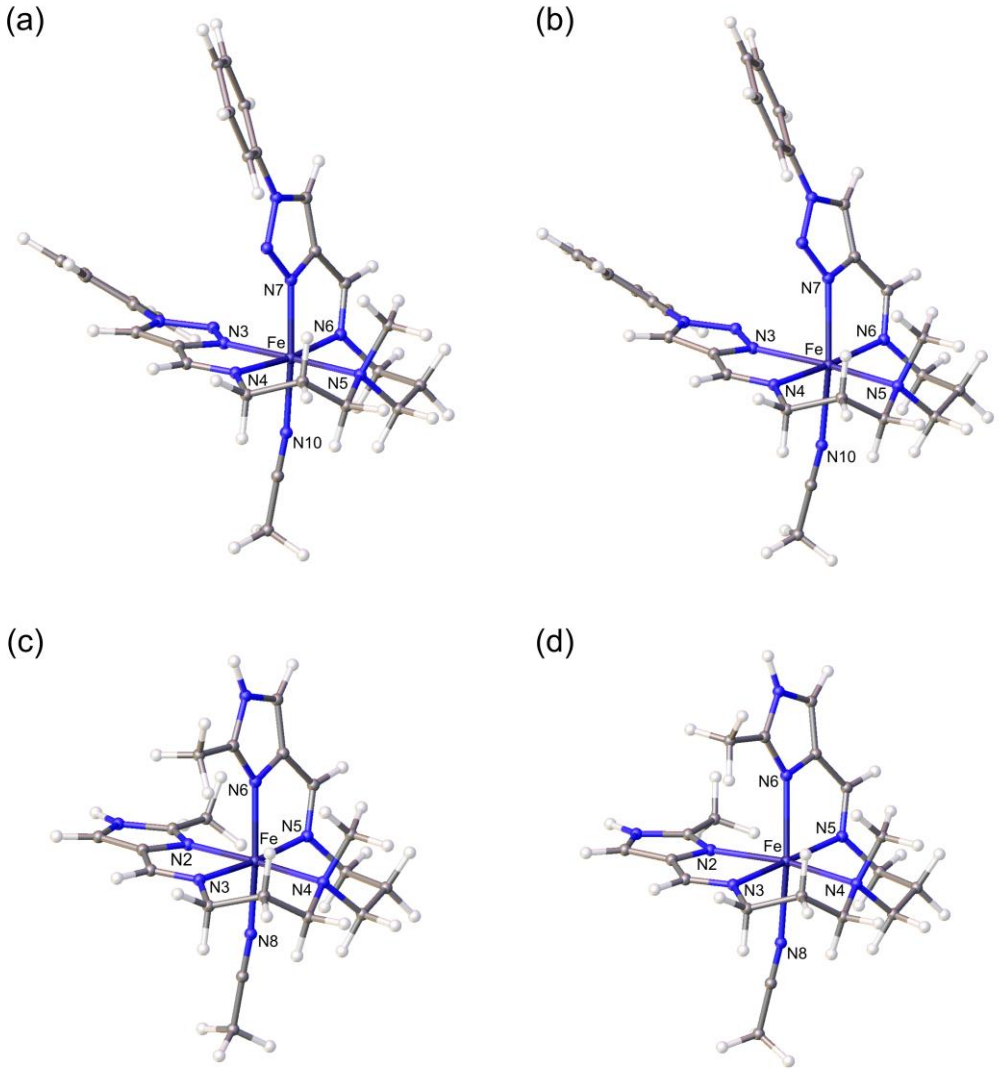
Table S7. Cartesian coordinates (Å) of DFT optimized geometry of **2** (LS, in gas-phase).

