Supporting Information for

Role of Two Alternate Water Networks in Compound I Formation in P450eryF

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1. Complete references

25. Barry, S. M.; Kers, J. A.; Johnson, E. G.; Song, L.; Aston, P. R.; Patel, B.; Krasnoff, S. B.; Crane, B. R.; Gibson, D. M.; Loria, R.; Challis, G. L. Cytochrome P450–catalyzed L-tryptophan Nitration in Thaxtomin Phytotoxin Biosynthesis. *Nat. Chem. Biol.* **2012**, *8*, 814-816.

32. Nebert, D. W.; Nelson, D. R.; Coon, M. J.; Estabrook, R. W.; Feyereisen, R.; Fujii-Kuriyama, Y.; Gonzalez, F. J.; Guengerich, F. P.; Gunsalus, I. C.; Johnson, E. F.; Loper, J. C.; Sato, R.; Waterman, M. R.; Waxman, D. J. The P450 Superfamily: Update on New Sequences, Gene Mapping, and Recommended Nomenclature. *DNA Cell Biol.* **1991**, *10*, 1-14.

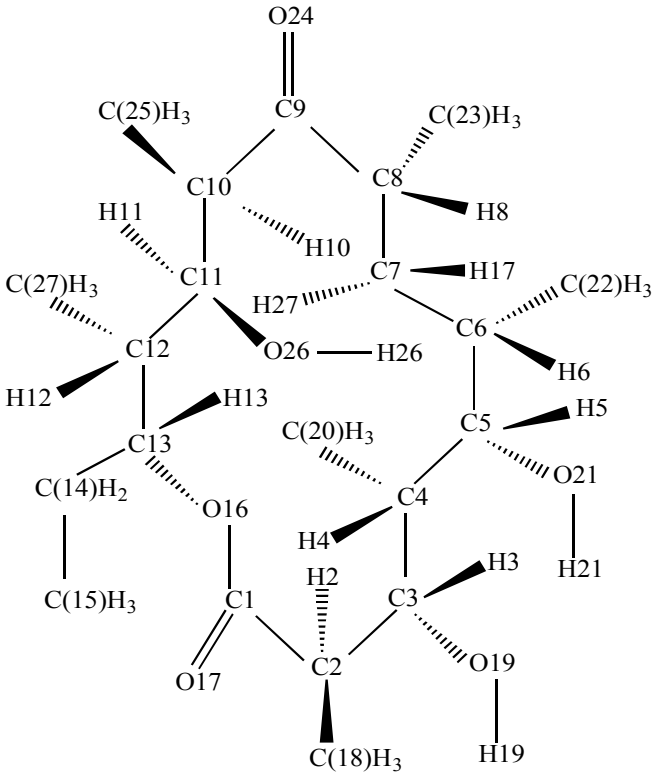
40. Zao, B.; Guengerich, F. P.; Bellamine, A.; Lamb, D. C.; Izumikawa, M.; Lei, L.; Podust, L. M.; Sundaramoorthy, M.; Kalaitzis, J. A.; Reddy, M.; Kelly, S. L.; Moore, B. S.; Stec, D.; Voehler, M.; Falck, J. R.; Shimada, T.; Waterman, M. R. Binding of Two Flaviolin Substrate Molecules, Oxidative Coupling, and Crystal Structure of *Streptomyces coelicolor* A3(2) Cytochrome P450 158A2. *J. Biol. Chem.* **2005**, *280*, 11599-11607.

50. MacKerell, A. D.; Bashford, D.; Dunbrack, R. L.; Evanseck, J. D.; Field, M. J.; Fischer, S.; Gao, J.; Guo, H.; Ha, S.; Joseph-McCarthy, D.; Kuchnir, L.; Kuczera, K.; Lau, F. T. K.; Mattos, C.; Michnick, S.; Ngo, T.; Nguyen, D. T.; Prodhom, B.; Reiher, W. E.; Roux, B.; Schlenkrich, M.; Smith, J. C.; Stote, R.; Straub, J.; Watanabe, M.; Wiórkiewicz-Kuczera, J.; Yin, D.; Karplus, M. All-Atom Empirical Potential for Molecular Modeling and Dynamics Studies of Proteins. *J. Phys. Chem. B* **1998**, *102*, 3586-3616.

58. Sherwood, P.; de Vries, A. H.; Guest, M. F.; Schreckenbach, G.; Catlow, C. R. A.; French, S. A.; Sokol, A. A.; Bromley, S. T.; Thiel, W.; Turner, A. J.; Billeter, S.; Terstegen, F.; Thiel, S.; Kendrick, J.; Rogers, S. C.; Casci, J.; Watson, M.; King, F.; Karlsen, E.; Sjøvoll, M.; Fahmi, A.; Schäfer, A.; Lennartz,C. QUASI: A General Purpose Implementation of the QM/MM Approach and its Application to Problems in Catalysis. *J. Mol. Struct.: THEOCHEM* **2003**, *632*, 1-28.

2. Partial charges and atom types of DEB

RESI DEB 0.000
GROUP
ATOM C13 CT1 0.500
ATOM H13 HA 0.050
ATOM O16 OS -0.550
GROUP
ATOM C1 CD 0.700
ATOM O17 OB -0.700
GROUP
ATOM C2 CT1 0.100
ATOM H2 HA 0.050
ATOM C18 CT3 -0.300
ATOM H118 HA 0.050
ATOM H218 HA 0.050
ATOM H318 HA 0.050
GROUP
ATOM C3 CT1 0.250
ATOM H3 HA 0.050
ATOM O19 OH1 -0.700
ATOM H19 H 0.400
GROUP
ATOM C4 CT1 0.200
ATOM H4 HA 0.050
ATOM C20 CT3 -0.400
ATOM H120 HA 0.050
ATOM H220 HA 0.050
ATOM H320 HA 0.050
GROUP
ATOM C5 CT1 0.150
ATOM H5 HA 0.050
ATOM O21 OH1 -0.600
ATOM H21 H 0.400
GROUP
ATOM C6 CT1 0.500
ATOM H6 HA 0.050
ATOM C22 CT3 -0.400
ATOM H122 HA 0.050
ATOM H222 HA 0.050
ATOM H322 HA 0.050
ATOM C7 CT2 -0.400
ATOM H17 HA 0.050
ATOM H27 HA 0.050
GROUP
ATOM C8 CT1 0.350
ATOM H8 HA -0.100
ATOM C23 CT3 -0.400
ATOM H123 HA 0.050
ATOM H223 HA 0.050
ATOM H323 HA 0.050
GROUP
ATOM C9 C 0.450
ATOM O24 O -0.450



The numbering of methyl H-atoms has been omitted for clarity. The methyl hydrogen atoms are numbered serially along with the number of the corresponding C atom.

GROUP ATOM C10 CT1 0.250 ATOM H10 HA 0.050 ATOM C25 CT3 -0.450 ATOM H125 HA 0.050 ATOM H225 HA 0.050 ATOM H325 HA 0.050	
GROUP ATOM C11 CT1 0.350 ATOM H11 HA 0.050 ATOM O26 OH1 -0.800 ATOM H26 H 0.400	
GROUP ATOM C12 CT1 -0.100 ATOM H12 HA 0.050 ATOM C27 CT3 -0.100 ATOM H127 HA 0.050 ATOM H227 HA 0.050 ATOM H327 HA 0.050	
GROUP ATOM C14 CT2 0.000 ATOM H114 HA 0.050 ATOM H214 HA 0.050 ATOM C15 CT3 -0.250 ATOM H115 HA 0.050 ATOM H215 HA 0.050 ATOM H315 HA 0.050	

Figure S1. Partial charges and atom types for 6-deoxyerythronolide B (DEB). These data were provided by R. C. Wade (ref. 53 of the main paper).

3. List of amino acids protonated for QM/MM calculations

The following amino acids were protonated to generate an overall neutral system for the QM/MM calculations.

Titrable amino acids were chosen that are at least 17.5 Å apart from the QM region and are not engaged in salt bridges or in H-bonds with polar residues.

E360 pathway:

D6, D10, E22, E25, D130, E131, D134, E201, E206, D221, D262, D270, E298, D328, D380, D382, D383, D403

E244 pathway:

D10, D15, E25, E127, E131, D134, D139, D198, E201, D221, D222, D262, E298, D328, E360 D380, D382, D383

4. Description of ABF setup

We utilized the adaptive biasing force (ABF) method to determine the barrier for a crucial crystal water molecule (CRW2) to traverse along the I-helix, from the region entered after 20 ns of the molecular dynamics (MD) simulation (see main paper) back to its initial position in the crystal structure. As starting point of the ABF calculation, we thus selected a random snapshot at 28.61 ns from the MD run. The potential of mean force (PMF) was calculated along a collective reaction coordinate ξ, which was defined as the projection of the distance of CRW2 from a reference point onto an axis perpendicular to the main axis of the I-helix. More precisely, the distance of CRW2 was measured from its center of mass at the current position to a reference position close to its crystallographic location, and the axis was taken as a constant vector formed by joining the mid point between the O3 and O5 atoms of substrate DEB and the midpoint of the Cα atoms of G242 and S246 (the i and i+4 position of the I-helix). With these conventions, the distance traversed by CRW2 during the ABF calculation was about 5.2 Å. To restrict the accessible range of distances during the simulation, a half-harmonic potential of 20 kcal/mol was added at the two boundaries (i.e., at 0 and 5.2 Å, respectively). We note that this may affect the computed PMF close to the boundaries (see Figure 4 of the main paper).

The following procedure was adopted for the ABF calculation. The snapshot at 28.61 ns was subjected first to 5000 steps of conjugate gradient (CG) minimization to eliminate any unphysical contacts. Next, water and ions were equilibrated in the NVT ensemble for 200 ps while keeping the protein, oxyheme, and DEB fixed. This was followed by 5000 steps of CG minimization and 200 ps equilibration in the NPT ensemble with the protein backbone harmonically restrained (5 kcal $\cdot$ mol^{-1} $\cdot$ Å^{-2}). During all these simulations, the oxyferrous complex, DEB, and the coordinated side chain of C351 were kept fixed at their positions in the

crystal structure. With the protein appropriately solvated, subsequent simulations were carried out for 5 ns allowing the protein, water, and the ions to relax around the oxyferrous and DEB moieties. This was followed by a 15 ns ABF calculation in the NPT ensemble. Utilizing the reaction coordinate and the conventions described above, simulations were performed at intervals of 5 ns until the PMF was converged to within 0.5 kcal/mol. No bias was applied in the first 500 steps of the ABF simulation to avoid non-equilibrium effects due to large fluctuations arising from rapidly varying biasing forces along the reaction coordinate.

