--Supporting Information--

Structures and Bonding in Hexacarbonyl Diiron Polyenes: Cycloheptatriene and 1,3,5-Cyclooctatriene

*Min Zhang[1], Guangchao Liang[2]**

[1] Department of Pharmacy, Medical School, Xi'an International University, Xi'an, Shaanxi 710077, P.R. China

[2] Academy of Advanced Interdisciplinary Research, Xidian University, Xi'an, Shaanxi 710071, P.R. China

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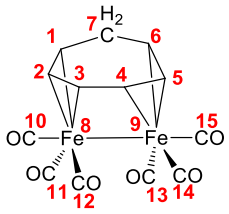
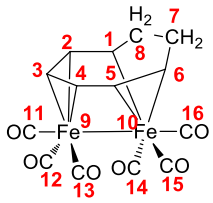
Table S1. Selected bond lengths (in Å) and angles (in °) for $(C_7H_8)Fe_2(CO)_6$ and $(C_8H_{10})Fe_2(CO)_6$

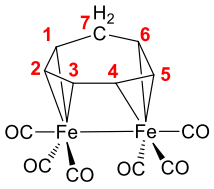


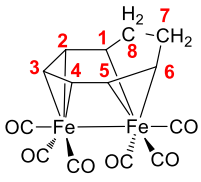


Parameter	$(C_7H_8)Fe_2(CO)_6$	
	Expt.	Compt.
Fe8-Fe9	2.866	2.868
Fe8-C1	2.142	2.125
Fe8-C2	2.043	2.043
Fe8-C3	2.177	2.199
Fe8-C10	1.790	1.754
Fe8-C11	1.786	1.770
Fe8-C12	1.778	1.772
Fe9-C4	2.168	2.165
Fe9-C5	2.041	2.041
Fe9-C6	2.117	2.128
Fe9-C13	1.786	1.773
Fe9-C14	1.801	1.776
Fe9-C15	1.782	1.750
C2-C3	1.402	1.426
C3-C4	1.459	1.462
C4-C5	1.397	1.422
C2-Fe8-C3	38.6	39.1
C2-Fe8-C10	88.1	86.9
C11-Fe8-C12	101.6	100.9
C4-Fe9-C5	38.6	39.4
C4-Fe9-C15	88.0	88.7
C13-Fe9-C14	103.3	103.3

Parameter	$(C_8H_{10})Fe_2(CO)_6$	
	Expt.	Compt.
Fe9-Fe10	2.767	2.705
Fe9-C2	2.173	2.146
Fe9-C3	2.062	2.053
Fe9-C4	2.124	2.118
Fe9-C11	1.798	1.760
Fe9-C12	1.799	1.776
Fe9-C13	1.800	1.771
Fe10-C1	2.085	2.098
Fe10-C5	2.221	2.211
Fe10-C6	2.181	2.196
Fe10-C14	1.788	1.760
Fe10-C15	1.814	1.797
Fe10-C16	1.790	1.755
C3-C4	1.409	1.435
C4-C5	1.460	1.463
C5-C6	1.411	1.413
C3-Fe9-C4	39.3	40.2
C3-Fe9-C11	88.7	90.0
C12-Fe9-C13	100.0	99.9
C5-Fe10-C6	37.4	37.4
C6-Fe10-C16	80.6	82.0
C14-Fe10-C15	92.4	92.6

Table S2. Computed proton chemical shifts of $(C_7H_8)Fe_2(CO)_6$ and $(C_8H_{10})Fe_2(CO)_6$

	Chemical shift (ppm)	H1	H6	H2	H5	H3	H4	7N	7X
	Experimental high temperature [a]	2.7		4.2		5.1		3.0	2.2
	Simulated high temperature [b]	1.9		3.5		4.1		2.3	1.8
	Computed low temperature limit [b]	1.8	2.0	3.6	3.3	4.1	4.1	2.3	1.8

	Chemical shift (ppm)	H1	H6	H2	H5	H3	H4	7N	8N	7X	8X
	Experimental high temperature [a]	2.65		3.92		4.53		1.53		2.04	
	Simulated high temperature [b]	2.86		3.97		4.52		1.56		2.34	
	Computed low temperature limit [b]	1.59	4.14	3.94	4.00	4.42	4.62	1.39	1.73	2.21	2.47

[a] Experiments in CS_2 solvent at 30℃. [b] Computed gas phase proton chemical shifts. 7N stands for the endo proton of the C7 and 7X for the exo proton.

