Supplementary Material (ESI) for New Journal of Chemistry

Neutral Homoleptic Tetranuclear Iron Carbonyls: Why Haven't They Been Synthesized as Stable Molecules?

Ting Ting Shi,[a] Qian-Shu Li,[*a,b] Yaoming Xie,[c] R. Bruce King,[*a,c]
and Henry F. Schaefer III[c]

[a]*Center for Computational Quantum Chemistry, South China Normal University, Guangzhou, 510631 China*
[b]*Institute of Chemical Physics, Beijing Institute of Technology, Beijing 100081, China*
[c]*Department of Chemistry and Center for Computational Chemistry University of Georgia, Athens, Georgia 30602, USA*

Supporting Information

Tables S1 to S9: Cartesian coordinates for the nine optimized $Fe_4(CO)_n$ (n = 16, 15, 14 structures,

Tables S10 to S18: Harmonic vibrational frequencies for the nine optimized $Fe_4(CO)_n$ (n = 16, 15, 14 structures,

Complete Gaussian reference (reference 27).

Table S1. Cartesian coordinates for the optimized $Fe_4(CO)_{16}$ structure **16-1**.

16-1	B3LYP			BP86		
	X	Y	Z	X	Y	Z
Fe	0.000000	2.070247	0.000000	0.000000	2.027989	0.000000
Fe	-2.070247	0.000000	0.000000	-2.027989	0.000000	0.000000
Fe	2.070247	0.000000	0.000000	2.027989	0.000000	0.000000
Fe	0.000000	-2.070247	0.000000	0.000000	-2.027989	0.000000
C	1.906720	0.583753	1.721529	1.864548	0.658343	1.690312
C	1.906720	-0.583753	-1.721529	1.864548	-0.658343	-1.690312
C	-1.906720	-0.583753	1.721529	-1.864548	-0.658343	1.690312
C	-1.906720	0.583753	-1.721529	-1.864548	0.658343	-1.690312
C	0.583753	1.906720	-1.721529	0.658343	1.864548	-1.690312
C	-0.583753	1.906720	1.721529	-0.658343	1.864548	1.690312
C	-0.583753	-1.906720	-1.721529	-0.658343	-1.864548	-1.690312
C	0.583753	-1.906720	1.721529	0.658343	-1.864548	1.690312
C	-1.241106	3.284065	-0.454163	-1.188885	3.258415	-0.500449
C	1.241106	3.284065	0.454163	1.188885	3.258415	0.500449
C	-1.241106	-3.284065	0.454163	-1.188885	-3.258415	0.500449
C	1.241106	-3.284065	-0.454163	1.188885	-3.258415	-0.500449
C	-3.284065	-1.241106	-0.454163	-3.258415	-1.188885	-0.500449
C	-3.284065	1.241106	0.454163	-3.258415	1.188885	0.500449
C	3.284065	-1.241106	0.454163	3.258415	-1.188885	0.500449
C	3.284065	1.241106	-0.454163	3.258415	1.188885	-0.500449
O	4.110779	-1.986776	0.757622	4.118734	-1.907593	0.831276
O	1.986776	-4.110779	-0.757622	1.907593	-4.118734	-0.831276
O	-1.986776	-4.110779	0.757622	-1.907593	-4.118734	0.831276
O	-4.110779	-1.986776	-0.757622	-4.118734	-1.907593	-0.831276
O	4.110779	1.986776	-0.757622	4.118734	1.907593	-0.831276
O	1.986776	4.110779	0.757622	1.907593	4.118734	0.831276
O	-4.110779	1.986776	0.757622	-4.118734	1.907593	0.831276
O	-1.986776	4.110779	-0.757622	-1.907593	4.118734	-0.831276
O	2.004163	0.899232	2.830611	1.994206	1.007761	2.800989
O	2.004163	-0.899232	-2.830611	1.994206	-1.007761	-2.800989
O	0.899232	-2.004163	2.830611	1.007761	-1.994206	2.800989
O	-0.899232	-2.004163	-2.830611	-1.007761	-1.994206	-2.800989
O	-2.004163	-0.899232	2.830611	-1.994206	-1.007761	2.800989
O	-2.004163	0.899232	-2.830611	-1.994206	1.007761	-2.800989
O	-0.899232	2.004163	2.830611	-1.007761	1.994206	2.800989
O	0.899232	2.004163	-2.830611	1.007761	1.994206	-2.800989

Table S2. Cartesian coordinates for the optimized $Fe_4(CO)_{16}$ structure **16-2**.

16-2	B3LYP			BP86		
	X	Y	Z	X	Y	Z
Fe	0.000000	2.076739	0.222036	0.000000	2.042588	0.216052
Fe	-2.076739	0.000000	-0.222036	-2.042588	0.000000	-0.216052
Fe	2.076739	0.000000	-0.222036	2.042588	0.000000	-0.216052
Fe	0.000000	-2.076739	0.222036	0.000000	-2.042588	0.216052
C	2.335606	0.000000	1.581859	2.318140	0.000000	1.577802
C	1.585332	0.000000	-1.977449	1.569763	0.000000	-1.967651
C	-2.335606	0.000000	1.581859	-2.318140	0.000000	1.577802
C	-1.585332	0.000000	-1.977449	-1.569763	0.000000	-1.967651
C	0.000000	2.335606	-1.581859	0.000000	2.318140	-1.577802
C	0.000000	1.585332	1.977449	0.000000	1.569763	1.967651
C	0.000000	-2.335606	-1.581859	0.000000	-2.318140	-1.577802
C	0.000000	-1.585332	1.977449	0.000000	-1.569763	1.967651
C	-1.322984	3.252810	0.496710	-1.298704	3.227386	0.493310
C	1.322984	3.252810	0.496710	1.298704	3.227386	0.493310
C	-1.322984	-3.252810	0.496710	-1.298704	-3.227386	0.493310
C	1.322984	-3.252810	0.496710	1.298704	-3.227386	0.493310
C	-3.252810	-1.322984	-0.496710	-3.227386	-1.298704	-0.493310
C	-3.252810	1.322984	-0.496710	-3.227386	1.298704	-0.493310
C	3.252810	-1.322984	-0.496710	3.227386	-1.298704	-0.493310
C	3.252810	1.322984	-0.496710	3.227386	1.298704	-0.493310
O	4.077658	-2.104591	-0.701645	4.078024	-2.072681	-0.706236
O	2.104591	-4.077658	0.701645	2.072681	-4.078024	0.706236
O	-2.104591	-4.077658	0.701645	-2.072681	-4.078024	0.706236
O	-4.077658	-2.104591	-0.701645	-4.078024	-2.072681	-0.706236
O	4.077658	2.104591	-0.701645	4.078024	2.072681	-0.706236
O	2.104591	4.077658	0.701645	2.072681	4.078024	0.706236
O	-4.077658	2.104591	-0.701645	-4.078024	2.072681	-0.706236
O	-2.104591	4.077658	0.701645	-2.072681	4.078024	0.706236
O	2.656495	0.000000	2.691886	2.676127	0.000000	2.691049
O	1.467920	0.000000	-3.126273	1.482626	0.000000	-3.133564
O	0.000000	-1.467920	3.126273	0.000000	-1.482626	3.133564
O	0.000000	-2.656495	-2.691886	0.000000	-2.676127	-2.691049
O	-2.656495	0.000000	2.691886	-2.676127	0.000000	2.691049
O	-1.467920	0.000000	-3.126273	-1.482626	0.000000	-3.133564
O	0.000000	1.467920	3.126273	0.000000	1.482626	3.133564
O	0.000000	2.656495	-2.691886	0.000000	2.676127	-2.691049

