Electronic Supporting Information

Synthesis, Structure, Magnetic Properties and Theoretical Calculations of Methoxy Bridged Dinuclear Iron(III) Complex Containing Hydrazone Based *O,N,N*-Donor Ligand

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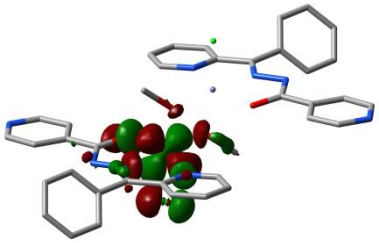
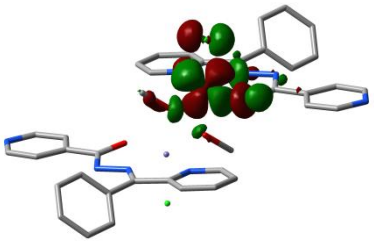
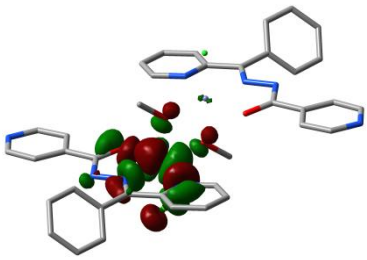
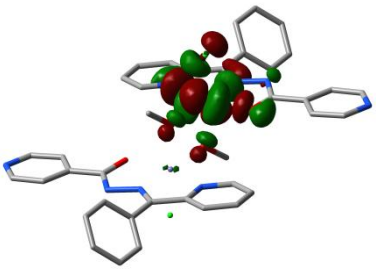
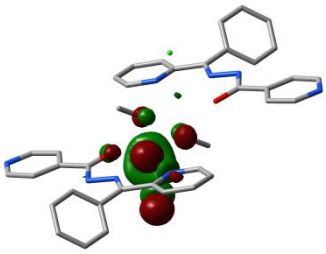
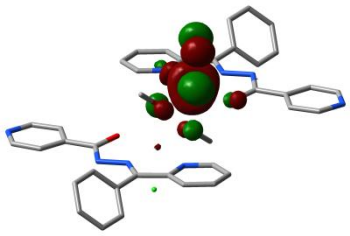
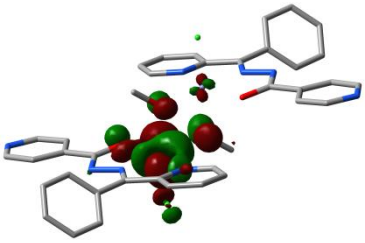
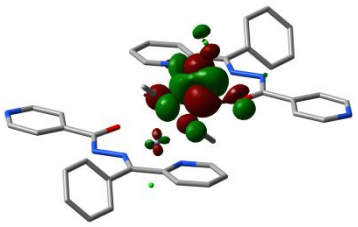
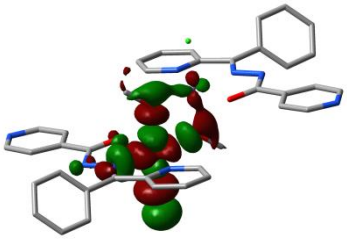
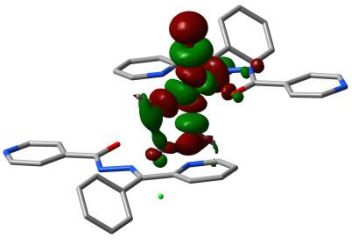
				overlap $S_{\alpha\beta}$
HOMO(α)		HOMO(β)		0.03899
HOMO-1(α)		HOMO-1(β)		0.06463
HOMO-2(α)		HOMO-2(β)		0.06675
HOMO-3(α)		HOMO-3(β)		0.11225
HOMO-4(α)		HOMO-4(β)		0.17990

Figure S1.The corresponding orbitals for broken-symmetry state calculated with B3LYP for **L_2Fe_2A**. The values of overlap $S_{\alpha\beta}$ between the corresponding orbitals are listed in right column.

Table S1. The BP86/def2-TZVP(-f) optimized structure of model compound **L_2Fe_2opt** – Cartesian coordinates in Å.

Fe	-0.059409	-0.024782	0.032949
Fe	3.181633	0.024782	-0.032953
O	1.639636	1.250019	0.029534
O	1.482589	-1.250019	-0.029540
Cl	-1.697364	-1.595011	-0.195189
C	-1.293493	1.301927	2.254670
Cl	4.819588	1.595011	0.195184
O	-0.381491	0.423898	2.026855
N	-1.945388	1.993909	1.303341
N	-1.479103	1.612784	0.091155
C	-1.968947	2.107017	-1.014311
C	-1.336023	1.582794	-2.229310
N	-0.358526	0.652627	-2.047527
C	0.291610	0.152399	-3.103554
H	1.086980	-0.560834	-2.880101
C	-0.007162	0.531930	-4.414302
H	0.548218	0.099449	-5.245541
C	-1.020761	1.467857	-4.620393
H	-1.286259	1.784854	-5.629978
C	-1.689067	2.003401	-3.521273
H	-2.476853	2.743500	-3.655661
C	1.511822	-2.666167	0.043494
H	0.499499	-3.071612	-0.103252
H	1.880833	-2.993586	1.031804
H	2.185386	-3.074336	-0.728902
C	4.415722	-1.301932	-2.254670
O	3.503719	-0.423904	-2.026858
N	5.067617	-1.993911	-1.303338
N	4.601329	-1.612784	-0.091153
C	5.091171	-2.107014	1.014315
C	4.458244	-1.582790	2.229311
N	3.480746	-0.652624	2.047524
C	2.830607	-0.152395	3.103549
H	2.035237	0.560837	2.880092
C	3.129376	-0.531925	4.414298
H	2.573993	-0.099442	5.245535
C	4.142974	-1.467850	4.620393
H	4.408470	-1.784845	5.629980
C	4.811285	-2.003395	3.521275
H	5.599071	-2.743493	3.655667
C	1.610402	2.666167	-0.043497
H	2.622727	3.071612	0.103242
H	1.241384	2.993588	-1.031804
H	0.936844	3.074336	0.728905
C	6.200038	-3.112104	1.062194
H	7.072870	-2.708738	1.599040
H	6.499452	-3.367765	0.040357
H	5.885174	-4.028843	1.584416
C	4.797067	-1.585648	-3.680017
H	5.573806	-2.356188	-3.728663
H	5.161117	-0.661432	-4.151492
H	3.913074	-1.915169	-4.245121
C	-1.674836	1.585639	3.680019
H	-2.038886	0.661423	4.151492
H	-2.451573	2.356180	3.728668
H	-0.790841	1.915158	4.245122
C	-3.077812	3.112108	-1.062186
H	-3.377224	3.367768	-0.040348
H	-3.950646	2.708744	-1.599031
H	-2.762949	4.028848	-1.584407