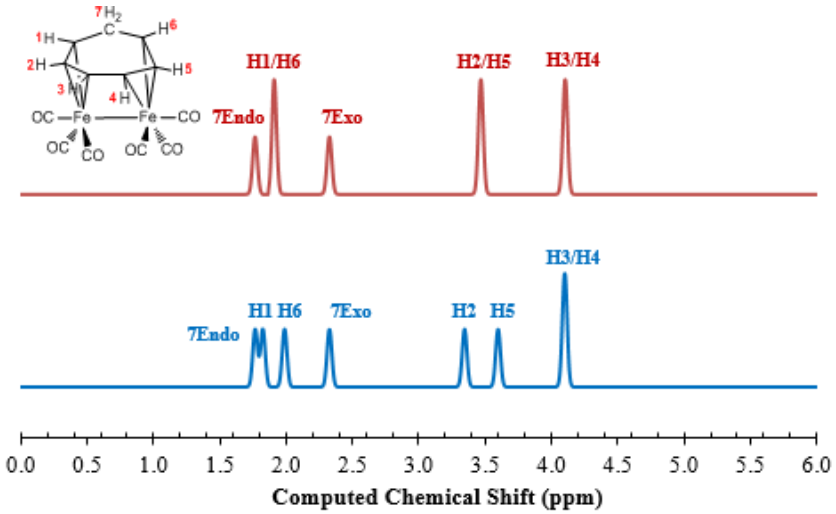


Figure S1. Simulated gas phase ^1H NMR spectra of $(C_7H_8)Fe_2(CO)_6$ at low temperature limit (bottom, bule) and high temperature fast exchange (top, red).

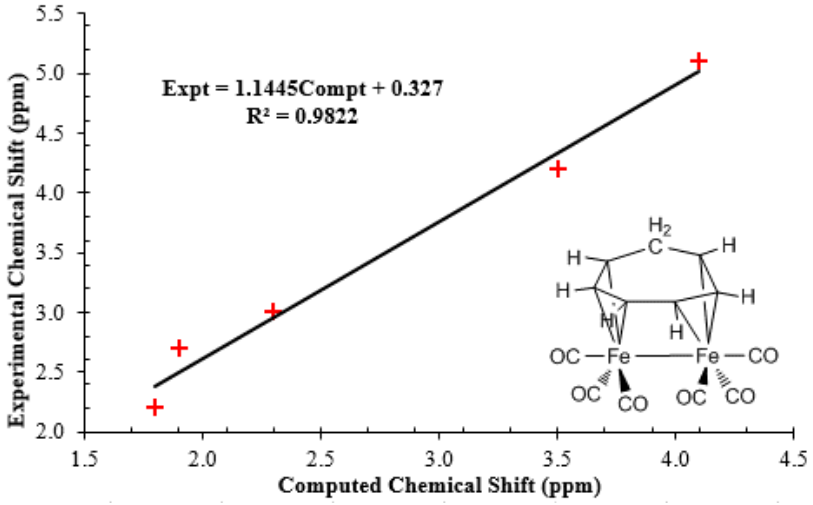


Figure S2. Linear fitting between the computed gas phase proton chemical shifts and experimental ^{1}H NMR of $(C_7H_8)Fe_2(CO)_6$.

Table S3. Cartesian coordinates of optimized structures and the computed energies.

