Electronic Supplementary Material (ESI) for New Journal of Chemistry

Binuclear Iron Boronyl Carbonyls

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Complete Gaussian 03 reference (Reference 25)

Table S1. Atomic charges and Wiberg bond indexes for $Fe_2(BO)_2(CO)_8$ by the BP86 method

structure	Natural charge on Fe_1/Fe_2	Wiberg bond index	Fe-Fe distance (Å)	Formal Fe-Fe bond order
28-1S(C_2)	-0.608/-0.608	0.13	2.878	1
28-2S(C_s)	-0.631/ -0.662	0.11	2.837	1
28-3S(C_2)	-0.597/-0.597	0.14	2.887	1
28-4S(C_{2h})	-0.568/-0.568	0.15	2.976	1
28-5S(C_1)	-0.381/-0.777	0.02	4.009	0
28-6S(D_2)	-0.671/-0.671	0.11	2.811	1
28-7S(C_{2v})	-0.566/ -0.566	0.15	3.059	1
28-8S(C_s)	-0.501/-0.762	0.09	2.776	1
28-9S(C_{2v})	-0.646/-0.646	0.08	2.693	1
28-10S(C_s)	-0.550/-0.480	0.06	4.923	0
28-11S(C_{2v})	-0.641/-0.641	0.08	2.764	1
28-12S(C_s)	-0.696/-0.534	0.11	2.909	1

Table S2. Atomic charges and Wiberg bond indexes for $Fe_2(BO)_2(CO)_8$ by the B3LYP method

structure	Natural charge on Fe_1/Fe_2	Wiberg bond index	Fe-Fe distance (Å)	Formal Fe-Fe bond order
28-1S(C_2)	-0.589/-0.589	0.15	2.925	1
28-2S(C_s)	-0.627/-0.626	0.13	2.874	1
28-3S(C_2)	-0.583/-0.583	0.16	2.931	1
28-4S(C_{2h})	-0.561/-0.561	0.17	3.039	1
28-5S(C_1)	-0.352/-0.771	0.02	4.028	0
28-6S(D_2)	-0.671/-0.671	0.11	2.821	1
28-7S(C_{2v})	-0.554/-0.554	0.17	3.059	1
28-8S(C_s)	-0.508/-0.628	0.12	2.992	1
28-9S(C_{2v})	-0.639/-0.639	0.08	2.725	1
28-10S(C_s)	-0.617/-0.393	0.02	4.896	0
28-11S(C_{2v})	-0.624/-0.624	0.08	2.714	1
28-12S(C_s)	-0.630/-0.512	0.12	3.002	1

Table S3. The total energies (E in Hartree), relative energies (ΔE in kcal/mol),and the number of imaginary vibrational frequencies (Nimag) for the $Fe(BO)_2(CO)_3$ and $Fe(CO)_5$ structures.

	BP86				**B3LYP**			
	E	Nimag	ΔE	$\langle S^2 \rangle$	E	Nimag	ΔE	$\langle S^2 \rangle$
$Fe(CO)_5(D_{3h})$	-1830.83755	0	0.0	0.00	-1830.58136	0	0.00	0.00
$Fe(BO)_2(CO)_3(C_s)$	-1804.35862	0	0.0	0.00	-1804.12782	0	0.00	0.00

Table S4. Theoretical Cartesian coordinates (in Å) for the structure **14-1D**(C_s) using the B3LYP/DZP and BP86/DZP methods

	B3LYP/DZP			BP86/DZP		
Fe	0.219752	0.045423	0.000000	0.228315	0.014367	0.000000
C	1.651959	-1.120704	0.000000	1.545851	-1.254824	0.000000
C	-1.134616	-1.218487	0.000000	-1.178297	-1.111586	0.000000
B	-1.076422	1.548092	0.000000	-0.938958	1.595688	0.000000
C	0.257300	0.424271	1.794793	0.273766	0.425460	1.767772
C	0.257300	0.424271	-1.794793	0.273766	0.425460	-1.767772
O	2.540478	-1.851754	0.000000	2.375800	-2.073231	0.000000
O	-2.002060	-1.974482	0.000000	-2.097982	-1.829651	0.000000
O	-1.868408	2.474159	0.000000	-1.666837	2.589199	0.000000
O	0.257300	0.677441	2.917091	0.273766	0.703151	2.900266
O	0.257300	0.677441	-2.917091	0.273766	0.703151	-2.900266

Table S5. Theoretical Cartesian coordinates (in Å) for the structure **14-2D**(C_{2v}) using the B3LYP/DZP and BP86/DZP methods

	B3LYP/DZP			BP86/DZP		
Fe	0.000000	0.000000	0.339776	0.000000	0.000000	0.340601
C	0.000000	1.816669	0.710246	0.000000	1.779170	0.768984
C	-1.802292	0.000000	0.088390	-1.772196	0.000000	0.015937
C	0.000000	-1.816669	0.710246	0.000000	-1.779170	0.768984
C	1.802292	0.000000	0.088390	1.772196	0.000000	0.015937
B	0.000000	0.000000	-1.631808	0.000000	0.000000	-1.603216
O	0.000000	2.951106	0.900700	0.000000	2.918116	1.018473
O	-2.935411	0.000000	-0.116497	-2.910281	0.000000	-0.242290
O	0.000000	-2.951106	0.900700	0.000000	-2.918116	1.018473
O	2.935411	0.000000	-0.116497	2.910281	0.000000	-0.242290
O	0.000000	0.000000	-2.850750	0.000000	0.000000	-2.834693

Table S6. Theoretical Cartesian coordinates (in Å) for the $Fe(BO)_2(CO)_3$ structure using the B3LYP/DZP and BP86/DZP methods

	B3LYP/DZP			BP86/DZP		
Fe	-0.115654	0.000000	-0.443172	-0.115654	0.000000	-0.457591
B	1.843628	0.000000	-0.309408	1.843628	0.000000	-0.324960
C	0.132763	1.808527	-0.334772	0.132763	1.784732	-0.337928
C	-1.939486	0.000000	-0.444753	-1.939486	0.000000	-0.423966
C	0.132763	-1.808527	-0.334772	0.132763	-1.784732	-0.337928
B	-0.085873	0.000000	1.466884	-0.085873	0.000000	1.436681
O	3.074302	0.000000	-0.293092	3.074302	0.000000	-0.295698
O	0.328101	2.937877	-0.223512	0.328101	2.924878	-0.210305
O	-3.100220	0.000000	-0.391157	-3.100220	0.000000	-0.334635
O	0.328101	-2.937877	-0.223512	0.328101	-2.924878	-0.210305
O	-0.097533	0.000000	2.683880	-0.097533	0.000000	2.668156

Table S7. Theoretical Cartesian coordinates (in Å) for the $Fe(CO)_5$ structure using the B3LYP/DZP and BP86/DZP methods.