Table S2. The BP86/def2-TZVP(-f) optimized structures of model compound **L_2Fe_2opt** under Fe-Fe distance constrain – Cartesian coordinates in Å.

d(Fe-Fe) = 2.900				d(Fe-Fe) = 2.956			
Fe	0.163230	0.008843	-0.128673	Fe	-0.027548	-0.004905	0.023360
Fe	3.051764	-0.008979	0.128340	Fe	2.927620	0.004921	-0.023441
O	1.677176	1.340287	-0.115632	O	1.501159	1.327770	0.010152
O	1.537835	-1.340423	0.115212	O	1.398912	-1.327755	-0.010229
Cl	-1.514294	-1.558519	-0.434335	Cl	-1.706268	-1.566560	-0.251031
C	-1.248598	1.347781	1.990385	C	-1.245287	1.147866	2.358881
Cl	4.729253	1.558403	0.434179	Cl	4.606341	1.566575	0.250927
O	-0.317738	0.473980	1.836798	O	-0.325301	0.302532	2.053753
N	-1.860766	2.001033	0.987629	N	-1.946983	1.872361	1.469857
N	-1.335925	1.588546	-0.188971	N	-1.524597	1.562871	0.222089
C	-1.793296	2.032859	-1.329152	C	-2.078758	2.095594	-0.834146
C	-1.117443	1.471774	-2.503041	C	-1.502098	1.641475	-2.103547
N	-0.116329	0.580142	-2.262384	N	-0.484657	0.739835	-2.022184
C	0.551775	0.036620	-3.285652	C	0.101172	0.294100	-3.138758
H	1.361464	-0.644951	-3.018167	H	0.931206	-0.400729	-2.997452
C	0.256833	0.335702	-4.617762	C	-0.299782	0.705894	-4.411871
H	0.828025	-0.130808	-5.419460	H	0.206503	0.316213	-5.294141
C	-0.773591	1.237855	-4.882976	C	-1.349699	1.618578	-4.514393
H	-1.036333	1.494228	-5.910343	H	-1.693851	1.961398	-5.491263
C	-1.464615	1.814729	-3.819918	C	-1.954237	2.095132	-3.353257
H	-2.269760	2.525462	-4.001361	H	-2.771206	2.813474	-3.406840
C	1.454227	-2.680434	0.575023	C	1.386690	-2.721867	0.255006
H	0.490738	-3.107790	0.260068	H	0.384956	-3.121395	0.038161
H	1.514215	-2.715796	1.675805	H	1.623630	-2.913903	1.315273
H	2.283708	-3.269335	0.152906	H	2.136793	-3.227132	-0.373931
C	4.463719	-1.347691	-1.990772	C	4.145338	-1.147886	-2.358958
O	3.532788	-0.473974	-1.837147	O	3.225367	-0.302535	-2.053836
N	5.075910	-2.000973	-0.988049	N	4.847028	-1.872380	-1.469928
N	4.551009	-1.588609	0.188569	N	4.424652	-1.562871	-0.222163
C	5.008392	-2.032964	1.328728	C	4.978811	-2.095589	0.834077
C	4.332477	-1.472007	2.502642	C	4.402161	-1.641448	2.103475
N	3.331307	-0.580427	2.262030	N	3.384729	-0.739799	2.022106
C	2.663144	-0.037026	3.285325	C	2.798909	-0.294044	3.138677
H	1.853409	0.644506	3.017874	H	1.968883	0.400793	2.997366
C	2.958082	-0.336183	4.617419	C	3.199865	-0.705826	4.411793
H	2.386841	0.130229	5.419139	H	2.693589	-0.316129	5.294061
C	3.988565	-1.238282	4.882589	C	4.249773	-1.618520	4.514321
H	4.251308	-1.494710	5.909942	H	4.593926	-1.961331	5.491194
C	4.679649	-1.815031	3.819502	C	4.854301	-2.095094	3.353189
H	5.484840	-2.525720	4.000907	H	5.671263	-2.813445	3.406777
C	1.760812	2.680272	-0.575506	C	1.513378	2.721882	-0.255082
H	2.724332	3.107607	-0.260615	H	2.515103	3.121417	-0.038210
H	1.700772	2.715583	-1.676288	H	1.276468	2.913918	-1.315356
H	0.931375	3.269226	-0.153378	H	0.763253	3.227142	0.373833
C	6.137730	-3.009423	1.452222	C	6.115538	-3.069596	0.780441
H	6.991576	-2.556788	1.980548	H	7.005902	-2.661950	1.284354
H	6.463246	-3.312693	0.451646	H	6.364857	-3.275541	-0.265751
H	5.833763	-3.902973	2.018925	H	5.855583	-4.014990	1.281288
C	4.919648	-1.670524	-3.385966	C	4.479421	-1.349587	-3.810156
H	5.715744	-2.422458	-3.369831	H	5.274398	-2.093950	-3.925816
H	5.283589	-0.754629	-3.873300	H	4.799934	-0.393132	-4.247604
H	4.072330	-2.043885	-3.979573	H	3.584260	-1.677697	-4.358416
C	-1.704461	1.670755	3.385567	C	-1.579380	1.349543	3.810080
H	-2.068452	0.754925	3.872986	H	-1.899876	0.393076	4.247515
H	-2.500502	2.422745	3.369397	H	-2.374372	2.093889	3.925746
H	-0.857097	2.044103	3.979118	H	-0.684228	1.677663	4.358348
C	-2.922560	3.009399	-1.452688	C	-3.215498	3.069586	-0.780504