5. Relevant active-site distances along MD trajectory

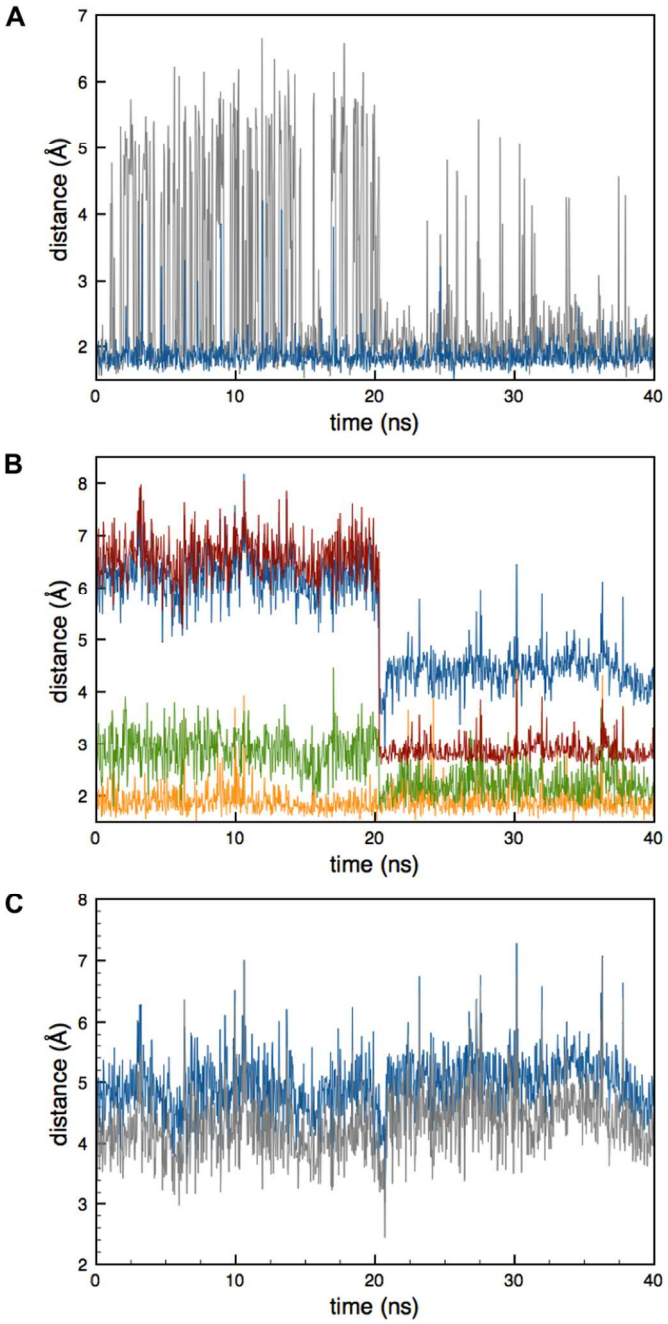


Figure S2. Time evolution of relevant active-site distances in the DEB-bound oxyferrous CYP107A1 MD simulation. (**A**) Distance between E360O−Ser246O-H (gray) and E360H−CRW1O (blue); (**B**) Distance between DEB3O−CRW2O (maroon), DEB5O−CRW2O (blue), A241O−CRW2H (orange) and A245N-H−CRW2O (green). (**C**) Distance between O_d−CRW2:center of mass (blue) and O_d−CRW2H (gray).

6. Relaxed potential energy surface scans

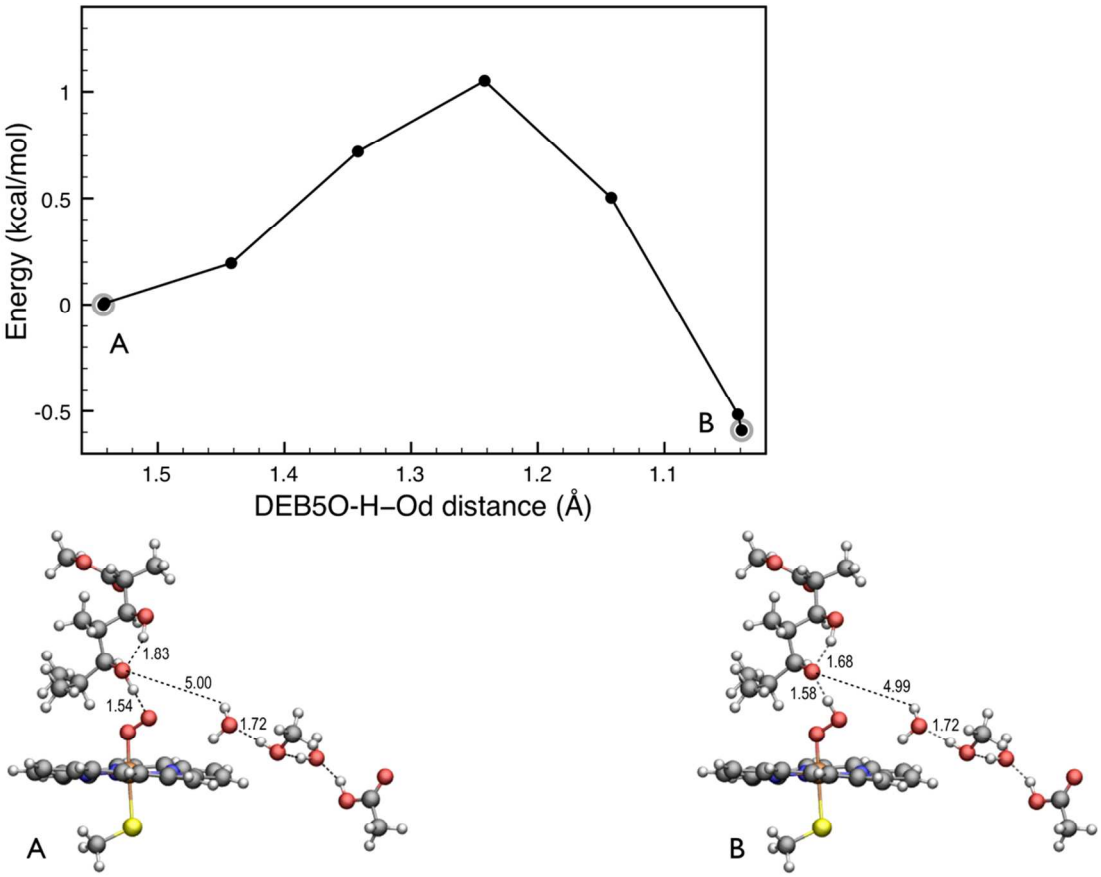


Figure S3. B3LYP/B1:CHARMM22 potential energy scan for transfer of the DEB-5OH hydrogen atom to the distal oxygen atom O_d. The data points from unconstrained full optimizations are surrounded with gray circles. The geometries of the fully optimized initial and final species are given below.

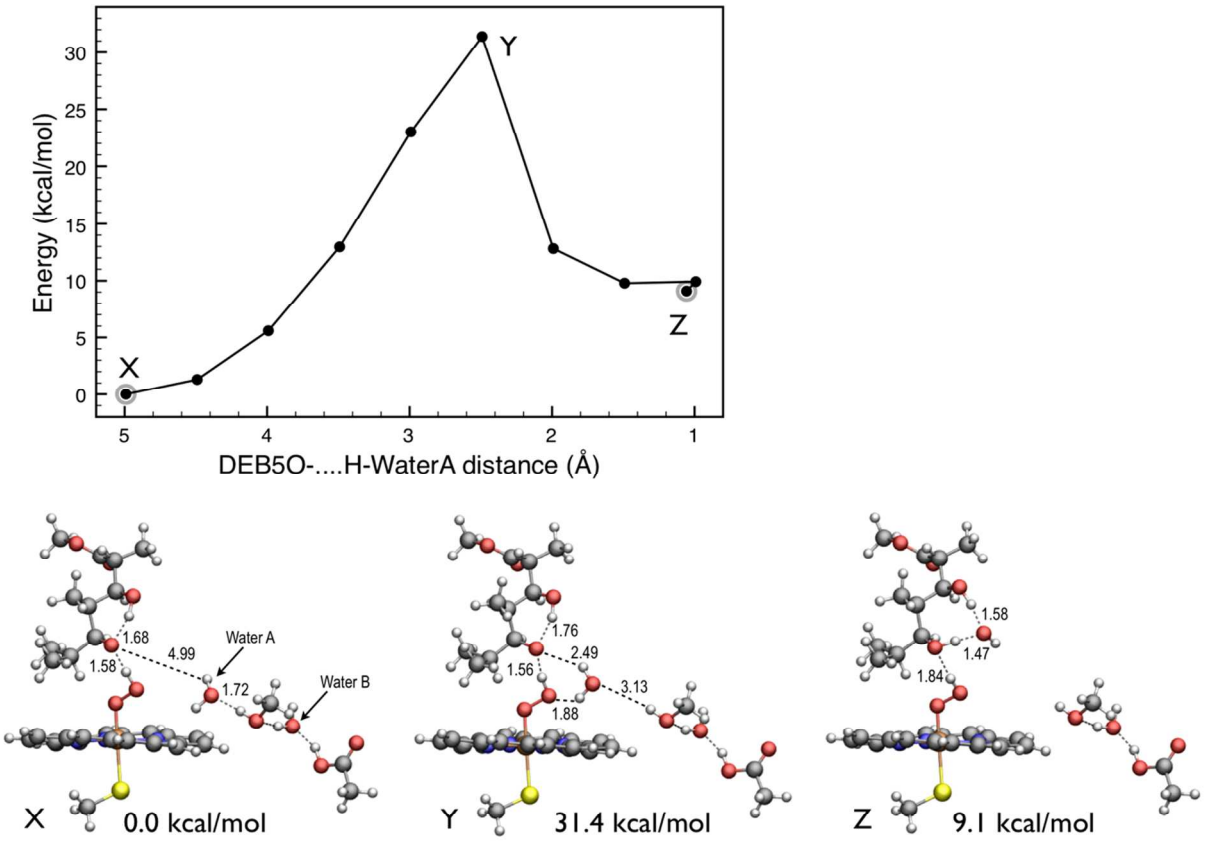


Figure S4. B3LYP/B1:CHARMM22 potential energy scan for transfer of a Water A hydrogen atom to DEB-5O$^-$. The data points from unconstrained full optimizations are surrounded with gray circles. The geometries of the reactant complex (X), the approximate transition state (Y), and the product (Z) are given below.

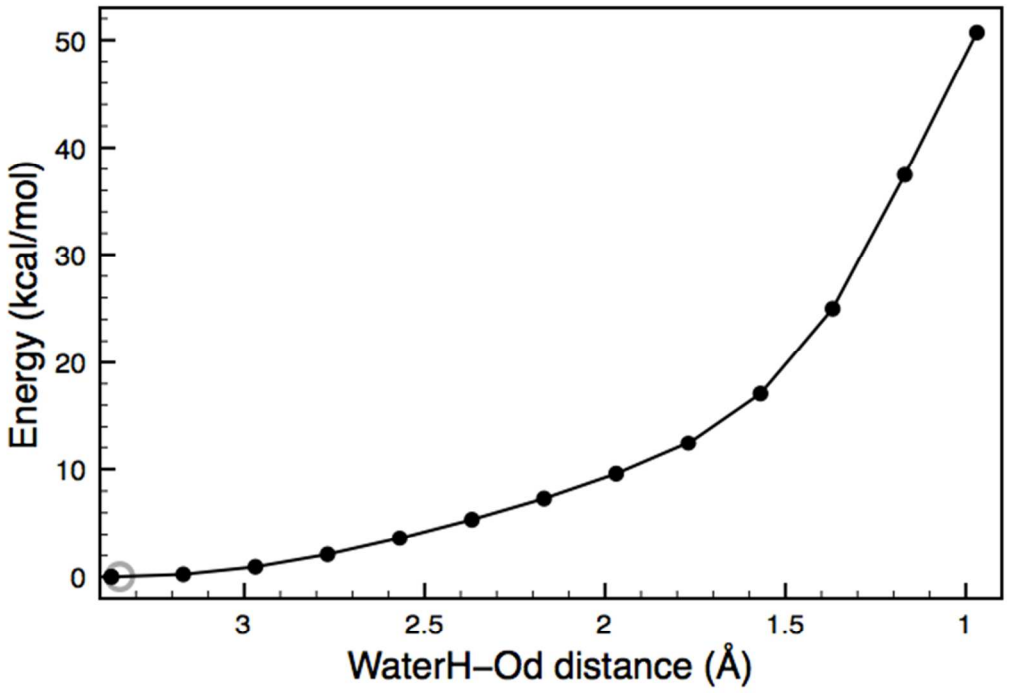


Figure S5. B3LYP/B1:CHARMM22 potential energy scan for transfer of a hydrogen atom of water molecule A (Figure 7) to distal oxygen atom O_d via E360 pathway. The data points from unconstrained full optimizations are surrounded with gray circles.