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Complex 1 with C8H10, el energy= -1236.78003096

Fe	0.365178	-1.137894	0.292607
Fe	-0.096376	1.529894	-0.272436
C	0.437042	-2.888194	0.184387
O	0.548548	-4.046050	0.111347
C	1.635261	-0.901588	-0.902984
O	2.493056	-0.885290	-1.691644
C	1.526607	-1.062942	1.661351
O	2.295725	-1.079008	2.533545
C	-0.502670	3.240349	-0.346940
O	-0.726675	4.382285	-0.391253
C	0.848108	1.627887	-1.773366
O	1.418263	1.785185	-2.774502
C	1.191471	1.794377	0.914535
O	2.024723	2.029654	1.692504
C	-2.624367	-1.943857	0.463080
C	-1.477448	-1.586845	1.398436
H	-1.213994	-2.319130	2.172275
C	-1.104518	-0.254887	1.689182
H	-0.600769	-0.076302	2.647930

C	-1.631721	0.962217	1.071256
H	-1.938488	1.751170	1.771400
C	-2.101102	1.086283	-0.278762
H	-2.754210	1.934773	-0.519819
C	-1.523514	0.346878	-1.353340
H	-1.780298	0.727090	-2.355841
C	-1.025756	-1.059545	-1.276083
H	-0.533617	-1.311785	-2.230968
C	-2.143935	-2.078805	-0.990385
H	-1.740791	-3.095630	-1.153461
H	-2.992481	-1.958196	-1.698597
H	-3.390136	-1.145644	0.531297
H	-3.107601	-2.876640	0.805252

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Complex 1i with C8H10, el energy= -1236.78003112

C	2.484188	-1.916585	4.517954
C	2.843527	0.091141	7.451824
C	2.218511	1.169308	6.757695
C	2.889825	2.091651	5.793163
C	3.978098	2.960789	6.449608
C	5.200053	2.099496	6.805311
C	0.527969	-0.107159	5.038861
C	1.187168	-1.891120	6.724748
C	4.510025	-0.240676	3.132691
C	2.349030	1.138538	3.333845
C	4.615136	2.293031	3.648694
C	5.430161	1.004994	5.772390
C	4.845314	-0.278414	5.864069
C	3.852545	-0.725971	6.841557
Fe	3.787470	0.898272	4.319580
Fe	2.044015	-0.711666	5.739328
O	2.742476	-2.751661	3.749275
O	-0.515254	0.239203	4.659663
O	0.606303	-2.692345	7.338572
O	4.996629	-0.924079	2.327273
O	1.469003	1.400047	2.616043
O	5.143588	3.201620	3.145122
H	2.383563	-0.268942	8.380979
H	1.289532	1.533451	7.226663
H	2.124188	2.742939	5.337843
H	4.276929	3.748175	5.732826
H	3.589668	3.484629	7.350113
H	6.107497	2.723222	6.895599
H	5.044733	1.619470	7.792024

H	6.363032	1.046984	5.195800
H	5.371447	-1.102775	5.365651
H	4.076537	-1.680384	7.337170

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Complex 2 with C8H10, el energy= -1236.75954294

Fe	2.649765	2.176486	1.825009
Fe	4.866698	1.370179	3.565986
C	1.714294	2.635741	0.419081
O	1.076366	2.890430	-0.523150
C	3.636705	1.205043	0.713356
O	4.175203	0.552659	-0.088551
C	1.504037	0.962034	2.404698
O	0.662586	0.208801	2.694064
C	6.107294	0.640967	4.562168
O	6.916598	0.119683	5.218635
C	6.012341	1.284119	2.205570
O	6.827391	1.234997	1.377399
C	3.906196	-0.118829	3.438525
O	3.394373	-1.165004	3.463688
C	2.245900	2.209911	5.290086
C	3.752632	2.035854	5.266679
H	4.084562	1.474334	6.153175
C	4.769696	2.961291	4.839189
H	5.655846	3.053666	5.483381
C	4.970461	3.503249	3.532957
H	5.987035	3.898989	3.395900
C	4.102726	3.831734	2.401531
H	4.690479	4.180494	1.541375
C	2.721801	4.158709	2.306044
H	2.448479	4.789903	1.450741
C	1.681894	3.589869	3.114834
H	0.681341	3.821033	2.723051
C	1.690421	3.474820	4.634686
H	0.641024	3.574892	4.968691
H	2.227149	4.349532	5.055426
H	1.967695	2.255998	6.364355
H	1.733036	1.314517	4.898051

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Complex 3 with C8H10, el energy= -1236.73779495

Fe	4.253763	1.594108	1.774354
Fe	3.005772	0.859361	4.022928
C	3.382179	2.747141	0.725660
O	2.940268	3.424434	-0.118984