Table S3. Cartesian coordinates for the optimized $Fe_4(CO)_{16}$ structure **16-3**.

16-3		B3LYP			BP86	
	X	Y	Z	X	Y	Z
Fe	0.188152	1.464582	0.000000	0.225575	1.415617	0.000000
Fe	-2.649131	0.135906	0.000000	-2.623389	0.202605	0.000000
Fe	2.649131	-0.135906	0.000000	2.623389	-0.202605	0.000000
Fe	-0.188152	-1.464582	0.000000	-0.225575	-1.415617	0.000000
C	2.609826	-0.067099	1.828223	2.614122	-0.109845	1.815238
C	2.609826	-0.067099	-1.828223	2.614122	-0.109845	-1.815238
C	-2.609826	0.067099	1.828223	-2.614122	0.109845	1.815238
C	-2.609826	0.067099	-1.828223	-2.614122	0.109845	-1.815238
C	0.044542	1.471091	-1.821418	0.050922	1.440415	-1.806153
C	0.044542	1.471091	1.821418	0.050922	1.440415	1.806153
C	-0.044542	-1.471091	-1.821418	-0.050922	-1.440415	-1.806153
C	-0.044542	-1.471091	1.821418	-0.050922	-1.440415	1.806153
C	-0.268401	3.178411	0.000000	-0.179205	3.128373	0.000000
C	2.005197	1.893508	0.000000	2.043779	1.842576	0.000000
C	-2.005197	-1.893508	0.000000	-2.043779	-1.842576	0.000000
C	0.268401	-3.178411	0.000000	0.179205	-3.128373	0.000000
C	-4.350781	-0.427701	0.000000	-4.336173	-0.273419	0.000000
C	-2.954139	1.932615	0.000000	-2.879882	1.999708	0.000000
C	2.954139	-1.932615	0.000000	2.879882	-1.999708	0.000000
C	4.350781	0.427701	0.000000	4.336173	0.273419	0.000000
O	3.330073	-3.024668	0.000000	3.244258	-3.110385	0.000000
O	0.493853	-4.310850	0.000000	0.371478	-4.282789	0.000000
O	-2.700109	-2.852772	0.000000	-2.767977	-2.791997	0.000000
O	-5.452890	-0.761268	0.000000	-5.469293	-0.551998	0.000000
O	5.452890	0.761268	0.000000	5.469293	0.551998	0.000000
O	2.700109	2.852772	0.000000	2.767977	2.791997	0.000000
O	-3.330073	3.024668	0.000000	-3.244258	3.110385	0.000000
O	-0.493853	4.310850	0.000000	-0.371478	4.282789	0.000000
O	2.690671	-0.023464	2.976435	2.734292	-0.055164	2.973981
O	2.690671	-0.023464	-2.976435	2.734292	-0.055164	-2.973981
O	0.044542	-1.601654	2.964796	0.050922	-1.611898	2.958489
O	0.044542	-1.601654	-2.964796	0.050922	-1.611898	-2.958489
O	-2.690671	0.023464	2.976435	-2.734292	0.055164	2.973981
O	-2.690671	0.023464	-2.976435	-2.734292	0.055164	-2.973981
O	-0.044542	1.601654	2.964796	-0.050922	1.611898	2.958489
O	-0.044542	1.601654	-2.964796	-0.050922	1.611898	-2.958489

Table S4. Cartesian coordinates for the optimized $Fe_4(CO)_{16}$ structure **16-4**

16-4	B3LYP			BP86		
	X	Y	Z	X	Y	Z
Fe	0.000000	2.112619	0.000000	0.000000	2.075617	0.000000
Fe	-2.112619	0.000000	0.000000	-2.075617	0.000000	0.000000
Fe	2.112619	0.000000	0.000000	2.075617	0.000000	0.000000
Fe	0.000000	-2.112619	0.000000	0.000000	-2.075617	0.000000
C	1.988842	0.000000	1.818722	1.971681	0.000000	1.812211
C	1.988842	0.000000	-1.818722	1.971681	0.000000	-1.812211
C	-1.988842	0.000000	1.818722	-1.971681	0.000000	1.812211
C	-1.988842	0.000000	-1.818722	-1.971681	0.000000	-1.812211
C	0.000000	1.988842	-1.818722	0.000000	1.971681	-1.812211
C	0.000000	1.988842	1.818722	0.000000	1.971681	1.812211
C	0.000000	-1.988842	-1.818722	0.000000	-1.971681	-1.812211
C	0.000000	-1.988842	1.818722	0.000000	-1.971681	1.812211
C	-1.303883	3.339482	0.000000	-1.279349	3.311214	0.000000
C	1.303883	3.339482	0.000000	1.279349	3.311214	0.000000
C	-1.303883	-3.339482	0.000000	-1.279349	-3.311214	0.000000
C	1.303883	-3.339482	0.000000	1.279349	-3.311214	0.000000
C	-3.339482	-1.303883	0.000000	-3.311214	-1.279349	0.000000
C	-3.339482	1.303883	0.000000	-3.311214	1.279349	0.000000
C	3.339482	-1.303883	0.000000	3.311214	-1.279349	0.000000
C	3.339482	1.303883	0.000000	3.311214	1.279349	0.000000
O	4.211778	-2.060301	0.000000	4.210897	-2.026644	0.000000
O	2.060301	-4.211778	0.000000	2.026644	-4.210897	0.000000
O	-2.060301	-4.211778	0.000000	-2.026644	-4.210897	0.000000
O	-4.211778	-2.060301	0.000000	-4.210897	-2.026644	0.000000
O	4.211778	2.060301	0.000000	4.210897	2.026644	0.000000
O	2.060301	4.211778	0.000000	2.026644	4.210897	0.000000
O	-4.211778	2.060301	0.000000	-4.210897	2.026644	0.000000
O	-2.060301	4.211778	0.000000	-2.026644	4.210897	0.000000
O	2.097610	0.000000	2.968849	2.117527	0.000000	2.972475
O	2.097610	0.000000	-2.968849	2.117527	0.000000	-2.972475
O	0.000000	-2.097610	2.968849	0.000000	-2.117527	2.972475
O	0.000000	-2.097610	-2.968849	0.000000	-2.117527	-2.972475
O	-2.097610	0.000000	2.968849	-2.117527	0.000000	2.972475
O	-2.097610	0.000000	-2.968849	-2.117527	0.000000	-2.972475
O	0.000000	2.097610	2.968849	0.000000	2.117527	2.972475
O	0.000000	2.097610	-2.968849	0.000000	2.117527	-2.972475

