Supporting Information

Iron Heme Enzyme-Catalyzed Cyclopropanations with Diazirines as Carbene Precursors: Computational Explorations of Diazirine Activation and Cyclopropanation Mechanism

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1. Density Functional Theory Calculations

1.1 Computational details

All density functional theory (DFT) calculations were performed with the Gaussian 16, Rev. A.03, program package.[1] Geometry optimizations were performed at the B3LYP level of theory[2, 3] including Grimme's D3 dispersion correction with Becke-Johnson damping function.[4, 5] Iron was described with the LANL2DZ basis set and associated effective core potential, while all other atoms were described with the 6-31G(d) basis set.[6] Analytical frequency calculations were performed at the same level of theory to characterize all stationary points as intermediates (no imaginary frequencies) or transition states (exactly one imaginary frequency). Transition states were located through one-dimensional relaxed energy surface scans and optimized using the Berny algorithm. Intrinsic reaction coordinate (IRC) calculations were performed at the same level of theory to confirm the intermediates linked by each transition state. The electronic energy was refined through single point calculations at the B3LYP-D3(BJ) level of theory, employing a def2-TZVP basis set.[7] In all single point calculations, solvent effects were taken into consideration through the use of the CPCM implicit solvent model for Et_2O as implemented in Gaussian.[8, 9] Et_2O was chosen as the solvent to model the hydrophobic environment in the active site of the enzyme. The stable=opt keyword was used in all oss, triplet and quintet single point calculations to confirm the stability of the wave function. GoodVibes[10] (v. 3.0.2) with quasi-harmonic entropy[11] and enthalpy[12] treatment (frequency cut-off value: 100 cm^{-1}) was used to obtain corrected Gibbs free energies and enthalpies at 298 K and 1 atm. 3D-visualizations of optimized structures were rendered with CYLview20.[13]

The ONIOM algorithm[14] implemented in Gaussian 16[1] was used in QM/MM calculations to calculate the stationary points (intermediates and transition states). A representative frame of the transition state **TS(C-D)** simulation was used as an initial structure. Water molecules and counterions within 5 Å from the enzyme were included in the QM/MM calculations. The representative structures from MD simulation were used as initial structure. The QM region includes the substrate, heme and the coordinated histidine. For the QM region, B3LYP/6-31G(d), LANL2DZ(Fe) level of theory was used in geometry optimization and vibrational frequency calculations, and B3LYP/def2-TZVP was used in single-point energy calculations. For the MM region, the same force field parameters from the classical MD simulations were used.

The mechanical embedding scheme were used in geometry optimization. Residues more than 10 Å away from the QM region were frozen during geometry optimization. Single-point energy calculations were performed with the electronic embedding scheme, which better describes electrostatic interactions between QM and MM regions.

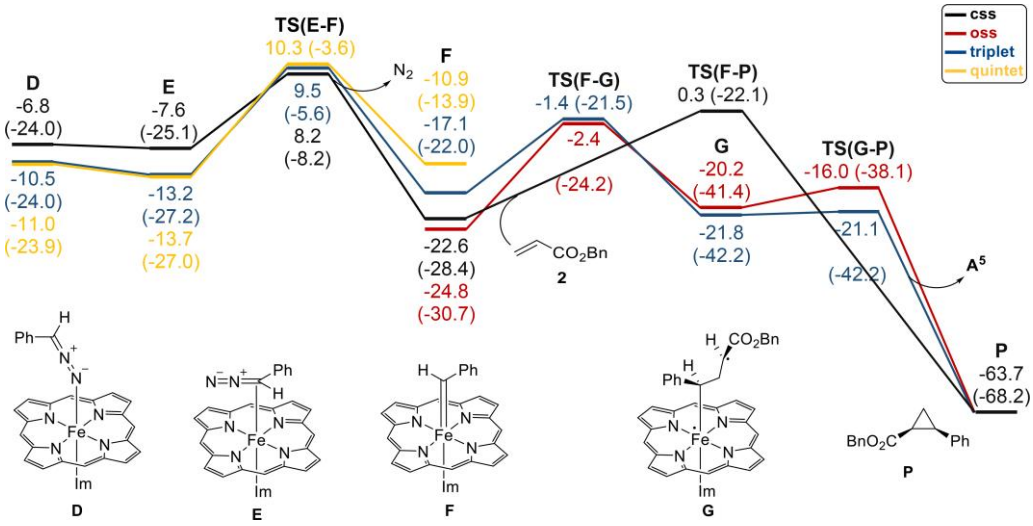

Figure S1. Calculated Gibbs free energy diagram (relative to $\mathbf{A^5}$, in kcal mol^{-1}) for the cyclopropanation with acrylate **2**. Values in parenthesis correspond to relative enthalpies ΔH (in kcal mol^{-1}).

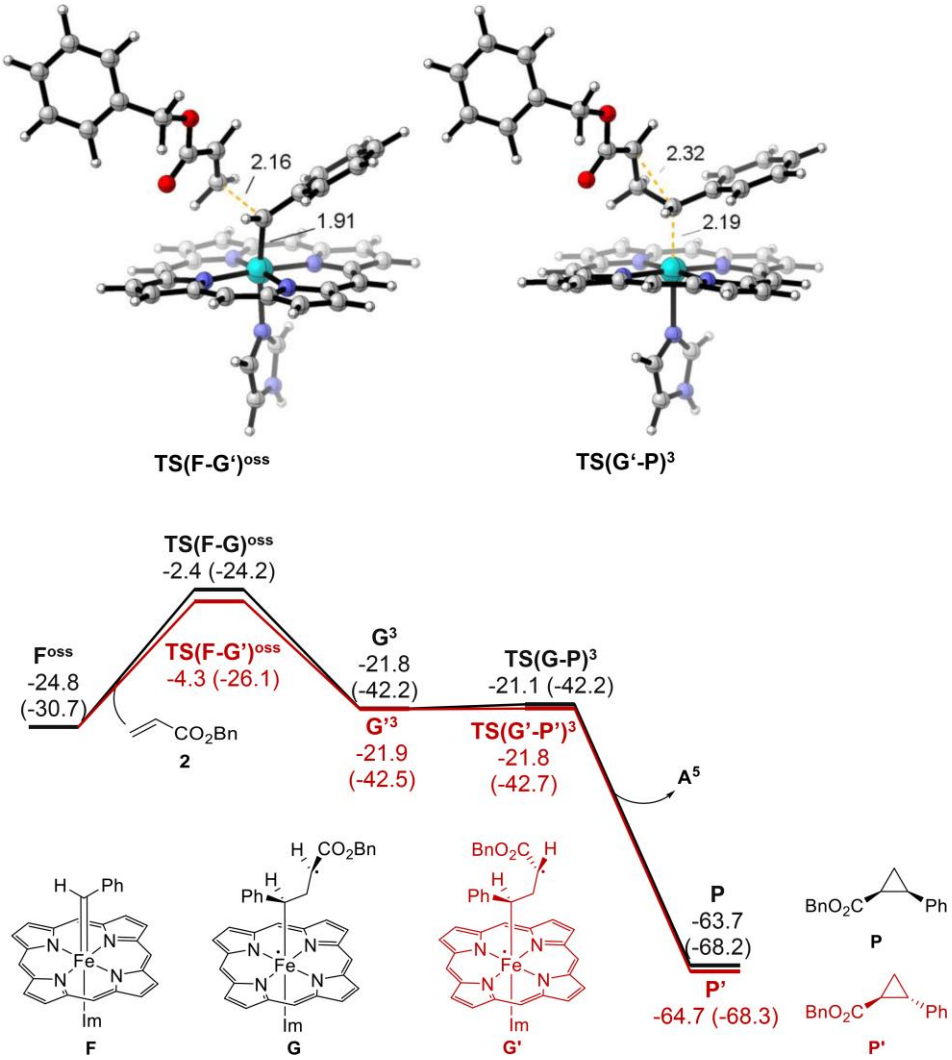

Figure S2. Calculated Gibbs free energy diagram (relative to **A**^{5}, in kcal mol^{-1}) for the formation of the *cis*- (in black) and *trans*-configured cyclopropane (in red) in the most favorable spin state. Values in parenthesis correspond to relative enthalpies ΔH (in kcal mol^{-1}). Superscripts correspond to the spin state. css = closed-shell singlet; oss = open-shell singlet.

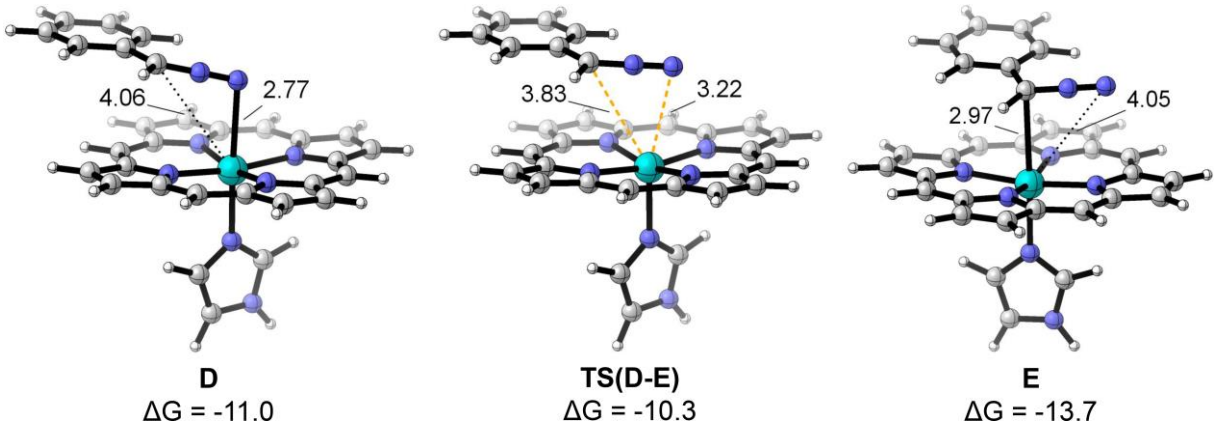

Figure S3. Optimized geometries for the coordination shift from intermediate **D** (left) to intermediate **E** (right) *via* transition state **TS(D-E)** (middle) on the quintet surface and Gibbs free energies (relative to $\mathbf{A^5}$, in kcal mol^{-1}). Distances are given in Å.

1.2 Additional analysis of intermediate C

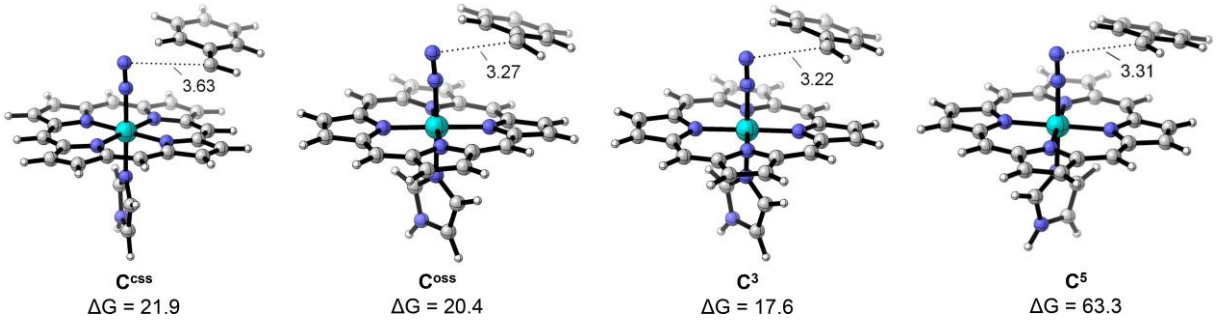

Figure S4. Optimized geometries for intermediate **C** and Gibbs free energies (relative to $\mathbf{A^5}$, in kcal mol^{-1}). Distances are given in Å.

When the free phenylcarbene was removed from intermediate **C** and calculated separately, the triplet spin state of phenylcarbene was found to be preferred over the singlet spin state by 3.5 kcal mol^{-1}, which is in good agreement with previous reports.[15] In addition, the dinitrogen-coordinated complex without phenylcarbene present (named intermediate **C***) displays a strong preference for a closed-shell singlet spin state. The corresponding open-shell singlet spin state was found to be unstable.

An alternative pathway involving decoordination of N_2 from intermediate **C** and subsequent coordination of phenylcarbene to the iron center, thus forming intermediate **F**, is not in line with previously reported, experimental observed formation of diazobenzene.[14]

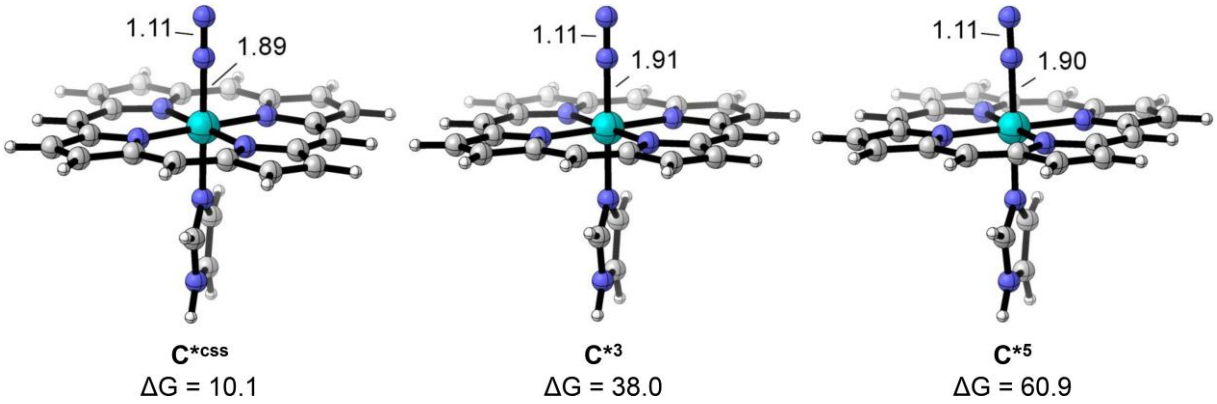

Figure S5. Optimized geometries for intermediate **C*** and Gibbs free energies (relative to $\mathbf{A}^5$, in kcal mol^{-1}). Distances are given in Å.

1.3 Spin state analysis

In our calculations, we found that not all intermediates and transition states represent stationary points (minima for intermediates or 1st order saddle points for transition states) in all four investigated spin states. Especially in cases of low-lying closed-shell singlet states, the corresponding open-shell singlet states tends to be unstable, consequently converging to the respective closed-shell singlet state and thus preventing optimization on the open-shell singlet surface. To provide an approximated Gibbs free energy of structures in a quintet or triplet spin state, which did not represent stable stationary points in these spin states, frequency and single point calculations were performed on the optimized geometries obtained in a different spin state (Figure S6).

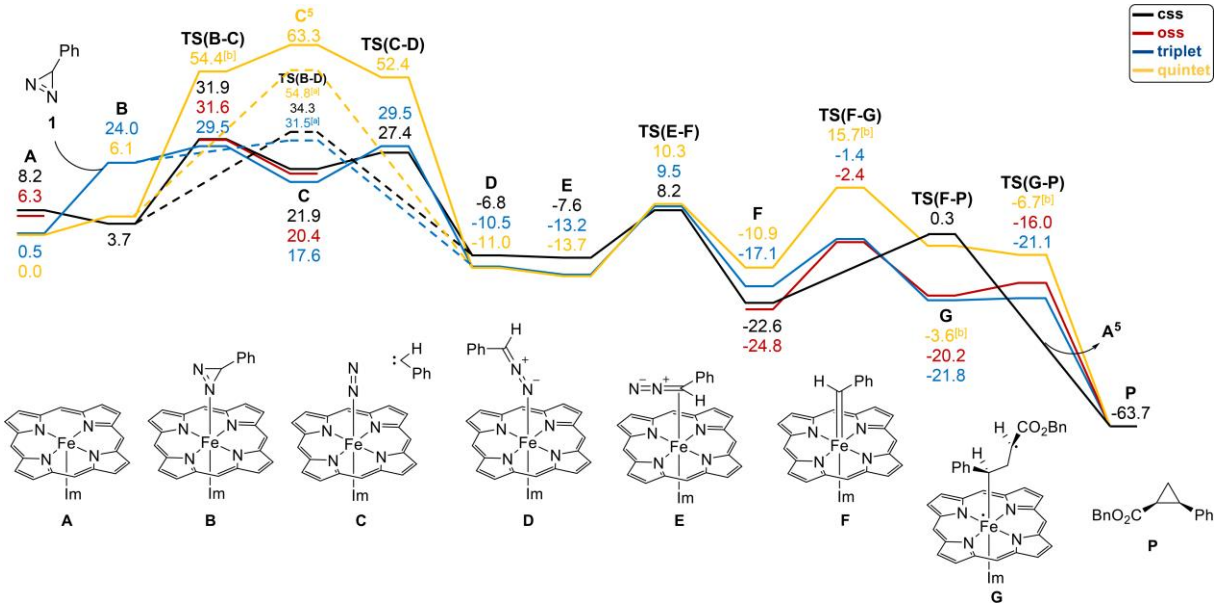

Figure S6. Calculated Gibbs free energy diagram (in kcal mol^{-1}) for the cyclopropanation of carbene precursor **1** with acrylate **2**, including estimated energies for all possible spin states. [a] estimated through frequency and single point calculations on the optimized css geometry; [b] estimated through frequency and single point calculations on the optimized triplet geometry.

1.4 Structures optimized using QM/MM

In our QM/MM calculations, we observed that the quintet and triplet intermediate **B**, although relatively lower in energy, are dissociated from the heme. Therefore, it can be assumed that the substrate first goes into the binding cavity with the singlet heme, and then directly binds with the Fe and undergoes a direct isomerization (the barrier is only 17.8 kcal mol^{-1} for the singlet pathway) instead of undergoing a spin-crossover to the triplet or quintet spin state.

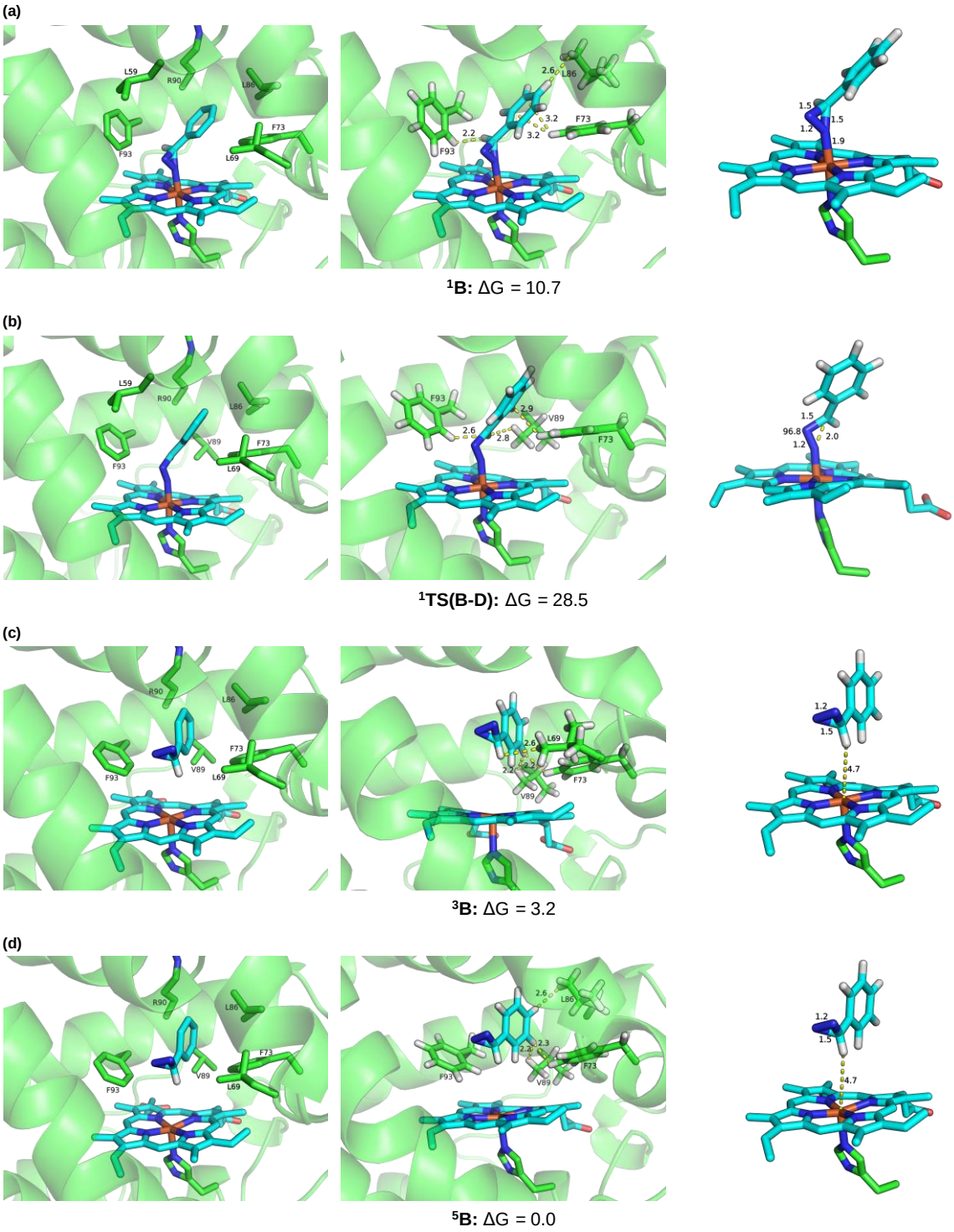

Figure S7. QM/MM optimized geometries for intermediate **B** and **TS(B-D**) and Gibbs free energies (in kcal mol^{-1}). Active site and surrounding residues (left column), shortest distances between substrate and peptide side chains (middle column) and close-up view of the iron-heme substrate complex (right column). Distances are given in Å and angles in °. Non-relevant hydrogen atoms are omitted for clarity.

Several attempts to find **TS(B-C)** have been made. Figure S8 shows a constraint optimization starting from a manually aligned **TS(B-C)** structure, where the C–N bond length is fixed. After the optimization, we found that the initial **TS(B-C)** structure cannot be maintained and is spontaneously transformed into a structure resembling **TS(B-D)**. This is likely caused by an incompatibility between **TS(B-C)** and the enzyme cavity, more specifically, unfavorable steric repulsion between **TS(B-C)** and residue L86.

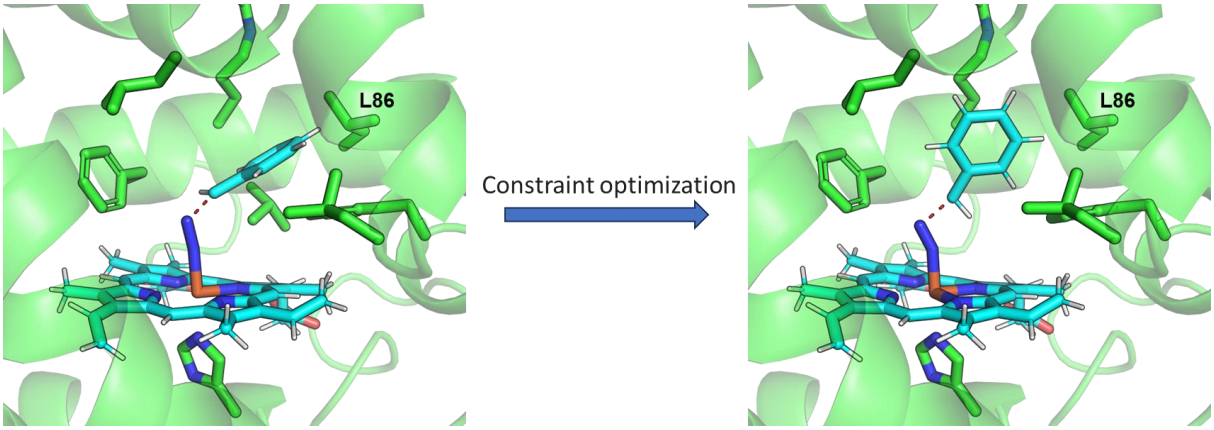

Figure S8. QM/MM constraint optimization from DFT optimized **TS(B-C)**.