C	5.836690	1.394533	1.010522
O	6.842276	1.259858	0.436014
C	3.573585	0.327492	0.753665
O	3.155943	-0.487480	0.036304
C	2.879768	-0.512567	5.117489
O	2.759866	-1.438996	5.813520
C	4.379676	-0.010744	3.044258
O	5.071755	-0.974806	3.069100
C	1.671121	0.292227	3.036341
O	0.751031	-0.084918	2.427457
C	2.184814	4.007703	3.160712
C	1.803609	2.780203	3.950649
H	0.733790	2.562126	3.809507
C	2.257401	2.389072	5.238674
H	1.520412	2.077503	5.990759
C	3.626028	2.132704	5.593356
H	3.763037	1.729622	6.605970
C	4.767258	1.983718	4.761236
H	5.548791	1.398357	5.265807
C	5.263918	2.542802	3.494601
H	6.311318	2.279507	3.314230
C	4.728990	3.583521	2.714454
H	5.430944	4.023922	1.996396
C	3.629148	4.509428	3.200919
H	3.672612	5.440708	2.608329
H	3.878380	4.793132	4.245120
H	1.542576	4.824901	3.559030
H	1.860080	3.872906	2.115973

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TS-1 with C8H10, el energy= -1236.76599278

Fe	1.459366	-0.052140	-0.371126
Fe	-0.524557	1.902686	0.038423
C	2.413150	-1.448999	-0.812900
O	3.100602	-2.342714	-1.107872
C	2.062700	0.887787	-1.738986
O	2.480332	1.409201	-2.691102
C	2.659082	0.524378	0.847315
O	3.473033	0.869677	1.600844
C	-1.258990	3.027306	-1.088867
O	-1.761765	3.784531	-1.817770
C	1.053714	2.687937	-0.098907
O	1.966783	3.418985	-0.124516
C	-0.931803	2.836751	1.468685
O	-1.237581	3.478693	2.392603

C	-0.442584	-2.460330	-0.059447
C	0.475304	-1.598173	0.797957
H	1.255348	-2.109708	1.376184
C	0.027327	-0.378996	1.372378
H	0.529249	-0.049291	2.291375
C	-1.264825	0.257217	1.149980
H	-1.838612	0.509508	2.051559
C	-1.929034	0.394038	-0.106057
H	-2.962564	0.761264	-0.103599
C	-1.215257	0.345583	-1.350624
H	-1.788745	0.733410	-2.207073
C	-0.081361	-0.552578	-1.696513
H	0.211104	-0.353783	-2.741038
C	-0.374473	-2.055891	-1.541638
H	0.440291	-2.615121	-2.038810
H	-1.312184	-2.332427	-2.069744
H	-1.478642	-2.344172	0.315713
H	-0.178415	-3.525728	0.065002

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TS-2 with C8H10, el energy= -1236.75783575

Fe	2.713583	2.145454	1.961013
Fe	4.717359	1.004872	3.577178
C	1.059027	1.619153	2.137764
O	-0.047728	1.254877	2.214719
C	2.378699	2.754093	0.350069
O	2.100529	3.151986	-0.710820
C	3.271508	0.642104	1.212591
O	3.472421	-0.306006	0.556752
C	5.830777	0.346905	4.762056
O	6.558940	-0.128692	5.535837
C	5.822781	0.546424	2.252063
O	6.587781	0.260190	1.426885
C	3.592092	-0.369657	3.724957
O	2.876589	-1.269814	3.889820
C	1.680956	3.862455	4.179863
C	2.210710	2.425432	4.063794
H	1.447590	1.715843	4.425218
C	3.455885	2.150999	4.836240
H	3.310900	1.724226	5.842296
C	4.737775	2.758888	4.637655
H	5.440940	2.779769	5.480539
C	5.245237	3.056519	3.336509
H	6.325631	3.245598	3.267996
C	4.444168	3.478532	2.185918

H	4.986067	3.468830	1.231736
C	3.247585	4.247579	2.251709
H	3.018104	4.809650	1.337688
C	2.675368	4.830670	3.535962
H	2.195484	5.802661	3.322103
H	3.508255	5.034667	4.239702
H	1.487205	4.130528	5.242338
H	0.712333	3.920815	3.649700

