Electronic Supplementary Material (ESI) for Dalton Transactions

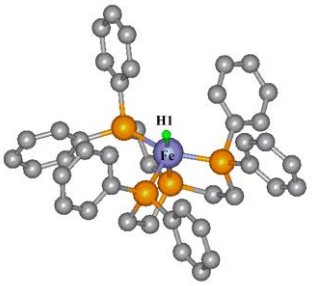
The reduction of carbon dioxide in iron catalyst catalytic hydrogenation reaction: a theoretical study

Longhua Yang[a,b], , *Hongming Wang**[a], *Ning Zhang*[b] *and Sanguo Hong*[b]

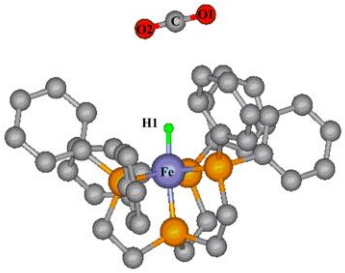
[a]Institute for Advanced Study, Nanchang University; [b]Department of Chemistry, Nanchang University, Nanchang, Jiangxi, 330031 China.

Email: hongmingwang@ncu.edu.cn

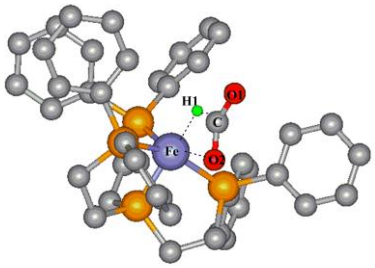
Contents



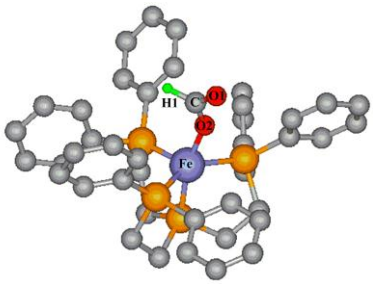
Complex 1



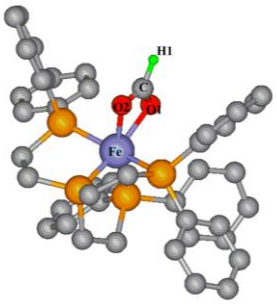
Complex 2



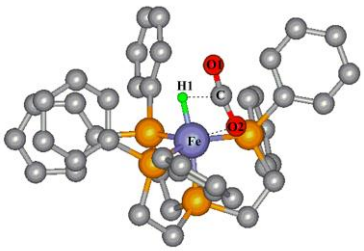
Complex 3



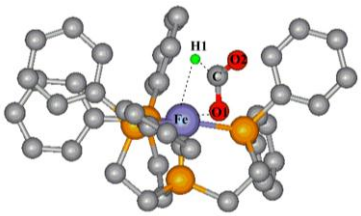
Complex 4



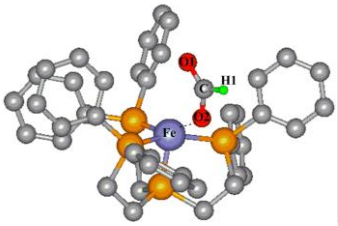
Complex 5



TS1

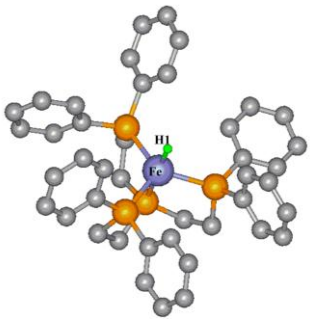


TS2

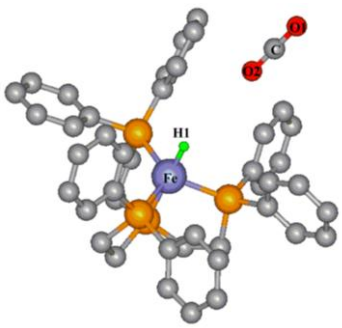


TS3

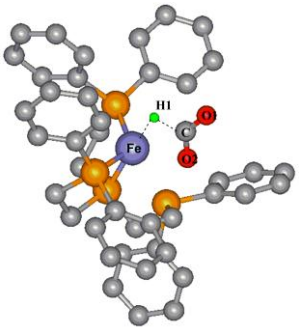
Figure S1. All structures of complexes and transition states of the CO_2 insertion step in singlet state (**1**, **2**, **3**, **4**, **5**, **TS1**, **TS2**, **TS3**). All H atoms not participating in the reaction directly are ignored. The concrete structural parameters are presented in Table S1 of support information.



Complex 1T



Complex 2T



Complex 3T

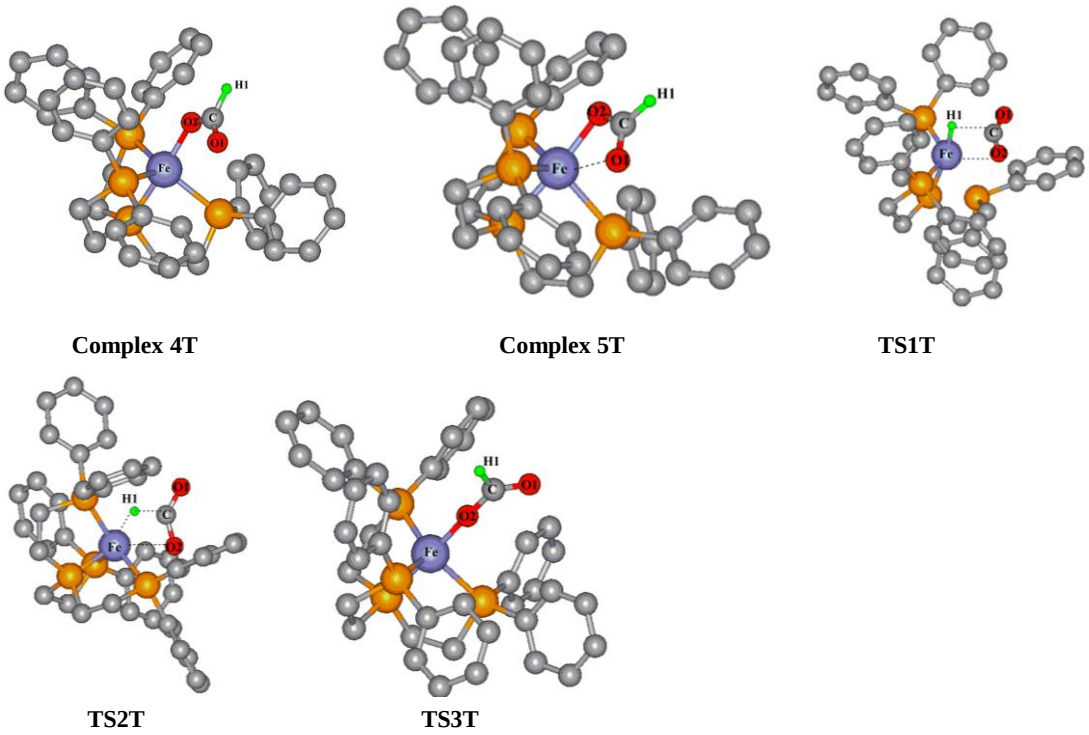


Figure S2. All structures of complexes and transition states of the CO_2 insertion step in triplet state (**1T**, **2T**, **3T**, **4T**, **5T**, **TS1T**, **TS2T**, **TS3T**). All H atoms not participating in the reaction directly are ignored. The concrete structural parameters are presented in Table S2 of support information.

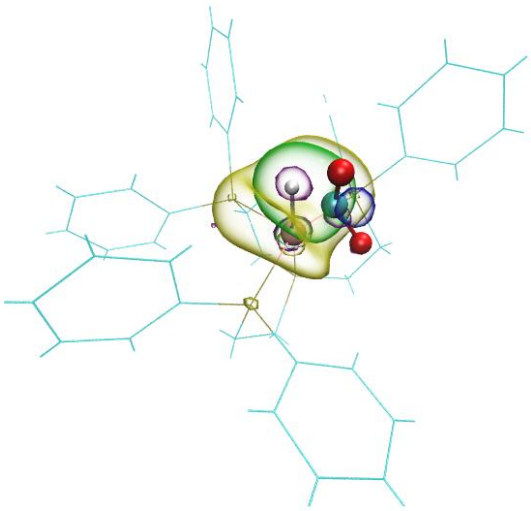


Figure S3. The orbital imagery of the favorable NBO donor-acceptor overlap of σ(C-H1)→LP*(Fe) in **3**.Yellow and purple represent the plus and minus isosurfaces of LP*(Fe), respectively; Green and blue represent the plus and minus isosurfaces of σ(C-H1), respectively.

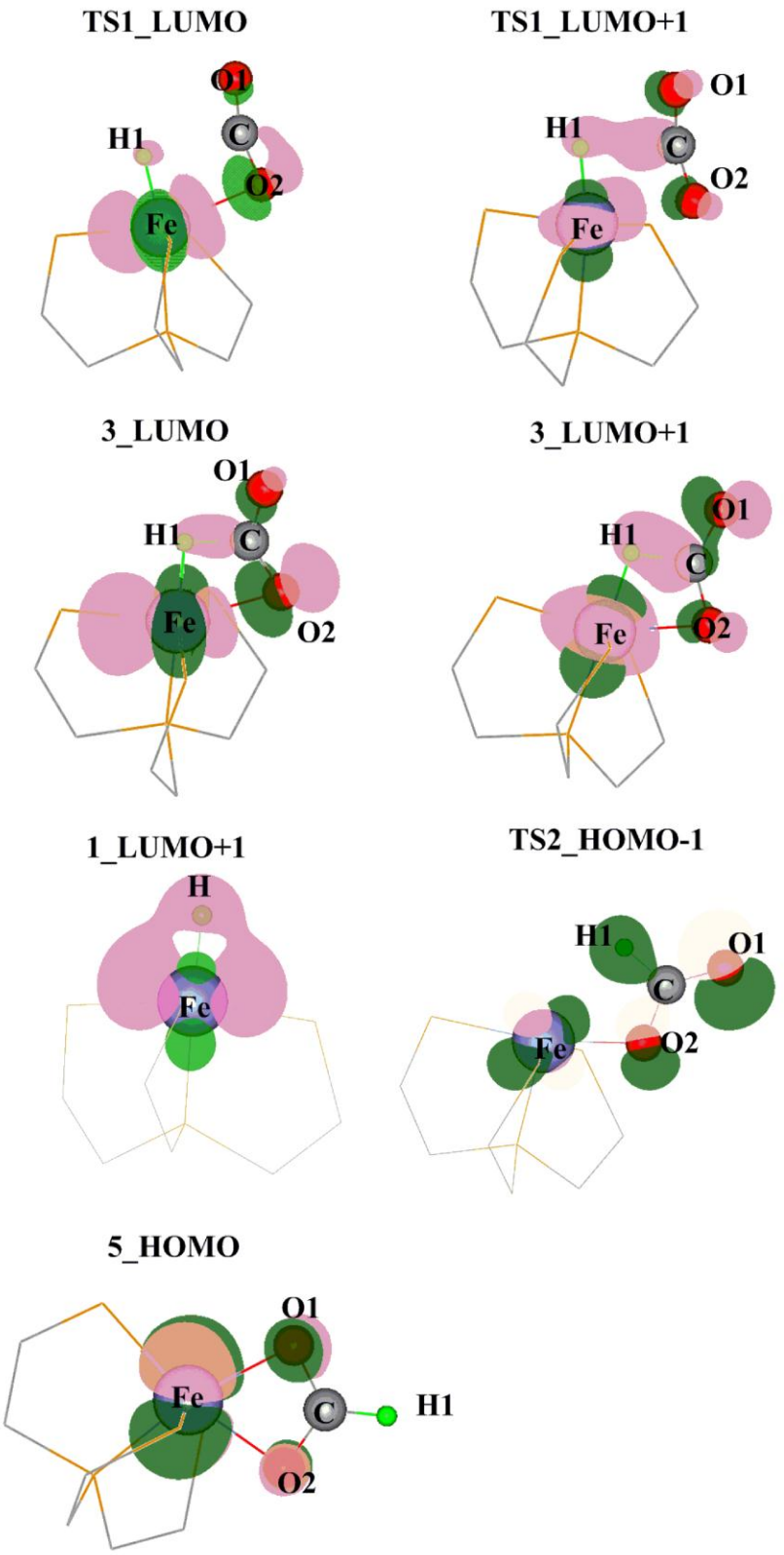


Figure S4. The molecular orbital figures of relative complexes and transition states during the reduction process of CO_2 in singlet state. Irrelated hydrogen atoms and the six phenyls on three P atoms are omitted.

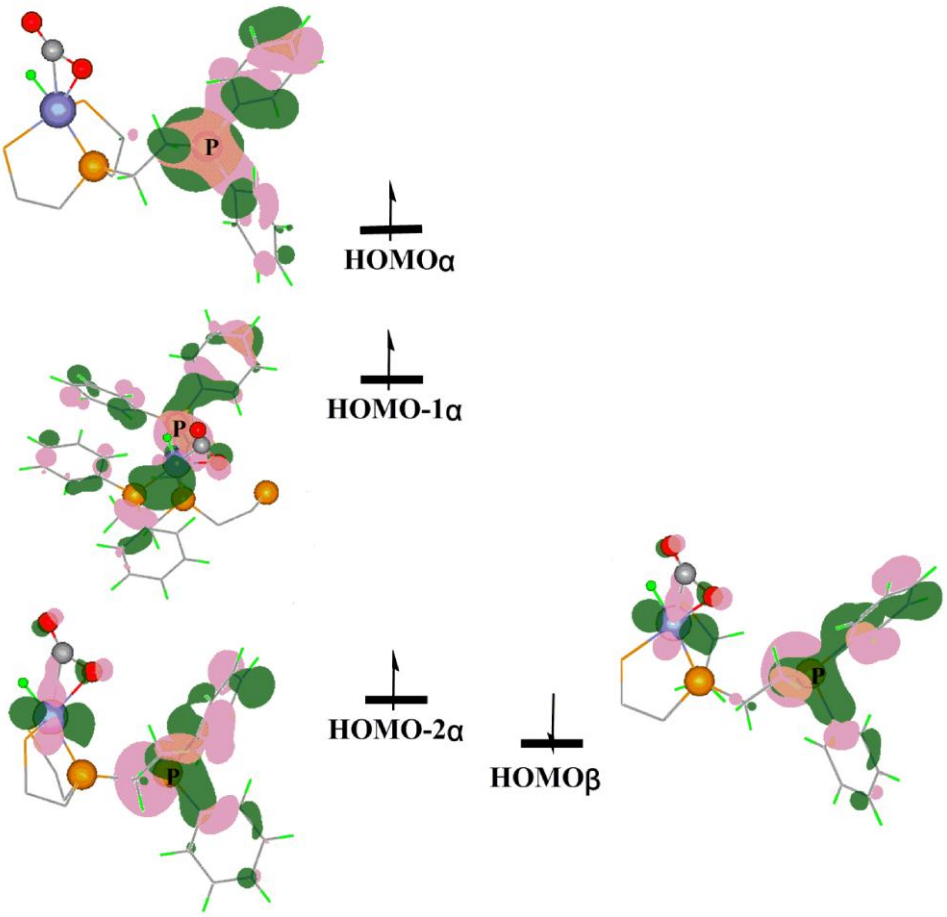


Figure S5. The relative frontier molecular orbital figures of **TS1T**. Irrelevant hydrogen atoms and the six phenyls on three P atoms are omitted.

