Electronic Supplementary Information for

Coupled Electron and Proton Transfer in the Piperidine Drug Metabolism Pathway by the Active Species of Cytochromes P450

Zhiqiang Fu,[a] Lili Yang,[c] Dongru Sun,[b] Zexing Qu,[c] Yufen Zhao,[b] Jiali Gao,*[d,e] and Yong Wang*[b]

a. Key Laboratory of Industrial Ecology and Environmental Engineering (MOE), School of Environmental Science and Technology, Dalian University of Technology, Dalian 116024, China.
b. Institute of Drug Discovery Technology, Ningbo 315211, China.
c. Laboratory of Theoretical and Computational Chemistry, Institute of Theoretical Chemistry, Jilin University, Changchun 130023, China.
d. Department of Chemistry and Supercomputing Institute, University of Minnesota, Minneapolis, Minnesota 55455, United States
e. School of Chemical Biology and Technology, Peking University Shenzhen Graduate School, Shenzhen 518055, China

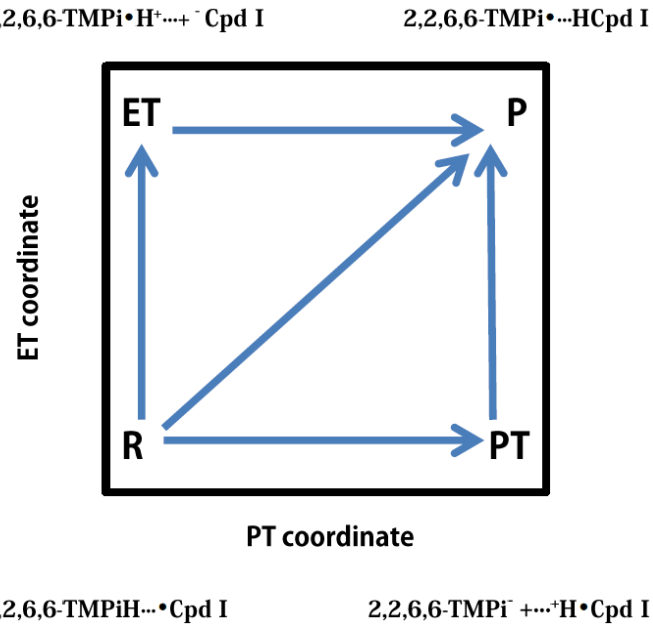
Email: yong@nbu.edu.cn, jiali@jialigao.org

Table of Contents

I. Full citation for reference 37.

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Milliam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian 09, revision C.01; Gaussian, Inc.: Wallingford CT, 2009.

II. Calculation details for the coupled electron proton transfer (CEPT) mechanism.



Scheme S1. Schematic representation of the mechanism for the coupled transfer of proton and electron as a function of electron transfer and proton transfer coordinates in the reaction of 2,2',6,6'-TMPiH and Cpd I.[1]

There have already been much work in CEPT reactions by theory and computation, usually we combine Marcus theory of electron transfer[2] and a generalized More O'Ferrall−'Ferrallner[3],[4] to represent the continuous variation of PT and ET reaction mechanisms.[5],[6] The four corners of the More O'Ferrall−Jencks plot in Scheme 1 show the effective VB states, namely diabatic states, which correspond to the electron and proton localized on the 2,2',6,6'-TMPiH and •Cpd I sites, respectively.

Diabatic and Adiabatic States.

The mechanisms of the concerted and sequential ET and PT processes can be characterized by the four VB states showed in Scheme 1.[5],[6] Each diabatic state of the corresponding Lewis configuration can be represented by a single determinant of block-localized Kohn−Sham (BLKS) orbitals in density functional theory (DFT):[7]-[9]

$$\Psi_R^{BLKS} = \hat{A}\{\Omega_R^1(\textbf{2,2',6,6'-TMPiH···•Cpd I}) - \Omega_R^2(\textbf{2,2',6,6'-TMPi}^- \textbf{ +···}^+\textbf{H•Cpd I})\} \quad (1)$$

$$\Psi_{PT}^{BLKS} = \hat{A}\{\Omega_{PT}^1(\textbf{2,2',6,6'-TMPi}^-) - \Omega_{PT}^2(^+\textbf{H•Cpd I})\} \quad (2)$$

$$\Psi_{ET}^{BLKS} = \hat{A}\{\Omega_{ET}^1(\textbf{2,2',6,6'-TMPi•H}^+\textbf{···+ }^-\textbf{Cpd I}) - \Omega_{ET}^2(^-\textbf{Cpd I})\} \quad (3)$$

$$\Psi_P^{BLKS} = \hat{A}\{\Omega_P^1(\textbf{2,2',6,6'-TMPi•···H Cpd I}) - \Omega_P^2(\textbf{H Cpd I})\} \quad (4)$$

In eqs 1-4, Â is the antisymmetrizer; and Ω denotes a product of the occupied BLKS orbitals for the *k*th (k = 1, 2) fragment specified in parentheses in the diabatic state.

Effective CEPT and HAT States.

Then we combine two of the diabatic configurations defined in eqs 1−4 to describe the CEPT and HAT mechanisms, respectively.[5] In hydrogen atom transfer, the electronic configuration is adiabatic according to the hydrogen nuclear position.[5],[10] So, combining the electronically localized configurations for a given proton configuration in eqs 1−4 will produce a lower energy state, the corresponding diabatic state for HAT. Particularly, at the given localized proton position on 2,2',6,6'-TMPiH site, the effective diabatic states for the HAT reactant and product are generated from the resonance of the initial(R, PT) and final (ET, P) electronic configurations:

$$\Phi_R^{\mathbf{HAT}} = \mathbf{c}_R\Psi_R^{\mathbf{BLKS}} + \mathbf{c}_{ET}\Psi_{ET}^{\mathbf{BLKS}} \quad (5)$$

$$\Phi_P^{\mathbf{HAT}} = \mathbf{c}_P\Psi_P^{\mathbf{BLKS}} + \mathbf{c}_{PT}\Psi_{PT}^{\mathbf{BLKS}} \quad (6)$$

where cγ are the configuration coefficients. The resonance of the HAT reactant (R) and product (P) VB diabatic states produces the adiabatic ground state potential surface for HAT. In the CEPT mechanism, electron transfer is separate from proton transfer by definition and each PCET diabatic state is stabilized by the accompanying proton tunnelling thus, a proton-coupled electron transfer. Consequently, the effective diabatic configuration for the CEPT process is a combination of the two localized proton configurations at the given electronic localization, in the reactant and product well, respectively:

$$\Phi_R^{\mathbf{CEPT}} = \mathbf{c}_R\Psi_R^{\mathbf{BLKS}} + \mathbf{c}_{PT}\Psi_{PT}^{\mathbf{BLKS}} \quad (7)$$

$$\Phi_P^{\mathbf{HAT}} = \mathbf{c}_P\Psi_P^{\mathbf{BLKS}} + \mathbf{c}_{PT}\Psi_{PT}^{\mathbf{BLKS}} \quad (8)$$

where the prime over the mixing coefficients distinguishes them from those in eqs. 5 and 6. Here, electron tunnelling can be treated by Marcus theory for electron transfer using eqs. 7 and 8 as the initial and final electron transfer diabatic states.

Reaction Coordinates.

The proton reaction coordinate is conveniently defined by the nuclear positions as follows:

$$\Delta R_P = R_{NH} - R_{OH} \quad (9)$$

where RNH and ROH are, respectively, the distance of the migrating hydrogen from the donor atom N(reactant state) and from the acceptor atom O (product state).

References

[1] A. Cembran, M. R. Provorse, C. Wang, W. Wu and J. Gao, *J. Chem. Theo. Comput.* 2012, **8**, 4347.

[2] R. A. Marcus, *J. Phys. Chem. B* 2007, **111**, 6643.

[3] R. A. More O'Ferrall, *J. Chem. Soc. B.* 1970, 274.

[4] W. P. Jencks, *Chem. Rev.* 1972, **72**, 705.

[5] R. I. Cukier and D. G. Nocera, *Annu. Rev. Phys. Chem.* 1998, **49**, 337.

[6] S. Hammes-Schiffer, *Acc. Chem. Res.* 2001, **34**, 273.
[7] L. Song and J. Gao, *J. Phys. Chem. A* 2008, **112**, 12925.
[8] A. Cembran, L. Song, Y. Mo and J. Gao, *J. Chem. Theo. Comput.* 2009, **5**, 2702.
[9] Y. Mo and J. Gao, *J. Comput. Chem.* 2000, **21**, 1458.
[10] R. I. Cukier, *J. Phys. Chem. B* 2002, **106**, 1746.

III. Kohn-Sham DFT Data for the relax scan points of the initial N-H activation process of 2,2',6,6'-TMPi by P450.

We carried out a relaxed energy-scan for hydrogen migration between the ring-N atom of the substrate and the oxygen atom of the Fe=O moiety (Fig. S2a, Table S1); both the doublet and quartet state of Cpd I were considered at the B3LYP-D2/B1 level of theory. Shown in Fig. S2 are the potential energy reaction profiles and the variations of Mulliken spin density along the O-H distance (r_{O-H}). The potential energy surfaces for both the doublet and quartet states (Fig. S2a) are very similar, with a flat transition state region, in which two maxima of essentially identical energies may be identified, corresponding to H-O separations at 1.28 and 1.46 Å on the doublet surface and 1.30 and 1.44 Å in the quartet state, respectively. However, it is important to note that the heavy atom donor-acceptor distance, R_{N-O}, was found to have little changes at values of 2.47-2.50 Å. Concomitantly, the computed spin densities in Figures S2b and S2c show that an electron is transferred from the substrate to the a_{2u} orbital of Cpd I (ρ_{FeO} does not vary significantly) in both electronic states. The highest energies of the two reaction profiles area ca. 6 kcal mol^{-1} above the encounter complex.

It is tempting to further examine the change in spin density along hydrogen migration path to gain mechanistic inspirations, although it should be kept in mind that the potential energy surfaces in Fig. S2a are not adequate to describe nonadiabatic electron transfer reactions. At the first maximum energy point, denoted as TS_{ET} in Fig. S2b, S2c, a large fraction of the electron spin density has already shifted (ρ_{sub} = -0.63/0.74 respectively on doublet and quartet states). When the second energy peak is reached, the electron transfer is virtually completed (ρ_{sub} = -0.97/1.02 on the LS/HS states), and this peak may be labeled by TS_{PT}. One may be concerned that the species at TS_{PT} arises from delocalization error in Kohn-Sham DFT, but calculations using the long-range corrected functional CAM-B3LYP attested to the steps. However, the optimization did not yield any distinct species, indicating that the process is not actually a stepwise ET/PT pathway. The significant electron transferred transition state is well consistent with the concerted PC_{ET}(ET) mechanism described in N-H bond activation of 1,2-diphenyl hydrazine by nonheme complexes. More interestingly, a clear difference is observed that the two asynchronous events herein involve, first ET and then PT, whereas in the nonheme study, where the iron(IV)-oxo reagents are more basic than Cpd I (P450), the sequence of events is reversed, i.e., first PT then ET.25 Furthermore, as also shown by Dandamudi et al., the HAT mechanism possesses a TS that has a singly occupied SNO, with a node on the H in transit between two σ-type lobes on the two heavy atoms O and N. However, for the PCET mechanism, the contributing orbitals on the substrates are π-type (or mixed π-lone pair type) orbitals that are perpendicular to the σ-lobes of the FeO orbital. Such a π type orbital is observed in this study (SNOs in Figure 2 in the main text). Thus, the current N-H activation transpires here via a novel PC_{ET} (ET) mechanism, electronic character of TS_{PT}. As can be seen, the electron transfer transpires within a span of 0.1 Å in r_{O-H}. Concerted but asynchronous

with the electron transfer, the proton transfer lags behind, namely, the N-H distance (Figure S2) varies negligibly from 1.019 Å (RC) to 1.078 Å (TS_{ET}), but significantly from 1.078 Å (TS_{ET}) to 1.192 Å (TS_{PT}). Therefore, the dual energy peaks represent the ET and PT events, respectively, in the N-H activation process. This electron/proton transfer features contrast with those of a "normal" HAT mechanism where the transfer of proton should be simultaneous with electron. We have further attempted to locate an ET intermediate in order to see whether the ET and PT are as real steps. However, the optimization did not yield any distinct species, indicating that the process is not actually a stepwise ET/PT pathway. The significant electron transferred transition state is well consistent with the concerted PCET(ET) mechanism described in N-H bond activation of 1,2-diphenyl hydrazine by nonheme complexes.

IV. Supplementary energy data for the initial N-H activation process of 2,2',6,6'-TMPi by P450.

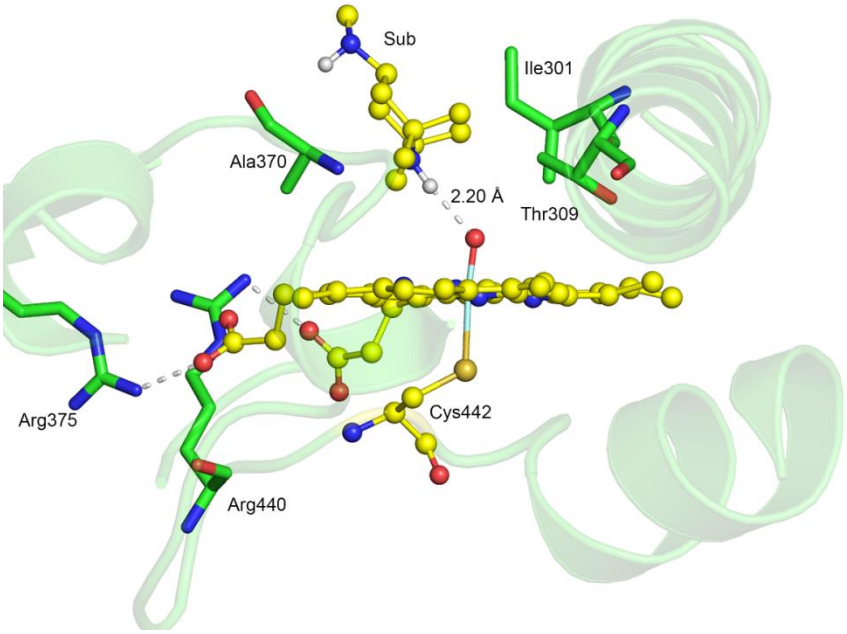


Fig. S1 The geometric information of the last snapshot in 100 ns MD simulations. The initial structures of P450 3A4 were taken from the Protein Data Bank (PDB ID: 1W0F). The protonation states of the ionizable residues and histidines were determined based on the pKa values calculated by H++ server. The GAFF was used to establish the potentials for the substrate, and the force field for Cpd I was taken from the literature (J. Comput. Chem., 2012, 33, 119.). MD simulations were carried out using AMBER 16 software package and ff14SB force field.

