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Open Chains versus Closed Rings: Comparison of Binuclear Butadiene Iron Carbonyls with their Cyclobutadiene Analogues

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Supporting Information

Tables S1 to S4: Fe-Fe distances (Å), total energies (E, in hartree), relative energies (ΔE, in kcal/mol), and numbers of imaginary frequencies (Nimag) for the singlet $(C_4H_6)_2Fe_2(CO)_n$ (n = 5, 4, 3; 7, 6,) structures at BP86 and B3LYP.

Tables S5 to S19: Atomic coordinates of the optimized structures for the $(C_4H_6)_2Fe_2(CO)_n$ (n = 7, 6, 5, 4, 3) complexes.

Tables S20 to S23: Atomic coordinates of the optimized structures for the mononuclear $C_4H_6Fe(CO)_n$ (n = 4, 3, 2, 1) complexes.

Tables S24 to S38: Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the $(C_4H_6)_2Fe_2(CO)_n$ (n = 7, 6, 5, 4, 3)) complexes.

Tables S39 to S42: Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the mononuclear $C_4H_6Fe(CO)_n$ (n = 4, 3, 2, 1) complexes.

Table S1. Fe-Fe distances (Å), total energies (E, in hartree), relative energies (ΔE, in kcal/mol), and numbers of imaginary frequencies (Nimag) for the singlet $(C_4H_6)_2Fe_2(CO)_5$ structures at BP86 and B3LYP levels

		5S-1, C_2	**5S-2, C_s**	**5S-3, C_{2v}**	**5S-4, C_1**
BP86	Fe-Fe	2.798	2.606	2.475	2.585
	E	-3406.89146	-3406.86058	-3406.86073	-3406.85531
	ΔE	0.0	19.4	19.3	22.7
	Nimag	none	none	none	none
B3LYP	Fe-Fe	2.844	2.643	2.480	2.621
	E	-3406.40062	-3406.36419	-3406.35625	-3406.36831
	ΔE	0.0	22.9	27.9	20.3
	Nimag	none	none	none	none

Table S2. Fe-Fe distances (Å), total energies (E, in hartree), relative energies (ΔE, in kcal/mol), numbers of imaginary frequencies (Nimag), and spin expectation values $\langle S^2 \rangle$ for the $(C_4H_6)_2Fe_2(CO)_4$ structures at BP86 and B3LYP levels

		trans-4T-1, C_1	**trans-4S-2, C_i**	**cis-4T-3, C_{2v}**	**cis-4S-4, C_s**
BP86	Fe-Fe	2.424	2.545	2.430	2.424
	E	-3293.50880	-3293.50955	-3293.50729	-3293.50612
	ΔE	0	-0.5	0.9	1.7
	Nimag	none	46i	none	none
	$\langle S^2 \rangle$	2.03	0.00	2.03	0.00
B3LYP	Fe-Fe	2.592	2.599	2.452	2.476
	E	-3293.03425	-3293.02712	-3293.02930	-3293.01360
	ΔE	0	4.5	3.1	13.0
	Nimag	none	none	17i,17i	none
	$\langle S^2 \rangle$	2.14	0.00	2.17	0.00

Table S3. Fe-Fe distances (Å), total energies (E in hartree), relative energies (ΔE, in kcal/mol), numbers of imaginary frequencies (Nimag), and spin expectation values $\langle S^2 \rangle$ for the $(C_4H_6)_2Fe_2(CO)_3$ structures at BP86 and B3LYP levels .

		3S-1, C_2	**3T-2, C_s**
BP86	Fe-Fe	2.151	2.332
	E	-3180.13285	-3180.12069
	ΔE	0.0	7.6
	Nimag	none	none
	$\langle S^2 \rangle$	0.00	2.05
B3LYP	Fe-Fe	2.195	2.383
	E	-3179.65470	-3179.66256
	ΔE	0.0	-4.9
	Nimag	1(82i)	none
	$\langle S^2 \rangle$	0.00	2.26

Table S4. Fe-Fe distances (Å), total energies (E in hartree), relative energies (kcal/mol), and numbers of imaginary frequencies (Nimag) for the $(C_4H_6)_2Fe_2(CO)_n$ (n = 7, 6) structures at BP86 and B3LYP levels.

		7S-1, C_2	**7S-2, C_2**	**6S-1, C_1**	**6S-2, C_2**	**6S-3, C_1**
BP86	Fe-Fe	2.517	2.732	2.762	2.473	2.606
	E	-3633.58223	-3633.57886	-3520.23562	-3520.20667	-3520.19474
	ΔE	0.0	2.1	0.0	18.2	25.7
	Nimag	none	none	none	none	none
B3LYP	Fe-Fe	2.522	2.765	2.795	2.475	2.642
	E	-3633.07568	-3633.08475	-3519.74376	-3519.70548	-3519.70537
	ΔE	0.0	-5.7	0.0	24.0	24.1
	Nimag	none	none	none	none	none

Table S5. Optimized coordinates of the **7S-1** for the $(\eta^2\text{-}C_4H_6)_2Fe_2(CO)_7$ structure

	BP86			M06-L			B3LYP		
	x	y	z	x	y	z	x	y	z
6	0.997164	4.141519	2.461842	1.163416	3.985955	2.413635	1.070391	4.141014	2.499525
1	1.130376	4.922932	1.702804	1.359563	4.725001	1.638815	1.148056	4.947286	1.771864
1	1.457742	4.315541	3.441484	1.660466	4.132559	3.367313	1.569279	4.288875	3.455252
6	0.280673	3.015703	2.222767	0.338329	2.946709	2.215172	0.375681	3.015816	2.252470
1	0.138160	2.290971	3.036198	0.146996	2.256137	3.034529	0.288354	2.261439	3.033837
6	-0.395678	2.698065	0.944421	-0.373092	2.676069	0.961996	-0.350138	2.735897	0.994503
1	-1.419596	2.305946	1.032861	-1.374767	2.254582	1.055331	-1.352442	2.320871	1.108439
6	0.000000	3.213426	-0.300559	0.000000	3.196019	-0.266264	0.000000	3.254670	-0.238372
1	-0.737345	3.322763	-1.103439	-0.726581	3.278440	-1.068504	-0.740286	3.332888	-1.029376
1	0.886122	3.857002	-0.358969	0.880924	3.830857	-0.338652	0.888242	3.875505	-0.332722
26	0.634497	1.087124	-0.347205	0.664417	1.063144	-0.356108	0.655346	1.077063	-0.363969
6	-1.177045	0.671479	-1.036265	-1.176720	0.688364	-1.039416	-1.162110	0.684111	-1.057018
8	-2.104345	1.212517	-1.557286	-2.079019	1.268588	-1.537026	-2.077313	1.239397	-1.559794
6	1.177045	-0.671479	-1.036265	1.176720	-0.688364	-1.039416	1.162110	-0.684111	-1.057018
8	2.104345	-1.212517	-1.557286	2.079019	-1.268588	-1.537026	2.077313	-1.239397	-1.559794
8	1.543388	2.135622	-2.978266	1.543468	2.115375	-2.994452	1.514962	2.139401	-2.997579
6	1.158150	1.717382	-1.954924	1.177459	1.699518	-1.976721	1.159971	1.723559	-1.979019
26	-0.634497	-1.087124	-0.347205	-0.664417	-1.063144	-0.356108	-0.655346	-1.077063	-0.363969
6	2.244079	1.313952	0.456566	2.270549	1.284403	0.472814	2.283561	1.272191	0.436242
6	-2.244079	-1.313952	0.456566	-2.270549	-1.284403	0.472814	-2.283561	-1.272191	0.436242
8	3.304410	1.458501	0.929188	3.304668	1.428409	0.974064	3.331037	1.393608	0.905906
8	-3.304410	-1.458501	0.929188	-3.304668	-1.428409	0.974064	-3.331037	-1.393608	0.905906
6	0.395678	-2.698065	0.944421	0.373092	-2.676069	0.961996	0.350138	-2.735897	0.994503
6	0.000000	-3.213426	-0.300559	0.000000	-3.196019	-0.266264	0.000000	-3.254670	-0.238372
1	1.419596	-2.305946	1.032861	1.374767	-2.254582	1.055331	1.352442	-2.320871	1.108439
6	-0.280673	-3.015703	2.222767	-0.338329	-2.946709	2.215172	-0.375681	-3.015816	2.252470
1	-0.886122	-3.857002	-0.358969	-0.880924	-3.830857	-0.338652	-0.888242	-3.875505	-0.332722
1	0.737345	-3.322763	-1.103439	0.726581	-3.278440	-1.068504	0.740286	-3.332888	-1.029376
1	-0.138160	-2.290971	3.036198	-0.146996	-2.256137	3.034529	-0.288354	-2.261439	3.033837
6	-0.997164	-4.141519	2.461842	-1.163416	-3.985955	2.413635	-1.070391	-4.141014	2.499525
1	-1.130376	-4.922932	1.702804	-1.359563	-4.725001	1.638815	-1.148056	-4.947286	1.771864
1	-1.457742	-4.315541	3.441484	-1.660466	-4.132559	3.367313	-1.569279	-4.288875	3.455252
6	0.000000	0.000000	1.227468	0.000000	0.000000	1.230589	0.000000	0.000000	1.212764
8	0.000000	0.000000	2.420449	0.000000	0.000000	2.412557	0.000000	0.000000	2.394844
6	-1.158150	-1.717382	-1.954924	-1.177459	-1.699518	-1.976721	-1.159971	-1.723559	-1.979019
8	-1.543388	-2.135622	-2.978266	-1.543468	-2.115375	-2.994452	-1.514962	-2.139401	-2.997579

Table S6. Optimized coordinates of the **7S-2** for the $(\eta^2\text{-}C_4H_6)_2Fe_2(CO)_7$ structure

	BP86			M06-L			B3LYP		
	x	y	z	x	y	z	x	y	z
6	0.000000	4.284744	2.513212	0.000000	4.136633	2.448988	-2.244339	3.637742	2.512938
1	-0.068575	5.089298	1.769981	0.026967	4.895295	1.668108	-2.753168	4.270540	1.787500
1	0.522594	4.513818	3.449458	0.518335	4.367566	3.374524	-1.891938	4.116768	3.424242
6	-0.547726	3.061537	2.304464	-0.644711	2.970240	2.286143	-2.065481	2.318628	2.313755
1	-0.485582	2.304818	3.099536	-0.661487	2.255882	3.108400	-1.583427	1.726017	3.091914
6	-1.293019	2.654289	1.090765	-1.374030	2.567656	1.078288	-2.521410	1.561530	1.126192
1	-2.236968	2.132201	1.305054	-2.296030	2.019588	1.273372	-3.034439	0.631827	1.375400
6	-1.147409	3.266406	-0.187477	-1.228779	3.187692	-0.182396	-2.762846	2.131083	-0.141192
1	-2.007050	3.335373	-0.864775	-2.071183	3.231132	-0.867853	-3.537904	1.723156	-0.786364
1	-0.398006	4.056116	-0.322624	-0.516061	4.003159	-0.297254	-2.553907	3.186552	-0.303587
26	-0.268326	1.339223	-0.338956	-0.289356	1.315382	-0.331355	-0.998044	0.956643	-0.344340
6	-1.896247	0.704708	-0.793762	-1.894140	0.600088	-0.808169	-2.071326	-0.467397	-0.725893
8	-2.979146	0.391437	-1.111757	-2.942706	0.224957	-1.129775	-2.808829	-1.319305	-0.979765
6	1.896247	-0.704708	-0.793762	1.894140	-0.600088	-0.808169	2.071326	0.467397	-0.725893
8	2.979146	-0.391437	-1.111757	2.942706	-0.224957	-1.129775	2.808829	1.319305	-0.979765
8	0.425489	1.818878	-3.196141	0.490415	1.675403	-3.185375	-0.727207	1.626103	-3.227337
6	0.157658	1.609248	-2.075501	0.178760	1.532990	-2.077718	-0.818377	1.345507	-2.108250
26	0.268326	-1.339223	-0.338956	0.289356	-1.315382	-0.331355	0.998044	-0.956643	-0.344340
6	1.326510	2.022018	0.187499	1.286293	2.063589	0.214122	0.000000	2.422800	0.111376
6	-1.326510	-2.022018	0.187499	-1.286293	-2.063589	0.214122	0.000000	-2.422800	0.111376
8	2.347805	2.495659	0.499347	2.276440	2.567913	0.531564	0.604035	3.368178	0.373784
8	-2.347805	-2.495659	0.499347	-2.276440	-2.567913	0.531564	-0.604035	-3.368178	0.373784
6	1.293019	-2.654289	1.090765	1.374030	-2.567656	1.078288	2.521410	-1.561530	1.126192
6	1.147409	-3.266406	-0.187477	1.228779	-3.187692	-0.182396	2.762846	-2.131083	-0.141192
1	2.236968	-2.132201	1.305054	2.296030	-2.019588	1.273372	3.034439	-0.631827	1.375400
6	0.547726	-3.061537	2.304464	0.644711	-2.970240	2.286143	2.065481	-2.318628	2.313755
1	0.398006	-4.056116	-0.322624	0.516061	-4.003159	-0.297254	2.553907	-3.186552	-0.303587
1	2.007050	-3.335373	-0.864775	2.071183	-3.231132	-0.867853	3.537904	-1.723156	-0.786364
1	0.485582	-2.304818	3.099536	0.661487	-2.255882	3.108400	1.583427	-1.726017	3.091914
6	0.000000	-4.284744	2.513212	0.000000	-4.136633	2.448988	2.244339	-3.637742	2.512938
1	0.068575	-5.089298	1.769981	-0.026967	-4.895295	1.668108	2.753168	-4.270540	1.787500
1	-0.522594	-4.513818	3.449458	-0.518335	-4.367566	3.374524	1.891938	-4.116768	3.424242
6	0.000000	0.000000	1.117686	0.000000	0.000000	1.162551	0.000000	0.000000	1.109357
8	0.000000	0.000000	2.314093	0.000000	0.000000	2.345355	0.000000	0.000000	2.292166
6	-0.157658	-1.609248	-2.075501	-0.178760	-1.532990	-2.077718	0.818377	-1.345507	-2.108250
8	-0.425489	-1.818878	-3.196141	-0.490415	-1.675403	-3.185375	0.727207	-1.626103	-3.227337

Table S7. Optimized coordinates of the **6S-1** for the (η^2, η^4-C_4H_6)$_2$Fe$_2$(CO)$_6$ structure

	BP86			M06-L			B3LYP		
	x	y	z	x	y	z	x	y	z
6	4.117565	2.076889	-0.072331	3.877446	2.117984	-0.026730	4.180068	2.026879	-0.120486
1	4.745330	1.470913	0.593283	4.460820	1.570878	0.712110	4.810707	1.425851	0.532637
1	4.295720	3.158616	-0.077961	3.996580	3.196677	-0.045530	4.368012	3.098460	-0.139023
6	3.167315	1.523850	-0.866752	3.049112	1.494763	-0.879557	3.215871	1.481901	-0.885139
1	2.596389	2.171936	-1.548183	2.510050	2.083674	-1.622643	2.642658	2.126653	-1.553671
6	2.852573	0.078814	-0.956994	2.814982	0.046033	-0.933831	2.880650	0.041350	-0.956803
1	2.726518	-0.278789	-1.988907	2.716103	-0.350446	-1.944386	2.744637	-0.318478	-1.977154
6	3.146864	-0.886561	0.048221	3.122980	-0.858311	0.105248	3.166093	-0.908931	0.043986
1	3.380657	-1.919432	-0.235740	3.386414	-1.886240	-0.128106	3.372026	-1.942111	-0.227035
1	3.598660	-0.561790	0.993638	3.553401	-0.483840	1.032664	3.622172	-0.589799	0.978833
26	1.043614	-0.592945	0.060549	1.033697	-0.618259	0.080681	1.059229	-0.586113	0.075786
6	1.251544	0.705028	1.315479	1.193072	0.736261	1.308859	1.292924	0.738244	1.327145
8	1.408077	1.493434	2.162475	1.306140	1.549916	2.121725	1.448977	1.531161	2.147705
6	-1.726659	-0.261220	1.668916	-1.641817	-0.090643	1.713859	-1.803468	-0.307376	1.650950
8	-1.914448	-0.619062	2.770393	-1.789492	-0.358328	2.834171	-2.027800	-0.688401	2.722572
8	0.217794	1.136632	-2.217724	0.237565	0.937384	-2.335823	0.245442	1.160510	-2.175389
6	0.025329	0.559565	-1.184799	0.065081	0.461885	-1.264014	0.070479	0.569282	-1.165753
26	-1.565287	0.310858	-0.023380	-1.517000	0.327135	-0.034757	-1.588077	0.304916	-0.024286
6	0.857044	-1.859252	-1.197639	0.864441	-1.935591	-1.144476	0.856017	-1.889252	-1.172760
6	-1.318641	2.028145	0.325926	-1.223003	2.077315	0.141461	-1.333975	2.029458	0.380052
8	0.761537	-2.696270	-2.013242	0.762545	-2.776100	-1.936590	0.756229	-2.722533	-1.966735
8	-1.237659	3.175859	0.561827	-1.091303	3.225552	0.257409	-1.257281	3.154057	0.645169
6	-2.368335	-0.707434	-1.674479	-2.312849	-0.802194	-1.584041	-2.364309	-0.657782	-1.732437
6	-2.359063	-1.628583	-0.582460	-2.283576	-1.625109	-0.430934	-2.383485	-1.613786	-0.687419
1	-1.766652	-0.879818	-2.575255	-1.713831	-1.029144	-2.463477	-1.744406	-0.802119	-2.615293
6	-3.015954	0.554890	-1.480739	-2.960124	0.457689	-1.476196	-2.990813	0.601477	-1.518713
1	-3.256259	-1.774874	0.029294	-3.171110	-1.727829	0.188209	-3.278567	-1.764983	-0.090833
1	-1.706325	-2.505285	-0.647344	-1.640326	-2.501419	-0.435213	-1.756741	-2.496006	-0.784321
1	-2.921408	1.347938	-2.232418	-2.872733	1.190338	-2.274580	-2.865309	1.403742	-2.243126
6	-3.612825	0.776364	-0.189440	-3.539846	0.755177	-0.205242	-3.616729	0.802863	-0.248545
1	-4.196607	-0.017135	0.293280	-4.113180	-0.006879	0.319709	-4.224058	0.016168	0.194068
1	-3.950586	1.790641	0.055267	-3.887135	1.769362	-0.025022	-3.955060	1.807802	-0.002127
6	0.785089	-1.832927	1.347001	0.679649	-1.817656	1.398118	0.769174	-1.799746	1.395913
8	0.665571	-2.669852	2.158169	0.462985	-2.623613	2.203746	0.632307	-2.602486	2.217690