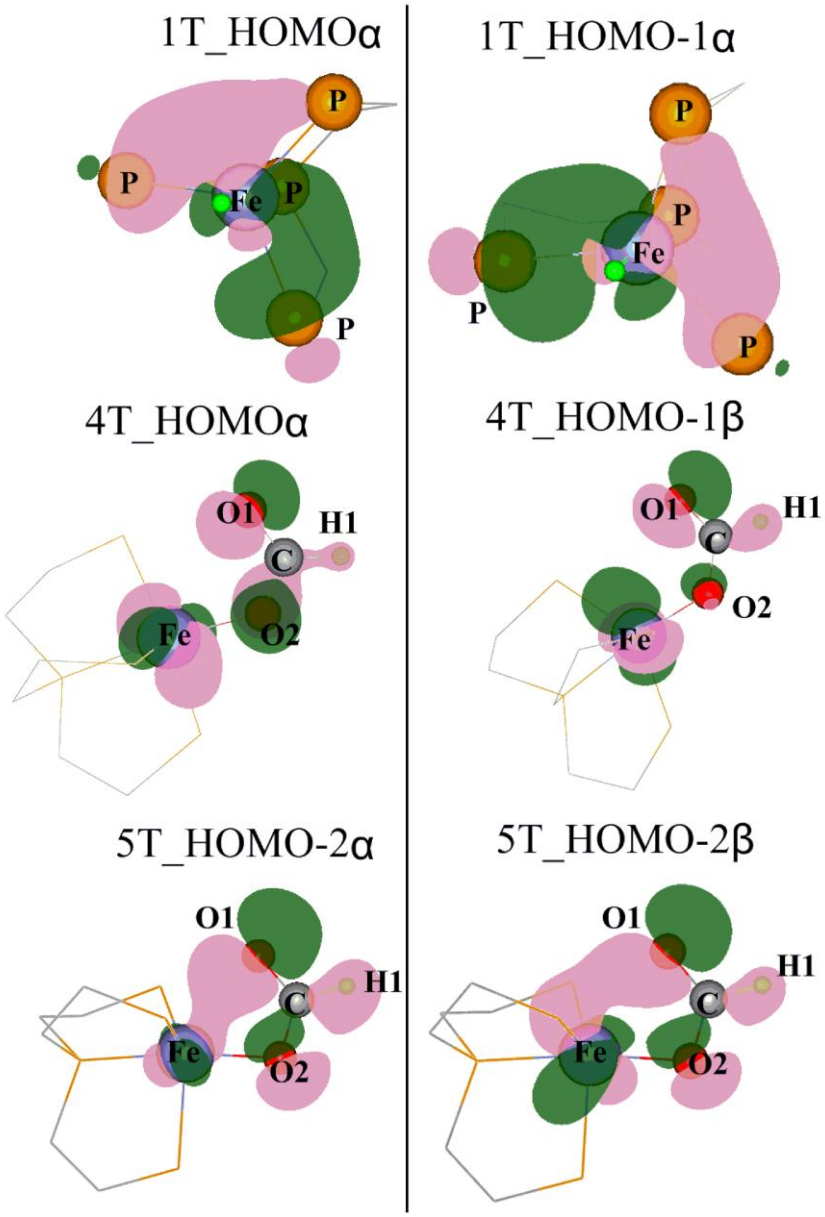
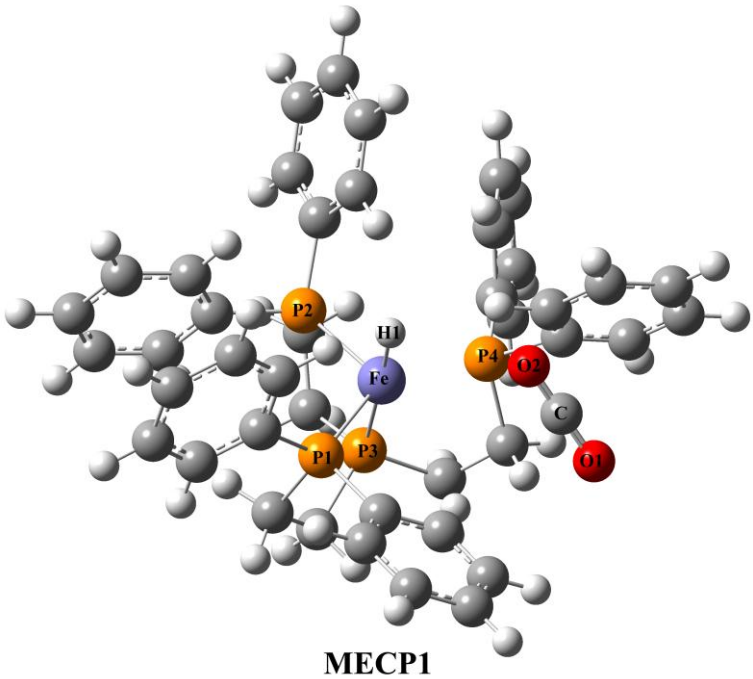
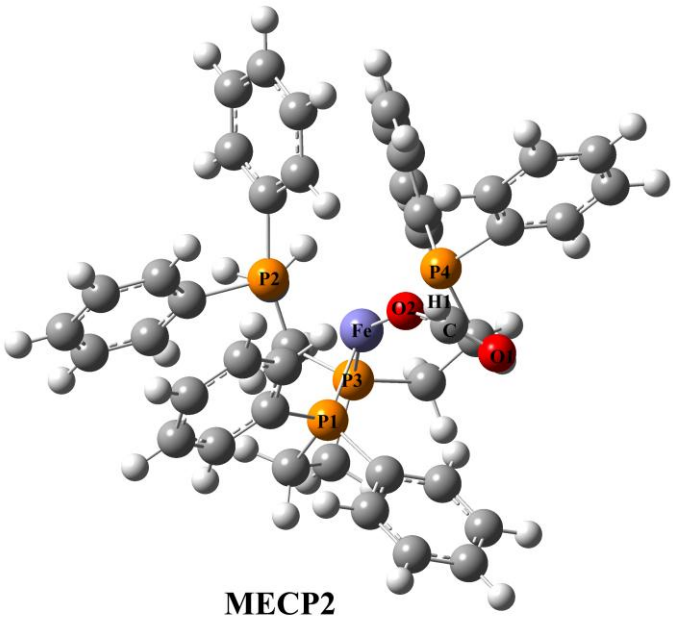


Figure S6. The molecular orbital figures of relative complexes of the reduction of CO_2 in triplet state. Irrelevant hydrogen atoms and the six phenyls on three P atoms are omitted.



MECP1



MECP2

Figure S7. The structures of MECPs.

$$-\Delta E^{(2)} = q_i \frac{F(i,j)^2}{E(j)-E(i)}$$

F(i,j) —— **Fock matrix element**

E(j)-E(i) —— **The energy difference between electron acceptor orbital (j) and electron donor orbital (i)**

q_i —— **Occupation number of electrons on electron donor orbital**

$\Delta E^{(2)}$ —— **Secondary perturbation energy**

Scheme S1. The calculation formula of the secondary perturbation energy.

Table S1. The structural parameters of complexes and transition states (Figure S1) in singlet state. Bond distances are measured in Å; angles and dihedral angles are measured in °.

	1	2	TS1	3	TS2	4	TS3	5
Fe-H1	1.525	1.524	1.530	1.628	2.574	3.423		3.540
Fe-O2			2.281	2.073	1.978	1.880	1.930	2.080
H1-C			2.083	1.264	1.134	1.113	1.111	1.103
Fe-O1						4.035	3.388	2.126
O1-C-O2		179.52	163.16	137.86	126.83	123.95	127.07	119.27
Fe-O2-C-O1						133.92	-10.97	-0.53
O1-Fe-O2								62.97
Fe-O2-C						144.82	132.34	89.84
Fe-O2-C-H1						-48.30		
C-O1		1.180	1.179	1.216	1.220	1.224	1.234	2.067
C-O2		1.177	1.203	1.268	1.313	1.323	1.307	2.060
Fe-P1	2.157	2.155	2.308	2.336	2.345	2.322	2.316	2.337
Fe-P2	2.310	2.308	2.209	2.257	2.291	2.205	2.231	2.291
Fe-P3	2.172	2.173	2.182	2.158	2.115	2.178	2.125	2.146
Fe-P4	2.221	2.231	2.395	2.428	2.447	2.508	2.460	2.438

Table S2. The structural parameters of complexes and transition states (Figure S2) in triplet state. Bond distances are measured in Å; angles and dihedral angles are measured in °.

	1T	2T	TS1T	3T	TS2T	4T	TS3T	5T
Fe-H1	1.536	1.533	1.526	1.679	1.803			
Fe-O2		5.162	2.130	2.036	2.471	1.913	1.873	2.021
H1-C		4.926	1.729	1.252	1.235	1.114	1.114	1.109
Fe-O1						3.197	4.028	2.601
O1-C-O2		179.91	148.66	137.29	137.45	127.61	126.04	123.21
Fe-O2-C						124.17	179.96	103.10
Fe-O2-C-O1						-2.90	-82.18	-0.94
Fe-O2-C-H1						177.50		
Fe-H1-C-O2				6.94	33.61			
C-O1		1.176	1.193	1.211	1.226	1.229	1.228	1.250
C-O2		1.181	1.239	1.280	1.255	1.313	1.309	1.290
Fe-P1	2.382	2.380	2.351	2.368	2.472	2.496	2.436	2.491
Fe-P2	2.376	2.379	2.356	2.369	2.434	2.495	2.475	2.539
Fe-P3	2.245	2.246	2.279	2.215	2.205	2.251	2.226	2.251
Fe-P4	2.384	2.390	5.227	5.129	2.556	2.505	2.473	2.523

Table S3. The bond orders of complexes and transition states of the CO_2 insertion step in singlet state.

	1	2	TS1	3	TS2	4	TS3	5
Fe-H1	0.6868	0.6843	0.6432	0.2832	0.0540	0.0171	0.0347	0.0393
C-H1		0.0003	0.0746	0.5406	0.8384	0.8832	0.8757	0.8780
Fe-O2		0.0004	0.2740	0.4750	0.4881	0.6237	0.5277	0.4393
Fe-O1						0.0541	0.0615	0.3900
C-O2		1.8675	1.6636	1.3613	1.1918	1.1439	1.2124	1.3827
C-O1		1.9224	1.7128	1.9146	1.7193	1.7060	1.6341	1.4248

Table S4. The bond orders of complexes and transition states of the CO_2 insertion step in triplet state.

	1T	2T	TS1T	3T	TS2T	4T	TS3T	5T
Fe-H1	0.7315	0.7315	0.5360	0.2519	0.2182	0.0385	0.0211	0.0428
C-H1			0.2242	0.5966	0.6203	0.8720	0.8804	0.8761
Fe-O2		0.0003	0.3392	0.4252	0.2101	0.5113	0.5443	0.4371
Fe-O1						0.0655	0.0569	0.1571
C-O2		1.8770	1.5159	1.3318	1.4542	1.2034	1.1825	1.3040
C-O1		1.9150	1.8430	1.7445	1.6427	1.6643	1.6807	1.5506

Table S5. The energies and relative energies of complexes and transition states in singlet and triplets using LanL2dz(f) basis set with polarization function.

Singlet state	1	2	TS1	3	TS2	4	TS3	5
Energy /a.u.	-3114.5997	-3303.1471	-3303.1234	-3303.1346	-3303.1207	-3303.1403	-3303.1384	-3303.1616
relative energy /kcal mol^{-1}		0.00	14.87	7.84	16.57	4.27	5.46	-9.10
Triplet state	1T	2T	TS1T	3T	TS2T	4T	TS3T	5T
Energy /a.u.	-3114.6083	-3303.1554	-3303.1189	-3303.1256	-3303.1173	-3303.1625	-3303.1535	-3303.1548
relative energy /kcal mol^{-1}		-5.21	17.70	13.49	18.70	-9.66	-4.02	-4.83

Table S6. The energies, relative energies and main structural parameters of MECPs.

	MECP1	MECP2
Energy/a.u.	-3303.1070	-3303.0964
relative energy/kcal mol^{-1}	7.97	14.75
Fe-H1	1.523	3.865
Fe-P1	2.269	2.290
Fe-P2	2.267	2.392
Fe-P3	2.198	2.174
Fe-P4	2.382	2.643
Fe-O2	5.807	1.889
Fe-O1	6.235	3.726
H1-C	5.101	1.114
C-O1	1.180	1.223
C-O2	1.177	1.321

List of Cartesian Coordinates for all optimized structures of complexes, transition states and MECPs

Complex 1 total energy:-3114.5723 a.u.