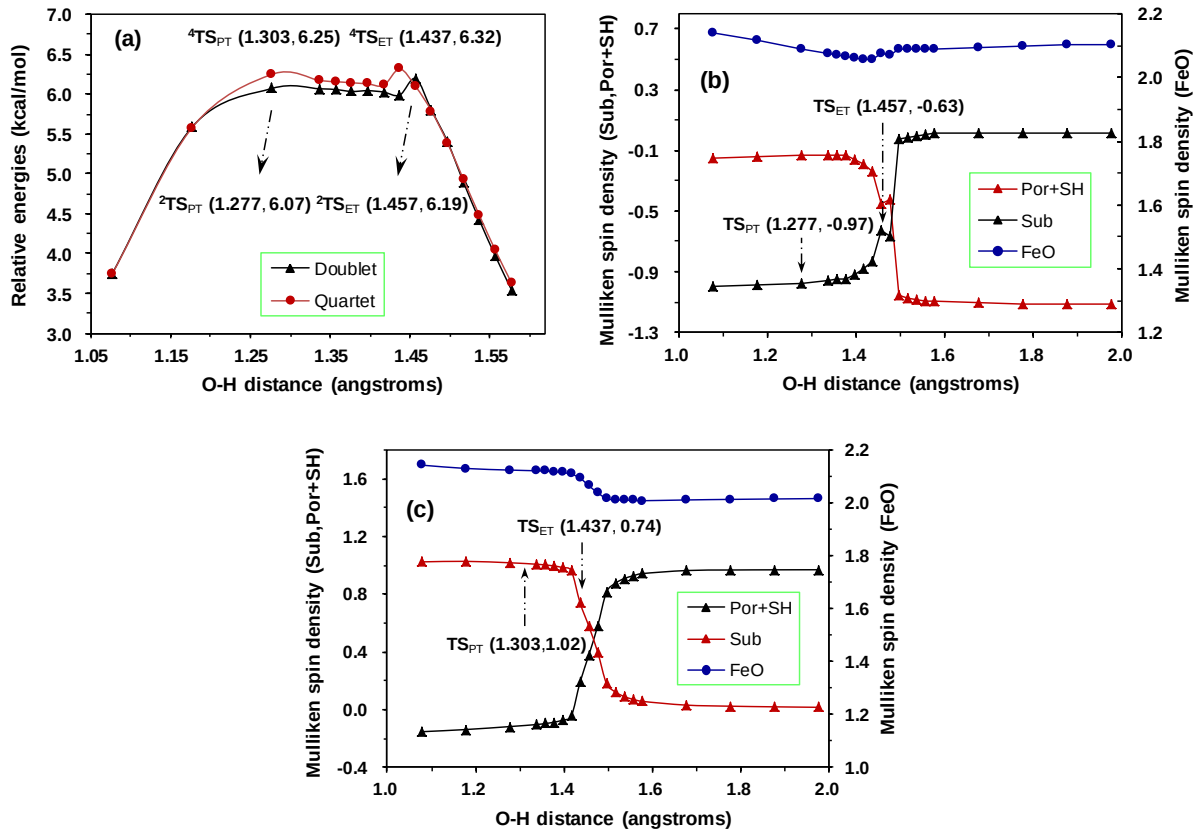


Fig. S2. Relaxed-scan SCF energies (kcal/mol) as a function of the distance between the migrating hydrogen and the oxygen atom of the Fe(IV)-oxo species (a), and the corresponding Mulliken spin densities in the low spin doublet (b) and high spin quartet states (c). All calculations were performed at the UB3LYP-D2/B1 level of theory. Step size used in the energy scan is 0.02 Å in regions with large spin variation, and 0.1 Å elsewhere. The transition state (TS_{PT}) and electron transfer point (TS_{ET}) are marked at the O-H distance of 1.277 Å and 1.457 Å, respectively.

Table S1. UB3LYP-D2 absolute (a.u.) and relative energies (**Δ*E***, kcal mol^{-1}) at various computational levels for species in the N-H bond activation of 2,2',6,6'-TMPi moiety by Cpd I of cytochrome P450. Energies with D3 corrections were also given at the B2 level.

	B1	ΔE	G	ΔE	ZPE	B2 +ZPE	ΔE	B2-D3	B2-D3 +ZPE	ΔE
^{2}**RC**	-2089.820780	**0.0**	-2089.283582	**0.0**	0.603890	-2089.656372	**0.0**	-2090.305743	-2089.701853	**0.0**
^{4}**RC**	-2089.820801	**0.0**	-2089.283800	**0.0**	0.604051	-2089.656213	**0.1**	-2090.305822	-2089.701771	**0.1**
^{2}**TS**$_{H}$	-2089.810958	**6.2**	-2089.277597	**3.9**	0.598678	-2089.656210	**0.1**	-2090.299266	-2089.700588	**0.8**
^{4}**TS**$_{H}$	-2089.810714	**6.3**	-2089.278035	**3.6**	0.598739	-2089.655478	**0.6**	-2090.298739	-2089.700000	**1.2**
^{2}**IM1**	-2089.815869	**3.1**	-2089.278999	**3.0**	0.602279	-2089.659958	**-2.3**	-2090.307365	-2089.705086	**-2.0**
^{4}**IM1**	-2089.815896	**3.1**	-2089.279866	**2.5**	0.602242	-2089.659934	**-2.2**	-2090.307351	-2089.705109	**-2.0**

Table S2. Mulliken charges and spin densities of key intermediates in the N-H bond activation of 2,2',6,6'-TMPi by Cpd I. Computations were performed at the UB3LYP-D2/B1 level.

	Spin density				Charge			
	FeO	Por+SH	H	Sub	FeO	Por+SH	H	Sub
^{2}**RC**	2.10	-1.11	0.00	0.01	-0.04	0.08	0.28	-0.32
^{4}**RC**	2.02	0.97	0.00	0.01	-0.04	0.08	0.28	-0.32
^{2}**TS**$_{H}$	2.09	-0.13	0.02	-0.97	-0.23	-0.48	0.46	0.24
^{4}**TS**$_{H}$	2.12	-0.11	-0.03	1.02	-0.23	-0.49	0.46	0.26
^{2}**IM1**	2.14	-0.16	0.01	-1.00	-0.22	-0.25	0.39	0.07
^{4}**IM1**	2.15	-0.15	-0.01	1.02	-0.22	-0.25	0.39	0.08

CAM-B3LYP derived Mulliken charges and spin densities for the **TS**$_{H}$ in the N-H bond activation of 2,2',6,6'-TMPi by Cpd I. Computations were performed at the UB3LYP-D2/B1 level.

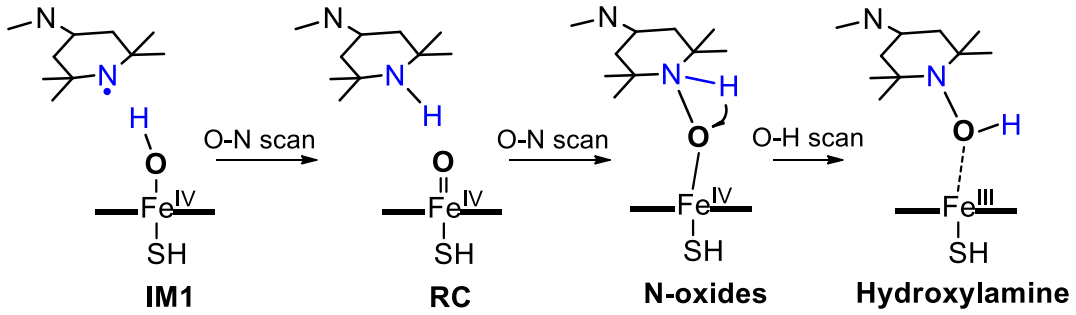
	Spin density				Charge			
	FeO	Por+SH	H	Sub	FeO	Por+SH	H	Sub
^{2}**TS**$_{H}$	2.15	-0.17	0.02	-1.00	-0.24	-0.48	0.46	0.25
^{4}**TS**$_{H}$	2.16	-0.16	-0.03	1.03	-0.24	-0.49	0.46	0.27

Table S3. UB3LYP-D2/B1 relative energies ($\boldsymbol{E}_{rel}$, kcal mol^{-1}) and spin densities for relax scan points in the N-H bond activation of 2,2',6,6'-TMPi moiety by Cpd I of cytochrome P450s. Results for both doublet and quartet states are given.

		Spin Density (doublet)				Spin Density (quartet)			
d(O-H)	$\boldsymbol{E}_{rel}$	FeO	Por+SH	H	Sub	FeO	Por+SH	H	Sub
1.977	**0.00**	2.10	-1.11	0.00	0.01	2.02	0.97	0.00	0.02
1.877	**0.23**	2.10	-1.11	0.00	0.01	2.02	0.97	0.00	0.02
1.777	**0.82**	2.10	-1.11	-0.01	0.02	2.01	0.97	-0.01	0.02
1.677	**1.87**	2.10	-1.11	-0.01	0.02	2.01	0.96	-0.01	0.03
1.577	**3.55**	2.09	-1.09	-0.01	0.01	2.01	0.94	-0.01	0.06
1.557	**3.97**	2.09	-1.09	-0.01	0.00	2.01	0.93	-0.01	0.07
1.537	**4.42**	2.09	-1.08	-0.01	0.00	2.01	0.91	-0.01	0.09
1.517	**4.89**	2.09	-1.07	-0.01	-0.01	2.01	0.88	-0.01	0.12
1.497	**5.40**	2.09	-1.06	-0.01	-0.03	2.02	0.82	-0.01	0.18
1.477	**5.80**	2.07	-0.42	0.01	-0.66	2.04	0.58	-0.02	0.40
1.457	**6.19**	2.07	-0.46	0.01	-0.63	2.07	0.38	-0.02	0.58
1.437	**5.99**	2.06	-0.24	0.01	-0.83	2.09	0.19	-0.03	0.74
1.417	**6.03**	2.06	-0.19	0.01	-0.88	2.11	-0.05	-0.03	0.96
1.397	**6.04**	2.06	-0.16	0.02	-0.92	2.12	-0.07	-0.03	0.99
1.377	**6.03**	2.07	-0.13	0.02	-0.95	2.12	-0.09	-0.03	1.00
1.357	**6.06**	2.07	-0.13	0.02	-0.95	2.12	-0.10	-0.03	1.00
1.337	**6.07**	2.07	-0.13	0.02	-0.96	2.12	-0.10	-0.03	1.01
1.277	**6.07**	2.09	-0.13	0.02	-0.97	2.12	-0.12	-0.03	1.02
1.177	**5.59**	2.12	-0.14	0.02	-0.99	2.13	-0.14	-0.02	1.03
1.077	**3.75**	2.14	-0.16	0.02	-1.00	2.14	-0.15	-0.02	1.03

d(O-H) refers to the distance (in unit of Å) between O of Cpd I and H of the N-H bond.

V. Supplementary energy data for C-C bond cleavage in the stepwise ring contraction process.



Scheme S1. Hydroxyl rebound pathway for H-abstracted 2,2',6,6'-TMPi **IM1**.

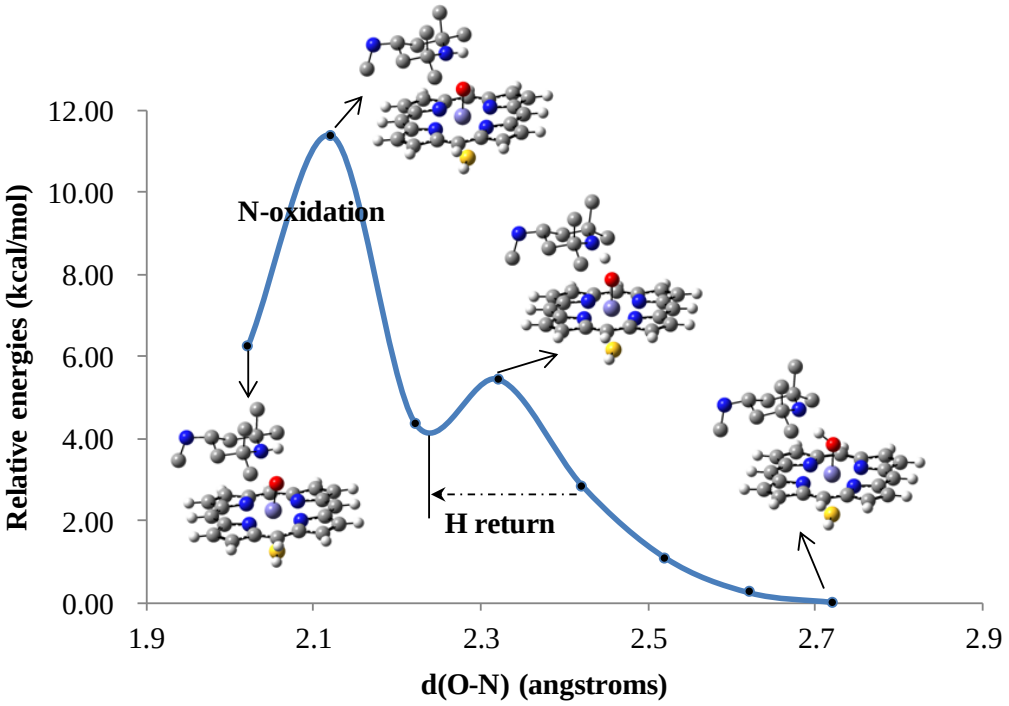
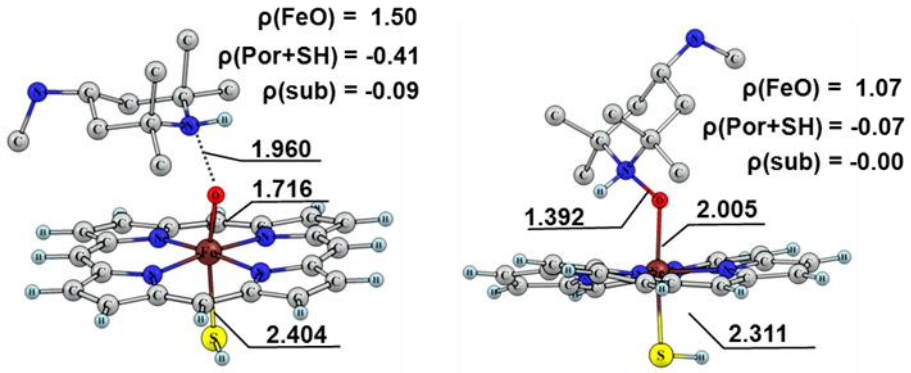


Fig. S3. Relative energies of the relaxed PES scan points versus the O-N distance (LS state, O-N scan process) in hydroxyl rebound on **IM1**. The scan span is 0.1 Å.