1.5 Summary of energies

Structure	E_SPC (au)	qh-H_SPC (au)	T.qh-S (au)	qh-G(T)_SPC (au)	im. freq. (cm^{-1})
Figure 1					
A^{css}	-2479.028280	-2478.658285	0.069874	-2478.728159	--
A^{oss}	-2479.029815	-2478.660346	0.070783	-2478.731129	--
A^{3}	-2479.034923	-2478.666150	0.074183	-2478.740333	--
A^{5}	-2479.033679	-2478.666254	0.074920	-2478.741174	--
B^{css}	-2859.013346	-2858.519496	0.086507	-2858.606003	--
B^{3}	-2858.976772	-2858.484970	0.088766	-2858.573736	--
B^{5}	-2858.998765	-2858.508832	0.093448	-2858.602280	--
$TS(B\text{-}C)^{css}$	-2858.963472	-2858.473875	0.087212	-2858.561087	-201.55
$TS(B\text{-}C)^{oss}$	-2858.963555	-2858.474406	0.087213	-2858.561619	-283.56

TS(B-C)^{3}	-2858.964657	-2858.476397	0.088576	-2858.564973	-437.21
TS(B-D)^{css}	-2858.961633	-2858.470708	0.086577	-2858.557285	-135.43
C^{css}	-2858.976333	-2858.487018	0.090026	-2858.577044	--
C^{oss}	-2858.977919	-2858.489239	0.090270	-2858.579509	--
C^{3}	-2858.981670	-2858.492830	0.091123	-2858.583953	--
C^{5}	-2858.903865	-2858.417399	0.093750	-2858.511149	--
TS(C-D)^{css}	-2858.970050	-2858.480320	0.087922	-2858.568242	-152.84
TS(C-D)^{3}	-2858.964667	-2858.476404	0.088577	-2858.564981	-437.13
TS(C-D)^{5}	-2858.923601	-2858.437476	0.090890	-2858.528366	-393.91
D^{css}	-2859.028789	-2858.535584	0.087126	-2858.622710	--
D^{3}	-2859.026676	-2858.535627	0.093132	-2858.628759	--
D^{5}	-2859.025308	-2858.535502	0.093986	-2858.629488	--
1	-379.951501	-379.831090	0.039676	-379.870767	--
Figure 2					
E^{css}	-2859.030763	-2858.537348	0.086647	-2858.623996	--
E^{3}	-2859.032054	-2858.540736	0.092250	-2858.632985	--
E^{5}	-2859.030469	-2858.540428	0.093354	-2858.633782	--
TS(E-F)^{css}	-2859.002533	-2858.510346	0.088480	-2858.598826	-470.94
TS(E-F)^{3}	-2858.996678	-2858.506306	0.090454	-2858.596760	-459.96
TS(E-F)^{5}	-2858.990274	-2858.503109	0.092383	-2858.595492	-461.32
F^{css}	-2749.459685	-2748.977666	0.083495	-2749.061160	--
F^{oss}	-2749.462720	-2748.981249	0.083541	-2749.064790	--
F^{3}	-2749.447575	-2748.967379	0.085114	-2749.052493	--
F^{5}	-2749.432574	-2748.954530	0.088065	-2749.042595	--
TS(F-G)^{oss}	-3287.232152	-3286.562837	0.106392	-3286.669228	-372.39
TS(F-G)^{3}	-3287.226721	-3286.558491	0.109093	-3286.667584	-163.99
TS(F-P)^{css}	-3287.229532	-3286.559454	0.105465	-3286.664919	-289.67

G^{oss}	-3287.261349	-3286.590255	0.107421	-3286.697676	--
G^{3}	-3287.262476	-3286.591477	0.108727	-3286.700204	--
TS(G-P)^{oss}	-3287.255004	-3286.584887	0.106094	-3286.690981	-467.72
TS(G-P)^{3}	-3287.261290	-3286.591395	0.107658	-3286.699053	-150.79
P	-808.263513	-807.966703	0.058994	-808.025697	--
2	-537.775866	-537.591836	0.048373	-537.640209	--
N_2	-109.573749	-109.564975	0.021754	-109.586729	--
Figure S2					
TS(F-G')^{oss}	-3287.235069	-3286.565753	0.106520	-3286.672272	-317.95
G'^{3}	-3287.262964	-3286.591865	0.108415	-3286.700280	--
TS(G'-P')^{3}	-3287.262359	-3286.592312	0.107820	-3286.700132	-100.72
P'	-808.263579	-807.966828	0.060468	-808.027297	--
Figure S5					
Phenylcarbene (singlet)	-270.350357	-270.243397	0.035825	-270.279223	--
Phenylcarbene (triplet)	-270.354665	-270.248109	0.036688	-270.284797	--
C*^{css}	-2588.616723	-2588.236410	0.074624	-2588.311034	--
C*^{3}	-2588.566914	-2588.188914	0.077673	-2588.266587	--
C*^{5}	-2588.525162	-2588.150946	0.079176	-2588.230122	--
Figure S6					
TS(B-D)^{3}	-2858.967723	-2858.477146	0.084639	-2858.561785	-49.82
TS(B-D)^{5}	-2858.929202	-2858.441090	0.083466	-2858.524555	-121.61
TS(B-C)^{5}	-2858.922308	-2858.437808	0.087488	-2858.525296	-416.06
TS(F-G)^{5}	-3287.202364	-3286.536244	0.104112	-3286.640356	-124.43
G^{5}	-3287.239299	-3286.579286	0.091853	-3286.671139	-4975.99
TS(G-P)^{5}	-3287.240952	-3286.588361	0.087729	-3286.676090	-4879.12
Additional data					

TS(D-E)^{5}	-2859.025696	-2858.536382	0.091970	-2858.628352	-22.74
TS(F-G')^{3}	-3287.225678	-3286.557693	0.109736	-3286.667430	-120.62
TS(F-P')^{css}	-3287.229369	-3286.559337	0.105666	-3286.665002	-255.17
G'^{oss}	-3287.261500	-3286.590176	0.107287	-3286.697464	--
TS(G'-P')^{oss}	-3287.256356	-3286.586128	0.105937	-3286.692065	-477.65

1.6 Cartesian coordinates

A^{css}

Fe	-0.457256	-0.048970	-1.205103
N	-0.443974	-2.059388	-1.206348
N	1.513007	-0.048382	-1.605038
N	-2.369237	-0.061868	-0.579556
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C	0.267875	4.164447	-1.042034
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C	-1.040968	4.159411	-0.666658
H	-1.792931	-5.120376	-1.045297
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H	-1.677368	5.001436	-0.425147
C	-2.798733	-2.476363	-0.658571
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H	2.636778	-3.225502	-2.040373
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H	0.358308	-1.386392	-3.947896
N	-1.963241	0.680147	-4.915336
H	-2.479171	1.560740	-3.006434
H	-0.919459	-0.609856	-6.299415
H	-2.591181	1.167851	-5.535883
N	-0.954565	0.064881	-3.070547

A^{oss}

Fe	-0.443105	-0.046795	-1.198491
N	-0.421939	-2.061299	-1.187484
N	1.535730	-0.045386	-1.576943
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N	-0.406638	1.957124	-0.976587
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C	3.682440	0.654109	-2.092467
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C	1.927089	-2.459307	-1.772378
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H	2.670021	-3.222039	-1.985849
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C	-1.860527	0.855164	-3.651159
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N	-1.935765	0.668573	-4.994673
H	-2.465942	1.550725	-3.090926
H	-0.879311	-0.621969	-6.368799
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N	-0.938841	0.059572	-3.139989

A[3]

Fe	-0.367905	-0.029874	-1.180943
N	-0.506582	-2.036150	-1.241935
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N	-2.300933	0.092304	-0.630012
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C	-4.500080	-0.452370	-0.162529
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H	-5.157915	1.621630	0.198863
H	-1.258139	5.091215	-0.434322
C	-2.892138	-2.288644	-0.721921
C	2.177822	2.222045	-1.545119
C	-2.507266	2.523756	-0.364419
C	1.808692	-2.595330	-1.832923
H	-3.699624	-3.004081	-0.601585
H	2.980473	2.939128	-1.686212
H	-3.189451	3.333983	-0.126285
H	2.493179	-3.406339	-2.061164
C	-0.410458	-0.575326	-4.431646
C	-1.749557	1.030697	-3.878200

C	-0.984841	-0.142909	-5.599450
H	0.313777	-1.359834	-4.270220
N	-1.837886	0.883177	-5.230441
H	-2.307392	1.761202	-3.310802
H	-0.874745	-0.454107	-6.626594
H	-2.420549	1.424717	-5.851322
N	-0.896004	0.163260	-3.374812

A^{5}

Fe	-0.388197	0.051514	-1.305864
N	-0.474190	-2.039043	-1.228001
N	1.666440	-0.065520	-1.551485
N	-2.309715	0.135716	-0.533403
N	-0.204982	2.119730	-0.998617
C	-1.585717	-2.791563	-0.961359
C	2.521642	0.997939	-1.689953
C	0.552108	-2.899747	-1.508733
C	2.378945	-1.208536	-1.809530
C	-3.163401	-0.928023	-0.390447
C	0.924945	2.867535	-1.194925
C	-3.021477	1.278472	-0.270691
C	-1.214013	2.975807	-0.647274
C	-1.256899	-4.199597	-1.104485
C	3.837608	0.506486	-2.036969
C	0.063192	-4.266400	-1.442486
C	3.749512	-0.855693	-2.110595
C	-4.470063	-0.439689	-0.006057
C	0.613156	4.270313	-0.983697
C	-4.382542	0.922511	0.067701
C	-0.707773	4.337178	-0.645492
H	-1.947816	-5.018985	-0.949854
H	4.709987	1.127111	-2.199497
H	0.662476	-5.151078	-1.618204
H	4.535920	-1.562165	-2.345193
H	-5.335585	-1.062562	0.182296
H	1.321325	5.085289	-1.068241
H	-5.162757	1.626781	0.328287
H	-1.288907	5.217414	-0.399925
C	-2.829473	-2.273316	-0.591133
C	2.177758	2.346037	-1.530354
C	-2.517248	2.583658	-0.328254
C	1.863848	-2.510850	-1.792830
H	-3.624410	-2.994766	-0.423224
H	2.981285	3.064999	-1.665247
H	-3.214854	3.378567	-0.078811
H	2.569498	-3.308270	-2.009132
C	-1.198309	-0.767877	-4.309009
C	-1.026182	1.381798	-4.059182
C	-1.483327	-0.217087	-5.530277
H	-1.172150	-1.802764	-4.003507
N	-1.369157	1.152229	-5.353455
H	-0.867035	2.359469	-3.629752
H	-1.748724	-0.651089	-6.481425
H	-1.514861	1.857213	-6.060935
N	-0.917226	0.238368	-3.409032

B^{css}

Fe	-0.599496	0.002894	-0.009882
N	-1.634458	-1.586188	-0.697235
N	-1.977116	1.240966	-0.816082
N	0.768883	-1.232003	0.833488
N	0.464132	1.595463	0.653971
C	-1.314464	-2.907274	-0.521559
C	-1.970015	2.611271	-0.770222
C	-2.787619	-1.566095	-1.439238
C	-3.091711	0.884325	-1.530543
C	0.751744	-2.603001	0.804052
C	0.150776	2.918029	0.466778
C	1.899299	-0.874589	1.524444
C	1.654157	1.575143	1.337814

C	-2.295840	-3.749636	-1.172870
C	-3.126987	3.137714	-1.463440
C	-3.210009	-2.917315	-1.742776
C	-3.822311	2.066483	-1.935983
C	1.902041	-3.129271	1.508614
C	1.178648	3.759388	1.041963
C	2.612482	-2.056822	1.956548
C	2.111922	2.925755	1.581567
H	-2.270010	-4.831949	-1.183845
H	-3.355930	4.190551	-1.570203
H	-4.090181	-3.174300	-2.318481
H	-4.739986	2.057848	-2.510456
H	2.122115	-4.182475	1.629984
H	1.170738	4.842070	1.026170
H	3.540501	-2.046485	2.513796
H	3.028805	3.182603	2.096949
C	-0.211569	-3.383792	0.176591
C	-0.984473	3.393113	-0.179755
C	2.319790	0.428917	1.757309
C	-3.471325	-0.419777	-1.827925
H	-0.087825	-4.461339	0.231240
H	-1.105533	4.470735	-0.240034
H	3.255833	0.562556	2.290334
H	-4.377869	-0.553797	-2.410477
C	-3.000716	-0.236116	1.835084
C	-1.145893	0.150847	2.902113
C	-3.325895	-0.183544	3.163815
H	-3.629162	-0.406087	0.976135
N	-2.136074	0.062434	3.827884
H	-0.108390	0.335323	3.130848
H	-4.263057	-0.294305	3.685621
H	-2.018380	0.160227	4.824820
N	-1.644119	-0.026580	1.691709
C	1.562238	0.682040	-2.202191
H	1.419378	1.701776	-2.547746
N	0.396028	0.060419	-1.601981
N	0.614917	-0.342420	-2.750927
C	2.900264	0.284172	-1.723573
C	3.866327	1.272575	-1.499832
C	3.204983	-1.053071	-1.439289
C	5.119253	0.931003	-0.995082
H	3.623201	2.312563	-1.701541
C	4.459242	-1.392057	-0.937763
H	2.452588	-1.821238	-1.583247
C	5.419256	-0.403448	-0.712516
H	5.859585	1.706462	-0.818930
H	4.678593	-2.429951	-0.706483
H	6.394957	-0.670465	-0.316090

B^3

Fe	0.599919	0.023323	-0.013473
N	-0.640014	1.589635	0.692136
N	1.841924	1.388454	-0.859533
N	-0.665940	-1.354806	0.824269
N	1.841465	-1.560693	-0.676141
C	-1.780605	1.438878	1.419967
C	3.010102	1.104790	-1.515335
C	-0.475630	2.916327	0.426907
C	1.662362	2.746394	-0.881575
C	-1.810450	-1.068598	1.523337
C	3.009215	-1.405112	-1.360368
C	-0.554488	-2.718955	0.738901
C	1.609030	-2.894741	-0.526764
C	-2.375821	2.745475	1.647317
C	3.605305	2.346344	-1.973243
C	-1.571334	3.660137	1.028977
C	2.773857	3.356464	-1.586728
C	-2.456898	-2.311267	1.897868
C	3.565327	-2.716799	-1.653005
C	-1.685790	-3.327715	1.413646

C	2.698140	-3.638788	-1.139519
H	-3.291689	2.926992	2.195934
H	4.534262	2.420650	-2.524589
H	-1.699644	4.734434	0.979167
H	2.890063	4.419395	-1.757525
H	-3.385849	-2.381871	2.449451
H	4.489476	-2.898512	-2.187750
H	-1.856201	-4.393941	1.497912
H	2.778106	-4.718470	-1.172376
C	-2.308959	0.205895	1.814922
C	3.549055	-0.169701	-1.735392
C	0.489499	-3.427186	0.125464
C	0.595637	3.447230	-0.302322
H	-3.242862	0.234598	2.368597
H	4.487179	-0.198881	-2.283037
H	0.419232	-4.510877	0.166773
H	0.609737	4.526294	-0.429322
C	2.085840	1.247827	2.333541
C	2.030574	-0.927418	2.398980
C	2.760052	0.879131	3.466100
H	1.883263	2.228826	1.935604
N	2.715422	-0.504944	3.492116
H	1.838515	-1.960133	2.154853
H	3.253376	1.452614	4.234494
H	3.119761	-1.101576	4.197864
N	1.641399	0.113849	1.685082
C	-1.541957	-0.756251	-2.186870
H	-1.369301	-1.773535	-2.526302
N	-0.639046	0.296679	-2.755848
N	-0.393248	-0.093121	-1.603431
C	-2.885595	-0.399149	-1.690030
C	-3.805890	-1.417755	-1.415413
C	-3.236744	0.933061	-1.437347
C	-5.059478	-1.110670	-0.890854
H	-3.525734	-2.452967	-1.591066
C	-4.492757	1.237657	-0.918364
H	-2.518446	1.725154	-1.620497
C	-5.406673	0.219011	-0.641464
H	-5.763071	-1.909168	-0.672565
H	-4.748017	2.273095	-0.713559
H	-6.383329	0.458999	-0.230324

B[5]

Fe	0.711594	0.021712	0.079801
N	1.996515	1.346673	-0.894159
N	1.680579	-1.579522	-0.817429
N	-0.508208	1.607204	0.625075
N	-0.740235	-1.310076	0.821140
C	1.889766	2.708992	-0.909523
C	1.361328	-2.904301	-0.681392
C	3.082274	1.002480	-1.649549
C	2.825041	-1.496015	-1.565498
C	-0.242865	2.932562	0.400078
C	-0.717011	-2.674621	0.710848
C	-1.653210	1.527399	1.372304
C	-1.858539	-0.966402	1.532103
C	2.988195	3.265196	-1.684064
C	2.347396	-3.701664	-1.379668
C	3.725629	2.211697	-2.139274
C	3.252255	-2.832037	-1.923697
C	-1.279215	3.731941	1.019663
C	-1.868699	-3.228227	1.404212
C	-2.147191	2.863966	1.623421
C	-2.570443	-2.173551	1.914018
H	3.152787	4.320494	-1.863073
H	2.342837	-4.782770	-1.443146
H	4.609948	2.237737	-2.763819
H	4.127019	-3.067457	-2.517048
H	-1.328215	4.813553	0.996111
H	-2.104627	-4.282889	1.476917

H	-3.044738	3.099725	2.181311
H	-3.496438	-2.197426	2.474699
C	0.860759	3.436322	-0.302923
C	0.256973	-3.405912	0.022367
C	-2.264182	0.342969	1.802295
C	3.472419	-0.309279	-1.937673
H	0.913349	4.517611	-0.397539
H	0.142381	-4.486626	0.026534
H	-3.186247	0.456520	2.364468
H	4.364183	-0.423920	-2.547970
C	3.026884	0.653944	2.244491
C	1.538561	-0.716856	3.027343
C	3.413582	0.362470	3.525980
H	3.488768	1.294693	1.508820
N	2.454518	-0.512057	4.010488
H	0.672153	-1.354291	3.119122
H	4.252200	0.681315	4.124856
H	2.437300	-0.925182	4.931165
N	1.862525	-0.024156	1.952378
C	-1.845963	-0.916677	-2.178639
H	-1.703696	-1.991042	-2.139872
N	-0.612228	-0.116088	-2.170095
N	-1.138218	-0.198874	-3.276788
C	-3.062596	-0.337091	-1.584988
C	-4.040957	-1.189975	-1.058520
C	-3.243739	1.050165	-1.497516
C	-5.180875	-0.666821	-0.453413
H	-3.890072	-2.264874	-1.100597
C	-4.384831	1.570340	-0.890857
H	-2.480097	1.722513	-1.873530
C	-5.357290	0.716247	-0.368102
H	-5.929362	-1.339190	-0.043223
H	-4.503038	2.646924	-0.812420
H	-6.245317	1.124777	0.106179

TS(B-C)^{css}

Fe	0.642136	0.011103	-0.039801
N	1.957844	1.387378	-0.730424
N	1.843946	-1.465418	-0.716375
N	-0.569446	1.489662	0.627478
N	-0.649408	-1.359503	0.696582
C	1.832395	2.749429	-0.648143
C	1.625300	-2.814085	-0.601928
C	3.130604	1.146613	-1.398496
C	3.024846	-1.322961	-1.399607
C	-0.359207	2.838293	0.494437
C	-0.511238	-2.723218	0.638834
C	-1.774489	1.348062	1.268927
C	-1.812194	-1.117624	1.382110
C	2.973025	3.391675	-1.266927
C	2.702364	-3.547968	-1.231333
C	3.778126	2.397474	-1.732933
C	3.570604	-2.623067	-1.726286
C	-1.471497	3.572248	1.060431
C	-1.621960	-3.363697	1.310734
C	-2.349137	2.647945	1.540268
C	-2.425650	-2.366761	1.777250
H	3.116610	4.462658	-1.333755
H	2.767410	-4.627561	-1.279604
H	4.719444	2.483109	-2.260842
H	4.495486	-2.786183	-2.264864
H	-1.552147	4.651806	1.078417
H	-1.751337	-4.434508	1.405564
H	-3.301046	2.809974	2.029581
H	-3.356830	-2.449719	2.323146
C	0.758230	3.427246	-0.084814
C	0.536237	-3.402657	0.028671
C	-2.347005	0.138873	1.641695
C	3.629475	-0.111370	-1.716517
H	0.790201	4.512431	-0.107879

H	0.502099	-4.487857	0.049069
H	-3.303270	0.176791	2.152657
H	4.570218	-0.151567	-2.257244
C	2.963990	-0.098035	1.895944
C	1.039237	0.104285	2.890089
C	3.226613	-0.059661	3.238629
H	3.640626	-0.189487	1.062353
N	1.993688	0.068638	3.855216
H	-0.018309	0.197712	3.077853
H	4.147023	-0.109606	3.798130
H	1.826224	0.127147	4.848120
N	1.601606	0.004543	1.698483
C	-2.114936	-0.929698	-2.662091
H	-1.617224	-1.814149	-2.236773
N	-0.198382	0.105407	-1.719069
N	-0.582523	0.335642	-2.760950
C	-3.144322	-0.409488	-1.805005
C	-3.902994	-1.314433	-1.025066
C	-3.560096	0.944120	-1.850736
C	-5.066058	-0.899384	-0.382887
H	-3.568709	-2.343001	-0.934900
C	-4.668751	1.368072	-1.134998
H	-2.975946	1.650556	-2.431674
C	-5.441311	0.444675	-0.416559
H	-5.651285	-1.615133	0.188209
H	-4.950962	2.416850	-1.148446
H	-6.326298	0.777200	0.118959

TS(B-C)^{oss}

Fe	0.640856	0.004907	-0.067612
N	1.968697	-1.346262	-0.759613
N	-0.525643	-1.497162	0.605682
N	1.833767	1.516693	-0.691291
N	-0.685377	1.360424	0.633714
C	3.189011	-1.076672	-1.322537
C	-1.660743	-1.371019	1.362486
C	1.826547	-2.710366	-0.778193
C	-0.332591	-2.842106	0.415664
C	3.075559	1.392694	-1.257741
C	-1.819947	1.092701	1.356366
C	1.554365	2.858750	-0.657605
C	-0.638657	2.722363	0.475897
C	3.843274	-2.310535	-1.703364
C	-2.201936	-2.677964	1.666271
C	2.994169	-3.323328	-1.374826
C	-1.386919	-3.591009	1.066114
C	3.607714	2.700731	-1.576454
C	-2.515925	2.324176	1.660642
C	2.660829	3.609647	-1.212276
C	-1.789268	3.334350	1.106931
H	4.818665	-2.373157	-2.168949
H	-3.098471	-2.853488	2.247175
H	3.130970	-4.388771	-1.509895
H	-1.468656	-4.670664	1.065270
H	4.573486	2.879640	-2.031911
H	-3.445302	2.384883	2.212016
H	2.691072	4.688105	-1.303427
H	-1.993024	4.397705	1.119876
C	3.717301	0.191522	-1.534035
C	-2.256650	-0.170686	1.728681
C	0.395052	3.424005	-0.136432
C	0.746587	-3.411105	-0.252491
H	4.699738	0.248480	-1.993102
H	-3.176957	-0.228402	2.300337
H	0.304908	4.505265	-0.180842
H	0.769473	-4.493882	-0.331031
C	2.041380	-1.065770	2.390242
C	1.854018	1.102290	2.388528
C	2.621587	-0.628328	3.550301
H	1.924221	-2.067228	2.009612

N	2.493869	0.750410	3.533336
H	1.616608	2.114846	2.103998
H	3.099354	-1.151251	4.363311
H	2.818739	1.388371	4.243866
N	1.571055	0.021839	1.683058
C	-2.145891	-0.974883	-2.605399
H	-1.657320	-1.877864	-2.217363
N	-0.196439	0.064162	-1.742786
N	-0.633135	0.245487	-2.777166
C	-3.154346	-0.434446	-1.742345
C	-3.928469	-1.322873	-0.956316
C	-3.525832	0.932821	-1.765598
C	-5.058818	-0.874821	-0.280855
H	-3.628446	-2.363667	-0.886996
C	-4.608008	1.384252	-1.026363
H	-2.927980	1.628026	-2.345852
C	-5.393137	0.481151	-0.296823
H	-5.653754	-1.576130	0.298216
H	-4.854503	2.441893	-1.023652
H	-6.254173	0.837308	0.261900