Fe	0.10184000	0.37942200	-0.24884600
P	0.10979300	-1.77392200	-0.37791200
P	-2.14703700	0.89087700	-0.37416800
P	0.06570600	0.49187700	-2.41739400
P	2.23523600	0.97209800	-0.42403700
C	1.73477600	-2.67003700	-0.23730000
C	2.40732200	-3.22116900	-1.34786900
C	3.61018300	-3.92163300	-1.18271800
C	4.16267800	-4.08493800	0.09261000
C	3.50480300	-3.54148600	1.20382300
C	2.30662500	-2.83891100	1.04156400
C	-0.91444100	-2.79150500	0.79263800
C	-1.18329300	-2.32678000	2.09296200
C	-1.86746900	-3.13268500	3.01271200
C	-2.30368300	-4.41045100	2.64209400
C	-2.04432300	-4.88174300	1.34842400
C	-1.34798200	-4.08503900	0.43196700
C	-3.58185000	-0.26832500	-0.62616600
C	-4.14048600	-0.91435900	0.49637300
C	-5.22552300	-1.78591500	0.35441700
C	-5.77679300	-2.03163500	-0.90965100
C	-5.23588000	-1.39355800	-2.03141600
C	-4.14871000	-0.51933200	-1.89271000
C	-2.81091900	1.98061500	0.97866300
C	-2.23983700	1.92299800	2.26399100
C	-2.74482800	2.71234200	3.30695400

C	-3.82304100	3.57478700	3.07712400
C	-4.40265900	3.63647700	1.80196300
C	-3.90761600	2.84233500	0.76136200
C	1.95026100	2.79025200	-0.18085300
C	1.00454900	3.17825000	0.79378700
C	0.70331000	4.53177800	1.00390300
C	1.36107300	5.51829800	0.26157400
C	2.31798600	5.14634600	-0.69511400
C	2.60729100	3.79629500	-0.92150300
C	3.70747100	0.58916100	0.62409500
C	4.99141200	0.34708300	0.09784200
C	6.07373200	0.10652900	0.95484400
C	5.89173200	0.11209900	2.34261700
C	4.61669200	0.34911200	2.87455500
C	3.53085000	0.57774100	2.02327600
C	-0.55453100	-2.22612700	-2.08429400
C	-0.05675300	-1.23513100	-3.14923000
C	-2.18858100	2.03428700	-1.88746600
C	-1.37941200	1.48815600	-3.08303700
C	1.64002300	1.19520500	-3.14857800
C	2.80373100	0.82986700	-2.20962100
H	0.17438100	0.15409000	1.25761400
H	1.99749900	-3.13618100	-2.35063500
H	4.10589500	-4.34922700	-2.05395100
H	5.09346400	-4.63616600	0.22044800
H	3.92309800	-3.66511300	2.20202600
H	1.80954100	-2.43230900	1.91872800
H	-0.85449300	-1.33010200	2.37586500
H	-2.06108800	-2.75832200	4.01785300
H	-2.83741400	-5.03706100	3.35582000
H	-2.37511400	-5.87648500	1.05142800
H	-1.13794400	-4.49066700	-0.55507800
H	-3.73985000	-0.73053200	1.48932000
H	-5.64261100	-2.26881700	1.23735400
H	-6.62437700	-2.70713500	-1.01807300
H	-5.66379700	-1.56393800	-3.01899100
H	-3.77163200	-0.02588400	-2.78398100
H	-1.39797800	1.25716900	2.43990300
H	-2.29352600	2.65128500	4.29713900
H	-4.21505900	4.19066800	3.88574200
H	-5.24854300	4.29793500	1.61725800
H	-4.39384400	2.89048600	-0.21077000
H	0.52025700	2.41511800	1.40130100
H	-0.03441900	4.80794900	1.75616600

H	1.14134100	6.57149800	0.43232600
H	2.84761500	5.91137200	-1.26225300
H	3.36322400	3.54158700	-1.66115800
H	5.16728700	0.34109400	-0.97504200
H	7.06065100	-0.08002300	0.53261500
H	6.73693200	-0.06844600	3.00576400
H	4.46552600	0.35136700	3.95364700
H	2.54125000	0.74291300	2.44566000
H	-0.31022000	-3.25859600	-2.35971900
H	-1.64425600	-2.16493900	-1.98743500
H	-0.71043400	-1.23764400	-4.03097300
H	0.94570900	-1.50532300	-3.50116400
H	-3.21792000	2.27400100	-2.18024300
H	-1.73061800	2.96463200	-1.52783700
H	-1.01540200	2.31345900	-3.70843700
H	-1.99070200	0.84995400	-3.73107400
H	1.81886800	0.83281700	-4.16972900
H	1.51907600	2.28351800	-3.20109500
H	3.68830200	1.44263800	-2.41886000
H	3.10069600	-0.21708200	-2.34646800

Complex 2 total energy:-3303.1199 a.u.

Fe	0.01679100	0.40325900	-0.51810500
P	0.01362900	-1.74348800	-0.70159700
P	-2.23353700	0.91602600	-0.51526500
P	-0.12353700	0.57754700	-2.67950900
P	2.14622800	1.01188500	-0.78947000
C	1.64028300	-2.63952500	-0.60108200
C	2.28853900	-3.18418400	-1.72893500
C	3.48540100	-3.90085200	-1.59100000
C	4.05552800	-4.08553200	-0.32640900
C	3.42373300	-3.54437300	0.80120200
C	2.23189600	-2.82544500	0.66675000
C	-0.99447900	-2.79520500	0.45284100
C	-1.31419300	-2.34071700	1.74415300
C	-1.98601100	-3.17258400	2.64965500
C	-2.36047900	-4.46733300	2.27210900
C	-2.05245300	-4.92868000	0.98547700
C	-1.36741300	-4.10552200	0.08444800
C	-3.68761100	-0.23847900	-0.66305900
C	-4.29186600	-0.75042400	0.50354300
C	-5.38349300	-1.62200100	0.42105500
C	-5.89626400	-2.00112200	-0.82560400
C	-5.31039700	-1.49612100	-1.99191300

C	-4.21602100	-0.62438900	-1.91250800
C	-2.78347200	2.01273800	0.88191300
C	-2.14498500	1.91712200	2.13333300
C	-2.56298200	2.70732900	3.21323800
C	-3.62064000	3.61049200	3.05457700
C	-4.26556600	3.71242500	1.81371200
C	-3.85750500	2.91716400	0.73657600
C	1.87656800	2.81826900	-0.46581100
C	1.00266700	3.17207100	0.58550900
C	0.72551500	4.51787700	0.86683200
C	1.33472900	5.52921100	0.11678400
C	2.22019200	5.19060900	-0.91801400
C	2.48656600	3.84929100	-1.21284900
C	3.69339200	0.60754600	0.13955300
C	4.88347700	0.19240500	-0.48899800
C	6.02988800	-0.07815200	0.27048800
C	6.00649800	0.06496200	1.66216800
C	4.82603700	0.47648300	2.29647300
C	3.67738500	0.74032700	1.54394400
C	-0.67912000	-2.16199300	-2.40519600
C	-0.22524200	-1.13345700	-3.45262200
C	-2.39341300	2.05601200	-2.02591600
C	-1.62359000	1.54519500	-3.26194400
C	1.39647300	1.33488100	-3.46684200
C	2.61020700	0.93589600	-2.60976300
H	0.15830000	0.11384300	0.97130700
H	1.86371900	-3.08218200	-2.72420000
H	3.96202500	-4.32445600	-2.47477500
H	4.98056700	-4.65075100	-0.21939300
H	3.85620100	-3.68407300	1.79125100
H	1.75567800	-2.42348800	1.55769500
H	-1.03555200	-1.32993000	2.02903900
H	-2.21844700	-2.80575200	3.64939500
H	-2.88412600	-5.11468300	2.97464400
H	-2.33521000	-5.93645700	0.68288400
H	-1.11546300	-4.50424000	-0.89575700
H	-3.92366600	-0.46018900	1.48362800
H	-5.83672500	-1.99936400	1.33704700
H	-6.74923800	-2.67566000	-0.88740900
H	-5.70804700	-1.77023700	-2.96874000
H	-3.79888300	-0.23995300	-2.83877700
H	-1.31528700	1.22534600	2.25662400
H	-2.05649500	2.61482600	4.17380300
H	-3.94538900	4.22810100	3.89126200

H	-5.09507700	4.40693300	1.68417500
H	-4.39349400	2.99869400	-0.20661200
H	0.55841900	2.38855500	1.19704400
H	0.04472300	4.76808800	1.67923900
H	1.13325000	6.57597400	0.34131600
H	2.71279500	5.97467600	-1.49245100
H	3.18951800	3.62001800	-2.01059200
H	4.93632400	0.07252400	-1.56799300
H	6.94230200	-0.39740500	-0.23213500
H	6.90078400	-0.14093500	2.24909500
H	4.80001000	0.59369000	3.37954800
H	2.76873900	1.05769600	2.05142400
H	-0.42265200	-3.18203700	-2.71349400
H	-1.76722300	-2.12794700	-2.28244400
H	-0.89483400	-1.12741700	-4.32262100
H	0.77609100	-1.37277800	-3.82969800
H	-3.44615700	2.24670900	-2.26618000
H	-1.95929500	3.00587900	-1.68926700
H	-1.30731900	2.38649800	-3.89213900
H	-2.24760600	0.90115200	-3.89218000
H	1.52078300	1.01924100	-4.51134800
H	1.26366900	2.42300900	-3.46337800
H	3.48663000	1.55259700	-2.84122400
H	2.89211000	-0.10566500	-2.80697100
C	1.14626300	-0.43261500	4.62727200
O	0.80126800	0.69445800	4.58330200
O	1.49010700	-1.55824900	4.66130600

Complex 3 total energy:-3303.1063 a.u.

Fe	-0.05164600	-0.51886700	-0.15612300
P	-2.35527700	-0.82464900	-0.39847300
P	0.10528900	1.71781100	-0.41655200
P	0.00632100	-0.67578600	-2.30799700
P	2.29647400	-1.09798400	-0.37258800
C	-2.95690500	-2.58261800	-0.22200200
C	-2.17712000	-3.65533900	-0.70252300
C	-2.66103400	-4.96775300	-0.66561400
C	-3.92787400	-5.23828700	-0.13436200
C	-4.70584900	-4.18488700	0.35858000
C	-4.22856500	-2.86839200	0.31662000
C	-3.60472500	0.12523500	0.57546700
C	-3.45420500	0.18504100	1.97770400
C	-4.42198300	0.81424700	2.76940200
C	-5.54919200	1.39886600	2.17708600

C	-5.70470700	1.34912500	0.78656400
C	-4.74269300	0.71544400	-0.01081800
C	-1.34519700	2.89358800	-0.50355400
C	-1.91730400	3.37291400	0.69316900
C	-2.94999500	4.31622600	0.66749900
C	-3.44165300	4.79640100	-0.55272100
C	-2.89246300	4.32208800	-1.74892800
C	-1.85439900	3.38041200	-1.72552600
C	1.14483500	2.63512300	0.82216600
C	1.18045200	2.22130600	2.16810200
C	1.88812000	2.96024200	3.12650400
C	2.57724500	4.12033200	2.75340900
C	2.54555100	4.54372800	1.41807000
C	1.82970700	3.81459900	0.46103700
C	3.72019400	-0.04368900	-0.95750100
C	4.28647700	0.89287400	-0.06572700
C	5.37973700	1.67794000	-0.44780600
C	5.93167000	1.54944500	-1.72878400
C	5.38342500	0.62321800	-2.62280000
C	4.28949500	-0.16644900	-2.24230600
C	3.09628400	-1.98351300	1.04996200
C	3.81130900	-3.18517900	0.86941500
C	4.45220500	-3.79905100	1.95249900
C	4.39823000	-3.22346600	3.22760600
C	3.69683900	-2.02723500	3.41565100
C	3.04870200	-1.41334700	2.33732000
C	-2.74712400	-0.48492000	-2.20638400
C	-1.64181900	-1.08948500	-3.08464400
C	0.97583300	1.97244600	-2.06051500
C	0.48762300	0.96094100	-3.10923500
C	1.24868900	-1.95209300	-2.89059400
C	2.10215900	-2.41749700	-1.69332900
H	-0.02343200	-0.36358700	1.46448100
H	-1.17566600	-3.47650600	-1.07773200
H	-2.03840400	-5.78066800	-1.03832900
H	-4.30062400	-6.26112800	-0.09686700
H	-5.69016300	-4.38174100	0.78204400
H	-4.85588300	-2.07240800	0.70608700
H	-2.59609500	-0.27428700	2.46215700
H	-4.29436300	0.84122800	3.85109700
H	-6.30329900	1.88528000	2.79481900
H	-6.57930500	1.79753600	0.31636900
H	-4.90075200	0.67995600	-1.08560900
H	-1.54711700	3.02935000	1.65548000

H	-3.36635400	4.67869700	1.60647500
H	-4.24023300	5.53695900	-0.57097200
H	-3.25852100	4.69249400	-2.70614400
H	-1.43896300	3.05848700	-2.67645500
H	0.65042900	1.32471500	2.48019000
H	1.89650700	2.62619100	4.16361500
H	3.12860600	4.69409200	3.49729300
H	3.07184400	5.44937900	1.11815600
H	1.80642000	4.18211500	-0.56228400
H	3.88855800	1.00703800	0.93808900
H	5.80220300	2.38738700	0.26280000
H	6.78517300	2.15849000	-2.02373700
H	5.81117600	0.50172100	-3.61754700
H	3.90864100	-0.88864200	-2.95829500
H	3.88491900	-3.65555000	-0.10732600
H	4.99603600	-4.72962000	1.79403600
H	4.89651600	-3.70530800	4.06773600
H	3.64090900	-1.57317300	4.40423400
H	2.49717700	-0.49417600	2.51145600
H	-3.72496500	-0.90516300	-2.46974100
H	-2.79896500	0.60190300	-2.33445900
H	-1.69686400	-0.72125400	-4.11799600
H	-1.73709000	-2.18061600	-3.12057000
H	0.85414100	2.99945600	-2.42176200
H	2.03891500	1.82137400	-1.85618200
H	1.25366300	0.79245300	-3.87615100
H	-0.40115800	1.33199300	-3.63188500
H	0.70952800	-2.80279600	-3.32570100
H	1.86141600	-1.52566500	-3.69291400
H	3.07274200	-2.79864700	-2.02941100
H	1.59232300	-3.23162100	-1.16698900
C	-0.15459000	-1.57987100	1.78388500
O	0.00457200	-2.35934800	0.79605700
O	-0.36723200	-1.66919400	2.97763200

Complex 4 total energy:-3303.1132 a.u.