Table S4. Supplementary data of UB3LYP-D2 absolute (a.u.) and relative energies (kcal mol^{-1}) for the relaxed PES scanning points in in hydroxyl rebound on **IM1** (O-N scan process)

Scan step	d(O-N)/angstroms	HF(UB3LYP-D2/B1)	E_{rel}
1	2.722	-2089.815869	**0.00**
2	2.622	-2089.815494	**0.24**
3	2.522	-2089.814157	**1.07**
4	2.422	-2089.811343	**2.84**
5	2.322	-2089.807197	**5.44**
6	2.222	-2089.808911	**4.37**
7	2.122	-2089.797729	**11.38**
8	2.022	-2089.805891	**6.26**



^{2}**TS** ^{2}**IM**

Fig. S4. Geometric and electronic information of the N-oxidation species ^{2}**TS** and ^{2}**IM** for hydroxyl rebound from the H-abstracted **IM1**(O-N scan process).

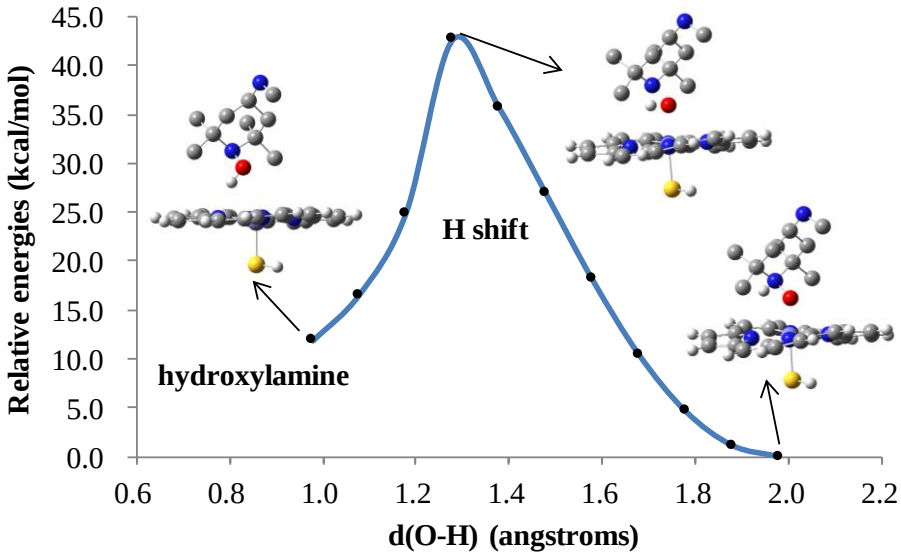


Fig. S5. Relative energies of the relaxed PES scan points versus the O-H distance (LS state, O-H scan process) in hydroxyl rebound on **IM1**. The scan span is 0.1 Å.

Table S5. Supplementary data of UB3LYP-D2 absolute (a.u.) and relative energies (kcal mol^{-1}) for the relaxed PES scanning points in in hydroxyl rebound on **IM1** (O-H scan process)

Scan step	d(O-N)/angstroms	HF(UB3LYP-D2/B1)	E_{rel}
1	1.979	-2089.864099	**0.00**
2	1.879	-2089.862272	**1.15**
3	1.779	-2089.856706	**4.64**
4	1.679	-2089.847503	**10.41**
5	1.579	-2089.835261	**18.10**
6	1.479	-2089.821205	**26.92**
7	1.379	-2089.807304	**35.64**
8	1.279	-2089.796151	**42.64**
9	1.179	-2089.824376	**24.93**
10	1.079	-2089.837696	**16.57**
11	0.979	-2089.845236	**11.84**

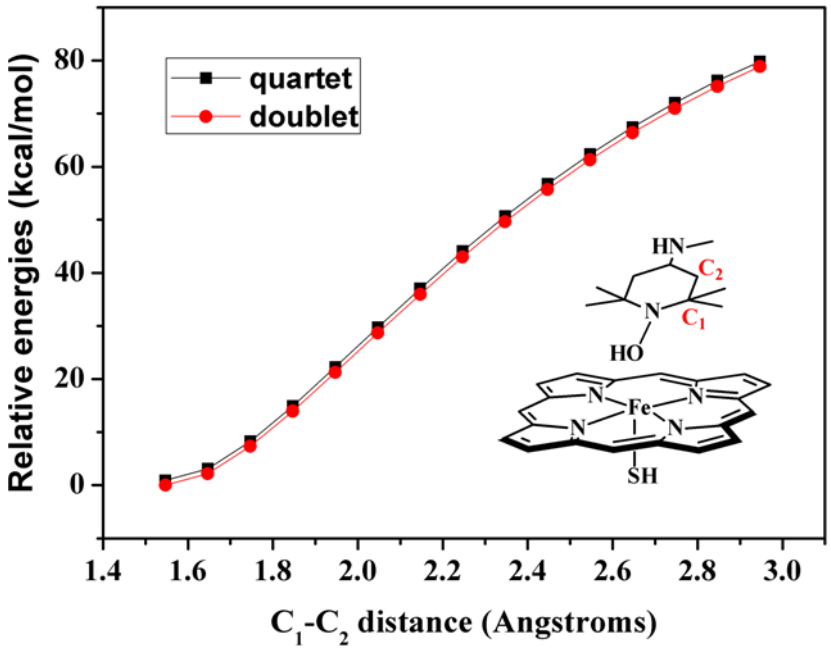


Fig. S6. Relative energies of the rigid PES scan points versus the C-C distance in C-C bond cleavage on hydroxylamine. The scan span is 0.1 angstrom.

Table S6. Supplementary data of UB3LYP-D2 absolute (a.u.) and relative energies (kcal mol^{-1}) for the rigid PES scanning points in in C-C bond cleavage on hydroxylamine

		Doublet State		**Quartet State**	
Step	C_1-C_2 distance	HF(UB3LYP-D2/B1)	E_{rel}	HF(UB3LYP-D2/B1)	E_{rel}
1	1.546	-2089.85072	**0.0**	-2089.849259	**0.9**
2	1.646	-2089.84725	**2.2**	-2089.845759	**3.1**
3	1.746	-2089.839045	**7.3**	-2089.837511	**8.3**
4	1.846	-2089.828466	**14.0**	-2089.826892	**15.0**
5	1.946	-2089.816859	**21.2**	-2089.815249	**22.3**
6	2.046	-2089.805017	**28.7**	-2089.803349	**29.7**
7	2.146	-2089.793375	**36.0**	-2089.791655	**37.1**
8	2.246	-2089.782186	**43.0**	-2089.78046	**44.1**
9	2.346	-2089.771635	**49.6**	-2089.769947	**50.7**
10	2.446	-2089.761911	**55.7**	-2089.760254	**56.8**
11	2.546	-2089.753005	**61.3**	-2089.751343	**62.4**
12	2.646	-2089.744899	**66.4**	-2089.743221	**67.5**
13	2.746	-2089.737602	**71.0**	-2089.735879	**72.1**
14	2.846	-2089.730989	**75.1**	-2089.729224	**76.2**
15	2.946	-2089.725042	**78.9**	-2089.723547	**79.8**

Table S7. UB3LYP-D2 absolute (a.u.) and relative energies (kcal mol^{-1}) at various levels for species of C-C bond cleavage in the stepwise ring contraction process of 2,2',6,6'-TMPi moiety by Cpd I of cytochrome P450. Energies with D3 corrections were also given at the B2 level.

	B1	ΔE	G	ΔE	ZPE	B2+ZPE	ΔE	B2-D3	B2-D3+ZPE	ΔE
^{2}**IM1**	-2089.815869	**3.1**	-2089.278999	**3.0**	0.602279	-2089.659958	**-2.3**	-2090.307365	-2089.705086	**-2.0**
^{4}**IM1**	-2089.815896	**3.1**	-2089.279866	**2.5**	0.602242	-2089.659934	**-2.2**	-2090.307351	-2089.705109	**-2.0**
^{2}**TS**$_{CC}$	-2089.773436	**29.7**	-2089.240955	**26.9**	0.598307	-2089.622719	**21.1**	-2090.267414	-2089.669107	**20.5**
^{4}**TS**$_{CC}$	-2089.773710	**29.5**	-2089.242793	**25.7**	0.595940	-2089.623167	**20.8**	-2090.267475	-2089.669557	**20.3**
^{2}**IM2**	-2089.783951	**23.1**	-2089.253175	**19.2**	0.598294	-2089.633729	**14.2**	-2090.278184	-2089.679805	**13.8**
^{4}**IM2**	-2089.783947	**23.1**	-2089.253839	**18.8**	0.599221	-2089.633728	**14.2**	-2090.278188	-2089.679811	**13.8**
^{4}**TS3**	-2089.777160	**27.4**	-2089.244738	**24.5**	0.597678	-2089.627373	**18.2**	-2090.278138	-2089.678871	**14.4**
^{2}**PC**	-2089.901163	**-50.4**	-2089.358262	**-46.7**	0.606788	-2089.735449	**-49.7**	-2090.386966	-2089.779772	**-48.9**
^{4}**PC**	-2089.890095	**-43.5**	-2089.352416	**-43.1**	0.605309	-2089.730218	**-47.5**	-2090.366564	-2089.761606	**-37.5**

Table S8. Mulliken charges and spin densities of key intermediates in stepwise ring contraction process of 2,2',6,6'-TMPi by Cpd I. Computations were performed at the UB3LYP-D2/B1 level.

	Spin density (ρ)						**Charge (Q)**					
	Fe	OH	Por+SH	Sub	N	C2	Fe	OH	Por+SH	Sub	N	C2
^{2}**IM1**	1.80	0.35	-0.16	-1.00	-0.91	-0.04	0.40	-0.23	-0.25	0.08	-0.37	-0.16
^{4}**IM1**	1.80	0.34	-0.16	1.02	0.92	0.04	0.40	-0.23	-0.25	0.08	-0.37	-0.16
^{2}**TS**$_{CC}$	1.77	0.37	-0.14	-1.00	-0.35	-0.81	0.41	-0.22	-0.28	0.09	-0.44	-0.22
^{4}**TS**$_{CC}$	1.76	0.36	-0.14	1.02	0.36	0.82	0.41	-0.22	-0.29	0.10	-0.44	-0.22
^{2}**IM2**	1.78	0.34	-0.14	-0.98	0.01	-1.06	0.41	-0.22	-0.27	0.08	-0.44	-0.24
^{4}**IM2**	1.78	0.34	-0.13	1.01	0.01	1.06	0.41	-0.22	-0.27	0.08	-0.44	-0.24
^{4}**TS3**	2.77	0.16	0.07	0.00	0.00	0.00	0.44	-0.39	-0.95	0.89	-0.40	-0.03
^{2}**PC**	1.08	0.00	-0.08	0.00	0.00	0.00	0.27	-0.19	-0.43	0.36	-0.44	-0.20
^{4}**PC**	2.62	0.02	0.35	0.01	0.00	0.00	0.48	-0.20	-0.60	0.32	-0.44	-0.21

VI. Data for the relax scan points of the C-C bond cleavage in the stepwise ring contraction process.

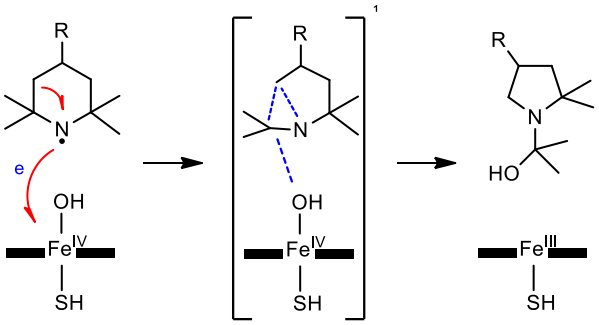
Table S9. UB3LYP-D2/B1 relative energies (E_{rel}, kcal mol^{-1}), charge and spin densities for relax scan points of C-C bond cleavage in stepwise ring contraction process of 2,2',6,6'-TMPi moiety by Cpd I of cytochrome P450.

		Spin Density				Charge			
d(C_1-C_2)	E_{rel}	FeO	Por+SH	H	Sub	FeO	Por+SH	H	Sub
1.55083	**0.0**	2.12	-0.13	0.01	-1.00	-0.23	-0.22	0.38	0.07
1.60083	**0.6**	2.12	-0.13	0.01	-1.00	-0.23	-0.22	0.38	0.07
1.65083	**2.0**	2.12	-0.13	0.01	-1.00	-0.23	-0.22	0.38	0.07
1.70083	**4.2**	2.11	-0.13	0.01	-1.00	-0.24	-0.23	0.39	0.07
1.75083	**6.8**	2.12	-0.13	0.01	-1.00	-0.24	-0.23	0.39	0.07
1.80083	**9.6**	2.12	-0.13	0.01	-1.00	-0.24	-0.23	0.39	0.07
1.85083	**12.5**	2.11	-0.12	0.01	-1.00	-0.24	-0.23	0.39	0.07
1.90083	**15.4**	2.11	-0.12	0.01	-1.00	-0.24	-0.24	0.39	0.08
1.95083	**18.2**	2.11	-0.12	0.01	-1.00	-0.24	-0.24	0.40	0.08
2.00083	**20.7**	2.10	-0.12	0.01	-1.00	-0.23	-0.24	0.40	0.08
2.05083	**22.8**	2.11	-0.12	0.01	-1.00	-0.23	-0.25	0.40	0.08
2.10083	**24.4**	2.11	-0.12	0.01	-1.00	-0.23	-0.25	0.40	0.08
2.15083	**25.6**	2.11	-0.12	0.01	-0.99	-0.23	-0.25	0.40	0.08
2.20083	**26.3**	2.11	-0.12	0.01	-0.99	-0.23	-0.25	0.40	0.08
2.25083	**26.5**	2.10	-0.12	0.01	-0.99	-0.23	-0.25	0.40	0.08
2.30083	**26.5**	2.10	-0.11	0.01	-0.99	-0.23	-0.25	0.40	0.08
2.35083	**26.3**	2.10	-0.11	0.00	-0.99	-0.23	-0.25	0.40	0.08
2.40083	**25.9**	2.09	-0.11	0.00	-0.99	-0.23	-0.25	0.40	0.08
2.45083	**25.4**	2.09	-0.11	0.00	-0.99	-0.23	-0.25	0.40	0.08
2.50083	**24.9**	2.10	-0.11	0.00	-0.99	-0.23	-0.25	0.40	0.08
2.55083	**24.3**	2.10	-0.11	0.00	-0.99	-0.23	-0.25	0.40	0.08
2.60083	**23.5**	2.10	-0.11	0.00	-0.99	-0.23	-0.23	0.40	0.07
2.65083	**23.0**	2.09	-0.11	0.00	-0.99	-0.23	-0.23	0.40	0.07

d(C_1-C_2) refers to the distance (in unit of Å) between C1 and C2 atoms (relative to N) of the 2,2',6,6'-TMPi moiety. No electron transfer is observed in the C1-C2 bond cleavage.