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TS-3 with C8H10, el energy= -1236.76328661

Fe	2.731900	1.890659	2.093046
Fe	4.963129	1.183562	3.714106
C	1.368489	2.618517	1.296732
O	0.452266	3.086343	0.747614
C	3.544403	1.438757	0.571638
O	3.982631	1.179199	-0.475167
C	1.935299	0.308127	2.293236
O	1.330601	-0.684238	2.362269
C	6.337670	0.781064	4.734497
O	7.249667	0.494547	5.398736
C	5.815650	0.733125	2.230032
O	6.440099	0.424375	1.298171
C	4.205709	-0.398093	3.952525
O	3.765494	-1.454925	4.159760
C	1.800989	4.127060	3.864128
C	1.944469	2.600414	3.900009
H	0.987118	2.096616	4.097942
C	2.991046	2.033940	4.736337
H	2.671805	1.220696	5.405325
C	4.270225	2.584897	5.081142
H	4.644628	2.421894	6.098947
C	5.157777	3.208533	4.131539
H	6.160656	3.487125	4.476932
C	4.862063	3.348602	2.734515
H	5.760536	3.390980	2.100658
C	3.628821	3.783917	2.097902
H	3.826035	4.091369	1.060554
C	2.751871	4.795194	2.846769
H	2.158587	5.343672	2.092705
H	3.395361	5.551627	3.340646
H	1.954345	4.539103	4.882405
H	0.753734	4.356558	3.595772

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TS-1-2 with C8H10, el energy= -1236.73115006

Fe	0.028855	-0.159296	-0.164489
Fe	-2.857324	-0.208164	-0.254738
C	1.723779	0.108869	-0.365713
O	2.873408	0.287767	-0.473676
C	-0.214610	1.604469	-0.245804
O	-0.242946	2.771054	-0.287419
C	0.256576	-0.517325	1.566403
O	0.478735	-0.681179	2.701941
C	-4.588393	-0.181447	0.041766
O	-5.734233	-0.145197	0.242973
C	-2.934194	1.321550	-1.152957
O	-3.070708	2.305382	-1.755497
C	-2.483210	0.496240	1.331258
O	-2.373628	0.971842	2.386963
C	-0.658145	-3.209208	0.445282
C	-1.855025	-2.300201	0.645371
H	-2.177800	-2.273635	1.697369
C	-2.958047	-2.272715	-0.273162
H	-3.929397	-2.663975	0.060780
C	-2.901736	-1.771133	-1.624660
H	-3.828091	-1.844616	-2.208708
C	-1.880557	-0.932258	-2.184485
H	-2.257414	-0.383592	-3.060398
C	-0.430266	-0.860040	-2.065443
H	0.034728	-0.221289	-2.825834
C	0.404478	-1.818342	-1.387050
H	1.435866	-1.816185	-1.766162
C	-0.061223	-3.199932	-0.950355
H	0.793985	-3.898936	-0.977476
H	-0.806154	-3.586771	-1.677923
H	-1.046603	-4.229670	0.682747
H	0.119766	-2.989138	1.194226

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TS-1-3 with C8H10, el energy= -1236.73708438

Fe	3.048745	2.055213	1.600779
Fe	4.413883	1.215670	3.785416
C	1.386722	2.666314	1.419304
O	0.326779	3.030648	1.084584
C	3.601624	2.279627	-0.066263
O	3.880625	2.364056	-1.193858
C	2.327388	0.461330	1.395780
O	1.841189	-0.582806	1.228482
C	5.952062	0.477789	4.175839

O	6.964933	-0.028670	4.448718
C	4.724449	0.920841	1.927013
O	5.484816	0.348533	1.217502
C	3.615907	-0.324682	4.081454
O	3.106502	-1.346860	4.309300
C	1.672233	3.393540	4.250674
C	2.512121	2.187101	4.634428
H	1.856827	1.377864	4.990225
C	3.710770	2.310075	5.414895
H	3.801667	1.807574	6.387534
C	4.896888	2.915079	4.902541
H	5.770570	2.901173	5.568421
C	5.200279	3.201472	3.527749
H	6.282983	3.276281	3.356231
C	4.437636	3.652552	2.355088
H	5.074566	3.803843	1.476832
C	3.148170	4.203030	2.305874
H	2.916412	4.767652	1.394329
C	2.369042	4.564025	3.554296
H	1.609441	5.325424	3.303146
H	3.075416	5.041479	4.264959
H	1.242934	3.770999	5.206444
H	0.810973	3.059388	3.650132