Fe	0.08374000	0.31781600	-0.19514500
P	-0.02465600	-1.87834800	-0.35980200
P	-2.33142700	0.96472500	-0.39203400
P	-0.03433800	0.37923600	-2.36894700
P	2.31686500	0.84957500	-0.54122300
C	1.51947200	-2.91071400	-0.29503700
C	2.09345900	-3.50912400	-1.43631400
C	3.21356900	-4.34392300	-1.31947100

C	3.78088100	-4.59247400	-0.06400400
C	3.22494800	-3.99684300	1.07598100
C	2.10809200	-3.16286900	0.96305200
C	-1.06419900	-2.77751600	0.88804100
C	-1.48079500	-2.15861300	2.07996800
C	-2.20565900	-2.88169600	3.03835700
C	-2.53528000	-4.22255200	2.81039900
C	-2.12986500	-4.84462400	1.62117500
C	-1.39142500	-4.13364200	0.66912200
C	-3.73456000	-0.17998200	-0.80610200
C	-4.29555600	-0.94520300	0.23942000
C	-5.35970200	-1.81991200	-0.00246800
C	-5.88966400	-1.95049800	-1.29302700
C	-5.35174200	-1.19016100	-2.33738600
C	-4.28507600	-0.31187600	-2.09798100
C	-3.14355700	2.10290900	0.83639800
C	-2.46668700	2.56298300	1.98220500
C	-3.09060200	3.46579400	2.85573000
C	-4.38753500	3.92183000	2.59829300
C	-5.06864700	3.46729800	1.46020400
C	-4.45704800	2.56235200	0.58658900
C	2.38886300	2.71017700	-0.52216000
C	1.44643800	3.46174900	0.20836900
C	1.50949900	4.86279900	0.22317200
C	2.50999700	5.53264700	-0.48882600
C	3.46408600	4.79410200	-1.20327300
C	3.40897000	3.39630400	-1.21800000
C	3.83287300	0.38112700	0.41317100
C	4.74817800	-0.57973500	-0.06232800
C	5.89602500	-0.89310700	0.67652300
C	6.14179600	-0.26427700	1.90268300
C	5.23414400	0.68710700	2.38647100
C	4.09036800	1.01289800	1.64959500
C	-0.82833600	-2.29122100	-2.00544300
C	-0.35330900	-1.32764100	-3.10080500
C	-2.17393100	2.11156500	-1.87490400
C	-1.37114900	1.51005200	-3.04024100
C	1.55136600	0.91710500	-3.19683300
C	2.71737400	0.43968200	-2.32411600
H	1.66475800	-3.36010000	-2.42409000
H	3.63051500	-4.81024600	-2.21175300
H	4.64411600	-5.25068700	0.02626700
H	3.65512300	-4.18651900	2.05856700
H	1.67988700	-2.73050700	1.86430000

H	-1.23910100	-1.11532200	2.25505100
H	-2.51155900	-2.39124700	3.96219800
H	-3.09882000	-4.78330800	3.55527200
H	-2.37765500	-5.88950100	1.43703500
H	-1.05997400	-4.64929300	-0.22993600
H	-3.91403500	-0.84813100	1.25190100
H	-5.77732700	-2.39534900	0.82283400
H	-6.72029800	-2.62971700	-1.48037200
H	-5.76706500	-1.26703000	-3.34186800
H	-3.91504000	0.28119900	-2.92910600
H	-1.46365700	2.21659200	2.20291400
H	-2.55314200	3.80483200	3.74085700
H	-4.86918500	4.62263100	3.27943900
H	-6.08103600	3.81241300	1.25221700
H	-5.01289100	2.21061800	-0.28017400
H	0.69063900	2.96001200	0.80404300
H	0.77921500	5.42434800	0.80501000
H	2.55875700	6.62082500	-0.47633400
H	4.26144800	5.30533500	-1.74179500
H	4.18312600	2.85112400	-1.75406400
H	4.58527500	-1.09080200	-1.00682500
H	6.59797200	-1.62990200	0.28732900
H	7.03543100	-0.51011600	2.47513400
H	5.41616400	1.18645800	3.33732700
H	3.41092900	1.76459900	2.04198500
H	-0.65588000	-3.33688800	-2.28463100
H	-1.90327000	-2.17749000	-1.83237500
H	-1.08300600	-1.26394700	-3.91803800
H	0.58827100	-1.66860500	-3.54711000
H	-3.16172200	2.46236600	-2.19826100
H	-1.64808200	2.98688700	-1.47307400
H	-0.90301200	2.30431300	-3.63525100
H	-2.00808700	0.93799100	-3.72293300
H	1.61507100	0.52531500	-4.22085500
H	1.54546600	2.01173000	-3.25866000
H	3.66816500	0.88475000	-2.63720700
H	2.83162000	-0.64795600	-2.39068600
O	0.96776600	1.62609200	3.51760700
O	0.10765400	0.75006900	1.63382400
C	0.81270200	0.68463700	2.75090500
H	1.23202500	-0.32346000	2.96551700

Complex 5 total energy:-3303.1335 a.u.

Fe	-0.05174500	-0.56029600	-0.15396000

P	0.07457100	1.71451800	-0.39674600
P	2.31821800	-1.09218500	-0.36225900
P	0.02796700	-0.66743500	-2.29563500
P	-2.35678100	-0.86623600	-0.38935000
C	-1.37970000	2.88786900	-0.48442700
C	-1.95671200	3.27941100	-1.71078900
C	-2.99980200	4.21434000	-1.75173700
C	-3.48978200	4.77635000	-0.56768800
C	-2.93049500	4.39243000	0.65718200
C	-1.88991100	3.45790200	0.70012800
C	1.11393400	2.62595800	0.84159500
C	1.18314400	2.15985400	2.16940800
C	1.89414000	2.88246200	3.13883500
C	2.54945600	4.07106100	2.79531700
C	2.48372500	4.54198200	1.47670600
C	1.76562200	3.83174000	0.50754800
C	3.72153300	0.00808000	-0.91488600
C	4.26855700	0.93466100	-0.00110500
C	5.34149600	1.75533200	-0.36589800
C	5.89135800	1.67466600	-1.65165700
C	5.36163400	0.75970500	-2.56802600
C	4.28904500	-0.06638700	-2.20439900
C	3.14570600	-1.99937500	1.03448900
C	3.07430800	-1.47607800	2.34180700
C	3.74112100	-2.10601900	3.40047000
C	4.48219500	-3.27183700	3.17534600
C	4.55629600	-3.80250800	1.88168400
C	3.89806900	-3.17244400	0.81833600
C	-3.00097700	-2.60308800	-0.12859300
C	-2.36708100	-3.70326100	-0.74618700
C	-2.88649200	-4.99633000	-0.62258700
C	-4.03944700	-5.22607500	0.13876500
C	-4.66561500	-4.14934800	0.77488900
C	-4.15540100	-2.85050700	0.64287200
C	-3.58558600	0.13757800	0.55569100
C	-4.79230900	0.59715300	-0.01050500
C	-5.73932800	1.26004100	0.78059900
C	-5.50225900	1.46378300	2.14580700
C	-4.30511500	1.01241600	2.71631100
C	-3.34913300	0.35945900	1.92865300
C	0.93598500	1.99854000	-2.04188700
C	0.48098500	0.97797000	-3.09670800
C	2.16912000	-2.38019300	-1.72033800
C	1.28972800	-1.91578300	-2.90002000

C	-1.60913800	-1.11867200	-3.08386600
C	-2.74840000	-0.57441900	-2.20753600
H	-1.59024300	2.88462500	-2.65440700
H	-3.41778000	4.50998500	-2.71375800
H	-4.29398200	5.51035100	-0.59966600
H	-3.29873300	4.82516200	1.58662300
H	-1.46403500	3.19223000	1.66391000
H	0.68040600	1.23756800	2.44561600
H	1.93220800	2.51348800	4.16366900
H	3.10167300	4.63117200	3.54912500
H	2.98424000	5.46977700	1.20104000
H	1.71321300	4.23365100	-0.50194500
H	3.86937400	1.01547500	1.00545500
H	5.74854300	2.45680400	0.36142500
H	6.72809800	2.31256100	-1.93346800
H	5.78703300	0.67582700	-3.56772500
H	3.92220500	-0.77686400	-2.93934500
H	2.48907800	-0.58467900	2.54475400
H	3.67426400	-1.68449400	4.40310600
H	4.99796800	-3.76287300	3.99959000
H	5.13243600	-4.70775400	1.69295600
H	3.99005500	-3.60536300	-0.17408300
H	-1.44385000	-3.56803700	-1.29830200
H	-2.37842100	-5.82725800	-1.11144600
H	-4.43896000	-6.23434300	0.24089400
H	-5.55866400	-4.31192400	1.37751700
H	-4.67014800	-2.03643000	1.14301800
H	-5.01577100	0.43275200	-1.06195000
H	-6.66740300	1.60777700	0.32794500
H	-6.24627100	1.96976400	2.76014500
H	-4.11154500	1.16799900	3.77739200
H	-2.42100200	0.01719700	2.37932000
H	0.77857200	3.02332500	-2.39568600
H	2.00352100	1.88207500	-1.83895500
H	1.25909700	0.82500900	-3.85457500
H	-0.40799900	1.33135200	-3.63091100
H	3.15184700	-2.71136900	-2.07281400
H	1.69293900	-3.22725800	-1.21730200
H	0.76446100	-2.77273900	-3.33988900
H	1.88497100	-1.46792100	-3.70409400
H	-1.67093700	-0.73270000	-4.11043800
H	-1.66281500	-2.21075800	-3.14810600
H	-3.70152300	-1.04548900	-2.47546900
H	-2.85956000	0.50745200	-2.34154700

O	0.03226700	-2.52422100	0.52449300
C	-0.09919200	-2.11139100	1.72499200
H	-0.13215900	-2.83895800	2.55367400
O	-0.19731200	-0.86459800	1.94550600

TS1 total energy:-3303.0953 a.u.

Fe	-0.06411300	-0.48931900	-0.18655600
P	-2.34310900	-0.73347800	-0.45410400
P	0.15751500	1.70057200	-0.37851800
P	0.00233600	-0.62927600	-2.36318300
P	2.24379400	-1.09342800	-0.40188700
C	-2.97366600	-2.48787800	-0.24534000
C	-2.33386400	-3.56176500	-0.90276900
C	-2.83542300	-4.86486000	-0.81457100
C	-3.97946600	-5.13125800	-0.05181700
C	-4.61278600	-4.08174500	0.62171300
C	-4.11828300	-2.77351600	0.52735700
C	-3.59515000	0.23009800	0.50497300
C	-3.37613500	0.41318900	1.88572900
C	-4.34344400	1.03434400	2.68472800
C	-5.53644400	1.49775600	2.11504500
C	-5.75745000	1.33475400	0.74178800
C	-4.79903700	0.69967300	-0.05858700
C	-1.27941300	2.89758700	-0.40785500
C	-1.77763500	3.42248700	0.80216300
C	-2.79560300	4.38241100	0.80395500
C	-3.34418500	4.83698600	-0.40149100
C	-2.86593100	4.32086800	-1.61088900
C	-1.84478400	3.36119100	-1.61429100
C	1.24040100	2.59431900	0.84321100
C	1.32135800	2.16680100	2.18182200
C	2.05956500	2.89525200	3.12493400
C	2.73577100	4.06014200	2.74328900
C	2.65970300	4.49791000	1.41453400
C	1.91299000	3.77875900	0.47373400
C	3.70141600	-0.03845400	-0.89883300
C	4.31264000	0.78459900	0.07080300
C	5.42990600	1.56314400	-0.25050400
C	5.96134300	1.54043500	-1.54624700
C	5.36787600	0.72660500	-2.51757100
C	4.24977100	-0.05623500	-2.19847700
C	3.01650100	-2.05717800	0.99021200
C	3.83287900	-3.18400200	0.76094400
C	4.43887200	-3.85147000	1.83250400

C	4.25142600	-3.40223200	3.14591500
C	3.45138500	-2.27871300	3.38363300
C	2.83566800	-1.61416600	2.31507800
C	-2.75505000	-0.42001900	-2.27099600
C	-1.64731300	-0.98754700	-3.17429400
C	0.99333500	2.01005400	-2.03793000
C	0.50266800	1.02831900	-3.11310300
C	1.25170500	-1.88389600	-2.98573100
C	2.10586900	-2.36453100	-1.79240400
H	-0.11190600	-0.12560500	1.29892500
H	-1.42204000	-3.39673400	-1.46788900
H	-2.32352400	-5.67392200	-1.33515700
H	-4.36705700	-6.14656700	0.02153600
H	-5.49929600	-4.27330600	1.22541800
H	-4.63800300	-1.98112800	1.05639100
H	-2.45051900	0.06521200	2.33783100
H	-4.16177700	1.15730900	3.75209500
H	-6.28909800	1.98195900	2.73630300
H	-6.68170000	1.69303900	0.28955000
H	-5.01051400	0.56694100	-1.11674400
H	-1.35862900	3.10197800	1.75200400
H	-3.15476400	4.77930100	1.75271400
H	-4.13064300	5.59065600	-0.39863900
H	-3.27521400	4.67204500	-2.55785100
H	-1.48447600	3.00521800	-2.57530900
H	0.79966800	1.26246700	2.48511900
H	2.10346200	2.54958000	4.15754800
H	3.31143200	4.62601900	3.47484400
H	3.17577300	5.40692700	1.10703100
H	1.85721000	4.15940300	-0.54326800
H	3.93032600	0.81277600	1.08678400
H	5.88684000	2.18448300	0.51881700
H	6.83354500	2.14409100	-1.79387900
H	5.77812100	0.68827000	-3.52632100
H	3.83071200	-0.68841900	-2.97579100
H	4.01404400	-3.54988500	-0.24644400
H	5.06283100	-4.72277800	1.63612200
H	4.72572100	-3.92408900	3.97605700
H	3.29704700	-1.92028100	4.40091700
H	2.20916600	-0.74960800	2.51476300
H	-3.72531300	-0.86506700	-2.52140100
H	-2.84302300	0.66489100	-2.39728300
H	-1.69835300	-0.56232500	-4.18560000
H	-1.75286300	-2.07282300	-3.27643500

H	0.85083500	3.04660100	-2.36262300
H	2.06212600	1.87003900	-1.85641000
H	1.27166600	0.87461900	-3.88018800
H	-0.37801300	1.42190900	-3.63298900
H	0.72049900	-2.73149000	-3.43682000
H	1.86495200	-1.44251900	-3.77973700
H	3.09420300	-2.69961800	-2.12615100
H	1.61936300	-3.22092700	-1.31245900
C	-0.31966000	-2.13602700	1.80208600
O	-0.05971600	-2.58409000	0.71622100
O	-0.59501700	-2.03283000	2.94399700

TS2 total energy:-3303.0948 a.u.