	B3LYP/DZP			BP86/DZP		
Fe	0.000000	0.000016	0.000000	0.000000	0.000137	0.000000
C	0.000000	-1.815688	0.000000	0.000000	1.805247	0.000000
C	0.000000	0.909214	-1.571817	0.000000	-0.904432	-1.562241
C	0.000000	0.909214	1.571817	0.000000	-0.904432	1.562241
C	-1.822518	-0.001157	0.000000	1.805386	0.001682	0.000000
C	1.822518	-0.001157	0.000000	-1.805386	0.001682	0.000000
O	0.000000	-2.971987	0.000000	0.000000	2.975377	0.000000
O	0.000000	1.488029	-2.572795	0.000000	-1.490859	-2.574794
O	0.000000	1.488029	2.572795	0.000000	-1.490859	2.574794
O	-2.974916	-0.002221	0.000000	2.972721	0.003043	0.000000
O	2.974916	-0.002221	0.000000	-2.972721	0.003043	0.000000

Table S8. Theoretical Cartesian coordinates (in Å) for the structure **28-1S** (C_2) using the B3LYP/DZP and BP86/DZP methods

	B3LYP/DZP			BP86/DZP		
Fe	0.126839	-1.456797	-0.042606	0.201791	-1.424927	-0.048440
Fe	-0.126839	1.456797	-0.042606	-0.201791	1.424927	-0.048440
C	1.694626	1.342015	0.689548	1.913523	-1.353381	-0.721338
C	-1.694626	-1.342015	0.689548	-1.913523	1.353381	-0.721338
C	-0.726450	-1.291458	-1.638031	0.685162	1.290489	-1.615820
C	0.726450	1.291458	-1.638031	0.105496	-3.204301	-0.012555
C	0.018333	3.247515	0.003085	0.685162	-1.309206	1.699793
C	-0.643896	1.333988	1.709688	-0.685162	-1.290489	-1.615820
C	0.643896	-1.333988	1.709688	-0.105496	3.204301	-0.012555
O	1.854640	-1.404668	-0.723617	2.990749	-1.402090	-1.154701
O	-0.018333	-3.247515	0.003085	-2.990749	1.402090	-1.154701
O	-1.854640	1.404668	-0.723617	-0.030797	4.367358	0.008748
O	-1.295107	-1.244697	-2.639331	0.030797	-4.367358	0.008748
O	1.295107	1.244697	-2.639331	0.959913	-1.328957	2.829978
O	-2.915164	1.449739	-1.158476	-1.284669	-1.283998	-2.616741
O	-0.931644	1.335020	2.821695	1.284669	1.283998	-2.616741
B	0.931644	-1.335020	2.821695	1.616514	1.356439	0.688165
B	2.915164	-1.449739	-1.158476	-1.616514	-1.356439	0.688165
C	-0.126839	-4.392329	0.031995	-0.685162	1.309206	1.699793
O	0.126839	4.392329	0.031995	-0.959913	1.328957	2.829978
O	2.824972	1.262480	1.138275	2.758659	1.337529	1.147484
O	-2.824972	-1.262480	1.138275	-2.758659	-1.337529	1.147484

Table S9. Theoretical Cartesian coordinates (in Å) for the structure **28-2S**(C_s) using the B3LYP/DZP and BP86/DZP methods

	B3LYP/DZP			BP86/DZP		
Fe	0.100518	1.528650	0.000000	0.100213	1.515388	0.000000
Fe	0.015968	-1.344091	0.000000	0.025030	-1.320670	0.000000
C	-1.293229	-1.436538	1.294306	-1.267698	-1.464205	1.277319
C	1.939275	1.485084	0.000000	1.926235	1.535761	0.000000
C	-0.097521	1.329315	1.792989	-0.131317	1.318779	1.779189
C	1.306919	-1.341422	1.295561	1.303716	-1.305091	1.283312
C	-0.101336	3.315547	0.000000	-0.128107	3.285726	0.000000
C	1.306919	-1.341422	-1.295561	1.303716	-1.305091	-1.283312
C	-0.097521	1.329315	-1.792989	-0.131317	1.318779	-1.779189
C	-1.293229	-1.436538	-1.294306	-1.267698	-1.464205	-1.277319
B	0.085138	-3.290745	0.000000	0.147588	-3.259002	0.000000
B	-1.853118	1.315258	0.000000	-1.844273	1.258598	0.000000
O	-3.062318	1.160479	0.000000	-3.065646	1.099916	0.000000
O	-2.092672	-1.566055	2.105122	-2.075195	-1.640009	2.092986
O	3.090638	1.491949	0.000000	3.090484	1.599406	0.000000
O	-0.253296	1.254324	2.933264	-0.315859	1.257793	2.930511
O	2.118619	-1.386589	2.107985	2.126283	-1.356968	2.105355
O	-0.240183	4.457900	0.000000	-0.284076	4.441302	0.000000
O	2.118619	-1.386589	-2.107985	2.126283	-1.356968	-2.105355
O	-0.253296	1.254324	-2.933264	-0.315859	1.257793	-2.930511
O	-2.092672	-1.566055	-2.105122	-2.075195	-1.640009	-2.092986
O	0.140260	-4.506328	0.000000	0.236524	-4.485177	0.000000

Table S10. Theoretical Cartesian coordinates (in Å) for the structure **28-3S**(C_2) using the B3LYP/DZP and BP86/DZP methods

	B3LYP/DZP			BP86/DZP		
Fe	-0.072514	-1.463755	-0.103930	-0.066667	-1.441976	-0.116787
Fe	0.072514	1.463755	-0.103930	0.066667	1.441976	-0.116787
C	-0.832185	-1.340564	-1.778753	-0.818790	-1.344337	-1.780621
C	0.832185	1.340564	-1.778753	0.818790	1.344337	-1.780621
C	1.657240	-1.314472	-0.636822	1.664739	-1.265106	-0.598307
C	1.623418	1.316172	0.859368	1.585150	1.339402	0.877907
C	-1.623418	-1.316172	0.859368	-1.585150	-1.339402	0.877907
C	-0.053691	-3.260867	-0.039340	-0.018549	-3.223766	-0.085513
C	-1.657240	1.314472	-0.636822	-1.664739	1.265106	-0.598307
C	0.053691	3.260867	-0.039340	0.018549	3.223766	-0.085513
O	-1.300165	-1.313558	-2.829458	-1.292091	-1.350306	-2.845329
O	1.300165	1.313558	-2.829458	1.292091	1.350306	-2.845329
O	0.034534	4.409725	0.004336	-0.018549	4.388369	-0.067336
O	2.591458	1.307042	1.476722	2.546251	1.368019	1.532226
O	-2.591458	-1.307042	1.476722	-2.546251	-1.368019	1.532226
O	-0.034534	-4.409725	0.004336	0.018549	-4.388369	-0.067336
O	-2.766459	1.278241	-0.946904	-2.796414	1.232195	-0.880121
O	2.766459	-1.278241	-0.946904	2.796414	-1.232195	-0.880121
B	-0.753129	1.486751	1.689717	-0.742372	1.469570	1.678774
B	0.753129	-1.486751	1.689717	0.742372	-1.469570	1.678774
O	1.300165	-1.560417	2.773662	1.279289	-1.556412	2.780782
O	-1.300165	1.560417	2.773662	-1.279289	1.556412	2.780782

Table S11. Theoretical Cartesian coordinates (in Å) for the structure **28-4S**(C_{2h}) using the B3LYP/DZP and BP86/DZP methods