Table S5. Cartesian coordinates for the optimized $Fe_4(CO)_{15}$ structure **15-1**

15-1		B3LYP			BP86	
	X	Y	Z	X	Y	Z
Fe	-1.329271	0.039418	0.000000	-1.342218	0.017306	0.000000
Fe	-0.088809	-2.376918	0.000000	-0.007288	-2.370168	0.000000
Fe	-0.053167	2.424401	0.000000	-0.002789	2.349128	0.000000
Fe	1.532151	-0.002827	0.000000	1.404071	0.031345	0.000000
C	0.102313	2.569280	1.820746	0.049086	2.558943	1.805667
C	0.102313	2.569280	-1.820746	0.049086	2.558943	-1.805667
C	-0.088684	-2.349853	1.822689	-0.032707	-2.344835	1.814305
C	-0.088684	-2.349853	-1.822689	-0.032707	-2.344835	-1.814305
C	-1.403206	0.061582	-1.821789	-1.429858	0.013835	-1.808869
C	-1.403206	0.061582	1.821789	-1.429858	0.013835	1.808869
C	1.474066	-0.036124	-1.819129	1.411898	-0.027992	-1.811888
C	1.474066	-0.036124	1.819129	1.411898	-0.027992	1.811888
C	-3.031488	-0.475349	0.000000	-2.996737	-0.601486	0.000000
C	2.908580	-1.145302	0.000000	2.974299	-0.802447	0.000000
C	2.458358	1.540106	0.000000	2.113666	1.746718	0.000000
C	1.122434	-3.715199	0.000000	1.296688	-3.593704	0.000000
C	-1.624991	-3.294533	0.000000	-1.414684	-3.458643	0.000000
C	0.075291	4.190175	0.000000	0.016933	4.108598	0.000000
C	-1.866337	2.132185	0.000000	-1.898269	1.938744	0.000000
O	0.129888	5.346315	0.000000	0.018759	5.280921	0.000000
O	3.254921	2.383668	0.000000	3.016164	2.510537	0.000000
O	3.842800	-1.825512	0.000000	4.027495	-1.310366	0.000000
O	1.865239	-4.596814	0.000000	2.127227	-4.414998	0.000000
O	-2.937636	2.614520	0.000000	-2.920587	2.545004	0.000000
O	-2.600596	-3.911427	0.000000	-2.325717	-4.189951	0.000000
O	-4.139523	-0.799922	0.000000	-4.101701	-0.987500	0.000000
O	0.208766	2.789386	2.946720	0.080993	2.841746	2.937793
O	0.208766	2.789386	-2.946720	0.080993	2.841746	-2.937793
O	1.604197	-0.024491	2.966778	1.597975	-0.011923	2.966007
O	1.604197	-0.024491	-2.966778	1.597975	-0.011923	-2.966007
O	-0.097711	-2.523745	2.963791	-0.059282	-2.554589	2.963679
O	-0.097711	-2.523745	-2.963791	-0.059282	-2.554589	-2.963679
O	-1.600828	0.121120	2.958200	-1.657918	0.061444	2.955469
O	-1.600828	0.121120	-2.958200	-1.657918	0.061444	-2.955469

Table S6. Cartesian coordinates for the optimized $Fe_4(CO)_{15}$ structure **15-2**

15-2	B3LYP			BP86		
	X	Y	Z	X	Y	Z
Fe	0.000000	0.000000	-1.296971	0.000000	0.000000	-1.423809
Fe	0.000000	2.397892	-0.123317	0.000000	2.322325	0.093927
Fe	0.000000	-2.397892	-0.123317	0.000000	-2.322325	0.093927
Fe	0.000000	0.000000	1.562292	0.000000	0.000000	1.463182
C	1.823274	-2.429913	-0.028902	1.806053	-2.490804	0.196200
C	-1.823274	-2.429913	-0.028902	-1.806053	-2.490804	0.196200
C	1.823274	2.429913	-0.028902	1.806053	2.490804	0.196200
C	-1.823274	2.429913	-0.028902	-1.806053	2.490804	0.196200
C	-1.818022	0.000000	-1.389948	-1.814968	0.000000	-1.436664
C	1.818022	0.000000	-1.389948	1.814968	0.000000	-1.436664
C	-1.818308	0.000000	1.499497	-1.812671	0.000000	1.448841
C	1.818308	0.000000	1.499497	1.812671	0.000000	1.448841
C	0.000000	0.000000	-3.073457	0.000000	0.000000	-3.192331
C	0.000000	1.373394	2.710202	0.000000	1.382194	2.600791
C	0.000000	-1.373394	2.710202	0.000000	-1.382194	2.600791
C	0.000000	3.958849	0.769563	0.000000	4.063878	0.369793
C	0.000000	2.835678	-1.850145	0.000000	2.217147	-1.731824
C	0.000000	-3.958849	0.769563	0.000000	-4.063878	0.369793
C	0.000000	-2.835678	-1.850145	0.000000	-2.217147	-1.731824
O	0.000000	-4.990796	1.286568	0.000000	-5.223850	0.534336
O	0.000000	-2.169639	3.550223	0.000000	-2.150827	3.487292
O	0.000000	2.169639	3.550223	0.000000	2.150827	3.487292
O	0.000000	4.990796	1.286568	0.000000	5.223850	0.534336
O	0.000000	-3.248669	-2.933137	0.000000	-2.803002	-2.763981
O	0.000000	3.248669	-2.933137	0.000000	2.803002	-2.763981
O	0.000000	0.000000	-4.228297	0.000000	0.000000	-4.358714
O	2.961023	-2.609982	0.028338	2.941029	-2.762411	0.236254
O	-2.961023	-2.609982	0.028338	-2.941029	-2.762411	0.236254
O	2.966471	0.000000	1.627714	2.968496	0.000000	1.622570
O	-2.966471	0.000000	1.627714	-2.968496	0.000000	1.622570
O	2.961023	2.609982	0.028338	2.941029	2.762411	0.236254
O	-2.961023	2.609982	0.028338	-2.941029	2.762411	0.236254
O	2.952187	0.000000	-1.612735	2.974865	0.000000	-1.577991
O	-2.952187	0.000000	-1.612735	-2.974865	0.000000	-1.577991