Fe	-0.04951100	-0.50379300	-0.18267900
P	0.08812100	1.77350000	-0.38680000
P	2.32796700	-1.03433600	-0.40980300
P	0.01231300	-0.57839600	-2.29558300
P	-2.37000600	-0.78430400	-0.37256800
C	-1.32159400	3.00040300	-0.46805700
C	-1.83478600	3.47738500	-1.69266100
C	-2.84847300	4.44486800	-1.72138900
C	-3.37001700	4.95600200	-0.52774100
C	-2.87359500	4.48761500	0.69487100
C	-1.86395300	3.51929100	0.72581200
C	1.10622800	2.55866300	0.94490400
C	1.06321000	2.01015400	2.24204000
C	1.75944900	2.61336800	3.29823500
C	2.51423500	3.77031900	3.06813300
C	2.56152200	4.32570000	1.78190000
C	1.85755400	3.73152000	0.72764900
C	3.73586900	0.05724500	-0.96108100
C	4.35809800	0.89502800	-0.01020200
C	5.43091600	1.71719200	-0.37167800
C	5.90686000	1.72329000	-1.68943000
C	5.30334900	0.89485300	-2.64236600
C	4.22840900	0.06986200	-2.28315800
C	3.14332700	-1.93447800	0.98822400
C	2.85742100	-1.58299600	2.31998200
C	3.51479200	-2.21555600	3.38223200
C	4.46223700	-3.21326000	3.12827100
C	4.75648600	-3.56876800	1.80576000
C	4.10903900	-2.93180200	0.74109000
C	-3.08483700	-2.50402100	-0.27149800
C	-2.39290700	-3.60102400	-0.82819600

C	-2.97192400	-4.87483400	-0.84932200
C	-4.24476700	-5.08291800	-0.30541000
C	-4.93413200	-4.00616200	0.26356700
C	-4.36338700	-2.72733500	0.28199000
C	-3.54345300	0.19930500	0.66186900
C	-4.67198900	0.85781000	0.13359100
C	-5.57139500	1.51741200	0.98153500
C	-5.36196700	1.52735200	2.36596000
C	-4.24334600	0.87613000	2.90240600
C	-3.33992000	0.22041600	2.05823300
C	1.00183500	2.06528300	-1.99551100
C	0.53380900	1.06523200	-3.06573100
C	2.15820100	-2.31690500	-1.76771900
C	1.21883700	-1.87291000	-2.90954000
C	-1.65372200	-0.93514200	-3.06155900
C	-2.73848000	-0.32858400	-2.15783500
H	-1.44118100	3.12583100	-2.64258400
H	-3.21743800	4.80625700	-2.68088800
H	-4.15008100	5.71590000	-0.55028300
H	-3.26666900	4.87968000	1.63206200
H	-1.48842700	3.18707300	1.68979500
H	0.47183400	1.11588700	2.43583900
H	1.71001400	2.18023200	4.29679500
H	3.05723400	4.24074800	3.88690600
H	3.14071500	5.23013200	1.59856400
H	1.89268100	4.19470300	-0.25628000
H	4.02112500	0.89440200	1.02310500
H	5.89977600	2.34779300	0.38292700
H	6.74579000	2.35968600	-1.96807000
H	5.67335900	0.87812000	-3.66714700
H	3.79903200	-0.57332300	-3.04653900
H	2.11484900	-0.82030400	2.53627000
H	3.27425600	-1.93615800	4.40729200
H	4.96694100	-3.71265000	3.95415900
H	5.49391100	-4.34314700	1.59766200
H	4.37235900	-3.21688500	-0.27468700
H	-1.38072500	-3.47840300	-1.19493300
H	-2.41430300	-5.70899100	-1.27393200
H	-4.68954400	-6.07724500	-0.31317000
H	-5.92098800	-4.15584600	0.70023000
H	-4.92354000	-1.91218000	0.72964200
H	-4.87125600	0.85407900	-0.93507000
H	-6.44067300	2.01749500	0.55579400
H	-6.06817900	2.03391300	3.02275100

H	-4.07541700	0.87112000	3.97889900
H	-2.48694100	-0.29443900	2.49679100
H	0.88286100	3.09761200	-2.34231100
H	2.06024200	1.91217300	-1.77200800
H	1.31880600	0.89371300	-3.81243100
H	-0.33664000	1.44801400	-3.61051900
H	3.13625100	-2.61466800	-2.15947600
H	1.72423300	-3.17423800	-1.24562200
H	0.64619500	-2.73053300	-3.28304100
H	1.76997500	-1.46526000	-3.76557300
H	-1.70597900	-0.53781900	-4.08441400
H	-1.77255000	-2.02226800	-3.12588800
H	-3.73150600	-0.69009200	-2.44975100
H	-2.73569900	0.76506200	-2.22333500
O	-0.18968600	-3.55838700	2.28391200
O	0.07752500	-2.40337100	0.35339400
C	-0.22254300	-2.53210300	1.62488600
H	-0.52901100	-1.55685400	2.11663600

TS3 total energy:-3303.1107 a.u.

Fe	0.03645600	0.47669200	-0.22464900
P	-0.00813500	-1.74260900	-0.44494500
P	-2.37073600	0.95494900	-0.39529400
P	-0.06146200	0.50445900	-2.34738800
P	2.30624900	0.88063300	-0.44334300
C	1.49702900	-2.84397500	-0.50958900
C	2.03489100	-3.30902800	-1.72881100
C	3.12040900	-4.19439800	-1.74479600
C	3.69179700	-4.63125900	-0.54403100
C	3.17213700	-4.17228800	0.67237400
C	2.08946900	-3.28634900	0.69193800
C	-0.95024900	-2.53932900	0.93130800
C	-0.89320500	-1.96346000	2.21695000
C	-1.53022700	-2.59198300	3.29673400
C	-2.22973000	-3.79002000	3.10518100
C	-2.28602400	-4.36733100	1.82876700
C	-1.64568800	-3.75232500	0.74650500
C	-3.74697600	-0.15406900	-0.98336400
C	-4.26191800	-1.11158800	-0.08200100
C	-5.31893900	-1.94954700	-0.45355800
C	-5.88463600	-1.85274800	-1.73172900
C	-5.38977700	-0.90317800	-2.63250500
C	-4.33222600	-0.06015400	-2.26294500
C	-3.22922800	1.83373900	0.99243300

C	-3.00201000	1.43473800	2.32310600
C	-3.70463400	2.03635800	3.37477500
C	-4.63766300	3.04675800	3.11448100
C	-4.87194500	3.44875600	1.79337800
C	-4.17975200	2.84400000	0.73740300
C	2.76185200	2.68344900	-0.31664000
C	1.85319700	3.67953500	-0.73108100
C	2.21700900	5.03125200	-0.72263100
C	3.49071500	5.41654900	-0.28673600
C	4.39687000	4.43889300	0.13996500
C	4.03950200	3.08442700	0.12541200
C	3.62824700	0.04434600	0.54015100
C	4.82341800	-0.42472300	-0.04445800
C	5.83340900	-0.97699000	0.75387900
C	5.66814500	-1.06552400	2.14175400
C	4.48242000	-0.60509300	2.72858800
C	3.46466800	-0.05739100	1.93785100
C	-0.91648900	-2.15202600	-2.03672000
C	-0.52786900	-1.14777500	-3.13370500
C	-2.17880000	2.25448800	-1.73180900
C	-1.33285500	1.76108400	-2.92316200
C	1.56178800	0.99678400	-3.13486600
C	2.71541100	0.51635600	-2.24331000
H	1.60639500	-3.01220100	-2.68219300
H	3.50796100	-4.55063000	-2.69887000
H	4.52985700	-5.32693200	-0.55660300
H	3.60534500	-4.50653800	1.61415400
H	1.69991600	-2.95738400	1.65116700
H	-0.34916400	-1.03463900	2.38649600
H	-1.47280100	-2.14182800	4.28737700
H	-2.72280500	-4.27680100	3.94592000
H	-2.82104000	-5.30398600	1.67473000
H	-1.68544100	-4.23089500	-0.22988600
H	-3.85218900	-1.19647800	0.92090400
H	-5.70362700	-2.67480700	0.26261200
H	-6.70949200	-2.50368500	-2.01861400
H	-5.83188500	-0.80520700	-3.62361600
H	-3.99533900	0.68147100	-2.98162400
H	-2.26577500	0.67014600	2.54808200
H	-3.51101000	1.71880900	4.39880600
H	-5.17935700	3.51780000	3.93379400
H	-5.59923800	4.23104200	1.57876800
H	-4.40180600	3.16302200	-0.27817200
H	0.84635000	3.40845100	-1.02987100

H	1.49754300	5.78439300	-1.04353200
H	3.77057300	6.46920200	-0.27156900
H	5.38765600	4.72576700	0.49072700
H	4.76172000	2.34767300	0.46520300
H	4.99010700	-0.35561100	-1.11646400
H	6.75222000	-1.33066100	0.28701100
H	6.45919100	-1.48824500	2.76035400
H	4.34388400	-0.66828900	3.80756100
H	2.55091700	0.29317700	2.41275100
H	-0.72661400	-3.18432100	-2.35032400
H	-1.98080300	-2.06817500	-1.80312300
H	-1.34385400	-1.01011700	-3.85312800
H	0.34162200	-1.49421100	-3.70401100
H	-3.14527200	2.63999100	-2.07551900
H	-1.66658700	3.07569600	-1.21762800
H	-0.81132500	2.60343900	-3.39443100
H	-1.95356500	1.30198900	-3.70077800
H	1.63943400	0.59740900	-4.15535000
H	1.57234600	2.09031400	-3.20982400
H	3.65139800	1.00997100	-2.53067000
H	2.86038000	-0.56541100	-2.33678900
O	-0.07093900	1.96904500	0.99511700
C	0.24762000	2.10020600	2.25594300
H	0.20178900	3.15935400	2.58794000
O	0.54354300	1.19939100	3.04626900

Complex 1T total energy:-3114.5786 a.u.

Fe	0.00400100	0.12059800	0.12851500
P	0.41838800	-2.20412900	0.44498800
P	1.89652500	1.53361800	0.38787400
P	-0.02669800	0.17305500	2.37301300
P	-2.26968600	0.80316600	0.34966100
C	-1.03727600	-3.34936300	0.30954100
C	-1.48630400	-4.17181900	1.36219900
C	-2.56417800	-5.04785400	1.17201700
C	-3.20425100	-5.12165000	-0.07033300
C	-2.76551100	-4.30783100	-1.12312700
C	-1.69812000	-3.42386700	-0.93459000
C	1.66740500	-3.04113200	-0.63267000
C	1.85855100	-2.56207600	-1.94317600
C	2.73348800	-3.21859300	-2.81835200
C	3.43883700	-4.35007400	-2.39176200
C	3.26080100	-4.82891600	-1.08667100
C	2.37572500	-4.18649700	-0.21310500

C	3.56274100	0.72601900	0.28256200
C	4.03328500	0.33798600	-0.98991200
C	5.28273500	-0.27401700	-1.13198100
C	6.08370600	-0.51786800	-0.00864200
C	5.62847600	-0.13679500	1.25851500
C	4.37848300	0.48054600	1.40541200
C	2.08873200	2.98128700	-0.74950900
C	1.35518300	3.00898900	-1.95128400
C	1.50443200	4.07510200	-2.84894500
C	2.38248700	5.12457100	-2.55387900
C	3.11866300	5.10377500	-1.36032600
C	2.97990700	4.03799800	-0.46437300
C	-2.72712100	2.60055700	0.26054000
C	-1.72759000	3.58134300	0.13713500
C	-2.06131600	4.94251200	0.10357300
C	-3.40038800	5.33823500	0.19366100
C	-4.40592400	4.36760800	0.30963000
C	-4.07568100	3.00851800	0.33954700
C	-3.50029300	0.00993900	-0.77584400
C	-4.67935400	-0.61761200	-0.32662000
C	-5.59377200	-1.14932500	-1.24643100
C	-5.34716000	-1.05913100	-2.62146900
C	-4.17459400	-0.44052300	-3.07695500
C	-3.25482100	0.08484600	-2.16321000
C	1.05607600	-2.39546900	2.19729200
C	0.23881400	-1.51318000	3.15328900
C	1.79656700	2.29314200	2.10718600
C	1.28754100	1.27384400	3.13973500
C	-1.66396800	0.76579800	3.06235200
C	-2.78345900	0.34660200	2.09820600
H	0.00598200	0.10683000	-1.40768500
H	-0.99999300	-4.15906300	2.33452400
H	-2.89279900	-5.67974300	1.99671800
H	-4.03610300	-5.80927400	-0.21793300
H	-3.25697900	-4.35531800	-2.09401100
H	-1.37618900	-2.79512300	-1.76169800
H	1.32269200	-1.67379700	-2.27159300
H	2.86607600	-2.84059300	-3.83186200
H	4.12168100	-4.85893000	-3.07127100
H	3.80351500	-5.71124400	-0.74887500
H	2.23708400	-4.59537000	0.78566000
H	3.43047800	0.52521700	-1.87597900
H	5.62993000	-0.55987000	-2.12411200
H	7.05673900	-0.99416800	-0.12123800

H	6.24785000	-0.30883300	2.13836200
H	4.06836300	0.78226400	2.40224600
H	0.66977400	2.19328900	-2.17398000
H	0.93187000	4.08380200	-3.77598100
H	2.49800400	5.95406300	-3.25065600
H	3.80879800	5.91468000	-1.12951900
H	3.57910800	4.02972600	0.44438200
H	-0.68888200	3.28123500	0.04753900
H	-1.27337000	5.68787400	-0.00099900
H	-3.66285700	6.39517500	0.16582400
H	-5.45145500	4.66829100	0.36965600
H	-4.87315000	2.27119500	0.40830600
H	-4.90243800	-0.69795400	0.73472400
H	-6.50135400	-1.63046600	-0.88312100
H	-6.06277500	-1.46841100	-3.33365400
H	-3.97299700	-0.36879000	-4.14538200
H	-2.33961000	0.54908500	-2.52641200
H	1.06289000	-3.44022300	2.52942800
H	2.10166700	-2.06487500	2.16179500
H	0.72578700	-1.42387400	4.13384400
H	-0.75356300	-1.94709200	3.32507600
H	2.75444400	2.72896800	2.41656800
H	1.08614200	3.12355600	2.01097500
H	0.89692300	1.77777200	4.03409700
H	2.09911600	0.61768000	3.47369700
H	-1.83624100	0.37828000	4.07579300
H	-1.61451800	1.86039900	3.13322600
H	-3.73413500	0.81973900	2.37248600
H	-2.92677600	-0.74107600	2.12123300

Complex 2T total energy:-3303.1259 a.u.