Table S8. Optimized coordinates of the **6S-2** for the $(\eta^2\text{-}C_4H_6)_2Fe_2(CO)_6$ structure

	BP86			M06-L			B3LYP		
	x	y	z	x	y	z	x	y	z
6	0.685814	3.656855	2.786120	0.724000	3.437365	2.774928	0.520779	3.563925	2.887680
1	0.722185	4.533087	2.126947	0.847703	4.286881	2.105565	0.570761	4.465923	2.280330
1	1.217856	3.729449	3.741620	1.261846	3.473710	3.716779	1.014083	3.593329	3.856831
6	0.003771	2.528842	2.450629	-0.056269	2.388238	2.456260	-0.131283	2.458233	2.475886
1	-0.029481	1.700579	3.174440	-0.162778	1.577035	3.176727	-0.181176	1.598836	3.147080
6	-0.775987	2.318448	1.216899	-0.837167	2.246202	1.229808	-0.865653	2.309411	1.205936
1	-1.679473	1.710203	1.353433	-1.728765	1.629978	1.322645	-1.763434	1.699399	1.277349
6	-0.685814	3.084316	0.030538	-0.724000	3.041032	0.087553	-0.714683	3.097519	0.067085
1	-1.556469	3.142649	-0.631812	-1.564076	3.107275	-0.597124	-1.530328	3.163188	-0.647348
1	0.023044	3.918875	-0.029299	-0.018630	3.869443	0.064706	0.011631	3.906913	0.049454
26	0.347173	1.186937	-0.353623	0.345482	1.175224	-0.370432	0.353902	1.185922	-0.387386
6	-1.405346	0.413050	-0.646495	-1.412618	0.404518	-0.681380	-1.391402	0.396740	-0.714381
8	-2.517082	0.777052	-0.910153	-2.512431	0.780432	-0.923797	-2.486362	0.767432	-0.983306
6	1.405346	-0.413050	-0.646495	1.412618	-0.404518	-0.681380	1.391402	-0.396740	-0.714381
8	2.517082	-0.777052	-0.910153	2.512431	-0.780432	-0.923797	2.486362	-0.767432	-0.983306
8	0.652923	2.533022	-2.946101	0.616446	2.564286	-2.941002	0.714683	2.514160	-2.980599
6	0.531278	2.014647	-1.900400	0.516772	2.029674	-1.915521	0.576142	2.011716	-1.947163
26	-0.347173	-1.186937	-0.353623	-0.345482	-1.175224	-0.370432	-0.353902	-1.185922	-0.387386
6	1.932746	1.779915	0.285126	1.926427	1.781888	0.299186	1.919068	1.777927	0.338354
6	-1.932746	-1.779915	0.285126	-1.926427	-1.781888	0.299186	-1.919068	-1.777927	0.338354
8	2.991693	2.147594	0.621801	2.964155	2.152657	0.656917	2.940371	2.134848	0.742400
8	-2.991693	-2.147594	0.621801	-2.964155	-2.152657	0.656917	-2.940371	-2.134848	0.742400
6	0.775987	-2.318448	1.216899	0.837167	-2.246202	1.229808	0.865653	-2.309411	1.205936
6	0.685814	-3.084316	0.030538	0.724000	-3.041032	0.087553	0.714683	-3.097519	0.067085
1	1.679473	-1.710203	1.353433	1.728765	-1.629978	1.322645	1.763434	-1.699399	1.277349
6	-0.003771	-2.528842	2.450629	0.056269	-2.388238	2.456260	0.131283	-2.458233	2.475886
1	-0.023044	-3.918875	-0.029299	0.018630	-3.869443	0.064706	-0.011631	-3.906913	0.049454
1	1.556469	-3.142649	-0.631812	1.564076	-3.107275	-0.597124	1.530328	-3.163188	-0.647348
1	0.029481	-1.700579	3.174440	0.162778	-1.577035	3.176727	0.181176	-1.598836	3.147080
6	-0.685814	-3.656855	2.786120	-0.724000	-3.437365	2.774928	-0.520779	-3.563925	2.887680
1	-0.722185	-4.533087	2.126947	-0.847703	-4.286881	2.105565	-0.570761	-4.465923	2.280330
1	-1.217856	-3.729449	3.741620	-1.261846	-3.473710	3.716779	-1.014083	-3.593329	3.856831
6	-0.531278	-2.014647	-1.900400	-0.516772	-2.029674	-1.915521	-0.576142	-2.011716	-1.947163
8	-0.652923	-2.533022	-2.946101	-0.616446	-2.564286	-2.941002	-0.714683	-2.514160	-2.980599

Table S9. Optimized coordinates of the **6S-3** for the $(\eta^2\text{-}C_4H_6)_2Fe_2(CO)_6$ structure

	BP86			M06-L			B3LYP		
	x	y	z	x	y	z	x	y	z
6	4.046816	-2.408262	-0.805064	3.842120	-2.405355	-0.828248	3.893779	-2.520306	-0.906669
1	4.622130	-2.222060	0.110477	4.368581	-2.274784	0.115971	4.560946	-2.322613	-0.069281
1	4.134100	-3.403660	-1.255937	3.894371	-3.387579	-1.287622	3.904080	-3.526894	-1.319674
6	3.267016	-1.452410	-1.372327	3.157335	-1.402476	-1.403429	3.094414	-1.568745	-1.425090
1	2.741006	-1.685542	-2.310614	2.665804	-1.582170	-2.360291	2.471826	-1.817227	-2.287248
6	3.089034	-0.069243	-0.877097	3.028936	-0.039327	-0.878685	3.001695	-0.163727	-0.969600
1	3.124368	0.678435	-1.683146	3.061531	0.725067	-1.655908	2.995875	0.544939	-1.798923
6	3.358140	0.386840	0.455982	3.338159	0.365464	0.450603	3.395123	0.322386	0.303429
1	3.711836	1.412286	0.617869	3.716062	1.368426	0.633558	3.789156	1.331834	0.400743
1	3.703596	-0.329586	1.211716	3.700040	-0.375067	1.162580	3.767049	-0.370938	1.055063
26	1.258303	0.346321	0.221010	1.254196	0.357501	0.263777	1.275166	0.361245	0.249923
6	1.355945	-1.325708	0.911972	1.366878	-1.336925	0.934570	1.360661	-1.304811	0.999897
8	1.475151	-2.379540	1.403249	1.504206	-2.384432	1.405247	1.470201	-2.333999	1.508345
6	-1.481096	2.089231	-0.344970	-1.438930	2.099903	-0.339772	-1.475016	2.113422	-0.440426
8	-1.663320	3.213816	-0.621281	-1.596117	3.215140	-0.612264	-1.632214	3.214897	-0.751807
8	0.312425	1.533156	2.765437	0.005160	1.409968	2.740338	0.483151	1.598669	2.810978
6	0.646100	1.045908	1.745541	0.501997	0.987671	1.769437	0.783161	1.105717	1.800536
26	-1.347894	0.374759	0.198146	-1.326804	0.365243	0.187660	-1.365521	0.401605	0.185498
6	1.410676	1.957895	-0.571541	1.429581	2.018564	-0.448785	1.435586	1.980791	-0.564301
6	-1.507741	-1.115830	1.242664	-1.481554	-1.193679	1.173334	-1.524611	-1.065892	1.307584
8	1.600054	3.003016	-1.065045	1.638326	3.069119	-0.889785	1.627886	2.997764	-1.077779
8	-1.680919	-1.982555	2.008617	-1.636741	-2.082103	1.896541	-1.682382	-1.874741	2.113596
6	-3.043226	-0.135800	-1.001284	-2.978555	-0.106466	-1.036419	-3.038579	-0.168304	-1.013094
6	-3.442948	0.410545	0.260665	-3.406457	0.398232	0.218245	-3.479783	0.436268	0.184695
1	-2.972526	0.547054	-1.860681	-2.904382	0.586950	-1.875056	-2.946113	0.456718	-1.902615
6	-3.142914	-1.558889	-1.377017	-3.026915	-1.516675	-1.420495	-3.113473	-1.612923	-1.308616
1	-3.863620	-0.254824	1.025404	-3.836520	-0.286852	0.947870	-3.901690	-0.178401	0.977684
1	-3.829521	1.436803	0.306522	-3.797919	1.410903	0.285204	-3.850015	1.459916	0.173235
1	-2.562882	-1.854813	-2.263137	-2.465221	-1.781966	-2.315781	-2.479001	-1.955763	-2.127039
6	-3.912743	-2.493430	-0.757927	-3.712878	-2.476593	-0.773365	-3.913769	-2.504087	-0.689546
1	-4.543720	-2.250985	0.106420	-4.310655	-2.259500	0.110646	-4.597750	-2.215452	0.106846
1	-3.935038	-3.529547	-1.115505	-3.696450	-3.507467	-1.112862	-3.909815	-3.552832	-0.979694
6	-0.181075	-0.209398	-1.134730	-0.132996	-0.177390	-1.164744	-0.150294	-0.223026	-1.097586
8	-0.139923	-0.640436	-2.245556	-0.093306	-0.567318	-2.277471	-0.150229	-0.683584	-2.182997

Table S10. Optimized coordinates of the **5S-1** for the $(\eta^4\text{-}C_4H_6)_2Fe_2(CO)_5$ structure

	BP86			M06-L			B3LYP		
	x	y	z	x	y	z	x	y	z
6	0.000000	3.494933	-0.028797	0.000000	3.441081	-0.097434	0.000000	3.513622	-0.010193
1	-0.530619	3.814382	-0.934483	-0.545783	3.729003	-0.994442	-0.532390	3.842343	-0.900330
1	0.905230	4.075518	0.186598	0.887918	4.039904	0.089163	0.895607	4.094572	0.203701
6	-0.732199	2.946315	1.083143	-0.711404	2.922889	1.028164	-0.720062	2.965729	1.097709
1	-0.440799	3.118654	2.126330	-0.420658	3.120869	2.056771	-0.419178	3.130888	2.130326
6	-1.754463	1.994793	0.765383	-1.716115	1.961364	0.737946	-1.750414	2.031064	0.796203
1	-2.239449	1.427461	1.569260	-2.183840	1.405884	1.548302	-2.214593	1.471020	1.605912
6	-1.956345	1.657042	-0.607946	-1.899319	1.588714	-0.616962	-1.987586	1.686364	-0.556917
1	-1.947372	2.432627	-1.381810	-1.896830	2.344009	-1.398598	-1.977506	2.444802	-1.334571
1	-2.577244	0.784835	-0.839185	-2.516776	0.720005	-0.831840	-2.630273	0.834575	-0.764048
26	0.106805	1.394829	-0.001076	0.132263	1.375160	-0.006053	0.101232	1.418398	-0.005392
6	1.764626	1.542831	0.578792	1.784994	1.516706	0.627396	1.787995	1.571414	0.554151
8	2.875380	1.686051	0.940842	2.873047	1.630031	1.023992	2.886443	1.722065	0.892967
6	0.517389	1.321200	-1.742785	0.611168	1.246036	-1.736633	0.481350	1.352776	-1.760576
8	0.803272	1.379055	-2.879487	0.935672	1.246407	-2.851456	0.735752	1.416612	-2.889122
8	0.000000	0.000000	2.588972	0.000000	0.000000	2.601258	0.000000	0.000000	2.570347
6	0.000000	0.000000	1.389260	0.000000	0.000000	1.415949	0.000000	0.000000	1.388267
26	-0.106805	-1.394829	-0.001076	-0.132263	-1.375160	-0.006053	-0.101232	-1.418398	-0.005392
6	-0.517389	-1.321200	-1.742785	-0.611168	-1.246036	-1.736633	-0.481350	-1.352776	-1.760576
6	-1.764626	-1.542831	0.578792	-1.784994	-1.516706	0.627396	-1.787995	-1.571414	0.554151
8	-0.803272	-1.379055	-2.879487	-0.935672	-1.246407	-2.851456	-0.735752	-1.416612	-2.889122
8	-2.875380	-1.686051	0.940842	-2.873047	-1.630031	1.023992	-2.886443	-1.722065	0.892967
6	0.732199	-2.946315	1.083143	0.711404	-2.922889	1.028164	0.720062	-2.965729	1.097709
6	0.000000	-3.494933	-0.028797	0.000000	-3.441081	-0.097434	0.000000	-3.513622	-0.010193
1	0.440799	-3.118654	2.126330	0.420658	-3.120869	2.056771	0.419178	-3.130888	2.130326
6	1.754463	-1.994793	0.765383	1.716115	-1.961364	0.737946	1.750414	-2.031064	0.796203
1	0.530619	-3.814382	-0.934483	0.545783	-3.729003	-0.994442	0.532390	-3.842343	-0.900330
1	-0.905230	-4.075518	0.186598	-0.887918	-4.039904	0.089163	-0.895607	-4.094572	0.203701
1	2.239449	-1.427461	1.569260	2.183840	-1.405884	1.548302	2.214593	-1.471020	1.605912
6	1.956345	-1.657042	-0.607946	1.899319	-1.588714	-0.616962	1.987586	-1.686364	-0.556917
1	1.947372	-2.432627	-1.381810	1.896830	-2.344009	-1.398598	1.977506	-2.444802	-1.334571
1	2.577244	-0.784835	-0.839185	2.516776	-0.720005	-0.831840	2.630273	-0.834575	-0.764048

Table S11. Optimized coordinates of the **5S-2** for the $(\eta^4\text{-}C_4H_6)_2Fe_2(CO)_5$ structure

	BP86			M06-L			B3LYP		
	x	y	z	x	y	z	x	y	z
6	0.779571	2.761081	1.486524	0.745284	2.767750	1.461959	0.754442	2.858288	1.506374
1	1.813553	2.936983	1.171513	1.760204	2.943117	1.117316	1.782807	2.988040	1.184595
1	0.632645	2.560564	2.553830	0.630817	2.574984	2.524166	0.603640	2.685043	2.569039
6	-0.304607	3.238808	0.729423	-0.347184	3.208022	0.724134	-0.316825	3.267914	0.727817
1	-1.256509	3.449130	1.234197	-1.296026	3.379827	1.226568	-1.272226	3.453230	1.216826
6	-0.304607	3.238808	-0.729423	-0.347184	3.208022	-0.724134	-0.316825	3.267914	-0.727817
1	-1.256509	3.449130	-1.234197	-1.296026	3.379827	-1.226568	-1.272226	3.453230	-1.216826
6	0.779571	2.761081	-1.486524	0.745284	2.767750	-1.461959	0.754442	2.858288	-1.506374
1	1.813553	2.936983	-1.171513	1.760204	2.943117	-1.117316	1.782807	2.988040	-1.184595
1	0.632645	2.560564	-2.553830	0.630817	2.574984	-2.524166	0.603640	2.685043	-2.569039
26	-0.023939	1.268581	0.000000	-0.027982	1.256111	0.000000	-0.022520	1.262416	0.000000
6	-1.839125	1.162576	0.000000	-1.849310	1.104048	0.000000	-1.857433	1.172364	0.000000
8	-3.003825	1.039207	0.000000	-2.995779	0.931435	0.000000	-3.008080	1.073025	0.000000
6	-0.268802	-0.227074	1.463335	-0.239671	-0.226729	1.482897	-0.267922	-0.256634	1.452467
8	-0.441352	-0.090344	2.640311	-0.367544	-0.086366	2.652652	-0.417254	-0.094088	2.615395
8	2.897993	0.685705	0.000000	2.891495	0.644112	0.000000	2.908311	0.725100	0.000000
6	1.735923	0.874749	0.000000	1.744697	0.845195	0.000000	1.764173	0.917682	0.000000
26	-0.006326	-1.337013	0.000000	-0.009854	-1.327282	0.000000	-0.017752	-1.380203	0.000000
6	-1.631804	-2.039779	0.000000	-1.651212	-2.012206	0.000000	-1.645776	-2.086817	0.000000
6	-0.268802	-0.227074	-1.463335	-0.239671	-0.226729	-1.482897	-0.267922	-0.256634	-1.452467
8	-2.676079	-2.579756	0.000000	-2.689567	-2.536381	0.000000	-2.678240	-2.618166	0.000000
8	-0.441352	-0.090344	-2.640311	-0.367544	-0.086366	-2.652652	-0.417254	-0.094088	-2.615395
6	1.757990	-2.210147	0.718921	1.750235	-2.146736	0.712497	1.762485	-2.226148	0.713516
6	0.665809	-2.861304	1.370981	0.670889	-2.815607	1.347303	0.688470	-2.878606	1.374666
1	2.490931	-1.612341	1.274359	2.459915	-1.534922	1.265414	2.482752	-1.619762	1.259339
6	1.757990	-2.210147	-0.718921	1.750235	-2.146736	-0.712497	1.762485	-2.226148	-0.713516
1	0.276433	-3.816609	1.001164	0.321087	-3.775093	0.973880	0.308273	-3.831602	1.016230
1	0.520111	-2.686807	2.443760	0.521786	-2.659744	2.412828	0.561561	-2.709427	2.442051
1	2.490931	-1.612341	-1.274359	2.459915	-1.534922	-1.265414	2.482752	-1.619762	-1.259339
6	0.665809	-2.861304	-1.370981	0.670889	-2.815607	-1.347303	0.688470	-2.878606	-1.374666
1	0.276433	-3.816609	-1.001164	0.321087	-3.775093	-0.973880	0.308273	-3.831602	-1.016230
1	0.520111	-2.686807	-2.443760	0.521786	-2.659744	-2.412828	0.561561	-2.709427	-2.442051