TS(B-C)^3

Fe	0.725453	0.023853	-0.116009
N	1.972161	1.462729	-0.783834
N	2.034703	-1.401681	-0.695019
N	-0.578339	1.443959	0.488179
N	-0.512046	-1.416709	0.587155
C	1.734867	2.812149	-0.816684
C	1.856168	-2.760954	-0.644834
C	3.223791	1.277140	-1.309631
C	3.278563	-1.194095	-1.232442
C	-0.477898	2.796598	0.284332
C	-0.359883	-2.774282	0.452368
C	-1.735242	1.244031	1.196814
C	-1.684114	-1.222976	1.271651
C	2.874881	3.504307	-1.380950
C	3.026864	-3.434972	-1.164557
C	3.802040	2.552549	-1.678674
C	3.912453	-2.462905	-1.520761
C	-1.614811	3.473256	0.874056
C	-1.479841	-3.460359	1.060709
C	-2.388021	2.510974	1.448828
C	-2.294563	-2.497393	1.578656
H	2.940040	4.576161	-1.519303
H	3.139729	-4.509399	-1.237193
H	4.783819	2.681510	-2.116506
H	4.899864	-2.575805	-1.950339
H	-1.776769	4.543550	0.848954
H	-1.603983	-4.535717	1.089610
H	-3.324448	2.624148	1.979408
H	-3.231113	-2.618939	2.107510
C	0.586799	3.436754	-0.340801
C	0.733551	-3.404377	-0.133258
C	-2.242041	0.010663	1.582093
C	3.842685	0.047694	-1.500897
H	0.534924	4.517807	-0.429567
H	0.725622	-4.489999	-0.162727
H	-3.189174	0.007638	2.111453
H	4.839088	0.056150	-1.932715
C	1.943513	1.232009	2.384001
C	1.977604	-0.943131	2.385816
C	2.532068	0.857648	3.561924
H	1.736307	2.215850	1.995654
N	2.545751	-0.526997	3.547172
H	1.851380	-1.975064	2.099558
H	2.931097	1.427431	4.385871
H	2.913187	-1.127595	4.269407
N	1.606486	0.101617	1.668113
C	-2.441845	-1.360543	-2.049389
H	-2.209308	-2.415803	-1.993241

N	-0.145701	-0.108434	-1.781176
N	-0.878131	-0.368867	-2.613615
C	-3.492618	-0.628783	-1.494874
C	-4.539182	-1.300940	-0.791647
C	-3.556368	0.792171	-1.576357
C	-5.568220	-0.586314	-0.200113
H	-4.501272	-2.382529	-0.708391
C	-4.594573	1.489767	-0.980063
H	-2.765438	1.325992	-2.090534
C	-5.605845	0.812875	-0.286510
H	-6.350434	-1.117454	0.336180
H	-4.609205	2.573943	-1.039163
H	-6.414562	1.367244	0.180630

TS(B-D)^{css}

Fe	0.703917	0.029030	-0.040200
N	0.781296	2.027744	0.277227
N	2.138250	0.203175	-1.455370
N	-0.654515	-0.164841	1.445753
N	0.661207	-1.979284	-0.317670
C	0.045888	2.739245	1.186276
C	2.690769	-0.813392	-2.188378
C	1.533692	2.941636	-0.412033
C	2.715190	1.363329	-1.902679
C	-1.194610	0.852289	2.191288
C	1.417862	-2.693630	-1.210760
C	-1.257158	-1.320822	1.874938
C	-0.112129	-2.895048	0.350544
C	0.349304	4.151149	1.076823
C	3.662065	-0.281169	-3.120602
C	1.272346	4.276908	0.084080
C	3.675933	1.068769	-2.944574
C	-2.167794	0.322272	3.121241
C	1.104902	-4.103084	-1.112078
C	-2.206271	-1.025203	2.926275
C	0.155400	-4.228463	-0.143715
H	-0.098092	4.927446	1.684432
H	4.240992	-0.877045	-3.814651
H	1.740888	5.177681	-0.291639
H	4.269675	1.810818	-3.463074
H	-2.740910	0.918805	3.819417
H	1.561255	-4.879545	-1.712803
H	-2.815471	-1.763125	3.432821
H	-0.328653	-5.128327	0.214235
C	-0.870491	2.198093	2.079396
C	2.362402	-2.158653	-2.077480
C	-1.007009	-2.594308	1.373041
C	2.434983	2.638788	-1.426318
H	-1.386959	2.887885	2.739928
H	2.884716	-2.851580	-2.730158
H	-1.559391	-3.419989	1.811507
H	2.968873	3.467410	-1.881617
C	3.291483	0.553359	1.475537
C	2.195434	-1.159414	2.247466
C	4.031431	0.060674	2.516088
H	3.484348	1.393112	0.828558
N	3.320580	-1.026604	2.995432
H	1.449485	-1.923652	2.395413
H	4.969120	0.370731	2.948945
H	3.586674	-1.620879	3.765849
N	2.155690	-0.216129	1.323405
C	-2.458156	-0.638436	-1.352055
H	-2.028851	-1.310267	-0.619647
N	-0.585971	0.306972	-1.300702
N	-1.494061	0.188139	-2.081876
C	-3.774573	-0.132436	-1.166300
C	-4.634773	-0.796627	-0.254267
C	-4.296700	0.955745	-1.910559
C	-5.969671	-0.432930	-0.147449
H	-4.231833	-1.601768	0.353652

C	-5.632806	1.311442	-1.790893
H	-3.631896	1.511163	-2.563611
C	-6.479662	0.620329	-0.915609
H	-6.616638	-0.959017	0.549501
H	-6.019416	2.144945	-2.371234
H	-7.520778	0.913747	-0.817482

C^{css}

Fe	0.792359	0.017898	-0.130748
N	2.597924	-0.369887	-0.953151
N	0.475840	-1.961306	0.088419
N	1.105430	2.006960	-0.353287
N	-0.996846	0.413842	0.727486
C	3.528451	0.554290	-1.355514
C	-0.612599	-2.552753	0.664367
C	3.136470	-1.600570	-1.221512
C	1.284198	-2.982074	-0.346363
C	2.236076	2.603269	-0.853013
C	-1.847749	-0.500044	1.286837
C	0.240025	3.024024	-0.041382
C	-1.568580	1.646986	0.929212
C	4.697794	-0.115180	-1.882600
C	-0.492967	-3.995088	0.599753
C	4.452272	-1.452953	-1.804490
C	0.681329	-4.262021	-0.032200
C	2.079407	4.040766	-0.857047
C	-2.988225	0.170422	1.873419
C	0.838231	4.302225	-0.358030
C	-2.822636	1.501131	1.640336
H	5.576159	0.387708	-2.266933
H	-1.227104	-4.692103	0.983105
H	5.088623	-2.274457	-2.108289
H	1.116304	-5.224017	-0.271596
H	2.827500	4.742220	-1.204234
H	-3.814699	-0.329574	2.360541
H	0.360113	5.262180	-0.208699
H	-3.478789	2.318939	1.909122
C	3.367428	1.933217	-1.303036
C	-1.686691	-1.881119	1.241323
C	-1.011032	2.860399	0.550156
C	2.520218	-2.821060	-0.956370
H	4.189846	2.541466	-1.667930
H	-2.461241	-2.486146	1.702025
H	-1.582737	3.759449	0.761008
H	3.059788	-3.721267	-1.234818
C	2.526728	-0.826230	2.193036
C	1.443231	1.022572	2.569571
C	2.878210	-0.424246	3.453412
H	2.839597	-1.690196	1.630000
N	2.181144	0.751024	3.676890
H	0.797652	1.878915	2.457845
H	3.538770	-0.850109	4.191653
H	2.212167	1.313201	4.513715
N	1.635880	0.083463	1.660499
C	-2.974717	-1.981654	-1.291874
H	-3.371376	-2.910832	-0.826102
N	0.035539	-0.047403	-1.871317
N	-0.351613	-0.072976	-2.910694
C	-3.965467	-0.951357	-1.056155
C	-5.214437	-1.166115	-0.416112
C	-3.680614	0.357169	-1.516906
C	-6.131300	-0.135832	-0.257802
H	-5.443950	-2.164091	-0.049941
C	-4.587455	1.397503	-1.342557
H	-2.728810	0.522047	-2.006168
C	-5.812456	1.148589	-0.719230
H	-7.087606	-0.316151	0.225768
H	-4.347475	2.397594	-1.691458
H	-6.526008	1.958256	-0.588452

C^{oss}

Fe	0.733387	0.007229	-0.121818
N	1.958643	-1.512123	-0.632008
N	-0.630867	-1.324961	0.543381
N	2.108651	1.346658	-0.753749
N	-0.492478	1.527344	0.398256
C	3.234474	-1.402967	-1.121358
C	-1.777173	-1.038983	1.238939
C	1.677718	-2.853512	-0.578708
C	-0.556495	-2.692958	0.463832
C	3.367774	1.064647	-1.217410
C	-1.679830	1.422253	1.076646
C	1.967720	2.709816	-0.818240
C	-0.294275	2.865789	0.168582
C	3.781931	-2.718393	-1.377874
C	-2.448787	-2.264472	1.613961
C	2.813181	-3.617675	-1.050340
C	-1.701206	-3.290634	1.118977
C	4.051310	2.290059	-1.571927
C	-2.256693	2.734453	1.272455
C	3.180131	3.309866	-1.332633
C	-1.404028	3.629550	0.699286
H	4.774095	-2.908506	-1.767225
H	-3.377597	-2.311925	2.167518
H	2.847622	-4.698080	-1.110739
H	-1.882575	-4.355407	1.194302
H	5.059263	2.343179	-1.963646
H	-3.197954	2.923685	1.772285
H	3.327820	4.371875	-1.483235
H	-1.494898	4.707088	0.642822
C	3.901269	-0.209565	-1.372185
C	-2.262501	0.235355	1.500762
C	0.841559	3.419759	-0.413686
C	0.500157	-3.407955	-0.089205
H	4.913013	-0.279389	-1.760454
H	-3.207676	0.307285	2.028400
H	0.867680	4.499700	-0.524993
H	0.420220	-4.490805	-0.094208
C	1.831642	-1.031427	2.494944
C	1.878721	1.139118	2.348131
C	2.372527	-0.577981	3.667846
H	1.634970	-2.039153	2.167280
N	2.395194	0.802152	3.558104
H	1.771604	2.149092	1.985973
H	2.733075	-1.090755	4.545209
H	2.736079	1.450223	4.251729
N	1.531602	0.047998	1.689261
C	-2.867951	-1.790389	-2.055671
H	-2.925354	-2.787873	-1.594603
N	0.039887	-0.007230	-1.889303
N	-0.291902	0.014245	-2.948127
C	-3.727151	-0.826293	-1.447952
C	-4.771537	-1.186668	-0.553873
C	-3.566939	0.549061	-1.756639
C	-5.616339	-0.225526	-0.014683
H	-4.896232	-2.234305	-0.296646
C	-4.387262	1.512420	-1.184740
H	-2.774251	0.830677	-2.440237
C	-5.417601	1.126703	-0.320844
H	-6.418587	-0.517357	0.657900
H	-4.228312	2.563217	-1.405738
H	-6.067227	1.880308	0.116534

C^{3}

Fe	0.748996	0.008142	-0.121464
N	2.069590	-1.417282	-0.671373
N	-0.516772	-1.425447	0.525652
N	2.024857	1.447422	-0.744475
N	-0.567963	1.434817	0.440119
C	3.330487	-1.213815	-1.169556

C	-1.697266	-1.229819	1.193774
C	1.883287	-2.775904	-0.632839
C	-0.358428	-2.782916	0.406824
C	3.293832	1.257995	-1.229299
C	-1.748959	1.236408	1.108953
C	1.797795	2.800165	-0.771395
C	-0.454321	2.788836	0.248791
C	3.966013	-2.484337	-1.445858
C	-2.305405	-2.503759	1.510020
C	3.065259	-3.453140	-1.121147
C	-1.482015	-3.468013	1.010624
C	3.892171	2.532560	-1.563322
C	-2.404964	2.504313	1.344417
C	2.961769	3.488555	-1.286766
C	-1.607865	3.466786	0.802810
H	4.965784	-2.600144	-1.844860
H	-3.245686	-2.622858	2.032505
H	3.175040	-4.527771	-1.194136
H	-1.600035	-4.543638	1.051113
H	4.889148	2.659299	-1.966084
H	-3.360040	2.617618	1.840177
H	3.039486	4.561230	-1.411995
H	-1.765503	4.537744	0.776698
C	3.910375	0.026056	-1.411588
C	-2.263883	0.004093	1.485819
C	0.637370	3.428065	-0.329878
C	0.745975	-3.416158	-0.152667
H	4.920194	0.031387	-1.810939
H	-3.221910	0.002355	1.994091
H	0.595090	4.510120	-0.411548
H	0.737716	-4.501749	-0.178541
C	1.939810	-1.002551	2.464301
C	1.853735	1.169083	2.354162
C	2.464271	-0.536433	3.639650
H	1.800879	-2.014774	2.121369
N	2.402123	0.844166	3.553230
H	1.681045	2.176482	2.010667
H	2.864098	-1.040714	4.504823
H	2.709312	1.500252	4.255026
N	1.566701	0.069814	1.680073
C	-2.932735	-1.793401	-1.972384
H	-2.787782	-2.852404	-1.804773
N	0.008863	-0.040276	-1.858361
N	-0.384223	-0.055749	-2.897040
C	-3.785553	-0.834895	-1.434123
C	-4.817054	-1.205355	-0.514885
C	-3.656110	0.548557	-1.756795
C	-5.643989	-0.245889	0.047743
H	-4.932291	-2.252808	-0.254128
C	-4.490458	1.493166	-1.181675
H	-2.877800	0.851514	-2.448014
C	-5.488028	1.109485	-0.275335
H	-6.419847	-0.550507	0.745804
H	-4.356118	2.542722	-1.426053
H	-6.137620	1.856259	0.171837

C[5]

Fe	0.753197	0.011550	-0.094221
N	2.117538	1.417149	-0.749119
N	2.123496	-1.510072	-0.583245
N	-0.620192	1.536019	0.369535
N	-0.604863	-1.388820	0.562708
C	1.925787	2.771853	-0.740345
C	1.905161	-2.846416	-0.417637
C	3.359658	1.166174	-1.267495
C	3.357290	-1.345533	-1.142598
C	-0.408786	2.871723	0.195159
C	-0.410037	-2.742982	0.565008
C	-1.869797	1.366401	0.890584
C	-1.842702	-1.134932	1.085200

C	3.112775	3.417562	-1.270743
C	3.068712	-3.577077	-0.890420
C	3.996281	2.428719	-1.595168
C	3.966904	-2.649941	-1.337693
C	-1.596480	3.597563	0.619275
C	-1.590448	-3.385469	1.116612
C	-2.498326	2.667136	1.048973
C	-2.470374	-2.393791	1.441005
H	3.239871	4.487314	-1.381415
H	3.174370	-4.654942	-0.881718
H	4.985680	2.532445	-2.023217
H	4.946898	-2.824221	-1.764654
H	-1.713561	4.673846	0.587197
H	-1.714307	-4.454342	1.240010
H	-3.500353	2.828930	1.424595
H	-3.459548	-2.490413	1.869546
C	0.768824	3.435945	-0.310733
C	0.737256	-3.408025	0.114550
C	-2.425419	0.129967	1.235863
C	3.929086	-0.102182	-1.449640
H	0.788752	4.519948	-0.385114
H	0.716125	-4.492361	0.184935
H	-3.436256	0.147413	1.628654
H	4.925482	-0.121303	-1.882951
C	0.812940	0.271360	2.901379
C	2.789717	0.063079	2.007395
C	1.710453	0.312974	3.933296
H	-0.262839	0.331260	2.915736
N	2.958828	0.181625	3.348014
H	3.590785	-0.044104	1.293657
H	1.582942	0.415621	4.998954
H	3.845691	0.177150	3.828480
N	1.501410	0.115821	1.715111
C	-3.001149	-1.852929	-2.132542
H	-2.954516	-2.932360	-2.074440
N	0.070431	-0.080483	-1.856229
N	-0.295713	-0.103436	-2.904031
C	-3.796910	-0.883295	-1.529677
C	-4.905881	-1.248884	-0.704286
C	-3.516624	0.506465	-1.679039
C	-5.651704	-0.279991	-0.050825
H	-5.141650	-2.301181	-0.579378
C	-4.264543	1.459827	-1.008366
H	-2.691361	0.800505	-2.315872
C	-5.333544	1.078931	-0.186285
H	-6.487651	-0.580587	0.575955
H	-4.007628	2.509716	-1.111234
H	-5.915305	1.831370	0.337983

TS(C-D)^{css}

Fe	-0.737797	0.026822	-0.044804
N	-1.023985	-1.970285	0.065246
N	-2.205042	0.153577	-1.425798
N	0.714817	-0.093609	1.364024
N	-0.450581	2.027221	-0.146416
C	-0.374881	-2.844712	0.898000
C	-2.680307	1.299318	-2.009187
C	-1.888845	-2.723822	-0.685374
C	-2.922160	-0.881885	-1.968024
C	1.100790	-1.223097	2.040248
C	-1.161273	2.913664	-0.913675
C	1.477907	0.934037	1.858245
C	0.487077	2.767496	0.529513
C	-0.847212	-4.194020	0.668996
C	-3.738801	0.979228	-2.943775
C	-1.783303	-4.119910	-0.316149
C	-3.885500	-0.374157	-2.921990
C	2.134723	-0.897951	2.998960
C	-0.658525	4.256536	-0.716931
C	2.369604	0.440673	2.884594

C	0.366989	4.165577	0.174743
H	-0.491130	-5.069575	1.196705
H	-4.280203	1.706757	-3.535139
H	-2.357516	-4.921353	-0.763300
H	-4.573799	-0.987596	-3.489488
H	2.610021	-1.611825	3.659756
H	-1.047403	5.138960	-1.209176
H	3.072967	1.051582	3.436524
H	0.992089	4.957808	0.567084
C	0.598746	-2.501736	1.826593
C	-2.205850	2.582667	-1.768594
C	1.390215	2.263746	1.458906
C	-2.769986	-2.223704	-1.637574
H	1.017731	-3.304865	2.425233
H	-2.677821	3.395649	-2.312206
H	2.068790	2.970068	1.927730
H	-3.404467	-2.938483	-2.152812
C	-3.298401	-0.340473	1.519088
C	-1.961409	1.127466	2.409145
C	-3.928422	0.122588	2.642559
H	-3.620813	-1.073448	0.797902
N	-3.065743	1.053509	3.195893
H	-1.118057	1.772878	2.595649
H	-4.881133	-0.114586	3.088409
H	-3.224428	1.588520	4.036078
N	-2.079443	0.294070	1.390640
C	3.035054	-1.677726	-2.263944
H	3.143484	-1.534610	-3.355218
N	0.539656	-0.245011	-1.402476
N	1.320827	-0.447470	-2.173498
C	4.032452	-0.866189	-1.589473
C	5.124830	-0.264729	-2.260615
C	3.975952	-0.758245	-0.178996
C	6.133276	0.381077	-1.553331
H	5.170187	-0.325272	-3.345075
C	4.955432	-0.069299	0.524385
H	3.144523	-1.225515	0.337286
C	6.039961	0.489639	-0.161478
H	6.977223	0.820871	-2.077614
H	4.883124	0.018238	1.603373
H	6.817001	1.012069	0.390703

TS(C-D)^3

Fe	0.726003	0.011260	-0.115898
N	2.031394	-1.421151	-0.678996
N	-0.515161	-1.415452	0.602555
N	1.976941	1.442275	-0.799309
N	-0.574647	1.444069	0.472017
C	3.275457	-1.223223	-1.218694
C	-1.686450	-1.211667	1.284741
C	1.848047	-2.778722	-0.616011
C	-0.367000	-2.774224	0.481128
C	3.228325	1.247160	-1.323107
C	-1.732861	1.254415	1.182059
C	1.744784	2.792749	-0.844244
C	-0.469552	2.794976	0.255910
C	3.905177	-2.497182	-1.494984
C	-2.300718	-2.481418	1.604730
C	3.016134	-3.462179	-1.129889
C	-1.489135	-3.451352	1.095934
C	3.811060	2.516749	-1.703634
C	-2.381641	2.525480	1.421339
C	2.887600	3.475185	-1.414084
C	-1.604473	3.480416	0.838773
H	4.892609	-2.617528	-1.922398
H	-3.236832	-2.594958	2.136077
H	3.125297	-4.537650	-1.190793
H	-1.615298	-4.526036	1.136455
H	4.792864	2.638044	-2.143681
H	-3.318909	2.646533	1.948739

H	2.956708	4.545365	-1.563555
H	-1.764083	4.550813	0.802613
C	3.843351	0.013590	-1.500938
C	-2.242213	0.026289	1.580934
C	0.599324	3.426046	-0.372276
C	0.722855	-3.413348	-0.100340
H	4.839767	0.014190	-1.932805
H	-3.189542	0.031055	2.109922
H	0.551114	4.506461	-0.471255
H	0.711569	-4.499106	-0.118920
C	2.004891	-0.953828	2.458165
C	1.916419	1.214880	2.312324
C	2.569116	-0.467891	3.606888
H	1.853908	-1.971842	2.137945
N	2.504862	0.911115	3.498141
H	1.733289	2.216337	1.956838
H	2.997774	-0.957067	4.466955
H	2.836694	1.579126	4.177120
N	1.606149	0.104488	1.667868
C	-2.447135	-1.381439	-2.031139
H	-2.217658	-2.436382	-1.958955
N	-0.145421	-0.135623	-1.780038
N	-0.879940	-0.402304	-2.608622
C	-3.495180	-0.637960	-1.487183
C	-4.543724	-1.296113	-0.773723
C	-3.554012	0.781868	-1.589369
C	-5.569857	-0.569317	-0.192047
H	-4.509453	-2.376466	-0.674611
C	-4.589382	1.491724	-1.002684
H	-2.761619	1.305278	-2.111940
C	-5.602603	0.828589	-0.298743
H	-6.353565	-1.089858	0.352384
H	-4.600425	2.574976	-1.077779
H	-6.409134	1.392533	0.160668

TS(C-D)[5]

Fe	0.713407	0.023368	-0.064997
N	1.907943	1.461136	-0.935922
N	2.078523	-1.471400	-0.656555
N	-0.635333	1.515739	0.551835
N	-0.472999	-1.406910	0.816928
C	1.632490	2.797992	-0.998157
C	1.909461	-2.815479	-0.494476
C	3.083742	1.238089	-1.595499
C	3.224719	-1.266109	-1.370519
C	-0.494918	2.853655	0.335707
C	-0.272493	-2.760380	0.755354
C	-1.723534	1.325577	1.357362
C	-1.613419	-1.176424	1.536086
C	2.690116	3.465187	-1.737227
C	3.026403	-3.509290	-1.111488
C	3.586566	2.504538	-2.103550
C	3.841122	-2.552339	-1.649366
C	-1.554518	3.561385	1.034639
C	-1.356814	-3.425896	1.453930
C	-2.309400	2.617572	1.671345
C	-2.176505	-2.448377	1.944474
H	2.730331	4.527882	-1.941319
H	3.156171	-4.584173	-1.138682
H	4.503410	2.627364	-2.666707
H	4.763054	-2.696884	-2.199085
H	-1.693150	4.635511	1.034355
H	-1.458690	-4.498502	1.563474
H	-3.189339	2.769440	2.283474
H	-3.083195	-2.566590	2.524635
C	0.536719	3.438456	-0.408641
C	0.816686	-3.404891	0.153054
C	-2.174432	0.079545	1.804569
C	3.693436	-0.010385	-1.783401
H	0.495658	4.518207	-0.523993