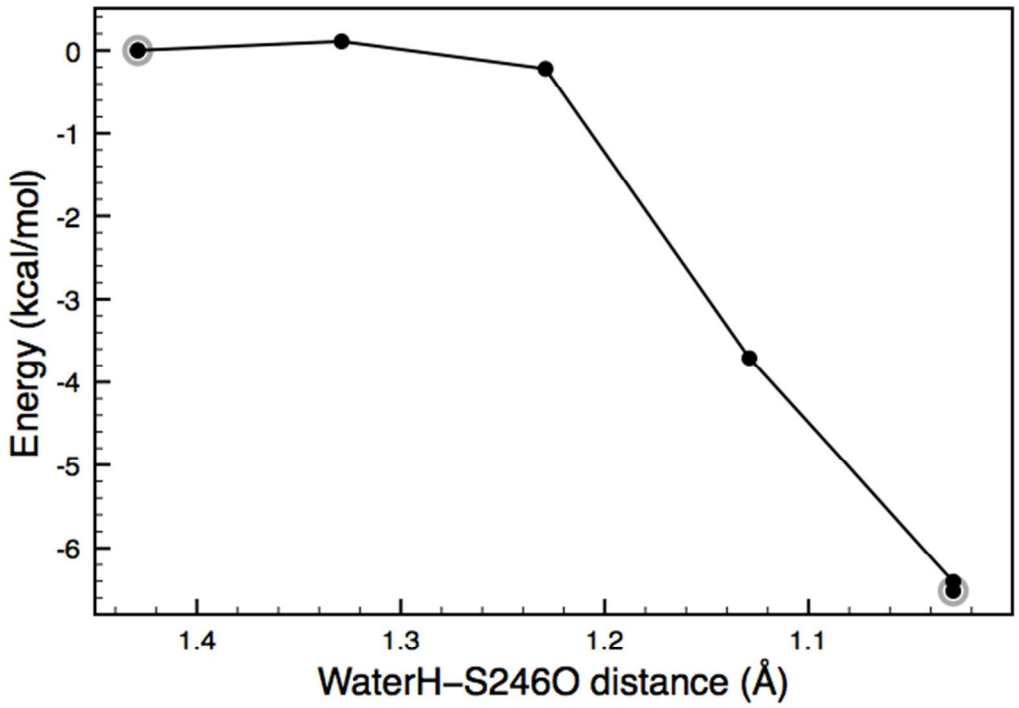


Figure S6. B3LYP/B1:CHARMM22 potential energy scan for proton transfer from water molecule B (Figure 7) to S246O$^-$ via E360 pathway. The data points from unconstrained full optimizations are surrounded with gray circles.

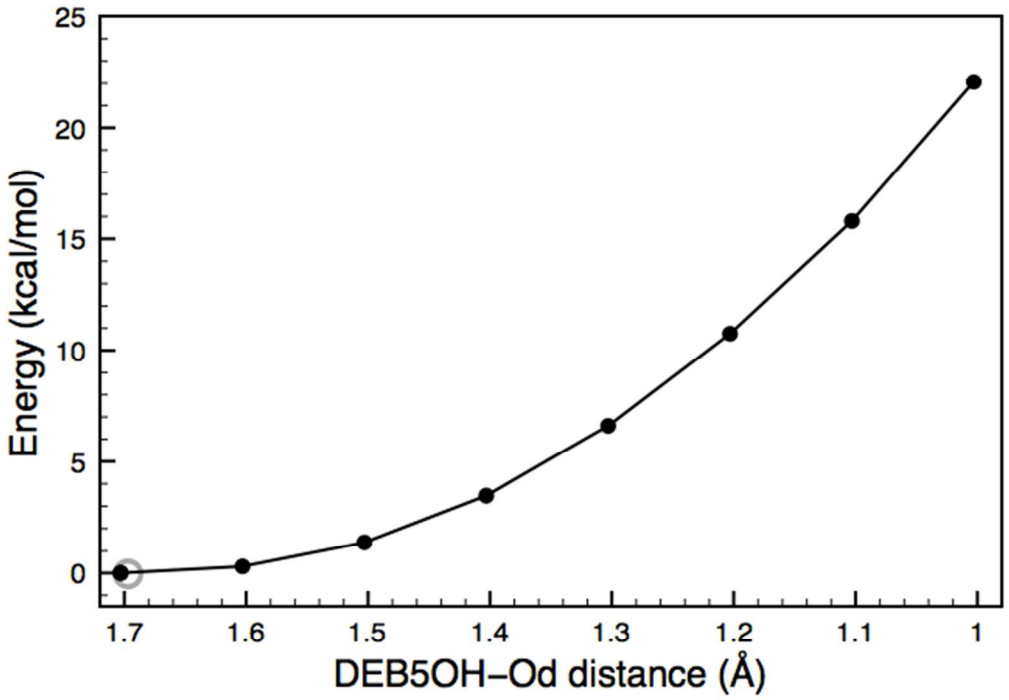


Figure S7. B3LYP/B1:CHARMM22 potential energy scans for transfer of the DEB-5OH hydrogen atom to the distal oxygen atom O_d via E244 pathway. The data points from unconstrained full optimizations are surrounded with gray circles.

7. Energy tables for all stationary points

All energies in Tables S1-S3 were evaluated at QM(UB3LYP/B1)/CHARMM optimized geometries. Except for the first entry in each Table, all data are thus single-point (SP) energies.

Table S1: Energies in kcal/mol for species illustrated in Figure 6. Conversion of peroxo species to Cpd 0 via E360 channel.

		PEROXO	**^{PEROXO}TS**	**CPD 0**
QM(B3LYP/B1)/CHARMM		0.00	19.30	-34.40
QM(B3LYP/B2)/CHARMM	SP	0.00	21.37	-30.29
QM(B3LYP+D/B2)/CHARMM	SP	0.00	11.49	-29.04
QM(PBE0/B2)/CHARMM	SP	0.00	22.28	-29.92
QM(M06/B2)/CHARMM	SP	0.00	21.81	-27.58
QM(^{4}B3LYP/B1)/CHARMM[a]	SP	16.16	31.96	-17.67

[a] quartet energies given with respect to PEROXO doublet calculated at the same level

Table S2: Energies in kcal/mol for species illustrated in Figure 7. Conversion of Cpd 0 to Cpd I via E360 channel.

		^{360}**CPD 0**	^{360}**TS1**	^{360}**IC1**	^{360}**TS2**	^{360}**IC2**	^{360}**TS3**	^{360}**CPD I**
QM(B3LYP/B1)/CHARMM		0.00	17.59	14.66	14.95	-4.02	-3.92	-10.54
QM(B3LYP/B2)/CHARMM	SP	0.00	17.72	17.82	18.92	-0.33	-0.33	-5.52
QM(B3LYP+D/B2)/CHARMM	SP	0.00	19.82	21.86	22.75	8.19	8.00	3.30
QM(PBE0/B2)/CHARMM	SP	0.00	22.44	25.49	26.39	5.52	5.20	1.15
QM(M06/B2)/CHARMM	SP	0.00	16.99	20.63	22.49	4.60	4.74	-1.22
QM(^{4}B3LYP/B1)/CHARMM[a]	SP	18.80	19.73	14.70	14.99	-3.94	-3.84	-10.44

[a] quartet energies given with respect to ^{360}Cpd 0 doublet calculated at the same level

Table S3: Energies in kcal/mol for species illustrated in Figure 8. Conversion of Cpd 0 to Cpd I via E244 channel.

		^{244}**CPD 0**	^{244}**TS1**	^{244}**IC1**	^{244}**TS2**	^{244}**CPD I**
QM(B3LYP/B1)/CHARMM		0.00	19.66	7.84	8.70	-23.94
QM(B3LYP/B2)/CHARMM	SP	0.00	21.21	13.77	14.38	-17.01
QM(B3LYP+D/B2)/CHARMM	SP	0.00	25.48	24.48	25.05	-7.81
QM(PBE0/B2)/CHARMM	SP	0.00	27.70	20.71	20.96	-10.02
QM(M06/B2)/CHARMM	SP	0.00	22.10	20.18	20.97	-14.56
QM(^{4}B3LYP/B1)/CHARMM[a]	SP	18.15	21.59	7.90	8.76	-23.80

[a] quartet energies given with respect to ^{244}Cpd 0 doublet calculated at the same level

Comments on the results in Tables S1-S3

First vs. second line: Extension of the basis from B1 to B2 generally increases the energies relative to Cpd 0 in a rather uniform manner, typically by 2-4 kcal/mol (Tables S1-S3), with a larger increase for the last three species in the E244 channel (Table S3).

Second vs. third line: Inclusion of D3 dispersion corrections lowers the barrier for Cpd 0 formation substantially without affecting the exothermicity much (Table S1). In the conversion of Cpd 0 to Cpd I, the D3 corrections raise the initial barrier to homolytic O-O cleavage by 2-4 kcal/mol, and even more strongly the relative energies of the subsequent species (by 4-9 kcal/mol in the E360 channel and by 9-11 kcal/mol in the E244 channel, see Tables S2-S3). Given these large changes in the single-point energies, geometry reoptimization appears necessary for a proper assessment of the effects of dispersion.

Second vs. fourth vs. fifth line: The B3LYP, PBE0, and M06 single-point relative energies are similar for Cpd 0 formation (Table S1). For both pathways towards Cpd I, the PBE0 relative energies of all species are higher than their B3LYP counterparts rather uniformly, by about 6-7 kcal/mol, implying that the Cpd 0 reference system is predicted to be more stable in B3LYP by this amount (Tables S2-S3). The M06 results are close to the B3LYP results for the initial barrier to homolytic O-O cleavage of Cpd 0 (within 1 kcal/mol), but resemble more the PBE0 results as the conversion to Cpd I proceeds (Tables S2-S3). The B3LYP, PBE0, and M06 single-point calculations predict **TS1** (**TS2**) to be rate-limiting in the E244 (E360) channel.

First vs. last line: The doublet state is well below the quartet state during the conversion of the peroxo species to Cpd 0 (Table S1). In the transition state for homolytic O-O cleavage in Cpd 0 (TS1), the doublet remains slightly below the quartet (by about 2 kcal/mol), whereas thereafter the two spin states become nearly degenerate on both pathways towards Cpd I (Tables S2-S3).

References for Tables S1-S3

D3 dispersion correction: Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. *J. Chem. Phys.* **2010**, *132*, 154104.
PBE0 functional: (a) Perdew, J. P. *Phys. Rev. B* **1986,** *33*, 8822-8824. (b) Perdew, J. P.; Burke, K.; Ernzerhof, M. *Phys. Rev. Lett.* **1996**, *77*, 3865. (c) Perdew, J. P.; Ernzerhof, M.; Burke, K. *J. Chem. Phys.* **1996**, *105*, 9982.
M06 functional: Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc.*, **2008,** *120,* 215.
Code used for M06 calculations: Gaussian 09, Revision **A.1**, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