Table S7. Cartesian coordinates for the optimized $Fe_4(CO)_{14}$ structure **14-1**

14-1		B3LYP			BP86	
	X	Y	Z	X	Y	Z
Fe	1.332237	0.000000	0.910378	1.305208	0.000000	0.921109
Fe	-1.332237	0.000000	0.910378	-1.305208	0.000000	0.921109
Fe	0.000000	1.332237	-0.910378	0.000000	1.305208	-0.921109
Fe	0.000000	-1.332237	-0.910378	0.000000	-1.305208	-0.921109
C	-1.299517	2.241616	-1.762933	-1.270531	2.247323	-1.751682
C	0.000000	2.414565	0.509574	0.000000	2.347766	0.532005
C	1.299517	2.241616	-1.762933	1.270531	2.247323	-1.751682
C	0.000000	-2.414565	0.509574	0.000000	-2.347766	0.532005
C	1.299517	-2.241616	-1.762933	1.270531	-2.247323	-1.751682
C	-1.299517	-2.241616	-1.762933	-1.270531	-2.247323	-1.751682
C	0.000000	0.000000	-2.431830	0.000000	0.000000	-2.452885
C	2.241616	-1.299517	1.762933	2.247323	-1.270531	1.751682
C	2.241616	1.299517	1.762933	2.247323	1.270531	1.751682
C	2.414565	0.000000	-0.509574	2.347766	0.000000	-0.532005
C	-2.241616	1.299517	1.762933	-2.247323	1.270531	1.751682
C	-2.241616	-1.299517	1.762933	-2.247323	-1.270531	1.751682
C	-2.414565	0.000000	-0.509574	-2.347766	0.000000	-0.532005
O	0.000000	0.000000	2.431830	0.000000	0.000000	2.452885
O	-2.890976	-2.088599	2.296819	-2.936140	-2.049320	2.284347
O	-2.890976	2.088599	2.296819	-2.936140	2.049320	2.284347
O	-3.282075	0.000000	-1.283795	-3.234559	0.000000	-1.305277
O	0.000000	0.000000	3.599019	0.000000	0.000000	3.634533
O	2.890976	-2.088599	2.296819	2.936140	-2.049320	2.284347
O	2.890976	2.088599	2.296819	2.936140	2.049320	2.284347
O	3.282075	0.000000	-1.283795	3.234559	0.000000	-1.305277
O	-2.088599	-2.890976	-2.296819	-2.049320	-2.936140	-2.284347
O	2.088599	-2.890976	-2.296819	2.049320	-2.936140	-2.284347
O	0.000000	-3.282075	1.283795	0.000000	-3.234559	1.305277
O	0.000000	0.000000	-3.599019	0.000000	0.000000	-3.634533
O	-2.088599	2.890976	-2.296819	-2.049320	2.936140	-2.284347
C	2.088599	2.890976	-2.296819	2.049320	2.936140	-2.284347
O	0.000000	3.282075	1.283795	0.000000	3.234559	1.305277

Table S8. Cartesian coordinates for the optimized $Fe_4(CO)_{14}$ structure **14-2**

14-2		B3LYP			BP86	
	X	Y	Z	X	Y	Z
Fe	1.595489	-0.129768	0.000000	0.086332	1.552510	0.000121
Fe	-0.170232	2.353391	0.000000	-2.336143	-0.168011	-0.000115
Fe	-0.470657	-2.190096	0.000000	2.186381	-0.431007	0.000063
Fe	-1.169940	0.211958	0.000000	-0.188309	-1.153550	-0.000085
C	-1.322467	-0.999403	1.398864	1.008490	-1.335339	1.397860
C	-0.424349	2.034377	1.770455	-2.015202	-0.460831	1.759556
C	-0.424349	2.034377	-1.770455	-2.015040	-0.460538	-1.759806
C	1.460090	-0.152274	-1.817765	0.121306	1.417477	-1.808757
C	1.460090	-0.152274	1.817765	0.121159	1.417178	1.808980
C	-1.322467	-0.999403	-1.398864	1.008607	-1.335125	-1.397959
C	2.868549	1.137417	0.000000	-1.141370	2.855053	0.000176
C	2.693373	-1.545052	0.000000	1.482553	2.662289	0.000266
C	-2.885019	0.638076	0.000000	-0.642531	-2.844913	-0.000233
C	-1.463344	3.582237	0.000000	-3.599295	-1.404107	-0.000280
C	1.165273	3.596906	0.000000	-3.564430	1.157250	-0.000062
C	-1.886935	-3.297791	0.000000	3.313322	-1.804817	0.000006
C	0.368627	-3.044657	1.369949	3.043314	0.395706	1.358545
O	-2.793869	-4.007492	0.000000	4.062513	-2.700566	-0.000025
O	-4.010861	0.905521	0.000000	-0.915100	-3.986980	-0.000335
O	-2.306226	4.369380	0.000000	-4.435545	-2.220405	-0.000395
O	0.870580	-3.628170	2.227104	3.654822	0.888100	2.222160
O	3.464766	-2.404972	0.000000	2.332518	3.465133	0.000340
O	1.976375	4.415733	0.000000	-4.403048	1.970330	-0.000032
O	3.775348	1.852749	0.000000	-1.834591	3.796203	0.000216
O	-1.676019	-1.038057	2.522232	1.080079	-1.719972	2.522490
O	-1.676019	-1.038057	-2.522232	1.080285	-1.719590	-2.522643
O	-0.632075	1.982159	2.907342	-1.973636	-0.716757	2.901191
O	-0.632075	1.982159	-2.907342	-1.973362	-0.716282	-2.901479
O	1.488785	-0.200758	2.969699	0.182376	1.465326	2.973576
O	1.488785	-0.200758	-2.969699	0.182618	1.465816	-2.973341
C	0.368627	-3.044657	-1.369949	3.043423	0.395910	-1.358224
O	0.870580	-3.628170	-2.227104	3.654996	0.888432	-2.221722

Table S9. Cartesian coordinates for the optimized $Fe_4(CO)_{14}$ structure **14-3**