H	-3.248034	3.312757	-0.452125	H	-3.464828	3.275513	0.265689
H	-3.776451	2.556801	-1.980972	H	-4.105853	2.661938	-1.284430
H	-2.618530	3.902891	-2.019451	H	-2.955550	4.014992	-1.281334
d(Fe-Fe) = 3.011				d(Fe-Fe) = 3.067			
Fe	-0.027647	-0.001318	0.020250	Fe	-0.027779	0.000029	0.000377
Fe	2.983190	0.001313	-0.020244	Fe	3.038888	-0.000031	-0.000375
O	1.537248	1.309504	0.015692	O	1.568534	1.293185	-0.001333
O	1.418296	-1.309508	-0.015686	O	1.442575	-1.293186	0.001335
Cl	-1.700552	-1.562822	-0.245555	Cl	-1.686187	-1.569475	-0.267573
C	-1.270016	1.200227	2.316430	C	-1.290566	1.237625	2.264277
Cl	4.656095	1.562818	0.245566	Cl	4.697295	1.569475	0.267576
O	-0.348677	0.346534	2.039757	O	-0.368712	0.377636	2.010018
N	-1.953699	1.913596	1.404505	N	-1.960114	1.941191	1.334593
N	-1.510767	1.583403	0.169037	N	-1.500995	1.593997	0.109804
C	-2.043309	2.102371	-0.904910	C	-2.017568	2.099479	-0.978571
C	-1.443550	1.627951	-2.156091	C	-1.399333	1.608050	-2.214591
N	-0.434765	0.720454	-2.040692	N	-0.395446	0.699110	-2.070901
C	0.174734	0.258412	-3.137783	C	0.232342	0.222151	-3.151160
H	0.996657	-0.439942	-2.969206	H	1.048509	-0.477013	-2.959516
C	-0.193742	0.658204	-4.424504	C	-0.112010	0.608241	-4.448721
H	0.331004	0.255870	-5.290136	H	0.426911	0.194832	-5.300308
C	-1.235700	1.575360	-4.562051	C	-1.148968	1.526263	-4.615360
H	-1.554950	1.908587	-5.550630	H	-1.449520	1.848684	-5.613343
C	-1.864266	2.069234	-3.421029	C	-1.796657	2.035261	-3.491723
H	-2.675226	2.791821	-3.501963	H	-2.604260	2.758693	-3.595660
C	1.414423	-2.713438	0.190556	C	1.436479	-2.694461	0.225718
H	0.406811	-3.107252	-0.008963	H	0.432883	-3.094078	0.018140
H	1.687198	-2.949325	1.233481	H	1.695632	-2.917727	1.275084
H	2.143230	-3.193111	-0.482364	H	2.174731	-3.183286	-0.430470
C	4.225565	-1.200224	-2.316424	C	4.301675	-1.237621	-2.264277
O	3.304222	-0.346535	-2.039750	O	3.379820	-0.377634	-2.010016
N	4.909249	-1.913593	-1.404500	N	4.971225	-1.941187	-1.334595
N	4.466315	-1.583404	-0.169032	N	4.512107	-1.593995	-0.109805
C	4.998857	-2.102372	0.904915	C	5.028682	-2.099477	0.978569
C	4.399094	-1.627959	2.156096	C	4.410448	-1.608052	2.214590
N	3.390307	-0.720464	2.040697	N	3.406558	-0.699114	2.070903
C	2.780802	-0.258429	3.137788	C	2.778770	-0.222158	3.151163
H	1.958878	0.439924	2.969211	H	1.962600	0.477004	2.959521
C	3.149275	-0.658225	4.424509	C	3.123126	-0.608248	4.448724
H	2.624523	-0.255897	5.290140	H	2.584204	-0.194841	5.300311
C	4.191235	-1.575378	4.562055	C	4.160086	-1.526267	4.615360
H	4.510483	-1.908609	5.550634	H	4.460640	-1.848688	5.613341
C	4.819807	-2.069245	3.421034	C	4.807774	-2.035262	3.491721
H	5.630768	-2.791831	3.501967	H	5.615379	-2.758692	3.595656
C	1.541122	2.713435	-0.190543	C	1.574631	2.694460	-0.225711
H	2.548736	3.107245	0.008970	H	2.578229	3.094075	-0.018138
H	1.268338	2.949327	-1.233465	H	1.315472	2.917730	-1.275075
H	0.812321	3.193105	0.482386	H	0.836383	3.183284	0.430482
C	6.131936	-3.081756	0.886924	C	6.160174	-3.080513	0.989710
H	7.014084	-2.670893	1.402528	H	7.035331	-2.664266	1.512882
H	6.400579	-3.303444	-0.151238	H	6.443481	-3.315939	-0.041514
H	5.857947	-4.018944	1.395649	H	5.877362	-4.010695	1.506407
C	4.582511	-1.426082	-3.758546	C	4.675883	-1.483796	-3.698703
H	5.375197	-2.176267	-3.849681	H	5.466981	-2.237786	-3.769914
H	4.915463	-0.478132	-4.205134	H	5.017645	-0.543095	-4.153883
H	3.694599	-1.757581	-4.316429	H	3.793715	-1.819691	-4.263060
C	-1.626960	1.426090	3.758552	C	-1.664774	1.483803	3.698702
H	-1.959913	0.478141	4.205144	H	-2.006539	0.543103	4.153883
H	-2.419644	2.176276	3.849686	H	-2.455872	2.237793	3.769911
H	-0.739046	1.757589	4.316433	H	-0.782606	1.819698	4.263059