8. NPA spin densities and charges for all species

Table S4: NPA spin densities (charges) for species illustrated in Figure 6

B3LYP/B1:CHARMM			
	PEROXO	**^{PEROXO}TS**	**CPD0**
Fe	0.28 (1.12) [2.17 (1.36)]	0.89 (1.28) [2.48 (1.50)]	1.01 (1.29) [2.61 (1.54)]
O_p-O_d	0.76 (-0.77) [0.87 (-0.90)]	0.16 (-1.04) [0.45 (-1.17)]	0.05 (-0.48)[a] [0.28 (-0.61)][a]
Porphyrin	-0.05 (-1.34) [-0.12 (-1.38)]	-0.04 (-1.11) [-0.02 (-1.13)]	-0.05 (-1.03) [-0.01 (-1.05)]
SCH_3	0.00 (-0.82) [0.07 (-0.89)]	-0.01 (-0.79) [0.08 (-0.87)]	0.01 (-0.70) [0.12 (-0.81)]
DEB	0.00 (-0.14) [0.00 (-0.15)]	0.00 (-0.09) [0.00 (-0.09]	0.00 (-0.07) [0.00 (-0.07)]
E360	0.00 (-0.06) [0.00 (-0.06)]	0.00 (-0.07) [0.00 (-0.07)]	0.00 (-0.92) [0.00 (-0.92)]
S246	0.00 (-0.01) [0.00 (-0.01)]	0.00 (-0.03) [0.00 (-0.03)]	0.00 (-0.04) [0.00 (-0.04)]
Water	0.00 (0.04) [0.00 (0.04)]	0.00 (-0.14) [0.00 (-0.14)]	0.00 (-0.04) [0.00 (-0.04)]
B3LYP/B2//B1:CHARMM			
Fe	0.20 (0.80)	0.75 (0.98)	0.86 (0.97)
O_p-O_d	0.81 (-0.74)	0.22 (-1.00)	0.09 (-0.46)[a]
Porphyrin	-0.03 (-1.18)	0.01 (-0.96)	0.02 (-0.87)
SCH_3	0.01 (-0.72)	0.02 (-0.69)	0.03 (-0.58)
DEB	0.00 (-0.14)	0.00 (-0.07)	0.00 (-0.06)
E360	0.00 (-0.06)	0.00 (-0.06)	0.00 (-0.93)
S246	0.00 (0.00)	0.00 (-0.03)	0.00 (-0.04)
Water	0.00 (0.04)	0.00 (-0.16)	0.00 (-0.03)
PBE0/B2//B3LYP/B1:CHARMM			
Fe	0.15 (0.81)	0.81 (1.01)	0.90 (1.00)
O_p-O_d	0.86 (-0.72)	0.17 (-1.02)	0.07 (-0.48)[a]
Porphyrin	-0.02 (-1.20)	0.01 (-0.96)	0.01 (-0.88)
SCH_3	0.01 (-0.73)	0.02 (-0.69)	0.02 (-0.59)
DEB	0.00 (-0.14)	0.00 (-0.08)	0.00 (-0.06)
E360	0.00 (-0.06)	0.00 (-0.06)	0.00 (-0.93)
S246	0.00 (0.00)	0.00 (-0.03)	0.00 (-0.04)
Water	0.00 (0.04)	0.00 (-0.16)	0.00 (-0.03)
B3LYP+D/B2//B3LYP/B1:C			
Fe	0.20 (0.80)	0.75 (0.98)	0.86 (0.97)
O_p-O_d	0.81 (-0.74)	0.22 (-1.00)	0.09 (-0.46)[a]
Porphyrin	-0.03 (-1.18)	0.01 (-0.96)	0.02 (-0.87)
SCH_3	0.01 (-0.72)	0.02 (-0.69)	0.03 (-0.58)
DEB	0.00 (-0.14)	0.00 (-0.08)	0.00 (-0.06)
E360	0.00 (-0.06)	0.00 (-0.06)	0.00 (-0.93)
S246	0.00 (0.00)	0.00 (-0.03)	0.00 (-0.04)
Water	0.00 (0.04)	0.00 (-0.16)	0.00 (-0.03)
M06/B2//B3LYP/B1:CHARMM			
Fe	0.22 (0.24)	0.85 (0.43)	0.94 (0.38)
O_p-O_d	0.83 (-0.66)	0.18 (-0.93)	0.08 (-0.38)[a]
Porphyrin	-0.04 (-0.86)	-0.02 (-0.63)	-0.01 (-0.52)
SCH_3	0.00 (-0.58)	-0.02 (-0.56)	-0.01 (-0.44)
DEB	0.00 (-0.13)	0.00 (-0.07)	0.00 (-0.05)
E360	0.00 (-0.05)	0.00 (-0.06)	0.00 (-0.93)
S246	0.00 (0.00)	0.00 (-0.03)	0.00 (-0.04)
Water	0.00 (0.04)	0.00 (-0.16)	0.00 (-0.02)

[a] The spin and charge of the transferred proton is added to O_p-O_d. The quartet spin and charges for B1 level given in square brackets.

Table S5: NPA spin densities (charges) for species illustrated in Figure 7

A) Doublet State

B3LYP/B1:CHARMM							
	^{360}CPD 0	^{360}TS1	^{360}IC1	^{360}TS2	^{360}IC2	^{360}TS3	^{360}CPD I
FeO	1.06 (0.83)	1.89 (0.73)	2.05 (0.71)	2.05 (0.73)	2.06 (0.68)	2.06 (0.68)	2.06 (0.68)
O_d-H	0.00 (-0.05)	-0.74 (-0.20)	-0.33 (-0.52)	-0.13 (-0.64)	-[a]	-[a]	-[a]
Porphyrin	-0.05 (-1.01)	-0.11 (-0.76)	-0.66 (-0.33)	-0.84 (-0.16)	-0.93 (-0.03)	-0.94 (-0.02)	-0.95 (-0.01)
SCH_3	-0.01 (-0.68)	-0.04 (-0.70)	-0.07 (-0.71)	-0.08 (-0.69)	-0.12 (-0.64)	-0.12 (-0.63)	-0.12 (-0.63)
DEB	0.00 (-0.06)	0.00 (-0.06)	0.00 (-0.08)	0.00 (-0.09)	0.00 (-0.06)	0.00 (-0.06)	0.00 (-0.06)
E360	0.00 (-0.06)	0.00 (-0.06)	0.00 (-0.06)	0.00 (-0.06)	0.00 (-0.10)	0.00 (-0.13)	0.00 (-0.90)
S246	0.00 (0.00)	0.00 (0.00)	0.00 (0.00)	0.00 (-0.01)	-0.01 (-0.74)	0.00 (-0.72)	0.00 (-0.03)
Water	0.00 (0.03)	0.00 (0.04)	0.00 (-0.01)	0.00 (-0.06)	0.00 (-0.11)	0.00 (-0.12)	0.00 (-0.05)
B3LYP/B2//B1:CHARMM							
FeO	0.96 (-0.53)	1.75 (0.47)	1.93 (0.46)	1.93 (0.48)	1.94 (0.43)	1.94 (0.43)	1.94 (0.43)
O_d-H	-0.01 (-0.06)	-0.76 (-0.19)	-0.39 (-0.48)	-0.19 (-0.60)	-[a]	-[a]	-[a]
Porphyrin	0.01 (-0.85)	-0.01 (-0.64)	-0.52 (-0.25)	-0.70 (-0.09)	-0.82 (0.07)	-0.84 (0.09)	-0.82 (0.08)
SCH_3	0.04 (-0.55)	0.02 (-0.59)	-0.02 (-0.60)	-0.05 (-0.59)	-0.08 (-0.53)	-0.09 (-0.52)	-0.09 (-0.52)
DEB	0.00 (-0.04)	0.00 (-0.05)	0.01 (-0.07)	0.01 (-0.08)	0.00 (-0.05)	0.00 (-0.05)	0.00 (-0.05)
E360	0.00 (-0.05)	0.00 (-0.05)	0.00 (-0.06)	0.00 (-0.06)	0.00 (-0.10)	0.00 (-0.13)	-0.04 (-0.86)
S246	0.00 (0.00)	0.00 (0.00)	0.00 (0.00)	0.00 (-0.01)	-0.03 (-0.72)	-0.01 (-0.70)	0.00 (-0.04)
Water	0.00 (0.04)	0.00 (0.05)	0.00 (0.00)	0.00 (-0.06)	0.00 (-0.10)	0.00 (-0.12)	0.01 (-0.04)
PBE0/B2//B3LYP/B1:CHARMM							
FeO	0.97 (0.55)	1.81 (0.46)	1.94 (0.47)	1.95 (0.50)	1.96 (0.45)	1.96 (0.45)	1.96 (0.44)
O_d-H	-0.01 (-0.06)	-0.83 (-0.13)	-0.45 (-0.43)	-0.18 (-0.61)	-[a]	-[a]	-[a]
Porphyrin	0.00 (-0.87)	-0.01 (-0.68)	-0.49 (-0.30)	-0.73 (-0.09)	-0.87 (0.09)	-0.87 (0.09)	-0.88 (0.10)
SCH_3	0.03 (-0.56)	0.02 (-0.60)	-0.02 (-0.61)	-0.05 (-0.60)	-0.08 (-0.53)	-0.09 (-0.53)	-0.09 (-0.52)
DEB	0.00 (-0.04)	0.00 (-0.05)	0.01 (-0.07)	0.01 (-0.08)	0.00 (-0.05)	0.00 (-0.05)	0.00 (-0.05)
E360	0.00 (-0.05)	0.00 (-0.05)	0.00 (-0.06)	0.00 (-0.06)	0.00 (-0.10)	0.00 (-0.13)	0.00 (-0.90)
S246	0.00 (0.00)	0.00 (0.00)	0.00 (0.00)	0.00 (-0.01)	-0.01 (-0.74)	0.00 (-0.71)	0.00 (-0.04)
Water	0.00 (0.04)	0.00 (0.05)	0.00 (0.00)	0.00 (-0.06)	0.00 (-0.11)	0.00 (-0.12)	0.01 (-0.04)
B3LYP+D/B2//B3LYP/B1:CHARMM							
FeO	0.96 (-0.53)	1.75 (0.47)	1.93 (0.46)	1.93 (0.48)	1.94 (0.43)	1.94 (0.43)	1.94 (0.43)
O_d-H	-0.01 (-0.06)	-0.76 (-0.19)	-0.39 (-0.48)	-0.19 (-0.60)	-[a]	-[a]	-[a]
Porphyrin	0.01 (-0.85)	-0.01 (-0.64)	-0.52 (-0.25)	-0.70 (-0.09)	-0.82 (0.07)	-0.84 (0.09)	-0.82 (0.08)
SCH_3	0.04 (-0.55)	0.02 (-0.59)	-0.02 (-0.60)	-0.05 (-0.59)	-0.08 (-0.53)	-0.09 (-0.52)	-0.09 (-0.52)
DEB	0.00 (-0.04)	0.00 (-0.05)	0.01 (-0.07)	0.01 (-0.08)	0.00 (-0.05)	0.00 (-0.05)	0.00 (-0.05)
E360	0.00 (-0.05)	0.00 (-0.05)	0.00 (-0.06)	0.00 (-0.06)	0.00 (-0.10)	0.00 (-0.13)	-0.04 (-0.86)
S246	0.00 (0.00)	0.00 (0.00)	0.00 (0.00)	0.00 (-0.01)	-0.03 (-0.72)	-0.01 (-0.70)	0.00 (-0.04)
Water	0.00 (0.04)	0.00 (0.05)	0.00 (0.00)	0.00 (-0.06)	0.00 (-0.10)	0.00 (-0.12)	0.01 (-0.04)
M06/B2//B3LYP/B1:CHARMM							
FeO	1.02 (0.01)	1.89 (-0.06)	2.04 (-0.06)	2.04 (-0.04)	2.06 (-0.09)	2.06 (-0.09)	2.06 (-0.10)
O_d-H	-0.01 (-0.05)	-0.80 (-0.15)	-0.41 (-0.48)	0.16 (-0.64)	-[a]	-[a]	-[a]
Porphyrin	-0.02 (-0.51)	-0.06 (-0.29)	-0.59 (0.13)	-0.82 (0.33)	-0.93 (0.48)	-0.94 (0.49)	-0.94 (0.50)
SCH_3	0.01 (-0.40)	-0.04 (-0.45)	-0.05 (-0.48)	-0.08 (-0.46)	-0.12 (-0.39)	-0.13 (-0.39)	-0.13 (-0.38)
DEB	0.00 (-0.04)	0.01 (-0.04)	0.01 (-0.06)	0.00 (-0.07)	0.00 (-0.05)	0.00 (-0.05)	0.00 (-0.04)
E360	0.00 (-0.05)	0.00 (-0.05)	0.00 (-0.06)	0.00 (-0.06)	0.00 (-0.10)	0.00 (-0.12)	0.00 (-0.91)
S246	0.00 (0.00)	0.00 (0.00)	0.00 (0.00)	0.00 (-0.01)	-0.01 (-0.75)	0.00 (-0.72)	0.00 (-0.03)
Water	0.00 (0.03)	0.00 (0.04)	0.00 (0.00)	0.00 (-0.05)	0.00 (-0.10)	0.00 (-0.12)	0.00 (-0.03)

[a] Since Od-H gets protonated to form water, it is considered with the rest of the water molecules.