14-3		B3LYP			BP86	
	X	Y	Z	X	Y	Z
Fe	0.000000	1.343269	0.917966	0.000000	1.325608	0.880998
Fe	-1.380939	0.000000	-0.887128	-1.400568	0.000000	-0.851510
Fe	0.000000	-1.343269	0.917966	0.000000	-1.325608	0.880998
Fe	1.380939	0.000000	-0.887128	1.400568	0.000000	-0.851510
C	3.190561	0.000000	-0.932796	3.185770	0.000000	-0.944844
C	1.362246	1.341130	-2.078292	1.370724	1.331306	-2.037218
C	1.362246	-1.341130	-2.078292	1.370724	-1.331306	-2.037218
C	-1.828364	-1.386688	0.920400	-1.840720	-1.376027	0.887584
C	-3.190561	0.000000	-0.932796	-3.185770	0.000000	-0.944844
C	1.828364	-1.386688	0.920400	1.840720	-1.376027	0.887584
C	-1.362246	1.341130	-2.078292	-1.370724	1.331306	-2.037218
C	-1.362246	-1.341130	-2.078292	-1.370724	-1.331306	-2.037218
C	1.828364	1.386688	0.920400	1.840720	1.376027	0.887584
C	-1.828364	1.386688	0.920400	-1.840720	1.376027	0.887584
C	0.000000	-3.086252	0.473285	0.000000	-3.069658	0.487182
C	0.000000	3.086252	0.473285	0.000000	3.069658	0.487182
C	0.000000	1.476388	2.702826	0.000000	1.467137	2.659868
O	-4.335764	0.000000	-1.030897	-4.344748	0.000000	-1.066335
O	4.335764	0.000000	-1.030897	4.344748	0.000000	-1.066335
O	-2.882924	-1.728046	1.293251	-2.886811	-1.755936	1.289140
O	2.882924	-1.728046	1.293251	2.886811	-1.755936	1.289140
O	1.484118	-2.200026	-2.839916	1.499134	-2.191087	-2.819015
O	-1.484118	-2.200026	-2.839916	-1.499134	-2.191087	-2.819015
O	0.000000	-4.215111	0.232450	0.000000	-4.222270	0.288516
O	-1.484118	2.200026	-2.839916	-1.499134	2.191087	-2.819015
O	1.484118	2.200026	-2.839916	1.499134	2.191087	-2.819015
O	2.882924	1.728046	1.293251	2.886811	1.755936	1.289140
O	0.000000	4.215111	0.232450	0.000000	4.222270	0.288516
O	-2.882924	1.728046	1.293251	-2.886811	1.755936	1.289140
O	0.000000	1.638441	3.845904	0.000000	1.646212	3.814530
C	0.000000	-1.476388	2.702826	0.000000	-1.467137	2.659868
O	0.000000	-1.638441	3.845904	0.000000	-1.646212	3.814530

Table S10. Harmonic vibrational frequencies for the optimized $Fe_4(CO)_{16}$ structure **16-1**.

16-1	B3LYP	13(0), 9(0), 43(0), 43(0), 44(0), 54(0), 58(0), 58(0), 65(0), 67(0), 69(0), 79(0), 79(0), 79(0), 89(0), 90(1), 98(0), 98(0), 104(0), 104(0), 104(0), 108(0), 109(0), 116(1), 116(1), 119(0), 126(0), 129(0), 131(0), 131(0), 136(0), 144(5), 144(5), 149(0), 153(0), 155(0), 159(0), 159(0), 378(0), 382(2), 382(2), 387(0), 399(0), 405(3), 405(33), 405(33), 413(3), 416(1), 416(1), 421(0), 422(0), 426(9), 426(9), 430(0), 456(1), 474(16), 474(16), 477(0), 477(0), 479(9), 479(9), 481(0), 509(3), 509(3), 511(0), 516(0), 523(0), 532(0), 532(0), 539(9), 549(0), 552(73), 552(21), 552(21), 562(0), 595(27), 595(27), 597(132), 599(0), 608(325), 608(325), 620(0), 621(0), 630(251), 630(251), 641(0), 2026(0), 2028(0), 2043(3), 2043(3), 2055(15), 2055(15), 2061(18), 2072(4), 2072(4), 2081(0), 2086(0), 2087(3486), 2092(0), 2115(3836), 2115(3836), 2170(0)
	BP86	29(0), 29(0), 29(0), 36(0), 41(0), 53(0), 58(0), 58(0), 59(0), 67(0), 74(0), 77(0), 77(0), 78(0), 86(0), 87(1), 94(0), 94(0), 96(0), 99(0), 99(0), 105(0), 109(0), 111(1), 111(1), 115(0), 121(0), 129(0), 129(1), 129(1), 131(0), 143(6), 143(6), 147(0), 155(0), 156(0), 162(0), 162(0), 368(0), 373(1), 373(1), 380(0), 397(4), 401(0), 402(25), 402(25), 417(1), 417(0), 417(0), 418(0), 426(0), 433(10), 433(10), 437(0), 459(1), 485(7), 485(7), 486(0), 493(0), 494(1), 494(1), 498(0), 513(0), 513(7), 513(7), 517(0), 525(0), 530(0), 530(0), 534(0), 535(0), 539(30), 539(30), 550(0), 562(75), 587(8), 587(8), 588(106), 589(0), 601(258), 601(258), 618(0), 619(0), 626(200), 626(200), 632(0), 1942(0), 1960(21), 1960(21), 1962(0), 1977(18), 1979(75), 1979(75), 1991(9), 1991(9), 2001(2870), 2002(0), 2005(0), 2012(0), 2038(2631), 2038(2631), 2081(0)

Table S11. Harmonic vibrational frequencies for the optimized $Fe_4(CO)_{16}$ structure **16-2**.