VII. Supplementary energy data and population analysis results in the concerted ring contraction process.

Mechanistic scheme for the concerted ring contraction process on H-abstracted 2,2',6,6'-TMPi:



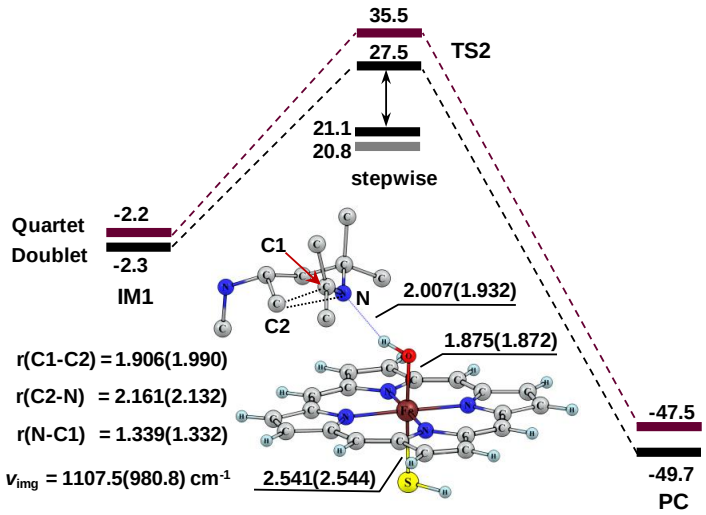


Fig. S7. Energy profiles (in kcal mol-1) for concerted ring contraction 2,2',6,6'-TMPi by Cpd I. Energy values were computed at the UB3LYP-D2/B2//B1+ZPE(B1) level. Optimized TS2 geometries obtained at the UB3LYP-D2/B1 level are also shown. Bond lengths are in Å unit. Hydrogen atoms in the 2,2',6,6'-TMPi moiety are omitted for clarity.

Table S10. UB3LYP-D2 absolute (a.u.) and relative energies (**ΔE**, kcal mol^{-1}) at various levels for species in the concerted ring contraction process on H-abstracted 2,2',6,6'-TMPi.

	B1	ΔE	G	ΔE	ZPE	B2+ZPE	ΔE
^{2}IM	-2089.815869	**3.1**	-2089.278999	**3.0**	0.602279	-2089.659958	**-2.3**
^{4}IM	-2089.815896	**3.1**	-2089.279866	**2.5**	0.602242	-2089.659934	**-2.2**
^{2}TS2	-2089.768274	**33.0**	-2089.233534	**31.5**	0.600305	-2089.612592	**27.5**
^{4}TS2	-2089.747782	**45.8**	-2089.220156	**39.9**	0.596491	-2089.599797	**35.5**
^{2}PC	-2089.900144	**-49.8**	-2089.359203	**-47.3**	0.606788	-2089.735579	**-49.7**
^{4}PC	-2089.892655	**-45.1**	-2089.356842	**-45.8**	0.605309	-2089.732127	**-47.5**

Table S11. UB3LYP-D2/B1 charge and spin densities for species in the concerted ring contraction on H-abstracted 2,2',6,6'-TMPi.

	Spin Density				Charge			
	FeO	Por+SH	H	Sub	FeO	Por+SH	H	Sub
^{2}IM	2.14	-0.16	0.01	-1.00	-0.22	-0.24	0.39	0.07
^{4}IM	2.15	-0.15	-0.01	1.02	-0.22	-0.24	0.39	0.08
^{2}TS2	1.05	0.13	0.00	-0.18	-0.41	-0.68	0.34	0.74
^{4}TS2	2.80	0.01	0.00	0.19	-0.26	-0.85	0.35	0.74
^{2}PC	1.08	-0.07	0.00	0.00	-0.26	-0.43	0.34	0.35
^{4}PC	2.64	0.35	0.00	0.01	-0.05	-0.60	0.33	0.31

VIII. Cartesian coordinates for various reaction species in the ring contraction of 2,2',6,6'-TMPi moiety by Cpd I.

N-H bond activation process

I. ^{2}RC

Fe	1.44826900	-0.01190200	0.26019600
N	0.47441600	1.53654600	1.09758900
C	-0.62918200	1.47476000	1.90584000
C	-1.10481600	2.79802400	2.21961000
C	-0.27189600	3.66926900	1.58543600
C	0.70863200	2.87031600	0.89513300
H	-1.96490800	3.00735000	2.84158300
H	-0.29729100	4.75077400	1.57563200
C	1.76457300	3.39068100	0.15516500
H	1.83392400	4.47108000	0.08126700
N	2.80858500	1.27396200	-0.48788600
C	2.75018800	2.64439900	-0.47414600
C	3.86364800	3.20662800	-1.19887700
C	4.59539100	2.15695100	-1.66172200
C	3.92359200	0.95899100	-1.21964900
H	4.04109100	4.26680500	-1.32207600
H	5.50401500	2.16753700	-2.24906700
C	4.34691700	-0.32974000	-1.51360000
H	5.24557800	-0.43164200	-2.11328000
N	2.57837000	-1.56184100	-0.35217900
C	3.71987400	-1.50029900	-1.10594700
C	4.18608900	-2.82616500	-1.43184500
C	3.30314900	-3.69682000	-0.87128800
C	2.30570800	-2.89717500	-0.20347600
H	5.07396500	-3.03714200	-2.01298900
H	3.30846700	-4.77858500	-0.88976300
C	1.23178900	-3.41563100	0.50511100
H	1.13534100	-4.49567300	0.54426600
N	0.24897200	-1.29911000	1.23975100
C	0.28348400	-2.66583400	1.19246100
C	-0.78091800	-3.23089000	1.98216000
C	-1.45917200	-2.18146100	2.52370700
C	-0.81044900	-0.98515200	2.04820900
H	-0.96018400	-4.29115700	2.10055700
H	-2.31534000	-2.19414700	3.18440500
C	-1.21866100	0.30373700	2.36363300
H	-2.08330900	0.40529000	3.00890100
O	0.55229000	0.01102000	-1.10673500
S	2.96380300	0.00869400	2.28204900
H	3.01266100	1.35305900	2.35526600
C	-1.82595900	-2.26121700	-1.79386500
C	-4.63012800	-0.08155900	-0.25083800
C	-3.78705100	1.20125000	-0.32442600
C	-3.69760800	-1.28028000	-0.44536000
C	-3.03871800	1.32851200	-1.67511700
C	-4.02390100	1.72972700	-2.78896000
C	-2.95327300	-1.21732500	-1.80142700
C	-1.98307300	2.43743700	-1.55542000
C	-3.91420500	-1.57349100	-2.95099500
H	-5.35005200	-0.06858900	-1.07777100
H	-4.42309200	2.08387900	-0.16747900
H	-1.42254600	0.09699000	-1.53516500
H	-6.14325800	0.52129300	0.95586800
H	-4.22001300	-2.62301200	-2.86341500
H	-3.40557800	-1.43035900	-3.90969600
H	-4.82153300	-0.96538900	-2.94975200
H	-2.23745500	-3.25872800	-1.60238200
H	-1.09210200	-2.02483700	-1.01738400
H	-1.31138700	-2.27016800	-2.76150400
H	-3.50569200	1.73107300	-3.75331200
H	-4.41295900	2.73638000	-2.59321700
H	-4.87789400	1.05278500	-2.85998500
H	-1.46392800	2.57124100	-2.51142800
H	-1.24296100	2.17613300	-0.79345100
H	-2.45781400	3.38401700	-1.27412700
H	-4.26854900	-2.21418200	-0.37064500
H	-2.94772700	-1.28451200	0.35507900
H	-3.04212400	1.18331600	0.48028600
N	-2.31133000	0.09353500	-2.03309300
N	-5.45254600	-0.22568000	0.96275900
C	-4.72209100	-0.15519900	2.22637100
H	-5.42886500	-0.27573000	3.05471100
H	-4.16903100	0.78687800	2.38558700
H	-4.00047900	-0.97642000	2.27662400

II. ^{4}RC

Fe	1.45900700	-0.01001800	0.26204000
N	0.47736500	1.53850700	1.09133100
C	-0.62682100	1.47595200	1.89897500
C	-1.10536800	2.79917800	2.20937200
C	-0.27395700	3.67079500	1.57392200
C	0.70900000	2.87234700	0.88626000
H	-1.96654500	3.00817700	2.82995200
H	-0.30178900	4.75221000	1.56174800
C	1.76567900	3.39209700	0.14706800
H	1.83512900	4.47241300	0.07195400
N	2.81160100	1.27464600	-0.49233100
C	2.75389300	2.64509000	-0.47799400
C	3.87222100	3.20717000	-1.19517800
C	4.60770000	2.15743100	-1.65213400
C	3.93288300	0.95957100	-1.21472100

H	4.05058800	4.26732800	-1.31718000
H	5.52072900	2.16802300	-2.23262700
C	4.35877100	-0.32917600	-1.50549100
H	5.26153900	-0.43070300	-2.09902100
N	2.58419100	-1.56106500	-0.35432400
C	3.72974400	-1.50011200	-1.10148200
C	4.19761200	-2.82609600	-1.42454300
C	3.31178200	-3.69634200	-0.86782500
C	2.31137300	-2.89626100	-0.20474700
H	5.08831200	-3.03746500	-2.00120900
H	3.31722000	-4.77812100	-0.88562600
C	1.23601700	-3.41491300	0.50200000
H	1.13968100	-4.49500300	0.54058100
N	0.25425100	-1.29905400	1.23838100
C	0.28656900	-2.66557600	1.18836300
C	-0.78143000	-3.23033300	1.97383200
C	-1.45955000	-2.18069300	2.51497800
C	-0.80711500	-0.98451500	2.04349900
H	-0.96325900	-4.29047100	2.08944200
H	-2.31828500	-2.19291400	3.17236900
C	-1.21568400	0.30481400	2.35743700
H	-2.08180300	0.40659200	3.00069500
O	0.54610100	0.00079000	-1.09572000
S	2.94339900	0.00806400	2.28160100
H	3.01256900	1.35188100	2.34735800
C	-1.84260700	-2.27148200	-1.78402900
C	-4.63645700	-0.07472800	-0.24642000
C	-3.78840300	1.20453500	-0.32610600
C	-3.70886900	-1.27781100	-0.43744000
C	-3.04115000	1.32349000	-1.67826800
C	-4.02620200	1.72388200	-2.79261300
C	-2.96578800	-1.22314600	-1.79455200
C	-1.98092100	2.42864100	-1.56448300
C	-3.92963300	-1.57969300	-2.94145300
H	-5.35744700	-0.06200100	-1.07243600
H	-4.42066900	2.09034400	-0.17185600
H	-1.43000900	0.08629400	-1.53473200
H	-6.14489700	0.53897800	0.96080500
H	-4.23901200	-2.62782700	-2.85009700
H	-3.42197700	-1.44121000	-3.90129400
H	-4.83460400	-0.96817200	-2.94038200
H	-2.25779000	-3.26659200	-1.58816800
H	-1.10701100	-2.03515300	-1.00912000
H	-1.32906500	-2.28639800	-2.75217600
H	-3.50959400	1.71793200	-3.75784000
H	-4.41011500	2.73334700	-2.60126000
H	-4.88357100	1.05071400	-2.85888000
H	-1.46319500	2.55703300	-2.52200200
H	-1.24035300	2.16708800	-0.80302100
H	-2.45129400	3.37811200	-1.28564100
H	-4.28329300	-2.20922800	-0.35861000
H	-2.95812800	-1.28173200	0.36213600
H	-3.04242400	1.18672000	0.47761700
N	-2.31901400	0.08424900	-2.03198000
N	-5.45774800	-0.21124900	0.96872800
C	-4.72555100	-0.14134000	2.23135200
H	-5.43240600	-0.25419700	3.06067300
H	-4.16609500	0.79756400	2.38680600
H	-4.00945600	-0.96731100	2.28404500

III. $^{2}TS_{ET}$

Fe	-1.30943900	0.00004800	0.37424000
N	-0.48083000	-1.68747200	1.10283700
C	0.57344600	-1.77113300	1.97145000
C	0.91376100	-3.15197400	2.21334600
C	0.04039200	-3.90262800	1.48609100
C	-0.83048800	-2.97789300	0.80282200
H	1.71633500	-3.47869000	2.86177100
H	-0.02923200	-4.97973100	1.40768300
C	-1.87765100	-3.35301100	-0.02746800
H	-2.04106300	-4.41495700	-0.17801000
N	-2.69277600	-1.11062100	-0.58231100
C	-2.74260200	-2.47514500	-0.66686900
C	-3.83863200	-2.88406300	-1.51382100
C	-4.44694000	-1.74392900	-1.94153900
C	-3.71808400	-0.64194400	-1.35803400
H	-4.08933200	-3.91343200	-1.73499400
H	-5.30503700	-1.63309900	-2.59176800
C	-4.01906200	0.69479400	-1.57612100
H	-4.86370100	0.91634200	-2.22010700
N	-2.24431500	1.68944700	-0.20828500
C	-3.32230500	1.77230400	-1.04605700
C	-3.64833800	3.15473900	-1.30782400
C	-2.74851700	3.90549300	-0.61564000
C	-1.87720600	2.97921300	0.06797400
H	-4.46302800	3.48103700	-1.94112700
H	-2.66459400	4.98272400	-0.55427400
C	-0.83300900	3.35534600	0.89938700
H	-0.66659700	4.41703200	1.04781700
N	-0.04157200	1.11001600	1.48278100
C	0.00767000	2.47543900	1.56913600
C	1.05263400	2.88395600	2.47379400
C	1.62416400	1.74286600	2.95037900
C	0.93383500	0.64140900	2.32540900
H	1.29168900	3.91304900	2.70795200
H	2.43236400	1.63459600	3.66138700
C	1.22690200	-0.69407200	2.55301100
H	2.03796500	-0.91586500	3.23668400
O	-0.36172100	0.00107200	-0.98883200
S	-2.78270600	-0.03828600	2.31345100
H	-3.07419400	-1.34847700	2.19869800
C	1.51532600	2.41051500	-1.71459800
C	4.32684300	0.02289900	-0.48643500
C	3.43433800	-1.22495000	-0.59520800