	B3LYP/DZP			BP86/DZP		
Fe	1.492739	-0.284802	0.000000	1.456799	-0.302973	0.000000
B	1.041166	-2.198931	0.000000	1.035086	-2.218881	0.000000
B	-1.041166	2.198931	0.000000	-1.035086	2.218881	0.000000
Fe	-1.492739	0.284802	0.000000	-1.456799	0.302973	0.000000
O	0.808928	-3.394420	0.000000	0.838923	-3.433112	0.000000
O	-0.808928	3.394420	0.000000	-0.838923	3.433112	0.000000
C	1.331061	-0.483937	1.802278	1.285317	-0.570095	1.780980
C	-1.331061	0.483937	1.802278	-1.285317	0.570095	1.780980
C	1.873890	1.537522	0.000000	1.840289	1.497999	0.000000
C	-1.873890	-1.537522	0.000000	-1.840289	-1.497999	0.000000
C	3.219708	-0.771550	0.000000	3.180174	-0.745897	0.000000
C	-3.219708	0.771550	0.000000	-3.180174	0.745897	0.000000
O	1.331061	-0.678292	2.937167	1.285317	-0.822292	2.919491
O	-1.331061	0.678292	2.937167	-1.285317	0.822292	2.919491
O	2.244834	2.621931	0.000000	2.231189	2.591936	0.000000
O	4.323665	-1.094095	0.000000	4.308327	-1.038609	0.000000
O	-2.244834	-2.621931	0.000000	-2.231189	-2.591936	0.000000
O	-4.323665	1.094095	0.000000	-4.308327	1.038609	0.000000
C	-1.331061	0.483937	-1.802278	-1.285317	0.570095	-1.780980
C	1.331061	-0.483937	-1.802278	1.285317	-0.570095	-1.780980
O	-1.331061	0.678292	-2.937167	-1.285317	0.822292	-2.919491
O	1.331061	-0.678292	-2.937167	1.285317	-0.822292	-2.919491

Table S12. Theoretical Cartesian coordinates (in Å) for the structure **28-5S**(C_1) using the B3LYP/DZP and BP86/DZP methods

	B3LYP/DZP			BP86/DZP		
Fe	2.059462	0.023511	-0.107416	2.037307	0.032603	-0.119717
B	-1.549576	-1.767854	0.438399	-1.454793	-1.660198	0.659945
B	-0.030981	0.039718	-0.660969	-0.027024	0.072604	-0.667267
Fe	-1.967473	0.096940	-0.032292	-1.970477	0.097426	-0.048675
O	-1.286715	-2.917618	0.738408	-1.129696	-2.757757	1.108810
O	0.708451	0.069889	-1.689261	0.697961	0.130350	-1.725164
C	1.820864	1.820598	0.101287	1.843358	1.811959	0.135567
C	-2.028797	1.853580	-0.563894	-2.101193	1.753805	-0.792433
C	3.682848	0.152518	-0.954594	3.674572	0.173508	-0.906965
C	-1.306057	0.438826	1.631863	-1.338686	0.631247	1.558894
C	2.378665	-0.111609	1.647833	2.298995	-0.155701	1.623496
C	-2.252904	-0.577503	-1.699575	-2.178347	-0.821757	-1.587655
O	1.653807	2.954683	0.236301	1.715614	2.959403	0.314518
O	-2.043512	2.949777	-0.906270	-2.161693	2.810663	-1.275114
O	4.720187	0.247274	-1.448513	4.744875	0.273651	-1.362244
O	2.596785	-0.200397	2.781151	2.494281	-0.281541	2.771698
O	-0.867411	0.630495	2.675084	-0.914835	0.949445	2.594145
O	-2.415998	-1.024183	-2.744071	-2.304224	-1.435640	-2.567343
C	1.991592	-1.820970	-0.200589	1.990070	-1.785469	-0.258118
C	-3.708084	-0.118828	0.521489	-3.697563	-0.106965	0.498652
O	1.981590	-2.967103	-0.276570	1.996226	-2.945125	-0.355057
O	-4.791894	-0.281657	0.864031	-4.797975	-0.259267	0.844020

Table S13. Theoretical Cartesian coordinates (in Å) for the structure **28-6S**(D_2) using the B3LYP/DZP and BP86/DZP methods

	B3LYP/DZP			BP86/DZP		
Fe	0.000000	0.000000	-1.410382	0.000000	0.000000	1.405659
Fe	0.000000	0.000000	1.410382	0.000000	0.000000	-1.405659
C	-0.722893	1.678416	-1.422159	-1.610503	0.819049	1.249567
C	-1.678412	0.722902	1.422225	-0.796409	1.606333	-1.637596
C	0.722893	-1.678416	-1.422159	1.610503	-0.819049	1.249567
C	1.678412	-0.722902	1.422225	0.796409	-1.606333	-1.637596
B	0.000000	0.000000	-3.357265	0.000000	0.000000	3.347980
B	0.000000	0.000000	3.357265	0.000000	0.000000	-3.347980
C	-1.678412	-0.722902	-1.422225	0.796409	1.606333	1.637596
C	-0.722893	-1.678416	1.422159	1.610503	0.819049	-1.249567
C	1.678412	0.722902	-1.422225	-0.796409	-1.606333	1.637596
C	0.722893	1.678416	1.422159	-1.610503	-0.819049	-1.249567
O	-1.177359	2.733624	-1.475108	-2.646181	1.352520	1.215703
O	-2.733591	1.177428	1.475230	-1.300453	2.634699	-1.850678
O	1.177359	-2.733624	-1.475108	2.646181	-1.352520	1.215703
O	2.733591	-1.177428	1.475230	1.300453	-2.634699	-1.850678
O	0.000000	0.000000	-4.574552	0.000000	0.000000	4.577670
O	0.000000	0.000000	4.574552	0.000000	0.000000	-4.577670
O	-2.733591	-1.177428	-1.475230	1.300453	2.634699	1.850678
O	-1.177359	-2.733624	1.475108	2.646181	1.352520	-1.215703
O	2.733591	1.177428	-1.475230	-1.300453	-2.634699	1.850678
O	1.177359	2.733624	1.475108	-2.646181	-1.352520	-1.215703

Table S14. Theoretical Cartesian coordinates (in Å) for the structure **28-7S**(C_{2v}) using the B3LYP/DZP and BP86/DZP methods

	B3LYP/DZP			BP86/DZP		
Fe	0.000000	1.529677	0.119836	0.000000	1.500765	0.133482
Fe	0.000000	-1.529677	0.119836	0.000000	-1.500765	0.133482
C	1.802282	1.423397	-0.116061	1.786244	1.410755	-0.142834
C	1.802282	-1.423397	-0.116061	1.786244	-1.410755	-0.142834
C	-1.802282	1.423397	-0.116061	-1.786244	1.410755	-0.142834
C	-1.802282	-1.423397	-0.116061	-1.786244	-1.410755	-0.142834
C	0.000000	3.322569	0.038604	0.000000	3.278862	0.074595
C	0.000000	-3.322569	0.038604	0.000000	-3.278862	0.074595
C	0.000000	1.467695	1.961277	0.000000	1.457525	1.960426
C	0.000000	-1.467695	1.961277	0.000000	-1.457525	1.960426
B	0.000000	1.575080	-1.858325	0.000000	1.548012	-1.839433
B	0.000000	-1.575080	-1.858325	0.000000	-1.548012	-1.839433
O	2.938357	1.476642	-0.292623	2.930299	1.492378	-0.350051
O	2.938357	-1.476642	-0.292623	2.930299	-1.492378	-0.350051
O	-2.938357	1.476642	-0.292623	-2.930299	1.492378	-0.350051
O	-2.938357	-1.476642	-0.292623	-2.930299	-1.492378	-0.350051
O	0.000000	4.470852	-0.017520	0.000000	4.443420	0.036324
O	0.000000	-4.470852	-0.017520	0.000000	-4.443420	0.036324
O	0.000000	1.531196	3.110036	0.000000	1.552606	3.121859
O	0.000000	-1.531196	3.110036	0.000000	-1.552606	3.121859
O	0.000000	1.751298	-3.061103	0.000000	1.730347	-3.054267
O	0.000000	-1.751298	-3.061103	0.000000	-1.730347	-3.054267