Fe	-0.12871200	0.25682800	-0.40002100
P	-0.02101900	-2.02949200	-1.04967400
P	-2.32418500	1.17523300	-0.32147500
P	-0.32543000	0.63088300	-2.60585100
P	1.88938500	1.51095000	-0.65462600
C	1.67603900	-2.77370600	-1.15931200
C	2.23330100	-3.26950000	-2.35492700
C	3.51075700	-3.84665100	-2.36080300
C	4.24790100	-3.94207000	-1.17510300
C	3.70239200	-3.45192700	0.01877800
C	2.43205500	-2.86641600	0.02823300
C	-0.93883500	-3.29291000	-0.05762600
C	-1.09902600	-3.07829600	1.32522000

C	-1.71789700	-4.04728100	2.12571100
C	-2.19698900	-5.23256000	1.55516300
C	-2.04789100	-5.45067100	0.17886700
C	-1.41617600	-4.49329500	-0.62352900
C	-3.73590100	-0.02871300	-0.28635500
C	-3.97964200	-0.72928600	0.91400300
C	-5.03106900	-1.64684500	1.00422600
C	-5.85593400	-1.88960100	-0.10191600
C	-5.62606800	-1.19942100	-1.29725100
C	-4.57638500	-0.27501300	-1.39089400
C	-2.77135600	2.33011500	1.05568200
C	-2.02251000	2.29733900	2.24859300
C	-2.36271500	3.13051600	3.32322300
C	-3.44908300	4.00705300	3.21755000
C	-4.20216700	4.04346300	2.03519100
C	-3.87233800	3.20788500	0.96222900
C	1.86861900	3.33395100	-0.30588900
C	0.72094800	3.92898600	0.24548400
C	0.68382900	5.30594800	0.50619300
C	1.79586200	6.10432700	0.21664300
C	2.95000900	5.51917500	-0.32434300
C	2.99103400	4.14432100	-0.58012800
C	3.39376000	0.93310900	0.24877200
C	4.65189000	0.76791100	-0.36437300
C	5.76613500	0.38772100	0.39565900
C	5.64162700	0.17233900	1.77340400
C	4.39264600	0.32879500	2.38962400
C	3.27469300	0.69959600	1.63459000
C	-0.74669700	-2.12916000	-2.77634000
C	-0.26982000	-0.94266900	-3.62796900
C	-2.54258300	2.19398200	-1.88589700
C	-1.92156900	1.48817700	-3.10219400
C	1.05161100	1.69441200	-3.29832800
C	2.32488600	1.44311900	-2.47937100
H	-0.00156500	0.04501300	1.11286000
H	1.68200200	-3.23168300	-3.29108500
H	3.92153900	-4.22988700	-3.29449400
H	5.23778200	-4.39671300	-1.18042700
H	4.26830900	-3.51960000	0.94709500
H	2.02863200	-2.48759400	0.96464300
H	-0.73996800	-2.15262900	1.76993200
H	-1.82930600	-3.87058600	3.19544700
H	-2.68130400	-5.98437800	2.17740100
H	-2.41447700	-6.37235400	-0.27195000

H	-1.29203200	-4.69956200	-1.68455800
H	-3.35574800	-0.55214500	1.78729500
H	-5.20477700	-2.17234700	1.94244900
H	-6.67457400	-2.60448600	-0.03025100
H	-6.26905100	-1.36867600	-2.16060400
H	-4.44537500	0.25903100	-2.32821600
H	-1.17243400	1.62138100	2.32637400
H	-1.77476300	3.09432600	4.23993200
H	-3.71234800	4.65628300	4.05185200
H	-5.05362200	4.71788600	1.94976000
H	-4.48643300	3.23668800	0.06414200
H	-0.13893900	3.31332600	0.48677600
H	-0.21278800	5.74760400	0.94020800
H	1.77000400	7.17465900	0.41796900
H	3.82389000	6.13288500	-0.54076100
H	3.90701200	3.70942700	-0.97616900
H	4.78207200	0.93504100	-1.43115600
H	6.73225900	0.26485500	-0.09289100
H	6.51134300	-0.11701200	2.36229500
H	4.28451400	0.15736300	3.46020700
H	2.30544400	0.79761000	2.11954800
H	-0.52646400	-3.08344000	-3.26912200
H	-1.83341500	-2.08796400	-2.63048500
H	-0.86756700	-0.84147200	-4.54401500
H	0.77217300	-1.08585500	-3.93836700
H	-3.59369400	2.44903200	-2.06862000
H	-2.01499900	3.13423600	-1.68055900
H	-1.73793500	2.19882400	-3.91928400
H	-2.59514800	0.71870000	-3.49602400
H	1.21045100	1.49482900	-4.36691000
H	0.73911300	2.74252500	-3.20280500
H	3.10424300	2.16958500	-2.73777300
H	2.72049900	0.43910100	-2.67719300
C	1.74207000	-2.25528800	5.10469400
O	1.36403800	-1.67537300	4.14837000
O	2.12049000	-2.83322000	6.05679700

Complex 3T total energy:-3303.0980 a.u.

Fe	1.08629000	-0.01357200	-0.52373100
P	2.81017700	-1.53135000	0.05204300
P	0.51997300	2.01410900	0.56215600
P	-0.10649200	-1.03666200	1.03727800
P	-3.92171000	-0.24467000	0.55943200
C	2.80547000	-3.12554800	-0.87630500

C	1.81830500	-3.37646300	-1.84963200
C	1.80479900	-4.59661300	-2.53939500
C	2.77209700	-5.57080100	-2.26708600
C	3.76198700	-5.32350900	-1.30473300
C	3.78474500	-4.10760500	-0.61368800
C	4.54621600	-0.92717600	0.00739400
C	5.04694800	-0.46986800	-1.23155600
C	6.35883800	0.00343900	-1.33112800
C	7.18447500	0.03778100	-0.19833100
C	6.69281600	-0.40616300	1.03498200
C	5.38067500	-0.88649300	1.14228600
C	2.01774200	2.65333300	1.42089800
C	3.13101400	3.00371700	0.62382000
C	4.29968500	3.49489700	1.21406600
C	4.38295000	3.63254700	2.60658000
C	3.28845400	3.28105600	3.40611100
C	2.11176700	2.79448100	2.82064600
C	-0.19636400	3.42484100	-0.37492600
C	-0.99190800	3.15063500	-1.50640800
C	-1.60648400	4.19744100	-2.20323200
C	-1.42566300	5.52222500	-1.78564600
C	-0.63065800	5.80034400	-0.66558900
C	-0.01632900	4.75999700	0.04125600
C	-4.99379800	-1.51506300	1.39184500
C	-4.96946000	-1.57410900	2.80024200
C	-5.73855600	-2.51951900	3.49375000
C	-6.55221200	-3.41276400	2.78713800
C	-6.59578500	-3.35673700	1.38621000
C	-5.82397400	-2.41718600	0.69349400
C	-4.99242600	0.38825600	-0.81432300
C	-6.04234800	1.25673000	-0.43905900
C	-6.88073600	1.83000700	-1.40007300
C	-6.67619500	1.56601600	-2.76169500
C	-5.63174100	0.71978300	-3.15014200
C	-4.79808700	0.13184200	-2.18715800
C	2.41707200	-2.00735900	1.81820800
C	0.92134200	-2.34521200	1.90884800
C	-0.76244100	1.58418700	1.84827900
C	-0.53907900	0.17394900	2.40579000
C	-1.63168700	-2.01093600	0.55728800
C	-2.69073000	-1.34785100	-0.34758800
H	1.91004900	0.74321100	-1.77549000
H	1.07221400	-2.62068600	-2.08336900
H	1.04174900	-4.77738500	-3.29563100

H	2.76248700	-6.51662600	-2.80734800
H	4.52286400	-6.07482100	-1.09649100
H	4.57195500	-3.92339600	0.11565200
H	4.41751900	-0.48284100	-2.12059800
H	6.73404100	0.34672100	-2.29444400
H	8.20579300	0.40812900	-0.27773000
H	7.32971800	-0.38494800	1.91858200
H	5.02663000	-1.22982000	2.11162600
H	3.08267700	2.90383800	-0.45950900
H	5.14540600	3.76749000	0.58419000
H	5.29425800	4.01428400	3.06511100
H	3.34239600	3.39276100	4.48849900
H	1.27265100	2.54661600	3.46635100
H	-1.12756600	2.12708100	-1.84845300
H	-2.21952400	3.97451500	-3.07547600
H	-1.89888000	6.33621700	-2.33338400
H	-0.48583100	6.82954300	-0.33918200
H	0.59981800	4.99145600	0.90755800
H	-4.35841800	-0.86490600	3.35942000
H	-5.71010800	-2.54885900	4.58277600
H	-7.15752900	-4.14297300	3.32335900
H	-7.23686600	-4.04283600	0.83295700
H	-5.88223600	-2.37655000	-0.39320900
H	-6.20881300	1.48319500	0.61424300
H	-7.68990700	2.48855600	-1.08551300
H	-7.32455500	2.01747700	-3.51180400
H	-5.46463000	0.50585900	-4.20572900
H	-4.00464200	-0.53003300	-2.52716200
H	3.03024300	-2.85459900	2.15013300
H	2.66123700	-1.14569100	2.45275000
H	0.59992000	-2.44867200	2.95394300
H	0.72232500	-3.30347800	1.41361400
H	-0.79911800	2.33894400	2.64379600
H	-1.72728900	1.62906700	1.32742900
H	-1.42528300	-0.17576800	2.94993800
H	0.30779700	0.15904800	3.10390700
H	-1.21359900	-2.87419000	0.02021900
H	-2.07532600	-2.40796500	1.48216400
H	-3.22628900	-2.15056400	-0.87184900
H	-2.19522900	-0.74325000	-1.11423700
C	1.20079600	0.35018600	-2.72945300
O	0.16238500	-0.27661900	-2.31901100
O	1.68210600	0.67462500	-3.79225700

Complex 4T total energy:-3303.1350 a.u.

Fe	0.06309100	-0.01148700	-0.07180400
P	-0.05562700	2.45259900	-0.45114200
P	2.24566200	-1.16935000	-0.42077900
P	0.07283100	-0.04398100	-2.32255600
P	-2.10056900	-1.22471300	-0.41789600
C	-1.76603500	3.16212800	-0.38876500
C	-2.34912400	3.90058600	-1.43804400
C	-3.62401200	4.46364800	-1.28716200
C	-4.32802900	4.30631300	-0.08734300
C	-3.75626700	3.57219600	0.96047000
C	-2.49047200	2.99568700	0.81049500
C	0.89550100	3.65796200	0.58962700
C	1.13122700	3.36164500	1.94798700
C	1.79636300	4.28381300	2.76769100
C	2.23805500	5.50568900	2.24597700
C	2.00628400	5.80762100	0.89731400
C	1.33522400	4.89551400	0.07394100
C	3.72196900	-0.05202900	-0.52331200
C	3.72373300	1.14382100	0.21979900
C	4.84264200	1.98799600	0.21299700
C	5.97176300	1.65089000	-0.54211600
C	5.98377000	0.45861900	-1.27927400
C	4.87287200	-0.39234400	-1.26529000
C	2.85669300	-2.52400100	0.68079000
C	3.24189400	-2.18971800	1.99577700
C	3.71939700	-3.17194500	2.86763100
C	3.81705200	-4.50448800	2.44516600
C	3.43800100	-4.84679700	1.14241000
C	2.95902900	-3.86607900	0.26305300
C	-2.10234600	-3.07943200	-0.50537000
C	-0.99141600	-3.82370100	-0.06889100
C	-1.00050700	-5.22361500	-0.15136300
C	-2.11384900	-5.89432600	-0.66865200
C	-3.23285900	-5.16077300	-1.08896900
C	-3.23226900	-3.76491200	-1.00312600
C	-3.58368800	-0.86972100	0.63026900
C	-4.70773000	-0.16600200	0.15292000
C	-5.81928000	0.04118800	0.98082700
C	-5.82271700	-0.44065100	2.29477000
C	-4.70697900	-1.13665900	2.77880100
C	-3.59512500	-1.35298000	1.95773100
C	0.57741200	2.71809600	-2.18603800
C	0.00411400	1.64962600	-3.12328600

C	2.11461500	-1.92295000	-2.12326900
C	1.57435300	-0.86040400	-3.08508100
C	-1.38582300	-0.93791900	-3.07361300
C	-2.60143600	-0.75469300	-2.16062200
H	-1.81896400	4.06404700	-2.37351300
H	-4.05807900	5.03572900	-2.10673400
H	-5.31398600	4.75417600	0.03084500
H	-4.29783200	3.43969400	1.89609200
H	-2.06705100	2.41742100	1.62941200
H	0.80215700	2.40989000	2.35729200
H	1.96926500	4.04214400	3.81617000
H	2.75536100	6.22057600	2.88482800
H	2.34042200	6.75852100	0.48342400
H	1.15389300	5.16843300	-0.96317300
H	2.85446900	1.41414300	0.81145000
H	4.82481300	2.90729700	0.79702900
H	6.84104900	2.30739700	-0.55202300
H	6.86385800	0.18291800	-1.85937200
H	4.92499000	-1.32558000	-1.82211300
H	3.17522100	-1.16047900	2.34230500
H	4.01347500	-2.89547100	3.87935500
H	4.18803300	-5.26924700	3.12622400
H	3.51911000	-5.87844500	0.80126700
H	2.67939200	-4.16481200	-0.74405600
H	-0.14854200	-3.31675300	0.38778800
H	-0.13847200	-5.78581600	0.20582700
H	-2.12015000	-6.98205200	-0.73045800
H	-4.11259500	-5.67569000	-1.47375700
H	-4.12513300	-3.22045200	-1.30530400
H	-4.74062900	0.22284500	-0.86141400
H	-6.68359700	0.57792600	0.59081400
H	-6.68945700	-0.27994700	2.93489800
H	-4.70120700	-1.52134600	3.79816600
H	-2.74444500	-1.90496800	2.34815900
H	0.36724300	3.72339700	-2.56903300
H	1.66857400	2.62555000	-2.11121600
H	0.54121100	1.62648500	-4.08141300
H	-1.04750300	1.86018000	-3.35036500
H	3.06986500	-2.32939500	-2.47413200
H	1.41057200	-2.75989900	-2.04544400
H	1.31276600	-1.29271600	-4.06030000
H	2.32813800	-0.08257000	-3.26037400
H	-1.57654100	-0.56571200	-4.08963400
H	-1.12591300	-2.00078200	-3.15538900

H	-3.44883800	-1.35401400	-2.51165500
H	-2.91881600	0.29483000	-2.14938500
O	0.07966600	0.24851700	1.82322700
O	-0.23583800	-1.91336500	2.48025000
C	-0.04399600	-0.71965900	2.70165900
H	0.04038700	-0.33173700	3.74249200

Complex 5T total energy:-3303.1279 a.u.