C	3.42898400	1.26387300	-0.52905200
C	2.60014100	-1.23562000	-1.90416700
C	3.50525500	-1.53924200	-3.12154900
C	2.59606200	1.32734600	-1.83980700
C	1.52753200	-2.33062600	-1.82272200
C	3.50369300	1.69281000	-3.03877700
H	4.99197600	0.05024700	-1.35659900
H	4.03975000	-2.13928400	-0.55983000
H	0.88972200	0.04069300	-1.73396500
H	5.91318700	-0.68720400	0.55065300
H	3.81378800	2.73675100	-2.92601900
H	2.94474500	1.59043600	-3.97390900
H	4.40376100	1.08097000	-3.10003200
H	1.99030700	3.37234900	-1.49815300
H	0.81837200	2.16391400	-0.91345200
H	0.95505600	2.49973700	-2.65211700
H	2.94473700	-1.39526000	-4.05025500
H	3.82082300	-2.58593600	-3.05969600
H	4.40209200	-0.91995400	-3.15378400
H	0.95871700	-2.38148700	-2.75792500
H	0.83613600	-2.12582100	-1.00459000
H	2.01236600	-3.29737700	-1.65559700
H	4.03465200	2.17291900	-0.44861900
H	2.72751800	1.24210300	0.31283200
H	2.73758800	-1.24669100	0.24986700
N	1.92000700	0.05000900	-2.05114500
N	5.22529100	0.05133800	0.67498500
C	4.57696800	-0.13694900	1.97283700
H	5.34210300	-0.11257500	2.75621600
H	4.01293900	-1.07906500	2.07123800
H	3.87925900	0.68479600	2.15553400

IV. $^{4}TS_{ET}$

Fe	1.36304700	0.00254000	-0.34933400
N	0.46537200	-1.64376300	-1.11453500
C	-0.64104400	-1.67327500	-1.92078100
C	-1.02759400	-3.03820100	-2.18508500
C	-0.13223900	-3.83164700	-1.53336800
C	0.79544600	-2.94869400	-0.86902900
H	-1.87269600	-3.32666700	-2.79675800
H	-0.08548400	-4.91213700	-1.49218800
C	1.86366500	-3.37170900	-0.08834200
H	2.01171300	-4.44101600	0.02055100
N	2.73176200	-1.16281400	0.53335900
C	2.75886600	-2.53284500	0.55925600
C	3.86812800	-2.99394200	1.36107200
C	4.50623500	-1.88357700	1.82179900
C	3.78620400	-0.74517600	1.30090600
H	4.10582300	-4.03574500	1.53350100
H	5.38178600	-1.81524600	2.45450500
C	4.12465700	0.57537700	1.55732400
H	4.98857100	0.75648000	2.18816200
N	2.34694600	1.64709600	0.25512300
C	3.44564500	1.68347900	1.06820200
C	3.82008300	3.05112100	1.34417600
C	2.93198300	3.84000600	0.68020900
C	2.01618800	2.95312200	0.00142000
H	4.65836200	3.34237800	1.96378500
H	2.88248700	4.92028400	0.63528800
C	0.97084800	3.38139600	-0.80168300
H	0.84018100	4.45122000	-0.92586600
N	0.08184900	1.17995500	-1.40002500
C	0.07753100	2.54527300	-1.46196800
C	-0.99998800	3.00587500	-2.30248600
C	-1.64169500	1.89322000	-2.75757000
C	-0.95516600	0.75772600	-2.18896300
H	-1.21460200	4.04636000	-2.50881900
H	-2.49145500	1.82495600	-3.42389700
C	-1.30258300	-0.56374500	-2.42822400
H	-2.15960100	-0.74487400	-3.06661900
O	0.38918500	-0.00509100	1.00706500
S	2.71081100	-0.01503900	-2.36846700
H	2.96445000	-1.33714100	-2.31444800
C	-1.53886800	2.36780500	1.67265200
C	-4.43607800	0.04182900	0.50825800
C	-3.56065600	-1.22306000	0.55040800
C	-3.52534400	1.27415700	0.55319800
C	-2.65323100	-1.27839500	1.81059100
C	-3.49181100	-1.58694100	3.07400200
C	-2.62195500	1.29159900	1.81685500
C	-1.60070700	-2.38204100	1.65106300
C	-3.45756900	1.61243400	3.07924800
H	-5.07580600	0.05249600	1.39783200
H	-4.18240000	-2.12675300	0.53612900
H	-0.90759500	-0.01158400	1.62621200
H	-6.05682300	-0.61989300	-0.51221600
H	-3.74191600	2.66851100	3.03077800
H	-2.85789200	1.45197300	3.97995000
H	-4.37018500	1.02159000	3.15114500
H	-2.01697200	3.33495100	1.48923200
H	-0.87365800	2.12976500	0.84370200
H	-0.94489600	2.43789000	2.59028500
H	-2.88491400	-1.45028300	3.97387500
H	-3.80587200	-2.63427600	3.01887100
H	-4.38683000	-0.97043300	3.15361900
H	-0.99002400	-2.46319900	2.55682300
H	-0.94686300	-2.16614700	0.80690000
H	-2.10669200	-3.33750700	1.48255900
H	-4.12591400	2.18986500	0.54103600
H	-2.87218400	1.28349200	-0.32611000
H	-2.91215800	-1.24463700	-0.33158900
N	-1.95011700	-0.00237700	1.93461000
N	-5.36346800	0.11456600	-0.62864200
C	-4.75537300	-0.02842500	-1.95213400

H	-5.54276800	0.04088000	-2.70993000
H	-4.21132600	-0.97474700	-2.10779100
H	-4.04942000	0.78938300	-2.12215800

V. $^{2}TS_{PT}$

Fe	1.34853400	0.00382700	-0.34722400
N	0.49942100	-1.67356200	-1.08118200
C	-0.62149400	-1.74678500	-1.86494600
C	-0.96245800	-3.12607400	-2.11450000
C	-0.02532200	-3.88302600	-1.47822700
C	0.88355000	-2.96589600	-0.83512900
H	-1.80836600	-3.44848200	-2.70795200
H	0.06186800	-4.96099800	-1.43422400
C	1.97931000	-3.35276100	-0.07644200
H	2.16507300	-4.41625500	0.03035300
N	2.77661400	-1.11559500	0.53047600
C	2.85293200	-2.48112700	0.55804600
C	3.98477700	-2.89857800	1.35291300
C	4.58145500	-1.76339000	1.80971100
C	3.81604100	-0.65366300	1.28988200
H	4.26373900	-3.93020500	1.52499900
H	5.45737100	-1.66051400	2.43726600
C	4.11014800	0.67954100	1.53755500
H	4.96911300	0.89381200	2.16471600
N	2.30354300	1.68907200	0.21974400
C	3.40245500	1.76021000	1.03126800
C	3.74791300	3.14109200	1.27933300
C	2.84579100	3.89859900	0.59726400
C	1.94716800	2.97957600	-0.06175900
H	4.58004200	3.46198200	1.89275800
H	2.77556400	4.97661800	0.52920200
C	0.88965700	3.36725100	-0.87136100
H	0.73845800	4.42993000	-1.02796900
N	0.02748200	1.12803700	-1.38533000
C	0.00818600	2.49447900	-1.49364200
C	-1.08219400	2.91049100	-2.33893000
C	-1.71266100	1.77537400	-2.75250100
C	-1.00736700	0.66702000	-2.15585400
H	-1.31168600	3.94069100	-2.57844300
H	-2.56268300	1.67441700	-3.41396700
C	-1.33047200	-0.66525800	-2.36792700
H	-2.19110400	-0.87769400	-2.99218200
O	0.42250500	-0.02356400	1.06269800
S	2.73844000	0.01967700	-2.32326000
H	2.97030300	-1.30707700	-2.29666100
C	-1.52266700	2.35069100	1.63969000
C	-4.47087400	0.04332600	0.54353800
C	-3.60590500	-1.23080400	0.55016100
C	-3.55082100	1.27023300	0.57028700
C	-2.64565000	-1.29660100	1.77316600
C	-3.43205700	-1.57686900	3.07733600
C	-2.59834300	1.26878700	1.79917500
C	-1.61302900	-2.41401600	1.58192300
C	-3.37839600	1.55038100	3.10636300
H	-5.08176900	0.05084700	1.45263500
H	-4.23393200	-2.12934400	0.57249400
H	-0.78295300	-0.03751600	1.48330100
H	-6.11498400	-0.61032900	-0.44272700
H	-3.61493900	2.61873400	3.11739400
H	-2.75963700	1.32301400	3.97907700
H	-4.31354400	0.99739100	3.17767200
H	-2.01154700	3.31822300	1.48987100
H	-0.88172900	2.13365000	0.78775800
H	-0.90086100	2.40733500	2.53926500
H	-2.80618500	-1.38408800	3.95329000
H	-3.70161000	-2.63751200	3.07084100
H	-4.34949400	-0.99583200	3.15875100
H	-0.97856900	-2.50440500	2.46991700
H	-0.98027900	-2.20822200	0.72136600
H	-2.13769900	-3.36151600	1.42697700
H	-4.14230900	2.19099400	0.60064400
H	-2.93331000	1.29250700	-0.33372600
H	-2.99413700	-1.26539900	-0.35705200
N	-1.92302600	-0.02773700	1.83148400
N	-5.43083900	0.13184600	-0.56294400
C	-4.86436000	0.03174800	-1.90887800
H	-5.67974400	0.09822000	-2.63644600
H	-4.30444400	-0.89721900	-2.10579200
H	-4.18523800	0.87027700	-2.08583300

VI. $^{4}TS_{PT}$

Fe	1.35200300	0.00430500	-0.34352400
N	0.49315100	-1.66625400	-1.07861300
C	-0.63224600	-1.73314200	-1.85658700
C	-0.97662500	-3.11026700	-2.11332200
C	-0.03660600	-3.87264200	-1.48781700
C	0.87719200	-2.96115100	-0.84366100
H	-1.82643700	-3.42767700	-2.70389800
H	0.04939800	-4.95101500	-1.45173800
C	1.97589300	-3.35539300	-0.09305400
H	2.15946300	-4.42009000	0.00559000
N	2.78147300	-1.12494700	0.52396800
C	2.85474500	-2.49020100	0.54356700
C	3.98873800	-2.91513800	1.33192300
C	4.58948100	-1.78385600	1.79301600
C	3.82452000	-0.66946900	1.28163200
H	4.26618600	-3.94833300	1.49700400
H	5.46810900	-1.68646500	2.41767600
C	4.12369600	0.66210200	1.53313300
H	4.98571000	0.87100600	2.15799900
N	2.31776000	1.68438900	0.22401700
C	3.41958800	1.74770500	1.03207900
C	3.77361200	3.12641600	1.28160600
C	2.87385500	3.89013700	0.60335700

C	1.96795900	2.97688600	-0.05418400
H	4.60953100	3.44167700	1.89281800
H	2.80967800	4.96865600	0.53708600
C	0.90921700	3.37105000	-0.85962800
H	0.76350900	4.43468600	-1.01515900
N	0.03059500	1.13684700	-1.36964400
C	0.01962500	2.50394800	-1.47795800
C	-1.07402800	2.92725700	-2.31537100
C	-1.71518700	1.79643800	-2.72424200
C	-1.01221400	0.68327700	-2.13367600
H	-1.29846000	3.95897200	-2.55318900
H	-2.57024700	1.70109300	-3.38004300
C	-1.34254300	-0.64701200	-2.34801900
H	-2.20811300	-0.85399600	-2.96733800
O	0.44818200	-0.02468900	1.08264100
S	2.74165600	0.02255000	-2.32232900
H	2.95130400	-1.30815700	-2.31435500
C	-1.52936900	2.34787200	1.62947500
C	-4.48784800	0.04445700	0.54559000
C	-3.62675400	-1.23314100	0.54539100
C	-3.56834500	1.27258200	0.57092000
C	-2.65437500	-1.30095600	1.76242300
C	-3.42987100	-1.57387200	3.07331800
C	-2.60351700	1.26545500	1.79315900
C	-1.62691400	-2.42146100	1.56375200
C	-3.37173100	1.53725300	3.10806400
H	-5.09521200	0.05050500	1.45695600
H	-4.25722800	-2.12966100	0.57693200
H	-0.80428200	-0.04186000	1.44128400
H	-6.13688900	-0.60372300	-0.43679700
H	-3.59817600	2.60749700	3.13427000
H	-2.74927000	1.29387700	3.97372000
H	-4.31200600	0.99326200	3.17973300
H	-2.01982700	3.31526400	1.48448200
H	-0.89284100	2.13347000	0.77392700
H	-0.90278100	2.40318300	2.52569200
H	-2.79802400	-1.37271000	3.94300200
H	-3.69511100	-2.63554400	3.07715600
H	-4.34941300	-0.99691000	3.15837300
H	-0.98635200	-2.51351700	2.44713100
H	-0.99999900	-2.21898300	0.69850400
H	-2.15603900	-3.36716800	1.41353900
H	-4.16013000	2.19261400	0.61436600
H	-2.95862300	1.30170500	-0.33784200
H	-3.02236400	-1.27148600	-0.36639300
N	-1.93280700	-0.03233700	1.78596500
N	-5.45146100	0.13711700	-0.55743100
C	-4.89087700	0.04117400	-1.90621800
H	-5.70955800	0.11164400	-2.62961000
H	-4.33356200	-0.88804000	-2.10935500
H	-4.21139300	0.87944400	-2.08360400