Table S15. Theoretical Cartesian coordinates (in Å) for the structure **28-8S**(C_s) using the B3LYP/DZP and BP86/DZP methods

	B3LYP/DZP			BP86/DZP		
Fe	-0.044725	1.525428	0.000000	0.034360	-1.386524	0.000000
Fe	-0.132234	-1.465702	0.000000	0.148135	1.387193	0.000000
C	-1.834254	1.140142	0.000000	1.556773	-0.224540	0.000000
B	1.392450	-1.293750	1.214598	-1.297034	0.817037	1.199228
B	1.392450	-1.293750	-1.214598	-1.297034	0.817037	-1.199228
C	1.824587	1.469385	0.000000	-1.776039	-1.856136	0.000000
C	-0.020185	1.308535	-1.835166	0.073351	-1.461472	-1.832380
C	-0.192450	3.344120	0.000000	0.912954	-2.938509	0.000000
C	-0.020185	1.308535	1.835166	0.073351	-1.461472	1.832380
C	0.205956	-3.201651	0.000000	-0.768911	2.915899	0.000000
C	-1.269015	-1.538568	1.431821	1.120006	1.884537	1.454724
C	-1.269015	-1.538568	-1.431821	1.120006	1.884537	-1.454724
O	2.304171	-1.114213	2.006934	-2.201781	0.566174	2.001904
O	2.304171	-1.114213	-2.006934	-2.201781	0.566174	-2.001904
O	-2.976266	0.993319	0.000000	2.743234	-0.220894	0.000000
O	2.964671	1.542042	0.000000	-2.863434	-2.255234	0.000000
O	-0.033328	1.254415	-2.980268	0.151964	-1.602224	-2.981418
O	-0.305913	4.487398	0.000000	1.486143	-3.954150	0.000000
O	-0.033328	1.254415	2.980268	0.151964	-1.602224	2.981418
O	0.440346	-4.330433	0.000000	-1.351204	3.925100	0.000000
O	-1.949526	-1.634299	2.357444	1.689732	2.248336	2.404358
O	-1.949526	-1.634299	-2.357444	1.689732	2.248336	-2.404358

Table S16. Theoretical Cartesian coordinates (in Å) for the structure **28-9S**(C_{2v}) using the B3LYP/DZP and BP86/DZP methods

	B3LYP/DZP			BP86/DZP		
Fe	0.000000	1.362685	0.088048	0.000000	1.346488	0.094470
Fe	0.000000	-1.362685	0.088048	0.000000	-1.346488	0.094470
C	0.000000	0.000000	-1.417873	0.000000	0.000000	-1.409445
C	0.000000	0.000000	1.596444	0.000000	0.000000	1.610489
C	-1.803483	1.564301	-0.145444	-1.775280	1.589551	-0.183675
C	-1.803483	-1.564301	-0.145444	-1.775280	-1.589551	-0.183675
C	0.000000	2.608055	1.421052	0.000000	2.553596	1.445968
C	0.000000	-2.608055	1.421052	0.000000	-2.553596	1.445968
C	1.803483	1.564301	-0.145444	1.775280	1.589551	-0.183675
C	1.803483	-1.564301	-0.145444	1.775280	-1.589551	-0.183675
B	0.000000	-2.766511	-1.286611	0.000000	-2.771621	-1.245400
B	0.000000	2.766511	-1.286611	0.000000	2.771621	-1.245400
O	0.000000	3.670111	-2.099746	0.000000	3.697967	-2.051819
O	0.000000	0.000000	-2.589700	0.000000	0.000000	-2.594325
O	0.000000	0.000000	2.767578	0.000000	0.000000	2.795156
O	-2.925277	1.749889	-0.311191	-2.902218	1.812044	-0.376319
O	-2.925277	-1.749889	-0.311191	-2.902218	-1.812044	-0.376319
O	0.000000	3.415919	2.236575	0.000000	3.352095	2.291034
O	0.000000	-3.415919	2.236575	0.000000	-3.352095	2.291034
O	2.925277	1.749889	-0.311191	2.902218	1.812044	-0.376319
O	2.925277	-1.749889	-0.311191	2.902218	-1.812044	-0.376319
O	0.000000	-3.670111	-2.099746	0.000000	-3.697967	-2.051819

Table S17. Theoretical Cartesian coordinates (in Å) for the structure **28-10S**(C_s) using the B3LYP/DZP and BP86/DZP methods

	B3LYP/DZP			BP86/DZP		
Fe	-0.054721	-2.612073	0.000000	-0.092584	2.623159	0.000000
Fe	0.222079	2.275944	0.000000	-0.140120	-2.299591	0.000000
C	-1.795022	-3.093731	0.000000	1.674098	2.948610	0.000000
C	2.075127	2.720958	0.000000	-1.891129	-2.930033	0.000000
C	0.043635	2.084981	1.839651	0.047645	-2.081078	1.807828
C	1.085670	-4.016100	0.000000	-0.980803	4.204378	0.000000
C	0.043635	-2.338257	-1.765785	-0.284483	2.331220	-1.753530
C	0.043635	-2.338257	1.765785	-0.284483	2.331220	1.753530
C	-0.376262	3.992982	0.000000	0.596857	-3.926694	0.000000
O	-2.916713	-3.384474	0.000000	2.827253	3.150817	0.000000
O	3.189728	2.966718	0.000000	-2.970193	-3.353339	0.000000
O	-0.780243	5.065904	0.000000	1.097664	-4.977957	0.000000
O	1.838612	-4.898071	0.000000	-1.578288	5.211612	0.000000
O	0.117054	-2.116967	-2.905033	-0.412895	2.103481	-2.898820
O	0.117054	-2.116967	2.905033	-0.412895	2.103481	2.898820
O	-0.090026	1.920505	2.961947	0.202503	-1.944911	2.949159
B	-1.686493	1.738962	0.000000	1.689925	-1.564317	0.000000
B	0.438114	-0.825350	0.000000	-0.525020	0.811013	0.000000
C	0.043635	2.084981	-1.839651	0.047645	-2.081078	-1.807828
O	-0.090026	1.920505	-2.961947	0.202503	-1.944911	-2.949159
O	-2.868180	1.460918	0.000000	2.841103	-1.137526	0.000000
O	0.846025	0.380176	0.000000	-0.962542	-0.388938	0.000000

Table S18. Theoretical Cartesian coordinates (in Å) for the structure **28-11S**(C_{2v}) using the B3LYP/DZP and BP86/DZP methods