C	-3.176385	3.081758	-0.886919	C	-3.149057	3.080517	-0.989714
H	-3.445024	3.303449	0.151243	H	-3.432363	3.315948	0.041508
H	-4.058535	2.670896	-1.402520	H	-4.024215	2.664271	-1.512886
H	-2.902395	4.018943	-1.395648	H	-2.866243	4.010698	-1.506414
d(Fe-Fe) = 3.122				d(Fe-Fe) = 3.178			
Fe	0.000018	-0.000737	0.004303	Fe	-0.027773	-0.002392	0.004541
Fe	3.122206	0.000738	-0.004306	Fe	3.149971	0.002391	-0.004539
O	1.632149	1.278010	0.001234	O	1.635517	1.262661	0.004695
O	1.490075	-1.278009	-0.001239	O	1.486682	-1.262662	-0.004690
Cl	-1.653016	-1.568498	-0.253285	Cl	-1.670199	-1.573563	-0.254336
C	-1.266978	1.279184	2.239608	C	-1.290059	1.290562	2.232797
Cl	4.775242	1.568498	0.253282	Cl	4.792397	1.573562	0.254335
O	-0.347437	0.411145	2.004338	O	-0.374036	0.417765	2.001272
N	-1.923897	1.974952	1.294993	N	-1.940679	1.987847	1.284923
N	-1.454584	1.610546	0.078896	N	-1.468115	1.618815	0.071358
C	-1.954384	2.108544	-1.020522	C	-1.962427	2.114849	-1.031610
C	-1.323103	1.601364	-2.243411	C	-1.326821	1.602126	-2.250376
N	-0.330860	0.683937	-2.077007	N	-0.339691	0.680647	-2.075593
C	0.312269	0.195702	-3.142980	C	0.308965	0.187743	-3.136055
H	1.118762	-0.509311	-2.932828	H	1.110905	-0.520221	-2.918683
C	-0.005893	0.577249	-4.448600	C	0.001204	0.568443	-4.444423
H	0.544676	0.154732	-5.288160	H	0.555872	0.142498	-5.279538
C	-1.032356	1.502449	-4.638729	C	-1.020416	1.497178	-4.643211
H	-1.312713	1.821358	-5.643693	H	-1.292598	1.815256	-5.650683
C	-1.695077	2.023927	-3.529613	C	-1.688646	2.023613	-3.539679
H	-2.494076	2.754025	-3.651841	H	-2.483802	2.756753	-3.668722
C	1.489809	-2.685712	0.174147	C	1.492665	-2.672116	0.159946
H	0.483597	-3.083089	-0.025591	H	0.487923	-3.073870	-0.038068
H	1.771482	-2.945176	1.209700	H	1.780374	-2.938549	1.192219
H	2.215030	-3.152522	-0.512480	H	2.216979	-3.131305	-0.532963
C	4.389204	-1.279186	-2.239609	C	4.412255	-1.290564	-2.232796
O	3.469665	-0.411146	-2.004340	O	3.496233	-0.417767	-2.001269
N	5.046122	-1.974954	-1.294992	N	5.062876	-1.987848	-1.284921
N	4.576808	-1.610546	-0.078896	N	4.590313	-1.618816	-0.071357
C	5.076608	-2.108542	1.020523	C	5.084627	-2.114848	1.031612
C	4.445324	-1.601362	2.243411	C	4.449021	-1.602125	2.250378
N	3.453081	-0.683934	2.077005	N	3.461890	-0.680647	2.075595
C	2.809951	-0.195699	3.142977	C	2.813234	-0.187744	3.136057
H	2.003459	0.509314	2.932824	H	2.011294	0.520220	2.918685
C	3.128111	-0.577246	4.448598	C	3.120997	-0.568442	4.444425
H	2.577542	-0.154728	5.288157	H	2.566329	-0.142498	5.279540
C	4.154573	-1.502446	4.638729	C	4.142617	-1.497177	4.643213
H	4.434928	-1.821355	5.643694	H	4.414800	-1.815254	5.650685
C	4.817296	-2.023925	3.529614	C	4.810847	-2.023612	3.539681
H	5.616294	-2.754023	3.651844	H	5.606004	-2.756751	3.668724
C	1.632415	2.685714	-0.174146	C	1.629532	2.672116	-0.159934
H	2.638628	3.083090	0.025592	H	2.634274	3.073869	0.038079
H	1.350740	2.945182	-1.209697	H	1.341820	2.938554	-1.192205
H	0.907196	3.152521	0.512485	H	0.905220	3.131300	0.532980
C	6.199486	-3.098754	1.055223	C	6.204192	-3.108303	1.073856
H	7.069566	-2.687100	1.590271	H	7.072806	-2.698138	1.612433
H	6.496965	-3.342641	0.029967	H	6.505961	-3.355294	0.050595
H	5.900314	-4.023604	1.572341	H	5.899713	-4.031163	1.591447
C	4.774984	-1.544786	-3.667407	C	4.801150	-1.560255	-3.658925
H	5.561269	-2.305140	-3.722479	H	5.583568	-2.324821	-3.710519
H	5.127731	-0.611915	-4.130284	H	5.160287	-0.629873	-4.121926
H	3.895557	-1.880647	-4.235978	H	3.921749	-1.892118	-4.229878
C	-1.652758	1.544781	3.667407	C	-1.678955	1.560253	3.658926
H	-2.005495	0.611908	4.130285	H	-2.038089	0.629870	4.121928
H	-2.439048	2.305130	3.722480	H	-2.461375	2.324817	3.710520