Fe	0.00311200	-0.04334700	-0.00455600
P	0.54677900	2.34744800	-0.44673600
P	1.93561300	-1.65637900	-0.33466200
P	-0.01814900	-0.16294800	-2.25212200
P	-2.40771000	-0.68922000	-0.37510800
C	-0.90578200	3.49838200	-0.40448500
C	-1.24110900	4.37989400	-1.45154400
C	-2.30735100	5.27839500	-1.30902100
C	-3.04345500	5.31785500	-0.11863500
C	-2.71810700	4.44341700	0.92671700
C	-1.66586100	3.53215400	0.78383600
C	1.79037300	3.28841000	0.55871900
C	1.93288300	2.99307200	1.93053800
C	2.82033900	3.73347600	2.72345000
C	3.57692500	4.76974500	2.16301300
C	3.43974300	5.06920200	0.80098800
C	2.55005600	4.33946700	0.00331400
C	3.62597600	-0.92943200	-0.57894000
C	3.94787700	0.27694700	0.07096700
C	5.23200600	0.82923300	-0.03835300
C	6.20981500	0.18514100	-0.80457200
C	5.90358700	-1.02185500	-1.44894500
C	4.62612100	-1.58126600	-1.33173200
C	2.29438200	-3.05617100	0.82081400
C	2.89992100	-2.75903400	2.05980900
C	3.18419500	-3.77681200	2.97531600
C	2.86733600	-5.10810400	2.67304700
C	2.26703000	-5.41335800	1.44664700
C	1.97914100	-4.39678500	0.52577900
C	-2.92422100	-2.47004600	-0.53655100
C	-2.02241400	-3.52826400	-0.32809000
C	-2.43361200	-4.85720300	-0.50594300
C	-3.74694800	-5.14598000	-0.89172000
C	-4.65749200	-4.09818400	-1.08799000
C	-4.25302800	-2.77094100	-0.90942400
C	-3.72261100	0.00031100	0.72247000

C	-4.56164300	1.06559800	0.33988600
C	-5.55323900	1.53493200	1.21210400
C	-5.71307800	0.95932400	2.47787100
C	-4.87781700	-0.09616600	2.86916500
C	-3.89102000	-0.57511500	2.00150300
C	1.21132700	2.37608700	-2.18975200
C	0.35304800	1.47890800	-3.08585600
C	1.54750500	-2.45238800	-1.98210300
C	1.22129500	-1.35233800	-2.99621000
C	-1.66816500	-0.61625500	-3.01011800
C	-2.78332800	-0.07860000	-2.10553100
H	-0.67337500	4.39391300	-2.37901500
H	-2.55134300	5.95555000	-2.12710800
H	-3.86331100	6.02630900	-0.00611000
H	-3.28717400	4.46274100	1.85520800
H	-1.43399700	2.84979500	1.59937400
H	1.35792200	2.18497800	2.37540300
H	2.91830300	3.49534000	3.78231300
H	4.26574300	5.34347400	2.78204700
H	4.01951700	5.87753400	0.35633100
H	2.45302400	4.60900900	-1.04592500
H	3.19914600	0.78287200	0.67281500
H	5.46084900	1.76187500	0.47561400
H	7.20721700	0.61401000	-0.89435900
H	6.66345900	-1.53641800	-2.03630400
H	4.42835900	-2.53513200	-1.81640300
H	3.16253300	-1.73317900	2.31222600
H	3.65659500	-3.52848300	3.92510200
H	3.08989600	-5.90035400	3.38657900
H	2.02401000	-6.44594700	1.19777600
H	1.51886900	-4.67096000	-0.42011500
H	-1.01985800	-3.31422700	0.02088600
H	-1.72605800	-5.66633900	-0.32635000
H	-4.06562200	-6.17906000	-1.02618800
H	-5.68719200	-4.31272400	-1.37236000
H	-4.98414900	-1.97558000	-1.04394700
H	-4.46303900	1.53507100	-0.63544500
H	-6.20266100	2.35025800	0.89478500
H	-6.48559400	1.32609100	3.15272400
H	-4.99877500	-0.55562900	3.84962900
H	-3.26319900	-1.40700200	2.31214400
H	1.28078100	3.38767300	-2.60559000
H	2.23524900	1.98923300	-2.11699500
H	0.83852200	1.29658400	-4.05458400

H	-0.61070100	1.95809400	-3.29596000
H	2.36488700	-3.09036800	-2.33707400
H	0.67287700	-3.09484100	-1.83369000
H	0.82584400	-1.76942800	-3.93213300
H	2.12381000	-0.78113400	-3.24726100
H	-1.73363800	-0.21304100	-4.02981100
H	-1.72755200	-1.70916400	-3.08330900
H	-3.76877500	-0.41399200	-2.44855300
H	-2.78146800	1.01806300	-2.09998100
O	0.05201100	0.29650900	1.98661400
O	-0.56278400	-1.84193100	1.78718700
C	-0.28081900	-0.84495600	2.48611300
H	-0.34133900	-1.00273300	3.58177400

TS1T total energy:-3303.0908 a.u.

Fe	1.12617300	0.02225300	-0.56466900
P	2.79728100	-1.52791100	0.01170000
P	0.57377600	2.04373200	0.51097100
P	-0.17126900	-1.02700300	0.98820900
P	-3.97753000	-0.23099900	0.53396600
C	2.73822200	-3.13979800	-0.88824400
C	1.72723600	-3.38444600	-1.83849300
C	1.66719200	-4.61559500	-2.50551700
C	2.61407300	-5.61001700	-2.23372600
C	3.62842400	-5.37031900	-1.29573100
C	3.69597400	-4.14269400	-0.62811400
C	4.56574100	-1.02003400	0.00102700
C	5.09356200	-0.51617500	-1.20720100
C	6.43560400	-0.13126700	-1.28602800
C	7.26541700	-0.22963400	-0.16016600
C	6.74714100	-0.71829300	1.04485900
C	5.40519700	-1.11419500	1.12912000
C	2.03763800	2.61667300	1.47274200
C	3.24428400	2.83926600	0.77268000
C	4.38313100	3.29308400	1.44618100
C	4.34187200	3.52075600	2.82846200
C	3.15237900	3.29902900	3.53330700
C	2.00571900	2.85212000	2.86311600
C	-0.05770800	3.49856300	-0.42124600
C	-0.93107300	3.27587900	-1.50650500
C	-1.46417200	4.35855300	-2.21469100
C	-1.12806800	5.67003800	-1.85400200
C	-0.25894900	5.89675200	-0.77923800
C	0.27681600	4.81956300	-0.06264300

C	-5.05951600	-1.45443000	1.42223600
C	-5.05318800	-1.43302700	2.83184900
C	-5.83607000	-2.33377400	3.56810100
C	-6.64428800	-3.26314600	2.90317900
C	-6.66931000	-3.28755300	1.50086400
C	-5.88481900	-2.39163000	0.76591700
C	-5.05575500	0.36783000	-0.84999600
C	-6.04762000	1.31231400	-0.50160000
C	-6.89250400	1.86057800	-1.47163200
C	-6.75140400	1.49424000	-2.81743000
C	-5.76422900	0.57135800	-3.18070000
C	-4.92535900	0.00884100	-2.20727500
C	2.36694500	-1.96321800	1.78532000
C	0.87139900	-2.30363700	1.88686400
C	-0.78163700	1.62874500	1.73031300
C	-0.59543100	0.22591600	2.32303500
C	-1.70377500	-2.01935300	0.56644400
C	-2.77038800	-1.38113100	-0.34806400
H	2.13076700	0.82622100	-1.38420000
H	0.99444500	-2.61520600	-2.07159300
H	0.88448600	-4.79055000	-3.24289200
H	2.56895900	-6.56506200	-2.75561300
H	4.37389700	-6.13704100	-1.08789000
H	4.50183500	-3.96598900	0.08207500
H	4.45772600	-0.41831900	-2.08544000
H	6.83057100	0.24977100	-2.22706600
H	8.30975700	0.07385800	-0.22252400
H	7.38542000	-0.79695600	1.92424000
H	5.03207800	-1.49450600	2.07725500
H	3.29196400	2.66037300	-0.29927400
H	5.30373000	3.46160700	0.88896500
H	5.23032300	3.87076100	3.35264000
H	3.10958700	3.48044200	4.60669100
H	1.09344700	2.70594500	3.43605000
H	-1.19226000	2.26276900	-1.80645600
H	-2.13445400	4.17388300	-3.05309100
H	-1.53864700	6.51142400	-2.41076200
H	0.00667200	6.91444000	-0.49545400
H	0.95184700	5.01268500	0.76784500
H	-4.44448400	-0.69663800	3.35728600
H	-5.82157900	-2.30074200	4.65728800
H	-7.25971600	-3.95914900	3.47237700
H	-7.30657500	-4.00159200	0.97949300
H	-5.93094200	-2.41185500	-0.32194600

H	-6.16236300	1.61928300	0.53820300
H	-7.65632400	2.57979300	-1.17717600
H	-7.40418800	1.92613500	-3.57518000
H	-5.64689100	0.27835500	-4.22394100
H	-4.17807200	-0.71466700	-2.52595300
H	2.97765000	-2.80188000	2.14300000
H	2.61120200	-1.08657200	2.39974600
H	0.55983000	-2.38930900	2.93651300
H	0.67760400	-3.27452900	1.41438500
H	-0.86161700	2.39443400	2.51224600
H	-1.71780700	1.67114300	1.15938300
H	-1.49616600	-0.08730200	2.86504300
H	0.24006500	0.21378300	3.03486300
H	-1.29344700	-2.89968700	0.05116200
H	-2.14120400	-2.38773200	1.50531900
H	-3.31910000	-2.19720500	-0.83701300
H	-2.28308000	-0.80462000	-1.14261400
C	1.25133600	0.36929000	-2.80071000
O	0.17852000	-0.15173400	-2.46401700
O	1.97278400	0.74273600	-3.67439200

TS2T total energy:-3303.0911 a.u.

Fe	0.10970100	-0.04702900	-0.15951100
P	-0.02352200	2.39911300	-0.49357400
P	2.23797300	-1.19873100	-0.41773500
P	0.11549700	-0.10872100	-2.36371300
P	-2.13734700	-1.21751400	-0.49940400
C	-1.73912300	3.07341900	-0.30933400
C	-2.42886800	3.73751000	-1.34338100
C	-3.69690200	4.28734200	-1.11129600
C	-4.28821000	4.18895000	0.15363300
C	-3.61068500	3.52748200	1.18613700
C	-2.35041400	2.96487300	0.95838400
C	0.98471900	3.62933200	0.46395100
C	1.21244000	3.42550500	1.84090600
C	1.92080000	4.37561400	2.58852900
C	2.41623700	5.53400800	1.97833300
C	2.19353000	5.74457000	0.61142300
C	1.47997700	4.80436700	-0.14189800
C	3.78701800	-0.17825100	-0.47482800
C	3.77093800	1.16570000	-0.06527400
C	4.94212400	1.93641600	-0.09535100
C	6.14265100	1.37058100	-0.53776800
C	6.17300700	0.02575300	-0.93507800

C	5.00813700	-0.74751700	-0.89800500
C	2.72866000	-2.57196000	0.71625100
C	3.06409400	-2.24475400	2.04746300
C	3.46068300	-3.24014200	2.94514400
C	3.52890600	-4.57757000	2.53202800
C	3.19989700	-4.91279500	1.21367000
C	2.79736800	-3.91971500	0.30961700
C	-2.17966600	-3.06929100	-0.40675200
C	-1.08511300	-3.78923100	0.10370600
C	-1.13052800	-5.18901400	0.17412600
C	-2.26383700	-5.88230000	-0.26445600
C	-3.36439300	-5.17067400	-0.76326000
C	-3.32793600	-3.77409200	-0.82923000
C	-3.63365300	-0.72806100	0.46813200
C	-4.78667600	-0.17556600	-0.12589700
C	-5.91003300	0.12628400	0.65532700
C	-5.89735000	-0.11202100	2.03459700
C	-4.75214000	-0.65455200	2.63326500
C	-3.62666500	-0.96127300	1.86121600
C	0.49119100	2.67185900	-2.26986600
C	-0.06563500	1.56866600	-3.17253800
C	2.17379100	-1.94134400	-2.13407500
C	1.66333300	-0.85944300	-3.09002800
C	-1.28110700	-1.09494800	-3.12071200
C	-2.55601800	-0.89458400	-2.29530900
H	-1.98798800	3.85521800	-2.33049500
H	-4.21328200	4.80397600	-1.91985500
H	-5.26932000	4.62641000	0.33414800
H	-4.06364800	3.44162000	2.17278400
H	-1.84658800	2.45143900	1.77482300
H	0.84247100	2.53776000	2.34735100
H	2.08321900	4.20166700	3.65163800
H	2.96801800	6.26969100	2.56229300
H	2.56765200	6.64576900	0.12661500
H	1.31123500	5.00945100	-1.19603400
H	2.84849300	1.60777600	0.29599100
H	4.91006500	2.97467600	0.23234700
H	7.05369900	1.96730500	-0.56337500
H	7.10789700	-0.42630700	-1.26473300
H	5.06466600	-1.79785200	-1.17849400
H	3.02621100	-1.21222000	2.38821600
H	3.71551000	-2.96861200	3.96868300
H	3.83894400	-5.35182100	3.23258700
H	3.25991700	-5.94830300	0.87992900

H	2.55203200	-4.21367900	-0.70788700
H	-0.22167900	-3.25518100	0.48415800
H	-0.28062300	-5.73191900	0.58568200
H	-2.29869000	-6.96966600	-0.20625500
H	-4.25780600	-5.70156700	-1.09048700
H	-4.20688200	-3.24117300	-1.18776300
H	-4.83361100	0.01805400	-1.19462900
H	-6.79626800	0.54430800	0.17875600
H	-6.77377800	0.12115700	2.63825800
H	-4.73141900	-0.84435600	3.70585200
H	-2.74732200	-1.38344900	2.34187600
H	0.20005600	3.66117800	-2.64051000
H	1.58780600	2.64412700	-2.25762600
H	0.43354000	1.56086500	-4.15150100
H	-1.13512100	1.72197400	-3.35762200
H	3.15151800	-2.32192400	-2.45030600
H	1.47563700	-2.78647600	-2.10525700
H	1.45343500	-1.26148600	-4.09067200
H	2.40890800	-0.06163800	-3.20114000
H	-1.41933400	-0.79570300	-4.16941200
H	-0.98580200	-2.15175600	-3.11719100
H	-3.35538300	-1.55367100	-2.65240400
H	-2.91488900	0.13790700	-2.38454400
O	-0.25054200	-1.28832500	1.94684200
C	0.12347700	-0.15338200	2.33034100
H	0.76935100	0.42448300	1.45049400
O	0.03051000	0.53432100	3.34044900

TS3T total energy:-3303.1254 a.u.