Table S12. Optimized coordinates of the **5S-3** for the $(\eta^4\text{-}C_4H_6)_2Fe_2(CO)_5$ structure

	BP86			M06-L			B3LYP		
	x	Y	z	x	y	z	x	y	z
6	-1.454740	2.325221	1.312514	-1.423552	2.299526	1.310237	-1.463782	2.337803	1.328457
1	-1.090699	2.079585	2.314023	-1.039846	2.066931	2.298924	-1.108422	2.049041	2.310666
1	-2.532008	2.208451	1.147831	-2.493631	2.174704	1.172578	-2.533306	2.240251	1.156246
6	-0.729009	3.167821	0.452226	-0.723205	3.139805	0.446149	-0.725979	3.171722	0.493581
1	-1.243850	3.719360	-0.344915	-1.239537	3.672339	-0.348641	-1.229338	3.732576	-0.292543
6	0.729009	3.167821	0.452226	0.723205	3.139805	0.446149	0.725979	3.171722	0.493581
1	1.243850	3.719360	-0.344915	1.239537	3.672339	-0.348641	1.229338	3.732576	-0.292543
6	1.454740	2.325221	1.312514	1.423552	2.299526	1.310237	1.463782	2.337803	1.328457
1	1.090699	2.079585	2.314023	1.039846	2.066931	2.298924	1.108422	2.049041	2.310666
1	2.532008	2.208451	1.147831	2.493631	2.174704	1.172578	2.533306	2.240251	1.156246
26	0.000000	1.237566	-0.000800	0.000000	1.233464	-0.001447	0.000000	1.240042	-0.011232
6	0.000000	1.719969	-1.736188	0.000000	1.693366	-1.750559	0.000000	1.776749	-1.742684
8	0.000000	2.008847	-2.873646	0.000000	1.949788	-2.883384	0.000000	2.102646	-2.853411
6	-1.426119	0.000000	-0.491917	-1.436448	0.000000	-0.486082	-1.409386	0.000000	-0.534495
8	-2.562743	0.000000	-0.865385	-2.568036	0.000000	-0.836097	-2.534990	0.000000	-0.902056
8	0.000000	0.000000	2.783493	0.000000	0.000000	2.778101	0.000000	0.000000	2.763577
6	0.000000	0.000000	1.585650	0.000000	0.000000	1.592852	0.000000	0.000000	1.577112
26	0.000000	-1.237566	-0.000800	0.000000	-1.233464	-0.001447	0.000000	-1.240042	-0.011232
6	0.000000	-1.719969	-1.736188	0.000000	-1.693366	-1.750559	0.000000	-1.776749	-1.742684
6	1.426119	0.000000	-0.491917	1.436448	0.000000	-0.486082	1.409386	0.000000	-0.534495
8	0.000000	-2.008847	-2.873646	0.000000	-1.949788	-2.883384	0.000000	-2.102646	-2.853411
8	2.562743	0.000000	-0.865385	2.568036	0.000000	-0.836097	2.534990	0.000000	-0.902056
6	0.729009	-3.167821	0.452226	0.723205	-3.139805	0.446149	0.725979	-3.171722	0.493581
6	1.454740	-2.325221	1.312514	1.423552	-2.299526	1.310237	1.463782	-2.337803	1.328457
1	1.243850	-3.719360	-0.344915	1.239537	-3.672339	-0.348641	1.229338	-3.732576	-0.292543
6	-0.729009	-3.167821	0.452226	-0.723205	-3.139805	0.446149	-0.725979	-3.171722	0.493581
1	1.090699	-2.079585	2.314023	1.039846	-2.066931	2.298924	1.108422	-2.049041	2.310666
1	2.532008	-2.208451	1.147831	2.493631	-2.174704	1.172578	2.533306	-2.240251	1.156246
1	-1.243850	-3.719360	-0.344915	-1.239537	-3.672339	-0.348641	-1.229338	-3.732576	-0.292543
6	-1.454740	-2.325221	1.312514	-1.423552	-2.299526	1.310237	-1.463782	-2.337803	1.328457
1	-1.090699	-2.079585	2.314023	-1.039846	-2.066931	2.298924	-1.108422	-2.049041	2.310666
1	-2.532008	-2.208451	1.147831	-2.493631	-2.174704	1.172578	-2.533306	-2.240251	1.156246

Table S13. Optimized coordinates of the **5S-4** for the $(\eta^4\text{-}C_4H_6)_2Fe_2(CO)_5$ structure

	BP86			M06-L			B3LYP		
	x	y	z	x	y	z	x	y	z
6	-4.271965	-1.399417	-0.800300	-4.066193	-1.453799	-0.811189	-4.291213	-1.389677	-0.832246
1	-4.742891	-1.242882	0.178343	-4.473042	-1.377624	0.196191	-4.794117	-1.227005	0.119540
1	-4.595074	-2.275598	-1.374666	-4.348272	-2.328074	-1.389202	-4.593931	-2.262325	-1.407540
6	-3.338280	-0.545207	-1.297334	-3.253746	-0.511008	-1.322693	-3.345796	-0.549073	-1.297371
1	-2.930816	-0.729782	-2.301873	-2.895084	-0.623121	-2.345677	-2.905656	-0.741152	-2.277064
6	-2.839871	0.670422	-0.625771	-2.807136	0.693821	-0.624610	-2.862485	0.668907	-0.615811
1	-2.689790	1.522010	-1.305543	-2.666421	1.560641	-1.271504	-2.718074	1.515214	-1.289184
6	-2.942186	0.937154	0.776941	-2.934778	0.910499	0.771971	-2.986573	0.930025	0.767245
1	-3.041468	1.973885	1.123796	-3.046074	1.924795	1.149733	-3.073402	1.955831	1.121497
1	-3.429570	0.200820	1.429053	-3.430615	0.156507	1.382893	-3.458807	0.194884	1.416445
26	-0.949089	0.451635	0.363922	-0.955929	0.446683	0.359897	-0.971993	0.449233	0.361525
6	-1.368560	-1.225437	0.972536	-1.365026	-1.275512	0.921726	-1.386955	-1.258936	0.969748
8	-1.650332	-2.243023	1.471219	-1.620127	-2.300602	1.387551	-1.649991	-2.265653	1.461958
6	1.032727	0.274163	1.579786	1.006179	0.276439	1.604089	1.097904	0.269826	1.612745
8	0.850035	0.584352	2.710059	0.730593	0.606200	2.697019	0.887724	0.583126	2.720118
8	-0.319856	-0.064226	-2.424578	-0.300943	0.034608	-2.436873	-0.322038	-0.046115	-2.398018
6	-0.080003	-0.000772	-1.255168	-0.086991	0.041155	-1.274168	-0.094432	0.011981	-1.241652
26	1.512490	-0.216831	-0.054311	1.502610	-0.212885	-0.027359	1.533940	-0.210104	-0.032974
6	-0.695439	2.225250	0.190311	-0.684633	2.234084	0.212225	-0.708065	2.248749	0.196934
6	1.304686	-1.983527	-0.056107	1.280883	-1.989970	-0.036610	1.311471	-1.994176	-0.039260
8	-0.629288	3.395232	0.146410	-0.603126	3.389652	0.179321	-0.627192	3.400174	0.161450
8	1.252436	-3.158300	-0.054257	1.218193	-3.151317	-0.036638	1.256246	-3.151912	-0.037930
6	2.730191	0.735397	-1.470844	2.678463	0.726433	-1.454981	2.707970	0.775273	-1.471184
6	2.294051	1.743749	-0.558089	2.254305	1.714863	-0.527181	2.327218	1.748919	-0.510216
1	2.429051	0.750919	-2.525814	2.353671	0.742348	-2.492569	2.365724	0.837900	-2.502735
6	3.381867	-0.417510	-0.930148	3.337110	-0.415063	-0.935142	3.354741	-0.403426	-1.015373
1	2.920034	2.043421	0.290209	2.907328	2.017021	0.288802	2.991286	2.005473	0.311149
1	1.649662	2.537702	-0.950928	1.613287	2.508251	-0.903623	1.700824	2.569279	-0.851117
1	3.616392	-1.274179	-1.574468	3.554246	-1.266142	-1.576092	3.541616	-1.224736	-1.705085
6	3.533045	-0.468600	0.501533	3.501024	-0.460710	0.484100	3.567070	-0.528548	0.395842
1	3.855203	0.421107	1.055905	3.834426	0.427517	1.017185	3.935347	0.318284	0.970688
1	3.845293	-1.418607	0.951198	3.829334	-1.396567	0.929611	3.895435	-1.495035	0.774036

Table S14. Optimized coordinates of the **4T-1** for the $(\eta^4\text{-}C_4H_6)_2Fe_2(CO)_4$ structure

	BP86			M06-L			B3LYP		
	x	y	z	x	y	z	x	y	z
6	0.067168	-0.106091	1.501564	-0.115914	-0.231517	-1.508446	-0.008690	0.315903	1.368572
26	1.219001	0.018787	0.001835	-1.225177	0.007492	-0.011890	1.279090	0.042232	-0.080982
26	-1.204269	-0.034956	-0.016512	1.192106	-0.064570	0.052973	-1.309091	-0.101278	-0.044004
6	2.838020	-0.350561	-1.377108	-2.818682	-0.233319	1.404920	3.043846	-0.729819	-1.334965
6	-2.768236	0.457709	-1.416889	2.732945	0.565668	1.379658	-2.861556	0.139370	-1.478230
6	2.447514	-1.524895	-0.660880	-2.516051	-1.429075	0.715110	2.590016	-1.617676	-0.360642
6	-2.145315	1.622336	-0.865638	2.014907	1.661386	0.833418	-2.101956	1.342360	-1.330104
6	2.458199	-1.463047	0.774620	-2.548966	-1.405064	-0.713021	2.545115	-1.264011	1.043634
6	-2.115914	1.751012	0.564543	1.939892	1.755361	-0.586300	-1.987914	1.880025	-0.019285
6	2.857443	-0.228273	1.378562	-2.886008	-0.180875	-1.342074	2.987749	-0.025872	1.505801
6	-2.714455	0.709309	1.339080	2.587895	0.749833	-1.344010	-2.641168	1.183155	1.037421
6	-0.090082	-0.380230	-1.481527	0.181049	-0.480194	1.528378	-0.434737	-0.978088	-1.331555
8	0.005013	-0.642723	-2.642139	-0.012707	-0.772874	2.652130	-0.109414	-1.586185	-2.277315
6	1.611489	1.757404	-0.094193	-1.446536	1.802517	0.032408	1.717598	1.803419	-0.407230
6	-1.953164	-1.640863	0.180817	2.017960	-1.644439	-0.200924	-2.040975	-1.490731	0.794935
8	1.898349	2.896862	-0.142620	-1.566459	2.959497	0.042144	1.917530	2.929079	-0.604725
8	-2.478165	-2.684765	0.302122	2.598349	-2.637851	-0.358741	-2.560987	-2.382286	1.323813
1	3.698302	0.243037	-1.048933	-3.628286	0.409095	1.069348	3.796412	0.023794	-1.126076
1	2.616680	-0.300165	-2.449428	-2.589297	-0.176784	2.465723	2.884975	-0.969788	-2.383771
1	1.987473	-2.380160	-1.171725	-2.080413	-2.281296	1.231973	2.091348	-2.535966	-0.667874
1	2.014432	-2.274051	1.365849	-2.154619	-2.244415	-1.280980	2.013974	-1.932723	1.720042
1	3.711636	0.333613	0.984577	-3.681062	0.441713	-0.939889	3.767550	0.531480	0.996072
1	2.661783	-0.086866	2.447680	-2.720026	-0.085327	-2.411682	2.763730	0.276882	2.525318
8	0.013867	-0.172443	2.693133	-0.024653	-0.375237	-2.676819	0.014430	0.595121	2.515830
1	-1.551553	2.302536	-1.489302	1.390996	2.301817	1.453107	-1.512955	1.755897	-2.146852
1	-3.710368	0.080891	-1.003144	3.677217	0.254505	0.939652	-3.810173	0.020706	-0.960654
1	-2.608993	0.236613	-2.478615	2.640637	0.367174	2.443932	-2.810141	-0.377629	-2.434658
1	-1.494206	2.524917	1.031835	1.251725	2.460547	-1.047484	-1.297241	2.698056	0.177936
1	-3.671686	0.269781	1.036826	3.571011	0.390724	-1.050172	-3.645476	0.791920	0.898218
1	-2.505050	0.671949	2.414308	2.370775	0.676304	-2.406100	-2.398404	1.458534	2.060989

Table S15. Optimized coordinates of the **4S-2** for the $(\eta^4\text{-}C_4H_6)_2Fe_2(CO)_4$ structure

	BP86			M06-L			B3LYP		
	x	y	z	x	y	z	x	y	z
6	-0.892762	-0.761882	-1.063768	-0.925504	-0.799326	-1.089011	-0.938253	-0.878208	-1.057309
26	-1.162472	0.019393	0.517106	-1.173690	-0.002699	0.486351	-1.208943	-0.027782	0.475393
26	1.162472	-0.019393	-0.517106	1.173690	0.002699	-0.486351	1.208943	0.027782	-0.475393
6	-3.119585	-0.703615	0.554872	-3.103781	-0.699397	0.559385	-3.175102	-0.674156	0.584307
6	0.867648	1.709243	-1.865800	0.862710	1.692871	-1.785701	0.918257	1.754798	-1.798685
6	-2.748804	-0.122929	1.819957	-2.720854	-0.116972	1.808414	-2.748735	-0.126947	1.840094
6	1.593959	0.659498	-2.479275	1.563231	0.652869	-2.430394	1.593222	0.696912	-2.442856
6	-1.593959	-0.659498	2.479275	-1.563231	-0.652869	2.430394	-1.593222	-0.696912	2.442856
6	2.748804	0.122929	-1.819957	2.720854	0.116972	-1.808414	2.748735	0.126947	-1.840094
6	-0.867648	-1.709243	1.865800	-0.862710	-1.692871	1.785701	-0.918257	-1.754798	1.798685
6	3.119585	0.703615	-0.554872	3.103781	0.699397	-0.559385	3.175102	0.674156	-0.584307
6	0.892762	0.761882	1.063768	0.925504	0.799326	1.089011	0.938253	0.878208	1.057309
8	1.122694	1.315958	2.089076	1.107172	1.356020	2.105496	1.089533	1.486501	2.044278
6	-1.692040	1.586193	-0.083095	-1.695408	1.579439	-0.125338	-1.764007	1.551246	-0.162340
6	1.692040	-1.586193	0.083095	1.695408	-1.579439	0.125338	1.764007	-1.551246	0.162340
8	-2.111535	2.621056	-0.460377	-2.097488	2.603307	-0.508221	-2.199359	2.551132	-0.555531
8	2.111535	-2.621056	0.460377	2.097488	-2.603307	0.508221	2.199359	-2.551132	0.555531
1	-3.094376	-1.791862	0.412155	-3.093936	-1.782451	0.440807	-3.204641	-1.752827	0.437561
1	-3.884984	-0.191640	-0.040459	-3.874850	-0.200424	-0.022319	-3.950161	-0.138776	0.038232
1	-3.239205	0.775587	2.215094	-3.191050	0.779547	2.204602	-3.194372	0.771897	2.262600
1	-1.162951	-0.111428	3.327838	-1.106694	-0.110196	3.256494	-1.121243	-0.172430	3.273788
1	-1.370809	-2.501358	1.300640	-1.393377	-2.489787	1.269837	-1.462684	-2.539136	1.279467
1	0.111359	-1.976780	2.276673	0.113311	-1.969555	2.173781	0.053488	-2.050575	2.184310
8	-1.122694	-1.315958	-2.089076	-1.107172	-1.356020	-2.105496	-1.089533	-1.486501	-2.044278
1	1.162951	0.111428	-3.327838	1.106694	0.110196	-3.256494	1.121243	0.172430	-3.273788
1	1.370809	2.501358	-1.300640	1.393377	2.489787	-1.269837	1.462684	2.539136	-1.279467
1	-0.111359	1.976780	-2.276673	-0.113311	1.969555	-2.173781	-0.053488	2.050575	-2.184310
1	3.239205	-0.775587	-2.215094	3.191050	-0.779547	-2.204602	3.194372	-0.771897	-2.262600
1	3.094376	1.791862	-0.412155	3.093936	1.782451	-0.440807	3.204641	1.752827	-0.437561
1	3.884984	0.191640	0.040459	3.874850	0.200424	0.022319	3.950161	0.138776	-0.038232