H	-0.773332	1.880651	4.235976	H	-0.799556	1.892119	4.229880
C	-3.077261	3.098758	-1.055219	C	-3.081991	3.108305	-1.073854
H	-3.374733	3.342650	-0.029962	H	-3.383755	3.355301	-0.050593
H	-3.947346	2.687101	-1.590258	H	-3.950607	2.698141	-1.612426
H	-2.778092	4.023604	-1.572345	H	-2.777512	4.031164	-1.591449
d(Fe-Fe) = 3.233				d(Fe-Fe) = 3.289			
Fe	-0.027531	-0.017773	0.022058	Fe	-0.027771	-0.004951	0.002480
Fe	3.205292	0.017774	-0.022060	Fe	3.261090	0.004951	-0.002478
O	1.669058	1.252438	0.018871	O	1.713886	1.239222	0.002779
O	1.508704	-1.252438	-0.018871	O	1.519433	-1.239223	-0.002780
Cl	-1.666430	-1.587007	-0.216591	Cl	-1.667912	-1.566797	-0.232767
C	-1.279103	1.313127	2.230403	C	-1.282746	1.383101	2.170833
Cl	4.844192	1.587008	0.216587	Cl	4.901231	1.566797	0.232771
O	-0.366656	0.433208	2.010936	O	-0.381383	0.485812	1.977318
N	-1.922784	2.003957	1.272998	N	-1.903042	2.067889	1.193463
N	-1.447958	1.619474	0.064935	N	-1.417266	1.656081	-0.001138
C	-1.930664	2.110842	-1.044947	C	-1.875972	2.135631	-1.126343
C	-1.290115	1.583474	-2.254735	C	-1.223891	1.578908	-2.316743
N	-0.314432	0.653116	-2.064709	N	-0.265785	0.637437	-2.094469
C	0.341417	0.149359	-3.115456	C	0.401760	0.107732	-3.124926
H	1.134319	-0.564608	-2.885518	H	1.179634	-0.613774	-2.868848
C	0.051212	0.526224	-4.428956	C	0.140791	0.468053	-4.449155
H	0.611121	0.091193	-5.255824	H	0.709282	0.012367	-5.258856
C	-0.959917	1.462877	-4.643482	C	-0.852862	1.415232	-4.696682
H	-1.218528	1.778064	-5.655423	H	-1.088584	1.717873	-5.718000
C	-1.634703	2.001500	-3.549800	C	-1.539311	1.980998	-3.624136
H	-2.421011	2.741913	-3.690928	H	-2.311985	2.730319	-3.791197
C	1.527852	-2.666431	0.092680	C	1.527449	-2.651985	0.126519
H	0.519598	-3.070814	-0.081945	H	0.519078	-3.053950	-0.052975
H	1.856432	-2.969313	1.102851	H	1.844202	-2.945047	1.143577
H	2.228465	-3.096938	-0.642387	H	2.232732	-3.096920	-0.595698
C	4.456866	-1.313130	-2.230402	C	4.516070	-1.383101	-2.170828
O	3.544419	-0.433210	-2.010936	O	3.614705	-0.485812	-1.977315
N	5.100547	-2.003958	-1.272996	N	5.136364	-2.067888	-1.193457
N	4.625720	-1.619474	-0.064933	N	4.650586	-1.656080	0.001143
C	5.108425	-2.110840	1.044950	C	5.109290	-2.135630	1.126349
C	4.467876	-1.583471	2.254736	C	4.457207	-1.578908	2.316748
N	3.492192	-0.653113	2.064709	N	3.499100	-0.637437	2.094472
C	2.836341	-0.149356	3.115454	C	2.831555	-0.107731	3.124928
H	2.043439	0.564611	2.885514	H	2.053681	0.613775	2.868848
C	3.126544	-0.526220	4.428955	C	3.092522	-0.468051	4.449157
H	2.566633	-0.091188	5.255822	H	2.524030	-0.012364	5.258857
C	4.137674	-1.462872	4.643483	C	4.086174	-1.415229	4.696686
H	4.396284	-1.778058	5.655424	H	4.321895	-1.717870	5.718005
C	4.812462	-2.001495	3.549802	C	4.772624	-1.980997	3.624142
H	5.598770	-2.741908	3.690931	H	5.545299	-2.730318	3.791204
C	1.649910	2.666433	-0.092676	C	1.705871	2.651984	-0.126526
H	2.658164	3.070815	0.081950	H	2.714242	3.053949	0.052966
H	1.321330	2.969317	-1.102846	H	1.389118	2.945042	-1.143586
H	0.949297	3.096937	0.642392	H	1.000588	3.096923	0.595690
C	6.217308	-3.115369	1.102633	C	6.201383	-3.155798	1.217795
H	7.084049	-2.712577	1.649612	H	7.065718	-2.757369	1.771731
H	6.527429	-3.369138	0.083531	H	6.523219	-3.431141	0.207954
H	5.897411	-4.033342	1.619685	H	5.859300	-4.060096	1.744647
C	4.848293	-1.599713	-3.652398	C	4.921387	-1.699124	-3.582514
H	5.625284	-2.370412	-3.693978	H	5.686487	-2.482507	-3.601312
H	5.215665	-0.676526	-4.123288	H	5.309459	-0.789666	-4.063423
H	3.968244	-1.930486	-4.222927	H	4.043639	-2.025307	-4.159183
C	-1.670531	1.599708	3.652399	C	-1.688059	1.699126	3.582520
H	-2.037903	0.676520	4.123287	H	-2.076129	0.789669	4.063431