VII. ^{2}IM1

Fe	1.45158800	0.00695800	-0.31346300
N	0.40509600	-1.52432400	-1.09387200
C	-0.73787100	-1.43580800	-1.84645500
C	-1.20746600	-2.75382800	-2.18792400
C	-0.32760100	-3.63937300	-1.64156700
C	0.67584200	-2.86320000	-0.95954000
H	-2.09648500	-2.95054300	-2.77280100
H	-0.34039900	-4.72082500	-1.67869500
C	1.74650500	-3.40694100	-0.26651100
H	1.83064800	-4.48781800	-0.23867700
N	2.78159200	-1.30091600	0.44664600
C	2.71899200	-2.66836800	0.38949600
C	3.82863100	-3.24491000	1.10838000
C	4.55791100	-2.20627800	1.60213400
C	3.89603400	-0.99533300	1.18126500
H	4.00384900	-4.30812900	1.20941000
H	5.46224500	-2.23169800	2.19608800
C	4.34527100	0.28075900	1.48354900
H	5.24902000	0.36721900	2.07695600
N	2.58970600	1.54436000	0.32359700
C	3.73204200	1.45418200	1.07412400
C	4.22763400	2.77393200	1.38173900
C	3.37261200	3.65988800	0.80058300
C	2.35284600	2.88115800	0.14157100
H	5.11735000	2.97018200	1.96584400
H	3.40771200	4.74158100	0.80343200
C	1.29896900	3.42501800	-0.57540500
H	1.24224400	4.50548100	-0.64887500
N	0.21323100	1.31546600	-1.20918800
C	0.31277000	2.68480400	-1.20807900
C	-0.78104900	3.25986900	-1.94643000
C	-1.53932900	2.22239700	-2.39994800
C	-0.90503500	1.01237500	-1.94356300
H	-0.93100900	4.32255200	-2.08495900
H	-2.44115700	2.25006200	-2.99743000
C	-1.36220800	-0.26195300	-2.23728900
H	-2.26685600	-0.34742700	-2.82738800
O	0.55823600	-0.01119600	1.19473900
S	2.73548800	0.00547900	-2.30830700
H	2.87296700	-1.33408800	-2.34349100
C	-1.74573300	2.33195700	1.58494900
C	-4.67601200	0.04484200	0.42980800
C	-3.80944500	-1.22575900	0.44148100
C	-3.76327200	1.27259200	0.50196800
C	-2.86046000	-1.28905300	1.66892700
C	-3.65888100	-1.59135700	2.96246100
C	-2.81333800	1.23761400	1.72731700
C	-1.83431800	-2.41526900	1.48144200
C	-3.59622900	1.51094100	3.03668000
H	-5.31476600	0.03641200	1.32036700
H	-4.43954400	-2.12421300	0.44115300

H	-0.44849200	-0.03390700	1.27596700
H	-6.28265500	-0.60009000	-0.62736600
H	-3.81285600	2.58343600	3.08210000
H	-2.99013000	1.24393300	3.90789400
H	-4.54376800	0.97532600	3.08795500
H	-2.22663500	3.30860600	1.46213800
H	-1.11392200	2.13379600	0.72098400
H	-1.11109500	2.36037900	2.47742600
H	-3.04262400	-1.39860500	3.84595800
H	-3.92582300	-2.65345000	2.95309500
H	-4.57928300	-1.01380200	3.04180200
H	-1.19951800	-2.49837300	2.37051800
H	-1.19967200	-2.21084400	0.62178000
H	-2.34974500	-3.36925200	1.32555600
H	-4.36221200	2.18905200	0.54261400
H	-3.14225600	1.31856600	-0.39807600
H	-3.18989100	-1.25034400	-0.46067600
N	-2.10576500	-0.04094400	1.75172300
N	-5.60261200	0.15154400	-0.70772000
C	-4.99174900	0.07824400	-2.03575600
H	-5.78317800	0.14245400	-2.78963100
H	-4.41178600	-0.84052400	-2.22785900
H	-4.32038000	0.93072100	-2.18280500

VIII. ^{4}IM1

Fe	1.44901400	0.00678000	-0.31485000
N	0.40478900	-1.52344300	-1.09732900
C	-0.73910000	-1.43538000	-1.84889400
C	-1.20854600	-2.75340300	-2.19005300
C	-0.32846900	-3.63884900	-1.64386700
C	0.67521500	-2.86280700	-0.96238600
H	-2.09763100	-2.95029400	-2.77474100
H	-0.34141900	-4.72031300	-1.68072400
C	1.74493800	-3.40719200	-0.26863200
H	1.82867600	-4.48812400	-0.24146000
N	2.77833300	-1.30226300	0.44796300
C	2.71649400	-2.66920900	0.38968100
C	3.82570200	-3.24604100	1.10934600
C	4.55411400	-2.20742400	1.60431600
C	3.89204200	-0.99645900	1.18318300
H	4.00125900	-4.30926600	1.20980800
H	5.45802700	-2.23283300	2.19891100
C	4.34101500	0.27991100	1.48478300
H	5.24405300	0.36672400	2.07925900
N	2.58807400	1.54432200	0.32083800
C	3.72896200	1.45341000	1.07346500
C	4.22444000	2.77297900	1.38209000
C	3.37057400	3.65938400	0.79979500
C	2.35151600	2.88105600	0.13928200
H	5.11322900	2.96888600	1.96772000
H	3.40599400	4.74106900	0.80308200
C	1.29789000	3.42476300	-0.57851600
H	1.24158300	4.50518400	-0.65296600
N	0.21019300	1.31500400	-1.20938200
C	0.31141400	2.68447100	-1.21029500
C	-0.78149200	3.25979400	-1.94983600
C	-1.54053300	2.22266200	-2.40265000
C	-0.90776400	1.01249100	-1.94454400
H	-0.93017300	4.32246600	-2.08983400
H	-2.44160400	2.25047000	-3.00123900
C	-1.36464000	-0.26180700	-2.23878800
H	-2.26934600	-0.34743600	-2.82883900
O	0.56352700	-0.01183000	1.19802300
S	2.74703100	0.00809200	-2.30120000
H	2.84489400	-1.33394400	-2.36388000
C	-1.74836400	2.33802500	1.57762500
C	-4.67611800	0.04090100	0.43419500
C	-3.80663600	-1.22807600	0.44642300
C	-3.76709400	1.27197100	0.50240500
C	-2.85358700	-1.28621400	1.67161100
C	-3.64773800	-1.58400400	2.96859400
C	-2.81232100	1.24087800	1.72488700
C	-1.82665500	-2.41182600	1.48506000
C	-3.59095200	1.51184500	3.03687100
H	-5.31355700	0.03242100	1.32571300
H	-4.43496900	-2.12774000	0.45078400
H	-0.44482000	-0.02938000	1.27497900
H	-6.28381800	-0.60939600	-0.61815300
H	-3.80571200	2.58454600	3.08592100
H	-2.98313000	1.24167100	3.90588200
H	-4.53928600	0.97789100	3.08929200
H	-2.23219300	3.31345200	1.45673700
H	-1.12017700	2.14077300	0.71100300
H	-1.10981700	2.36845000	2.46729400
H	-3.03036000	-1.38342400	3.84957300
H	-3.91014900	-2.64727700	2.96654800
H	-4.57071400	-1.01048900	3.04716900
H	-1.19213600	-2.49473300	2.37437000
H	-1.19130800	-2.20658000	0.62618400
H	-2.34140200	-3.36614500	1.32915700
H	-4.36890000	2.18645800	0.54497900
H	-3.14903300	1.31945200	-0.39955000
H	-3.18968600	-1.25383500	-0.45744400
N	-2.10154700	-0.03577100	1.73802800
N	-5.60496100	0.14292600	-0.70195000
C	-4.99657800	0.06708000	-2.03096700
H	-5.78945300	0.12953000	-2.78347100
H	-4.41665000	-0.85189600	-2.22229800
H	-4.32588400	0.91956300	-2.18094700

Stepwise ring contraction process via C-C bond cleavage and C-N bond formation

I. $^{2}TS_{CC}$

Fe	1.42873400	-0.02870900	-0.33893500
N	0.22274600	-1.44248800	-1.11197400
C	-0.88759000	-1.23604500	-1.88802000
C	-1.49817200	-2.49764200	-2.22283100
C	-0.73795700	-3.46901900	-1.64348900
C	0.33860200	-2.80135300	-0.95805400
H	-2.39119300	-2.60021800	-2.82544900
H	-0.87352300	-4.54242300	-1.66604500
C	1.34127100	-3.45357800	-0.25723900
H	1.30167400	-4.53653000	-0.21375200
N	2.61943600	-1.46988200	0.41043200
C	2.40081900	-2.82179800	0.37540300
C	3.45411700	-3.51213200	1.07883200
C	4.31014000	-2.55750400	1.53752400
C	3.77769400	-1.28413900	1.11625300
H	3.50922400	-4.58708400	1.19212000
H	5.22011300	-2.67848100	2.11092000
C	4.36445900	-0.06188900	1.40699400
H	5.28657700	-0.07176300	1.97792700
N	2.71035800	1.38302200	0.31182200
C	3.85588700	1.17186900	1.03236600
C	4.47123400	2.43411300	1.36517900
C	3.67993400	3.40791600	0.83656900
C	2.58355500	2.74003500	0.17826200
H	5.38767700	2.53500800	1.93209900
H	3.80663000	4.48216600	0.87246300
C	1.56894700	3.39430700	-0.50302700
H	1.60113300	4.47778800	-0.53733400
N	0.31965300	1.40503700	-1.21463400
C	0.52643600	2.76028900	-1.16068900
C	-0.50584800	3.44742300	-1.89307300
C	-1.33145000	2.49008500	-2.40157800
C	-0.80453500	1.21762900	-1.97675500
H	-0.56859400	4.52305600	-1.99412500
H	-2.21888200	2.61026100	-3.00952400
C	-1.37182300	-0.00444900	-2.29942100
H	-2.26553300	0.00198000	-2.91144200
O	0.54208300	0.04254400	1.15946600
S	2.70523900	-0.14248000	-2.33946900
H	2.73733200	-1.48889100	-2.36851400
C	-1.56006700	2.55870600	1.58582300
C	-4.61827100	0.05159000	0.35211000
C	-3.66874300	-1.14002200	0.59588900
C	-3.86640000	1.33601500	0.12038900
C	-2.78932200	-1.03122400	1.86952600
C	-3.62874400	-1.18611000	3.15697300
C	-2.49990300	1.41869700	1.92624400
C	-1.75688800	-2.17123900	1.84787100
C	-3.60273300	1.84945800	2.89263800
H	-5.25277800	0.17423300	1.23788900
H	-4.26533100	-2.05897500	0.66959600
H	-0.48669800	0.08340400	1.21257900
H	-6.15424100	-0.97245700	-0.50010600
H	-3.81089700	2.91235600	2.74358300
H	-3.23390600	1.71572400	3.91700700
H	-4.53619500	1.30274200	2.79343700
H	-2.09919200	3.34798300	1.05202900
H	-0.72283500	2.21455100	0.98181000
H	-1.17430800	2.99726800	2.51619600
H	-3.05733400	-0.84477000	4.02622000
H	-3.86117900	-2.24727900	3.29782900
H	-4.57609900	-0.64685100	3.12882300
H	-1.13003700	-2.13327800	2.74591500
H	-1.11148500	-2.08266500	0.97392300
H	-2.27008800	-3.13860200	1.81898000
H	-4.39883700	2.27285700	0.26131900
H	-3.06930900	1.33948900	-0.61454800
H	-3.00080100	-1.24781000	-0.26350200
N	-2.02487100	0.21349400	1.73278800
N	-5.57802300	-0.17359200	-0.75708100
C	-4.96629300	-0.44166300	-2.05988000
H	-5.76015000	-0.64027400	-2.78730700
H	-4.26505700	-1.29261400	-2.07481600
H	-4.41867200	0.44678000	-2.39231400

II. $^{4}TS_{CC}$

Fe	1.41272300	-0.02579100	-0.34327400
N	0.08767900	1.14533100	-1.30784500
C	0.09153100	2.51520400	-1.37812800
C	-1.00006700	2.97214700	-2.19850600
C	-1.64744700	1.85967700	-2.64695200
C	-0.96099200	0.72370200	-2.08527900
H	-1.21585800	4.01264600	-2.40307800
H	-2.50989800	1.79147100	-3.29684700
C	-1.32803500	-0.59334600	-2.30720800
H	-2.19794100	-0.77469600	-2.92697400
N	0.44638600	-1.66509700	-0.99384800
C	-0.67731900	-1.69723100	-1.77763600
C	-1.10824600	-3.05858800	-1.96820800
C	-0.23039300	-3.84821000	-1.28791700
C	0.74072600	-2.97010200	-0.68682700
H	-1.97528300	-3.34754600	-2.54795300
H	-0.22067600	-4.92596900	-1.19025800
C	1.81942600	-3.39985100	0.07110300
H	1.92877700	-4.46729300	0.22898100
N	2.80661200	-1.20081500	0.51584000
C	2.78330500	-2.56601700	0.61668400
C	3.93232400	-3.02708600	1.35810800
C	4.64876100	-1.92016000	1.69810200
C	3.93299400	-0.78302000	1.17060200

H	4.14249700	-4.06655300	1.57430000
H	5.57348100	-1.85319300	2.25644200
C	4.33407800	0.53388000	1.33692500
H	5.25216000	0.71264000	1.88630200
N	2.46950900	1.61442800	0.16077000
C	3.63967100	1.64032500	0.87289100
C	4.04990100	3.00508700	1.09993900
C	3.10847200	3.80018200	0.52063800
C	2.12669100	2.92105100	-0.06642500
H	4.94355000	3.29134600	1.63921800
H	3.06337300	4.88069900	0.47763200
C	1.01977300	3.35392000	-0.77984200
H	0.88504200	4.42300000	-0.90226000
O	0.53096900	0.01010600	1.15533000
S	2.69833600	-0.09513200	-2.33767700
H	2.71366800	-1.43975100	-2.41520100
C	-1.50535200	2.49893200	1.73639500
C	-4.58330500	0.09491900	0.35141900
C	-3.64869400	-1.11737300	0.54249500
C	-3.81958400	1.38396700	0.19526600
C	-2.78468900	-1.08624000	1.83039400
C	-3.64051500	-1.29608300	3.09863300
C	-2.45998100	1.35520000	2.01958300
C	-1.76455900	-2.23571800	1.76320500
C	-3.56496700	1.74720100	2.99862000
H	-5.22865000	0.17806900	1.23400400
H	-4.25344700	-2.03388000	0.55693900
H	-0.50254700	0.04645300	1.22924100
H	-6.15875200	-0.82145400	-0.55500600
H	-3.75638700	2.81976100	2.90910800
H	-3.20931900	1.54866400	4.01702500
H	-4.50478600	1.22036900	2.85780400
H	-2.04527000	3.33469600	1.27926600
H	-0.69020700	2.18823400	1.08468200
H	-1.08679500	2.86038500	2.68564800
H	-3.07696400	-1.00297400	3.99018500
H	-3.88333600	-2.36081300	3.18421200
H	-4.58302500	-0.74775000	3.08574200
H	-1.15746500	-2.25627900	2.67522600
H	-1.09985600	-2.10730900	0.90927900
H	-2.28830500	-3.19308100	1.66946800
H	-4.34586800	2.31535400	0.38577500
H	-3.01559400	1.42395200	-0.53038500
H	-2.96925000	-1.18267500	-0.31275100
N	-2.00445200	0.15537700	1.76377900
N	-5.52934000	-0.05443200	-0.78180700
C	-4.90177000	-0.33236900	-2.07510600
H	-5.68057000	-0.38759200	-2.84305700
H	-4.31568300	-1.26589200	-2.11124600
H	-4.22792900	0.49126100	-2.33219300