Table S16. Optimized coordinates of the **4T-3** for the $(\eta^4\text{-}C_4H_6)_2Fe_2(CO)_4$ structure

	BP86			M06-L			B3LYP		
	x	y	z	x	y	z	x	y	z
6	-1.491877	0.000000	-0.203232	-1.496262	0.000000	-0.352403	-1.501942	0.000000	-0.229509
26	0.000000	1.214809	-0.010718	0.000000	1.201599	-0.016078	0.000000	1.225906	-0.010170
26	0.000000	-1.214809	-0.010718	0.000000	-1.201599	-0.016078	0.000000	-1.225906	-0.010170
6	-1.380243	2.834229	-0.374284	-1.366603	2.817776	-0.290263	-1.395269	2.857354	-0.382751
6	1.380243	-2.834229	-0.374284	1.366603	-2.817776	-0.290263	1.395269	-2.857354	-0.382751
6	-0.718250	2.401675	-1.565930	-0.712939	2.453883	-1.493535	-0.714885	2.445610	-1.553963
6	0.718250	-2.401675	-1.565930	0.712939	-2.453883	-1.493535	0.714885	-2.445610	-1.553963
6	0.718250	2.401675	-1.565930	0.712939	2.453883	-1.493535	0.714885	2.445610	-1.553963
6	-0.718250	-2.401675	-1.565930	-0.712939	-2.453883	-1.493535	-0.714885	-2.445610	-1.553963
6	1.380243	2.834229	-0.374284	1.366603	2.817776	-0.290263	1.395269	2.857354	-0.382751
6	-1.380243	-2.834229	-0.374284	-1.366603	-2.817776	-0.290263	-1.395269	-2.857354	-0.382751
6	1.491877	0.000000	-0.203232	1.496262	0.000000	-0.352403	1.501942	0.000000	-0.229509
8	2.675474	0.000000	-0.373939	2.641356	0.000000	-0.645146	2.662926	0.000000	-0.427781
6	0.000000	1.727274	1.705328	0.000000	1.598217	1.755817	0.000000	1.703739	1.742134
6	0.000000	-1.727274	1.705328	0.000000	-1.598217	1.755817	0.000000	-1.703739	1.742134
8	0.000000	2.115465	2.813013	0.000000	1.895443	2.877329	0.000000	2.030514	2.852738
8	0.000000	-2.115465	2.813013	0.000000	-1.895443	2.877329	0.000000	-2.030514	2.852738
1	-1.020265	3.710879	0.175739	-1.001139	3.654234	0.300076	-1.038193	3.701700	0.200060
1	-2.451925	2.628775	-0.272352	-2.431956	2.621809	-0.202970	-2.462518	2.662690	-0.309156
1	-1.270424	1.924603	-2.385361	-1.259418	2.013734	-2.324278	-1.251835	1.975669	-2.376113
1	1.270424	1.924603	-2.385361	1.259418	2.013734	-2.324278	1.251835	1.975669	-2.376113
1	1.020265	3.710879	0.175739	1.001139	3.654234	0.300076	1.038193	3.701700	0.200060
1	2.451925	2.628775	-0.272352	2.431956	2.621809	-0.202970	2.462518	2.662690	-0.309156
8	-2.675474	0.000000	-0.373939	-2.641356	0.000000	-0.645146	-2.662926	0.000000	-0.427781
1	1.270424	-1.924603	-2.385361	1.259418	-2.013734	-2.324278	1.251835	-1.975669	-2.376113
1	1.020265	-3.710879	0.175739	1.001139	-3.654234	0.300076	1.038193	-3.701700	0.200060
1	2.451925	-2.628775	-0.272352	2.431956	-2.621809	-0.202970	2.462518	-2.662690	-0.309156
1	-1.270424	-1.924603	-2.385361	-1.259418	-2.013734	-2.324278	-1.251835	-1.975669	-2.376113
1	-1.020265	-3.710879	0.175739	-1.001139	-3.654234	0.300076	-1.038193	-3.701700	0.200060
1	-2.451925	-2.628775	-0.272352	-2.431956	-2.621809	-0.202970	-2.462518	-2.662690	-0.309156

Table S17. Optimized coordinates of the **4S-4** for the $(\eta^4\text{-}C_4H_6)_2Fe_2(CO)_4$ structure

	BP86			M06-L			B3LYP		
	x	y	z	x	y	z	x	y	z
6	-1.048801	1.018534	0.000000	-0.999229	1.093482	0.000000	-1.028081	1.051976	0.000000
26	0.046485	0.026527	1.212217	0.053889	0.005560	1.212941	0.036763	-0.007186	1.238211
26	0.046485	0.026527	-1.212217	0.053889	0.005560	-1.212941	0.036763	-0.007186	-1.238211
6	-0.657043	1.218443	2.883188	-0.525182	1.229931	2.834032	-0.434516	1.351427	2.829747
6	1.234522	-0.862078	-2.835482	1.084887	-0.972303	-2.781384	1.075458	-0.980270	-2.844525
6	0.681458	1.511382	2.489017	0.829912	1.416940	2.463746	0.928072	1.424562	2.449779
6	1.656895	0.447051	-2.482033	1.679649	0.272011	-2.456025	1.712753	0.231857	-2.472058
6	1.656895	0.447051	2.482033	1.679649	0.272011	2.456025	1.712753	0.231857	2.472058
6	0.681458	1.511382	-2.489017	0.829912	1.416940	-2.463746	0.928072	1.424562	-2.449779
6	1.234522	-0.862078	2.835482	1.084887	-0.972303	2.781384	1.075458	-0.980270	2.844525
6	-0.657043	1.218443	-2.883188	-0.525182	1.229931	-2.834032	-0.434516	1.351427	-2.829747
6	1.298168	-0.774896	0.000000	1.365851	-0.732177	0.000000	1.313378	-0.785505	0.000000
8	2.309194	-1.427252	0.000000	2.391720	-1.332806	0.000000	2.311711	-1.420861	0.000000
6	-1.277990	-1.011361	1.756252	-1.412173	-0.912702	1.651330	-1.437503	-0.889374	1.722914
6	-1.277990	-1.011361	-1.756252	-1.412173	-0.912702	-1.651330	-1.437503	-0.889374	-1.722914
8	-2.134728	-1.727857	2.122073	-2.331547	-1.537906	1.989095	-2.361332	-1.485861	2.089281
8	-2.134728	-1.727857	-2.122073	-2.331547	-1.537906	-1.989095	-2.361332	-1.485861	-2.089281
1	-0.855436	0.555350	3.733177	-0.775773	0.592761	3.679004	-0.736730	0.755988	3.687268
1	-1.437860	1.956941	2.669473	-1.231934	2.031024	2.636383	-1.080089	2.197559	2.607039
1	0.929847	2.474541	2.024058	1.168873	2.347367	2.012742	1.328159	2.317120	1.969706
1	2.637715	0.614745	2.020776	2.676308	0.331002	2.027195	2.710924	0.233787	2.040695
1	0.537187	-1.027885	3.663902	0.399352	-1.051567	3.621680	0.394044	-1.012671	3.690601
1	1.889472	-1.705418	2.588876	1.637286	-1.879710	2.549984	1.594127	-1.914026	2.636802
8	-1.910914	1.855588	0.000000	-1.808039	1.957962	0.000000	-1.860986	1.887697	0.000000
1	2.637715	0.614745	-2.020776	2.676308	0.331002	-2.027195	2.710924	0.233787	-2.040695
1	0.537187	-1.027885	-3.663902	0.399352	-1.051567	-3.621680	0.394044	-1.012671	-3.690601
1	1.889472	-1.705418	-2.588876	1.637286	-1.879710	-2.549984	1.594127	-1.914026	-2.636802
1	0.929847	2.474541	-2.024058	1.168873	2.347367	-2.012742	1.328159	2.317120	-1.969706
1	-0.855436	0.555350	-3.733177	-0.775773	0.592761	-3.679004	-0.736730	0.755988	-3.687268
1	-1.437860	1.956941	-2.669473	-1.231934	2.031024	-2.636383	-1.080089	2.197559	-2.607039

Table S18. Optimized coordinates of the **3S-1** for the $(\eta^4\text{-}C_4H_6)_2Fe_2(CO)_3$ structure

	BP86			M06-L			B3LYP		
	x	y	z	x	y	z	x	y	z
6	0.000000	0.000000	1.627224	0.000000	0.000000	1.633119	0.000000	0.000000	1.632844
26	0.000000	1.075470	-0.015019	0.000000	1.081902	-0.020665	0.000000	1.097311	-0.025661
26	0.000000	-1.075470	-0.015019	0.000000	-1.081902	-0.020665	0.000000	-1.097311	-0.025661
6	0.942103	2.698950	0.915255	0.901343	2.691782	0.903110	0.802287	2.764231	0.948152
6	-0.942103	-2.698950	0.915255	-0.901343	-2.691782	0.903110	-0.802287	-2.764231	0.948152
6	-0.489436	2.820341	0.955402	-0.520066	2.775667	0.973299	-0.625658	2.782566	0.995113
6	0.489436	-2.820341	0.955402	0.520066	-2.775667	0.973299	0.625658	-2.782566	0.995113
6	-1.171901	2.731784	-0.302178	-1.215005	2.682535	-0.262358	-1.324272	2.659022	-0.237099
6	1.171901	-2.731784	-0.302178	1.215005	-2.682535	-0.262358	1.324272	-2.659022	-0.237099
6	-0.343972	2.541292	-1.459430	-0.404116	2.526678	-1.422655	-0.544406	2.539191	-1.424985
6	0.343972	-2.541292	-1.459430	0.404116	-2.526678	-1.422655	0.544406	-2.539191	-1.424985
6	1.467144	0.382834	-0.812759	1.466683	0.425790	-0.841546	1.486701	0.654279	-0.880340
8	2.498713	0.295462	-1.391176	2.476655	0.310475	-1.425145	2.494544	0.582088	-1.463403
6	-1.467144	-0.382834	-0.812759	-1.466683	-0.425790	-0.841546	-1.486701	-0.654279	-0.880340
8	-2.498713	-0.295462	-1.391176	-2.476655	-0.310475	-1.425145	-2.494544	-0.582088	-1.463403
1	1.531996	3.245297	0.169321	1.452063	3.266301	0.161059	1.339721	3.361656	0.214813
1	1.466226	2.504007	1.859434	1.444611	2.514389	1.829245	1.335038	2.623219	1.887666
1	-1.051966	2.786373	1.897673	-1.059116	2.705586	1.916088	-1.167086	2.692912	1.936117
1	-2.263694	2.620793	-0.338013	-2.292645	2.530536	-0.280675	-2.394496	2.454076	-0.234402
1	0.566220	3.135518	-1.606532	0.472958	3.152833	-1.575075	0.303317	3.197188	-1.603360
1	-0.826620	2.201794	-2.385402	-0.889489	2.195650	-2.339323	-1.049810	2.198940	-2.328248
8	0.000000	0.000000	2.816000	0.000000	0.000000	2.807171	0.000000	0.000000	2.799561
1	1.051966	-2.786373	1.897673	1.059116	-2.705586	1.916088	1.167086	-2.692912	1.936117
1	-1.531996	-3.245297	0.169321	-1.452063	-3.266301	0.161059	-1.339721	-3.361656	0.214813
1	-1.466226	-2.504007	1.859434	-1.444611	-2.514389	1.829245	-1.335038	-2.623219	1.887666
1	2.263694	-2.620793	-0.338013	2.292645	-2.530536	-0.280675	2.394496	-2.454076	-0.234402
1	-0.566220	-3.135518	-1.606532	-0.472958	-3.152833	-1.575075	-0.303317	-3.197188	-1.603360
1	0.826620	-2.201794	-2.385402	0.889489	-2.195650	-2.339323	1.049810	-2.198940	-2.328248

Table S19. Optimized coordinates of the **3T-2** for the $(\eta^4\text{-}C_4H_6)_2Fe_2(CO)_3$ structure

	BP86			M06-L			B3LYP		
	x	y	z	x	y	z	x	y	z
6	0.484173	2.835751	1.444275	0.517665	2.823822	1.435453	0.482919	2.893704	1.474140
1	1.439595	3.228605	1.069357	1.472417	3.176072	1.047155	1.470201	3.178156	1.110535
1	0.446339	2.643142	2.521568	0.484138	2.647728	2.505531	0.405757	2.737408	2.546674
6	-0.720482	2.988773	0.725105	-0.670486	2.990544	0.720317	-0.676735	3.105075	0.721571
1	-1.685475	2.900496	1.243259	-1.628644	2.915701	1.232130	-1.645289	3.085165	1.222435
6	-0.720482	2.988773	-0.725105	-0.670486	2.990544	-0.720317	-0.676735	3.105075	-0.721571
1	-1.685475	2.900496	-1.243259	-1.628644	2.915701	-1.232130	-1.645289	3.085165	-1.222435
6	0.484173	2.835751	-1.444275	0.517665	2.823822	-1.435453	0.482919	2.893704	-1.474140
1	1.439595	3.228605	-1.069357	1.472417	3.176072	-1.047155	1.470201	3.178156	-1.110535
1	0.446339	2.643142	-2.521568	0.484138	2.647728	-2.505531	0.405757	2.737408	-2.546674
26	0.184493	1.252686	0.000000	0.166571	1.233596	0.000000	0.126343	1.282785	0.000000
6	0.649858	-0.027532	-1.429061	0.680924	-0.076160	-1.429846	0.663329	-0.076793	-1.422030
8	1.109766	-0.060945	-2.534031	1.163494	-0.107312	-2.509458	1.162615	-0.072756	-2.489007
8	-2.988325	-0.620873	0.000000	-2.951596	-0.401745	0.000000	-2.990332	-0.706447	0.000000
6	-1.816224	-0.744761	0.000000	-1.806942	-0.627710	0.000000	-1.831172	-0.799407	0.000000
26	-0.069421	-1.065358	0.000000	-0.082241	-1.081742	0.000000	-0.073211	-1.091792	0.000000
6	0.649858	-0.027532	1.429061	0.680924	-0.076160	1.429846	0.663329	-0.076793	1.422030
8	1.109766	-0.060945	2.534031	1.163494	-0.107312	2.509458	1.162615	-0.072756	2.489007
6	0.963980	-2.721052	0.717076	0.893308	-2.745994	0.710208	0.960479	-2.757844	0.710961
6	-0.311329	-2.684847	1.371593	-0.375947	-2.661974	1.349940	-0.301370	-2.703099	1.373759
1	1.900935	-2.584566	1.271301	1.823819	-2.635195	1.261933	1.895040	-2.633431	1.254918
6	0.963980	-2.721052	-0.717076	0.893308	-2.745994	-0.710208	0.960479	-2.757844	-0.710961
1	-1.138660	-3.308294	1.013839	-1.207754	-3.264517	0.992263	-1.129794	-3.316936	1.029204
1	-0.332039	-2.455861	2.443792	-0.393793	-2.446712	2.415681	-0.304438	-2.493466	2.441479
1	1.900935	-2.584566	-1.271301	1.823819	-2.635195	-1.261933	1.895040	-2.633431	-1.254918
6	-0.311329	-2.684847	-1.371593	-0.375947	-2.661974	-1.349940	-0.301370	-2.703099	-1.373759
1	-1.138660	-3.308294	-1.013839	-1.207754	-3.264517	-0.992263	-1.129794	-3.316936	-1.029204
1	-0.332039	-2.455861	-2.443792	-0.393793	-2.446712	-2.415681	-0.304438	-2.493466	-2.441479

Table S20. Optimized coordinates of the $(\eta^2\text{-}C_4H_6)Fe(CO)_4$ structure

	BP86			M06-L			B3LYP		
	x	y	z	x	y	z	x	y	z
6	1.523084	-1.350558	-0.259509	1.552734	-1.321495	-0.300306	1.540484	-1.356355	-0.260344
8	2.249154	-2.253943	-0.416772	2.263420	-2.210487	-0.507620	2.244129	-2.254992	-0.431239
26	0.421241	0.053525	-0.008263	0.421615	0.063690	0.003739	0.428040	0.060699	0.001888
6	-0.671357	1.480399	0.187745	-0.743808	1.451530	0.182114	-0.690109	1.492084	0.202024
8	-1.338383	2.429358	0.321915	-1.461612	2.351574	0.277696	-1.363859	2.417693	0.331608
6	-1.249074	-1.238439	-0.564689	-1.181774	-1.252476	-0.603564	-1.235028	-1.233915	-0.570878
6	-0.746379	-0.535096	-1.700038	-0.690278	-0.512151	-1.706599	-0.733364	-0.542258	-1.697062
1	-0.878283	-2.260920	-0.400980	-0.793152	-2.261204	-0.464029	-0.870816	-2.248509	-0.403168
6	-2.531891	-0.958679	0.123328	-2.462516	-1.008595	0.071538	-2.524723	-0.960170	0.104104
1	-1.310640	0.310569	-2.110756	-1.278955	0.311306	-2.106425	-1.287900	0.296103	-2.112433
1	-0.112942	-1.055182	-2.427621	-0.046594	-0.993592	-2.437251	-0.097054	-1.058234	-2.412224
1	-2.634367	-1.405286	1.124397	-2.590572	-1.514957	1.029236	-2.627578	-1.394880	1.101165
6	-3.576857	-0.258516	-0.385557	-3.469011	-0.253359	-0.397736	-3.565703	-0.277862	-0.409449
1	-3.550523	0.179160	-1.391296	-3.407929	0.255379	-1.358272	-3.541184	0.149977	-1.410137
1	-4.494537	-0.115517	0.196663	-4.386405	-0.124980	0.167746	-4.479591	-0.139432	0.164422
6	0.523657	-0.145848	1.771330	0.478748	-0.195854	1.787866	0.519861	-0.154038	1.789890
8	0.603108	-0.259253	2.935573	0.514449	-0.355283	2.936903	0.588764	-0.278420	2.939458
6	1.684139	1.141607	-0.662623	1.680645	1.216017	-0.568516	1.685859	1.162829	-0.667131
8	2.523259	1.852125	-1.070155	2.502889	1.955497	-0.921603	2.504894	1.870084	-1.080282