H	0.812031	-4.490629	0.199522
H	-3.079795	0.080581	2.404507
H	4.626864	-0.005424	-2.339963
C	1.297928	0.940265	2.774445
C	2.954960	-0.130842	1.851089
C	2.303378	0.909231	3.702431
H	0.310060	1.364349	2.835831
N	3.346974	0.228873	3.099392
H	3.562042	-0.673406	1.145185
H	2.371508	1.291529	4.708381
H	4.246983	0.031218	3.509972
N	1.719524	0.286032	1.633737
C	-2.496041	-1.725412	-1.558990
H	-2.267688	-2.699701	-1.148790
N	-0.190963	-0.337201	-1.680693
N	-0.869891	-0.903763	-2.390859
C	-3.578562	-0.869420	-1.365987
C	-4.637720	-1.264620	-0.490332
C	-3.671247	0.412274	-1.979576
C	-5.706336	-0.419057	-0.241786
H	-4.572950	-2.230068	0.001385
C	-4.753584	1.240193	-1.725326
H	-2.873356	0.740865	-2.635574
C	-5.775830	0.838947	-0.855763
H	-6.495896	-0.737288	0.434418
H	-4.796874	2.218832	-2.193124
H	-6.616438	1.497841	-0.659419

D^{css}

Fe	-0.763870	0.005991	-0.086054
N	0.171657	-1.577539	0.760824
N	-2.115546	-1.243065	-0.911483
N	0.588106	1.255761	0.757912
N	-1.683690	1.588468	-0.938813
C	1.265148	-1.539064	1.589056
C	-3.207513	-0.884746	-1.658026
C	-0.135818	-2.904094	0.592829
C	-2.133453	-2.612495	-0.835370
C	1.603556	0.909143	1.613418
C	-2.829037	1.558622	-1.689365
C	0.671176	2.616661	0.591080
C	-1.294715	2.902263	-0.883172
C	1.662268	-2.882218	1.953288
C	-3.945437	-2.064674	-2.059980
C	0.795472	-3.729999	1.332005
C	-3.275964	-3.137055	-1.554912
C	2.348677	2.086110	2.003300
C	-3.178655	2.896520	-2.121464
C	1.775173	3.145033	1.364217
C	-2.223168	3.730300	-1.625838
H	2.498586	-3.125159	2.596579
H	-4.849050	-2.053796	-2.656384
H	0.770938	-4.812100	1.364121
H	-3.517599	-4.188409	-1.647984
H	3.205186	2.081336	2.665269
H	-4.040002	3.144000	-2.729125
H	2.057341	4.189760	1.403710
H	-2.139002	4.803783	-1.740211
C	1.919417	-0.386228	2.004378
C	-3.549583	0.414633	-2.011922
C	-0.194364	3.384561	-0.181905
C	-1.205109	-3.390674	-0.152750
H	2.773723	-0.509922	2.662885
H	-4.443109	0.544935	-2.615420
H	-0.007005	4.453585	-0.223772
H	-1.338586	-4.468015	-0.186369
C	-2.541875	-0.818008	2.224124
C	-2.245563	1.333527	2.108191
C	-3.247792	-0.276335	3.264724
H	-2.427423	-1.847959	1.927723

N	-3.048553	1.091000	3.177279
H	-1.920410	2.312939	1.795426
H	-3.855390	-0.720241	4.037145
H	-3.430978	1.790358	3.795234
N	-1.926862	0.195708	1.518230
C	2.563643	-1.297761	-1.765214
H	2.594029	-2.330351	-2.095076
N	0.401105	-0.163140	-1.653050
N	1.405451	-0.744546	-1.725359
C	3.769715	-0.588037	-1.350574
C	4.999340	-1.266941	-1.375089
C	3.734604	0.746300	-0.909540
C	6.165879	-0.627622	-0.962695
H	5.033407	-2.299514	-1.713136
C	4.903764	1.377001	-0.498042
H	2.792206	1.281747	-0.873542
C	6.124433	0.696704	-0.521352
H	7.109139	-1.166380	-0.984718
H	4.853243	2.403343	-0.147067
H	7.034396	1.193210	-0.197048

D^3

Fe	0.775009	-0.005731	-0.096777
N	-0.535374	-1.438570	0.440950
N	-0.452748	1.386469	0.690193
N	1.937091	-1.386656	-0.985433
N	2.016447	1.444711	-0.739044
C	-0.430672	-2.785367	0.181520
C	-0.294010	2.751288	0.630585
C	-1.676191	-1.283272	1.193740
C	-1.621707	1.168229	1.382669
C	1.703239	-2.738943	-1.052379
C	1.852508	2.800492	-0.581549
C	3.139212	-1.175361	-1.617585
C	3.208728	1.279162	-1.403391
C	-1.542632	-3.493651	0.775401
C	-1.398948	3.409309	1.290667
C	-2.309364	-2.563737	1.408719
C	-2.217043	2.427620	1.762965
C	2.786992	-3.397704	-1.746390
C	2.973426	3.507506	-1.158578
C	3.680282	-2.429791	-2.090743
C	3.817422	2.564582	-1.661269
H	-1.695146	-4.563335	0.708921
H	-1.511050	4.482540	1.378695
H	-3.230953	-2.705697	1.957688
H	-3.147852	2.525041	2.306344
H	2.838536	-4.462395	-1.935131
H	3.081859	4.584570	-1.167780
H	4.615746	-2.533099	-2.625720
H	4.760322	2.706525	-2.173879
C	0.600972	-3.391729	-0.520026
C	0.773937	3.412238	0.040536
C	3.744737	0.060746	-1.797472
C	-2.179752	-0.073387	1.646111
H	0.549977	-4.468529	-0.648340
H	0.771733	4.497177	0.080761
H	4.696359	0.079405	-2.319764
H	-3.116577	-0.095094	2.192791
C	1.405193	-0.355520	3.142147
C	3.227771	-0.283754	1.980668
C	2.431805	-0.481505	4.042695
H	0.338912	-0.343532	3.312042
N	3.590450	-0.433967	3.286341
H	3.929010	-0.217629	1.161685
H	2.452662	-0.596925	5.115212
H	4.533913	-0.499462	3.638184
N	1.916615	-0.233756	1.868438
C	-2.577562	1.423906	-1.756654
H	-2.555757	2.501211	-1.659831

N	-1.478613	0.874079	-2.169571
N	-0.514083	0.344569	-2.498483
C	-3.689322	0.616733	-1.283883
C	-4.789779	1.259270	-0.688423
C	-3.688457	-0.787478	-1.361867
C	-5.851807	0.517465	-0.179326
H	-4.794506	2.343157	-0.611833
C	-4.754123	-1.521208	-0.851505
H	-2.837063	-1.305698	-1.793073
C	-5.841909	-0.877637	-0.255925
H	-6.690719	1.032050	0.281755
H	-4.724940	-2.605451	-0.907851
H	-6.670865	-1.454989	0.142834

D[5]

Fe	0.835768	0.006460	0.023043
N	-0.509017	1.442113	0.756296
N	1.971185	1.523864	-0.814980
N	-0.539977	-1.476193	0.487852
N	2.013365	-1.411740	-0.964334
C	-1.690668	1.187723	1.399212
C	3.125231	1.353989	-1.532527
C	-0.380709	2.799869	0.640654
C	1.762578	2.869149	-0.666233
C	-1.687196	-1.311140	1.219492
C	3.153627	-1.153348	-1.674228
C	-0.377198	-2.818599	0.260394
C	1.793536	-2.760769	-1.001297
C	-2.336338	2.445999	1.728110
C	3.678356	2.653439	-1.851961
C	-1.529424	3.442233	1.257635
C	2.835196	3.589202	-1.319921
C	-2.289562	-2.605210	1.453872
C	3.707251	-2.406773	-2.160079
C	-1.483205	-3.536119	0.859564
C	2.866713	-3.399120	-1.745975
H	-3.289554	2.540721	2.232758
H	4.587151	2.821078	-2.416501
H	-1.690278	4.511969	1.311932
H	2.924330	4.667520	-1.364858
H	-3.215417	-2.769050	1.990143
H	4.607440	-2.501291	-2.754740
H	-1.617724	-4.610246	0.827406
H	2.946976	-4.462377	-1.935643
C	-2.213181	-0.084856	1.642074
C	3.673784	0.122065	-1.914907
C	0.694630	-3.406251	-0.425281
C	0.677043	3.453602	-0.000185
H	-3.165277	-0.126267	2.162513
H	4.592090	0.167250	-2.494205
H	0.660586	-4.487516	-0.528634
H	0.647515	4.539920	0.005878
C	1.765065	0.527054	3.075545
C	2.984600	-0.973642	2.091062
C	2.681245	0.110277	4.004790
H	0.976420	1.259326	3.157625
N	3.450326	-0.845764	3.361418
H	3.390443	-1.649367	1.353351
H	2.857571	0.390670	5.031367
H	4.221230	-1.358135	3.763691
N	1.968377	-0.155441	1.895068
C	-2.567152	1.348352	-1.732915
H	-2.567828	2.425395	-1.627689
N	-0.456877	0.319588	-2.409851
N	-1.443841	0.823475	-2.108221
C	-3.677232	0.517151	-1.295970
C	-4.805044	1.137357	-0.729320
C	-3.646750	-0.886303	-1.375788
C	-5.866054	0.374305	-0.250062
H	-4.831835	2.220789	-0.650737

C	-4.710545	-1.641627	-0.893747
H	-2.773824	-1.387182	-1.783382
C	-5.826358	-1.020141	-0.327377
H	-6.726885	0.871581	0.189084
H	-4.657508	-2.725030	-0.948395
H	-6.653803	-1.614248	0.049387

TS(D-E)[5]

Fe	0.765384	0.002735	0.117490
N	-0.794867	-1.253139	0.662596
N	-0.376360	1.643875	0.762104
N	1.681148	-1.606513	-0.862484
N	2.024073	1.308844	-0.885887
C	-0.812502	-2.617911	0.523947
C	-0.084310	2.964964	0.552693
C	-1.886729	-0.898931	1.413899
C	-1.566375	1.583883	1.436334
C	1.285685	-2.915652	-0.817095
C	1.995207	2.677527	-0.819447
C	2.804438	-1.538322	-1.641220
C	3.106760	0.951356	-1.645860
C	-1.972362	-3.149671	1.206477
C	-1.129067	3.785398	1.139853
C	-2.634648	-2.088105	1.756372
C	-2.043403	2.931100	1.688193
C	2.223323	-3.726102	-1.576038
C	3.112341	3.213118	-1.567764
C	3.161497	-2.875450	-2.084298
C	3.800358	2.146815	-2.075799
H	-2.241306	-4.197780	1.249766
H	-1.154983	4.867979	1.121996
H	-3.554903	-2.097655	2.325759
H	-2.963929	3.178824	2.201915
H	2.151686	-4.798075	-1.712452
H	3.331642	4.266565	-1.689459
H	4.006721	-3.116481	-2.716993
H	4.689182	2.161215	-2.694164
C	0.143553	-3.380391	-0.159425
C	1.024445	3.437425	-0.156337
C	3.473006	-0.358989	-1.978572
C	-2.238894	0.405946	1.770819
H	-0.033498	-4.451989	-0.193898
H	1.131294	4.516721	-0.223762
H	4.355596	-0.465240	-2.603420
H	-3.168767	0.517525	2.319764
C	1.869416	0.561854	3.089808
C	2.800173	-1.169857	2.169248
C	2.738538	0.055655	4.019592
H	1.210548	1.414821	3.146750
N	3.322695	-1.046770	3.417164
H	3.066632	-1.943083	1.464445
H	2.992296	0.361415	5.022390
H	4.015054	-1.653373	3.831161
N	1.921236	-0.210317	1.948648
C	-2.217221	1.409112	-1.827637
H	-2.152865	2.458766	-1.572626
N	-0.261465	0.417621	-2.909948
N	-1.169704	0.904182	-2.406076
C	-3.316822	0.563448	-1.396210
C	-4.399608	1.153782	-0.719851
C	-3.324059	-0.829074	-1.595086
C	-5.452976	0.373476	-0.252325
H	-4.394649	2.226468	-0.546931
C	-4.379358	-1.601347	-1.122577
H	-2.485724	-1.309725	-2.090130
C	-5.450775	-1.009318	-0.448655
H	-6.278628	0.848460	0.271359
H	-4.355312	-2.677381	-1.267562
H	-6.271127	-1.618017	-0.079696

E^{css}

Fe	0.458558	0.078558	0.118744
N	-0.945011	-1.024345	1.053956
N	-0.669821	1.730046	0.394327
N	1.541736	-1.586098	-0.240371
N	1.805078	1.160958	-0.934299
C	-0.929994	-2.382724	1.245348
C	-0.397197	2.996571	-0.061453
C	-2.105181	-0.572020	1.634899
C	-1.855235	1.819413	1.080469
C	1.229203	-2.866904	0.144982
C	1.742328	2.507580	-1.205048
C	2.754120	-1.669667	-0.884264
C	2.975931	0.714103	-1.498132
C	-2.119088	-2.802463	1.958063
C	-1.443532	3.910646	0.345661
C	-2.845462	-1.677964	2.203571
C	-2.344370	3.180383	1.060965
C	2.272403	-3.782487	-0.265111
C	2.903006	2.919133	-1.964035
C	3.221000	-3.039394	-0.898376
C	3.671347	1.807698	-2.140987
H	-2.348519	-3.826049	2.226410
H	-1.467320	4.967073	0.109464
H	-3.798332	-1.586368	2.709058
H	-3.263696	3.512359	1.526614
H	2.260736	-4.850367	-0.087015
H	3.090293	3.928918	-2.307035
H	4.146283	-3.371529	-1.352050
H	4.616255	1.717806	-2.662103
C	0.078261	-3.241727	0.825723
C	0.716539	3.358312	-0.810303
C	3.428735	-0.601171	-1.462615
C	-2.521407	0.751328	1.669054
H	-0.041907	-4.296877	1.053289
H	0.797085	4.400411	-1.105785
H	4.376085	-0.814923	-1.948837
H	-3.465390	0.963761	2.161128
C	0.873418	0.726389	3.028059
C	2.731575	0.329644	1.964072
C	1.879792	0.859575	3.946442
H	-0.191630	0.839715	3.146731
N	3.051858	0.604688	3.255412
H	3.445002	0.091250	1.191525
H	1.873306	1.104750	4.996499
H	3.984957	0.618336	3.637877
N	1.421122	0.397459	1.803985
C	-0.791296	-0.111763	-2.105842
H	-0.331842	0.837340	-2.352109
N	0.389522	-2.084938	-2.962765
N	-0.157553	-1.154652	-2.604505
C	-2.222771	-0.219953	-1.800559
C	-2.991009	0.952542	-1.750660
C	-2.834574	-1.449591	-1.511467
C	-4.340094	0.894975	-1.411783
H	-2.517720	1.909867	-1.946608
C	-4.183693	-1.500114	-1.176467
H	-2.242927	-2.360158	-1.508926
C	-4.944593	-0.329459	-1.123244
H	-4.916730	1.814651	-1.364514
H	-4.637616	-2.457590	-0.937744
H	-5.996399	-0.372087	-0.855170

E^{3}

Fe	-0.443911	0.056937	0.078887
N	0.971621	-0.856574	1.167218
N	-1.356779	-1.709795	-0.197707
N	0.529723	1.806952	0.259083
N	-1.789742	0.946458	-1.126292
C	2.011749	-0.249670	1.830127

C	-2.555605	-1.922230	-0.836750
C	1.099691	-2.202960	1.408286
C	-0.929461	-2.944955	0.229448
C	1.622899	2.053277	1.054487
C	-2.927835	0.374782	-1.644634
C	0.245031	2.992332	-0.378834
C	-1.776866	2.247928	-1.575518
C	2.813850	-1.241196	2.509863
C	-2.897476	-3.326084	-0.799614
C	2.256288	-2.452606	2.239155
C	-1.883923	-3.961357	-0.151438
C	2.034005	3.431029	0.920100
C	-3.652965	1.341909	-2.435883
C	1.189240	4.010459	0.021362
C	-2.933860	2.498547	-2.403654
H	3.696339	-1.019289	3.095761
H	-3.790258	-3.752435	-1.238579
H	2.578309	-3.433163	2.565729
H	-1.775372	-5.016937	0.062085
H	2.874089	3.874573	1.439034
H	-4.581421	1.139373	-2.954332
H	1.185551	5.030368	-0.341701
H	-3.154141	3.443788	-2.883225
C	2.295677	1.105839	1.811063
C	-3.303003	-0.951784	-1.485822
C	-0.818200	3.197547	-1.248258
C	0.225133	-3.182725	0.960398
H	3.159706	1.441378	2.375344
H	-4.228133	-1.267940	-1.957513
H	-0.928178	4.188076	-1.678898
H	0.443273	-4.210990	1.231422
C	-2.023055	-0.377089	2.936795
C	-2.235232	1.651403	2.217653
C	-2.787837	0.276015	3.869200
H	-1.686809	-1.403118	2.917902
N	-2.915263	1.571251	3.396517
H	-2.160891	2.548625	1.620784
H	-3.240809	-0.042318	4.795222
H	-3.421058	2.320851	3.844353
N	-1.689680	0.490722	1.920546
N	0.421067	-1.376573	-2.748573
H	0.499256	0.641898	-2.699474
C	2.353544	-0.258998	-1.837039
C	3.018939	0.969586	-1.689405
C	2.983191	-1.429526	-1.379004
C	4.276943	1.023982	-1.097511
H	2.530441	1.882802	-2.015918
C	4.240083	-1.366144	-0.787332
H	2.471429	-2.384142	-1.458022
C	4.896849	-0.141164	-0.642751
H	4.767661	1.986390	-0.980677
H	4.702722	-2.278710	-0.422533
H	5.876295	-0.096108	-0.175339
C	1.021836	-0.265533	-2.427950
N	-0.090106	-2.369158	-3.001038

E[5]

Fe	0.515257	0.135497	0.182270
N	-0.839937	-1.039351	1.211404
N	-0.779597	1.769533	0.359050
N	1.645235	-1.577047	-0.250086
N	1.616828	1.187936	-1.233463
C	-0.722162	-2.379744	1.465055
C	-0.640427	2.986135	-0.251339
C	-1.974458	-0.591833	1.835964
C	-1.923861	1.805919	1.106585
C	1.404865	-2.841256	0.215758
C	1.430341	2.500483	-1.586436
C	2.760174	-1.630792	-1.042736
C	2.748261	0.740768	-1.865437

C	-1.839610	-2.806558	2.281295
C	-1.738470	3.850034	0.149715
C	-2.610192	-1.701489	2.512784
C	-2.528143	3.121577	0.991772
C	2.439437	-3.735979	-0.274247
C	2.484493	2.899960	-2.493271
C	3.278183	-2.988309	-1.047904
C	3.299975	1.814787	-2.662688
H	-2.006490	-3.819302	2.626580
H	-1.882008	4.870506	-0.183219
H	-3.531072	-1.637867	3.078544
H	-3.445753	3.428824	1.477688
H	2.494496	-4.797087	-0.065407
H	2.583872	3.882574	-2.937412
H	4.150853	-3.319520	-1.596875
H	4.191292	1.741588	-3.273329
C	0.315750	-3.205502	1.012470
C	0.386214	3.321950	-1.139793
C	3.277273	-0.553709	-1.767851
C	-2.457910	0.720652	1.805864
H	0.256188	-4.251555	1.300374
H	0.370731	4.333713	-1.535877
H	4.173351	-0.749347	-2.350508
H	-3.384813	0.901074	2.342138
C	1.633426	1.807985	2.706369
C	2.777179	-0.000603	2.344346
C	2.613827	1.778340	3.662572
H	0.854502	2.534666	2.532941
N	3.333151	0.619912	3.417755
H	3.128925	-0.929400	1.921224
H	2.864132	2.447477	4.470748
H	4.130568	0.292844	3.942966
N	1.750060	0.697169	1.897849
C	-1.026799	-0.478598	-2.280468
H	-0.508836	0.428858	-2.561104
N	0.119066	-2.579601	-2.790890
N	-0.406607	-1.589066	-2.565193
C	-2.380919	-0.484418	-1.742509
C	-3.094477	0.724824	-1.696875
C	-2.988115	-1.648857	-1.241067
C	-4.379125	0.766043	-1.164144
H	-2.623564	1.635097	-2.055593
C	-4.272759	-1.599305	-0.710752
H	-2.438034	-2.585256	-1.236444
C	-4.978105	-0.393671	-0.668793
H	-4.907324	1.714682	-1.124972
H	-4.718766	-2.506320	-0.312527
H	-5.979511	-0.358569	-0.249360

TS(E-F)^{css}

Fe	0.346253	0.016547	-0.066573
N	-1.092172	-0.822345	1.124662
N	-0.432804	1.880268	0.328615
N	1.196610	-1.794018	-0.322482
N	1.878763	0.889633	-1.106210
C	-1.250385	-2.155127	1.394699
C	0.023744	3.074835	-0.165742
C	-2.110181	-0.163885	1.766129
C	-1.543741	2.156616	1.080984
C	0.729552	-2.996092	0.154346
C	2.019549	2.226256	-1.386811
C	2.378040	-2.063903	-0.974133
C	2.954709	0.249970	-1.667010
C	-2.413262	-2.352474	2.236723
C	-0.835734	4.150010	0.287506
C	-2.944551	-1.118442	2.467583
C	-1.803341	3.581361	1.062072
C	1.633638	-4.061027	-0.228334
C	3.228011	2.438193	-2.156641
C	2.655585	-3.484018	-0.919465

C	3.809688	1.215464	-2.325694
H	-2.760956	-3.312169	2.598132
H	-0.698279	5.196306	0.044794
H	-3.817618	-0.862046	3.054288
H	-2.620877	4.067399	1.579542
H	1.495374	-5.106101	0.018791
H	3.576660	3.401122	-2.508629
H	3.522501	-3.960429	-1.359668
H	4.728225	0.975802	-2.846707
C	-0.413594	-3.168038	0.930236
C	1.150804	3.233965	-0.969715
C	3.189577	-1.121938	-1.600738
C	-2.320295	1.211633	1.746739
H	-0.656494	-4.184137	1.227970
H	1.390715	4.246629	-1.281617
H	4.088598	-1.492729	-2.084664
H	-3.180047	1.583625	2.296262
C	1.354311	-0.090694	3.216297
C	2.867186	0.822627	1.964689
C	2.386007	0.247840	4.054612
H	0.410673	-0.564912	3.438744
N	3.344230	0.829539	3.241782
H	3.401958	1.214326	1.112640
H	2.528367	0.135502	5.118052
H	4.236583	1.193821	3.539963
N	1.671558	0.273222	1.927355
C	-0.809443	0.152491	-1.639664
H	-0.523485	1.028602	-2.226857
N	0.207887	-1.999664	-2.984514
N	-0.296260	-1.027019	-2.771275
C	-2.284519	-0.005941	-1.575408
C	-3.081699	1.142884	-1.674398
C	-2.895460	-1.235594	-1.285768
C	-4.457514	1.070507	-1.457968
H	-2.611911	2.099923	-1.883350
C	-4.270280	-1.311134	-1.095052
H	-2.282540	-2.125032	-1.183661
C	-5.055811	-0.156530	-1.172578
H	-5.060378	1.972364	-1.517989
H	-4.729364	-2.268255	-0.865139
H	-6.128504	-0.216028	-1.010481

TS(E-F)^3

Fe	-0.347915	0.074761	-0.047787
N	1.095940	-0.657374	1.168030
N	-1.130917	-1.793994	-0.215213
N	0.362449	1.947293	0.236984
N	-1.886953	0.810346	-1.125470
C	2.093601	0.063532	1.781296
C	-2.290238	-2.141641	-0.859394
C	1.326630	-1.977028	1.469831
C	-0.594572	-2.957931	0.272232
C	1.450972	2.309740	0.989720
C	-2.935377	0.101296	-1.658104
C	-0.121406	3.097849	-0.335790
C	-2.062417	2.118309	-1.508147
C	2.969701	-0.828941	2.503379
C	-2.494496	-3.571260	-0.773479
C	2.496817	-2.091793	2.308565
C	-1.439120	-4.078480	-0.082276
C	1.662365	3.735200	0.889230
C	-3.805641	0.992039	-2.391640
C	0.693144	4.222466	0.064420
C	-3.261613	2.238135	-2.305381
H	3.835745	-0.512811	3.070236
H	-3.335081	-4.098535	-1.205505
H	2.892804	-3.025849	2.685874
H	-1.236291	-5.108610	0.180835
H	2.456198	4.275109	1.389103
H	-4.706542	0.683919	-2.906335