III. ^{2}IM2

Fe	1.45262400	-0.10558300	-0.32841700
N	0.12414100	-1.48196600	-0.95112500
C	-1.00080700	-1.25563400	-1.70082400
C	-1.68865000	-2.49810800	-1.94540600
C	-0.97121500	-3.47500500	-1.32276000
C	0.16278500	-2.83229400	-0.71020400
H	-2.60616300	-2.58403500	-2.51163300
H	-1.16983800	-4.53768700	-1.27342700
C	1.14967900	-3.50101900	-0.00186000
H	1.04214900	-4.57337800	0.11936700
N	2.58512200	-1.56853000	0.46509500
C	2.27637100	-2.90140700	0.53855300
C	3.31735900	-3.61268000	1.23930500
C	4.25863500	-2.69084200	1.58382400
C	3.79041600	-1.41575000	1.09714100
H	3.30752400	-4.67835000	1.42800800
H	5.18859800	-2.83533200	2.11827900
C	4.47328400	-0.22088800	1.26443300
H	5.42369300	-0.25469200	1.78602600
N	2.85422600	1.25538500	0.15688800
C	4.02588500	1.01570800	0.82616700
C	4.73930700	2.25232900	1.03293600
C	3.98072800	3.24047500	0.48279600
C	2.80561300	2.60717300	-0.06279000
H	5.69274600	2.32898000	1.53934900
H	4.17710000	4.30383300	0.43700700
C	1.79027800	3.28424100	-0.71988800
H	1.88793500	4.35892400	-0.82770400
N	0.37332800	1.34382200	-1.21596900
C	0.66526600	2.68238900	-1.26106800
C	-0.37307900	3.39206300	-1.96319900
C	-1.29102000	2.46257100	-2.35176500
C	-0.80944800	1.18492100	-1.89137900
H	-0.37632900	4.46166900	-2.12789000
H	-2.21112900	2.60269200	-2.90378200
C	-1.45079600	-0.01870000	-2.13390500
H	-2.38172800	0.01182300	-2.68816600
O	0.63679800	0.10921700	1.20306800
S	2.60313500	-0.41952900	-2.37636600
H	2.42578200	-1.75481700	-2.39640800
C	-1.09943700	2.87762600	1.50251600
C	-4.77868400	0.06125900	0.23503400
C	-3.66896400	-0.90061800	0.72018900
C	-4.25384100	1.23165000	-0.53447900
C	-2.81249300	-0.50982200	1.94845500
C	-3.67508500	-0.36843100	3.21818500
C	-2.17761700	1.88222400	1.85457300
C	-1.83171500	-1.67750000	2.19333500
C	-3.43972500	2.51186800	2.41396900
H	-5.32555500	0.42416900	1.12259400
H	-4.15503500	-1.84968400	0.98326900
H	-0.37321100	0.27371400	1.21791600

H	-6.28203300	-1.29674900	0.03362600
H	-3.43990200	3.58425800	2.20036600
H	-3.47711900	2.38299100	3.50125100
H	-4.33861700	2.07194600	1.98391200
H	-1.41226400	3.44698900	0.61763900
H	-0.14922200	2.38943200	1.28918900
H	-0.97844200	3.59694100	2.32211000
H	-3.06649800	0.01206800	4.04545300
H	-4.04593800	-1.36058200	3.49669500
H	-4.53989900	0.28435500	3.09547900
H	-1.19930700	-1.46249300	3.06143900
H	-1.18483300	-1.82310000	1.32534900
H	-2.39110500	-2.59968300	2.38427900
H	-4.95598700	1.84444500	-1.09199300
H	-3.20114100	1.47771400	-0.54782000
H	-2.99155600	-1.11088600	-0.10916600
N	-1.94090800	0.64400100	1.63829200
N	-5.82033200	-0.61886800	-0.56893400
C	-5.30013100	-1.32195200	-1.74420600
H	-6.13488500	-1.76940200	-2.29423100
H	-4.57150400	-2.11671300	-1.51427000
H	-4.80550500	-0.59744500	-2.40178300

IV. ^{4}IM2

Fe	1.45263500	-0.10547300	-0.32816600
N	0.12472500	-1.48246900	-0.95053100
C	-1.00046900	-1.25671100	-1.70004900
C	-1.68795000	-2.49946800	-1.94416800
C	-0.96997700	-3.47598700	-1.32155200
C	0.16391600	-2.83274500	-0.70937200
H	-2.60559700	-2.58586300	-2.51012000
H	-1.16820400	-4.53873100	-1.27196200
C	1.15120700	-3.50099000	-0.00114500
H	1.04410600	-4.57336500	0.12031200
N	2.58596000	-1.56782300	0.46515800
C	2.27777700	-2.90082800	0.53888700
C	3.31918700	-3.61157400	1.23952600
C	4.26013600	-2.68930000	1.58376600
C	3.79131400	-1.41447600	1.09699000
H	3.30982300	-4.67722200	1.42838000
H	5.19025200	-2.83333700	2.11807700
C	4.47375500	-0.21934600	1.26399600
H	5.42425900	-0.25269500	1.78544400
N	2.85393300	1.25606600	0.15642600
C	4.02580700	1.01697800	0.82554800
C	4.73882500	2.25389600	1.03190100
C	3.97978300	3.24164900	0.48170000
C	2.80480000	2.60780300	-0.06351500
H	5.69233700	2.33100300	1.53810700
H	4.17576500	4.30506800	0.43564200
C	1.78908000	3.28438100	-0.72049600
H	1.88629200	4.35908400	-0.82850900
N	0.37279000	1.34330300	-1.21593800
C	0.66418700	2.68198700	-1.26129300
C	-0.37457900	3.39115400	-1.96329200
C	-1.29225000	2.46126000	-2.35151500
C	-0.81008000	1.18386000	-1.89107000
H	-0.37826700	4.46073200	-2.12815600
H	-2.21252700	2.60095800	-2.90335400
C	-1.45101700	-0.02003400	-2.13326900
H	-2.38210300	0.01005300	-2.68729100
O	0.63699500	0.10933200	1.20347400
S	2.60319000	-0.41945800	-2.37658400
H	2.42627800	-1.75481500	-2.39593400
C	-1.09978100	2.87712600	1.50319400
C	-4.77901400	0.06135600	0.23458800
C	-3.66944900	-0.90073500	0.71967200
C	-4.25397100	1.23195300	-0.53447500
C	-2.81293300	-0.51038400	1.94806300
C	-3.67545900	-0.36945100	3.21788300
C	-2.17792000	1.88165400	1.85519200
C	-1.83225300	-1.67823200	2.19247600
C	-3.43980800	2.51115700	2.41526800
H	-5.32607600	0.42400000	1.12213100
H	-4.15567100	-1.84980900	0.98245100
H	-0.37302100	0.27345900	1.21812700
H	-6.28206600	-1.29685200	0.03225000
H	-3.43992700	3.58366100	2.20223800
H	-3.47690300	2.38170200	3.50249300
H	-4.33888300	2.07159100	1.98524600
H	-1.41280400	3.44683200	0.61860300
H	-0.14967200	2.38893200	1.28941800
H	-0.97849800	3.59613000	2.32302100
H	-3.06676600	0.01054200	4.04531000
H	-4.04646600	-1.36168000	3.49591500
H	-4.54015300	0.28355300	3.09555500
H	-1.19979800	-1.46357300	3.06062900
H	-1.18541200	-1.82356600	1.32441500
H	-2.39170200	-2.60044600	2.38310800
H	-4.95597700	1.84478900	-1.09211800
H	-3.20127500	1.47812000	-0.54738800
H	-2.99199100	-1.11087200	-0.10965800
N	-1.94132200	0.64352400	1.63829500
N	-5.82047100	-0.61849300	-0.56985200
C	-5.30000700	-1.32066100	-1.74555900
H	-6.13458700	-1.76815500	-2.29581000
H	-4.57100500	-2.11524000	-1.51613900
H	-4.80575400	-0.59553700	-2.40273800

V. ^{4}TS3

Fe	1.39357000	0.12767400	-0.45268900
N	0.50080500	-1.34677400	-1.44113600
C	-0.64763600	-1.25839800	-2.19007000
C	-0.99995000	-2.57158600	-2.67878000

C	-0.06170200	-3.44121900	-2.20409800
C	0.88082100	-2.66868500	-1.42898600
H	-1.86232000	-2.78237100	-3.29894800
H	0.00432200	-4.51106700	-2.35745300
C	1.99830700	-3.22455300	-0.79703900
H	2.13322100	-4.29497300	-0.92333100
N	2.90678300	-1.21228100	0.20025500
C	2.95657800	-2.54360600	-0.04207700
C	4.14411400	-3.11197600	0.57913700
C	4.79296100	-2.07754100	1.18896000
C	3.99520900	-0.88614200	0.93842600
H	4.43107400	-4.15589500	0.54267500
H	5.71790000	-2.10439900	1.75213500
C	4.26903400	0.41229500	1.37298700
H	5.16788400	0.55966500	1.96478100
N	2.32479600	1.63613300	0.42468700
C	3.49251700	1.55393000	1.14192000
C	3.81112900	2.85659100	1.68148900
C	2.81818300	3.70628300	1.29036600
C	1.88314800	2.93400800	0.50336200
H	4.68389300	3.07169400	2.28522900
H	2.71049900	4.76202300	1.50576900
C	0.72333200	3.47537100	-0.06256200
H	0.56830900	4.53874400	0.09618700
N	-0.17056800	1.47032800	-1.09881000
C	-0.22726600	2.80049100	-0.83275500
C	-1.36078900	3.38844600	-1.52349000
C	-1.95152000	2.37802200	-2.23105300
C	-1.18434300	1.17447200	-1.95072900
H	-1.64201100	4.43406000	-1.49028300
H	-2.80728900	2.43976600	-2.89050500
C	-1.40587600	-0.11138600	-2.45567200
H	-2.24030700	-0.24725100	-3.13774300
O	0.40223400	-0.23263300	1.09315900
S	2.73040400	0.65926300	-2.47409300
H	2.40242400	-0.47954100	-3.11548900
C	-1.40214600	1.37188300	3.21133500
C	-4.74383500	0.10357200	0.49204000
C	-4.00063500	-1.17312600	0.17185400
C	-3.82654200	1.21465300	0.68864400
C	-3.17289900	-1.52272600	1.45701300
C	-4.11025100	-2.19173600	2.47889500
C	-1.84177900	-0.03921100	2.91731700
C	-2.03522200	-2.46916700	1.03369300
C	-1.11008800	-1.09353500	3.70984800
H	-5.50860200	-0.01785000	1.25753600
H	-4.66010500	-2.00741000	-0.08102500
H	-0.47729500	0.11737900	0.89898700
H	-6.04590000	1.54320700	-0.30738700
H	-0.86146200	-0.71239100	4.70483100
H	-0.17810400	-1.27346200	3.16037700
H	-1.65443700	-2.03126700	3.80521800
H	-1.51311100	1.60023400	4.27771000
H	-1.95704100	2.09831400	2.61327800
H	-0.33690100	1.43861200	2.95729300
H	-3.57912700	-2.45743400	3.39506700
H	-4.52356700	-3.10852200	2.04501300
H	-4.93974800	-1.53052000	2.75056500
H	-1.57464200	-2.95698700	1.89493600
H	-1.25714400	-1.92158600	0.49533100
H	-2.44363600	-3.24735400	0.37943800
H	-4.04689300	2.02699500	1.37052200
H	-2.95922600	1.29431300	0.04417800
H	-3.30829100	-1.00569900	-0.66043400
N	-2.68521800	-0.22067900	1.97414500
N	-5.17486100	1.07864500	-0.53789600
C	-4.97322400	0.81596400	-1.96321500
H	-5.17648700	1.73086700	-2.52318700
H	-5.63577700	0.01181900	-2.30502600
H	-3.93719400	0.52568600	-2.12541200

VI. ^{2}PC

Fe	1.22756700	0.20355400	0.62226700
N	0.72432100	2.12692500	0.36974000
C	-0.31333900	2.81021900	0.95195400
C	-0.30343600	4.19130400	0.53465300
C	0.76660200	4.33965800	-0.29482800
C	1.40086800	3.04680800	-0.38895200
H	-1.02582300	4.93225700	0.85221700
H	1.10882100	5.22814700	-0.80969800
C	2.50341800	2.77946800	-1.18717800
H	2.93007900	3.60797200	-1.74310400
N	2.68328500	0.37217900	-0.74113600
C	3.08444100	1.53074200	-1.35671700
C	4.19646600	1.26942100	-2.23843400
C	4.46660600	-0.06252300	-2.14505900
C	3.52341600	-0.61085500	-1.20130400
H	4.68830800	2.02140900	-2.84207800
H	5.22946700	-0.63843400	-2.65301500
C	3.50557500	-1.93955200	-0.79979000
H	4.23740800	-2.60789800	-1.24142100
N	1.64493500	-1.76598500	0.78557600
C	2.63369700	-2.47040800	0.14053700
C	2.63552800	-3.84431500	0.57684000
C	1.63620000	-3.96463600	1.49615200
C	1.02266500	-2.66532000	1.61740400
H	3.31760200	-4.60210300	0.21309100
H	1.32276800	-4.84287900	2.04581800
C	-0.06857300	-2.38871800	2.42897000
H	-0.46795200	-3.20497000	3.02193000
N	-0.34953900	-0.01545400	1.85832800
C	-0.70521000	-1.15871000	2.52678400
C	-1.86442700	-0.91667400	3.35283700