Atom	X	Y	Z	Atom	X	Y	Z
Fe	-0.30959	0.086273	0.018397	H	3.568163	-3.350799	0.040089
N	2.981901	2.725545	-0.214158	H	3.452663	2.966267	1.86669
N	1.267374	1.378766	-0.055978	H	1.242565	1.342724	3.338415
N	-0.029621	0.382757	1.990213	H	0.481716	-1.362065	-3.463872
N	-1.993054	-1.208236	0.175064	H	2.963487	-2.956156	-2.384087
N	-0.409219	-0.277031	-1.91475	H	0.86871	1.99189	-2.687788
N	1.109426	-1.374803	-0.12766	H	2.310897	3.005219	-2.793724
N	2.81816	-2.738928	-0.253385	H	2.462393	1.253258	-2.85548
N	-1.485893	1.627233	-0.002036	H	-0.329461	-0.223126	3.986244
C	1.912916	2.074696	-2.384104	H	-1.610209	0.748998	3.280873
C	2.027922	2.036925	-0.910964	H	-1.027355	-2.166459	2.548245
C	2.818965	2.506644	1.122982	H	-2.302052	-1.582659	3.570691
C	1.739508	1.664563	1.215354	H	-3.106327	-0.135806	1.587549
C	0.986004	1.118052	2.299215	H	-3.439313	-1.860695	1.561198
C	-0.907466	-0.069029	3.065661	H	-3.924698	-1.48034	-0.629472
C	-1.693731	-1.310376	2.702302	H	-3.3935	0.187874	-0.522602
C	-2.627879	-1.119921	1.523006	H	-2.477266	-1.87923	-2.595801
C	-1.623434	-2.615848	-0.07958	H	-3.618449	-0.583709	-2.830483
C	-3.065232	-0.816227	-0.801506	H	-1.835952	1.117935	-2.507412
C	-2.713344	-0.856996	-2.277387	H	-1.380162	-0.033438	-3.775111
C	-1.57915	0.071585	-2.701294	H	1.185128	-1.910416	2.552426
C	0.477813	-1.077603	-2.408209	H	2.496539	-3.079372	2.391526
C	1.389173	-1.643854	-1.464694	H	2.852937	-1.356591	2.422242
C	2.456244	-2.500781	-1.546749	H	-3.659787	3.821024	-0.619944
C	1.99259	-2.049418	0.589685	H	-3.269295	3.985415	1.099688
C	2.137161	-2.102542	2.060091	H	-2.204971	4.699675	-0.122088
C	-2.083597	2.618818	0.049566	H	-2.513806	-3.257388	-0.07342
C	-2.841529	3.840822	0.104471	H	-1.131535	-2.713953	-1.046161
H	3.689834	3.318298	-0.626889	H	-0.932685	-2.973654	0.681916

Table S8. Cartesian coordinates (Å) of DFT optimized geometry of **2** (HS, in gas-phase).

Atom	X	Y	Z	Atom	X	Y	Z
Fe	-0.319462	0.012317	0.003116	H	4.070921	-3.041417	0.66034
N	2.884573	2.93877	-0.692757	H	2.988873	3.870344	1.239677
N	1.247389	1.530356	-0.333681	H	0.791405	2.613445	2.872943
N	-0.247733	1.091655	1.893867	H	0.560824	-2.647587	-2.895425
N	-2.05867	-1.256664	0.592771	H	3.178548	-3.53742	-1.653567
N	-0.412167	-1.152866	-1.810151	H	1.334587	0.922583	-2.911853
N	1.408866	-1.404364	0.170473	H	2.360167	2.297998	-3.339311
N	3.232974	-2.616017	0.285062	H	3.090348	0.810539	-2.747058
N	-1.764777	1.60457	-0.696869	H	-0.6625	1.106247	3.965267
C	2.229807	1.477661	-2.629317	H	-1.947183	1.693406	2.921576
C	2.102328	1.961959	-1.239265	H	-1.068485	-1.229476	3.132037
C	2.512987	3.135221	0.60735	H	-2.442973	-0.516354	3.913954
C	1.486842	2.250014	0.826076	H	-3.249456	0.192524	1.520415
C	0.6544	2.005952	1.970528	H	-3.515775	-1.443457	2.101087
C	-1.171171	0.919245	3.010297	H	-3.961571	-1.860029	-0.085456
C	-1.827407	-0.44772	3.011431	H	-3.441966	-0.271847	-0.629763
C	-2.730516	-0.727316	1.816364	H	-2.430147	-2.969899	-1.693663
C	-1.564188	-2.620355	0.858372	H	-3.619018	-1.935044	-2.428339
C	-3.100152	-1.300829	-0.482213	H	-1.927216	-0.165777	-2.8264
C	-2.710352	-1.917176	-1.816615	H	-1.455596	-1.70586	-3.568422
C	-1.621152	-1.195788	-2.610224	H	1.817435	-0.675997	2.667662
C	0.543455	-1.987117	-2.019367	H	2.845668	-2.073536	3.016886
C	1.57367	-2.096067	-1.021869	H	3.557108	-0.602743	2.36421
C	2.712287	-2.85902	-0.953989	H	-4.205404	3.489214	-1.321281
C	2.423434	-1.734644	0.944613	H	-2.916144	4.541465	-0.712876
C	2.675571	-1.250384	2.317443	H	-2.897215	3.998839	-2.401159
C	-2.372182	2.542913	-0.997881	H	-2.391718	-3.300196	1.102497
C	-3.135248	3.70235	-1.377021	H	-1.037249	-3.011448	-0.011331
H	3.614697	3.446598	-1.175067	H	-0.862598	-2.616817	1.692114

Figure S3. DFT optimized structures of LS **1** (**a**), HS **1** (**b**), LS **2** (**c**), and HS **2** (**d**) in gas-phase.



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