16-2	B3LYP	-17(0), 33(0), 34(0), 34(0), 38(0), 57(0), 57(0), 59(0), 66(0), 73(0), 73(0), 76(0), 85(0), 90(1), 96(0), 99(0), 99(0), 103(0), 107(0), 107(0), 113(0), 114(0), 116(2), 116(2), 117(0), 126(0), 126(0), 126(0), 131(0), 132(0), 137(0), 140(0), 140(0), 141(0), 155(0), 155(0), 159(0), 164(0), 400(0), 400(0), 400(0), 401(0), 404(0), 404(1), 404(1), 408(0), 410(0), 411(2), 412(2), 412(2), 416(31), 416(31), 418(0), 425(0), 453(0), 471(31), 471(31), 479(0), 479(2), 481(9), 481(9), 481(0), 521(0), 522(1), 522(1), 526(0), 529(0), 529(0), 535(34), 535(0), 553(0), 559(0), 559(0), 563(0), 576(0), 601(9), 601(9), 602(140), 603(0), 606(0), 613(219), 613(219), 633(365), 633(365), 633(29), 642(0), 2044(0), 2050(43), 2053(21), 2053(21), 2055(0), 2060(17), 2060(17), 2070(0), 2070(0), 2073(38), 2090(0), 2099(0), 2105(3280), 2112(3939), 2112(3939), 2174(0)
	BP86	-18(0), 24(0), 24(0), 25(0), 34(0), 52(0), 52(0), 56(0), 63(0), 66(0), 70(0), 70(0), 81(0), 87(1), 92(0), 96(0), 96(0), 102(0), 103(0), 103(0), 108(0), 110(0), 111(3), 111(3), 116(0), 121(0), 121(0), 123(0), 127(0), 129(0), 136(0), 138(0), 138(0), 139(0), 152(0), 153(0), 153(0), 158(0), 395(0), 395(0), 397(0), 397(0), 401(0), 401(0), 401(0), 403(0), 405(0), 409(0), 409(0), 413(0), 427(0), 430(21), 430(21), 437(0), 462(0), 482(15), 482(15), 488(0), 492(0), 493(0), 493(0), 495(0), 524(0), 526(1), 526(1), 528(0), 534(0), 534(0), 539(15), 539(0), 540(0), 546(0), 546(0), 549(0), 591(0), 592(134), 592(6), 592(6), 596(0), 601(0), 610(149), 610(149), 629(307), 629(307), 630(20), 634(0), 1961(0), 1971(27), 1971(27), 1971(0), 1979(80), 1982(76), 1982(76), 1993(78), 1993(78), 2004(0), 2007(168), 2017(0), 2020(2500), 2038(2621), 2038(2621), 2086(0)

Table S12. Harmonic vibrational frequencies for the optimized $Fe_4(CO)_{16}$ structure **16-3**.

16-3	B3LYP	13(0), 32(0), 43(0), 52(0), 55(0), 56(0), 60(0), 63(0), 66(0), 69(0), 81(0), 83(0), 84(0), 86(1), 90(0), 90(0), 94(2), 97(0), 97(2), 104(0), 106(0), 106(0), 114(0), 115(0), 118(0), 118(0), 120(0), 125(1), 128(0), 129(0), 136(0), 136(0), 136(0), 140(0), 149(0), 160(0), 239(12), 241(0), 363(0), 369(72), 380(0), 380(1), 393(0), 396(0), 403(0), 405(0), 409(0), 412(32), 413(0), 414(10), 423(0), 423(0), 432(0), 440(3), 447(28), 450(0), 465(38), 467(0), 478(16), 478(0), 486(0), 490(35), 493(5), 497(0), 503(0), 504(1), 506(0), 518(27), 523(0), 532(59), 557(7), 557(0), 564(0), 565(0), 597(36), 599(105), 599(0), 610(0), 621(0), 623(0), 625(122), 627(335), 629(417), 636(0), 661(154), 662(0), 1866(815), 1872(0), 2052(0), 2055(24), 2061(2), 2062(0), 2069(65), 2073(0), 2085(0), 2096(0), 2098(179), 2104(3072), 2111(0), 2113(3314), 2128(3459), 2177(0)
	BP86	9(0), 20(0), 41(0), 43(0), 48(0), 51(0), 56(0), 60(0), 64(0), 68(0), 78(0), 79(0), 80(0), 81(1), 86(0), 89(0), 92(1), 92(0), 92(1), 100(0), 103(0), 103(0), 109(0), 111(0), 115(0), 115(0), 116(0), 121(1), 127(0), 129(0), 132(0), 133(0), 136(0), 137(0), 148(1), 163(0), 238(10), 239(0), 364(0), 376(64), 377(1), 378(0), 389(3), 389(0), 400(0), 404(0), 413(0), 424(0), 425(0), 429(0), 430(20), 432(4), 434(0), 438(0), 454(24), 456(0), 469(14), 469(0), 475(0), 490(4), 494(0), 495(15), 500(33), 507(0), 511(0), 513(18), 514(0), 515(2), 517(0), 521(63), 542(0), 542(6), 548(0), 549(1), 588(21), 590(0), 596(38), 604(0), 613(0), 613(125), 618(0), 621(318), 629(361), 631(0), 653(162), 655(0), 1824(691), 1828(0), 1961(0), 1966(45), 1980(2), 1981(0), 1991(184), 1996(0), 1999(0), 2014(346), 2017(0), 2022(2761), 2025(2294), 2028(0), 2052(2470), 2090(0)

Table S13. Harmonic vibrational frequencies for the optimized $Fe_4(CO)_{16}$ structure **16-4**.

16-4	B3LYP	-23(0), -19(0), 32(0), 41(0), 41(0), 41(0), 60(0), 60(0), 61(0), 68(0), 76(0), 76(0), 80(0), 89(0), 90(1), 102(0), 102(0), 107(0), 109(0), 118(0), 118(3), 118(3), 122(0), 125(0), 129(0), 129(0), 130(0), 136(0), 136(0), 142(0), 147(0), 147(0), 150(0), 152(0), 155(0), 157(0), 157(0), 158(0), 402(0), 402(0), 404(0), 405(0), 405(0), 408(0), 409(2), 409(2), 410(0), 412(0), 413(0), 413(0), 416(34), 416(34), 416(1), 424(0), 454(0), 473(35), 473(35), 479(0), 481(0), 482(0), 483(11), 483(11), 529(3), 529(3), 530(0), 531(0), 533(0), 533(0), 536(35), 537(0), 556(0), 561(0), 561(0), 564(0), 580(0), 605(160), 605(0), 605(0), 606(0), 608(0), 616(237), 616(237), 633(0), 635(367), 635(367), 642(0), 2038(0), 2043(0), 2055(0), 2059(0), 2059(0), 2060(33), 2060(33), 2070(0), 2070(0), 2073(0), 2091(0), 2100(0), 2103(3364), 2114(4020), 2114(4020), 2174(0)
	BP86	-25(0), -22(0), 23(0), 31(0), 31(0), 40(0), 51(0), 56(0), 56(0), 65(0), 72(0), 72(0), 77(0), 85(0), 87(1), 99(0), 99(0), 103(0), 108(0), 113(3), 113(3), 116(0), 121(0), 122(0), 127(0), 127(0), 127(0), 131(0), 131(0), 138(0), 142(0), 142(0), 145(0), 147(0), 150(0), 154(0), 154(0), 155(0), 397(0), 397(0), 401(0), 401(0), 402(0), 405(0), 407(1), 407(1), 409(0), 409(0), 409(0), 413(0), 425(0), 430(21), 430(21), 436(0), 463(0), 483(18), 483(18), 489(0), 491(0), 496(0), 496(0), 499(0), 534(2), 534(2), 535(0), 535(0), 538(0), 538(0), 540(17), 543(0), 543(0), 548(0), 548(0), 550(0), 594(143), 596(0), 596(0), 596(0), 600(0), 600(0), 613(156), 613(156), 631(314), 631(314), 632(0), 634(0), 1955(0), 1971(0), 1972(0), 1976(0), 1976(0), 1980(21), 1980(21), 1994(126), 1994(126), 2005(0), 2009(0), 2016(2765), 2018(0), 2039(2671), 2039(2671), 2086(0)

Table S14. Harmonic vibrational frequencies for the optimized $Fe_4(CO)_{15}$ structure **15-1**.