Fe	-0.02647000	0.12073400	0.20446600
P	1.60461700	1.91335200	0.44907600
P	-2.46327100	0.42652300	0.51188600
P	-0.05269500	0.21685100	2.42811500
P	0.88102100	-2.13943200	0.63222100
C	3.35834600	1.35934800	0.25075200
C	4.30661800	1.35746700	1.29361900
C	5.62640100	0.94992700	1.05378300
C	6.01794900	0.54087300	-0.22597000
C	5.08184500	0.53761300	-1.26878300
C	3.76237000	0.93586600	-1.03381300
C	1.55424900	3.43951600	-0.59837100
C	0.61690600	3.55599000	-1.64158600
C	0.58189100	4.71016800	-2.43664200
C	1.47992700	5.75675300	-2.19830200

C	2.42187200	5.64569500	-1.16519900
C	2.46531400	4.49401600	-0.37263900
C	-3.20841100	2.12216000	0.36228600
C	-2.38797200	3.26242800	0.42877600
C	-2.94357700	4.54878200	0.39305300
C	-4.32958000	4.71051000	0.28826400
C	-5.15707700	3.58089100	0.21755700
C	-4.60511200	2.29551800	0.25291200
C	-3.61935200	-0.60951000	-0.48365600
C	-3.65950100	-0.39498500	-1.87831100
C	-4.53199500	-1.13024700	-2.68656400
C	-5.37875200	-2.09184700	-2.11838000
C	-5.34587400	-2.31347900	-0.73671300
C	-4.47129200	-1.58149700	0.07786400
C	-0.35363800	-3.50678300	0.42180200
C	-1.07006100	-3.56742400	-0.79246000
C	-1.94895400	-4.62849900	-1.04027600
C	-2.14552300	-5.62767100	-0.07900100
C	-1.45143400	-5.56521100	1.13545300
C	-0.55586400	-4.51705500	1.38435700
C	2.35512200	-2.75759200	-0.30355200
C	3.48373300	-3.29956500	0.34604200
C	4.55480900	-3.80752000	-0.40033800
C	4.51454700	-3.78727400	-1.79942100
C	3.39592900	-3.25205300	-2.45054100
C	2.32377700	-2.73507600	-1.71377100
C	1.45016400	2.56904100	2.19676600
C	1.16907100	1.42428000	3.17591600
C	-2.81078600	0.02061500	2.30755400
C	-1.71246100	0.66613400	3.15839100
C	0.35252900	-1.40918500	3.25863200
C	1.39424600	-2.16024300	2.42611000
H	4.04386700	1.68924600	2.29541400
H	6.34827800	0.96333600	1.86992000
H	7.04512100	0.22908300	-0.41056500
H	5.37590500	0.21974600	-2.26811000
H	3.04887600	0.92260000	-1.85543400
H	-0.07872000	2.74431400	-1.83346800
H	-0.14660100	4.78614100	-3.24327400
H	1.45316600	6.65257800	-2.81760400
H	3.12997100	6.45292900	-0.98086700
H	3.22169100	4.41532900	0.40632800
H	-1.31111700	3.14501500	0.48960200
H	-2.29053100	5.41992300	0.43656200

H	-4.76394900	5.70899000	0.25567600
H	-6.23675800	3.69868100	0.13083200
H	-5.26387600	1.43235900	0.18809600
H	-3.01561600	0.35191500	-2.33580700
H	-4.54745500	-0.95101700	-3.76084100
H	-6.06016600	-2.66214000	-2.74851100
H	-6.00329300	-3.05513300	-0.28431200
H	-4.47663800	-1.77590600	1.14732100
H	-0.94117000	-2.79944300	-1.55135700
H	-2.48445800	-4.66492300	-1.98795000
H	-2.83209400	-6.45066700	-0.27440300
H	-1.59324100	-6.33925600	1.88920300
H	-0.01408400	-4.51627500	2.32720100
H	3.54375900	-3.34936900	1.43023300
H	5.41610600	-4.22746000	0.11839300
H	5.34638900	-4.18954000	-2.37666900
H	3.34984300	-3.23372900	-3.53902300
H	1.47049900	-2.32643100	-2.24795200
H	2.33001700	3.15063600	2.49664600
H	0.60647000	3.26920800	2.17124100
H	0.78657900	1.79595500	4.13644700
H	2.08484200	0.86109300	3.39056000
H	-3.80616000	0.37321800	2.60287200
H	-2.78895400	-1.06994700	2.41958800
H	-1.76293800	0.34234400	4.20730800
H	-1.80583800	1.75914800	3.14504800
H	0.69944900	-1.23235800	4.28638300
H	-0.57784100	-1.98636200	3.32369300
H	1.55668700	-3.17410700	2.80832200
H	2.36204300	-1.64612000	2.47103700
O	-0.07967800	-0.00019900	-1.66362300
O	-0.16330300	-1.12171000	-3.62450800
C	-0.11787800	-0.08482400	-2.96908200
H	-0.10619200	0.90687900	-3.47741200

MECP1 total energy:-3303.1070 a.u.

Fe	0.02997300	0.08125100	-0.40269300
P	2.21705500	0.58809700	-0.73204600
P	-0.05151700	-2.17100200	-0.15964200
P	-0.07193000	-0.26927900	-2.57053700
P	-2.22038800	0.80978000	-0.68030300
C	2.42015300	2.42718200	-0.90182400
C	1.36914600	3.17318100	-1.47096400
C	1.48246700	4.55406200	-1.66008400

C	2.65090300	5.21937100	-1.26927400
C	3.69658500	4.49343500	-0.68158400
C	3.58621000	3.10874200	-0.49569700
C	3.55944100	0.09842900	0.42774300
C	3.32941600	0.24161200	1.81106700
C	4.32845800	-0.08199300	2.73362800
C	5.56812900	-0.56420700	2.29034800
C	5.80676700	-0.70887000	0.91839000
C	4.81164800	-0.37611700	-0.00970900
C	1.49815500	-3.18983800	-0.00351300
C	2.10320300	-3.33854300	1.26250700
C	3.25878700	-4.10986500	1.41808000
C	3.84329900	-4.74429700	0.31390200
C	3.25244200	-4.60974200	-0.94774600
C	2.09209500	-3.84162200	-1.10478500
C	-1.03945300	-2.84347000	1.25372200
C	-1.16133000	-2.08664300	2.43301300
C	-1.82663900	-2.61066100	3.55029300
C	-2.38836400	-3.89310500	3.49478700
C	-2.27890300	-4.65040100	2.32202100
C	-1.60252700	-4.13721300	1.20932800
C	-3.68212300	-0.33579300	-0.73234100
C	-4.08209200	-0.94334600	0.47744200
C	-5.16657700	-1.82505800	0.51002300
C	-5.88176500	-2.11369700	-0.66149700
C	-5.50682000	-1.49971500	-1.86346600
C	-4.41540100	-0.61824200	-1.90292400
C	-2.85135100	2.13013600	0.45818700
C	-4.02884500	2.85630800	0.17504500
C	-4.55647300	3.73721800	1.12482600
C	-3.92719600	3.89735900	2.37042100
C	-2.75187900	3.19087200	2.64958600
C	-2.20880200	2.31883500	1.69775400
C	2.71191100	-0.08110000	-2.42280100
C	1.55858600	0.12569400	-3.41820300
C	-0.90429000	-2.82237700	-1.70757300
C	-0.44213700	-2.07282100	-2.97226600
C	-1.41209700	0.74633500	-3.42959300
C	-2.16707800	1.60996400	-2.39163600
H	0.17451200	0.29795000	1.09814300
H	0.45426500	2.66843600	-1.75956900
H	0.65551100	5.11020400	-2.10406500
H	2.74247100	6.29670000	-1.41311400
H	4.60253000	5.00587900	-0.36450700

H	4.40730300	2.56586200	-0.03210600
H	2.36243000	0.60111000	2.16161700
H	4.13629400	0.03722700	3.79848700
H	6.34320800	-0.82661200	3.01153600
H	6.76929800	-1.07702100	0.56440200
H	5.02838700	-0.48654800	-1.06971300
H	1.66388700	-2.86627700	2.13601600
H	3.70264400	-4.21655300	2.40694000
H	4.74303000	-5.34607100	0.43715000
H	3.68644300	-5.11112800	-1.81319100
H	1.64867500	-3.78110600	-2.09599600
H	-0.73900400	-1.08528600	2.46504200
H	-1.90855300	-2.01685300	4.45701200
H	-2.90562000	-4.30152400	4.36357100
H	-2.71343700	-5.64829600	2.27252900
H	-1.50911100	-4.75547600	0.31835600
H	-3.54996700	-0.72781500	1.39944200
H	-5.44853500	-2.29033100	1.45287300
H	-6.72519900	-2.80031000	-0.63506300
H	-6.06595700	-1.70221100	-2.77748100
H	-4.16766100	-0.15202800	-2.85015500
H	-4.55478800	2.72110700	-0.76787800
H	-5.47080100	4.28406100	0.90143000
H	-4.35967100	4.56201300	3.11702000
H	-2.25737400	3.30680200	3.61384900
H	-1.29707700	1.76544800	1.91265700
H	3.63180700	0.39268600	-2.79044400
H	2.91793300	-1.14872400	-2.28115400
H	1.70036300	-0.47819200	-4.32471300
H	1.51754100	1.17647700	-3.72914200
H	-0.76493700	-3.90363700	-1.81836500
H	-1.97047100	-2.64499900	-1.53138400
H	-1.19697000	-2.14673700	-3.76591000
H	0.47789900	-2.50655600	-3.37713200
H	-0.96607500	1.38112600	-4.20652000
H	-2.09725300	0.06051400	-3.93833000
H	-3.17107000	1.86811300	-2.74769600
H	-1.64930300	2.56219500	-2.23820300
C	0.51589800	5.17745100	2.54581700
O	0.29542200	5.95000700	1.68511100
O	0.73901000	4.40439800	3.40851600

MECP2 total energy:-3303.0964 a.u.

Fe	-0.1759109	-0.4709461	-0.1427726

P	0.0229010	1.9054715	-0.3283918
P	2.3624767	-1.1521965	-0.4243045
P	-0.0084521	-0.5219567	-2.3093455
P	-2.4081337	-0.8471103	-0.4879758
C	-1.3500475	3.1755760	-0.4329282
C	-1.8442721	3.6411919	-1.6712865
C	-2.8814056	4.5787132	-1.7268867
C	-3.4540078	5.0751863	-0.5492428
C	-2.9540492	4.6448550	0.6846793
C	-1.9187609	3.7067457	0.7489500
C	1.0927038	2.6789452	0.9876962
C	1.1241683	2.1073060	2.2784218
C	1.8756195	2.6987352	3.3055012
C	2.6231747	3.8547167	3.0633892
C	2.5941264	4.4325506	1.7882243
C	1.8311233	3.8628830	0.7610865
C	3.7696013	-0.0656968	-0.9994291
C	4.3525656	0.8063330	-0.0525536
C	5.3926099	1.6690777	-0.4116134
C	5.8776860	1.6873038	-1.7258898
C	5.3163283	0.8249116	-2.6733770
C	4.2749469	-0.0453216	-2.3174143
C	3.1974356	-2.0869884	0.9384068
C	2.9306376	-1.7019484	2.2652134
C	3.6046673	-2.3059482	3.3357865
C	4.5465145	-3.3112364	3.0957092
C	4.8222878	-3.7002080	1.7791553
C	4.1617038	-3.0910098	0.7036093
C	-3.0802933	-2.5780350	-0.3398066
C	-2.3159316	-3.6709680	-0.7928592
C	-2.8445070	-4.9663659	-0.7850050
C	-4.1391726	-5.1929064	-0.2973622
C	-4.9057393	-4.1165314	0.1638635
C	-4.3880938	-2.8165929	0.1383637
C	-3.5368760	0.1477217	0.5678586
C	-4.6761283	0.8055890	0.0639482
C	-5.5409850	1.4816515	0.9303704
C	-5.2890552	1.5118686	2.3089039
C	-4.1550624	0.8638090	2.8156177
C	-3.2799785	0.1935126	1.9554200
C	0.9761206	2.0966890	-1.9326847
C	0.4531917	1.1507179	-3.0270152
C	2.0792555	-2.3839151	-1.8114789
C	1.2216248	-1.7956249	-2.9526502

C	-1.6273152	-0.9446021	-3.1475241
C	-2.7784172	-0.4165139	-2.2807394
H	-1.4162738	3.3053822	-2.6117798
H	-3.2247843	4.9381893	-2.6952379
H	-4.2689655	5.7936232	-0.5974750
H	-3.3647156	5.0568280	1.6072551
H	-1.5525756	3.4097168	1.7284513
H	0.5697456	1.1958533	2.4881725
H	1.8791700	2.2543575	4.3008686
H	3.2163697	4.3083508	3.8577992
H	3.1636512	5.3416172	1.5958959
H	1.8216848	4.3579115	-0.2079924
H	4.0089179	0.8079756	0.9788776
H	5.8287609	2.3258387	0.3401733
H	6.6822832	2.3651777	-2.0081252
H	5.6912090	0.8173031	-3.6960605
H	3.8873651	-0.7140922	-3.0806777
H	2.1866203	-0.9392403	2.4699943
H	3.3853283	-1.9901225	4.3542410
H	5.0659709	-3.7868630	3.9293024
H	5.5630809	-4.4753469	1.5846426
H	4.4198027	-3.4001410	-0.3076448
H	-1.2842940	-3.5218428	-1.1118559
H	-2.2400524	-5.8050161	-1.1320961
H	-4.5497656	-6.2014060	-0.2642966
H	-5.9092038	-4.2807874	0.5581226
H	-5.0062638	-1.9990141	0.5015018
H	-4.9034076	0.7923889	-1.0002498
H	-6.4200590	1.9775255	0.5220999
H	-5.9722923	2.0308718	2.9785754
H	-3.9498563	0.8739998	3.8857360
H	-2.3948466	-0.2854372	2.3633662
H	0.9610427	3.1327117	-2.2860959
H	2.0120248	1.8507050	-1.6795596
H	1.1838750	1.0490179	-3.8406695
H	-0.4674163	1.5351260	-3.4789759
H	3.0204237	-2.7772037	-2.2167819
H	1.5596196	-3.2235155	-1.3297525
H	0.6446858	-2.5850807	-3.4497447
H	1.8511551	-1.3400730	-3.7252239
H	-1.6627763	-0.5412063	-4.1696506
H	-1.6783585	-2.0359901	-3.2169524
H	-3.7395023	-0.8399801	-2.5982199
H	-2.8406885	0.6743422	-2.3559844

O	-0.3922825	-3.6015092	1.8668413
O	-0.2872024	-1.3489313	1.5260591
C	-0.5418166	-2.4413535	2.2241829
H	-0.9333526	-2.1879650	3.2364026