Table S21. Optimized coordinates of the $(\eta^4\text{-}C_4H_6)Fe(CO)_3$ structure

	BP86			M06-L			B3LYP		
	x	y	z	x	y	z	x	y	z
6	-0.280767	-1.598551	1.371980	-0.275133	-1.573007	1.349039	-0.268425	-1.588709	1.374347
1	-1.124167	-2.201892	1.016000	-1.097634	-2.188489	0.990886	-1.111571	-2.182000	1.028713
1	-0.290744	-1.395556	2.449416	-0.294070	-1.384394	2.419287	-0.263620	-1.402477	2.446725
6	0.998874	-1.683861	0.715435	0.999979	-1.653640	0.708642	0.995814	-1.680960	0.710296
1	1.942891	-1.596163	1.267571	1.933019	-1.556961	1.258006	1.936063	-1.597232	1.252861
6	0.998874	-1.683861	-0.715435	0.999979	-1.653640	-0.708642	0.995814	-1.680960	-0.710296
1	1.942891	-1.596163	-1.267571	1.933019	-1.556961	-1.258006	1.936063	-1.597232	-1.252861
6	-0.280767	-1.598551	-1.371980	-0.275133	-1.573007	-1.349039	-0.268425	-1.588709	-1.374347
1	-1.124167	-2.201892	-1.016000	-1.097634	-2.188489	-0.990886	-1.111571	-2.182000	-1.028713
1	-0.290744	-1.395556	-2.449416	-0.294070	-1.384394	-2.419287	-0.263620	-1.402477	-2.446725
26	0.010980	0.000319	0.000000	0.009731	0.006556	0.000000	0.007013	0.011079	0.000000
6	0.616828	1.097737	-1.265719	0.619129	1.095094	-1.288117	0.619480	1.101125	-1.294176
8	0.998874	1.829178	-2.100804	0.999979	1.790526	-2.136525	0.995814	1.791921	-2.143732
6	0.616828	1.097737	1.265719	0.619129	1.095094	1.288117	0.619480	1.101125	1.294176
8	0.998874	1.829178	2.100804	0.999979	1.790526	2.136525	0.995814	1.791921	2.143732
8	-2.874621	0.621716	0.000000	-2.880531	0.584746	0.000000	-2.873056	0.624677	0.000000
6	-1.724277	0.392409	0.000000	-1.736462	0.390248	0.000000	-1.735848	0.404958	0.000000

Table S22. Optimized coordinates of the $(\eta^4\text{-}C_4H_6)Fe(CO)_2$ structure

	BP86			M06-L			B3LYP		
	x	y	z	x	y	z	x	y	z
6	1.849839	0.998028	-0.459934	1.901202	0.836966	-0.457333	1.905504	0.898165	-0.484627
1	1.933075	1.557300	0.480436	2.039333	1.390398	0.469658	2.014955	1.478876	0.429117
1	2.134037	1.568018	-1.353472	2.257382	1.358516	-1.342601	2.237900	1.411499	-1.385734
6	2.014763	-0.426723	-0.493084	1.951438	-0.587559	-0.458945	1.989179	-0.525186	-0.464631
1	2.380278	-0.908805	-1.413021	2.288736	-1.124927	-1.345926	2.339683	-1.055341	-1.352989
6	1.396769	-1.252408	0.495145	1.263339	-1.307087	0.545505	1.330408	-1.275680	0.542131
1	1.387776	-2.342854	0.372921	1.159392	-2.386886	0.474022	1.269635	-2.359266	0.453676
6	0.628226	-0.575711	1.532132	0.564743	-0.512117	1.527948	0.587787	-0.539947	1.542283
1	1.058533	0.288996	2.059511	1.085028	0.317334	2.010402	1.051547	0.311428	2.042572
1	-0.025740	-1.192067	2.161399	-0.134576	-1.023234	2.185668	-0.073752	-1.112196	2.191404
26	-0.009146	0.012412	-0.294487	-0.005412	0.017769	-0.321328	-0.014438	0.025723	-0.310042
6	-1.397058	-1.070622	-0.280212	-1.448150	-1.020805	-0.280337	-1.436968	-1.061714	-0.292072
8	-2.334126	-1.786592	-0.304971	-2.393549	-1.701859	-0.256386	-2.358378	-1.767291	-0.286697
8	-1.446288	2.490291	0.359538	-1.258949	2.587501	0.337936	-1.349074	2.554479	0.351845
6	-0.890347	1.506954	0.024678	-0.788339	1.577547	-0.001685	-0.843402	1.564145	0.017225

Table S23. Optimized coordinates of the $(\eta^4\text{-}C_4H_6)Fe(CO)$ structure

	BP86			M06-L			B3LYP		
	x	y	z	x	y	z	x	y	z
6	-0.876592	-0.234018	1.404948	-0.896825	-0.210061	1.386329	-0.900410	-0.251078	1.424000
1	-1.652517	0.517619	1.197057	-1.649016	0.541756	1.143058	-1.634609	0.521808	1.194728
1	-0.559956	-0.244842	2.460733	-0.633543	-0.219769	2.445001	-0.637361	-0.295202	2.482622
6	-0.876592	-1.516671	0.710297	-0.896825	-1.481382	0.704335	-0.900410	-1.503409	0.705823
1	-0.619520	-2.448970	1.237683	-0.654173	-2.406921	1.229051	-0.643362	-2.432188	1.220609
6	-0.876592	-1.516671	-0.710297	-0.896825	-1.481382	-0.704335	-0.900410	-1.503409	-0.705823
1	-0.619520	-2.448970	-1.237683	-0.654173	-2.406921	-1.229051	-0.643362	-2.432188	-1.220609
6	-0.876592	-0.234018	-1.404948	-0.896825	-0.210061	-1.386329	-0.900410	-0.251078	-1.424000
1	-1.652517	0.517619	-1.197057	-1.649016	0.541756	-1.143058	-1.634609	0.521808	-1.194728
1	-0.559956	-0.244842	-2.460733	-0.633543	-0.219769	-2.445001	-0.637361	-0.295202	-2.482622
26	0.526714	-0.199079	0.000000	0.522326	-0.218181	0.000000	0.531140	-0.195271	0.000000
8	0.952476	2.688916	0.000000	1.022984	2.653603	0.000000	1.007875	2.680372	0.000000
6	0.897974	1.504231	0.000000	0.938817	1.485178	0.000000	0.927974	1.516515	0.000000

Table S24. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **7S-1** of $(\eta^2\text{-}C_4H_6)_2Fe_2(CO)_7$ structure

BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP
45(0)	43(0)	46(1)	418(0)	413(0)	416(0)	1041(10)	1065(6)	1079(12)
46(0)	44(0)	46(0)	437(15)	436(12)	431(11)	1079(1)	1105(2)	1115(1)
61(1)	54(0)	61(1)	437(1)	437(0)	441(1)	1080(1)	1105(2)	1115(0)
65(1)	57(0)	67(1)	461(15)	452(24)	450(38)	1220(7)	1261(4)	1271(9)
68(0)	61(1)	68(4)	470(6)	460(25)	467(28)	1220(2)	1261(9)	1271(2)
71(0)	70(0)	72(1)	474(10)	465(1)	470(5)	1282(10)	1323(10)	1325(12)
76(0)	73(1)	76(0)	482(3)	474(5)	482(10)	1282(0)	1324(0)	1326(0)
76(0)	76(1)	79(0)	487(4)	481(4)	486(0)	1369(3)	1401(2)	1424(3)
86(0)	78(0)	79(0)	497(7)	498(4)	500(5)	1369(0)	1401(1)	1424(1)
87(0)	82(0)	88(0)	534(1)	544(4)	552(2)	1408(0)	1443(0)	1458(0)
93(1)	84(1)	91(0)	544(6)	554(93)	558(9)	1408(23)	1443(16)	1459(23)
99(1)	89(1)	95(1)	551(52)	560(12)	561(90)	1503(4)	1560(10)	1579(8)
108(2)	103(1)	103(1)	552(65)	563(42)	565(55)	1504(10)	1561(7)	1580(11)
111(0)	104(3)	110(1)	571(5)	569(4)	583(2)	1623(0)	1686(0)	1680(0)
112(1)	106(1)	110(1)	583(6)	581(12)	588(9)	1623(11)	1686(14)	1680(10)
117(0)	115(0)	117(0)	603(32)	596(38)	614(24)	1825(513)	1899(553)	1869(685)
135(0)	135(0)	132(0)	618(114)	618(110)	625(105)	1829(689)	1904(815)	1874(921)
158(9)	151(15)	150(19)	624(73)	627(48)	634(61)	1858(1)	1934(1)	1919(0)
174(7)	166(6)	158(6)	648(87)	658(71)	666(62)	1981(162)	2060(186)	2065(169)
178(7)	170(7)	161(1)	651(5)	660(4)	667(5)	1985(959)	2064(1134)	2071(1181)
206(0)	213(0)	207(0)	685(744)	695(724)	706(742)	2004(1411)	2083(1698)	2088(1851)
210(0)	216(0)	208(1)	800(2)	799(1)	815(2)	2030(247)	2114(280)	2119(211)
238(1)	238(1)	229(3)	800(9)	799(10)	816(9)	3078(2)	3136(13)	3156(5)
248(2)	243(6)	230(1)	870(3)	895(2)	891(3)	3078(0)	3136(4)	3156(0)
252(5)	255(2)	252(1)	870(3)	895(2)	891(1)	3081(11)	3143(29)	3162(1)
291(0)	291(1)	291(1)	902(15)	920(59)	956(21)	3081(0)	3143(0)	3162(1)
304(11)	304(7)	308(7)	902(80)	920(13)	956(82)	3086(1)	3148(1)	3171(11)
307(2)	305(1)	308(0)	930(1)	947(6)	982(1)	3086(6)	3148(12)	3171(2)
339(5)	333(6)	338(7)	930(2)	947(6)	983(0)	3108(4)	3182(4)	3191(4)
361(0)	355(0)	357(0)	971(18)	964(0)	1004(20)	3108(6)	3182(11)	3191(4)
387(0)	378(0)	381(0)	971(6)	964(6)	1005(7)	3176(1)	3245(2)	3251(1)
390(3)	390(4)	384(3)	991(7)	1020(7)	1033(10)	3176(6)	3245(2)	3251(12)
405(2)	402(2)	400(0)	991(27)	1020(24)	1033(26)	3177(0)	3245(3)	3262(0)
410(0)	409(0)	401(6)	1041(14)	1065(11)	1078(12)	3177(8)	3245(27)	3262(0)

Table S25. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **7S-2** of $(\eta^2\text{-}C_4H_6)_2Fe_2(CO)_7$ structure

BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP
24(0)	39(1)	24(0)	443(1)	439(9)	446(3)	1032(8)	1059(4)	1071(9)
40(1)	40(0)	43(1)	449(81)	443(2)	448(1)	1072(0)	1104(0)	1115(1)
54(0)	62(1)	56(0)	454(0)	443(123)	452(13)	1072(1)	1104(1)	1115(0)
54(0)	67(0)	61(0)	456(11)	450(42)	454(8)	1202(19)	1236(37)	1246(42)
58(0)	70(0)	65(0)	469(2)	459(25)	460(26)	1202(5)	1236(9)	1246(10)
65(0)	71(0)	68(0)	471(4)	471(14)	468(5)	1274(6)	1318(6)	1321(7)
70(0)	76(0)	74(0)	471(10)	477(3)	470(15)	1274(0)	1319(0)	1322(1)
74(0)	79(0)	82(0)	478(2)	483(11)	484(6)	1369(2)	1404(5)	1422(6)
80(0)	89(0)	82(0)	499(49)	491(0)	491(2)	1369(2)	1405(1)	1422(3)
82(0)	90(1)	86(1)	510(6)	494(20)	496(27)	1406(1)	1446(2)	1455(1)
85(0)	93(0)	87(0)	537(8)	550(2)	555(10)	1406(15)	1446(9)	1455(11)
93(0)	97(0)	95(0)	538(17)	556(16)	557(21)	1488(5)	1531(18)	1548(15)
93(0)	110(0)	98(0)	551(25)	562(40)	567(27)	1488(3)	1531(1)	1548(1)
105(0)	111(0)	109(0)	562(1)	564(4)	573(0)	1619(1)	1688(4)	1676(2)
106(0)	117(0)	110(0)	584(91)	573(86)	586(89)	1619(20)	1688(29)	1676(25)
113(0)	119(0)	112(0)	609(414)	611(342)	618(330)	1814(375)	1896(406)	1878(460)
114(0)	120(0)	119(0)	623(125)	617(113)	624(124)	1956(28)	2041(6)	2047(128)
141(1)	138(3)	143(3)	630(190)	627(220)	631(161)	1972(156)	2050(98)	2051(0)
141(0)	139(0)	150(0)	630(2)	637(1)	636(0)	1983(1384)	2068(1237)	2074(1212)
146(1)	143(0)	151(2)	661(15)	681(14)	685(19)	1993(929)	2076(1093)	2076(1117)
175(3)	186(2)	175(2)	662(28)	681(36)	685(31)	2009(505)	2095(913)	2096(1017)
195(4)	205(5)	206(5)	790(2)	797(3)	815(2)	2052(244)	2140(267)	2137(261)
214(4)	228(3)	222(4)	790(5)	797(7)	816(6)	3070(4)	3132(18)	3148(1)
263(2)	260(17)	265(41)	858(7)	888(4)	881(4)	3070(6)	3132(12)	3148(5)
264(0)	290(5)	275(4)	858(3)	888(3)	881(2)	3077(7)	3158(34)	3155(9)
268(6)	291(0)	277(0)	886(14)	897(54)	932(4)	3077(0)	3158(0)	3155(1)
343(53)	337(111)	331(119)	886(29)	897(17)	932(6)	3080(5)	3163(0)	3159(3)
343(5)	338(8)	334(7)	891(52)	908(0)	940(76)	3080(1)	3163(8)	3159(0)
382(3)	367(12)	375(0)	891(7)	908(7)	940(20)	3103(2)	3200(3)	3184(2)
385(0)	369(0)	381(9)	950(2)	949(8)	986(4)	3103(8)	3200(17)	3184(7)
409(1)	400(115)	399(128)	950(4)	950(1)	986(3)	3157(0)	3229(2)	3234(1)
426(1)	404(0)	411(0)	984(9)	1018(5)	1029(8)	3157(6)	3229(18)	3234(6)
433(172)	419(3)	415(0)	985(29)	1018(26)	1029(26)	3175(1)	3256(2)	3249(1)
435(14)	433(26)	434(267)	1031(10)	1059(6)	1071(8)	3175(16)	3256(37)	3249(15)

Table S26. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **6S-1** of (η^2, η^4-$C_4H_6)_2Fe_2(CO)_6$ structure

BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP
8(8)	32(1)	28(0)	425(3)	464(10)	458(38)	1123(6)	1083(2)	1082(1)
21(0)	41(0)	44(1)	442(2)	466(4)	467(21)	1124(2)	1104(1)	1115(1)
32(0)	54(0)	56(0)	464(1)	479(61)	469(16)	1266(49)	1191(3)	1195(4)
60(0)	69(0)	66(0)	465(1)	485(11)	484(67)	1269(3)	1233(4)	1235(5)
62(7)	73(0)	77(0)	477(8)	490(7)	487(22)	1327(0)	1236(19)	1247(24)
79(8)	80(0)	81(0)	492(10)	498(32)	490(8)	1328(1)	1306(4)	1320(4)
80(0)	82(0)	85(0)	512(14)	502(29)	500(7)	1424(16)	1387(1)	1405(1)
82(0)	87(0)	93(0)	517(18)	525(11)	533(11)	1425(2)	1404(2)	1422(4)
90(0)	90(0)	95(0)	527(19)	552(24)	556(28)	1457(8)	1440(5)	1455(6)
94(3)	93(0)	99(0)	558(9)	563(72)	565(80)	1458(1)	1478(1)	1483(2)
106(0)	100(0)	104(0)	562(24)	574(113)	579(68)	1562(55)	1507(3)	1525(4)
106(13)	105(1)	106(0)	571(96)	597(95)	596(77)	1564(10)	1525(12)	1538(18)
115(5)	106(0)	113(0)	587(0)	614(60)	614(60)	1666(0)	1532(8)	1549(8)
115(0)	115(0)	122(0)	601(18)	632(46)	631(90)	1667(1)	1682(22)	1677(17)
122(0)	133(2)	134(3)	615(129)	639(207)	637(178)	1831(991)	1890(427)	1877(472)
155(1)	146(0)	151(0)	625(89)	667(10)	660(9)	1888(63)	2037(81)	2038(138)
160(2)	165(1)	164(1)	662(37)	683(23)	687(26)	2059(257)	2049(523)	2058(437)
171(4)	184(3)	179(5)	663(4)	790(3)	790(1)	2065(1142)	2065(1604)	2072(1559)
174(3)	206(2)	214(2)	801(48)	799(3)	813(2)	2077(2112)	2071(556)	2078(702)
216(56)	250(5)	252(16)	806(16)	812(4)	815(8)	2106(416)	2122(294)	2126(336)
221(0)	269(1)	275(2)	888(3)	880(3)	879(3)	3158(3)	3125(31)	3144(9)
260(0)	343(22)	308(21)	888(4)	894(41)	907(9)	3159(1)	3126(17)	3148(3)
261(9)	348(39)	336(52)	946(75)	897(3)	923(10)	3161(0)	3139(11)	3154(4)
285(0)	374(1)	356(0)	946(28)	912(7)	936(42)	3161(3)	3143(9)	3159(3)
288(13)	383(8)	374(4)	963(6)	919(2)	944(13)	3168(1)	3143(12)	3167(4)
318(5)	399(0)	394(146)	964(10)	944(3)	952(0)	3169(9)	3156(11)	3174(4)
384(24)	413(44)	395(1)	975(27)	945(1)	978(3)	3204(8)	3174(4)	3193(0)
386(0)	423(3)	413(4)	981(12)	961(3)	981(3)	3204(0)	3189(13)	3206(3)
397(1)	435(25)	420(51)	1017(6)	979(2)	992(2)	3255(1)	3220(11)	3228(4)
400(0)	447(6)	445(37)	1018(20)	1017(12)	1031(14)	3255(9)	3222(10)	3234(4)
418(19)	452(74)	448(71)	1073(7)	1053(5)	1069(5)	3261(2)	3234(9)	3248(8)
420(1)	460(64)	452(6)	1074(11)	1062(3)	1071(7)	3261(1)	3242(18)	3252(4)

Table S27. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **6S-2** of $(\eta^2\text{-}C_4H_6)_2Fe_2(CO)_6$ structure

BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP
16(0)	21(1)	8(8)	443(7)	435(5)	425(3)	1090(3)	1116(2)	1123(6)
26(1)	21(0)	21(0)	450(1)	440(2)	442(2)	1091(2)	1117(3)	1124(2)
27(0)	42(0)	32(0)	464(0)	462(0)	464(1)	1218(22)	1257(27)	1266(49)
59(0)	60(0)	60(0)	474(1)	466(0)	465(1)	1220(2)	1259(4)	1269(3)
64(0)	65(1)	62(7)	484(0)	483(7)	477(8)	1280(3)	1319(1)	1327(0)
79(0)	76(0)	79(8)	485(0)	496(2)	492(10)	1283(0)	1323(1)	1328(1)
79(0)	79(1)	80(0)	523(7)	513(16)	512(14)	1372(9)	1406(9)	1424(16)
85(0)	82(0)	82(0)	524(21)	524(24)	517(18)	1373(3)	1407(1)	1425(2)
87(0)	98(0)	90(0)	545(14)	525(3)	527(19)	1411(18)	1444(9)	1457(8)
97(1)	102(1)	94(3)	549(11)	557(11)	558(9)	1411(0)	1444(0)	1458(1)
109(0)	107(0)	106(0)	555(9)	562(18)	562(24)	1492(22)	1545(43)	1562(55)
109(1)	111(2)	106(13)	570(79)	569(79)	571(96)	1493(9)	1547(6)	1564(10)
115(0)	113(0)	115(5)	576(2)	579(1)	587(0)	1603(2)	1667(0)	1666(0)
118(0)	118(4)	115(0)	602(10)	601(25)	601(18)	1603(1)	1667(0)	1667(1)
120(4)	121(0)	122(0)	617(157)	613(164)	615(129)	1792(699)	1865(826)	1831(991)
157(0)	156(0)	155(1)	621(93)	621(78)	625(89)	1823(55)	1901(60)	1888(63)
161(4)	160(3)	160(2)	639(37)	656(35)	662(37)	1972(275)	2052(364)	2059(257)
170(1)	174(2)	171(4)	640(2)	658(4)	663(4)	1977(872)	2056(970)	2065(1142)
171(3)	183(4)	174(3)	787(35)	793(37)	801(48)	1997(1313)	2076(1625)	2077(2112)
225(0)	225(0)	216(56)	791(11)	797(13)	806(16)	2017(466)	2101(568)	2106(416)
240(6)	232(18)	221(0)	868(4)	893(1)	888(3)	3078(2)	3134(20)	3158(3)
263(0)	259(0)	260(0)	868(1)	893(2)	888(4)	3078(2)	3134(3)	3159(1)
277(1)	268(14)	261(9)	891(71)	910(54)	946(75)	3082(1)	3142(13)	3161(0)
281(1)	279(2)	285(0)	891(28)	910(20)	946(28)	3082(9)	3144(1)	3161(3)
299(19)	280(11)	288(13)	903(14)	931(4)	963(6)	3089(7)	3150(5)	3168(1)
335(5)	322(5)	318(5)	907(2)	932(13)	964(10)	3089(4)	3159(23)	3169(9)
389(1)	383(1)	384(24)	951(11)	945(24)	975(27)	3112(6)	3183(12)	3204(8)
393(16)	397(13)	386(0)	954(13)	950(1)	981(12)	3112(1)	3183(4)	3204(0)
407(1)	402(0)	397(1)	971(5)	1008(19)	1017(6)	3176(1)	3242(5)	3255(1)
414(2)	414(3)	400(0)	972(21)	1013(5)	1018(20)	3176(0)	3242(0)	3255(9)
427(0)	420(16)	418(19)	1034(9)	1061(7)	1073(7)	3182(2)	3247(3)	3261(2)
431(8)	430(0)	420(1)	1036(6)	1062(3)	1074(11)	3182(11)	3247(25)	3261(1)

Table S28. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **6S-3** of $(\eta^2\text{-}C_4H_6)_2Fe_2(CO)_6$ structure

BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP
28(0)	32(0)	8(8)	441(5)	419(14)	425(3)	1067(2)	1104(3)	1123(6)
33(0)	35(0)	21(0)	446(0)	439(12)	442(2)	1082(1)	1116(1)	1124(2)
43(0)	42(1)	32(0)	467(6)	456(14)	464(1)	1193(18)	1228(33)	1266(49)
53(0)	62(0)	60(0)	478(1)	465(5)	465(1)	1198(33)	1232(51)	1269(3)
66(1)	68(1)	62(7)	487(3)	480(5)	477(8)	1276(1)	1321(3)	1327(0)
70(0)	72(0)	79(8)	489(5)	489(35)	492(10)	1278(2)	1322(2)	1328(1)
73(0)	74(0)	80(0)	502(3)	500(4)	512(14)	1371(7)	1406(11)	1424(16)
82(0)	81(0)	82(0)	504(17)	511(1)	517(18)	1373(6)	1409(6)	1425(2)
88(0)	85(0)	90(0)	535(20)	541(14)	527(19)	1407(8)	1445(8)	1457(8)
89(0)	86(0)	94(3)	541(18)	551(14)	558(9)	1410(9)	1449(6)	1458(1)
90(0)	94(1)	106(0)	552(10)	554(39)	562(24)	1482(10)	1522(18)	1562(55)
94(0)	101(0)	106(13)	560(6)	565(13)	571(96)	1483(9)	1531(12)	1564(10)
102(0)	109(0)	115(5)	569(51)	569(11)	587(0)	1606(2)	1669(3)	1666(0)
109(0)	113(0)	115(0)	595(83)	602(81)	601(18)	1613(8)	1680(18)	1667(1)
118(0)	131(0)	122(0)	621(54)	619(55)	615(129)	1843(381)	1923(451)	1831(991)
132(0)	138(0)	155(1)	627(73)	628(68)	625(89)	1940(199)	1994(502)	1888(63)
152(0)	148(0)	160(2)	654(40)	679(42)	662(37)	1943(431)	2029(46)	2059(257)
163(0)	162(0)	171(4)	662(39)	682(38)	663(4)	1977(1761)	2064(2127)	2065(1142)
170(1)	182(2)	174(3)	782(9)	794(12)	801(48)	1993(313)	2075(342)	2077(2112)
191(1)	199(1)	216(56)	790(10)	804(19)	806(16)	2037(137)	2122(162)	2106(416)
212(1)	224(3)	221(0)	855(7)	882(46)	888(3)	3059(4)	3127(13)	3158(3)
233(0)	245(0)	260(0)	858(17)	884(4)	888(4)	3068(6)	3132(20)	3159(1)
268(0)	270(0)	261(9)	877(44)	889(11)	946(75)	3072(3)	3151(14)	3161(0)
277(0)	301(0)	285(0)	886(10)	901(1)	946(28)	3077(3)	3153(14)	3161(3)
330(10)	348(6)	288(13)	892(49)	907(47)	963(6)	3081(6)	3157(5)	3168(1)
359(18)	357(2)	318(5)	895(4)	910(4)	964(10)	3083(3)	3162(8)	3169(9)
368(1)	364(40)	384(24)	932(14)	943(16)	975(27)	3090(5)	3175(14)	3204(8)
381(5)	381(20)	386(0)	937(6)	951(29)	981(12)	3102(5)	3178(13)	3204(0)
389(11)	384(12)	397(1)	978(16)	1016(10)	1017(6)	3143(3)	3219(8)	3255(1)
397(7)	393(9)	400(0)	980(17)	1023(13)	1018(20)	3154(3)	3225(11)	3255(9)
418(3)	407(6)	418(19)	1029(5)	1057(2)	1073(7)	3177(8)	3255(19)	3261(2)
430(8)	418(7)	420(1)	1031(6)	1063(4)	1074(11)	3178(7)	3258(17)	3261(1)

Table S29. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **5S-1** of $(\eta^4\text{-}C_4H_6)_2Fe_2(CO)_5$ structure

BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP
35(1)	43(0)	29(0)	480(4)	487(0)	487(1)	1049(0)	1084(0)	1082(1)
46(1)	55(0)	43(1)	487(121)	496(17)	491(14)	1154(0)	1192(0)	1195(0)
61(0)	66(1)	61(0)	508(77)	499(10)	495(7)	1154(4)	1192(5)	1195(8)
68(0)	78(0)	71(0)	520(4)	507(1)	505(1)	1197(3)	1234(6)	1237(8)
81(0)	84(0)	85(0)	529(6)	528(8)	527(2)	1197(0)	1234(0)	1237(0)
83(0)	86(0)	87(0)	560(18)	540(39)	543(38)	1352(5)	1388(0)	1405(0)
89(0)	89(0)	92(0)	573(187)	569(224)	568(208)	1352(0)	1388(2)	1405(3)
91(0)	91(0)	95(0)	588(0)	599(3)	589(0)	1436(4)	1479(3)	1482(1)
116(0)	112(1)	119(0)	596(84)	603(135)	600(113)	1436(0)	1480(0)	1482(3)
116(0)	127(0)	119(0)	610(56)	608(49)	608(59)	1467(1)	1508(1)	1526(1)
131(1)	128(1)	131(1)	634(53)	638(59)	634(59)	1467(5)	1508(5)	1526(7)
133(1)	129(1)	133(0)	643(1)	667(1)	661(1)	1480(10)	1526(6)	1540(11)
146(0)	153(0)	146(0)	645(43)	669(24)	662(17)	1480(10)	1526(14)	1540(18)
165(4)	167(3)	170(4)	763(2)	788(1)	792(1)	1795(387)	1890(431)	1882(476)
181(1)	185(1)	179(1)	763(4)	788(6)	792(2)	1950(130)	2030(101)	2034(62)
255(1)	250(2)	251(9)	787(5)	810(5)	816(4)	1963(634)	2046(797)	2051(768)
326(13)	344(25)	306(26)	788(6)	811(4)	816(14)	1972(1099)	2057(1284)	2061(1404)
327(1)	347(0)	314(1)	875(5)	896(3)	907(6)	2009(465)	2094(447)	2093(499)
343(0)	370(0)	350(0)	875(20)	896(4)	907(8)	3066(16)	3123(47)	3144(16)
343(5)	372(8)	351(7)	895(2)	906(2)	923(5)	3066(5)	3123(13)	3144(3)
375(0)	381(0)	368(0)	897(21)	908(12)	925(19)	3085(4)	3141(14)	3165(3)
402(44)	414(8)	395(172)	919(1)	946(2)	953(0)	3085(4)	3141(10)	3165(3)
415(26)	426(0)	407(0)	919(0)	947(1)	953(0)	3118(1)	3172(6)	3194(1)
416(0)	426(76)	408(22)	945(2)	962(6)	982(4)	3118(0)	3172(1)	3194(0)
437(12)	454(1)	439(4)	945(2)	962(1)	982(1)	3129(4)	3188(11)	3206(3)
437(6)	459(107)	442(26)	949(1)	984(4)	999(3)	3129(4)	3188(18)	3207(3)
450(0)	468(2)	454(0)	949(4)	984(1)	999(2)	3155(4)	3218(14)	3228(5)
463(4)	469(16)	460(151)	1032(2)	1063(2)	1070(2)	3155(4)	3218(10)	3228(5)
468(49)	476(41)	475(22)	1032(5)	1064(4)	1070(7)	3174(1)	3233(1)	3251(1)
470(0)	484(29)	486(29)	1049(1)	1084(3)	1082(0)	3174(6)	3233(17)	3251(7)

Table S30. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **5S-2** of $(\eta^4\text{-}C_4H_6)_2Fe_2(CO)_5$ structure

BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP
28(1)	28(1)	33(1)	468(0)	489(0)	485(0)	1049(3)	1078(3)	1091(4)
58(0)	60(1)	56(1)	492(0)	493(37)	494(1)	1160(2)	1198(2)	1201(2)
59(1)	62(0)	60(1)	494(4)	499(2)	498(43)	1197(1)	1234(18)	1236(23)
79(0)	75(0)	65(1)	515(25)	507(1)	504(5)	1200(14)	1237(1)	1253(1)
94(0)	89(0)	93(1)	526(10)	519(27)	528(28)	1247(2)	1282(4)	1303(4)
94(0)	90(0)	96(1)	533(25)	542(36)	542(35)	1351(3)	1385(1)	1403(2)
109(1)	104(1)	100(0)	566(24)	576(23)	581(22)	1371(4)	1403(2)	1428(4)
110(1)	107(1)	112(1)	579(65)	586(66)	584(18)	1421(7)	1453(7)	1469(12)
122(0)	122(0)	115(0)	586(15)	589(16)	596(60)	1428(1)	1474(1)	1476(4)
126(0)	128(0)	122(0)	598(9)	596(40)	601(7)	1473(5)	1512(6)	1529(6)
130(3)	137(3)	137(1)	600(46)	617(5)	610(60)	1484(13)	1523(12)	1537(17)
144(0)	144(0)	145(1)	637(544)	646(564)	641(580)	1503(13)	1549(18)	1570(25)
179(1)	180(0)	174(2)	641(1)	667(2)	660(1)	1511(2)	1562(3)	1587(2)
190(1)	194(1)	178(1)	743(23)	755(19)	739(27)	1817(817)	1898(954)	1881(999)
202(0)	207(0)	183(7)	763(1)	782(1)	778(1)	1834(14)	1913(10)	1897(14)
217(2)	215(1)	201(2)	764(2)	787(3)	790(3)	1942(697)	2026(738)	2033(711)
235(3)	239(2)	210(4)	771(16)	805(14)	796(9)	1970(456)	2049(483)	2048(668)
239(10)	245(11)	236(5)	875(11)	902(6)	905(12)	2006(534)	2089(672)	2093(626)
300(13)	300(17)	277(9)	887(1)	903(0)	910(4)	3077(13)	3131(40)	3155(11)
325(5)	348(4)	322(6)	890(5)	905(8)	920(0)	3081(4)	3135(14)	3156(4)
357(2)	379(7)	358(2)	905(4)	915(0)	939(2)	3090(2)	3148(11)	3175(1)
371(9)	384(4)	377(8)	909(0)	931(1)	943(0)	3090(0)	3152(2)	3175(2)
376(3)	391(7)	381(4)	920(5)	935(0)	949(12)	3107(1)	3172(4)	3184(0)
394(9)	402(6)	393(6)	920(0)	953(0)	968(0)	3117(1)	3175(3)	3193(1)
404(4)	412(2)	399(5)	936(2)	965(4)	972(2)	3117(3)	3184(16)	3195(1)
425(0)	430(0)	418(1)	938(24)	967(13)	993(18)	3128(5)	3186(12)	3205(5)
439(11)	433(1)	425(0)	947(1)	974(1)	1003(1)	3167(3)	3227(7)	3243(3)
445(2)	464(28)	447(9)	1031(0)	1057(0)	1063(1)	3169(3)	3229(10)	3244(3)
456(2)	468(1)	462(1)	1035(3)	1066(2)	1072(3)	3183(1)	3250(3)	3270(0)
463(37)	474(10)	465(19)	1043(0)	1076(1)	1076(1)	3184(0)	3253(4)	3271(0)