H	0.524802	5.245091	-0.247766
H	-3.626938	3.164161	-2.730289
C	2.254500	1.439522	1.712494
C	-3.135961	-1.266033	-1.524104
C	-1.237089	3.179210	-1.158543
C	0.554676	-3.050286	1.043776
H	3.097717	1.867679	2.244722
H	-4.015425	-1.687979	-1.999859
H	-1.501430	4.160039	-1.540933
H	0.863155	-4.041135	1.362175
C	-3.048049	0.700776	2.008797
C	-1.334188	0.082602	3.173193
C	-3.473304	0.657209	3.312429
H	-3.596224	0.960282	1.115546
N	-2.367594	0.261159	4.044992
H	-0.343312	-0.231503	3.465702
H	-4.425038	0.862217	3.777379
H	-2.332759	0.127155	5.044590
N	-1.719831	0.342514	1.941464
N	0.313673	-1.098777	-3.038276
H	0.534206	0.981983	-2.254152
C	2.250378	-0.074180	-1.565862
C	3.075329	1.062344	-1.614709
C	2.844555	-1.318528	-1.290618
C	4.443095	0.966431	-1.361565
H	2.627531	2.029427	-1.826715
C	4.210020	-1.417515	-1.049358
H	2.217195	-2.202769	-1.252846
C	5.014947	-0.273797	-1.075901
H	5.062008	1.859546	-1.390348
H	4.650261	-2.386704	-0.830899
H	6.081186	-0.352499	-0.881035
C	0.786373	0.063956	-1.717864
N	-0.101022	-2.155630	-2.950622

TS(E-F)[5]

Fe	0.366217	0.056109	-0.023165
N	-0.984639	-0.950800	1.194884
N	-0.627764	1.859113	0.349715
N	1.436713	-1.714678	-0.287467
N	1.821618	1.099363	-1.099284
C	-0.996268	-2.293790	1.442043
C	-0.286963	3.086588	-0.149885
C	-2.081804	-0.396164	1.792819
C	-1.772921	1.997564	1.083412
C	1.088864	-2.946433	0.195094
C	1.815797	2.438011	-1.371263
C	2.616689	-1.844551	-0.969403
C	2.936027	0.552266	-1.668418
C	-2.160077	-2.613626	2.245864
C	-1.270732	4.061321	0.290858
C	-2.829578	-1.441284	2.462690
C	-2.185745	3.389802	1.051255
C	2.097775	-3.913761	-0.204655
C	2.986891	2.762070	-2.163104
C	3.041653	-3.233487	-0.918628
C	3.680307	1.597709	-2.344406
H	-2.424846	-3.604702	2.593182
H	-1.252822	5.116902	0.049372
H	-3.746796	-1.291868	3.018401
H	-3.059236	3.791266	1.549807
H	2.078449	-4.969610	0.035666
H	3.241102	3.750550	-2.525228
H	3.939354	-3.627046	-1.379056
H	4.607849	1.453338	-2.884401
C	-0.040236	-3.211103	0.979710
C	0.836879	3.347731	-0.943019
C	3.300611	-0.800911	-1.602903
C	-2.437016	0.958277	1.744703
H	-0.187993	-4.246325	1.275596

H	0.974136	4.379592	-1.254990
H	4.223595	-1.071287	-2.108798
H	-3.347572	1.231052	2.270659
C	1.590851	1.541794	2.688138
C	2.562318	-0.357956	2.320349
C	2.515008	1.388781	3.688891
H	0.899526	2.349932	2.505252
N	3.126645	0.171378	3.440696
H	2.843652	-1.306015	1.887971
H	2.790227	2.007340	4.528858
H	3.860604	-0.249380	3.990782
N	1.633862	0.449614	1.848723
C	-0.890014	0.045814	-1.734158
H	-0.663931	0.952454	-2.303052
N	0.351064	-2.075191	-3.054282
N	-0.279845	-1.150132	-2.998789
C	-2.333727	-0.178767	-1.603836
C	-3.225639	0.904016	-1.702307
C	-2.839927	-1.438927	-1.232616
C	-4.577804	0.740514	-1.407265
H	-2.840512	1.882614	-1.974814
C	-4.193462	-1.609434	-0.973222
H	-2.152719	-2.272244	-1.130712
C	-5.065378	-0.517298	-1.050210
H	-5.251101	1.591218	-1.465404
H	-4.569130	-2.586835	-0.685178
H	-6.121328	-0.649050	-0.830174

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Fe	-0.267708	0.000048	-0.049223
N	-1.287231	-1.421748	-1.066856
N	-1.287315	1.422588	-1.065717
N	0.621345	-1.415955	1.083423
N	0.621315	1.415192	1.084479
C	-1.121064	-2.776620	-0.945780
C	-1.121237	2.777375	-0.943568
C	-2.204327	-1.234046	-2.067993
C	-2.204418	1.235623	-2.066990
C	0.514012	-2.772236	0.909366
C	0.513959	2.771605	0.911457
C	1.422618	-1.234559	2.183098
C	1.422609	1.232978	2.184002
C	-1.970956	-3.469484	-1.891692
C	-1.971214	3.470936	-1.888891
C	-2.646145	-2.512267	-2.585518
C	-2.646353	2.514227	-2.583468
C	1.292271	-3.467918	1.912789
C	1.292251	3.466539	1.915371
C	1.848461	-2.513978	2.709185
C	1.848468	2.512004	2.711034
H	-2.030840	-4.545628	-1.994012
H	-2.031178	4.547157	-1.990348
H	-3.374502	-2.639271	-3.376528
H	-3.374740	2.641811	-3.374355
H	1.377544	-4.544489	1.989710
H	1.377515	4.543053	1.993100
H	2.489809	-2.644125	3.571847
H	2.489834	2.641505	3.573780
C	-0.274080	-3.406122	-0.042718
C	-0.274219	3.406209	-0.040072
C	1.786218	-0.000983	2.714011
C	-2.639016	0.000962	-2.535659
H	-0.251797	-4.491757	-0.059384
H	-0.251989	4.491857	-0.055885
H	2.429847	-0.001299	3.588669
H	-3.368525	0.001262	-3.340033
C	-3.223320	-0.000304	1.088843
C	-1.762947	-0.001386	2.689847
C	-3.939571	-0.000912	2.256199
H	-3.573165	0.000326	0.069215

N	-2.994208	-0.001596	3.268133
H	-0.835404	-0.001797	3.240405
H	-4.998723	-0.000928	2.460182
H	-3.181442	-0.002156	4.259387
N	-1.873476	-0.000609	1.375333
C	0.944309	0.000559	-1.371896
H	0.463276	0.000942	-2.359935
C	2.380222	0.000568	-1.519085
C	3.271859	0.000153	-0.422796
C	2.934847	0.001089	-2.823195
C	4.646692	0.000263	-0.624985
H	2.872314	-0.000268	0.577955
C	4.309389	0.001203	-3.024687
H	2.259329	0.001414	-3.674783
C	5.169538	0.000789	-1.921916
H	5.317085	-0.000061	0.229969
H	4.714339	0.001610	-4.032707
H	6.245678	0.000876	-2.073768

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Fe	0.269302	0.007447	-0.076240
N	1.255099	1.451210	-1.078472
N	1.261279	-1.398299	-1.130351
N	-0.578056	1.400881	1.094640
N	-0.572549	-1.434473	1.043361
C	1.027353	2.800940	-0.995090
C	1.039386	-2.751589	-1.095906
C	2.219987	1.279893	-2.036116
C	2.225133	-1.188084	-2.081569
C	-0.556098	2.757848	0.896457
C	-0.545126	-2.783828	0.796189
C	-1.271214	1.193233	2.260456
C	-1.267100	-1.271765	2.215852
C	1.880429	3.506897	-1.927486
C	1.895376	-3.419257	-2.053176
C	2.629595	2.564157	-2.563643
C	2.639955	-2.450339	-2.655288
C	-1.285654	3.426582	1.952706
C	-1.271599	-3.492871	1.827637
C	-1.713465	2.457155	2.808225
C	-1.704092	-2.556148	2.717311
H	1.897473	4.581758	-2.055908
H	1.916339	-4.488545	-2.221784
H	3.384255	2.705032	-3.327073
H	3.393932	-2.560095	-3.424527
H	-1.422388	4.498100	2.024977
H	-1.405408	-4.566749	1.860795
H	-2.282557	2.567726	3.722575
H	-2.274349	-2.701966	3.626028
C	0.156450	3.412591	-0.101337
C	0.172294	-3.399167	-0.223517
C	-1.561913	-0.049946	2.809264
C	2.695746	0.054884	-2.486733
H	0.082655	4.495230	-0.138272
H	0.102777	-4.480094	-0.299981
H	-2.123545	-0.067622	3.738337
H	3.459634	0.070730	-3.258303
C	2.536465	1.074023	1.879797
C	2.469762	-1.091989	1.815999
C	3.524690	0.637885	2.722792
H	2.237547	2.079535	1.628222
N	3.469649	-0.744907	2.671254
H	2.195614	-2.108501	1.579170
H	4.240984	1.160765	3.336764
H	4.064320	-1.384233	3.176642
N	1.893472	-0.012277	1.327258
C	-1.000372	0.027729	-1.370373
H	-0.557788	0.049821	-2.374303
C	-2.437759	0.021887	-1.429746
C	-3.267873	-0.002041	-0.283496

C	-3.072971	0.040883	-2.698699
C	-4.651797	-0.006768	-0.405075
H	-2.813107	-0.016188	0.693614
C	-4.456693	0.035858	-2.817715
H	-2.450319	0.059647	-3.589630
C	-5.253136	0.011922	-1.667859
H	-5.269434	-0.025057	0.488875
H	-4.919038	0.050642	-3.800934
H	-6.336269	0.008064	-1.756040

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Fe	0.291403	0.006371	-0.031432
N	1.187839	1.459002	-1.106012
N	1.199020	-1.417661	-1.140442
N	-0.514845	1.411014	1.133835
N	-0.503866	-1.435403	1.100563
C	0.952863	2.807020	-1.039493
C	0.972218	-2.768787	-1.107485
C	2.091960	1.271874	-2.118917
C	2.100651	-1.199674	-2.149781
C	-0.532608	2.769280	0.917542
C	-0.513029	-2.788371	0.851162
C	-1.170475	1.202844	2.321245
C	-1.162263	-1.260148	2.292150
C	1.740688	3.498334	-2.034409
C	1.763748	-3.429937	-2.119603
C	2.459266	2.546968	-2.694051
C	2.475331	-2.457523	-2.756525
C	-1.240452	3.432024	1.987783
C	-1.216563	-3.481217	1.904881
C	-1.618877	2.463244	2.867451
C	-1.602372	-2.536097	2.807359
H	1.738155	4.569784	-2.187874
H	1.767035	-4.497108	-2.300830
H	3.163613	2.676570	-3.505845
H	3.178465	-2.562461	-3.572963
H	-1.402052	4.500439	2.050058
H	-1.372590	-4.551737	1.940773
H	-2.165274	2.571854	3.795581
H	-2.149956	-2.670653	3.731424
C	0.122454	3.425740	-0.113485
C	0.147653	-3.415469	-0.194981
C	-1.434638	-0.036351	2.889776
C	2.543665	0.043388	-2.584115
H	0.025713	4.505495	-0.164876
H	0.057139	-4.494233	-0.273155
H	-1.969571	-0.049194	3.834072
H	3.257215	0.056193	-3.402271
C	2.670060	1.094669	1.777155
C	2.625211	-1.073765	1.700797
C	3.706091	0.663451	2.562203
H	2.345959	2.097886	1.548390
N	3.663458	-0.720367	2.502752
H	2.348874	-2.091180	1.470044
H	4.448786	1.189319	3.141179
H	4.291485	-1.355939	2.971885
N	2.011720	0.003818	1.252210
C	-1.058074	0.015856	-1.402354
H	-0.599321	0.031059	-2.391146
C	-2.467859	0.008863	-1.385064
C	-3.270656	-0.009186	-0.204876
C	-3.176497	0.020056	-2.631080
C	-4.655228	-0.015457	-0.272249
H	-2.785158	-0.017737	0.758472
C	-4.560075	0.013555	-2.685485
H	-2.597211	0.034074	-3.551368
C	-5.319714	-0.004351	-1.506201
H	-5.231414	-0.029123	0.650402
H	-5.059336	0.022555	-3.651777
H	-6.405177	-0.009329	-1.549385

F[5]

Fe	0.333018	0.002227	-0.211465
N	1.310974	1.779139	-0.723824
N	1.854380	-1.103019	-1.113788
N	-0.996820	1.099292	0.955675
N	-0.495392	-1.770724	0.516924
C	0.923917	3.044010	-0.389046
C	1.940930	-2.463407	-1.170493
C	2.432488	1.871471	-1.498454
C	2.890004	-0.579629	-1.834397
C	-1.064603	2.463032	1.030946
C	-0.076823	-3.040004	0.211268
C	-2.057599	0.583346	1.646689
C	-1.629954	-1.864108	1.277745
C	1.843774	3.998561	-0.987474
C	3.096395	-2.830885	-1.966818
C	2.775364	3.274331	-1.672675
C	3.682822	-1.666606	-2.376891
C	-2.223082	2.833957	1.819162
C	-0.990433	-3.989879	0.818731
C	-2.838062	1.672957	2.196341
C	-1.947734	-3.266164	1.472569
H	1.778075	5.074854	-0.887201
H	3.410325	-3.845288	-2.179485
H	3.619252	3.643088	-2.242388
H	4.567572	-1.546616	-2.989607
H	-2.522353	3.849807	2.045553
H	-0.902414	-5.067052	0.749667
H	-3.735898	1.557412	2.790444
H	-2.790374	-3.638382	2.041803
C	-0.176633	3.356496	0.417250
C	1.047222	-3.354863	-0.558833
C	-2.348138	-0.779234	1.790036
C	3.150755	0.785881	-2.011524
H	-0.367577	4.412959	0.585266
H	1.246877	-4.412701	-0.706454
H	-3.236588	-1.021535	2.366221
H	4.023464	1.030044	-2.611307
C	2.716372	0.865953	1.987591
C	1.658603	-0.913649	2.618951
C	3.288341	0.486382	3.174198
H	2.951072	1.701541	1.346751
N	2.602480	-0.651250	3.565042
H	0.972917	-1.746014	2.659429
H	4.092086	0.901153	3.762324
H	2.771188	-1.191025	4.400781
N	1.707513	-0.013360	1.658259
C	-0.945585	-0.370731	-1.693629
H	-0.715636	-1.367125	-2.091932
C	-2.368126	-0.128573	-1.632925
C	-2.859205	1.188095	-1.479104
C	-3.305227	-1.184842	-1.708269
C	-4.223238	1.435598	-1.400892
H	-2.143202	1.999760	-1.419831
C	-4.671047	-0.938420	-1.615279
H	-2.936680	-2.201790	-1.812455
C	-5.131675	0.372664	-1.461981
H	-4.584307	2.452995	-1.281321
H	-5.378448	-1.761959	-1.661364
H	-6.198690	0.567006	-1.391578

TS(F-G)[oss]

C	-2.105504	-1.442938	0.738732
C	-0.973920	-1.729088	0.019180
C	-0.113113	0.093657	0.586210
Fe	1.771133	-0.197408	0.021522
N	1.609829	1.062531	-1.552421
C	1.671488	2.431225	-1.509408
C	1.474696	2.981793	-2.834327

C	1.288897	1.926618	-3.674484
C	1.384335	0.730568	-2.862658
C	1.849638	3.197404	-0.364554
C	1.970888	2.710160	0.930333
N	1.970334	1.385813	1.282912
C	2.059688	1.346423	2.652112
C	2.119905	2.692043	3.182111
C	2.072197	3.536694	2.113843
C	1.293532	-0.569524	-3.348826
C	1.477046	-1.722033	-2.592681
N	1.723100	-1.753730	-1.241032
C	1.912100	-3.076214	-0.918361
C	1.777203	-3.901727	-2.099011
C	1.496673	-3.063424	-3.135313
C	2.145769	-3.569608	0.360022
C	2.188261	-2.811523	1.525035
N	2.048245	-1.448881	1.584038
C	2.130979	-1.112494	2.911978
C	2.309740	-2.302481	3.718272
C	2.354635	-3.356044	2.856559
C	2.112460	0.185447	3.415441
H	1.472727	4.038703	-3.068659
H	1.876704	-4.979747	-2.112410
H	1.108674	1.936921	-4.742090
H	1.324309	-3.311017	-4.175144
H	2.095164	4.619018	2.109466
H	2.483458	-4.406977	3.082799
H	2.196988	2.938665	4.233559
H	2.400583	-2.309770	4.797200
H	1.856339	4.276040	-0.488472
H	2.266743	-4.644026	0.461611
H	2.185724	0.301585	4.492713
H	1.106247	-0.695032	-4.411111
H	-0.979271	-1.628023	-1.059549
H	-0.208233	-2.361850	0.441955
H	-2.155220	-1.615830	1.808702
N	3.803527	-0.116532	-0.220815
C	4.439191	-0.213801	-1.373182
C	4.761420	-0.005125	0.764950
H	3.970775	-0.317354	-2.339318
C	6.004745	-0.035905	0.191737
H	4.480962	0.089665	1.801651
H	6.997920	0.025327	0.607625
H	6.489642	-0.226537	-1.885716
N	5.782338	-0.170491	-1.168738
C	-0.939698	1.235773	0.167880
C	-1.309695	2.200111	1.125070
C	-1.333121	1.439059	-1.166093
C	-2.014674	3.343133	0.758374
H	-1.012508	2.053076	2.159728
C	-2.059320	2.568049	-1.530691
H	-1.075791	0.697442	-1.910580
C	-2.396117	3.528142	-0.573023
H	-2.274278	4.083890	1.509901
H	-2.357379	2.701386	-2.566450
H	-2.955962	4.413741	-0.861985
H	-0.167172	-0.056569	1.666306
C	-3.229641	-0.733440	0.116506
O	-3.413490	-0.637797	-1.086058
O	-4.011932	-0.152028	1.054678
C	-5.066762	0.711245	0.557302
H	-5.190425	1.455931	1.345790
H	-4.709357	1.199178	-0.350774
C	-6.346149	-0.047680	0.318913
C	-7.284273	-0.186908	1.347876
C	-6.605166	-0.638552	-0.924791
C	-8.464175	-0.902118	1.142615
H	-7.087970	0.271038	2.314521
C	-7.784735	-1.352978	-1.131867
H	-5.865020	-0.548314	-1.712661

C	-8.716485	-1.485937	-0.099985
H	-9.186118	-1.000550	1.948653
H	-7.977606	-1.806493	-2.100261
H	-9.635971	-2.041284	-0.263919

TS(F-G)^3

C	2.460133	-0.901752	-1.616239
C	1.300252	-1.496109	-1.239401
C	-0.238000	0.333488	-0.948992
Fe	-1.880434	-0.178648	-0.017640
N	-1.465923	0.918112	1.617383
C	-1.603014	2.276956	1.756009
C	-1.144407	2.690716	3.061368
C	-0.731724	1.566402	3.707567
C	-0.925603	0.463662	2.793930
C	-2.118061	3.136792	0.798357
C	-2.609128	2.745282	-0.437714
N	-2.650348	1.453854	-0.902990
C	-3.243595	1.504413	-2.141029
C	-3.596240	2.868428	-2.460534
C	-3.197280	3.637062	-1.409384
C	-0.546903	-0.843053	3.061417
C	-0.647480	-1.903780	2.174569
N	-1.178544	-1.838934	0.911850
C	-1.097266	-3.108246	0.395571
C	-0.483121	-3.997265	1.356327
C	-0.205629	-3.250967	2.459610
C	-1.558668	-3.496969	-0.852623
C	-2.176537	-2.657269	-1.769016
N	-2.407357	-1.315407	-1.593382
C	-3.051339	-0.882527	-2.725230
C	-3.237164	-1.984926	-3.640381
C	-2.691897	-3.083842	-3.049444
C	-3.448797	0.422113	-2.982146
H	-1.142262	3.713574	3.414657
H	-0.295651	-5.049664	1.187402
H	-0.315924	1.472125	4.702273
H	0.258807	-3.561476	3.386357
H	-3.285664	4.708352	-1.283552
H	-2.634768	-4.096374	-3.427498
H	-4.077862	3.178007	-3.379045
H	-3.719820	-1.906546	-4.605947
H	-2.147098	4.194510	1.037730
H	-1.436204	-4.538588	-1.131096
H	-3.935560	0.615598	-3.932630
H	-0.106444	-1.044897	4.032301
H	1.172165	-1.810944	-0.212642
H	0.586148	-1.865468	-1.963983
H	2.648053	-0.590846	-2.638626
N	-3.815615	-0.591201	0.849363
C	-4.644809	0.317562	1.323934
C	-4.422811	-1.817131	1.018503
H	-4.464411	1.381445	1.341798
C	-5.646798	-1.642049	1.608810
H	-3.933751	-2.725827	0.704166
H	-6.417973	-2.335632	1.904986
H	-6.561542	0.197069	2.212890
N	-5.773297	-0.276345	1.797099
C	0.619976	1.440851	-0.551993
C	0.793392	2.549444	-1.408122
C	1.328201	1.444593	0.667527
C	1.606389	3.622897	-1.051659
H	0.263354	2.562651	-2.357474
C	2.148084	2.509981	1.020508
H	1.257607	0.580570	1.314895
C	2.287179	3.610175	0.167894
H	1.713588	4.468030	-1.727295
H	2.686984	2.480059	1.963925
H	2.927471	4.442882	0.447183
H	-0.450547	0.353692	-2.022482

C	3.433566	-0.493793	-0.604847
O	3.434053	-0.836934	0.570330
O	4.359525	0.351742	-1.135846
C	5.304190	0.929838	-0.210872
H	5.498020	1.930396	-0.604261
H	4.823723	1.010714	0.765985
C	6.579618	0.128503	-0.130684
C	7.723290	0.547508	-0.817993
C	6.634304	-1.050668	0.626081
C	8.905500	-0.191845	-0.753506
H	7.686409	1.460598	-1.407712
C	7.813317	-1.791686	0.688948
H	5.741084	-1.378070	1.147874
C	8.952070	-1.364467	0.000974
H	9.786953	0.146988	-1.291305
H	7.845558	-2.704246	1.278347
H	9.870660	-1.942789	0.053688

TS(F-G')^{oss}

C	-2.256027	1.066691	-1.276739
C	-1.216974	0.232074	-1.593565
C	0.125010	0.896740	-0.036906
Fe	1.455643	-0.467023	0.026442
N	2.889723	0.753439	-0.728729
C	3.596186	1.702529	-0.035445
C	4.493954	2.405126	-0.926343
C	4.316047	1.869353	-2.165900
C	3.315061	0.833429	-2.028056
C	3.461609	1.982282	1.317599
C	2.573104	1.368815	2.190319
N	1.701941	0.361577	1.863348
C	0.969871	0.095236	2.993442
C	1.398348	0.957410	4.072134
C	2.397159	1.741279	3.576223
C	2.866336	0.017989	-3.061598
C	1.962795	-1.027015	-2.917174
N	1.342635	-1.389824	-1.743105
C	0.599834	-2.509699	-2.033288
C	0.751033	-2.858438	-3.427538
C	1.586810	-1.933780	-3.978044
C	-0.219893	-3.192255	-1.142840
C	-0.454830	-2.827979	0.176585
N	0.128953	-1.766494	0.815985
C	-0.397331	-1.748166	2.082646
C	-1.351963	-2.824781	2.243199
C	-1.379889	-3.501448	1.064017
C	-0.023334	-0.872148	3.094026
H	5.158917	3.204925	-0.626371
H	0.265730	-3.698655	-3.907688
H	4.807901	2.134731	-3.093240
H	1.934342	-1.863351	-5.001039
H	2.965428	2.510298	4.083686
H	-1.973753	-4.365553	0.795168
H	0.982897	0.946503	5.071804
H	-1.913908	-3.020336	3.147412
H	4.080844	2.777001	1.722052
H	-0.754199	-4.057048	-1.524007
H	-0.525621	-0.972404	4.051296
H	3.281541	0.186182	-4.050774
H	-0.563134	0.444504	-2.429941
H	-1.249811	-0.790712	-1.248503
H	-2.336691	2.068497	-1.683628
N	2.994426	-1.774471	0.569752
C	4.065214	-2.039844	-0.153888
C	3.078198	-2.537778	1.715000
H	4.296817	-1.602330	-1.112249
C	4.227798	-3.281049	1.679903
H	2.309205	-2.490527	2.469163
H	4.655837	-3.990599	2.370218
H	5.717152	-3.325167	0.141148