15-1	B3LYP	20(0), 35(0), 38(0), 39(0), 52(0), 57(0), 60(0), 66(0), 71(0), 75(0), 78(0), 81(0), 84(0), 87(0), 90(0), 91(1), 94(1), 99(0), 100(0), 106(0), 107(0), 110(0), 112(0), 118(0), 120(3), 130(1), 135(0), 135(0), 139(0), 141(1), 146(0), 153(0), 158(0), 161(0), 171(0), 208(11), 315(14), 357(1), 393(1), 398(0), 402(0), 407(1), 409(9), 411(15), 411(0), 415(0), 417(0), 422(0), 424(1), 430(2), 447(22), 460(0), 461(13), 464(25), 475(10), 479(9), 485(2), 486(1), 486(22), 494(8), 499(3), 504(13), 511(21), 520(18), 531(14), 536(20), 556(11), 565(1), 566(0), 589(34), 603(11), 606(29), 609(22), 612(88), 613(63), 619(40), 621(74), 631(84), 641(117), 643(313), 653(61), 1940(431), 2038(240), 2045(0), 2050(6), 2060(77), 2062(136), 2069(155), 2071(343), 2072(14), 2074(507), 2096(19), 2102(2798), 2105(3364), 2117(2917), 2172(31)
	BP86	-22(0), 17(0), 26(1), 41(4), 46(0), 53(1), 54(0), 59(0), 62(1), 70(0), 75(1), 79(0), 82(1), 83(1), 85(0), 88(0), 91(1), 94(0), 96(0), 102(0), 106(1), 107(0), 113(1), 117(0), 125(1), 127(1), 130(0), 132(0), 140(0), 152(5), 156(0), 157(1), 162(0), 167(2), 184(0), 237(13), 305(26), 345(34), 389(0), 395(0), 404(0), 406(15), 408(0), 416(0), 421(0), 422(4), 426(6), 428(0), 432(4), 434(1), 436(8), 443(11), 460(1), 462(0), 463(12), 475(0), 481(1), 495(9), 497(6), 500(3), 506(10), 516(9), 526(16), 528(4), 533(0), 538(34), 541(8), 542(0), 548(0), 591(2), 593(35), 594(2), 594(8), 601(49), 609(94), 611(40), 618(22), 632(27), 636(237), 639(135), 647(99), 1854(443), 1897(395), 1956(2), 1964(13), 1981(90), 1983(6), 1985(134), 1992(265), 1995(33), 2003(16), 2014(2817), 2019(267), 2024(1938), 2041(2268), 2085(39)

Table S15. Harmonic vibrational frequencies for the optimized $Fe_4(CO)_{15}$ structure **15-2**.

15-2	B3LYP	-33(4), 16(0), 38(0), 40(0), 45(0), 50(0), 53(0), 64(0), 69(0), 77(0), 77(0), 78(0), 82(0), 86(1), 90(0), 93(1), 94(0), 95(0), 95(0), 102(0), 106(0), 112(0), 114(0), 115(0), 116(6), 123(2), 129(0), 134(0), 138(0), 142(0), 145(0), 146(0), 153(0), 156(0), 161(1), 195(1), 350(24), 365(0), 372(18), 398(0), 399(0), 409(4), 412(15), 412(7), 413(0), 414(0), 416(0), 420(0), 426(0), 428(25), 431(2), 465(15), 473(0), 477(45), 478(28), 478(0), 487(7), 490(7), 502(0), 504(13), 505(3), 507(0), 509(42), 509(0), 513(3), 538(18), 568(0), 574(7), 575(0), 580(99), 602(30), 603(0), 608(5), 611(75), 614(56), 616(80), 626(88), 629(95), 642(352), 642(140), 651(14), 2041(57), 2042(20), 2048(41), 2049(0), 2055(13), 2057(107), 2059(15), 2072(21), 2074(0), 2082(330), 2095(830), 2098(2651), 2105(3323), 2111(3549), 2173(0)
	BP86	27(0), 28(3), 39(0), 40(1), 45(0), 48(0), 53(0), 53(0), 60(2), 73(0), 76(0), 78(0), 80(0), 84(0), 87(0), 91(0), 91(0), 94(1), 103(0), 104(0), 105(0), 107(0), 112(1), 114(0), 119(0), 119(0), 133(0), 135(0), 136(0), 143(0), 149(0), 156(0), 160(0), 175(18), 182(0), 184(10), 316(10), 329(9), 344(1), 400(0), 403(0), 411(0), 415(0), 417(0), 424(2), 426(0), 431(0), 433(8), 433(0), 438(1), 451(1), 457(14), 458(0), 479(5), 479(10), 491(6), 495(27), 499(0), 499(1), 500(0), 515(1), 517(22), 518(11), 520(2), 527(0), 534(11), 546(18), 548(0), 556(0), 586(23), 590(0), 599(0), 603(6), 604(79), 609(87), 609(51), 613(47), 624(79), 639(116), 651(217), 656(17), 1876(124), 1877(465), 1964(13), 1967(17), 1967(79), 1976(235), 1984(0), 1989(120), 1991(686), 2006(167), 2015(23), 2016(2812), 2034(1490), 2036(2321), 2085(1)

Table S16. Harmonic vibrational frequencies for the optimized $Fe_4(CO)_{14}$ structure **14-1**.