	B3LYP/DZP			BP86/DZP		
Fe	0.000000	1.381778	0.100438	0.000000	1.357158	-0.105338
Fe	0.000000	-1.381778	0.100438	0.000000	-1.357158	-0.105338
C	1.488430	0.000000	0.051654	-1.485246	0.000000	-0.280990
C	-1.488430	0.000000	0.051654	1.485246	0.000000	-0.280990
B	0.000000	1.539420	-1.886011	0.000000	1.445377	1.879418
B	0.000000	-1.539420	-1.886011	0.000000	-1.445377	1.879418
C	-1.344943	2.579086	-0.112926	1.340333	2.512759	0.233309
C	-1.344943	-2.579086	-0.112926	1.340333	-2.512759	0.233309
C	0.000000	1.541276	1.946371	0.000000	1.669407	-1.910125
C	0.000000	-1.541276	1.946371	0.000000	-1.669407	-1.910125
C	1.344943	-2.579086	-0.112926	-1.340333	-2.512759	0.233309
C	1.344943	2.579086	-0.112926	-1.340333	2.512759	0.233309
O	2.185783	3.348217	-0.254463	-2.194096	3.276711	0.435702
O	2.660061	0.000000	0.029994	-2.657086	0.000000	-0.458066
O	-2.660061	0.000000	0.029994	2.657086	0.000000	-0.458066
O	0.000000	1.778159	-3.077104	0.000000	1.690304	3.083267
O	0.000000	-1.778159	-3.077104	0.000000	-1.690304	3.083267
O	-2.185783	3.348217	-0.254463	2.194096	3.276711	0.435702
O	-2.185783	-3.348217	-0.254463	2.194096	-3.276711	0.435702
O	0.000000	1.733175	3.079239	0.000000	1.968177	-3.035520
O	0.000000	-1.733175	3.079239	0.000000	-1.968177	-3.035520
O	2.185783	-3.348217	-0.254463	-2.194096	-3.276711	0.435702

Table S19. Theoretical Cartesian coordinates (in Å) for the structure **28-12S**(C_s) using the B3LYP/DZP and BP86/DZP methods

	B3LYP/DZP			BP86/DZP		
Fe	-0.000044	-1.460558	0.000000	-0.000024	-1.410525	0.000000
Fe	-0.000033	1.541252	0.000000	0.000003	1.498035	0.000000
C	1.813716	-1.421717	0.000000	1.799158	-1.392429	0.000000
C	-1.296920	1.316039	1.296500	-1.285198	1.287442	1.288315
C	-1.296920	1.316039	-1.296500	-1.285198	1.287442	-1.288315
C	-1.813800	-1.421470	0.000000	-1.799182	-1.392382	0.000000
B	-0.000028	-1.430985	-1.982283	0.000145	-1.396415	-1.974988
C	-0.000150	-3.232415	0.000000	-0.000104	-3.160984	0.000000
B	-0.000028	-1.430985	1.982283	0.000145	-1.396415	1.974988
C	-0.000069	3.367238	0.000000	-0.000062	3.308462	0.000000
C	1.296973	1.316004	1.296373	1.285188	1.287519	1.288336
C	1.296973	1.316004	-1.296373	1.285188	1.287519	-1.288336
O	-2.122908	1.257740	2.089356	-2.119649	1.248931	2.093566
O	-2.122908	1.257740	-2.089356	-2.119649	1.248931	-2.093566
O	2.966259	-1.430989	0.000000	2.966556	-1.438101	0.000000
O	-2.966346	-1.430529	0.000000	-2.966587	-1.438051	0.000000
O	-0.000045	-1.345381	-3.199767	0.000190	-1.342728	-3.207121
O	-0.000223	-4.384486	0.000000	-0.000154	-4.329513	0.000000
O	-0.000045	-1.345381	3.199767	0.000190	-1.342728	3.207121
O	-0.000078	4.515833	0.000000	-0.000139	4.471824	0.000000
O	2.123364	1.257568	2.088801	2.119645	1.249053	2.093587
O	2.123364	1.257568	-2.088801	2.119645	1.249053	-2.093587

Table S20. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **14-1D**(C_s). using the B3LYP/DZP and BP86/DZP methods

B3LYP/DZP	BP86/DZP
47(2), 74(1), 76(1), 91(1), 95(3), 99(2), 103(0), 324(0), 340(0), 349(0), 355(4), 388(1), 400(2), 420(7), 439(5), 449(6), 485(2), 507(2), 526(8), 589(72), 597(91), 600(100), 1925(265), 2099(1453), 2102(808), 2109(549), 2168(105)	45(2), 71(1), 74(0), 88(1), 93(2), 96(1), 100(0), 329(1), 350(0), 353(0), 375(2), 397(1), 419(0), 430(1), 457(1), 476(3), 480(1), 502(2), 520(1), 597(83), 604(83), 613(92), 1845(182), 2006(1216), 2010(708), 2018(516), 2075(96)

Table S21. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **14-2D**(C_{2v}) using the B3LYP/DZP and BP86/DZP methods

B3LYP/DZP	BP86/DZP
40(0), 64(3), 85(1), 94(0), 97(4), 100(3), 112(0), 330(0), 356(1), 358(7), 360(0), 390(0), 405(7), 425(1), 441(3), 452(0), 457(25), 508(6), 556(0), 594(83), 626(81), 635(79), 1919(205), 2093(1571), 2098(1448), 2107(96), 2170(32)	49(0), 60(2), 82(0), 90(0), 94(3), 96(2), 107(0), 332(0), 363(0), 365(0), 387(3), 392(1), 415(0), 433(0), 453(1), 471(10), 474(0), 495(1), 544(0), 602(80), 621(77), 634(81), 1848(186), 1998(1303), 2007(1203), 2016(138), 2079(21)

Table S22. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the $Fe(BO)_2(CO)_3$ structure using the B3LYP/DZP and BP86/DZP methods.

B3LYP/DZP	BP86/DZP
54(2), 72(3), 75(0), 93(4), 97(6), 104(1), 110(1), 311(5), 346(1), 353(0), 360(7), 387(3), 420(6), 422(9), 425(0), 458(4), 470(1), 491(0), 542(7), 605(97), 615(79), 626(50), 1926(219), 1934(182), 2121(1280), 2128(601), 2180(105)	46(2), 63(2), 69(0), 89(4), 93(3), 99(0), 105(1), 306(4), 349(0), 355(0), 362(4), 392(1), 428(1), 434(0), 445(0), 448(3), 470(2), 485(0), 531(6), 611(74), 612(96), 629(46), 1844(162), 1853(155), 2018(1140), 2028(576), 2085(70)

Table S23. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the $Fe(CO)_5$ structure using the B3LYP/DZP and BP86/DZP methods.