B) Quartet State

B3LYP/B1:CHARMM							
	^{360}CPD 0	**^{360}TS1**	**^{360}IC1**	**^{360}TS2**	**^{360}IC2**	**^{360}TS3**	**^{360}CPD I**
FeO	2.84 (1.11)	2.13 (0.71)	2.03 (0.71)	2.02 (0.73)	2.03 (0.68)	2.03 (0.68)	2.03 (0.68)
O_d-H	-0.01 (-0.04)	0.75 (-0.21)	0.35 (-0.52)	0.14 (-0.64)	-[a]	-[a]	-[a]
Porphyrin	0.24 (-1.33)	0.09 (-0.72)	0.58 (-0.32)	0.76 (-0.16)	0.85 (-0.03)	0.86 (-0.02)	0.86 (-0.01)
SCH_3	-0.06 (-0.65)	0.03 (-0.70)	0.04 (-0.71)	0.06 (-0.70)	0.09 (-0.64)	0.09 (-0.64)	0.09 (-0.63)
DEB	0.00 (-0.06)	0.00 (-0.06)	0.00 (-0.08)	0.00 (-0.09)	0.00 (-0.06)	0.00 (-0.06)	0.00 (-0.06)
E360	0.00 (-0.06)	0.00 (-0.06)	0.00 (-0.06)	0.00 (-0.06)	0.00 (-0.10)	0.00 (-0.13)	0.00 (-0.90)
S246	0.00 (0.00)	0.00 (0.00)	0.00 (0.00)	0.00 (-0.01)	0.01 (-0.74)	0.00 (-0.72)	0.00 (-0.03)
Water	0.00 (0.03)	0.00 (0.04)	0.00 (-0.01)	0.00 (-0.06)	0.02 (-0.11)	0.02 (-0.12)	0.01 (-0.05)

[a] Since Od-H gets protonated to form water, it is considered with the rest of the water molecules.

Table S6: NPA spin densities (charges) for species illustrated in Figure 8

B3LYP/B1:CHARMM					
	^{244}CPD 0	**^{244}TS1**	**^{244}IC2[b]**	**^{244}TS3[b]**	**^{244}CPD I**
FeO	1.07 (0.81) [2.91(1.09)]	1.89 (0.77) [2.08 (0.74)]	2.06 (0.75) [2.02 (0.75)]	2.06 (0.74) [2.02 (0.75)]	2.07 (0.69) [2.03 (0.69)]
O_d-H	0.00(-0.05) [-0.01(-0.04)]	-0.48(-0.38) [0.44(-0.43)]	-[a]	-[a]	-[a]
Porphyrin	-0.05(-1.04) [0.24(-1.37)]	-0.30(-0.63) [0.36(-0.55)]	-0.90(-0.12) [0.83(-0.12)]	-0.90(-0.12) [0.83(-0.12)]	-0.92(-0.07) [0.84(-0.07)]
SCH_3	-0.01(-0.65)[-0.09(-0.61)]	-0.10(-0.65) [0.10(-0.65)]	-0.16(-0.63) [0.14(-0.63)]	-0.16(-0.62) [0.14(-0.62)]	-0.16(-0.59) [0.13(-0.60)]
DEB	0.00 (-0.04) [0.00 (-0.04)]	0.00 (-0.07) [0.01 (-0.07)]	0.00 (-0.08) [0.00 (-0.08)]	0.00 (-0.07) [0.00 (-0.07)]	0.00(-0.07) [0.00(-0.07)]
E244	0.00 (-0.07) [0.00 (-0.07)]	0.00 (-0.07) [0.00 (-0.07)]	0.00 (-0.08) [0.00 (-0.08)]	0.00 (-0.10) [0.00 (-0.10)]	0.00(-0.97) [0.00(-0.97)]
Water	0.00 (0.03) [0.00 (0.03)]	-0.01 (0.03) [0.01 (0.02)]	0.00(-0.84) [0.00(-0.84)][b]	0.00(-0.83) [0.00(-0.83)][b]	0.01 (0.02) [0.01 (0.02)]
B3LYP/B2//B1:CHARMM					
FeO	0.96 (-0.51)	1.72 (0.53)	1.95 (0.52)	1.95 (0.52)	1.94 (0.44)
O_d-H	-0.01 (-0.05)	-0.54 (-0.34)	-[a]	-[a]	-[a]
Porphyrin	0.01 (-0.87)	-0.12 (-0.56)	-0.81 (-0.01)	-0.81 (-0.01)	-0.82 (0.05)
SCH_3	0.04 (-0.52)	-0.04 (-0.53)	-0.14 (-0.52)	-0.15 (-0.51)	-0.13 (-0.48)
DEB	0.00 (-0.04)	0.00 (-0.06)	0.00 (-0.07)	0.00 (-0.06)	0.00 (-0.06)
E244	0.00 (-0.06)	0.00 (-0.06)	0.00 (-0.08)	0.00 (-0.10)	-0.04 (-0.98)
Water	0.00 (0.04)	-0.02 (0.03)	0.00 (-0.85)[b]	0.00 (-0.84)[b]	0.01 (0.02)
PBE0/B2//B3LYP/B1:CHARMM					
FeO	0.97 (0.53)	1.71 (0.54)	1.96 (0.54)	1.97 (0.53)	1.96 (0.46)
O_d-H	-0.01 (-0.05)	-0.61 (-0.28)	-[a]	-[a]	-[a]
Porphyrin	0.00 (-0.88)	-0.06 (-0.63)	-0.83 (-0.02)	-0.83 (-0.02)	-0.84 (0.04)
SCH_3	0.03 (-0.53)	-0.01 (-0.55)	-0.14 (-0.52)	-0.14 (-0.52)	-0.13 (-0.48)
DEB	0.00 (-0.04)	0.00 (-0.06)	0.00 (-0.07)	0.00 (-0.06)	0.00 (-0.06)
E244	0.00 (-0.06)	0.00 (-0.06)	0.00 (-0.08)	0.00 (-0.09)	0.00 (-0.98)
Water	0.00 (0.04)	-0.02 (0.04)	0.00 (-0.85)[b]	0.00 (-0.84)[b]	0.01 (0.02)
B3LYP+D/B					
FeO	0.96 (-0.51)	1.72 (0.52)	1.95 (0.52)	1.95 (0.52)	1.94 (0.44)
O_d-H	-0.01 (-0.05)	-0.54 (-0.34)	-[a]	-[a]	-[a]
Porphyrin	0.01 (-0.87)	-0.12 (-0.56)	-0.81 (-0.01)	-0.81 (-0.01)	-0.82 (0.05)
SCH_3	0.04 (-0.52)	-0.04 (-0.53)	-0.14 (-0.52)	-0.15 (-0.51)	-0.13 (-0.48)
DEB	0.00 (-0.04)	0.00 (-0.06)	0.00 (-0.07)	0.00 (-0.06)	0.00 (-0.06)
E244	0.00 (-0.06)	0.00 (-0.06)	0.00 (-0.08)	0.00 (-0.10)	-0.04 (-0.98)
Water	0.00 (0.04)	-0.02 (0.03)	0.00 (-0.85)[b]	0.00 (-0.84)[b]	0.01 (0.02)
M06/B2//B3LYP/B1:CHARMM					
FeO	1.02 (-0.02)	1.80 (0.01)	2.06 (0.00)	2.06 (-0.01)	2.07 (-0.09)
O_d-H	-0.01 (-0.05)	-0.60 (-0.29)	-[a]	-[a]	-[a]
Porphyrin	-0.02 (-0.52)	-0.11 (-0.24)	-0.90 (0.39)	-0.90 (0.39)	-0.92 (0.45)
SCH_3	0.01 (-0.36)	-0.08 (-0.40)	-0.16 (-0.40)	-0.16 (-0.39)	-0.16 (-0.35)
DEB	0.00 (-0.04)	0.00 (-0.05)	0.00 (-0.06)	0.00 (-0.06)	0.00 (-0.06)
E244	0.00 (-0.06)	0.00 (-0.05)	0.00 (-0.07)	0.00 (-0.09)	0.00 (-0.98)
Water	0.00 (0.04)	-0.01 (0.03)	0.00 (-0.86)[b]	0.00 (-0.85)[b]	0.01 (0.02)

[a] Since Od-H gets protonated to form water, it is considered with the rest of the water molecules. [b] An OH^- intermediate is formed by proton transfer from water. The quartet spin densities and charges are given in square brackets.

9. Coordinates (Å) and total energies (au)

Cpd 0 formation via E360 pathway

Figures 5 and 6

Peroxo (**PEROXO**)

C	25.6658798	6.0187160	11.6628478
H	26.7507927	5.9205399	11.5640689
H	25.3625125	5.7133366	12.6718471
O	25.3512319	7.3895785	11.4119254
H	24.3949151	7.5512268	11.6266133
C	19.7657123	14.0624324	7.0090782
H	20.4028221	14.3048679	6.1482629
H	19.0195912	13.3335062	6.6749028
S	20.7942824	13.2854097	8.3146258
C	31.0470307	8.2338198	11.0904669
H	31.0194518	9.2745027	10.7620984
H	32.0370899	7.9912426	11.4869832
C	30.0289181	7.9924732	12.1835827
O	30.1399679	7.1025813	13.0160892
O	29.0115310	8.8483051	12.1285534
H	28.2862384	8.6598884	12.8030108
C	11.9341264	8.1269655	16.3037043
H	12.3626296	8.6011393	17.1877367
O	12.8856657	7.1962031	15.7245626
C	14.2113855	7.3825542	15.9402301
O	14.6519956	8.3131453	16.6003537
C	15.0570188	6.3348586	15.2418689
H	14.3816990	5.6036042	14.7872624
C	15.9723496	5.6387377	16.2601353
H	15.4158433	5.3157962	17.1437780
H	16.4406545	4.7740438	15.7909684
H	16.7748380	6.3164135	16.5579479
C	15.9198319	7.0239237	14.1579020
H	16.4345257	7.8477905	14.6768357
O	16.8853357	6.0865275	13.6927802
H	17.2782449	6.5235838	12.8982446
C	15.1481635	7.6373344	12.9641537
H	14.3343804	8.2400220	13.3873320
C	14.5151005	6.5666234	12.0551295
H	14.1040339	5.7406193	12.6468313
H	13.6957973	6.9832277	11.4625658
H	15.2554441	6.1529592	11.3668724
C	16.1204248	8.6196981	12.2566839
H	16.5684177	9.2177580	13.0673256
O	17.1616985	7.8603531	11.6480305
H	17.9726221	8.4926032	11.5013565
C	15.5338092	9.6621501	11.2645789
H	16.3863905	10.3055524	11.0197814
C	15.0479017	9.0596450	9.9382445
H	14.1085315	8.5053238	10.0432875
H	14.8892583	9.8487903	9.1964792
H	15.8113934	8.3792486	9.5503639
C	14.4024347	10.5464130	11.8429123
H	14.1218658	11.2938407	11.0939455
H	13.5168850	9.9233244	12.0293952
Fe	19.4522408	11.8422057	9.8627335
N	17.8197071	11.9251461	8.6463644
N	20.2117633	10.3043523	8.7952720
N	21.0715822	11.8458143	11.0814226
N	18.6731487	13.4479860	10.9027998
C	16.7743632	12.8153105	8.6826997
C	15.7492498	12.4518996	7.7106903
C	16.1879733	11.3021587	7.1033181
C	17.4959660	11.0036300	7.6872930
C	19.5977781	9.6329905	7.7765832
C	20.4652277	8.5663179	7.2668688
C	21.6223458	8.6017579	8.0128211
C	21.4282550	9.7187077	8.9584078
C	22.2104277	11.1175070	10.9081066
C	23.1957392	11.4158083	11.9504350
C	22.5905727	12.3188391	12.8046110
C	21.2572632	12.5769146	12.2276935
C	19.1466075	13.9423258	12.0862592
C	18.3035043	15.0376024	12.5735962
C	17.3222852	15.2192913	11.6287283
C	17.5489312	14.1842271	10.6184140
C	16.6784890	13.8890180	9.5690962
H	15.8042633	14.5258349	9.4677380
C	18.3247040	9.9488780	7.2947090
H	17.9255749	9.3272197	6.5015333
C	22.3686782	10.1585147	9.8999706
H	23.3558789	9.7126320	9.8178561
C	20.3244241	13.5087257	12.7006622
H	20.5576970	14.0125561	13.6369053
O	18.5327139	10.6311368	10.9364883
O	19.1468054	9.4764268	11.3073986
O	26.7407980	8.7064284	13.3731462
H	26.2204297	8.3510935	12.6076020
H	26.2737233	8.3230776	14.1504306
O	22.7071401	7.7908096	11.8242765
H	22.3482822	8.4990951	11.2382331
H	22.0770523	7.7827122	12.5877365
H	25.1649532	5.3751748	10.9396647
H	19.1863376	14.9556964	7.2424676
H	30.8662593	7.5868878	10.2320572
H	11.0856543	7.5343277	16.6456723
H	11.6300230	8.8861045	15.5830826
H	14.6545434	11.1139009	12.7387165
H	14.8016229	12.9711497	7.5676902
H	15.6525356	10.6565802	6.4071849
H	20.1855883	7.9070193	6.4451671
H	22.5188770	7.9818586	8.0176338
H	24.2152702	11.0307378	11.9318943
H	22.9359165	12.8222447	13.7075988
H	18.4599065	15.5494836	13.5231132
H	16.5119125	15.9477472	11.6019984