32

TS-2-3 with C8H10, el energy= -1236.73719230

Fe	2.744691	-0.429401	-0.825073
Fe	0.096228	-0.739209	-0.597685
C	3.666393	-1.294684	0.416996
O	4.427562	-1.747099	1.181505
C	3.926456	0.300177	-1.911288
O	4.764252	0.769406	-2.575176
C	2.843073	1.047077	0.143713
O	2.988031	2.014492	0.775358
C	-1.467362	0.067278	-0.497530
O	-2.473939	0.643573	-0.387105
C	0.861734	0.726670	-1.372861
O	0.815792	1.742559	-1.970437
C	0.595587	-0.427807	1.061379
O	0.781294	-0.238072	2.199002
C	1.576238	-3.540534	0.297442
C	0.250174	-2.827171	0.281537
H	-0.233689	-2.883530	1.268629
C	-0.698690	-2.662749	-0.756866
H	-1.760390	-2.765649	-0.496052

C	-0.467811	-2.144218	-2.083380
H	-1.387261	-1.975700	-2.658897
C	0.677779	-1.521595	-2.640422
H	0.394212	-0.897088	-3.500381
C	2.136532	-1.606872	-2.525354
H	2.642344	-1.172866	-3.394537
C	2.908267	-2.450147	-1.688259
H	3.957862	-2.533698	-1.996803
C	2.364326	-3.691877	-1.002915
H	3.217975	-4.358523	-0.784756
H	1.733212	-4.232298	-1.739868
H	1.350504	-4.565293	0.666961
H	2.214511	-3.089786	1.077388

29

Complex 1 with C7H8, el energy= -1197.52966929

C	0.994078	-0.522206	3.410443
C	1.540510	1.352928	0.821096
C	2.244872	-0.573961	-0.756575
C	4.116696	0.710461	0.179515
C	1.163917	-1.024850	1.996806
C	2.978357	2.197819	2.999171
C	4.507385	1.315111	4.863125
C	5.469020	1.010801	2.631862
C	2.177700	-1.903920	1.499229
C	3.560721	-1.777778	1.823626
C	4.126310	-1.431523	3.126263
C	3.418801	-1.042262	4.297301
C	2.213666	-0.263512	4.262158
Fe	2.652970	-0.022908	0.858223
Fe	3.872777	0.707086	3.349507
H	0.375855	0.394822	3.387015
H	0.367847	-1.271964	3.952485
H	0.200329	-1.124348	1.475789
H	1.922723	-2.583479	0.676017
H	4.249688	-2.316997	1.160865
H	5.153208	-1.784535	3.287259
H	3.945753	-1.160978	5.252907
H	1.938817	0.162903	5.238179
O	0.737828	2.187778	0.703859
O	1.966451	-0.889988	-1.843306
O	5.030003	1.186399	-0.363155
O	2.459392	3.239108	2.929009
O	4.912280	1.759982	5.861304
O	6.550046	1.211009	2.251024

29
Complex 2 with C7H8, el energy= -1197.52130053
C 2.293343 -1.056133 4.588573
C 1.591673 1.327133 0.382210
C 2.228615 -0.842537 -0.758287
C 4.178534 0.519037 0.162271
C 1.712057 -0.014687 3.614828
C 2.900238 2.343051 2.614986
C 3.733433 1.455600 4.836633
C 5.283049 1.260733 2.759304
C 1.212500 -0.601315 2.351327
C 1.861314 -1.705721 1.725483
C 3.295216 -1.808463 1.772946
C 4.144940 -1.327646 2.866438
C 3.759337 -1.066214 4.194282
Fe 2.622182 -0.069300 0.770047
Fe 3.593117 0.830430 3.199570
H 2.189726 -0.708085 5.631545
H 1.815422 -2.057602 4.513132
H 1.007795 0.700334 4.062065
H 0.163699 -0.423326 2.073747
H 1.297399 -2.376539 1.067166
H 3.765176 -2.550318 1.114137
H 5.221910 -1.421413 2.674762
H 4.546990 -1.069713 4.957920
O 0.875552 2.180383 0.048055
O 1.984641 -1.319529 -1.792525
O 5.185473 0.870690 -0.304345
O 2.462422 3.393511 2.365497
O 3.849879 1.928260 5.895459
O 6.382241 1.576064 2.548926