N	4.843964	-2.953317	0.483353
C	0.375304	2.327492	-0.264032
C	0.178924	3.230206	0.797121
C	0.859564	2.834532	-1.483214
C	0.493171	4.581160	0.659608
H	-0.196426	2.852375	1.744339
C	1.152563	4.185511	-1.629484
H	1.014340	2.154239	-2.312741
C	0.979858	5.064644	-0.555509
H	0.350554	5.257044	1.498728
H	1.528265	4.554835	-2.579863
H	1.217819	6.118844	-0.669158
H	-0.602078	0.735553	0.759921
C	-3.218056	0.677101	-0.244455
O	-3.172063	-0.350330	0.416388
O	-4.180784	1.625460	-0.090167
C	-5.194920	1.342551	0.902481
H	-4.727554	0.817534	1.738175
H	-5.533980	2.328210	1.228720
C	-6.337337	0.544649	0.325863
C	-6.289922	-0.855674	0.299049
C	-7.453454	1.198697	-0.207315
C	-7.344208	-1.583900	-0.251207
H	-5.414910	-1.359435	0.695763
C	-8.508677	0.471197	-0.758104
H	-7.494442	2.285283	-0.189497
C	-8.455318	-0.923384	-0.780209
H	-7.299007	-2.669495	-0.266852
H	-9.370774	0.991161	-1.166819
H	-9.276448	-1.493046	-1.206846

TS(F-G')[3]

C	-2.461050	1.438167	-1.452417
C	-1.420216	0.697354	-1.900857
C	0.268469	1.019478	-0.160659
Fe	1.523606	-0.443468	0.065956
N	3.151398	0.680182	-0.237826
C	3.720973	1.581596	0.631712
C	4.840288	2.236385	0.003619
C	4.945648	1.717627	-1.253075
C	3.880166	0.756798	-1.400119
C	3.305442	1.818763	1.933932
C	2.269561	1.148696	2.567767
N	1.501521	0.165886	1.994974
C	0.615278	-0.241882	2.960020
C	0.842914	0.494520	4.183870
C	1.864515	1.361437	3.938812
C	3.602386	0.079908	-2.580309
C	2.525335	-0.770700	-2.783843
N	1.595969	-1.115403	-1.836161
C	0.745877	-2.007766	-2.443021
C	1.131360	-2.206153	-3.822576
C	2.237999	-1.441600	-4.033189
C	-0.294875	-2.677187	-1.814664
C	-0.635089	-2.538002	-0.475488
N	-0.010495	-1.705403	0.419358
C	-0.664985	-1.868222	1.613132
C	-1.721467	-2.842708	1.471813
C	-1.704825	-3.256313	0.175279
C	-0.377242	-1.197155	2.793482
H	5.454350	2.992799	0.475030
H	0.616214	-2.855669	-4.518585
H	5.661479	1.965180	-2.026466
H	2.820074	-1.331976	-4.939322
H	2.314643	2.082254	4.609236
H	-2.356885	-3.966769	-0.315858
H	0.278877	0.357659	5.097654
H	-2.391020	-3.143026	2.267197
H	3.837742	2.576058	2.500359
H	-0.883920	-3.365259	-2.412528

H	-1.001351	-1.419411	3.653285
H	4.265693	0.255838	-3.421413
H	-0.764971	1.055123	-2.686333
H	-1.328425	-0.337773	-1.609639
H	-2.638516	2.456282	-1.781307
N	2.843957	-2.068621	0.621722
C	3.795711	-1.980591	1.530408
C	2.875008	-3.354420	0.126070
H	4.031393	-1.098205	2.105182
C	3.870019	-4.057761	0.751499
H	2.180972	-3.670502	-0.636657
H	4.214338	-5.075271	0.653711
H	5.215861	-3.364206	2.266545
N	4.447376	-3.167860	1.642600
C	0.598282	2.406935	-0.395190
C	0.058931	3.410089	0.443448
C	1.403844	2.827917	-1.477944
C	0.340144	4.757311	0.233616
H	-0.575515	3.108111	1.272632
C	1.682264	4.172162	-1.687253
H	1.794815	2.080671	-2.157842
C	1.159437	5.146990	-0.829015
H	-0.079914	5.506558	0.900159
H	2.307676	4.466953	-2.526210
H	1.380430	6.198020	-0.994191
H	-0.528153	0.879308	0.569115
C	-3.320575	0.909216	-0.395395
O	-3.156921	-0.149790	0.195882
O	-4.344546	1.763396	-0.111181
C	-5.244388	1.343883	0.937933
H	-4.669230	0.813435	1.700204
H	-5.631899	2.277720	1.351989
C	-6.371353	0.487939	0.413632
C	-6.204162	-0.893364	0.242170
C	-7.599300	1.070179	0.081275
C	-7.250220	-1.671498	-0.252251
H	-5.245170	-1.339052	0.483630
C	-8.646853	0.292316	-0.413209
H	-7.734273	2.141418	0.211658
C	-8.473409	-1.082188	-0.580587
H	-7.111355	-2.741673	-0.381205
H	-9.595723	0.757829	-0.665602
H	-9.287389	-1.691497	-0.964125

TS(F-P)^{css}

C	2.053341	-1.569002	-0.324890
C	0.946560	-1.696843	0.474798
C	0.179573	0.000475	-0.449289
Fe	-1.772622	-0.201706	-0.008569
N	-1.729514	1.323225	1.323460
C	-1.691686	2.666996	1.048809
C	-1.633261	3.427969	2.279497
C	-1.636500	2.524579	3.298137
C	-1.701916	1.211935	2.688329
C	-1.703350	3.230771	-0.222206
C	-1.756310	2.525804	-1.418916
N	-1.811509	1.159256	-1.528140
C	-1.834816	0.877147	-2.870796
C	-1.797176	2.106287	-3.635033
C	-1.751267	3.128186	-2.734548
C	-1.725504	0.015415	3.394870
C	-1.814904	-1.253452	2.836341
N	-1.860393	-1.531285	1.492706
C	-1.989937	-2.896128	1.390764
C	-2.015415	-3.496457	2.707675
C	-1.900841	-2.478258	3.604079
C	-2.061326	-3.609439	0.198578
C	-2.015600	-3.053415	-1.076527
N	-1.912227	-1.711671	-1.345428
C	-1.925642	-1.593687	-2.711876

C	-2.023430	-2.902452	-3.325290
C	-2.083673	-3.808392	-2.310298
C	-1.879204	-0.397905	-3.421460
H	-1.589488	4.508283	2.335461
H	-2.105736	-4.558038	2.900345
H	-1.600748	2.709680	4.364338
H	-1.881863	-2.530960	4.685300
H	-1.711982	4.193221	-2.925294
H	-2.167416	-4.886123	-2.371935
H	-1.808586	2.161397	-4.716333
H	-2.050346	-3.083693	-4.392438
H	-1.652049	4.313468	-0.285486
H	-2.150180	-4.689425	0.269260
H	-1.891299	-0.467291	-4.505305
H	-1.692514	0.077913	4.478631
H	0.979500	-1.368305	1.506682
H	0.167107	-2.392443	0.210300
H	2.072172	-1.974692	-1.330858
N	-3.810095	-0.085538	0.029003
C	-4.522357	1.026350	0.027386
C	-4.703648	-1.137782	0.046934
H	-4.122284	2.027286	0.013178
C	-5.981704	-0.646755	0.056996
H	-4.359665	-2.158890	0.052387
H	-6.944928	-1.131561	0.072809
H	-6.600980	1.403292	0.045464
N	-5.849021	0.731099	0.043778
C	0.993463	1.182766	-0.133916
C	1.506958	1.967979	-1.184121
C	1.240296	1.596006	1.186862
C	2.207351	3.143082	-0.926476
H	1.326413	1.655040	-2.208713
C	1.960269	2.756898	1.447738
H	0.863715	0.996349	2.005606
C	2.439479	3.538620	0.393827
H	2.578912	3.745113	-1.751333
H	2.141438	3.056036	2.475764
H	2.994597	4.449999	0.599882
H	0.301719	-0.298922	-1.491632
C	3.198024	-0.751910	0.097999
O	3.415481	-0.401264	1.245352
O	3.949351	-0.387421	-0.966140
C	5.012242	0.563541	-0.697355
H	5.114909	1.112875	-1.635207
H	4.672807	1.243215	0.086141
C	6.300745	-0.123169	-0.326420
C	6.580873	-0.446642	1.007663
C	7.229200	-0.458602	-1.318229
C	7.770981	-1.093367	1.339199
H	5.851279	-0.201634	1.772016
C	8.419832	-1.106130	-0.988160
H	7.016479	-0.208778	-2.355068
C	8.692622	-1.424199	0.343315
H	7.979968	-1.339268	2.376726
H	9.133707	-1.359150	-1.767213
H	9.620115	-1.926683	0.604009

TS(F-P')^{css}

C	-2.145946	0.961544	-1.238189
C	-1.146039	0.105215	-1.615598
C	0.046392	0.905991	-0.096170
Fe	1.438421	-0.488649	0.029031
N	2.834757	0.703968	-0.833550
C	3.500505	1.756677	-0.256797
C	4.385675	2.376164	-1.220198
C	4.244924	1.682106	-2.383516
C	3.277216	0.635415	-2.127498
C	3.357604	2.176504	1.060983
C	2.512618	1.605109	2.005265
N	1.688903	0.530604	1.780850

C	1.009630	0.308134	2.952224
C	1.421561	1.270436	3.951319
C	2.356282	2.071601	3.365266
C	2.860072	-0.300782	-3.066983
C	1.958238	-1.331866	-2.836942
N	1.303718	-1.570644	-1.652810
C	0.544857	-2.697914	-1.857031
C	0.718577	-3.178838	-3.210596
C	1.590093	-2.328345	-3.820295
C	-0.295060	-3.283615	-0.914869
C	-0.496091	-2.821493	0.380861
N	0.127695	-1.731595	0.931160
C	-0.335780	-1.637118	2.217241
C	-1.289269	-2.695316	2.484997
C	-1.385127	-3.433177	1.347166
C	0.062145	-0.688984	3.152615
H	5.018594	3.230585	-1.016350
H	0.227202	-4.051058	-3.622945
H	4.742761	1.845675	-3.331081
H	1.965909	-2.361557	-4.835173
H	2.893585	2.906841	3.796513
H	-1.999276	-4.303912	1.156188
H	1.039604	1.310587	4.963671
H	-1.806113	-2.835978	3.425779
H	3.943161	3.035455	1.374377
H	-0.849653	-4.165008	-1.222386
H	-0.399651	-0.740660	4.134250
H	3.294374	-0.235379	-4.060376
H	-0.503185	0.319165	-2.459382
H	-1.191170	-0.921823	-1.287089
N	2.965437	-1.710162	0.638389
C	4.134265	-1.316780	1.109746
C	2.967826	-3.090578	0.652377
H	4.448880	-0.292874	1.231238
C	4.165884	-3.536615	1.142547
H	2.113443	-3.651045	0.310389
H	4.557857	-4.527415	1.309186
H	5.829681	-2.364858	1.810134
N	4.896177	-2.396025	1.429501
C	0.297294	2.330377	-0.378707
C	0.087068	3.279839	0.637119
C	0.815958	2.774846	-1.607792
C	0.415565	4.620308	0.445590
H	-0.309108	2.947301	1.592641
C	1.117898	4.116408	-1.810763
H	0.998094	2.053909	-2.396645
C	0.927493	5.044004	-0.781594
H	0.263108	5.334563	1.250241
H	1.521311	4.438431	-2.766622
H	1.175222	6.090407	-0.938198
H	-0.641725	0.772921	0.739466
H	-2.207464	1.976987	-1.611189
C	-3.124091	0.556546	-0.218956
O	-3.128312	-0.510137	0.372929
O	-4.028630	1.545006	-0.002431
C	-5.059564	1.255378	0.974321
H	-5.353536	2.237970	1.349120
H	-4.617723	0.668262	1.781927
C	-6.232068	0.539900	0.353434
C	-6.268001	-0.859577	0.297920
C	-7.291545	1.271802	-0.194394
C	-7.349069	-1.511477	-0.294754
H	-5.436272	-1.424171	0.705648
C	-8.372764	0.620823	-0.788225
H	-7.267403	2.358256	-0.153936
C	-8.402929	-0.773921	-0.838462
H	-7.369031	-2.597191	-0.332419
H	-9.190551	1.200020	-1.208034
H	-9.244934	-1.283900	-1.298477

G^{oss}

C	2.468204	-0.046294	-1.136215
C	1.220738	-0.545306	-0.500942
C	0.028498	0.383415	-0.824961
Fe	-1.722528	-0.350840	-0.025899
N	-1.748438	0.939230	1.525613
C	-2.327838	2.182386	1.527187
C	-2.088844	2.841424	2.792261
C	-1.352154	1.983506	3.549901
C	-1.153051	0.794003	2.752063
C	-3.023038	2.750100	0.471095
C	-3.189464	2.181411	-0.784750
N	-2.728037	0.950534	-1.174458
C	-3.036766	0.825682	-2.506675
C	-3.711658	2.013661	-2.972482
C	-3.817361	2.849343	-1.899729
C	-0.492372	-0.346993	3.187236
C	-0.379294	-1.521171	2.455494
N	-0.853242	-1.710724	1.179060
C	-0.572501	-3.015671	0.857320
C	0.090361	-3.667985	1.962515
C	0.221032	-2.737422	2.949528
C	-0.827489	-3.622606	-0.365195
C	-1.369081	-2.993216	-1.478498
N	-1.785807	-1.687731	-1.530439
C	-2.215351	-1.473646	-2.818391
C	-2.055439	-2.676268	-3.603471
C	-1.540914	-3.622307	-2.769157
C	-2.775625	-0.293597	-3.287607
H	-2.435013	3.835882	3.042440
H	0.419076	-4.699382	1.961170
H	-0.972068	2.123454	4.553684
H	0.675072	-2.848019	3.925810
H	-4.261721	3.835356	-1.855317
H	-1.287577	-4.651081	-2.991324
H	-4.059528	2.168702	-3.985727
H	-2.317826	-2.769404	-4.649527
H	-3.423259	3.747840	0.619297
H	-0.538968	-4.663514	-0.472912
H	-3.071177	-0.257430	-4.331441
H	-0.061028	-0.331667	4.183021
H	1.386450	-0.635570	0.572842
H	0.985400	-1.545650	-0.883252
H	2.528541	0.066588	-2.214587
N	-3.638781	-1.085441	0.662355
C	-3.985464	-1.265465	1.921621
C	-4.716666	-1.455621	-0.112310
H	-3.358625	-1.066456	2.777192
C	-5.738454	-1.869398	0.700636
H	-4.671288	-1.394052	-1.188393
H	-6.733317	-2.230956	0.493323
H	-5.758152	-1.963675	2.840356
N	-5.256014	-1.742562	1.993312
C	0.263467	1.816453	-0.488715
C	-0.180151	2.823097	-1.362892
C	0.929244	2.217666	0.683453
C	0.001603	4.172841	-1.068779
H	-0.683982	2.536235	-2.281745
C	1.110298	3.565369	0.981234
H	1.308674	1.468070	1.367670
C	0.641507	4.553532	0.111675
H	-0.358213	4.927540	-1.763978
H	1.621739	3.844988	1.898709
H	0.784033	5.605179	0.346269
H	-0.207123	0.297779	-1.888397
C	3.593104	0.401317	-0.348057
O	3.665524	0.346259	0.877165
O	4.587239	0.906168	-1.134299
C	5.761390	1.388520	-0.444227
H	6.147714	2.182924	-1.086883

H	5.454649	1.808688	0.515845
C	6.789696	0.299849	-0.261838
C	7.818109	0.138262	-1.196522
C	6.719473	-0.574057	0.831606
C	8.764530	-0.875805	-1.045985
H	7.876833	0.813232	-2.047214
C	7.663936	-1.588700	0.982731
H	5.911820	-0.456184	1.546242
C	8.688503	-1.741896	0.045764
H	9.559804	-0.988338	-1.777853
H	7.601626	-2.260565	1.834570
H	9.424971	-2.531714	0.166913

G[3]

C	2.466916	-0.412472	-1.038519
C	1.221419	-0.784206	-0.328256
C	0.154972	0.267534	-0.708032
Fe	-1.744235	-0.324631	-0.020270
N	-1.837918	1.052906	1.446299
C	-2.278186	2.351548	1.351004
C	-2.117359	3.027410	2.617342
C	-1.569399	2.123926	3.475743
C	-1.401939	0.893061	2.735629
C	-2.798893	2.939949	0.208941
C	-2.908819	2.314755	-1.026313
N	-2.543081	1.019015	-1.291895
C	-2.771134	0.821390	-2.630490
C	-3.296245	2.029055	-3.226837
C	-3.389049	2.953223	-2.228701
C	-0.877812	-0.274656	3.273084
C	-0.738050	-1.480159	2.599218
N	-1.061333	-1.702965	1.284866
C	-0.800425	-3.032246	1.048576
C	-0.297940	-3.663357	2.246730
C	-0.250786	-2.698233	3.206660
C	-0.964848	-3.677939	-0.169113
C	-1.392395	-3.064353	-1.340504
N	-1.746230	-1.742617	-1.456414
C	-2.091773	-1.552277	-2.770992
C	-1.941897	-2.787089	-3.507374
C	-1.515251	-3.727342	-2.617992
C	-2.549032	-0.362521	-3.322982
H	-2.381251	4.060700	2.801384
H	-0.015077	-4.705414	2.322511
H	-1.293859	2.260418	4.513641
H	0.075747	-2.785549	4.234980
H	-3.734671	3.977316	-2.287210
H	-1.294777	-4.772327	-2.794381
H	-3.557624	2.137277	-4.271814
H	-2.148156	-2.903572	-4.563713
H	-3.101013	3.980143	0.273462
H	-0.713161	-4.732704	-0.216950
H	-2.775443	-0.364528	-4.384806
H	-0.569934	-0.248619	4.313664
H	1.395625	-0.817868	0.747876
H	0.870319	-1.766004	-0.651815
H	2.519593	-0.490620	-2.120138
N	-3.788437	-0.942950	0.505614
C	-4.793840	-0.119855	0.731566
C	-4.270300	-2.223136	0.679522
H	-4.745432	0.956847	0.678337
C	-5.596576	-2.169244	1.017565
H	-3.627530	-3.079403	0.549146
H	-6.324743	-2.934968	1.234264
H	-6.818166	-0.427368	1.264034
N	-5.914890	-0.821384	1.046602
C	0.464709	1.679603	-0.362519
C	0.186228	2.702500	-1.284561
C	1.023715	2.047082	0.874206
C	0.426357	4.040328	-0.978532

H	-0.235451	2.438649	-2.250643
C	1.264732	3.382169	1.182729
H	1.271846	1.280236	1.597289
C	0.961074	4.389167	0.262286
H	0.194451	4.809870	-1.710995
H	1.692077	3.638004	2.148595
H	1.149732	5.431382	0.506636
H	-0.070117	0.187174	-1.773658
C	3.571596	0.218146	-0.355198
O	3.656661	0.368305	0.860866
O	4.536314	0.627012	-1.229384
C	5.700349	1.252524	-0.644672
H	6.050239	1.946926	-1.411995
H	5.388750	1.809106	0.241630
C	6.770393	0.242484	-0.311140
C	7.790344	-0.033273	-1.228224
C	6.747262	-0.446787	0.909121
C	8.773970	-0.979058	-0.936967
H	7.813178	0.498651	-2.176530
C	7.728987	-1.392903	1.201209
H	5.946219	-0.242438	1.611551
C	8.744444	-1.661099	0.280254
H	9.562053	-1.181319	-1.657239
H	7.703016	-1.921069	2.150567
H	9.509983	-2.396976	0.511168

G'^{oss}

C	-2.295713	1.367018	-1.043845
C	-1.078248	0.536417	-1.227991
C	-0.037478	0.926355	-0.146306
Fe	1.433009	-0.478708	0.014735
N	2.892229	0.652058	-0.804651
C	3.723717	1.529048	-0.150217
C	4.594546	2.190151	-1.095016
C	4.272403	1.710109	-2.328202
C	3.211606	0.745813	-2.135405
C	3.720417	1.769310	1.214123
C	2.829718	1.210480	2.120483
N	1.846554	0.303906	1.815407
C	1.153387	0.077616	2.977585
C	1.714543	0.867777	4.047871
C	2.762838	1.561486	3.517904
C	2.632262	-0.004602	-3.149488
C	1.678066	-0.995803	-2.962034
N	1.116024	-1.351100	-1.759345
C	0.282047	-2.412385	-2.024807
C	0.317615	-2.731074	-3.430891
C	1.173181	-1.844279	-4.014615
C	-0.523937	-3.061058	-1.098922
C	-0.651625	-2.699230	0.234418
N	0.052732	-1.695348	0.846878
C	-0.408549	-1.638553	2.138265
C	-1.436330	-2.636751	2.344822
C	-1.577967	-3.303066	1.167455
C	0.086149	-0.801061	3.127110
H	5.337199	2.932410	-0.832467
H	-0.251391	-3.525530	-3.896443
H	4.700147	1.972652	-3.287454
H	1.454501	-1.765830	-5.057075
H	3.427503	2.259542	4.010361
H	-2.253596	-4.113728	0.927250
H	1.348261	0.873813	5.066540
H	-1.967255	-2.790067	3.275402
H	4.430612	2.495587	1.596096
H	-1.141930	-3.877112	-1.459637
H	-0.371377	-0.864149	4.109403
H	2.982024	0.166205	-4.162895
H	-0.665866	0.663482	-2.232162
H	-1.342267	-0.511344	-1.093467
H	-2.402169	2.334916	-1.520862

N	2.941763	-1.986518	0.446167
C	4.186902	-1.970684	0.010893
C	2.794925	-3.127161	1.206869
H	4.621219	-1.204613	-0.611723
C	3.979999	-3.813807	1.230174
H	1.852108	-3.361867	1.674603
H	4.277514	-4.735190	1.705731
H	5.819836	-3.290270	0.267899
N	4.855152	-3.065735	0.461493
C	0.483081	2.317789	-0.255938
C	0.608119	3.113448	0.895052
C	0.873383	2.883179	-1.482406
C	1.127008	4.405497	0.832071
H	0.301404	2.701719	1.852459
C	1.396279	4.171467	-1.549964
H	0.795674	2.292249	-2.390113
C	1.531140	4.941223	-0.391382
H	1.215368	4.994106	1.741757
H	1.705098	4.575756	-2.510780
H	1.938823	5.947132	-0.444709
H	-0.512473	0.788794	0.825087
C	-3.277843	0.976788	-0.058940
O	-3.209083	-0.033037	0.637623
O	-4.305336	1.872280	0.023135
C	-5.348146	1.549927	0.969634
H	-4.895055	1.078026	1.844202
H	-5.767772	2.518740	1.250120
C	-6.407001	0.664377	0.360220
C	-6.270281	-0.730330	0.375681
C	-7.533309	1.230769	-0.246816
C	-7.246758	-1.538804	-0.205350
H	-5.386433	-1.166003	0.829322
C	-8.510860	0.423042	-0.828391
H	-7.643609	2.312545	-0.262532
C	-8.368745	-0.965311	-0.807799
H	-7.132433	-2.619365	-0.187444
H	-9.381772	0.875781	-1.294456
H	-9.129168	-1.597521	-1.258272

G'[3]

C	-2.289701	1.359949	-0.995139
C	-1.092503	0.536609	-1.273572
C	-0.083881	0.992456	-0.198877
Fe	1.433743	-0.475265	0.050324
N	2.888982	0.626889	-0.794375
C	3.749780	1.470560	-0.137359
C	4.630944	2.113077	-1.085287
C	4.281910	1.658115	-2.319831
C	3.199233	0.720629	-2.127293
C	3.751198	1.721304	1.225957
C	2.828634	1.221257	2.132558
N	1.812454	0.349313	1.834334
C	1.073954	0.202114	2.982074
C	1.639583	1.011142	4.037343
C	2.736698	1.628408	3.515215
C	2.604789	-0.018331	-3.141147
C	1.657169	-1.013021	-2.943093
N	1.120967	-1.365027	-1.728361
C	0.320061	-2.455819	-1.960624
C	0.349470	-2.799847	-3.363610
C	1.164225	-1.895721	-3.975450
C	-0.467484	-3.096569	-1.013563
C	-0.623940	-2.688776	0.302810
N	0.040203	-1.644778	0.894455
C	-0.470312	-1.531585	2.163424
C	-1.490984	-2.532837	2.377080
C	-1.572908	-3.261077	1.231949
C	-0.014961	-0.648188	3.131129
H	5.396846	2.830655	-0.821497
H	-0.201427	-3.619653	-3.806296