TURBOMOLE (QM) and ChemShell Energies (MM and QM/MM)

	QM/MM	QM	MM
B3LYP/B1	-4168.023373	-4070.594117	-97.429256
B3LYP/B2*	-4168.903759	-4071.474503	-97.429256
PBE0/B2/*	-4167.261019	-4069.831763	-97.429256
B3LYP+D/B2*	-4169.387979	-4071.958723	-97.429256
[A]M06/B2/*	-4168.778237	-5491.148166	-97.429256
[4]B3LYP/B1	-4167.997618	-4070.568362	-97.429256

*B3LYP/B1 geometry

[A]Additional contribution to MM energy and charges: 1419.799185

Figure 6

TS for O_d-watH cleavage starting from **PEROXO** ($^{\mathbf{PEROXO}}$**TS**)

C	25.0223711	6.4153231	11.8235597
H	26.1158254	6.4352887	11.8540100
H	24.6472705	6.0496506	12.7864749
O	24.5899028	7.7527694	11.5539876
H	23.5768478	7.8988515	11.6241207
C	19.7096534	14.0663992	7.0260922
H	20.3291567	14.2992834	6.1504599
H	18.9643264	13.3257829	6.7165907
S	20.7761770	13.3267358	8.3194935
C	30.8935450	8.2724645	11.0614620
H	30.8964712	9.3011776	10.6948668
H	31.8533105	8.0484588	11.5354965
C	29.8030067	8.1012850	12.1013414
O	29.9566927	7.4409238	13.1191303
O	28.6802387	8.7497473	11.7918170
H	27.9498417	8.6333079	12.4830996
C	11.9587615	8.1213050	16.2521036
H	12.3784332	8.5894821	17.1436362
O	12.9157541	7.1930270	15.6782042
C	14.2396145	7.3823397	15.9069342
O	14.6712197	8.3096611	16.5775132
C	15.0948037	6.3398835	15.2161508
H	14.4286255	5.6171827	14.7354356
C	15.9690001	5.6267162	16.2598974
H	15.3697994	5.2679440	17.1007768
H	16.4757146	4.7855867	15.7888677
H	16.7417544	6.3063644	16.6243416
C	15.9999696	7.0260250	14.1639358
H	16.5159992	7.8311952	14.7095649
O	16.9475770	6.0667260	13.7154606
H	17.3706378	6.4798650	12.9264092
C	15.2845004	7.6767500	12.9568658
H	14.5061759	8.3280901	13.3720987
C	14.5960876	6.6480606	12.0392338
H	14.1587573	5.8292797	12.6211451
H	13.7868214	7.1078783	11.4647600
H	15.3074707	6.2172501	11.3321473
C	16.3095883	8.6128455	12.2549307
H	16.7850535	9.1876373	13.0643948
O	17.3124563	7.7998375	11.6413399
H	18.1598483	8.3316572	11.4803868
C	15.7539953	9.6756696	11.2660974
H	16.6140408	10.3197394	11.0496294
C	15.2914538	9.0919164	9.9218140
H	14.3596537	8.5226461	10.0067755
H	15.1265752	9.8937688	9.1966237
H	16.0681543	8.4316432	9.5262964
C	14.6032028	10.5557960	11.8221745
H	14.3758909	11.3318415	11.0844006
H	13.6999172	9.9423720	11.9413187
Fe	19.5592386	11.7568919	9.9098671
N	17.8820292	11.8268172	8.7200044
N	20.3463864	10.3298898	8.7646323
N	21.2238982	11.9297557	11.0014719
N	18.7211774	13.3624561	10.9592130
C	16.8337721	12.7201689	8.7488543
C	15.8266546	12.3697428	7.7589084
C	16.2793622	11.2298518	7.1396996
C	17.5770367	10.9247347	7.7333787
C	19.7177814	9.6257745	7.7793550
C	20.5900064	8.5601559	7.2821897
C	21.7502271	8.6178928	8.0202303
C	21.5790748	9.7712753	8.9202328
C	22.3806140	11.2362306	10.7993506
C	23.3454820	11.5356642	11.8496683
C	22.7117136	12.3795518	12.7427369
C	21.3739000	12.6158282	12.1812037
C	19.2051439	13.8800828	12.1272917
C	18.3631937	14.9776858	12.6054143
C	17.3815740	15.1544091	11.6580258
C	17.6002145	14.1011622	10.6663611
C	16.7292993	13.8010548	9.6224109
H	15.8598092	14.4412963	9.5084260
C	18.4266707	9.8987884	7.3193654
H	18.0378274	9.2753360	6.5229408
C	22.5359633	10.2698092	9.8052790
H	23.4751223	9.7372900	9.8216857
C	20.4074393	13.4822324	12.7087101
H	20.6371519	13.9683813	13.6539920
O	18.9533321	10.5043161	11.0898771
O	19.5770303	9.1814821	11.2185259
O	26.4998151	8.7645106	13.2346237
H	25.7636939	8.6030048	12.5837213
H	26.1718494	8.3092155	14.0433547
O	21.8620505	8.2291358	11.6749796
H	20.7653983	8.9215251	11.3912847
H	21.5793751	7.9299783	12.5685504
H	24.6910488	5.7348566	11.0391763
H	19.1309521	14.9616029	7.2536480
H	30.7681838	7.6035008	10.2100875
H	11.1046708	7.5299324	16.5820639
H	11.6681063	8.8858697	15.5316684
H	14.8077157	11.0906353	12.7496377
H	14.8824458	12.8920874	7.6049847
H	15.7533342	10.5975611	6.4244587
H	20.3048312	7.8796439	6.4799148
H	22.6310296	7.9770038	8.0591518
H	24.3727826	11.1714174	11.8430219
H	23.0370849	12.8467998	13.6721879
H	18.5225514	15.4996099	13.5489538
H	16.5691244	15.8803832	11.6271439

TURBOMOLE (QM) and ChemShell Energies (MM and QM/MM)

	QM/MM	QM	MM
B3LYP/B1	-4167.992608	-4070.583999	-97.408608
B3LYP/B2*	-4168.869711	-4071.461103	-97.408608
PBE0/B2/*	-4167.225505	-4069.816897	-97.408608
B3LYP+D/B2*	-4169.369663	-4071.961055	-97.408608
[A]M06/B2/*	-4168.743487	-5491.124221	-97.408608
[4]B3LYP/B1	-4167.972439	-4070.563831	-97.408608

*B3LYP/B1 geometry

[A]Additional contribution to MM energy and charges: 1419.789342

Figure 6

Compound 0 (**Cpd 0**)

C	25.7279928	5.9406794	11.5811971
H	26.8170732	5.8739445	11.4590752
H	25.4558863	5.6146108	12.5941401
O	25.2712506	7.2712325	11.3283386
H	23.5272692	7.4579241	12.0406689
C	19.7066651	14.0491222	7.0603628
H	20.3683512	14.2842006	6.2178405
H	18.9623242	13.3269160	6.7110345
S	20.7202664	13.2640177	8.3719355
C	31.0169099	8.2332823	11.1087144
H	30.9126694	9.2734110	10.7874638
H	32.0374257	8.0617464	11.4724933
C	30.0213056	7.9045000	12.2420483
O	30.2662792	6.8890252	12.9403651
O	29.0298679	8.6980837	12.3546346
H	27.5564181	8.6122224	13.0141874
C	11.9432739	8.1241994	16.3522572
H	12.3854484	8.6120958	17.2219711
O	12.8866837	7.1857781	15.7701761
C	14.2158891	7.3752819	15.9494820
O	14.6769170	8.3242845	16.5681991
C	15.0380067	6.3025752	15.2603113
H	14.3444670	5.5722211	14.8330483
C	15.9681609	5.6101906	16.2697915
H	15.4506814	5.3801439	17.2042981
H	16.3510206	4.6865956	15.8372756
H	16.8319994	6.2465757	16.4703562
C	15.8892849	6.9533205	14.1461016
H	16.4466938	7.7665206	14.6385965
O	16.8078397	5.9725027	13.6775154
H	17.2110012	6.3679347	12.8744534
C	15.0973762	7.5741267	12.9669629
H	14.3048359	8.1892053	13.4098312
C	14.4251769	6.5092974	12.0800735
H	13.9851034	5.7157284	12.6934906
H	13.6201056	6.9421364	11.4802992
H	15.1464993	6.0481538	11.4014494
C	16.0543574	8.5462212	12.2327585
H	16.5366468	9.1376219	13.0265028
O	17.0692949	7.7549134	11.5988177
H	17.8540233	8.3384111	11.4299191
C	15.4683110	9.5890341	11.2417521
H	16.3195613	10.2327054	10.9912907
C	14.9738591	8.9833252	9.9195786
H	14.0353836	8.4309575	10.0332226
H	14.8074538	9.7726224	9.1798375
H	15.7302655	8.2999424	9.5233545
C	14.3387563	10.4748257	11.8227224
H	14.0379317	11.2028114	11.0629998
H	13.4624421	9.8476569	12.0334428
Fe	19.4056950	11.8574519	9.8597218
N	17.7870187	11.9482036	8.6436892
N	20.1829738	10.3192668	8.8026042
N	21.0246918	11.8454021	11.0786156
N	18.6231859	13.4553147	10.8944873
C	16.7342213	12.8314955	8.6804660
C	15.7166146	12.4562810	7.7130111
C	16.1605434	11.3041366	7.1119804
C	17.4678589	11.0146704	7.6907050
C	19.5711127	9.6534432	7.7799322
C	20.4397828	8.5909880	7.2719264
C	21.5925279	8.6168315	8.0257141
C	21.3991629	9.7233883	8.9757397
C	22.1744614	11.1194689	10.9059928
C	23.1532851	11.4361541	11.9378069
C	22.5414659	12.3359446	12.7918101
C	21.2063355	12.5808805	12.2250134
C	19.0891067	13.9288283	12.0918103
C	18.2398391	15.0114409	12.5868136
C	17.2652317	15.2064260	11.6378196
C	17.4949607	14.1900182	10.6153821
C	16.6276872	13.9047567	9.5640840
H	15.7520086	14.5377884	9.4630540
C	18.2972827	9.9642030	7.2981073
H	17.9005178	9.3405512	6.5067244
C	22.3339127	10.1495208	9.9192345
H	23.2821700	9.6277475	9.9121055
C	20.2626021	13.4960890	12.7083328
H	20.4857256	13.9853951	13.6530373
O	18.4919114	10.7174403	10.9877930
O	19.1567479	9.4388851	11.2199904
O	26.5575977	8.7146039	13.1434000
H	25.7823521	7.8671220	11.9579319
H	26.2742753	8.3048637	13.9865279
O	22.6598662	7.1683167	12.4018714
H	19.8314182	9.6241451	11.9103754
H	22.0920140	7.9566009	12.5309504
H	25.2310999	5.2826966	10.8682998
H	19.1355417	14.9512060	7.2797472
H	30.8660565	7.5765960	10.2519340
H	11.1031668	7.5324684	16.7157693
H	11.6231218	8.8712247	15.6259500
H	14.5965612	11.0652058	12.7019575
H	14.7660063	12.9695153	7.5680939
H	15.6290076	10.6577489	6.4136115
H	20.1632099	7.9328694	6.4482433
H	22.4875238	7.9946991	8.0259305
H	24.1759348	11.0598341	11.9125602
H	22.8859637	12.8418888	13.6937016
H	18.3862392	15.5100645	13.5449409
H	16.4591354	15.9396133	11.6111418