14-1	B3LYP	-34(0), 13(0), 28(0), 28(0), 45(1), 58(0), 67(0), 71(0), 75(0), 80(0), 86(0), 86(0), 90(0), 92(0), 101(0), 103(0), 104(0), 106(0), 115(1), 119(0), 120(0), 122(0), 123(0), 125(1), 127(0), 128(0), 134(0), 146(0), 154(4), 162(6), 182(1), 193(2), 201(1), 220(0), 326(3), 342(1), 375(4), 384(1), 386(0), 393(6), 399(1), 409(2), 416(0), 421(7), 425(5), 426(1), 428(1), 445(17), 446(1), 451(17), 469(11), 470(12), 484(19), 487(21), 491(0), 492(18), 495(5), 500(0), 511(3), 523(18), 527(17), 532(3), 534(16), 560(0), 561(21), 565(157), 568(185), 585(12), 589(96), 590(1), 608(17), 613(3), 619(186), 622(246), 630(173), 641(29), 1965(247), 1976(930), 2000(167), 2021(278), 2024(55), 2037(72), 2078(3), 2087(77), 2089(305), 2090(192), 2104(2838), 2108(2996), 2108(2972), 2163(0)
	BP86	10(0), 16(0), 16(0), 43(0), 43(0), 56(0), 62(0), 67(0), 67(0), 76(0), 85(0), 85(0), 86(0), 90(0), 100(0), 100(0), 102(0), 106(0), 113(0), 119(0), 119(1), 120(0), 120(0), 121(0), 125(0), 125(0), 138(0), 142(0), 173(2), 173(2), 198(9), 198(9), 202(1), 228(0), 331(9), 331(9), 377(0), 377(0), 383(7), 384(0), 393(0), 393(0), 405(0), 416(3), 417(11), 417(11), 426(0), 439(36), 439(36), 444(0), 476(0), 476(0), 496(0), 501(2), 501(2), 505(0), 506(0), 507(0), 523(2), 523(2), 526(0), 531(0), 541(5), 550(87), 550(87), 555(70), 555(70), 579(0), 584(0), 589(65), 604(3), 604(3), 615(215), 615(215), 618(153), 633(0), 1888(0), 1892(792), 1947(94), 1947(94), 1950(0), 1950(155), 1991(0), 2000(0), 2003(467), 2003(467), 2026(1917), 2028(2119), 2028(2119), 2071(0)

Table S17. Harmonic vibrational frequencies for the optimized $Fe_4(CO)_{14}$ structure **14-2**

14-2	B3LYP	23(0), 42(0), 42(0), 48(0), 55(0), 56(0), 67(0), 68(0), 77(0), 79(0), 80(0), 84(0), 85(0), 86(0), 88(0), 94(0), 98(0), 100(1), 102(0), 103(0), 108(0), 109(0), 111(1), 113(0), 117(1), 128(3), 140(0), 144(1), 148(0), 152(0), 187(1), 201(0), 236(2), 281(1), 299(1), 385(0), 391(0), 402(25), 402(0), 404(0), 409(1), 410(0), 415(12), 419(1), 425(33), 431(5), 435(0), 455(12), 457(4), 466(3), 466(28), 471(6), 474(2), 479(5), 481(10), 504(6), 510(8), 513(6), 518(0), 520(2), 525(10), 531(22), 536(12), 547(4), 560(2), 565(2), 581(23), 593(151), 605(39), 606(209), 615(70), 615(45), 621(34), 624(272), 637(166), 676(169), 1894(518), 1925(142), 2047(271), 2056(155), 2063(11), 2067(236), 2076(37), 2080(373), 2091(115), 2098(624), 2102(1976), 2108(2273), 2121(3550), 2168(54)
	BP86	17(0), 38(0), 38(0), 45(0), 50(0), 50(0), 63(0), 65(0), 70(0), 76(0), 76(0), 81(0), 82(1), 83(0), 85(0), 91(0), 93(0), 97(0), 101(0), 102(0), 103(0), 106(0), 107(0), 109(0), 115(1), 127(3), 138(0), 142(1), 144(0), 152(0), 189(1), 212(0), 234(0), 278(2), 306(1), 371(0), 382(0), 396(0), 399(0), 401(16), 405(0), 409(7), 414(0), 427(23), 431(10), 432(0), 437(6), 452(0), 454(13), 473(4), 474(6), 481(1), 482(7), 491(2), 496(2), 498(2), 506(0), 510(3), 517(2), 521(3), 527(5), 537(1), 543(16), 547(3), 556(1), 559(10), 573(70), 586(72), 596(43), 606(141), 609(54), 611(37), 617(0), 623(227), 627(170), 660(127), 1841(340), 1857(89), 1967(195), 1976(273), 1983(58), 1987(14), 1995(132), 1995(235), 2006(96), 2013(741), 2014(1830), 2032(1293), 2041(2584), 2079(79)

Table S18. Harmonic vibrational frequencies for the optimized $Fe_4(CO)_{14}$ structure **14-3**

14-3	B3LYP	–29(0), 25(0), 34(1), 54(0), 55(0), 58(0), 60(0), 71(0), 73(0), 74(0), 84(0), 85(1), 86(1), 93(0), 98(0), 103(0), 103(0), 105(1), 106(0), 107(0), 109(1), 110(0), 115(0), 118(4), 135(0), 156(0), 159(0), 163(0), 165(0), 170(1), 190(0), 192(0), 198(2), 207(0), 370(2), 376(0), 378(4), 397(4), 399(9), 407(0), 409(0), 413(0), 416(16), 428(1), 429(0), 431(2), 437(0), 439(0), 460(2), 465(9), 480(5), 482(27), 485(40), 487(15), 488(18), 495(0), 505(2), 511(0), 520(17), 528(13), 531(0), 548(0), 552(6), 561(17), 575(41), 582(0), 583(108), 585(64), 601(0), 601(116), 607(33), 610(65), 618(97), 619(143), 642(215), 662(141), 1944(0), 1970(1348), 1971(261), 1996(155), 2058(0), 2063(0), 2064(184), 2078(136), 2079(28), 2105(3197), 2106(921), 2115(1805), 2122(2585), 2167(46)
	BP86	-31(0), 27(0), 28(0), 48(0), 55(0), 58(0), 60(0), 68(0), 69(0), 76(0), 79(0), 85(0), 87(0), 89(0), 94(0), 97(0), 99(0), 101(0), 102(0), 104(0), 105(0), 113(0), 126(3), 138(2), 140(0), 150(0), 152(0), 162(0), 170(1), 174(0), 191(0), 193(1), 200(4), 220(2), 362(0), 371(0), 376(1), 387(1), 391(9), 402(1), 402(0), 409(0), 416(20), 427(1), 429(0), 436(2), 436(0), 440(3), 457(0), 479(11), 486(0), 490(5), 494(6), 507(1), 507(7), 508(0), 511(0), 518(0), 519(1), 522(28), 531(2), 534(0), 543(2), 549(29), 572(6), 575(66), 578(0), 578(81), 589(157), 590(4), 593(0), 604(4), 610(145), 611(165), 627(147), 647(107), 1876(0), 1896(998), 1901(144), 1920(135), 1974(0), 1981(45), 1988(3), 1995(43), 2000(31), 2016(318), 2023(2503), 2034(1840), 2039(2017), 2077(48)

Complete Gaussian 03 reference (Reference 27)

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A. Gaussian 03, Revision C.02; Gaussian, Inc., Wallingford CT, **2004**.