B3LYP/DZP	BP86/DZP
54(0), 54(0), 95(0), 95(0), 104(0), 104(0), 107(1), 365(0), 366(0), 366(0), 413(0), 439(1), 439(14), 440(13), 473(7), 483(2), 483(2), 563(0), 563(0), 617(127), 660(132), 660(132), 2067(1275), 2067(1273), 2093(0), 2094(1474), 2169(0	53(0), 54(0), 90(0), 91(0), 99(0), 99(0), 103(0), 358(0), 369(0), 369(0), 434(6), 435(6), 435(0), 460(0), 488(0), 492(1), 492(1), 547(0), 547(0), 626(127), 662(125), 662(125), 1992(1080), 1992(1077), 2008(1264), 2012(0), 2089(0)

Table S24. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **28-1S** (C_2) using the B3LYP/DZP and BP86/DZP methods

B3LYP/DZP	BP86/DZP
44(1), 52(1), 56(1), 62(0), 65(0), 75(3), 75(0), 82(1), 83(1), 98(4), 98(1), 100(0), 101(0), 108(1), 109(0), 113(0), 115(0), 119(0), 122(2), 148(0), 356(0), 357(0), 358(0), 366(23), 375(14), 376(1), 402(1), 415(25), 415(0), 424(0), 432(1), 432(2), 442(2), 446(0), 453(5), 458(0), 474(1), 482(0), 525(1), 525(1), 532(5), 536(2), 544(1), 555(3), 618(146), 618(33), 625(544), 630(30), 634(168), 649(1), 1921(343), 1922(57), 2085(98), 2103(809), 2111(383), 2118(1), 2126(1122), 2134(1058), 2141(1789), 2189(6)	42(1), 46(0), 52(1), 55(0), 61(0), 69(0), 70(2), 76(1), 79(1), 93(3), 94(1), 96(0), 97(0), 105(0), 106(0), 108(0), 110(0), 114(0), 119(1), 150(0), 345(0), 355(0), 355(0), 356(9), 384(11), 386(1), 397(1), 410(0), 424(0), 425(1), 434(14), 439(0), 439(5), 442(0), 469(5), 469(1), 489(6), 499(0), 516(0), 517(0), 519(2), 524(2), 536(1), 548(2), 619(112), 620(30), 623(51), 626(147), 630(452), 647(0), 1851(48), 1851(290), 2002(108), 2017(667), 2021(618), 2027(51), 2039(600), 2043(887), 2062(1343), 2101(4)

Table S25. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **28-2S**(C_s) using the B3LYP/DZP and BP86/DZP methods

B3LYP/DZP	BP86/DZP
37(0), 49(0), 55(2), 58(0), 61(3), 63(0), 71(2), 81(3), 81(0), 92(1), 96(0), 98(2), 100(1), 104(0), 107(1), 109(1), 110(0), 115(1), 122(5), 154(1), 361(0), 362(3), 371(0), 373(0), 376(3), 382(13), 401(21), 407(0), 411(0), 418(0), 426(4), 433(7), 449(3), 453(0), 465(10), 465(15), 468(1), 480(0), 503(3), 506(7), 535(1), 536(3), 555(0), 567(2), 624(80), 634(45), 637(443), 637(86), 640(179), 663(41), 1919(213), 1935(279), 2081(453), 2094(14), 2097(121), 2120(1105), 2121(1312), 2136(1505), 2144(488), 2192(3)	30(0), 39(1), 44(0), 51(1), 54(0), 56(2), 64(1), 75(2), 76(0), 88(0), 91(0), 92(1), 97(1), 101(0), 103(1), 105(0), 106(0), 109(1), 119(5), 154(0), 350(5), 358(0), 368(1), 371(1), 377(0), 390(5), 401(0), 412(7), 420(0), 424(0), 439(9), 440(0), 445(1), 446(4), 478(4), 479(3), 482(2), 489(7), 493(7), 495(4), 523(1), 525(2), 545(0), 554(1), 625(72), 628(52), 636(400), 640(86), 640(112), 662(69), 1848(176), 1863(215), 1995(263), 2009(58), 2017(73), 2031(1334), 2031(1269), 2054(181), 2055(1029), 2107(6)

Table S26. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **28-3S**(C_2) using the B3LYP/DZP and BP86/DZP methods

B3LYP/DZP	BP86/DZP
40(0), 46(0), 57(1), 60(1), 62(0), 69(0), 73(4), 83(0), 83(0), 97(0), 97(0), 97(3), 101(1), 105(0), 109(0), 111(0), 114(1), 117(0), 122(2), 148(0), 349(3), 353(0), 359(3), 365(1), 376(15), 382(5), 398(0), 410(10), 416(19), 424(0), 434(0), 436(0), 444(3), 446(1), 464(3), 464(1), 475(0), 480(0), 522(7), 522(4), 533(3), 535(0), 548(0), 555(1), 622(156), 622(15), 625(385), 627(209), 630(164), 648(5), 1932(89), 1938(336), 2089(10), 2090(113), 2108(762), 2116(650), 2123(1216), 2124(522), 2137(1914), 2186(77)	35(0), 41(0), 51(0), 54(0), 55(1), 62(0), 66(3), 78(0), 79(0), 90(0), 93(2), 93(0), 96(0), 102(0), 105(0), 108(0), 109(1), 112(0), 118(2), 149(0), 344(3), 350(0), 354(1), 359(0), 384(5), 385(2), 393(1), 407(0), 427(0), 428(0), 430(8), 433(0), 437(12), 441(0), 477(4), 478(1), 488(7), 497(0), 514(2), 516(2), 521(2), 525(1), 537(0), 546(2), 619(37), 622(139), 623(137), 624(32), 629(449), 644(2), 1861(61), 1866(283), 2002(17), 2007(122), 2023(868), 2026(501), 2032(917), 2035(533), 2060(1246), 2098(61)

Table S27. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **28-4S**(C_{2h}) using the B3LYP/DZP and BP86/DZP methods

B3LYP/DZP	BP86/DZP
-29(2), 36(0), 38(0), 61(1), 65(3), 67(0), 79(0), 82(0), 88(5), 94(0), 98(3), 107(1), 107(0), 111(0), 118(0), 119(0), 130(0), 131(4), 147(0), 154(0), 358(0), 359(0), 360(0), 365(25), 374(0), 375(10), 402(0), 412(0), 415(32), 424(0), 430(0), 433(2), 446(0), 446(1), 455(5), 461(0), 482(4), 483(0), 527(5), 528(0), 529(0), 537(1), 548(0), 557(6), 619(0), 619(173), 627(0), 631(318), 632(430), 643(0), 1926(410), 1927(0), 2083(0), 2094(26), 2115(2067), 2117(0), 2124(1713), 2132(0), 2145(1674), 2188(0)	-28(1), 30(0), 32(0), 51(2), 61(2), 62(0), 74(0), 76(0), 83(4), 90(0), 95(1), 102(0), 104(0), 106(0), 114(0), 115(0), 127(0), 127(3), 140(0), 149(0), 354(0), 358(0), 359(0), 360(3), 382(10), 385(0), 398(0), 408(0), 419(0), 427(2), 433(21), 433(0), 436(1), 440(0), 475(8), 479(0), 496(2), 500(0), 511(2), 514(0), 518(0), 527(4), 542(0), 550(2), 618(0), 620(167), 621(158), 621(0), 634(457), 640(0), 1857(0), 1857(338), 1995(0), 2013(120), 2025(1746), 2028(0), 2034(969), 2038(0), 2061(1482), 2097(0)

Table S28. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **28-5S**(C_1) using the B3LYP/DZP and BP86/DZP methods