Table S31. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **5S-3** of $(\eta^4\text{-}C_4H_6)_2Fe_2(CO)_5$ structure

BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP
55(2)	58(3)	27(0)	471(11)	483(17)	467(17)	1049(7)	1077(6)	1099(2)
62(0)	61(0)	45(1)	472(0)	486(0)	470(16)	1194(0)	1229(0)	1191(2)
66(1)	65(1)	54(1)	484(0)	491(1)	485(11)	1195(3)	1230(3)	1224(33)
77(4)	73(3)	60(0)	496(14)	493(0)	489(3)	1242(5)	1274(12)	1232(11)
94(0)	89(0)	73(0)	534(27)	538(38)	505(1)	1243(5)	1275(6)	1318(2)
109(1)	106(2)	76(0)	546(13)	553(15)	530(2)	1369(0)	1400(0)	1388(1)
112(0)	117(10)	81(0)	565(16)	574(31)	545(39)	1370(3)	1400(1)	1404(9)
116(7)	119(0)	83(0)	570(0)	580(0)	552(27)	1421(8)	1456(9)	1448(6)
124(0)	122(0)	94(0)	577(28)	584(17)	577(21)	1422(7)	1457(6)	1481(3)
127(0)	130(0)	103(1)	595(42)	595(36)	580(77)	1502(1)	1542(8)	1503(3)
158(1)	163(1)	105(0)	598(0)	622(0)	600(33)	1504(22)	1544(22)	1521(13)
166(0)	171(0)	112(0)	610(15)	635(12)	610(33)	1510(0)	1552(0)	1524(10)
204(0)	207(0)	134(0)	700(657)	714(667)	670(6)	1511(6)	1553(7)	1676(4)
219(3)	220(2)	145(1)	748(59)	780(71)	676(41)	1799(458)	1884(499)	1908(408)
220(0)	222(0)	165(0)	752(4)	781(3)	770(1)	1821(780)	1900(917)	1965(565)
238(0)	248(0)	186(3)	762(0)	793(0)	793(18)	1847(28)	1928(55)	2035(104)
238(0)	259(0)	219(1)	765(1)	796(2)	803(4)	1964(212)	2042(245)	2047(1718)
251(15)	266(16)	241(0)	883(34)	902(14)	887(6)	1995(1073)	2078(1226)	2114(206)
265(0)	277(2)	284(0)	888(6)	908(4)	891(2)	3089(0)	3146(2)	3123(14)
267(0)	289(0)	335(3)	897(0)	911(0)	903(52)	3090(2)	3147(20)	3140(23)
299(5)	299(10)	361(2)	903(2)	917(0)	905(6)	3091(0)	3149(0)	3148(22)
348(3)	357(5)	367(10)	912(17)	938(1)	908(2)	3091(4)	3149(16)	3151(12)
369(0)	368(0)	377(6)	915(15)	940(5)	932(25)	3108(0)	3176(0)	3169(6)
374(1)	384(1)	387(26)	933(13)	961(6)	933(9)	3108(3)	3176(10)	3185(13)
386(1)	386(0)	404(23)	934(2)	962(3)	959(2)	3119(11)	3188(36)	3196(6)
400(1)	407(1)	411(10)	941(0)	970(0)	967(4)	3119(2)	3188(5)	3210(19)
420(1)	414(1)	420(16)	942(0)	971(0)	1016(12)	3187(0)	3250(0)	3215(10)
439(4)	453(5)	433(5)	1034(0)	1062(0)	1062(3)	3187(2)	3251(3)	3236(9)
448(3)	456(22)	454(13)	1034(0)	1062(0)	1064(5)	3189(0)	3253(0)	3242(13)
463(0)	459(1)	460(66)	1048(0)	1077(0)	1083(5)	3189(0)	3253(10)	3255(18)

Table S32. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **5S-4** of $(\eta^4\text{-}C_4H_6)_2Fe_2(CO)_5$ structure

BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP
34(0)	27(0)	40(0)	458(15)	467(17)	471(4)	1067(1)	1099(2)	1105(4)
46(1)	45(1)	50(1)	465(2)	470(16)	475(21)	1154(2)	1191(2)	1194(3)
51(1)	54(1)	59(1)	477(5)	485(11)	482(3)	1192(19)	1224(33)	1233(15)
59(1)	60(0)	66(0)	486(6)	489(3)	490(1)	1198(8)	1232(11)	1237(45)
75(0)	73(0)	77(0)	504(1)	505(1)	495(11)	1277(2)	1318(2)	1324(2)
81(0)	76(0)	81(0)	531(10)	530(2)	535(2)	1352(2)	1388(1)	1404(1)
87(0)	81(0)	84(0)	540(4)	545(39)	549(18)	1371(6)	1404(9)	1421(13)
91(0)	83(0)	92(0)	554(47)	552(27)	556(43)	1409(8)	1448(6)	1456(6)
100(0)	94(0)	94(0)	571(37)	577(21)	569(50)	1439(4)	1481(3)	1488(6)
103(0)	103(1)	104(0)	581(62)	580(77)	584(66)	1465(3)	1503(3)	1520(4)
103(0)	105(0)	106(0)	598(29)	600(33)	601(19)	1479(9)	1521(13)	1534(13)
107(0)	112(0)	109(0)	607(33)	610(33)	611(44)	1482(8)	1524(10)	1544(13)
139(0)	134(0)	142(1)	636(3)	670(6)	659(3)	1607(3)	1676(4)	1669(4)
142(1)	145(1)	148(1)	654(44)	676(41)	679(45)	1826(365)	1908(408)	1903(485)
168(0)	165(0)	171(0)	748(1)	770(1)	781(1)	1896(450)	1965(565)	1982(614)
183(2)	186(3)	180(5)	773(5)	793(18)	799(27)	1948(584)	2035(104)	2049(60)
215(0)	219(1)	218(1)	786(12)	803(4)	801(6)	1966(1049)	2047(1718)	2062(1728)
244(0)	241(0)	239(1)	857(17)	887(6)	879(18)	2025(173)	2114(206)	2118(226)
272(0)	284(0)	281(0)	870(7)	891(2)	903(7)	3058(4)	3123(14)	3139(3)
314(4)	335(3)	315(3)	887(10)	903(52)	927(0)	3073(9)	3140(23)	3147(9)
341(3)	361(2)	341(6)	892(42)	905(6)	931(12)	3076(3)	3148(22)	3153(5)
361(4)	367(10)	354(1)	893(1)	908(2)	944(44)	3081(3)	3151(12)	3156(2)
376(4)	377(6)	368(21)	910(2)	932(25)	949(19)	3082(3)	3169(6)	3159(5)
390(15)	387(26)	380(30)	925(1)	933(9)	949(11)	3102(5)	3185(13)	3179(5)
400(17)	404(23)	399(10)	927(15)	959(2)	967(2)	3112(2)	3196(6)	3189(1)
410(21)	411(10)	400(14)	935(3)	967(4)	985(2)	3125(5)	3210(19)	3203(5)
422(5)	420(16)	420(26)	982(18)	1016(12)	1027(14)	3142(3)	3215(10)	3223(3)
423(6)	433(5)	429(5)	1030(6)	1062(3)	1070(7)	3161(4)	3236(9)	3231(5)
439(43)	454(13)	439(4)	1033(7)	1064(5)	1070(8)	3170(3)	3242(13)	3245(4)
450(1)	460(66)	457(95)	1049(2)	1083(5)	1083(2)	3177(7)	3255(18)	3251(7)

Table S33. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **4T-1** of $(\eta^4\text{-}C_4H_6)_2Fe_2(CO)_4$ structure

BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP
25(1)	31(0)	17(1)	468(1)	478(0)	469(34)	1159(1)	1199(1)	1191(2)
39(1)	46(1)	38(1)	471(2)	481(18)	489(12)	1159(1)	1201(1)	1224(13)
63(0)	56(1)	63(1)	497(9)	497(47)	490(8)	1196(15)	1238(24)	1235(2)
76(0)	69(0)	66(0)	521(125)	506(32)	513(31)	1200(3)	1242(5)	1279(18)
82(0)	77(0)	77(0)	525(61)	520(168)	518(16)	1350(4)	1386(2)	1401(2)
83(0)	82(0)	82(0)	535(53)	526(38)	572(47)	1352(3)	1388(1)	1415(2)
86(0)	83(0)	92(0)	546(14)	542(16)	583(253)	1427(4)	1467(3)	1462(20)
110(2)	102(3)	104(0)	550(42)	560(39)	603(63)	1430(1)	1474(1)	1483(3)
124(2)	117(3)	116(1)	627(1)	648(3)	606(5)	1469(12)	1513(14)	1520(6)
140(0)	138(0)	130(0)	632(1)	651(2)	663(2)	1470(4)	1514(1)	1532(18)
153(0)	149(0)	140(2)	762(3)	773(2)	707(14)	1478(24)	1521(23)	1550(40)
193(0)	177(2)	143(4)	766(6)	780(3)	746(0)	1478(1)	1524(7)	1565(11)
222(0)	207(1)	170(1)	768(1)	783(2)	795(2)	1823(773)	1921(756)	1887(454)
227(1)	214(1)	199(8)	770(2)	790(5)	806(5)	1836(47)	1947(288)	1969(589)
296(0)	289(10)	246(4)	862(11)	886(14)	878(12)	1958(1317)	2034(1391)	2037(1268)
319(16)	327(8)	258(2)	873(1)	891(1)	890(1)	1978(246)	2066(399)	2066(568)
330(4)	334(2)	307(2)	891(1)	895(0)	896(11)	3081(11)	3137(38)	3151(9)
342(1)	354(2)	338(5)	892(0)	902(1)	929(1)	3082(11)	3138(23)	3160(7)
353(1)	366(0)	369(2)	907(6)	918(3)	930(0)	3084(3)	3140(11)	3172(0)
359(0)	368(0)	377(8)	910(5)	924(1)	947(0)	3085(3)	3143(12)	3174(1)
388(4)	402(4)	390(4)	919(0)	941(0)	948(4)	3112(0)	3172(3)	3185(0)
406(18)	404(22)	394(14)	921(0)	946(0)	967(0)	3113(0)	3173(2)	3188(1)
421(4)	431(18)	414(7)	932(0)	953(2)	971(2)	3125(3)	3186(9)	3198(1)
428(22)	435(2)	417(5)	934(1)	957(1)	978(0)	3126(3)	3186(16)	3202(5)
444(2)	454(9)	434(2)	1035(4)	1066(3)	1062(0)	3171(2)	3233(6)	3236(4)
449(14)	461(8)	444(0)	1036(0)	1068(1)	1068(4)	3173(2)	3236(6)	3248(2)
456(6)	465(14)	450(10)	1043(2)	1072(4)	1080(2)	3174(2)	3236(7)	3266(1)
462(1)	475(5)	465(7)	1044(1)	1077(3)	1088(3)	3176(2)	3240(7)	3270(1)

Table S34. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **4S-2** of $(\eta^4\text{-}C_4H_6)_2Fe_2(CO)_4$ structure

BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP
-46(7)	18(4)	28(7)	510(0)	495(0)	492(0)	1157(5)	1192(5)	1194(9)
43(0)	45(1)	46(1)	515(3)	497(20)	493(21)	1158(0)	1193(0)	1194(0)
49(1)	47(0)	64(0)	539(0)	528(0)	533(0)	1212(17)	1242(22)	1244(26)
65(1)	65(1)	69(1)	542(33)	534(38)	544(46)	1212(0)	1242(0)	1245(0)
79(0)	72(0)	77(0)	557(73)	564(76)	557(71)	1354(4)	1387(1)	1406(2)
81(4)	90(4)	95(4)	561(0)	570(0)	569(0)	1354(0)	1388(0)	1406(0)
99(0)	97(0)	100(0)	586(63)	592(75)	590(75)	1434(0)	1476(0)	1483(0)
102(1)	101(0)	107(0)	590(0)	599(0)	592(0)	1435(9)	1476(6)	1484(15)
131(0)	123(0)	126(0)	615(0)	642(0)	646(0)	1468(7)	1506(5)	1523(10)
133(0)	128(0)	131(0)	618(2)	645(3)	648(2)	1468(0)	1506(0)	1523(0)
151(0)	144(1)	139(0)	711(0)	737(0)	753(0)	1492(18)	1532(0)	1541(26)
154(1)	147(0)	148(1)	712(4)	738(5)	755(9)	1493(0)	1532(23)	1542(0)
164(0)	161(0)	149(0)	771(23)	800(0)	811(0)	1878(0)	1974(0)	1979(0)
190(0)	182(0)	172(0)	772(0)	800(18)	811(27)	1889(915)	1989(1166)	1996(1304)
240(17)	280(16)	265(14)	857(0)	868(0)	893(10)	1952(1187)	2038(1296)	2054(1325)
275(0)	302(0)	284(0)	857(17)	870(6)	894(0)	1965(0)	2053(0)	2065(0)
298(2)	330(1)	326(5)	880(0)	896(2)	912(0)	3064(0)	3117(57)	3138(19)
321(0)	341(0)	335(0)	881(0)	897(0)	913(2)	3064(17)	3117(0)	3138(0)
336(1)	362(3)	351(0)	912(0)	943(0)	951(0)	3090(0)	3141(0)	3165(0)
377(0)	403(0)	400(0)	913(4)	943(3)	951(4)	3090(3)	3141(14)	3165(3)
402(18)	419(9)	410(12)	933(0)	954(1)	976(2)	3106(3)	3165(9)	3180(3)
402(0)	421(0)	411(0)	933(1)	954(0)	976(0)	3106(0)	3165(0)	3180(0)
408(0)	438(0)	421(0)	935(6)	960(13)	982(9)	3119(9)	3182(36)	3197(7)
413(4)	442(1)	426(3)	936(0)	961(0)	984(0)	3119(0)	3182(0)	3197(0)
442(5)	459(1)	457(1)	1036(14)	1067(13)	1071(19)	3154(10)	3214(29)	3222(0)
448(0)	460(0)	459(0)	1037(0)	1067(0)	1072(0)	3154(0)	3214(0)	3222(12)
462(0)	482(0)	485(12)	1046(3)	1081(7)	1080(3)	3181(2)	3239(11)	3254(3)
467(1)	486(3)	486(0)	1046(0)	1081(0)	1080(0)	3182(0)	3239(0)	3254(0)

Table S35. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **4T-3** of $(\eta^4\text{-}C_4H_6)_2Fe_2(CO)_4$ structure

BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP
20(0)	-8(0)	-17(0)	462(0)	469(7)	468(0)	1159(0)	1199(0)	1206(0)
29(1)	44(1)	-17(3)	485(2)	482(4)	481(5)	1160(2)	1199(2)	1206(2)
69(1)	66(0)	30(1)	485(0)	492(2)	486(6)	1197(15)	1236(24)	1242(33)
81(0)	76(0)	72(0)	504(1)	495(0)	495(0)	1199(1)	1238(1)	1243(2)
82(0)	84(0)	82(0)	513(120)	500(2)	503(2)	1350(8)	1384(4)	1405(6)
82(0)	89(0)	88(0)	524(136)	519(270)	504(265)	1350(0)	1385(0)	1405(0)
87(0)	95(1)	92(0)	533(27)	537(38)	531(46)	1429(0)	1469(0)	1473(5)
120(0)	103(0)	99(0)	555(51)	547(55)	542(63)	1430(4)	1470(3)	1474(6)
125(0)	122(0)	121(0)	631(0)	652(0)	645(0)	1469(20)	1510(20)	1531(22)
136(0)	133(0)	125(3)	631(1)	652(3)	645(2)	1469(0)	1511(0)	1531(0)
157(3)	157(2)	137(0)	770(1)	787(1)	787(2)	1476(20)	1518(25)	1533(34)
208(0)	204(0)	166(5)	770(0)	787(0)	789(9)	1477(4)	1519(1)	1533(3)
215(0)	216(0)	202(0)	770(0)	789(0)	791(2)	1810(796)	1899(996)	1894(1079)
234(0)	216(2)	211(0)	772(10)	791(8)	791(0)	1823(65)	1920(175)	1920(101)
290(0)	309(7)	258(1)	869(1)	896(1)	903(3)	1959(341)	2036(331)	2037(465)
322(17)	315(0)	279(0)	876(12)	901(12)	910(25)	1989(1177)	2080(1278)	2081(1350)
333(6)	334(16)	298(18)	894(0)	903(0)	924(0)	3080(18)	3136(54)	3162(0)
346(2)	359(1)	340(2)	896(1)	903(0)	925(0)	3080(3)	3136(8)	3162(3)
348(1)	363(0)	346(0)	910(1)	925(0)	937(2)	3083(5)	3140(21)	3163(11)
376(0)	391(1)	372(1)	911(12)	925(4)	938(4)	3083(0)	3140(0)	3163(3)
390(3)	392(0)	377(0)	921(0)	946(1)	965(1)	3111(0)	3173(5)	3188(0)
408(2)	412(4)	387(18)	923(0)	947(0)	966(0)	3111(1)	3173(0)	3189(1)
417(6)	423(7)	402(0)	934(2)	954(4)	968(0)	3124(0)	3187(31)	3202(0)
418(1)	426(0)	423(3)	934(1)	954(0)	969(0)	3124(10)	3187(0)	3202(7)
445(0)	445(6)	431(1)	1035(0)	1066(0)	1075(5)	3172(3)	3235(7)	3252(0)
449(1)	457(3)	437(1)	1036(3)	1066(2)	1075(0)	3172(2)	3235(4)	3252(3)
453(0)	463(2)	455(7)	1044(3)	1075(8)	1075(0)	3173(0)	3237(0)	3254(3)
453(5)	464(0)	467(6)	1044(0)	1075(1)	1076(5)	3173(3)	3237(14)	3254(1)