H	-2.447522	2.370407	3.693981	H	-2.453159	2.482510	3.601319
H	-0.790482	1.930480	4.222929	H	-0.810309	2.025310	4.159185
C	-3.039547	3.115371	-1.102628	C	-2.968065	3.155798	-1.217786
H	-3.349664	3.369142	-0.083526	H	-3.289898	3.431143	-0.207945
H	-3.906289	2.712578	-1.649603	H	-3.832402	2.757368	-1.771719
H	-2.719651	4.033343	-1.619683	H	-2.625984	4.060095	-1.744641
d(Fe-Fe) = 3.344				d(Fe-Fe) = 3.400			
Fe	-0.027532	-0.026539	0.011282	Fe	0.000223	-0.028292	0.002370
Fe	3.316411	0.026540	-0.011281	Fe	3.399750	0.028264	-0.002370
O	1.754893	1.235187	0.007544	O	1.840905	1.229814	0.004520
O	1.533986	-1.235186	-0.007541	O	1.559069	-1.229842	-0.004516
Cl	-1.664907	-1.583101	-0.220066	Cl	-1.656370	-1.557105	-0.224960
C	-1.259235	1.391233	2.170084	C	-1.198521	1.441406	2.141709
Cl	4.953786	1.583103	0.220065	Cl	5.056345	1.557080	0.224956
O	-0.367734	0.483061	1.982582	O	-0.330959	0.507915	1.966750
N	-1.871740	2.076875	1.188475	N	-1.783006	2.138525	1.150703
N	-1.389311	1.653789	-0.003242	N	-1.303008	1.693390	-0.033936
C	-1.837233	2.135474	-1.131822	C	-1.719947	2.186083	-1.169665
C	-1.185531	1.568438	-2.317529	C	-1.071419	1.593309	-2.344522
N	-0.241578	0.614877	-2.087902	N	-0.164307	0.608464	-2.098178
C	0.428387	0.077411	-3.112490	C	0.503203	0.046489	-3.111142
H	1.195681	-0.652576	-2.849178	H	1.240012	-0.708951	-2.833881
C	0.182061	0.439988	-4.438887	C	0.291295	0.415343	-4.441714
H	0.751591	-0.022782	-5.243798	H	0.857961	-0.067500	-5.236777
C	-0.798477	1.398792	-4.694470	C	-0.651664	1.406517	-4.714394
H	-1.022982	1.703434	-5.717706	H	-0.848341	1.717334	-5.741502
C	-1.485909	1.973758	-3.627453	C	-1.336775	2.006232	-3.659561
H	-2.246945	2.733552	-3.800639	H	-2.068643	2.791097	-3.846139
C	1.552477	-2.648727	0.100168	C	1.561912	-2.642676	0.110454
H	0.545723	-3.058493	-0.073531	H	0.553073	-3.046881	-0.064646
H	1.882675	-2.956400	1.108985	H	1.885861	-2.948749	1.122069
H	2.252145	-3.079632	-0.636428	H	2.261293	-3.084703	-0.620183
C	4.548114	-1.391230	-2.170085	C	4.598483	-1.441438	-2.141711
O	3.656610	-0.483060	-1.982581	O	3.730926	-0.507943	-1.966751
N	5.160621	-2.076871	-1.188476	N	5.182975	-2.138553	-1.150706
N	4.678192	-1.653785	0.003240	N	4.702984	-1.693412	0.033935
C	5.126114	-2.135472	1.131820	C	5.119934	-2.186098	1.169663
C	4.474413	-1.568437	2.317527	C	4.471414	-1.593317	2.344522
N	3.530459	-0.614877	2.087902	N	3.564297	-0.608476	2.098176
C	2.860493	-0.077414	3.112491	C	2.896793	-0.046495	3.111140
H	2.093197	0.652572	2.849181	H	2.159982	0.708942	2.833877
C	3.106820	-0.439991	4.438887	C	3.108711	-0.415338	4.441713
H	2.537290	0.022778	5.243800	H	2.542049	0.067510	5.236777
C	4.087359	-1.398794	4.694469	C	4.051674	-1.406507	4.714395
H	4.311865	-1.703437	5.717705	H	4.248358	-1.717316	5.741504
C	4.774792	-1.973758	3.627451	C	4.736779	-2.006229	3.659562
H	5.535828	-2.733552	3.800636	H	5.468650	-2.791091	3.846141
C	1.736401	2.648729	-0.100155	C	1.838067	2.642648	-0.110435
H	2.743155	3.058494	0.073546	H	2.846905	3.046849	0.064680
H	1.406202	2.956408	-1.108970	H	1.514127	2.948732	-1.122050
H	1.036734	3.079629	0.636444	H	1.138690	3.084677	0.620204
C	6.203857	-3.170057	1.230745	C	6.157663	-3.258996	1.285748
H	7.068372	-2.784096	1.793083	H	7.024695	-2.906532	1.865810
H	6.530670	-3.448312	0.223314	H	6.492823	-3.546781	0.283735
H	5.844942	-4.070571	1.752931	H	5.756250	-4.147295	1.797956
C	4.949694	-1.720487	-3.579877	C	5.002703	-1.790463	-3.545882
H	5.706089	-2.512382	-3.594083	H	5.736948	-2.603062	-3.548762
H	5.347599	-0.818186	-4.066235	H	5.429425	-0.902603	-4.034368
H	4.068298	-2.040183	-4.154533	H	4.117654	-2.089289	-4.126130
C	-1.660817	1.720492	3.579876	C	-1.602748	1.790422	3.545880

H	-2.058722	0.818192	4.066235	H	-2.029479	0.902560	4.034355
H	-2.417211	2.512387	3.594080	H	-2.336997	2.603018	3.548761
H	-0.779421	2.040189	4.154532	H	-0.717703	2.089247	4.126134
C	-2.914976	3.170058	-1.230748	C	-2.757676	3.258982	-1.285752
H	-3.241789	3.448314	-0.223318	H	-3.092835	3.546770	-0.283739
H	-3.779491	2.784095	-1.793086	H	-3.624709	2.906515	-1.865811
H	-2.556062	4.070572	-1.752936	H	-2.356262	4.147284	-1.797953

Table S3. The B2PLYP/def2-TZVP(-f) calculated net Mulliken spin densities[a], the $<S^2>$ values and total energies of HS and BS states of the two geometrical extremes of **L_2Fe_2opt** model compound.

	d(Fe-Fe) = 2.900		d(Fe-Fe) = 3.400	
	HS (M_S = 5)	BS (M_S = 0)	HS (M_S = 5)	BS (M_S = 0)
ρ(Fe1)	4.24	4.25	4.26	4.25
ρ(Cl)	0.22	0.21	0.23	0.23
ρ(N_{ax})	0.06	0.06	0.04	0.05
ρ(N_{eq})	0.09	0.08	0.11	0.10
ρ(O_{ax})	0.11	0.11	0.11	0.11
ρ(O)	0.23	0.04	0.21	0.09
ρ(O(i))	0.23	-0.04	0.21	-0.09
ρ($O(i)_{ax}$)	0.11	-0.11	0.11	-0.11
ρ($N(i)_{eq}$)	0.09	-0.09	0.11	-0.09
ρ($N(i)_{ax}$)	0.06	-0.06	0.04	-0.05
ρ(Cl(i))	0.22	-0.21	0.23	-0.23
ρ(Fe1(i))	4.24	-4.25	4.26	-4.25
$<S^2>$	30.03	5.01	30.03	5.01
J (cm^{-1})	+9.7		-30.3	