B3LYP/DZP	BP86/DZP
6(0), 29(1), 37(0), 46(1), 55(0), 62(1), 67(1), 72(1), 79(1), 87(2), 89(0), 94(1), 101(0), 103(1), 109(1), 110(1), 115(0), 158(2), 160(1), 271(38), 342(1), 356(0), 364(4), 376(47), 382(7), 386(19), 401(6), 405(3), 417(41), 423(39), 431(2), 435(15), 440(5), 448(3), 459(0), 468(20), 471(12), 476(26), 479(16), 512(72), 531(10), 542(114), 547(24), 553(5), 606(33), 620(329), 632(89), 643(83), 647(121), 652(137), 1624(72), 1935(178), 2064(626), 2080(781), 2103(784), 2126(800), 2130(1259), 2135(544), 2149(553), 2187(135)	9(0), 26(1), 35(0), 40(0), 49(0), 57(1), 61(0), 69(0), 76(1), 83(1), 88(0), 91(1), 96(0), 98(0), 104(1), 107(1), 111(0), 152(0), 156(0), 271(15), 335(0), 355(0), 359(1), 374(1), 388(16), 392(8), 401(6), 417(24), 425(49), 432(3), 436(0), 440(15), 443(4), 448(1), 471(5), 476(9), 483(1), 487(12), 493(21), 510(50), 523(14), 533(111), 541(9), 542(12), 605(38), 625(402), 635(89), 644(77), 647(122), 654(103), 1544(78), 1864(153), 1989(555), 1998(717), 2016(547), 2034(722), 2036(1149), 2044(476), 2068(486), 2100(88)

Table S29. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **28-6S**(D_2) using the B3LYP/DZP and BP86/DZP methods

B3LYP/DZP	BP86/DZP
23(0), 39(0), 49(0), 50(3), 50(3), 53(3), 53(3), 78(0), 78(0), 88(1), 88(1), 92(0), 101(0), 101(0), 106(3), 106(3), 110(0), 110(0), 122(10), 160(0), 370(0), 370(0), 375(0), 376(1), 376(1), 376(0), 406(32), 410(2), 415(0), 418(0), 427(0), 427(0), 440(0), 440(0), 472(0), 472(0), 474(24), 474(24), 502(0), 502(0), 521(11), 521(11), 571(0), 571(0), 641(0), 641(0), 645(149), 645(149), 654(526), 674(0), 1932(581), 1934(0), 2094(0), 2094(0), 2115(621), 2117(0), 2118(0), 2119(2098), 2119(2098), 2191(0)	14(0), 24(0), 45(0), 45(1), 48(4), 48(5), 58(1), 69(0), 79(0), 88(1), 92(0), 93(0), 97(0), 101(0), 102(2), 102(2), 105(0), 108(0), 122(9), 158(0), 359(0), 367(2), 375(1), 375(2), 380(0), 380(0), 409(10), 415(0), 421(37), 441(0), 444(0), 445(1), 461(0), 462(0), 463(0), 472(1), 475(1), 486(3), 493(3), 494(10), 505(1), 506(15), 554(0), 554(0), 635(16), 639(89), 645(60), 647(136), 650(468), 667(0), 1861(445), 1862(0), 1997(8), 2006(58), 2027(1868), 2027(1749), 2031(0), 2032(41), 2052(420), 2105(0)

Table S30. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **28-7S**(C_{2v}) using the B3LYP/DZP and BP86/DZP methods

B3LYP/DZP	BP86/DZP
-31(0), 32(1), 38(0), 60(0), 61(4), 68(1), 79(0), 82(0), 88(0), 92(4), 95(0), 97(2), 108(0), 111(0), 116(0), 123(1), 123(0), 129(0), 150(0), 156(0), 347(6), 351(2), 354(0), 355(0), 376(10), 384(6), 403(0), 412(0), 416(41), 427(1), 434(0), 437(0), 444(1), 445(0), 466(2), 467(3), 482(0), 483(3), 531(0), 532(7), 533(2), 540(0), 550(0), 560(3), 622(0), 623(173), 627(2), 629(185), 637(567), 649(5), 1934(39), 1943(406), 2087(0), 2092(20), 2098(17), 2118(449), 2119(2039), 2124(511), 2133(2350), 2185(132)	-31(0), 23(1), 31(0), 53(3), 55(0), 64(1), 73(0), 77(0), 83(0), 87(3), 91(0), 94(1), 104(0), 106(0), 111(0), 118(1), 121(0), 127(0), 145(0), 152(0), 342(0), 342(6), 351(0), 352(0), 382(2), 387(3), 400(0), 409(0), 425(0), 429(3), 432(0), 433(0), 435(25), 442(1), 479(1), 479(0), 498(1), 501(0), 520(0), 520(3), 526(2), 530(2), 546(0), 553(2), 620(174), 620(0), 622(0), 622(158), 641(452), 646(2), 1860(16), 1868(333), 1999(0), 2005(20), 2016(78), 2027(360), 2030(1732), 2037(514), 2056(1549), 2097(91)

Table S31. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **28-8S**(C_s) using the B3LYP/DZP and BP86/DZP methods

B3LYP/DZP	BP86/DZP
42(0), 50(0), 52(0), 54(3), 61(3), 70(0), 72(0), 78(2), 80(0), 88(0), 98(1), 99(0), 105(1), 106(0), 108(0), 109(1), 113(0), 114(1), 118(0), 138(5), 349(0), 358(0), 359(2), 370(1), 372(16), 377(4), 382(17), 386(3), 393(0), 394(1), 407(1), 415(5), 451(3), 451(12), 458(8), 459(0), 465(0), 473(8), 492(5), 514(16), 529(5), 534(0), 542(1), 550(4), 615(185), 622(0), 624(94), 626(150), 628(291), 643(43), 1902(193), 1911(234), 2086(368), 2086(97), 2105(724), 2127(914), 2130(948), 2135(1274), 2160(497), 2199(132)	30(1), 37(1), 47(0), 58(0), 67(1), 74(0), 82(0), 86(0), 86(0), 92(1), 100(0), 101(1), 105(1), 107(1), 113(3), 113(0), 118(0), 120(2), 173(1), 211(9), 326(2), 330(7), 354(0), 360(20), 364(0), 370(20), 390(2), 398(1), 400(0), 411(5), 412(8), 428(9), 442(3), 452(0), 459(43), 463(11), 474(0), 481(2), 487(1), 510(3), 514(48), 525(10), 534(71), 546(1), 592(14), 615(170), 616(130), 621(236), 626(103), 653(90), 1817(163), 1825(195), 1873(363), 2015(349), 2024(100), 2024(951), 2042(1151), 2060(234), 2062(1114), 2106(106)

Table S32. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **28-9S**(C_{2v}) using the B3LYP/DZP and BP86/DZP methods

B3LYP/DZP	BP86/DZP
-80(0), 33(0), 42(0), 59(2), 65(1), 66(3), 73(0), 80(0), 90(0), 92(0), 98(1), 99(0), 105(0), 105(1), 109(5), 111(0), 128(0), 167(1), 199(2), 241(10), 310(8), 349(0), 362(1), 369(0), 372(0), 387(2), 387(0), 388(0), 409(0), 413(1), 414(13), 417(19), 432(0), 443(12), 451(7), 453(23), 473(0), 494(24), 502(71), 514(0), 519(0), 521(0), 570(0), 573(301), 583(0), 618(141), 625(336), 629(157), 642(10), 651(59), 1922(1194), 1939(304), 1939(62), 1974(30), 2101(0), 2121(68), 2124(2048), 2131(591), 2144(1024), 2182(104)	29(0), 29(0), 44(1), 54(2), 58(2), 60(0), 77(0), 81(0), 87(0), 91(0), 93(0), 95(0), 100(0), 102(0), 105(4), 109(0), 124(0), 179(0), 203(2), 241(9), 321(5), 356(0), 363(0), 369(0), 372(0), 383(1), 387(2), 388(3), 409(0), 412(0), 416(1), 434(0), 448(33), 454(0), 460(0), 462(1), 466(11), 492(17), 494(38), 501(0), 505(0), 519(0), 554(0), 569(294), 576(0), 614(144), 621(380), 623(167), 637(3), 646(80), 1863(793), 1867(246), 1869(92), 1896(52), 2005(0), 2026(1801), 2031(54), 2040(576), 2059(838), 2091(81)