29
Complex 3 with C7H8, el energy= -1197.50209099
C 0.884717 -0.512136 3.347133
C 2.769761 1.994155 1.096654
C 3.681031 0.310990 -0.561579
C 4.778170 0.193091 1.794281
C 0.972466 0.125489 1.963262
C 2.571912 1.548694 4.263456
C 4.923169 -0.195160 4.760653
C 4.869528 1.916067 3.506292
C 1.147853 -0.617471 0.766258
C 2.168500 -1.623586 0.707615

C	3.151371	-1.825043	1.716804
C	3.167158	-1.607775	3.176180
C	2.196204	-0.947927	3.952979
Fe	3.017371	0.252846	1.065373
Fe	3.833301	0.492768	3.551705
H	0.371964	0.185665	4.030508
H	0.227911	-1.407421	3.280947
H	0.367630	1.035713	1.857034
H	0.624367	-0.352040	-0.159875
H	2.344556	-2.125034	-0.252197
H	4.010003	-2.415722	1.370871
H	3.895964	-2.234777	3.701440
H	2.203349	-1.147103	5.031918
O	2.576290	3.143008	1.086660
O	4.107696	0.384191	-1.642783
O	5.905761	0.011798	1.472713
O	1.836885	2.271892	4.808779
O	5.613456	-0.602403	5.608490
O	5.554000	2.855726	3.522141

29

TS-1 with C7H8, el energy= -1197.52972015

C	2.226305	0.049957	0.000000
C	-0.046889	2.037439	1.367871
C	-0.620556	0.313293	3.187723
C	-2.285697	0.425120	1.403154
C	1.527814	-0.247529	1.305064
C	-0.046889	2.037439	-1.367871
C	-0.620556	0.313293	-3.187723
C	-2.285697	0.425120	-1.403154
C	0.646691	-1.342399	1.587554
C	-0.423565	-1.728176	0.730873
C	-0.423565	-1.728176	-0.730873
C	0.646691	-1.342399	-1.587554
C	1.527814	-0.247529	-1.305064
Fe	-0.514229	0.329940	1.439048
Fe	-0.514229	0.329940	-1.439048
H	2.540314	1.110705	0.000000
H	3.182211	-0.528370	0.000000
H	2.129663	0.066832	2.170417
H	0.649650	-1.773046	2.597226
H	-1.180365	-2.380538	1.185457
H	-1.180365	-2.380538	-1.185457
H	0.649650	-1.773046	-2.597226
H	2.129663	0.066832	-2.170417

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O            0.283626        3.148596        1.477604
O           -0.695611        0.349254        4.350260
O           -3.444949        0.485068        1.484631
O            0.283626        3.148596       -1.477604
O           -0.695611        0.349254       -4.350260
O           -3.444949        0.485068       -1.484631

29
TS-2 with C7H8,        el energy= -1197.51532834
C            0.126933       -0.056115       -0.427171
C           -1.370744        3.276372       -0.704261
C           -3.941659        2.839696       -0.670179
C           -3.011305        2.317752       -2.900663
C           -0.571747        0.601600        0.738568
C           -0.284677        2.524121       -2.950287
C            1.559198        1.085699       -2.190676
C           -0.078563        0.222869       -4.034337
C           -2.006545        1.049859        0.598860
C           -3.056706        0.389006       -0.120066
C           -2.895937       -0.123628       -1.438711
C           -1.703959       -0.722175       -2.022396
C           -0.432098       -0.932716       -1.409574
Fe          -2.504010        2.008416       -1.221275
Fe          -0.155830        0.854354       -2.386097
H            0.036294        1.464917        1.068212
H            1.170623       -0.294860       -0.176434
H           -0.530543       -0.115796        1.594581
H           -2.356274        1.587466        1.492654
H           -4.082573        0.451836        0.264572
H           -3.827542       -0.351033       -1.972492
H           -1.904781       -1.336876       -2.909064
H            0.210653       -1.703197       -1.852200
O           -0.708442        4.121911       -0.254321
O           -4.876670        3.432234       -0.306228
O           -3.389775        2.500055       -3.984872
O           -0.198797        3.569187       -3.468404
O            2.712445        1.226873       -2.083115
O            0.026334       -0.196963       -5.116121