[a] the net atomic spin densities are based on relaxed MP2 density population analysis

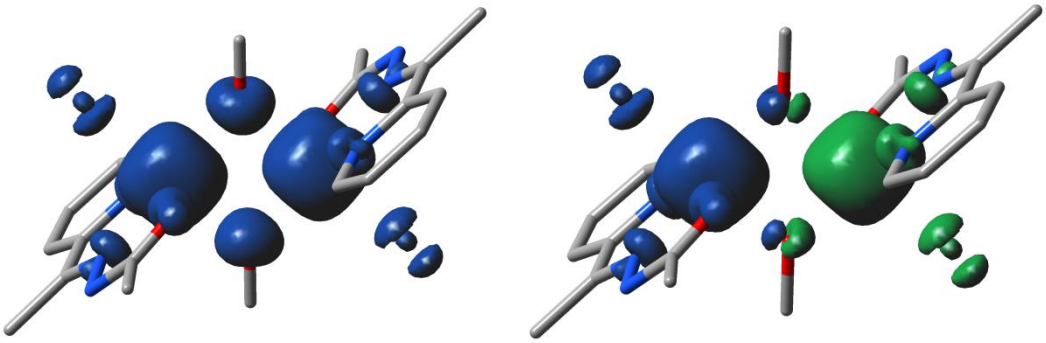


Figure S2. The calculated spin density distribution using B2PLYP for **L_2Fe_2opt** (d(Fe-Fe) = 2.900). Positive and negative spin densities are represented by dark blue and green surfaces, respectively. The isodensity surfaces are depicted with the cutoff values of 0.007 e·boh^{-3}.

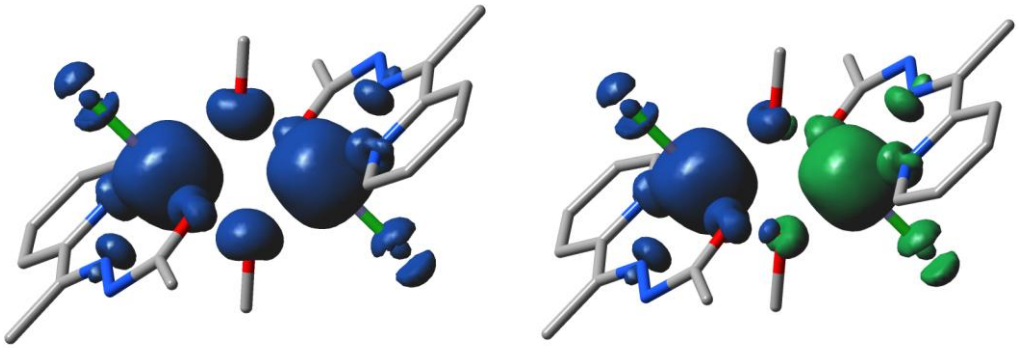


Figure S3. The calculated spin density distribution using B2PLYP for **L_2Fe_2opt** (d(Fe-Fe) = 3.400). Positive and negative spin densities are represented by dark blue and green surfaces, respectively. The isodensity surfaces are depicted with the cutoff values of 0.007 e·boh^{-3}.

Table S4. The BP86/def2-TZVP(-f) optimized structure of model compound **$L_2Fe_2optF_2$** and **$L_2Fe_2optBr_2$** – Cartesian coordinates in Å.