Table S36. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **4S-4** of $(\eta^4\text{-}C_4H_6)_2Fe_2(CO)_4$ structure

BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP
31(0)	32(1)	31(0)	493(14)	489(10)	483(4)	1169(0)	1200(0)	1204(0)
39(1)	37(0)	39(1)	495(2)	497(8)	487(25)	1170(2)	1201(2)	1204(3)
57(0)	78(1)	80(1)	521(38)	522(16)	527(18)	1209(1)	1237(2)	1239(2)
88(0)	83(0)	89(0)	536(9)	528(27)	528(68)	1209(18)	1239(23)	1241(31)
92(1)	88(1)	92(0)	540(8)	538(43)	536(56)	1356(0)	1386(3)	1405(5)
95(0)	92(1)	95(0)	565(1)	545(7)	543(59)	1356(8)	1387(0)	1405(0)
97(1)	94(0)	100(0)	616(59)	596(223)	569(142)	1422(5)	1469(5)	1474(7)
124(0)	111(0)	117(1)	618(61)	599(57)	605(59)	1424(1)	1471(0)	1476(6)
137(0)	144(0)	151(0)	625(1)	657(3)	649(3)	1481(2)	1512(15)	1524(8)
151(5)	153(1)	152(1)	640(176)	657(2)	649(1)	1481(16)	1512(0)	1524(21)
180(1)	177(0)	190(0)	755(0)	793(3)	794(0)	1484(6)	1521(2)	1529(17)
213(2)	221(1)	209(0)	756(8)	794(6)	794(6)	1485(24)	1522(25)	1529(10)
247(2)	238(0)	244(0)	784(0)	810(0)	805(2)	1789(769)	1879(741)	1876(640)
267(0)	269(3)	262(2)	785(5)	810(4)	805(2)	1815(56)	1904(243)	1893(422)
304(21)	347(11)	320(14)	879(9)	898(4)	907(19)	1965(214)	2043(258)	2045(341)
312(16)	358(7)	331(7)	880(4)	904(4)	913(3)	1990(1137)	2078(1282)	2078(1351)
322(0)	360(7)	332(3)	890(4)	914(3)	934(0)	3082(2)	3133(56)	3155(4)
332(2)	370(21)	345(23)	891(2)	915(0)	935(1)	3082(10)	3133(8)	3155(3)
346(1)	377(2)	349(2)	909(0)	936(0)	941(2)	3087(3)	3136(0)	3158(8)
371(1)	386(1)	359(2)	911(3)	936(7)	942(4)	3087(2)	3136(19)	3158(3)
402(1)	409(1)	380(8)	918(5)	953(6)	971(1)	3110(1)	3169(11)	3185(1)
405(3)	417(2)	394(3)	920(3)	953(2)	971(2)	3110(2)	3169(0)	3186(3)
438(11)	446(6)	429(5)	933(0)	959(0)	977(5)	3126(0)	3190(1)	3210(0)
440(4)	446(14)	439(2)	933(3)	959(2)	980(1)	3126(6)	3190(25)	3210(5)
453(0)	463(1)	458(1)	1037(2)	1066(0)	1073(0)	3176(1)	3231(7)	3244(2)
462(11)	472(3)	463(0)	1037(1)	1067(2)	1073(5)	3176(2)	3231(6)	3244(2)
462(2)	481(10)	471(5)	1043(1)	1077(8)	1078(5)	3180(0)	3234(1)	3249(2)
467(1)	483(14)	480(9)	1043(3)	1078(1)	1078(0)	3180(1)	3235(12)	3249(2)

Table S37. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **3S-1** of $(\eta^4\text{-}C_4H_6)_2Fe_2(CO)_3$ structure

BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP
45(1)	65(1)	-82(10)	504(0)	526(1)	500(16)	1152(3)	1191(4)	1193(4)
48(0)	65(1)	47(0)	533(29)	533(17)	520(28)	1189(0)	1227(0)	1227(0)
56(0)	73(0)	60(1)	533(23)	535(31)	528(26)	1190(16)	1228(25)	1228(27)
81(0)	80(1)	76(1)	559(7)	562(14)	571(17)	1346(1)	1383(0)	1400(1)
83(1)	90(3)	79(0)	565(40)	571(58)	575(48)	1347(2)	1384(1)	1401(1)
88(2)	97(0)	89(0)	645(2)	673(3)	664(2)	1430(1)	1475(1)	1479(0)
123(0)	109(3)	92(1)	645(1)	673(2)	665(2)	1431(4)	1476(3)	1481(7)
128(0)	122(0)	122(0)	746(0)	772(4)	780(2)	1462(3)	1502(4)	1517(10)
137(0)	135(0)	134(1)	747(0)	777(0)	784(0)	1462(7)	1502(10)	1517(4)
141(0)	163(1)	153(0)	760(9)	791(6)	793(5)	1472(3)	1515(0)	1523(2)
167(1)	164(0)	158(2)	769(3)	797(5)	797(4)	1472(10)	1515(13)	1523(20)
237(0)	242(0)	226(0)	868(0)	887(0)	899(3)	1867(737)	1960(898)	1980(942)
330(0)	350(0)	320(18)	868(7)	889(0)	900(1)	1900(864)	1990(976)	2013(1029)
331(4)	355(1)	334(0)	887(2)	905(2)	927(4)	1925(62)	2016(60)	2035(71)
353(9)	361(26)	338(8)	889(0)	908(1)	929(0)	3063(8)	3118(34)	3141(3)
368(8)	392(3)	368(3)	906(7)	930(7)	942(7)	3063(8)	3118(20)	3141(9)
390(63)	409(44)	394(53)	909(2)	932(2)	943(2)	3069(13)	3123(28)	3144(1)
398(0)	411(1)	411(5)	920(0)	946(1)	969(3)	3069(2)	3124(12)	3144(15)
408(1)	429(4)	419(1)	921(1)	947(1)	970(1)	3104(0)	3161(2)	3179(1)
420(10)	432(11)	424(3)	935(6)	959(7)	973(4)	3104(1)	3161(5)	3179(1)
424(3)	440(4)	427(6)	935(0)	959(0)	973(0)	3116(10)	3176(35)	3193(8)
426(1)	441(2)	436(1)	1028(1)	1059(1)	1066(2)	3116(2)	3176(7)	3193(2)
455(0)	471(2)	457(0)	1028(4)	1059(3)	1066(6)	3151(13)	3212(29)	3227(8)
456(6)	478(1)	481(0)	1046(8)	1082(15)	1079(11)	3151(0)	3212(0)	3227(1)
463(0)	479(1)	483(2)	1047(0)	1082(0)	1080(0)	3156(2)	3216(1)	3229(6)
463(2)	482(3)	488(33)	1152(1)	1190(1)	1193(2)	3156(6)	3216(19)	3229(6)

Table S38. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **3T-2** of $(\eta^4\text{-}C_4H_6)_2Fe_2(CO)_3$ structure

BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP
16(0)	36(0)	12(0)	476(5)	486(1)	488(1)	1175(3)	1216(3)	1220(4)
38(1)	44(1)	41(1)	504(46)	505(62)	506(63)	1193(8)	1229(12)	1228(13)
71(1)	75(0)	46(1)	535(41)	546(56)	551(66)	1228(12)	1267(15)	1273(30)
78(0)	79(1)	80(1)	563(197)	564(204)	559(305)	1347(2)	1384(1)	1400(1)
81(1)	87(1)	88(1)	581(1)	578(60)	583(60)	1358(1)	1392(0)	1411(1)
100(0)	94(0)	99(3)	585(45)	595(1)	589(1)	1421(7)	1457(4)	1465(20)
123(0)	116(0)	101(0)	642(2)	671(3)	663(2)	1431(2)	1479(1)	1482(4)
149(2)	136(1)	123(2)	670(7)	681(9)	675(16)	1463(8)	1504(8)	1518(9)
160(1)	144(3)	147(5)	690(1)	708(1)	710(0)	1474(11)	1519(12)	1529(18)
209(0)	202(0)	185(1)	761(1)	784(1)	798(2)	1492(25)	1539(31)	1541(53)
222(1)	213(0)	200(0)	773(7)	800(7)	805(3)	1497(4)	1545(5)	1555(5)
230(0)	219(0)	215(0)	845(16)	844(11)	860(15)	1810(793)	1899(958)	1901(1020)
263(11)	262(10)	221(10)	851(0)	846(0)	865(0)	1833(298)	1923(408)	1920(434)
283(3)	284(4)	264(3)	877(7)	896(4)	908(8)	1957(572)	2034(590)	2039(687)
339(7)	344(4)	321(7)	888(1)	903(0)	925(1)	3065(0)	3128(36)	3143(1)
345(4)	371(1)	336(2)	894(3)	918(2)	929(0)	3069(4)	3132(16)	3149(5)
352(1)	374(0)	356(0)	906(1)	924(1)	937(1)	3076(12)	3134(1)	3153(10)
380(4)	392(4)	380(5)	908(3)	931(3)	947(2)	3078(4)	3134(14)	3153(4)
398(0)	403(1)	386(1)	912(2)	933(1)	962(1)	3094(1)	3158(4)	3166(1)
411(13)	416(5)	398(1)	924(0)	954(0)	970(3)	3107(3)	3171(13)	3181(4)
414(6)	429(3)	399(13)	932(1)	962(3)	977(0)	3113(0)	3172(3)	3191(0)
427(14)	433(20)	417(19)	1032(1)	1059(5)	1061(4)	3125(7)	3186(24)	3204(6)
432(1)	444(9)	430(5)	1033(4)	1063(1)	1069(2)	3166(4)	3225(9)	3241(3)
457(17)	465(1)	444(21)	1039(8)	1071(7)	1079(9)	3167(2)	3226(11)	3242(4)
463(0)	468(1)	461(1)	1046(2)	1081(5)	1080(3)	3169(3)	3240(4)	3246(3)
470(0)	484(12)	477(18)	1156(1)	1193(2)	1196(2)	3171(2)	3240(12)	3248(2)

Table S39. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure $(\eta^2\text{-}C_4H_6)Fe(CO)_4$ structure

BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP
38(0)	38(0)	38(0)	466(5)	466(5)	466(5)	1104(1)	1104(1)	1104(1)
57(0)	57(0)	57(0)	484(8)	484(8)	484(8)	1235(27)	1235(27)	1235(27)
70(0)	70(0)	70(0)	490(25)	490(25)	490(25)	1317(1)	1317(1)	1317(1)
86(0)	86(0)	86(0)	493(5)	493(5)	493(5)	1406(2)	1406(2)	1406(2)
91(0)	91(0)	91(0)	555(11)	555(11)	555(11)	1442(7)	1442(7)	1442(7)
94(0)	94(0)	94(0)	565(3)	565(3)	565(3)	1528(11)	1528(11)	1528(11)
103(0)	103(0)	103(0)	594(73)	594(73)	594(73)	1679(27)	1679(27)	1679(27)
111(0)	111(0)	111(0)	641(108)	641(108)	641(108)	2053(1086)	2053(1086)	2053(1086)
143(0)	143(0)	143(0)	651(157)	651(157)	651(157)	2071(681)	2071(681)	2071(681)
197(2)	197(2)	197(2)	682(20)	682(20)	682(20)	2078(1043)	2078(1043)	2078(1043)
269(0)	269(0)	269(0)	790(5)	790(5)	790(5)	2142(286)	2142(286)	2142(286)
343(23)	343(23)	343(23)	880(2)	880(2)	880(2)	3132(20)	3132(20)	3132(20)
391(0)	391(0)	391(0)	892(39)	892(39)	892(39)	3138(13)	3138(13)	3138(13)
403(5)	403(5)	403(5)	909(3)	909(3)	909(3)	3142(14)	3142(14)	3142(14)
424(4)	424(4)	424(4)	932(2)	932(2)	932(2)	3153(14)	3153(14)	3153(14)
443(1)	443(1)	443(1)	1015(9)	1015(9)	1015(9)	3227(9)	3227(9)	3227(9)
455(10)	455(10)	455(10)	1054(2)	1054(2)	1054(2)	3244(21)	3244(21)	3244(21)

Table S40. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure $(\eta^4\text{-}C_4H_6)Fe(CO)_3$ structure

BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP
60(0)	71(1)	66(1)	515(0)	512(24)	514(1)	1150(2)	1188(2)	1190(3)
79(0)	77(0)	83(0)	524(13)	517(2)	523(23)	1187(4)	1224(7)	1223(9)
82(0)	79(0)	84(0)	587(76)	583(88)	581(94)	1345(2)	1384(0)	1398(1)
95(0)	90(0)	98(0)	627(61)	626(61)	625(65)	1436(3)	1483(3)	1483(5)
122(0)	117(0)	124(0)	636(101)	634(111)	633(115)	1459(3)	1500(3)	1516(4)
125(1)	123(0)	128(0)	649(6)	676(6)	667(5)	1476(8)	1519(8)	1529(11)
340(0)	368(0)	346(0)	768(2)	788(2)	795(2)	1967(682)	2049(805)	2056(805)
356(4)	381(3)	347(4)	785(4)	805(4)	807(2)	1977(897)	2057(1022)	2058(1015)
376(6)	383(2)	371(2)	876(8)	898(3)	906(8)	2030(532)	2114(621)	2112(700)
411(2)	419(3)	416(2)	893(0)	909(0)	925(1)	3076(11)	3129(28)	3151(8)
432(1)	465(2)	431(3)	912(4)	935(2)	944(3)	3080(4)	3134(16)	3152(5)
462(9)	469(0)	465(7)	927(0)	957(0)	968(1)	3115(1)	3176(4)	3188(1)
467(0)	475(8)	468(0)	934(0)	962(2)	974(0)	3128(8)	3191(24)	3202(8)
477(0)	487(1)	486(0)	1028(4)	1061(3)	1064(5)	3165(3)	3224(8)	3237(6)
507(0)	488(3)	487(9)	1044(0)	1081(1)	1077(1)	3166(5)	3226(18)	3238(4)

Table S41. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure $(\eta^4\text{-}C_4H_6)Fe(CO)_2$ structure

BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP
80(1)	80(0)	79(1)	580(35)	584(29)	566(35)	1198(4)	1228(6)	1233(8)
86(0)	85(1)	86(0)	614(38)	615(54)	609(60)	1345(1)	1381(0)	1396(0)
108(0)	106(0)	109(0)	630(13)	657(2)	650(2)	1431(5)	1472(6)	1481(4)
109(0)	109(0)	111(0)	713(2)	734(4)	734(4)	1457(4)	1491(3)	1508(4)
273(1)	306(1)	286(1)	762(10)	790(6)	788(11)	1472(9)	1519(8)	1520(15)
346(3)	371(2)	344(1)	837(5)	865(2)	877(5)	1937(893)	2022(1064)	2030(1101)
381(3)	399(2)	380(2)	865(6)	885(2)	895(4)	1986(663)	2074(785)	2079(843)
423(4)	440(5)	428(7)	917(2)	945(3)	948(3)	3042(15)	3098(34)	3121(13)
445(2)	467(1)	435(0)	931(1)	952(2)	974(1)	3071(2)	3129(13)	3146(3)
458(3)	472(1)	463(1)	953(3)	969(4)	981(4)	3077(5)	3143(15)	3155(5)
483(0)	492(4)	489(2)	1025(4)	1056(4)	1059(6)	3117(5)	3179(18)	3191(5)
519(5)	512(4)	504(7)	1036(3)	1073(4)	1069(3)	3140(6)	3202(17)	3210(8)
552(16)	541(39)	538(38)	1141(2)	1179(3)	1181(4)	3156(3)	3220(12)	3230(3)

Table S42. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure $(\eta^4\text{-}C_4H_6)Fe(CO)$ structure

BP86	M06-L	B3LYP	BP86	M06-L	B3LYP	BP86	M06-L	B3LYP
85(0)	92(0)	91(0)	686(11)	716(11)	719(8)	1340(1)	1382(0)	1396(0)
106(0)	106(0)	107(1)	735(10)	746(9)	746(17)	1431(8)	1466(8)	1486(6)
254(2)	270(2)	266(1)	813(7)	846(4)	862(4)	1434(1)	1480(2)	1497(3)
367(13)	394(8)	368(4)	893(0)	915(2)	928(6)	1461(4)	1519(3)	1513(6)
421(0)	444(0)	412(0)	912(6)	939(6)	939(9)	1932(848)	2025(1019)	2031(1093)
446(2)	463(0)	419(1)	919(8)	941(7)	958(1)	3025(5)	3090(23)	3118(12)
464(2)	476(6)	472(7)	936(2)	955(2)	965(4)	3025(18)	3094(34)	3118(5)
469(2)	489(2)	485(2)	1011(3)	1051(4)	1057(7)	3059(5)	3123(13)	3140(5)
545(1)	551(26)	539(2)	1028(5)	1067(8)	1059(5)	3074(17)	3140(41)	3158(14)
564(20)	559(3)	549(34)	1133(4)	1179(5)	1181(5)	3103(12)	3175(20)	3196(6)
636(1)	665(1)	652(2)	1180(2)	1219(4)	1228(5)	3103(4)	3178(19)	3197(8)