TURBOMOLE (QM) and ChemShell Energies (MM and QM/MM)

	QM/MM	QM	MM
B3LYP/B1	-4168.078191	-4070.639808	-97.438383
B3LYP/B2*	-4168.952025	-4071.513642	-97.438383
PBE0/B2/*	-4167.308704	-4069.870321	-97.438383
B3LYP+D/B2*	-4169.434257	-4071.995874	-97.438383
[A]M06/B2/*	-4168.822196	-5491.190857	-97.438383
[4]B3LYP/B1	-4168.051537	-4070.613154	-97.438383

*B3LYP/B1 geometry

[A]Additional contribution to MM energy and charges: 1419.807044

Cpd I formation via E360 pathway
Figure 7

Compound 0 (^{360}**Cpd 0**)

C	25.7188684	5.9535340	11.6150122
H	26.7999967	5.8670760	11.4783412
H	25.4533076	5.6549591	12.6361982
O	25.3753375	7.3199179	11.3658956
H	24.4313144	7.4602880	11.6202396
C	19.7134813	14.0379623	7.0705702
H	20.3810619	14.2808214	6.2355584
H	18.9703512	13.3216326	6.7082037
S	20.7208803	13.2370509	8.3780827
C	31.0506767	8.2293585	11.0969750
H	31.0332317	9.2716605	10.7735211
H	32.0362427	7.9774434	11.4985232
C	30.0249101	7.9884260	12.1813947
O	30.1074010	7.0819524	12.9972477
O	29.0230372	8.8692504	12.1419781
H	28.3033474	8.6744902	12.8132355
C	11.8592623	8.2261496	16.3073789
H	12.2873109	8.7178875	17.1818898
O	12.8062362	7.2693816	15.7572103
C	14.1302343	7.4439350	15.9645048
O	14.5938000	8.3988043	16.5733062
C	14.9598877	6.3459943	15.3239604
H	14.2761688	5.6007589	14.9067819
C	15.8649313	5.6962653	16.3814090
H	15.3042125	5.4323199	17.2813918
H	16.3231129	4.7962548	15.9716191
H	16.6727123	6.3841596	16.6405196
C	15.8320962	6.9661884	14.2098002
H	16.3697289	7.7977824	14.6919679
O	16.7733626	5.9822281	13.7874797
H	17.1829533	6.3586245	12.9797328
C	15.0659452	7.5501271	12.9954204
H	14.2612101	8.1731084	13.4045403
C	14.4157857	6.4620519	12.1217146
H	13.9430979	5.6973399	12.7470317
H	13.6390498	6.8813123	11.4773846
H	15.1550672	5.9668870	11.4880964
C	16.0312852	8.5142810	12.2633865
H	16.4904323	9.1210344	13.0584323
O	17.0763884	7.7237349	11.6674271
H	17.8495085	8.3135438	11.4963727
C	15.4635017	9.5360169	11.2435260
H	16.3221843	10.1662925	10.9855617
C	14.9715144	8.9078572	9.9314675
H	14.0240823	8.3723959	10.0480362
H	14.8189171	9.6826145	9.1735273
H	15.7195381	8.2052881	9.5524579
C	14.3424909	10.4483604	11.7980183
H	14.0653648	11.1698894	11.0234394
H	13.4490275	9.8450213	12.0063873
Fe	19.4158853	11.8320043	9.8351976
N	17.8034066	11.9142109	8.6215368
N	20.2013789	10.2899304	8.7879422
N	21.0257736	11.8041225	11.0820028
N	18.6293780	13.4139486	10.8786751
C	16.7530806	12.7996048	8.6495596
C	15.7383317	12.4249988	7.6774616
C	16.1781239	11.2665219	7.0886034
C	17.4832589	10.9755818	7.6757462
C	19.5830051	9.6099974	7.7757608
C	20.4555616	8.5508444	7.2694384
C	21.6205459	8.6021845	8.0039293
C	21.4286600	9.7191861	8.9424257
C	22.1885809	11.1077529	10.8958370
C	23.1543738	11.4097311	11.9449962
C	22.5287248	12.2919852	12.8093366
C	21.1966955	12.5336113	12.2369997
C	19.0772855	13.8751732	12.0885504
C	18.2053255	14.9328211	12.5982585
C	17.2316759	15.1244245	11.6517709
C	17.4913067	14.1374497	10.6072933
C	16.6375674	13.8635795	9.5422191
H	15.7618493	14.4959900	9.4399070
C	18.3085652	9.9167353	7.2951440
H	17.9091889	9.2888156	6.5089258
C	22.3697852	10.1675845	9.8766960
H	23.3685290	9.7535865	9.7842025
C	20.2479171	13.4465098	12.7130560
H	20.4653153	13.9389416	13.6572005
H	19.7849452	9.7621261	11.9972534
O	18.4752381	10.6583828	10.9076223
O	19.2146187	9.4476038	11.2715601
O	26.7110901	8.7039544	13.3472794
H	26.2363077	8.3182876	12.5708906
H	26.2017826	8.3476991	14.1100155
O	22.7187297	7.7403734	11.8209160
H	22.4030339	8.4008750	11.1662894
H	22.0886417	7.8476066	12.5740515
H	25.1978917	5.3034246	10.9121555
H	19.1439179	14.9392956	7.2969819
H	30.8709313	7.5865630	10.2352488
H	11.0065420	7.6450573	16.6584717
H	11.5634738	8.9688630	15.5664656
H	14.6018567	11.0440804	12.6731832
H	14.7887868	12.9392958	7.5293755
H	15.6456136	10.6179216	6.3930340
H	20.1823834	7.8864203	6.4496941
H	22.5219011	7.9893018	8.0043530
H	24.1595825	10.9882841	11.9471054
H	22.8631716	12.7901586	13.7193009
H	18.3229092	15.4112311	13.5705570
H	16.3984291	15.8270718	11.6444933

TURBOMOLE (QM) and ChemShell Energies (MM and QM/MM)

	QM/MM	QM	MM
B3LYP/B1	-4168.587310	-4071.118910	-97.468399
B3LYP/B2*	-4169.465020	-4071.996620	-97.468399
PBE0/B2/*	-4167.825309	-4070.356909	-97.468399
B3LYP+D/B2*	-4169.957279	-4072.488880	-97.468399
[A]M06/B2/*	-4169.338845	-5491.692907	-97.468399
[4]B3LYP/B1	-4168.557344	-4071.088945	-97.468399

*B3LYP/B1 geometry
[A]Additional contribution to MM energy and charges: 1419.822460

Figure 7

TS for O-O homolytic cleavage from Cpd 0 (^{360}**TS1**)

C	25.6583256	5.9963137	11.6182761
H	26.7428524	5.9409708	11.4946466
H	25.3900939	5.7074974	12.6415421
O	25.2758172	7.3483943	11.3379035
H	24.3177974	7.4649906	11.5512523
C	19.7258059	14.0592752	7.0513612
H	20.3901861	14.3026064	6.2144293
H	18.9843049	13.3393739	6.6917038
S	20.7315121	13.2785692	8.3709920
C	31.0237918	8.2385757	11.0917480
H	31.0152155	9.2774041	10.7566630
H	32.0012315	7.9883074	11.5135364
C	29.9755077	8.0166857	12.1589034
O	30.0578880	7.1474131	13.0141438
O	28.9524942	8.8676523	12.0550665
H	28.2235400	8.6879441	12.7231185
C	11.8760985	8.2225371	16.2865220
H	12.2979489	8.7124660	17.1651768
O	12.8236492	7.2607592	15.7473375
C	14.1475062	7.4319947	15.9657357
O	14.6075562	8.3864711	16.5779060
C	14.9783177	6.3299828	15.3374306
H	14.2962117	5.5815649	14.9236123
C	15.8749961	5.6892109	16.4082098
H	15.3040059	5.4282463	17.3026707
H	16.3417788	4.7892746	16.0083753
H	16.6761269	6.3821306	16.6747915
C	15.8632648	6.9294061	14.2199971
H	16.4253385	7.7460570	14.7012938
O	16.7709146	5.9160983	13.7991875
H	17.1607940	6.2542435	12.9640204
C	15.1182280	7.5381107	13.0048402
H	14.3586284	8.2138991	13.4140553
C	14.3946818	6.4799222	12.1521637
H	13.8777819	5.7561247	12.7909679
H	13.6410474	6.9380749	11.5058250
H	15.0973551	5.9315655	11.5206845
C	16.1309808	8.4297618	12.2388585
H	16.6557605	9.0075139	13.0151007
O	17.0869898	7.5617516	11.6108462
H	17.9518385	8.0352942	11.4845453
C	15.5909927	9.4866843	11.2349043
H	16.4620057	10.1088810	10.9951750
C	15.0991646	8.8883714	9.9079363
H	14.1518142	8.3502298	10.0133036
H	14.9443909	9.6804530	9.1683236
H	15.8471286	8.1934753	9.5162704
C	14.4750436	10.4120984	11.7837242
H	14.2339326	11.1533239	11.0150927
H	13.5639797	9.8243938	11.9568084
Fe	19.3554214	11.8400440	9.8904023
N	17.7961814	11.9527974	8.6183094
N	20.1575433	10.3264581	8.8111588
N	21.0173811	11.9094631	11.0620723
N	18.6300225	13.4869255	10.8729732
C	16.7458169	12.8409361	8.6515664
C	15.7304468	12.4632438	7.6844452
C	16.1632802	11.3000185	7.0986157
C	17.4654080	11.0057556	7.6803554
C	19.5463105	9.6338226	7.8025263
C	20.4252566	8.5793666	7.3067130
C	21.5890149	8.6435641	8.0414511
C	21.3969237	9.7700506	8.9664203
C	22.1651202	11.1892537	10.8833263
C	23.1237116	11.4677643	11.9447044
C	22.5039904	12.3494793	12.8114985
C	21.1825351	12.6152392	12.2303791
C	19.0659940	13.9427719	12.0912247
C	18.1798377	14.9835336	12.6011766
C	17.2066804	15.1657304	11.6522148
C	17.4793215	14.1894312	10.6032448
C	16.6277376	13.9065941	9.5402129
H	15.7469775	14.5312944	9.4393810
C	18.2779999	9.9378607	7.3102777
H	17.8764573	9.3031996	6.5311277
C	22.3424408	10.2433546	9.8738735
H	23.3254516	9.7916804	9.8176055
C	20.2348477	13.5207390	12.7157958
H	20.4445872	14.0006266	13.6672481
H	19.5414637	9.5586616	11.7876423
O	18.5838355	10.8066377	10.9184093
O	19.5945608	8.6643015	11.3822168
O	26.6542480	8.7353867	13.2870157
H	26.1437802	8.3634579	12.5261013
H	26.2096608	8.3258325	14.0639581
O	22.5885568	7.6927898	11.8229704
H	22.0119564	8.2142826	11.2265743
H	22.0542641	7.6631813	12.6552179
H	25.1644631	5.3211562	10.9194709
H	19.1541352	14.9587156	7.2799792
H	30.8549033	7.5885152	10.2332817
H	11.0154622	7.6477483	16.6285592
H	11.5944337	8.9670894	15.5419595
H	14.7159801	10.9887846	12.6767243
H	14.7784718	12.9741767	7.5403705
H	15.6285226	10.6505242	6.4056092
H	20.1553434	7.9082691	6.4913349
H	22.4889044	8.0285839	8.0495027
H	24.1140411	11.0126474	11.9582151
H	22.8353551	12.8306478	13.7316837
H	18.2931369	15.4624978	13.5737110
H	16.3719036	15.8664990	11.6404870