29
TS-1-3 with C7H8,      el energy= -1197.50106266
C           -0.654472        2.637015        0.372637
C            0.816323       -0.252369        1.744706
C            2.932539       -0.503126        0.249317
C            0.702226       -1.320162       -0.766681
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C	0.729727	2.198043	0.815618
C	-2.141080	0.287221	1.182313
C	-2.406980	-0.930185	-1.428188
C	-1.333816	-1.965057	0.522315
C	1.892802	2.156994	0.006367
C	1.857842	1.610594	-1.324221
C	0.726736	0.973409	-1.894545
C	-0.724173	1.119427	-1.704695
C	-1.379202	1.773797	-0.633852
Fe	1.308592	0.166716	0.104286
Fe	-1.265697	-0.360045	-0.212320
H	-1.287530	2.759909	1.268170
H	-0.562099	3.656447	-0.067144
H	0.932385	2.402618	1.875702
H	2.871711	2.414206	0.428553
H	2.810626	1.492932	-1.854037
H	0.973964	0.375019	-2.782264
H	-1.305148	0.932851	-2.614988
H	-2.426201	2.051105	-0.813541
O	0.615367	-0.503602	2.866068
O	3.988103	-0.976272	0.382227
O	0.867468	-2.290209	-1.416852
O	-2.823765	0.653844	2.056888
O	-3.228031	-1.289428	-2.176769
O	-1.442659	-3.014757	1.013399

29

TS-2-3 with C7H8, el energy= -1197.49476137

C	1.720505	-0.881744	4.187747
C	1.768725	0.879345	0.118185
C	3.365374	-0.881420	-0.642469
C	4.319633	0.723908	1.135731
C	1.316324	-0.376670	2.795104
C	3.174923	2.619110	2.318932
C	2.577770	1.758864	4.496553
C	5.154558	1.514250	3.591905
C	1.242428	-1.382381	1.760261
C	2.383996	-2.208019	1.557871
C	3.683139	-1.831181	2.072872
C	4.057260	-1.125552	3.317284
C	3.206238	-0.702397	4.349017
Fe	2.809128	-0.314415	0.907589
Fe	3.502093	1.085423	3.127512
H	1.177781	-0.308758	4.959638
H	1.433737	-1.950028	4.306373

H	0.527778	0.384761	2.777768
H	0.353023	-1.520373	1.133298
H	2.346369	-3.020130	0.821596
H	4.521918	-2.378035	1.623585
H	5.131822	-1.155210	3.533277
H	3.644197	-0.536487	5.341061
O	1.074945	1.644579	-0.417374
O	3.736113	-1.254269	-1.682278
O	5.324038	1.128588	0.657288
O	2.947758	3.641938	1.813730
O	2.140532	2.319189	5.423160
O	6.205896	1.868118	3.945783

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TMS, el energy= -163.340740233

Si	-0.000000	-0.000000	-0.000000
C	0.708611	-1.359138	-1.120902
C	-1.222033	1.063882	-0.990250
C	1.414391	1.092364	0.641908
C	-0.900969	-0.797109	1.469244
H	1.425506	-1.996923	-0.571196
H	-0.092976	-2.013327	-1.511258
H	1.240585	-0.925061	-1.987773
H	-1.652671	1.866286	-0.362888
H	-0.725612	1.542579	-1.854716
H	-2.059173	0.454313	-1.378201
H	1.959361	1.571585	-0.192501
H	1.032303	1.895292	1.299326
H	2.144282	0.499723	1.224076
H	-1.325694	-0.028975	2.141898
H	-1.732197	-1.440948	1.126585
H	-0.213715	-1.424544	2.066648