H	4.707811	1.916684	-3.280753
H	1.430702	-1.826980	-5.022350
H	3.419541	2.314001	4.000056
H	-2.228023	-4.092093	1.005500
H	1.243934	1.074088	5.042843
H	-2.056650	-2.646852	3.292431
H	4.486314	2.425636	1.601323
H	-1.064928	-3.937959	-1.349416
H	-0.509678	-0.664038	4.096820
H	2.949531	0.152515	-4.156058
H	-0.701739	0.686059	-2.282473
H	-1.325437	-0.517416	-1.140601
H	-2.356689	2.385652	-1.340930
N	2.916946	-1.994594	0.481897
C	3.863167	-2.405880	-0.337895
C	3.055882	-2.711310	1.650275
H	4.026781	-2.038339	-1.339531
C	4.112127	-3.576373	1.531584
H	2.386812	-2.548816	2.481177
H	4.542265	-4.298017	2.208196
H	5.402646	-3.848063	-0.155044
N	4.616230	-3.369747	0.258573
C	0.489767	2.350745	-0.349570
C	0.684010	3.160512	0.783989
C	0.886391	2.871321	-1.594941
C	1.274902	4.417722	0.685536
H	0.372258	2.785870	1.754757
C	1.479867	4.126009	-1.696707
H	0.755282	2.271196	-2.489403
C	1.683431	4.907426	-0.556237
H	1.415892	5.016634	1.581969
H	1.790526	4.494978	-2.670959
H	2.146938	5.886980	-0.636995
H	-0.534998	0.877192	0.786139
C	-3.262394	0.897407	-0.035077
O	-3.216917	-0.178496	0.557678
O	-4.267618	1.806360	0.151302
C	-5.310700	1.410529	1.066704
H	-4.864004	0.840129	1.884101
H	-5.707713	2.353501	1.450073
C	-6.393976	0.615804	0.379187
C	-6.292462	-0.776529	0.256505
C	-7.507872	1.266572	-0.162606
C	-7.291106	-1.499797	-0.394970
H	-5.417268	-1.275448	0.658817
C	-8.507471	0.544369	-0.814951
H	-7.590892	2.347089	-0.071356
C	-8.400488	-0.842414	-0.931483
H	-7.203852	-2.579384	-0.484274
H	-9.368319	1.062238	-1.229132
H	-9.178274	-1.408236	-1.437280

TS(G-P)^{oss}

C	2.368639	-0.761633	-0.852405
C	1.139785	-0.960981	-0.067265
C	0.280201	0.200731	-0.637133
Fe	-1.737830	-0.340068	0.017778
N	-1.809441	1.089974	1.439805
C	-2.186485	2.398382	1.258305
C	-2.087058	3.123767	2.507155
C	-1.640206	2.239856	3.439965
C	-1.481026	0.969266	2.763090
C	-2.577565	2.966628	0.056970
C	-2.599700	2.324343	-1.176106
N	-2.269008	1.014374	-1.393718
C	-2.360268	0.809024	-2.745680
C	-2.754131	2.032604	-3.406764
C	-2.914860	2.970411	-2.429156
C	-1.095117	-0.215299	3.380663
C	-1.041504	-1.454678	2.757086

N	-1.316085	-1.691777	1.428138
C	-1.202322	-3.052635	1.251363
C	-0.852232	-3.686358	2.500023
C	-0.740450	-2.695513	3.429911
C	-1.341261	-3.725756	0.045103
C	-1.561395	-3.125041	-1.189228
N	-1.727356	-1.779973	-1.392251
C	-1.880410	-1.614094	-2.748904
C	-1.790983	-2.893155	-3.420344
C	-1.604321	-3.831740	-2.451808
C	-2.148479	-0.409110	-3.385277
H	-2.318412	4.174082	2.628549
H	-0.700934	-4.750488	2.629361
H	-1.434857	2.410525	4.489096
H	-0.483907	-2.781660	4.478113
H	-3.204579	4.008241	-2.532427
H	-1.495804	-4.903097	-2.563045
H	-2.895033	2.140739	-4.474686
H	-1.874602	-3.035393	-4.490300
H	-2.840021	4.019746	0.069758
H	-1.218005	-4.804252	0.060545
H	-2.247985	-0.427882	-4.466346
H	-0.854780	-0.176525	4.438607
H	1.309900	-0.863324	1.004144
H	0.666395	-1.916957	-0.278066
H	2.397229	-1.060611	-1.895028
N	-3.800556	-0.617596	0.286462
C	-4.397338	-0.639218	1.462749
C	-4.761274	-0.888443	-0.663971
H	-3.914869	-0.464958	2.411923
C	-5.968008	-1.077048	-0.044383
H	-4.509253	-0.923415	-1.711980
H	-6.952306	-1.302534	-0.423351
H	-6.396879	-0.990718	2.052206
N	-5.718756	-0.916544	1.308706
C	0.633730	1.591583	-0.301114
C	0.505354	2.592779	-1.280903
C	1.067975	1.976644	0.980184
C	0.775812	3.927080	-0.990644
H	0.175689	2.313043	-2.277540
C	1.336563	3.309428	1.272355
H	1.187239	1.227294	1.751651
C	1.188223	4.293880	0.291848
H	0.662230	4.680503	-1.765944
H	1.661820	3.581321	2.272622
H	1.399097	5.334486	0.523978
H	0.118586	0.068439	-1.704938
C	3.470424	0.020690	-0.342314
O	3.584678	0.403430	0.818168
O	4.395267	0.279098	-1.311779
C	5.558106	1.028130	-0.892773
H	5.873600	1.563279	-1.791338
H	5.254203	1.743877	-0.126241
C	6.657626	0.123583	-0.394369
C	7.649602	-0.328925	-1.271256
C	6.690613	-0.291455	0.943738
C	8.660836	-1.179988	-0.824570
H	7.628386	-0.010291	-2.310861
C	7.700331	-1.142615	1.391607
H	5.910924	0.047606	1.617507
C	8.687571	-1.588361	0.509821
H	9.426727	-1.521714	-1.515526
H	7.717811	-1.457859	2.431410
H	9.474842	-2.249759	0.861437

TS(G-P)^3

C	-2.458232	-0.802695	0.834295
C	-1.226499	-0.994413	0.041521
C	-0.347572	0.130119	0.610107
Fe	1.766592	-0.297054	0.013502

N	1.870107	1.184612	-1.339257
C	2.316686	2.462129	-1.108036
C	2.213677	3.247908	-2.316678
C	1.685171	2.435472	-3.272090
C	1.482435	1.143948	-2.655073
C	2.750306	2.956063	0.112202
C	2.726331	2.261022	1.312220
N	2.331428	0.957129	1.468692
C	2.365306	0.699165	2.816585
C	2.783706	1.882240	3.534679
C	3.024018	2.843994	2.600487
C	1.020127	0.014780	-3.316734
C	0.953857	-1.255454	-2.761576
N	1.268140	-1.569316	-1.462239
C	1.180594	-2.936514	-1.364369
C	0.795162	-3.500277	-2.638485
C	0.636860	-2.457522	-3.499376
C	1.356438	-3.674835	-0.202593
C	1.576114	-3.139645	1.059498
N	1.728403	-1.804121	1.339862
C	1.845312	-1.705312	2.705756
C	1.749665	-3.016963	3.304895
C	1.600635	-3.906541	2.284076
C	2.104044	-0.532397	3.402834
H	2.493699	4.290167	-2.396170
H	0.652808	-4.556922	-2.824893
H	1.449512	2.668279	-4.302508
H	0.348519	-2.480673	-4.542369
H	3.354275	3.863540	2.751494
H	1.498632	-4.982785	2.337190
H	2.889223	1.944027	4.610132
H	1.808324	-3.213363	4.367715
H	3.062375	3.994738	0.145338
H	1.245228	-4.752035	-0.274860
H	2.170915	-0.596731	4.484185
H	0.746406	0.121164	-4.361532
H	-1.406065	-0.883149	-1.028056
H	-0.762247	-1.961998	0.227265
H	-2.488374	-1.122695	1.870675
N	3.888235	-0.733383	-0.380732
C	4.498663	-0.600166	-1.540623
C	4.826938	-1.194616	0.515941
H	4.038247	-0.254923	-2.454026
C	6.032618	-1.343069	-0.119045
H	4.562314	-1.382287	1.545379
H	7.001157	-1.672574	0.223175
H	6.490030	-0.949932	-2.173157
N	5.806927	-0.960747	-1.430410
C	-0.649850	1.537968	0.304223
C	-0.437322	2.521272	1.289483
C	-1.108881	1.962387	-0.956860
C	-0.647062	3.870628	1.022667
H	-0.092750	2.213384	2.272624
C	-1.316860	3.311197	-1.224819
H	-1.299890	1.229179	-1.729241
C	-1.082690	4.275367	-0.240990
H	-0.469192	4.607041	1.802370
H	-1.664363	3.611910	-2.209463
H	-1.246254	5.328296	-0.454869
H	-0.158462	-0.019123	1.672544
C	-3.548275	0.000611	0.343257
O	-3.656069	0.420244	-0.806777
O	-4.480560	0.238479	1.314807
C	-5.632428	1.009042	0.910515
H	-5.944228	1.531218	1.818218
H	-5.319956	1.735808	0.157764
C	-6.743673	0.129019	0.393234
C	-7.762002	-0.299556	1.251531
C	-6.762212	-0.286257	-0.945290
C	-8.784960	-1.126848	0.786707

H	-7.752295	0.019044	2.291351
C	-7.783103	-1.113992	-1.411117
H	-5.962780	0.035087	-1.604517
C	-8.796856	-1.535760	-0.547598
H	-9.571146	-1.449907	1.463790
H	-7.788974	-1.429551	-2.451021
H	-9.592858	-2.178823	-0.913399

TS(G'-P')^{oss}

C	-2.195795	1.336835	-0.984586
C	-1.025003	0.491639	-1.268156
C	-0.092345	1.042570	-0.161218
Fe	1.396524	-0.536001	0.017824
N	2.821892	0.577412	-0.889411
C	3.650920	1.485891	-0.277838
C	4.527660	2.095259	-1.254162
C	4.214168	1.546897	-2.460392
C	3.155158	0.590761	-2.217002
C	3.644609	1.804603	1.071467
C	2.759147	1.307433	2.020670
N	1.769504	0.391737	1.780229
C	1.083380	0.240690	2.956262
C	1.652380	1.094135	3.974226
C	2.702450	1.746008	3.395829
C	2.593269	-0.236530	-3.184441
C	1.656208	-1.228967	-2.932907
N	1.105392	-1.513633	-1.701904
C	0.273940	-2.592397	-1.894915
C	0.306234	-3.000940	-3.279232
C	1.153327	-2.149469	-3.924608
C	-0.533622	-3.174526	-0.926068
C	-0.671611	-2.724568	0.380773
N	0.018966	-1.677683	0.931560
C	-0.454343	-1.542774	2.215360
C	-1.477631	-2.532543	2.476583
C	-1.603787	-3.272988	1.343682
C	0.021100	-0.638428	3.153521
H	5.269230	2.850845	-1.028832
H	-0.261732	-3.825485	-3.691036
H	4.650178	1.752791	-3.429756
H	1.426697	-2.137010	-4.972120
H	3.373615	2.469391	3.840954
H	-2.272571	-4.101719	1.150018
H	1.292998	1.165411	4.992936
H	-2.016786	-2.629074	3.410080
H	4.359354	2.549836	1.406407
H	-1.149119	-4.014816	-1.231802
H	-0.443580	-0.646808	4.134681
H	2.944230	-0.126677	-4.206033
H	-0.604310	0.626913	-2.264314
H	-1.251433	-0.556942	-1.102802
H	-2.233479	2.365483	-1.324065
N	2.909530	-1.863564	0.584348
C	3.931763	-2.212810	-0.172931
C	2.998696	-2.589900	1.752477
H	4.144338	-1.821260	-1.155452
C	4.103455	-3.397118	1.697648
H	2.265664	-2.471851	2.534536
H	4.521480	-4.105355	2.395446
H	5.521576	-3.578176	0.102614
N	4.685136	-3.146034	0.465553
C	0.477012	2.391257	-0.338364
C	0.632108	3.233603	0.776750
C	0.903549	2.872652	-1.589585
C	1.211099	4.493974	0.654219
H	0.303117	2.881154	1.749946
C	1.484996	4.130046	-1.713666
H	0.809365	2.240865	-2.466211
C	1.646110	4.948277	-0.591892
H	1.324288	5.121412	1.534582

H	1.822436	4.470933	-2.688774
H	2.100859	5.930211	-0.690769
H	-0.535424	0.902131	0.820529
C	-3.181665	0.892664	-0.023923
O	-3.153175	-0.178219	0.575135
O	-4.172080	1.817385	0.145867
C	-5.233759	1.440951	1.050738
H	-4.803736	0.875734	1.880438
H	-5.625405	2.392675	1.417100
C	-6.313809	0.649642	0.355174
C	-6.229344	-0.745810	0.258147
C	-7.407274	1.306770	-0.219673
C	-7.224905	-1.466113	-0.401310
H	-5.370103	-1.250598	0.686658
C	-8.403563	0.587430	-0.880021
H	-7.476907	2.389694	-0.147969
C	-8.313702	-0.802511	-0.971168
H	-7.151147	-2.548102	-0.470686
H	-9.248619	1.109908	-1.320035
H	-9.089083	-1.366025	-1.483129

TS(G'-P')^3

C	-2.299231	1.355566	-0.975580
C	-1.111817	0.527812	-1.281166
C	-0.139499	1.010221	-0.195955
Fe	1.439758	-0.481909	0.043810
N	2.900979	0.648248	-0.773818
C	3.722023	1.524326	-0.108883
C	4.622819	2.169115	-1.039750
C	4.328623	1.678037	-2.274769
C	3.255046	0.723273	-2.097124
C	3.683532	1.783945	1.252430
C	2.767570	1.247519	2.148362
N	1.787778	0.336330	1.840183
C	1.066935	0.135281	2.991956
C	1.602518	0.948483	4.055814
C	2.665527	1.629168	3.534700
C	2.693103	-0.031846	-3.118034
C	1.725155	-1.013772	-2.944422
N	1.140531	-1.353147	-1.747866
C	0.309312	-2.414237	-2.012221
C	0.365464	-2.748857	-3.414128
C	1.233510	-1.870948	-3.995502
C	-0.507888	-3.053128	-1.086047
C	-0.654914	-2.683299	0.242932
N	0.033753	-1.672572	0.863686
C	-0.457910	-1.607684	2.143541
C	-1.486025	-2.609588	2.336567
C	-1.598524	-3.284922	1.162758
C	0.001879	-0.749003	3.131276
H	5.364292	2.908908	-0.766745
H	-0.197899	-3.547021	-3.880413
H	4.782440	1.926291	-3.225831
H	1.531451	-1.806931	-5.034358
H	3.319618	2.335815	4.029347
H	-2.266581	-4.099231	0.913721
H	1.213636	0.977970	5.065673
H	-2.037737	-2.756431	3.255990
H	4.389165	2.511438	1.640942
H	-1.120960	-3.873012	-1.446878
H	-0.480243	-0.799271	4.102532
H	3.067907	0.127393	-4.124520
H	-0.718319	0.688980	-2.286226
H	-1.338106	-0.526408	-1.148970
H	-2.357125	2.388771	-1.299201
N	2.974033	-1.988955	0.481615
C	4.151452	-2.094782	-0.101780
C	2.888817	-3.007125	1.406635
H	4.526142	-1.443201	-0.875971
C	4.043488	-3.744142	1.380125

H	2.005946	-3.127248	2.014968
H	4.369789	-4.607366	1.938717
H	5.761417	-3.447550	0.136683
N	4.837077	-3.150849	0.412446
C	0.450044	2.356684	-0.334506
C	0.624002	3.164707	0.803224
C	0.876825	2.867474	-1.574009
C	1.216260	4.421466	0.712309
H	0.296655	2.788696	1.768232
C	1.474289	4.120185	-1.666206
H	0.770420	2.259639	-2.466411
C	1.650265	4.905270	-0.523125
H	1.341457	5.022938	1.609059
H	1.811469	4.484301	-2.633078
H	2.116865	5.883827	-0.597066
H	-0.560124	0.846659	0.793789
C	-3.272459	0.879323	-0.019890
O	-3.229868	-0.207436	0.550732
O	-4.270619	1.789973	0.183862
C	-5.318956	1.381351	1.089471
H	-4.876634	0.792929	1.896304
H	-5.711066	2.319141	1.489862
C	-6.403907	0.606395	0.382891
C	-6.308370	-0.783548	0.231503
C	-7.513121	1.273788	-0.148197
C	-7.308256	-1.488201	-0.438179
H	-5.437380	-1.295483	0.626532
C	-8.513973	0.570103	-0.818554
H	-7.591517	2.352502	-0.034396
C	-8.412827	-0.814381	-0.964090
H	-7.225734	-2.566035	-0.549824
H	-9.371219	1.100508	-1.224184
H	-9.191577	-1.365776	-1.484082

P

C	-3.486364	-0.350654	-0.654795
C	-2.697011	-0.967234	0.454825
C	-1.330097	-1.541798	0.253058
C	-1.012997	-2.274787	-0.893475
C	0.256722	-2.831393	-1.052143
C	1.224066	-2.658288	-0.063108
C	0.916614	-1.926824	1.085191
C	-0.351517	-1.374263	1.240867
H	-0.583544	-0.786427	2.125117
H	1.673185	-1.764695	1.845966
H	2.217272	-3.079149	-0.189868
H	0.489726	-3.396843	-1.950478
H	-1.765984	-2.407030	-1.665254
H	-3.280851	-1.472003	1.223629
C	-2.945975	0.547847	0.438942
C	-1.819733	1.486656	0.199797
O	-1.552141	2.412869	0.941407
O	-1.125672	1.186950	-0.919379
C	0.053229	1.989889	-1.187800
C	1.287175	1.424193	-0.534799
C	1.604327	1.745379	0.791730
C	2.755320	1.228861	1.383907
C	3.603111	0.389470	0.657568
C	3.289297	0.060602	-0.660892
C	2.134819	0.574266	-1.250618
H	1.886669	0.311269	-2.275690
H	3.940950	-0.596557	-1.229867
H	4.504361	-0.006052	1.118193
H	2.995506	1.487542	2.411574
H	0.938596	2.394862	1.350470
H	-0.143504	3.009529	-0.851723
H	0.144381	1.970795	-2.275377
H	-3.633877	0.927066	1.186383
H	-3.006527	-0.262114	-1.623330
H	-4.560390	-0.507149	-0.684135

P'

C	1.256635	-0.650980	1.647802
C	2.056466	-0.824698	0.392859
C	3.407290	-0.227407	0.213533
C	3.785217	0.976401	0.825838
C	5.058602	1.506838	0.631088
C	5.982306	0.843427	-0.178866
C	5.618416	-0.354862	-0.792582
C	4.342327	-0.882461	-0.598102
H	4.063912	-1.816352	-1.079841
H	6.327408	-0.881522	-1.425421
H	6.975198	1.257348	-0.329180
H	5.330504	2.441245	1.114374
H	3.081103	1.508540	1.460227
H	1.903143	-1.769694	-0.120474
C	0.812131	0.071880	0.397464
C	-0.384227	-0.452161	-0.303752
O	-0.707836	-1.625751	-0.331021
O	-1.060610	0.539885	-0.920043
C	-2.273103	0.150995	-1.624059
C	-3.470564	0.173506	-0.711588
C	-4.219829	1.345828	-0.563914
C	-5.318110	1.382876	0.294390
C	-5.676985	0.242619	1.014770
C	-4.933919	-0.930915	0.873639
C	-3.835632	-0.966568	0.015482
H	-3.244217	-1.870291	-0.087996
H	-5.211126	-1.820725	1.432013
H	-6.533960	0.267959	1.682183
H	-5.894176	2.298085	0.398568
H	-3.940108	2.233369	-1.126538
H	-2.366956	0.894682	-2.417609
H	-2.118314	-0.837680	-2.059335
H	0.972395	1.141877	0.328976
H	1.678391	-0.049177	2.447037
H	0.639053	-1.485545	1.963729

1

C	0.488420	1.264948	-0.169679
H	-0.152889	0.452532	0.157654
N	0.915889	2.215510	0.887585
N	0.016596	2.632993	0.161550
C	1.343231	1.051166	-1.351263
C	2.197200	2.053625	-1.833877
C	1.302617	-0.185226	-2.009931
C	2.992482	1.818120	-2.953593
H	2.239253	3.016164	-1.334256
C	2.098871	-0.417117	-3.128935
H	0.642670	-0.966389	-1.640707
C	2.947110	0.584424	-3.604871
H	3.650027	2.602104	-3.318290
H	2.057045	-1.380258	-3.629517
H	3.568342	0.404377	-4.477340

2

C	-2.056410	-1.160261	-0.334395
C	-3.164631	-0.490324	-0.851399
C	-3.336389	0.870930	-0.595709
C	-2.397018	1.556905	0.176445
C	-1.289097	0.886059	0.692576
C	-1.111087	-0.480188	0.441069
C	0.093282	-1.208820	0.976556
H	-0.110671	-2.274788	1.094241
H	0.426757	-0.788386	1.926905
O	1.202658	-1.163791	0.038441
C	2.031091	-0.100061	0.141807
O	1.917375	0.780015	0.973716
C	3.092240	-0.170466	-0.892766
C	4.027257	0.777951	-0.971519

H	4.811727	0.746508	-1.721196
H	4.020345	1.612229	-0.276067
H	3.062173	-1.019347	-1.568752
H	-0.547182	1.415734	1.280966
H	-2.528047	2.616364	0.378228
H	-4.200352	1.394826	-0.995178
H	-3.893698	-1.029599	-1.449688
H	-1.922320	-2.221160	-0.532009

N_2

N	-1.863058	-0.290859	0.000000
N	-2.968555	-0.290859	-0.000000

Phenylcarbene (singlet)

C	0.286107	-0.409092	-0.036482
H	0.181069	-1.501185	0.163759
C	0.712205	0.188824	1.204767
C	0.938490	-0.517383	2.417625
C	0.918858	1.592837	1.209386
C	1.347253	0.142888	3.567724
H	0.784300	-1.593416	2.428486
C	1.327843	2.258831	2.358111
H	0.742319	2.118648	0.276350
C	1.540515	1.530512	3.533247
H	1.517779	-0.404540	4.490249
H	1.482670	3.333631	2.350415
H	1.860630	2.047633	4.434173

Phenylcarbene (triplet)

C	0.315736	-0.496912	0.075799
H	0.102641	-1.533464	-0.154379
C	0.720693	0.181396	1.222422
C	0.945683	-0.515071	2.451347
C	0.926304	1.593559	1.216845
C	1.348341	0.167121	3.588451
H	0.795905	-1.590353	2.481040
C	1.328973	2.257060	2.364404
H	0.760467	2.139088	0.293138
C	1.543540	1.554268	3.557804
H	1.513402	-0.382456	4.511351
H	1.479264	3.332832	2.336370
H	1.859087	2.081118	4.453218

C*^{CSS}

Fe	0.794810	0.023206	-0.130402
N	2.590926	-0.368914	-0.970821
N	0.475362	-1.960430	0.091531
N	1.118421	2.009466	-0.340772
N	-0.997514	0.417673	0.721767
C	3.518607	0.552606	-1.383367
C	-0.607948	-2.551757	0.688827
C	3.128547	-1.602594	-1.236698
C	1.295643	-2.981472	-0.316279
C	2.249200	2.603593	-0.840072
C	-1.878138	-0.501352	1.232500
C	0.262723	3.028876	-0.006590
C	-1.570919	1.649450	0.914188
C	4.681461	-0.119432	-1.922971
C	-0.466214	-3.991974	0.661999
C	4.437716	-1.456336	-1.836314
C	0.712403	-4.258853	0.034406
C	2.105590	4.043354	-0.817509
C	-3.042788	0.170296	1.767778
C	0.871834	4.307403	-0.304228
C	-2.854328	1.504259	1.566885
H	5.556304	0.382274	-2.316730
H	-1.186439	-4.690222	1.069223
H	5.071837	-2.278979	-2.141741
H	1.161026	-5.221046	-0.177866
H	2.857268	4.743524	-1.159438