C	-2.19981300	0.39218800	3.18197600
C	-1.24491500	0.94488300	2.25266900
H	-2.34133700	-1.66486900	3.97289600
H	-3.01212500	0.94975200	3.62888600
C	-1.23958200	2.26648100	1.83014800
H	-2.00957000	2.92288700	2.22100900
O	-0.04412900	-0.51388200	-0.92907800
S	2.61195100	0.75651600	2.31190200
H	3.52072400	-0.21258400	2.07919000
C	-2.05571500	-2.63975400	-0.78686300
C	-4.34485900	0.25022800	-1.11664700
C	-2.89737700	0.75344900	-1.21151400
C	-4.10970700	-1.21565400	-0.75848400
C	-0.82148400	-0.20505000	-2.15871100
C	-0.29795300	-1.14455100	-3.25216400
C	-2.88859600	-1.64081800	-1.61385900
C	-0.42873500	1.22758200	-2.51571000
C	-3.36969100	-2.30795200	-2.91372100
H	-4.77674700	0.29754000	-2.12360300
H	-2.83452200	1.69802800	-1.75976200
H	0.10012000	-1.46718400	-0.86956100
H	-5.52432600	1.83178100	-0.66414900
H	-3.89736000	-3.24195300	-2.68599800
H	-2.53296900	-2.53885100	-3.57798000
H	-4.05427000	-1.63896800	-3.44596500
H	-2.70587200	-3.47603600	-0.50571300
H	-1.68373000	-2.17506000	0.12962000
H	-1.21517100	-3.06725600	-1.34436700
H	0.77832800	-0.98634700	-3.36583600
H	-0.79885700	-0.91926400	-4.19732600
H	-0.46952700	-2.19641900	-3.01598000
H	0.64710400	1.26239200	-2.69740300
H	-0.65632900	1.91715900	-1.70459100
H	-0.96698000	1.53482000	-3.41736300
H	-4.98078000	-1.85054500	-0.94471100
H	-3.85583300	-1.28682800	0.30580100
H	-2.46699100	0.90666400	-0.21078300
N	-2.22888100	-0.32907100	-1.94335900
N	-5.27226600	0.94812900	-0.23101500
C	-4.78392300	1.21375900	1.12217300
H	-5.58342300	1.69127100	1.69958900
H	-3.89051200	1.85621200	1.16894100
H	-4.52651700	0.27329500	1.61873600

VII. ^{4}PC

Fe	1.29957300	0.23528900	0.62189700
N	0.66231700	2.11238100	0.32748100
C	-0.34938900	2.75695300	0.99854000
C	-0.43842400	4.12855900	0.57089700
C	0.53818900	4.31371000	-0.36232500
C	1.22437700	3.05633600	-0.50111400
H	-1.16036900	4.84102400	0.94842200
H	0.78788300	5.21031900	-0.91458800
C	2.28927800	2.84322000	-1.36120000
H	2.62413800	3.67995800	-1.96470500
N	2.66788000	0.47781700	-0.82761500
C	2.95249800	1.63425300	-1.51132700
C	4.03930000	1.41654700	-2.43120000
C	4.41111300	0.11196300	-2.29742700
C	3.54906800	-0.46562700	-1.29790800
H	4.44736300	2.17502600	-3.08656100
H	5.18975700	-0.42891500	-2.81955100
C	3.61529100	-1.78967000	-0.88846000
H	4.37575400	-2.41673700	-1.34155300
N	1.75333600	-1.73556100	0.70868700
C	2.77346900	-2.37515800	0.04611900
C	2.84215600	-3.75509000	0.45135000
C	1.84900300	-3.94681600	1.36653300
C	1.17816300	-2.68289000	1.52241600
H	3.56070100	-4.46972500	0.07133400
H	1.58051700	-4.85138700	1.89656800
C	0.09668700	-2.46882600	2.36401900
H	-0.26712000	-3.31313300	2.93953600
N	-0.23495300	-0.08031600	1.88293400
C	-0.55684300	-1.25574500	2.52117400
C	-1.68879000	-1.05785500	3.38891200
C	-2.04210200	0.25460300	3.28116600
C	-1.13081700	0.85376600	2.34131900
H	-2.13786700	-1.83391500	3.99489700
H	-2.84404000	0.78473900	3.77741500
C	-1.17852300	2.18368900	1.94997700
H	-1.93375100	2.81428000	2.40497600
O	-0.10416700	-0.63705600	-1.07253500
S	2.89901700	0.81432000	2.42379300
H	3.89629200	0.16123700	1.79443500
C	-2.24329200	-2.64599700	-0.59820900
C	-4.37419700	0.34415300	-0.95889800
C	-2.89972300	0.73402900	-1.14441500
C	-4.22459000	-1.12140200	-0.55510600
C	-0.97177600	-0.39280400	-2.22928100
C	-0.61606000	-1.42881500	-3.30277400
C	-3.07527300	-1.66254200	-1.44559100
C	-0.54072200	0.99404100	-2.71394300
C	-3.67013600	-2.38883800	-2.66448300
H	-4.84829100	0.38651100	-1.94682700
H	-2.79393500	1.66114600	-1.71495900
H	-0.07897600	-1.58089300	-0.87579600
H	-5.43847000	2.00948100	-0.51715000
H	-4.24242900	-3.26487800	-2.33610700
H	-2.89409800	-2.72634900	-3.35543200
H	-4.34173200	-1.71466100	-3.20659200
H	-2.91265000	-3.42469100	-0.21478900
H	-1.79435300	-2.13615300	0.25849600
H	-1.46048600	-3.15644400	-1.17020500

H	0.44855800	-1.34091900	-3.53818600
H	-1.20295900	-1.24501900	-4.20675100
H	-0.81063500	-2.44971800	-2.96868300
H	0.50381000	0.94934300	-3.03135900
H	-0.61559900	1.72460200	-1.90861900
H	-1.16897600	1.30689900	-3.55306300
H	-5.14510600	-1.69914300	-0.67879300
H	-3.93020500	-1.17174400	0.49987300
H	-2.40024100	0.86952500	-0.17266000
N	-2.37142800	-0.41150200	-1.89387200
N	-5.21288800	1.13104400	-0.05957600
C	-4.63898500	1.42358500	1.25323000
H	-5.38134700	1.96095800	1.85407000
H	-3.71665800	2.02342200	1.22227800
H	-4.39784600	0.49074800	1.77269400

Concerted ring contraction process

I. ^{2}TS2

Fe	1.49597400	0.01348000	-0.35603200
N	0.19495200	-1.27873800	-1.22167300
C	-0.91453800	-0.98577800	-1.96564800
C	-1.55672800	-2.20167200	-2.41143800
C	-0.81328200	-3.23513800	-1.92146100
C	0.28218600	-2.64600800	-1.18863000
H	-2.44668200	-2.23879200	-3.02746700
H	-0.96902800	-4.29960900	-2.04312000
C	1.27129400	-3.37804000	-0.54081000
H	1.19938100	-4.46007700	-0.59394000
N	2.62125700	-1.51820800	0.31554000
C	2.35423400	-2.84843700	0.15186200
C	3.37402800	-3.64926200	0.79651300
C	4.26193500	-2.77737700	1.34773400
C	3.77777800	-1.44849400	1.04005100
H	3.38828200	-4.73184300	0.80849600
H	5.16156800	-2.98869700	1.91188900
C	4.40700200	-0.27224400	1.43183000
H	5.32715600	-0.36237000	2.00069900
N	2.80743300	1.30392100	0.46259500
C	3.94364800	1.01044000	1.16122700
C	4.59946400	2.22678800	1.59226000
C	3.83325000	3.25832400	1.14368500
C	2.71552700	2.66662800	0.43819400
H	5.51953600	2.26075200	2.16196400
H	3.98871200	4.32298700	1.26443700
C	1.70532100	3.39964000	-0.17394800
H	1.77132900	4.48144100	-0.10991400
N	0.37383700	1.54008400	-1.06371300
C	0.62670700	2.87274300	-0.87517900
C	-0.39190900	3.67178600	-1.51761200
C	-1.25930700	2.80029800	-2.10537100
C	-0.76642000	1.47310900	-1.81639100
H	-0.41863100	4.75401100	-1.50998200
H	-2.14811400	3.01287200	-2.68621300
C	-1.37204300	0.29808800	-2.24741100
H	-2.25968500	0.39074000	-2.86227600
O	0.57337300	-0.00733100	1.22979600
S	2.80013700	0.05045600	-2.37220500
H	3.99108600	-0.07684500	-1.75400400
C	-1.96182600	2.35294300	1.54170900
C	-4.69635300	-0.07017200	0.33929500
C	-3.69835400	-1.21027900	0.37592500
C	-3.94425400	1.26044500	0.40947400
C	-2.65690500	-1.22079700	1.97168500
C	-3.61172200	-1.53536900	3.11935700
C	-3.02554800	1.24569100	1.67400200
C	-1.62077700	-2.30434100	1.73414400
C	-3.83466100	1.47597400	2.96468700
H	-5.36133800	-0.15290400	1.20374800
H	-4.10878900	-2.19214000	0.62499200
H	-0.36673000	0.10293000	1.01424600
H	-6.08149600	-1.05941500	-0.79641000
H	-4.06406900	2.54393500	3.02655300
H	-3.24428400	1.20669300	3.84470200
H	-4.78132400	0.93533900	2.99092400
H	-2.46726700	3.31976400	1.45517600
H	-1.34269000	2.18532000	0.66226800
H	-1.32032000	2.36676800	2.42800800
H	-3.15652100	-1.19347200	4.05397400
H	-3.73918100	-2.61914000	3.17775000
H	-4.59039800	-1.07211000	3.01864900
H	-1.07527600	-2.44812400	2.67457400
H	-0.90967300	-2.01072900	0.96458800
H	-2.10878700	-3.25071800	1.48225800
H	-4.63233600	2.10777500	0.47549800
H	-3.30809300	1.38394200	-0.47127200
H	-2.98327200	-1.24682600	-0.44209200
N	-2.30766100	-0.01125500	1.51533200
N	-5.55271800	-0.19397900	-0.84628700
C	-4.92372500	-0.05519400	-2.16150000
H	-5.69588700	-0.20775300	-2.92068400
H	-4.10376700	-0.76111200	-2.35858700
H	-4.53174100	0.95971700	-2.27764300

II. ^{4}TS2

Fe	1.47794300	0.05522400	-0.30938900
N	0.64206000	-1.56077300	-1.11221500
C	-0.48878700	-1.60630200	-1.89098600
C	-0.79910900	-2.97805400	-2.21155900
C	0.15246600	-3.75244800	-1.61441600
C	1.05555100	-2.86006800	-0.93077700
H	-1.64060300	-3.28850400	-2.81821900
H	0.25406700	-4.83014500	-1.62931500

C	2.16694600	-3.29160800	-0.20761000
H	2.34166900	-4.36274800	-0.18013200
N	2.99422700	-1.12114600	0.51447500
C	3.07772300	-2.47637000	0.45937800
C	4.25783400	-2.92817400	1.17363800
C	4.87521100	-1.80898000	1.64835500
C	4.06688000	-0.68101800	1.22284000
H	4.55961200	-3.96255100	1.28183900
H	5.78760500	-1.73565000	2.22702700
C	4.33372400	0.66090500	1.47932700
H	5.22232300	0.89391200	2.05781200
N	2.40317000	1.69243300	0.32197300
C	3.55838800	1.74268700	1.06274600
C	3.86974000	3.11572600	1.38181000
C	2.88707300	3.88461000	0.83262300
C	1.96934200	2.98742500	0.17185500
H	4.73192500	3.42856200	1.95701300
H	2.77462900	4.96101200	0.86055200
C	0.82990200	3.41942200	-0.50613100
H	0.65825800	4.49101900	-0.53323800
N	-0.01509500	1.24756300	-1.20555000
C	-0.08741100	2.60680700	-1.16626000
C	-1.23465000	3.06214100	-1.92469800
C	-1.82796400	1.94505500	-2.43930900
C	-1.04268800	0.81450600	-1.98345400
H	-1.52462100	4.09771100	-2.05123900
H	-2.69646000	1.88023900	-3.08151700
C	-1.26347600	-0.52237800	-2.30796000
H	-2.10014500	-0.74919200	-2.96137100
O	0.48743700	-0.10256700	1.27101100
S	2.82545400	0.21043100	-2.46106200
H	3.57153300	1.24371300	-2.02366300
C	-1.96388300	2.09755100	1.82747500
C	-4.73069500	-0.11126400	0.35611400
C	-3.72225300	-1.22778400	0.20352700
C	-3.98323300	1.19967800	0.60665700
C	-2.61458500	-1.48959500	1.83531600
C	-3.55114800	-1.95096900	2.94108300
C	-3.03958400	0.99496800	1.82601900
C	-1.59761200	-2.52569300	1.41295900
C	-3.81272000	1.04557800	3.15653600
H	-5.37602900	-0.33170000	1.21172400
H	-4.09244500	-2.24221100	0.36319300
H	-0.45712200	0.00439800	1.06335700
H	-6.08390700	-0.95872900	-0.92913200
H	-4.04496400	2.09411000	3.36585100
H	-3.20005400	0.66565400	3.97868900
H	-4.75734400	0.50054900	3.13331000
H	-2.45687700	3.07167400	1.90811500
H	-1.37796700	2.06000200	0.90927000
H	-1.28864500	1.96929800	2.67817500
H	-3.10020400	-1.69757300	3.90578200
H	-3.65365800	-3.03731800	2.88716400
H	-4.53955600	-1.49890700	2.89329000
H	-1.01712800	-2.79052400	2.30529100
H	-0.91600900	-2.13076300	0.66318000
H	-2.09682500	-3.43321800	1.06017200
H	-4.67371900	2.02354400	0.80735700
H	-3.37320700	1.45589800	-0.26525800
H	-3.01380600	-1.14655200	-0.61743200
N	-2.32816100	-0.23891400	1.47796200
N	-5.60095200	-0.07191800	-0.82357000
C	-5.00842200	0.35142300	-2.09440900
H	-5.77249700	0.25309600	-2.87039000
H	-4.12389600	-0.22195000	-2.40750800
H	-4.71931400	1.40428900	-2.03239800