Table S33. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **28-10S**(C_s) using the B3LYP/DZP and BP86/DZP methods

B3LYP/DZP	BP86/DZP
6(0), 16(0), 22(0), 28(0), 58(0), 62(0), 66(0), 72(3), 78(1), 80(1), 88(0), 89(1), 92(1), 99(0), 104(1), 106(1), 108(0), 140(3), 172(3), 246(4), 335(0), 340(20), 365(5), 374(8), 381(0), 387(4), 389(3), 397(23), 400(3), 418(5), 421(0), 429(1), 443(14), 475(0), 480(6), 485(3), 487(0), 491(9), 493(21), 513(3), 518(7), 549(16), 549(0), 571(0), 608(56), 612(82), 617(208), 634(126), 665(148), 680(132), 1620(956), 1954(136), 2027(1337), 2044(452), 2048(1057), 2106(910), 2146(584), 2169(924), 2179(364), 2212(295)	6(0), 19(0), 24(0), 28(0), 54(0), 60(0), 62(0), 67(0), 74(1), 75(1), 82(0), 85(1), 86(4), 94(0), 100(1), 101(0), 103(0), 130(0), 162(1), 221(15), 340(0), 356(8), 367(4), 370(48), 372(0), 384(56), 386(1), 403(0), 413(1), 413(0), 436(2), 444(7), 447(14), 452(1), 470(31), 481(6), 484(7), 491(22), 496(18), 506(12), 519(5), 520(1), 520(2), 548(0), 606(67), 609(81), 612(498), 634(103), 642(112), 657(80), 1570(35), 1872(119), 1964(965), 1982(421), 1985(853), 2028(1463), 2034(751), 2048(1036), 2058(440), 2102(412)

Table S34. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **28-11S**(C_{2v}) using the B3LYP/DZP and BP86/DZP methods

B3LYP/DZP	BP86/DZP
-100(0), 22(0), 40(1), 58(0), 67(8), 67(0), 69(2), 81(1), 91(0), 92(0), 95(3), 96(3), 97(0), 103(0), 110(0), 119(0), 136(0), 175(0), 200(0), 249(10), 325(0), 344(0), 347(0), 351(3), 354(0), 358(0), 368(0), 374(8), 377(6), 422(14), 431(0), 433(15), 435(24), 447(0), 460(15), 464(2), 478(0), 498(0), 498(1), 512(11), 533(0), 542(1), 546(22), 579(194), 582(152), 608(401), 612(173), 615(89), 629(70), 637(0), 1915(1035), 1937(16), 1944(359), 1969(30), 2107(15), 2124(896), 2125(0), 2128(1366), 2148(1711), 2182(181)	-43(0), 26(1), 45(0), 52(0), 56(6), 70(2), 71(0), 78(0), 83(0), 89(0), 91(0), 92(1), 94(2), 106(0), 106(0), 124(0), 132(0), 187(0), 204(0), 245(7), 331(0), 338(0), 339(0), 341(0), 351(0), 370(1), 372(0), 383(3), 385(1), 417(2), 424(0), 429(10), 444(5), 457(1), 458(5), 472(9), 481(0), 490(2), 494(1), 513(1), 514(0), 539(11), 539(0), 559(143), 587(69), 609(121), 611(177), 614(596), 628(40), 639(0), 1854(9), 1861(327), 1862(734), 1890(0), 2018(6), 2030(903), 2035(0), 2038(1215), 2063(1388), 2090(105)

Table S35. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **28-12S**(C_s) using the B3LYP/DZP and BP86/DZP methods

B3LYP/DZP	BP86/DZP
39(0), 41(0), 53(0), 54(3), 63(0), 65(2), 69(6), 69(1), 80(2), 90(0), 92(0), 97(2), 101(0), 104(0), 108(1), 111(0), 112(0), 114(2), 120(0), 136(6), 341(0), 349(2), 358(1), 358(0), 371(0), 374(0), 380(0), 391(16), 412(1), 418(0), 420(0), 422(10), 425(3), 436(4), 451(7), 452(13), 454(11), 501(0), 502(0), 520(33), 529(4), 536(0), 537(0), 551(1), 625(78), 626(69), 632(453), 634(60), 642(91), 650(1), 1905(355), 1918(8), 2084(535), 2099(198), 2127(6), 2131(1568), 2133(960), 2137(1471), 2142(0), 2197(120)	17(0), 43(0), 43(0), 48(3), 54(0), 60(2), 64(5), 64(1), 76(2), 88(0), 93(0), 95(2), 99(0), 102(0), 104(1), 108(0), 109(1), 109(0), 118(1), 142(3), 338(0), 354(1), 354(1), 361(0), 364(0), 376(0), 379(0), 403(4), 409(22), 420(2), 422(0), 429(1), 433(0), 460(4), 466(7), 466(6), 470(0), 477(0), 520(1), 521(12), 523(5), 523(0), 535(3), 537(6), 628(59), 629(77), 633(61), 635(398), 636(98), 656(23), 1831(302), 1845(2), 1989(553), 2010(243), 2039(299), 2046(811), 2049(1186), 2051(835), 2061(0), 2114(123)

Table S3. Theoretical Cartesian coordinates (in Å) for the $Fe(CO)_5$ structure using the B3LYP/DZP and BP86/DZP methods.

	B3LYP/DZP			BP86/DZP		
Fe	0.000000	0.000016	0.000000	0.000000	0.000137	0.000000
C	0.000000	-1.815688	0.000000	0.000000	1.805247	0.000000
C	0.000000	0.909214	-1.571817	0.000000	-0.904432	-1.562241
C	0.000000	0.909214	1.571817	0.000000	-0.904432	1.562241
C	-1.822518	-0.001157	0.000000	1.805386	0.001682	0.000000
C	1.822518	-0.001157	0.000000	-1.805386	0.001682	0.000000
O	0.000000	-2.971987	0.000000	0.000000	2.975377	0.000000
O	0.000000	1.488029	-2.572795	0.000000	-1.490859	-2.574794
O	0.000000	1.488029	2.572795	0.000000	-1.490859	2.574794
O	-2.974916	-0.002221	0.000000	2.972721	0.003043	0.000000
O	2.974916	-0.002221	0.000000	-2.972721	0.003043	0.000000

Table S4. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the $Fe(CO)_5$ structure using the B3LYP/DZP and BP86/DZP methods

B3LYP/DZP	BP86/DZP
54(0), 54(0), 95(0), 95(0), 104(0), 104(0), 107(1), 365(0), 366(0), 366(0), 413(0), 439(1), 439(14), 440(13), 473(7), 483(2), 483(2), 563(0), 563(0), 617(127), 660(132), 660(132), 2067(1275), 2067(1273), 2093(0), 2094(1474), 2169(0	53(0), 54(0), 90(0), 91(0), 99(0), 99(0), 103(0), 358(0), 369(0), 369(0), 434(6), 435(6), 435(0), 460(0), 488(0), 492(1), 492(1), 547(0), 547(0), 626(127), 662(125), 662(125), 1992(1080), 1992(1077), 2008(1264), 2012(0), 2089(0)

Complete Gaussian 03 reference (Reference 25)

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