$L_2Fe_2optF_2$				**$L_2Fe_2optBr_2$**			
Fe	-0.048319	0.059909	0.040662	Fe	-0.049162	-0.014607	0.024974
Fe	3.170543	-0.059907	-0.040661	Fe	3.171384	0.014607	-0.024974
O	1.668534	1.240537	0.031494	O	1.644079	1.258028	0.018122
O	1.453690	-1.240535	-0.031491	O	1.478142	-1.258028	-0.018121
F	-1.341735	-1.240711	-0.167088	Br	-1.816327	-1.692829	-0.238567
C	-1.332558	1.370282	2.247613	C	-1.292364	1.289719	2.251872
F	4.463959	1.240714	0.167089	Br	4.938549	1.692829	0.238566
O	-0.398481	0.512258	2.034551	O	-0.381365	0.411612	2.017313
N	-1.998605	2.037067	1.288108	N	-1.945041	1.985763	1.304521
N	-1.514098	1.662708	0.079908	N	-1.480695	1.608108	0.090177
C	-2.036542	2.108214	-1.030469	C	-1.965815	2.113539	-1.012758
C	-1.385750	1.596571	-2.243555	C	-1.334559	1.592904	-2.229569
N	-0.365891	0.715780	-2.056090	N	-0.358324	0.660208	-2.051032
C	0.302248	0.232569	-3.108063	C	0.289359	0.161251	-3.109666
H	1.132018	-0.440183	-2.880598	H	1.082860	-0.554961	-2.889297
C	-0.019602	0.581138	-4.422756	C	-0.011247	0.543935	-4.418757
H	0.551506	0.164757	-5.251632	H	0.541660	0.111886	-5.251858
C	-1.076443	1.466142	-4.634636	C	-1.023958	1.481798	-4.621386
H	-1.360978	1.758114	-5.646672	H	-1.291200	1.800521	-5.629930
C	-1.764367	1.984065	-3.538669	C	-1.689218	2.016360	-3.520070
H	-2.585760	2.685592	-3.678893	H	-2.476705	2.757277	-3.651548
C	1.350528	-2.653780	-0.074088	C	1.524590	-2.669725	0.114676
H	0.296244	-2.947620	-0.185148	H	0.525043	-3.096443	-0.058866
H	1.746707	-3.096473	0.857412	H	1.853025	-2.951731	1.130715
H	1.934497	-3.056786	-0.919934	H	2.235769	-3.097330	-0.611551
C	4.454780	-1.370281	-2.247613	C	4.414586	-1.289718	-2.251872
O	3.520703	-0.512257	-2.034551	O	3.503586	-0.411611	-2.017313
N	5.120828	-2.037065	-1.288109	N	5.067263	-1.985762	-1.304521
N	4.636323	-1.662706	-0.079908	N	4.602918	-1.608107	-0.090177
C	5.158766	-2.108212	1.030469	C	5.088037	-2.113538	1.012757
C	4.507974	-1.596570	2.243555	C	4.456782	-1.592903	2.229569
N	3.488116	-0.715778	2.056090	N	3.480547	-0.660208	2.051033
C	2.819977	-0.232568	3.108063	C	2.832865	-0.161250	3.109667
H	1.990208	0.440185	2.880598	H	2.039363	0.554962	2.889299
C	3.141826	-0.581137	4.422755	C	3.133474	-0.543933	4.418758
H	2.570717	-0.164756	5.251632	H	2.580567	-0.111884	5.251860
C	4.198667	-1.466142	4.634636	C	4.146184	-1.481796	4.621386
H	4.483200	-1.758115	5.646672	H	4.413429	-1.800518	5.629930
C	4.886591	-1.984065	3.538669	C	4.811443	-2.016358	3.520069
H	5.707984	-2.685592	3.678892	H	5.598931	-2.757275	3.651547
C	1.771696	2.653782	0.074091	C	1.597632	2.669725	-0.114674
H	2.825980	2.947622	0.185154	H	2.597179	3.096443	0.058864
H	1.375519	3.096475	-0.857409	H	1.269193	2.951731	-1.130712
H	1.187725	3.056788	0.919936	H	0.886455	3.097331	0.611555
C	6.321566	-3.050402	1.089367	C	6.191950	-3.123984	1.055144
H	7.167678	-2.597383	1.629253	H	7.069937	-2.723514	1.585879
H	6.639375	-3.294574	0.070246	H	6.484532	-3.382056	0.031955
H	6.054982	-3.980894	1.614402	H	5.876148	-4.038343	1.580756
C	4.850123	-1.658709	-3.668822	C	4.792229	-1.566850	-3.679134
H	5.649280	-2.406609	-3.706845	H	5.570275	-2.335701	-3.732934
H	5.187951	-0.729858	-4.150669	H	5.153078	-0.640045	-4.147951
H	3.977582	-2.020677	-4.232042	H	3.907311	-1.896092	-4.242978
C	-1.727904	1.658709	3.668821	C	-1.670007	1.566852	3.679134
H	-2.065734	0.729858	4.150666	H	-2.030860	0.640049	4.147950
H	-2.527060	2.406610	3.706844	H	-2.448051	2.335706	3.732933
H	-0.855363	2.020674	4.232044	H	-0.785089	1.896091	4.242979
C	-3.199343	3.050402	-1.089368	C	-3.069728	3.123985	-1.055145

H	-3.517150	3.294577	-0.070247	H	-3.362310	3.382057	-0.031956
H	-4.045455	2.597382	-1.629251	H	-3.947714	2.723514	-1.585880
H	-2.932760	3.980893	-1.614405	H	-2.753925	4.038344	-1.580757

Table S5. The B3LYP/def2-TZVP(-f) and B2PLYP/def2-TZVP(-f) calculated net Mulliken spin densities, the $<S^2>$ values and total energies of HS and BS states of the fluroro-model compound **$L_2Fe_2optF_2$**.

	B3LYP		B2PLYP[a]	
	HS (M_S = 5)	BS (M_S = 0)	HS (M_S = 5)	BS (M_S = 0)
ρ(Fe1)	4.24	4.23	4.34	4.33
ρ(F)	0.21	0.21	0.19	0.19
ρ(N_{ax})	0.08	0.08	0.05	0.05
ρ(N_{eq})	0.07	0.07	0.09	0.09
ρ(O_{ax})	0.11	0.11	0.10	0.10
ρ(O)	0.22	0.06	0.19	0.05
ρ(O(i))	0.22	-0.06	0.19	-0.05
ρ($O(i)_{ax}$)	0.11	-0.11	0.10	-0.10
ρ($N(i)_{eq}$)	0.07	-0.07	0.09	-0.09
ρ($N(i)_{ax}$)	0.08	-0.08	0.05	-0.05
ρ(F(i))	0.21	-0.21	0.19	-0.19
ρ(Fe1(i))	4.24	-4.23	4.34	-4.33
$<S^2>$	30.02	4.97	30.02	5.01
J (cm^{-1})	-32.3		-19.2	

[a] the net atomic spin densities are based on relaxed MP2 density population analysis

Table S6. The B3LYP/def2-TZVP(-f) and B2PLYP/def2-TZVP(-f) calculated net Mulliken spin densities, the $<S^2>$ values and total energies of HS and BS states of the bromo-model compound **$L_2Fe_2optBr_2$**.

	B3LYP		B2PLYP[a]	
	HS (M_S = 5)	BS (M_S = 0)	HS (M_S = 5)	BS (M_S = 0)
ρ(Fe1)	4.16	4.15	4.25	4.24
ρ(Br)	0.26	0.26	0.23	0.23
ρ(N_{ax})	0.08	0.08	0.05	0.05
ρ(N_{eq})	0.07	0.07	0.10	0.10
ρ(O_{ax})	0.12	0.11	0.11	0.11
ρ(O)	0.23	0.06	0.21	0.05
ρ(O(i))	0.23	-0.06	0.21	-0.05
ρ($O(i)_{ax}$)	0.12	-0.11	0.11	-0.11
ρ($N(i)_{eq}$)	0.07	-0.06	0.10	-0.09
ρ($N(i)_{ax}$)	0.08	-0.08	0.05	-0.05
ρ(Br(i))	0.26	-0.26	0.23	-0.23
ρ(Fe1(i))	4.16	-4.15	4.25	-4.24
$<S^2>$	30.02	4.97	30.03	5.01
J (cm^{-1})	-32.2		-20.0	

[a] the net atomic spin densities are based on relaxed MP2 density population analysis