H	-3.886306	-0.329578	2.226884
H	0.402700	5.268652	-0.136302
H	-3.510117	2.325091	1.828536
C	3.368986	1.932259	-1.315673
C	-1.697326	-1.879068	1.228419
C	-0.993195	2.866677	0.568792
C	2.525389	-2.821008	-0.945058
H	4.191274	2.538641	-1.683542
H	-2.484620	-2.483555	1.668815
H	-1.562753	3.766276	0.782268
H	3.069892	-3.722124	-1.210708
C	2.574533	-0.809317	2.166580
C	1.428542	0.992664	2.583937
C	2.917503	-0.419788	3.433131
H	2.915763	-1.650540	1.585894
N	2.180912	0.725714	3.682321
H	0.753510	1.828366	2.491615
H	3.596059	-0.836496	4.160168
H	2.195691	1.271976	4.530103
N	1.649832	0.078820	1.655603
N	-0.022740	-0.030357	-1.838641
N	-0.501726	-0.062141	-2.839972

C*[3]

Fe	0.751377	0.006771	-0.114634
N	2.107818	-1.461916	-0.690242
N	-0.556456	-1.473200	0.537965
N	2.056635	1.493951	-0.770540
N	-0.605985	1.482676	0.456868
C	3.342524	-1.235327	-1.228330
C	-1.769113	-1.257258	1.128141
C	1.932359	-2.812497	-0.581767
C	-0.350304	-2.822168	0.470609
C	3.299759	1.279458	-1.295644
C	-1.811052	1.257529	1.060292
C	1.838750	2.842610	-0.731323
C	-0.444355	2.832936	0.321071
C	3.991229	-2.511536	-1.475410
C	-2.369048	-2.538888	1.456797
C	3.120707	-3.484842	-1.077809
C	-1.494387	-3.504606	1.049907
C	3.907672	2.561108	-1.607828
C	-2.452499	2.533746	1.323951
C	3.006152	3.525841	-1.260470
C	-1.609799	3.506066	0.867246
H	4.979931	-2.634889	-1.899622
H	-3.332807	-2.670703	1.932712
H	3.259484	-4.558260	-1.112991
H	-1.603535	-4.579100	1.129093
H	4.892365	2.693880	-2.038570
H	-3.420501	2.658054	1.793320
H	3.110691	4.599871	-1.352175
H	-1.755152	4.579008	0.890677
C	3.888066	0.025210	-1.501877
C	-2.340698	-0.001688	1.369499
C	0.682772	3.458006	-0.230709
C	0.795578	-3.437658	-0.051422
H	4.885721	0.030764	-1.932605
H	-3.316169	-0.004973	1.848373
H	0.661718	4.543882	-0.266481
H	0.809470	-4.523972	-0.031195
C	1.942155	-1.001696	2.457057
C	1.874659	1.172978	2.334852
C	2.478235	-0.531956	3.624997
H	1.792612	-2.014633	2.121431
N	2.427521	0.848633	3.530348
H	1.708840	2.179763	1.986390
H	2.879690	-1.034738	4.490157
H	2.744908	1.506501	4.226025
N	1.573632	0.070732	1.669688

N	-0.045554	-0.055248	-1.843952
N	-0.509785	-0.091709	-2.851311

C*[5]

Fe	0.761827	0.017756	-0.085457
N	2.084957	1.446384	-0.747997
N	2.116754	-1.486308	-0.690497
N	-0.597235	1.519395	0.497928
N	-0.555714	-1.411504	0.576729
C	1.887060	2.785222	-0.687239
C	1.914804	-2.845400	-0.554545
C	3.304720	1.211613	-1.321383
C	3.332802	-1.304159	-1.278706
C	-0.401075	2.876017	0.360807
C	-0.354839	-2.752052	0.520556
C	-1.820425	1.331948	1.076698
C	-1.767599	-1.177185	1.157413
C	3.001603	3.442009	-1.223018
C	3.114827	-3.565370	-1.103705
C	3.911452	2.433333	-1.628570
C	3.956225	-2.652766	-1.532164
C	-1.612389	3.592918	0.894786
C	-1.461302	-3.408267	1.074955
C	-2.452880	2.677385	1.319084
C	-2.365552	-2.398057	1.486687
H	3.113234	4.516429	-1.302243
H	3.234874	-4.641248	-1.131489
H	4.883040	2.550660	-2.092356
H	4.923747	-2.811118	-1.992375
H	-1.739441	4.668151	0.911945
H	-1.570234	-4.482521	1.162193
H	-3.432237	2.827009	1.755083
H	-3.334818	-2.510725	1.955254
C	0.672210	3.446884	-0.147854
C	0.849390	-3.412517	-0.033689
C	-2.352276	0.153097	1.387236
C	3.880225	-0.120404	-1.563454
H	0.669589	4.533091	-0.180133
H	0.850430	-4.499005	-0.004133
H	-3.342969	0.168578	1.829469
H	4.860971	-0.138004	-2.031002
C	0.962020	0.205793	2.914161
C	2.892626	-0.028234	1.931133
C	1.902904	0.194626	3.907498
H	-0.109193	0.304016	2.975687
N	3.121206	0.045997	3.266165
H	3.658433	-0.147987	1.181564
H	1.823528	0.275937	4.979670
H	4.026690	-0.000329	3.708201
N	1.595134	0.066442	1.695296
N	-0.003187	-0.025992	-1.823628
N	-0.416980	-0.044383	-2.853472

2. Molecular Dynamics Simulations

Molecular dynamics (MD) simulations were prepared with the Amber 16[16] package and the AmberTools 21 package.[17] The structure of the structurally strongly related *Ape*Pgb GLVRSQL variant (PDB ID: 7UTE) was used as the starting point for the preparation of the MD simulations.[18] The V60A, G61V and F175L mutations contained in the most active *Ape*Pgb GLAVRSQLL variant were manually introduced using Pymol v.1.8.2.[19] The DFT-optimized geometries of the carbene intermediate and the C–C bond forming transition states served as initial starting geometries and were manually placed in the active site of the enzyme. Hydrogen atoms were added using H++ server.[20] A combination of the ff14SB force field for proteins, the General Amber Force Field (gaff)[21] for benzyl acrylate and TIP3P parameters[22] for water molecules was employed.[23] For benzyl acrylate, restrained electrostatic potential (RESP) atomic charges[24] were calculated at the B3LYP/6-31G(d)[2, 3] level of theory according to the Merz–Singh–Kollman scheme.[25, 26] Force field parameters and charges for the iron heme-carbene complex were generating using the MCPB.py program[27] with geometry optimizations, force constant and Merz–Singh–Kollman RESP charge calculations at the B3LYP/6-31G(d) level of theory in Gaussian 09, Rev. D.01.[28] The system was solvated in a 10 Å buffer water box and neutralized by addition of sodium ions.

Employing the GPU-accelerated pmemd[29] code implemented in Amber 16, the energy was minimized over 5,000 steps with positional restraints (500 kcal mol^{-1} $Å^{-2}$) applied to all atoms except water molecules and sodium ions, followed by an energy minimization over 5,000 steps with positional restraints (2.0 kcal mol^{-1} $Å^{-2}$) on all peptide backbone atoms (C, Cα, N) as well as all non-hydrogen atoms of the iron heme-carbene complex and the benzyl acrylate. Subsequently, the temperature was raised from 0 K to 300 K within 300 ps in an NVT ensemble with positional restraints (30 kcal mol^{-1} $Å^{-2}$) on all peptide backbone atoms (C, Cα, N) as well as all non-hydrogen atoms of the iron heme-carbene complex and the benzyl acrylate. Afterwards, the system was equilibrated at 300 K and 1 atm for 2 ns in an NPT ensemble with high positional restraints (30 kcal mol^{-1} $Å^{-2}$) on all peptide backbone atoms (C, Cα, N) as well as all non-hydrogen atoms of the iron heme-carbene complex and the benzyl acrylate, followed by an equilibration at 300 K and 1 atm for 2 ns in an NPT ensemble with low positional restraints (0.5 kcal mol^{-1} $Å^{-2}$) on all peptide backbone atoms (C, Cα, N) as well as all non-hydrogen atoms of the iron heme-carbene complex and the benzyl acrylate. Production runs were performed in an NPT ensemble for 1,000 ns. For each system, 3 independent replicas

were simulated. For the carbene formation/diazo formation transition state mimic (Figure S8), the distances between nitrogen not coordinated to iron and the carbene carbon (N–C1) were restrained in all simulations to the distance measured in the corresponding DFT-optimized structures, employing a harmonic potential with k = 100 kcal mol^{-1} Å^{-2}. For the cyclopropanation transition state mimics (Figure 4), the distances between iron and the carbene carbon (Fe–C1), the carbene carbon and the terminal alkene carbon (C1–C_{term}) and the carbene carbon and the internal alkene carbon (C1-$C_{internal}$) were restrained in all simulations to the distances measured in the corresponding DFT-optimized structures, employing a harmonic potential with k = 100 kcal mol^{-1} Å^{-2}. k-means clustering was performed using cpptraj to analyze each MD trajectory and obtain representative structures for the most populated clusters. Root Mean Square Deviation (RMSD) of the peptide backbone (C, Cα, N, O) was calculated using the pair-wise distance-based RMSD (DRMSD) method implemented in cpptraj with each previous frame as reference. Structures were visualized using Pymol v.1.8.2.[19]

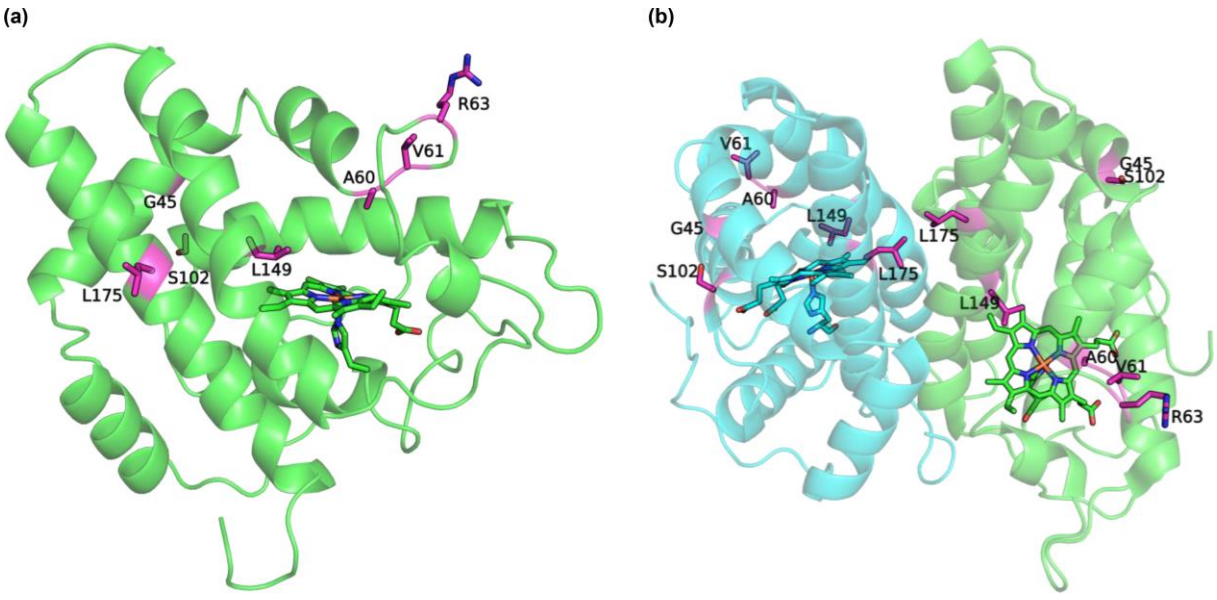

Figure S9. Mutations introduced during the directed evolution campaign (modified from PDB ID: 7UTE). (a) Monomeric structure employed in the MD simulations; (b) functional dimeric enzyme structure. Hydrogen atoms were omitted for clarity.

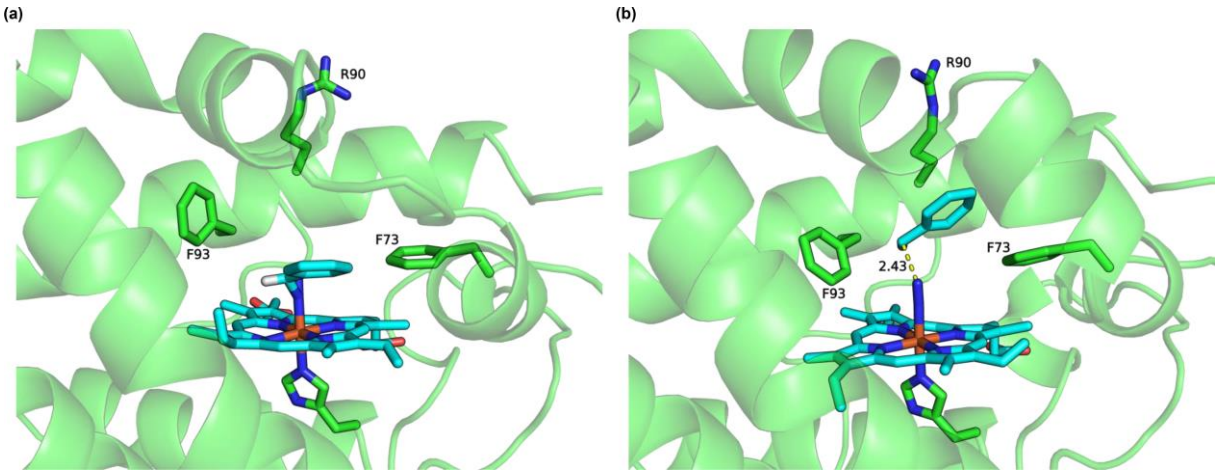

Figure S10. Most populated cluster of (a) the free carbene intermediate **C** and (b) the carbene formation/diazo formation transition state **TS(C-D)** mimic obtained from MD simulations. Non-relevant hydrogen atoms were omitted for clarity and distances are given in Å.

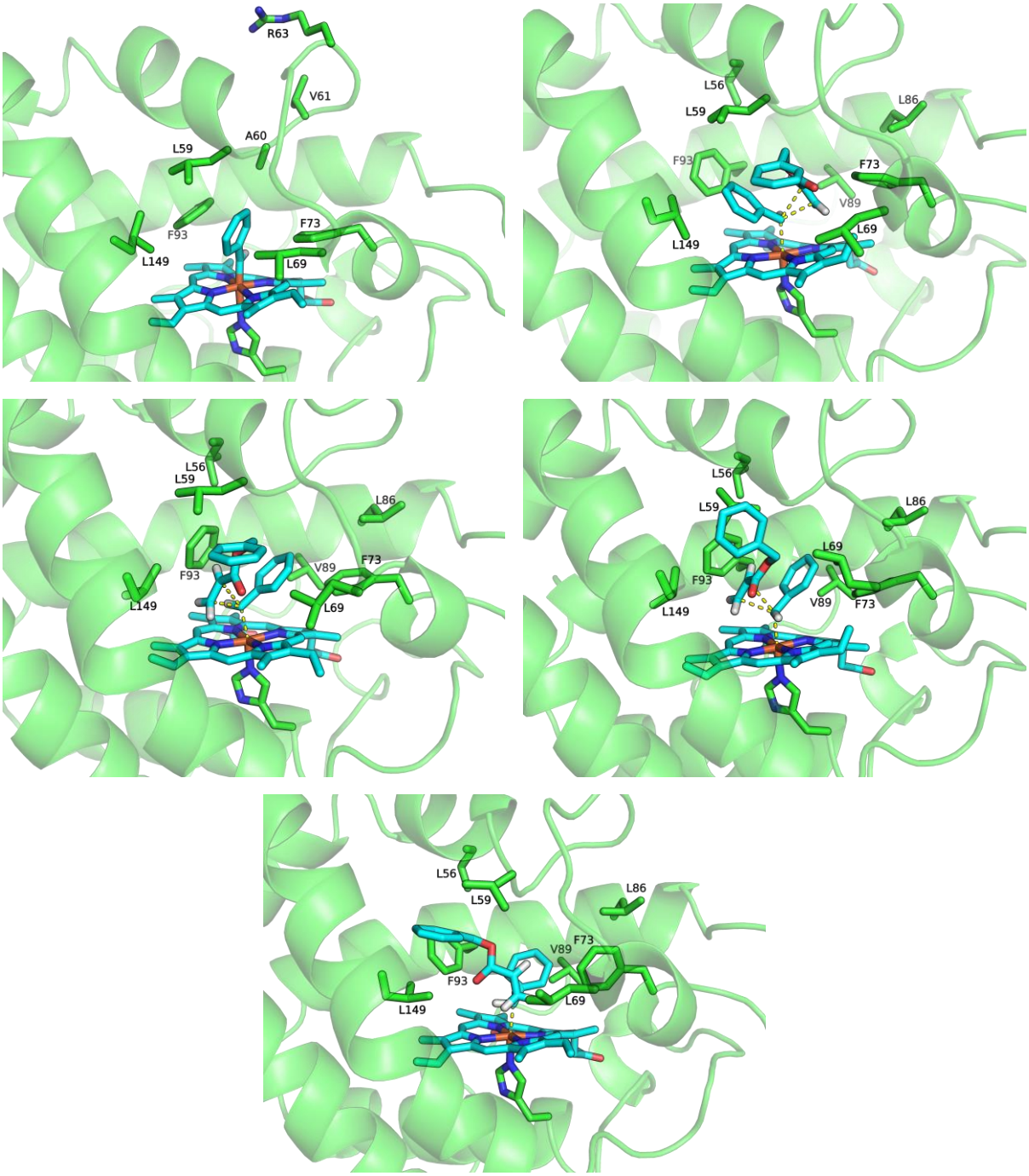

Figure S11. Structures prior to MD production runs of the carbene intermediate (top-left), C–C bond forming transition state mimics leading to the major product (1*R*,2*S*)-**4** (top-right), to (1*S*,2*R*)-**4** (middle-left), to (1*R*,2*R*)-**4** (middle-right) and (1*S*,2*S*)-**4** (bottom). Non-relevant hydrogen atoms were omitted for clarity.

2.1 Comparison to an experimentally-determined carbene intermediate structure

A comparison of the most populated cluster from the MD simulations of the key carbene intermediate shows a good agreement with the microED structure of the strongly related, albeit catalytically-less active, enzyme variant *Ape*Pgb GLVRSQL, which was reported by *Gonen et al.* (PDB: 8EUN).[30] The overall structure of the enzyme, the orientation of R63 towards the solvent as well as the positioning of key residues in the vicinity of the active site is well-reproduced by the MD simulations within the expected limits of these simulations (Figure S12).

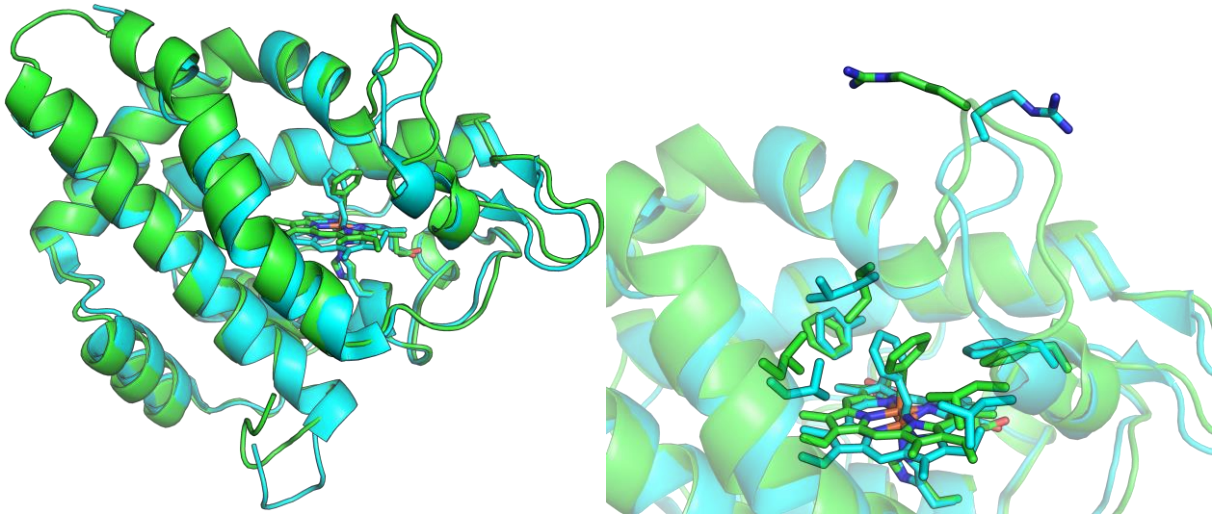

Figure S12. Overlay of the most populated cluster of the carbene intermediate structure obtained from MD simulations (in green, *Ape*Pgb GLAVRSQLL variant) and the corresponding microED structure (in blue, *Ape*Pgb GLVRSQL variant, PDB: 8EUN, A-chain).[30] Hydrogen atoms were omitted for clarity.

2.2 Flexibility of the open-loop

The flexibility of the open-loop region from residue 60 to residue 70 was analyzed by means of Root Mean Square Deviation (RMSD) analysis (Figure S13). Compared to a rigid helical region in the enzyme (residues #140-150), significantly larger fluctuations in RMSD values are observed for the open-loop, which highlights the considerably higher degree of flexibility of this peptide region.

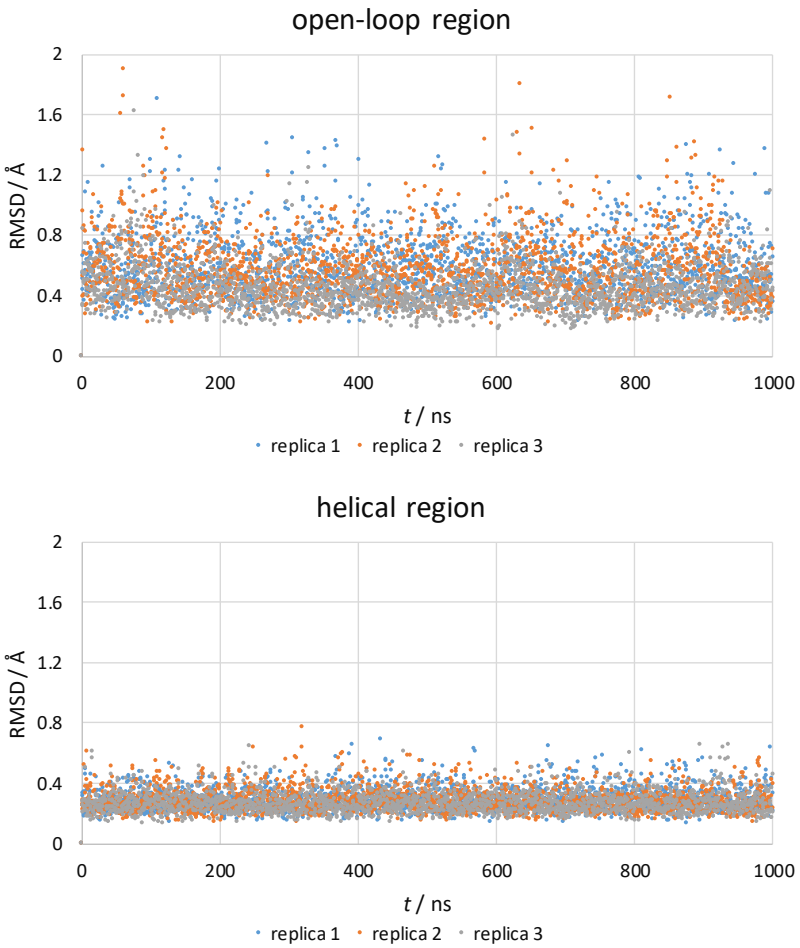

Figure S13. RMSD analysis of the open-loop (top, residues #60-70) of the MD trajectories of the key carbene intermediate and comparison with a rigid helical region (bottom, residues #140-150) with three independent replicas.

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