TURBOMOLE (QM) and ChemShell Energies (MM and QM/MM)

	QM/MM	QM	MM
B3LYP/B1	-4168.559274	-4071.095470	-97.463804
B3LYP/B2*	-4169.436782	-4071.972978	-97.463804
PBE0/B2/*	-4167.789549	-4070.325745	-97.463804
B3LYP+D/B2*	-4169.925701	-4072.461897	-97.463804
[A]M06/B2/*	-4169.311771	-5491.661373	-97.463804
[4]B3LYP/B1	-4168.555865	-4071.092061	-97.463804

*B3LYP/B1 geometry

[A]Additional contribution to MM energy and charges: 1419.813406

Figure 7

Compound I/OH radical intermediate (^{360}**IC1**)

C	25.5201672	6.0622318	11.6566020
H	26.6085030	6.0791426	11.5573705
H	25.2491534	5.7488848	12.6713972
O	25.0523196	7.3893835	11.3751671
H	24.0734044	7.4481850	11.5434519
C	19.7361127	14.0963476	7.0120102
H	20.4006096	14.3557836	6.1806182
H	19.0000922	13.3787549	6.6368990
S	20.7417876	13.3057528	8.3250174
C	30.9587567	8.2450707	11.0808027
H	30.9701399	9.2778596	10.7259841
H	31.9201273	7.9975831	11.5389985
C	29.8756559	8.0653066	12.1222746
O	29.9826797	7.3162016	13.0815279
O	28.7941487	8.8098282	11.8761113
H	28.0677243	8.6759711	12.5615869
C	11.9474770	8.1691170	16.3060689
H	12.3642691	8.6675511	17.1826348
O	12.9009021	7.2082880	15.7781577
C	14.2245160	7.3818955	16.0113953
O	14.6736160	8.3423652	16.6222736
C	15.0594596	6.2713916	15.4072711
H	14.3785217	5.5236528	14.9907454
C	15.9326483	5.6332049	16.5003387
H	15.3555744	5.4361820	17.4072409
H	16.3540484	4.6965653	16.1367067
H	16.7688819	6.2951717	16.7347781
C	15.9735762	6.8422279	14.2972313
H	16.5578402	7.6404249	14.7835434
O	16.8444127	5.7963832	13.8877564
H	17.2631484	6.1247646	13.0606775
C	15.2663291	7.4720152	13.0735522
H	14.5372682	8.1853707	13.4743371
C	14.4975321	6.4413514	12.2271794
H	13.9435424	5.7474517	12.8684426
H	13.7685138	6.9280433	11.5726025
H	15.1776319	5.8564182	11.6042600
C	16.3192761	8.3149533	12.3014030
H	16.8512288	8.8963306	13.0701218
O	17.2531260	7.4147383	11.6952453
H	18.1787152	7.8141613	11.6002812
C	15.7915346	9.3689501	11.2815241
H	16.6606242	9.9978118	11.0579346
C	15.3318884	8.7654590	9.9429888
H	14.3814184	8.2276982	10.0230595
H	15.1940354	9.5562813	9.1974394
H	16.0910356	8.0682155	9.5777132
C	14.6552012	10.2935878	11.7963674
H	14.4314404	11.0292119	11.0161823
H	13.7416856	9.7034300	11.9480051
Fe	19.3481202	11.9134837	9.8908583
N	17.7844490	12.0025827	8.6188302
N	20.1395886	10.3621983	8.8324425
N	21.0117455	11.9918527	11.0519670
N	18.6182874	13.5542449	10.8606369
C	16.7313366	12.8686767	8.6448240
C	15.7140236	12.4847177	7.6799799
C	16.1558126	11.3282941	7.0912142
C	17.4632394	11.0485769	7.6719197
C	19.5583183	9.6824182	7.8170497
C	20.4329420	8.6166964	7.3274979
C	21.5769554	8.6578629	8.0889857
C	21.3808338	9.7861268	9.0144950
C	22.1362150	11.2520377	10.9055462
C	23.0926858	11.5189911	11.9781730
C	22.4825544	12.4150615	12.8299809
C	21.1702394	12.6989350	12.2279318
C	19.0401712	14.0119529	12.0699753
C	18.1451583	15.0408009	12.5910659
C	17.1669222	15.2133357	11.6472601
C	17.4495982	14.2443038	10.5932443
C	16.6030063	13.9427540	9.5420418
H	15.7111160	14.5517888	9.4426670
C	18.2830531	9.9942681	7.3093560
H	17.8911554	9.3541725	6.5296635
C	22.3135582	10.2753768	9.9077225
H	23.2804945	9.7901123	9.8939483
C	20.2222193	13.5945505	12.7010342
H	20.4205478	14.0750431	13.6542587
H	19.6247427	9.2554958	11.2809806
O	18.6175827	10.8813420	10.9342290
O	19.7937989	8.3012170	11.4152194
O	26.5560559	8.7605769	13.2232815
H	25.9655779	8.4053052	12.5115840
H	26.2157659	8.3094885	14.0298560
O	22.3412737	7.5747137	11.8426031
H	21.4461100	7.9125657	11.4802809
H	22.0649301	7.4781203	12.7861779
H	25.0864045	5.3642688	10.9405266
H	19.1579806	14.9887612	7.2516509
H	30.8111930	7.5838858	10.2269139
H	11.0866048	7.5949131	16.6484946
H	11.6686566	8.9086644	15.5554722
H	14.8626715	10.8779157	12.6927955
H	14.7555868	12.9856155	7.5437197
H	15.6247290	10.6724378	6.4013815
H	20.1603932	7.9449158	6.5135603
H	22.4665512	8.0287212	8.1184225
H	24.0711563	11.0393503	12.0028028
H	22.8067681	12.8927563	13.7545130
H	18.2563091	15.5165273	13.5654356
H	16.3315682	15.9133386	11.6315740

TURBOMOLE (QM) and ChemShell Energies (MM and QM/MM)

	QM/MM	QM	MM
B3LYP/B1	-4168.563943	-4071.111263	-97.452680
B3LYP/B2*	-4169.436622	-4071.983942	-97.452680
PBE0/B2/*	-4167.784689	-4070.332009	-97.452680
B3LYP-D/B2*	-4169.922447	-4072.469767	-97.452680
[A]M06/B2/*	-4169.305969	-5491.657821	-97.452680
[4]B3LYP/B1	-4168.563883	-4071.111203	-97.452680

*B3LYP/B1 geometry

[A]Additional contribution to MM energy and charges: 1419.804532

Figure 7

TS for H-atom abstraction by the OH radical from its immediate neighboring water molecule (^{360}**TS2**)

C	25.4455641	6.1058675	11.6776577
H	26.5346334	6.1428982	11.5903333
H	25.1702797	5.7802942	12.6873182
O	24.9537641	7.4248941	11.3997493
H	23.9640599	7.4700316	11.5591148
C	19.7384296	14.1049016	7.0096835
H	20.4053066	14.3661770	6.1809539
H	19.0041317	13.3875296	6.6309678
S	20.7426582	13.3138731	8.3229380
C	30.9348859	8.2518527	11.0785400
H	30.9446442	9.2826348	10.7181878
H	31.8940006	8.0124149	11.5458864
C	29.8431542	8.0747372	12.1122141
O	29.9481846	7.3375747	13.0808265
O	28.7578229	8.8077416	11.8481172
H	28.0238983	8.6745138	12.5274610
C	11.9585923	8.1685226	16.2940183
H	12.3732482	8.6672732	17.1715353
O	12.9130036	7.2076695	15.7692048
C	14.2367349	7.3815689	16.0058317
O	14.6828817	8.3420897	16.6188094
C	15.0727354	6.2711266	15.4037386
H	14.3917251	5.5264727	14.9818245
C	15.9374458	5.6282350	16.5003872
H	15.3525499	5.4242652	17.4007246
H	16.3646133	4.6954658	16.1338972
H	16.7702831	6.2903035	16.7459932
C	15.9950048	6.8405710	14.2992177
H	16.5789442	7.6369683	14.7889230
O	16.8629110	5.7930148	13.8916731
H	17.2912726	6.1242451	13.0697715
C	15.2962936	7.4731775	13.0728995
H	14.5691033	8.1901770	13.4707339
C	14.5256860	6.4451086	12.2249480
H	13.9670522	5.7530757	12.8642769
H	13.8005164	6.9340959	11.5675523
H	15.2056613	5.8577055	11.6044765
C	16.3582394	8.3093357	12.3033981
H	16.8846755	8.8947289	13.0730446
O	17.2927213	7.4119933	11.7017943
H	18.2380133	7.7949773	11.6295452
C	15.8264403	9.3618904	11.2819198
H	16.6940342	9.9922841	11.0588899
C	15.3717814	8.7558568	9.9426829
H	14.4220794	8.2164342	10.0193846
H	15.2343777	9.5447564	9.1946285
H	16.1343121	8.0591553	9.5832811
C	14.6856497	10.2845166	11.7924720
H	14.4600933	11.0175959	11.0101300
H	13.7736249	9.6920867	11.9440927
Fe	19.3515083	11.9209959	9.8844243
N	17.7856963	12.0095005	8.6141625
N	20.1441553	10.3750778	8.8233717
N	21.0123983	11.9988610	11.0471433
N	18.6190787	13.5614807	10.8552097
C	16.7331086	12.8725785	8.6377024
C	15.7148099	12.4882995	7.6746245
C	16.1560810	11.3310504	7.0869199
C	17.4638643	11.0533526	7.6667855
C	19.5644306	9.6914778	7.8134608
C	20.4357121	8.6209924	7.3272452
C	21.5764385	8.6587271	8.0926003
C	21.3815069	9.7908457	9.0136324
C	22.1339624	11.2596832	10.9068101
C	23.0903465	11.5269625	11.9793622
C	22.4801832	12.4224122	12.8307428
C	21.1689761	12.7061532	12.2267413
C	19.0357280	14.0175513	12.0639365
C	18.1414882	15.0449911	12.5871251
C	17.1641394	15.2194514	11.6425626
C	17.4483455	14.2532809	10.5873185
C	16.6034219	13.9481416	9.5380554
H	15.7098486	14.5548950	9.4384407
C	18.2843851	10.0006424	7.3076361
H	17.8914735	9.3555479	6.5326274
C	22.3091002	10.2743768	9.9116086
H	23.2696047	9.7777737	9.9099462
C	20.2194415	13.5970120	12.6976221
H	20.4138834	14.0747888	13.6529614
H	19.6916048	9.1967895	11.2952926
O	18.6230147	10.8884756	10.9251667
O	19.8232342	8.2473300	11.4650899
O	26.5238672	8.7642302	13.2046481
H	25.9028857	8.4225153	12.5105088
H	26.2098899	8.3047448	14.0172890
O	22.2572847	7.5850518	11.8243858
H	21.2603052	7.9073699	11.5339764
H	22.0446937	7.4707390	12.7808591
H	25.0339076	5.4036765	10.9527211
H	19.1596953	14.9967989	7.2497922
H	30.7966974	7.5862403	10.2265244
H	11.0964716	7.5953082	16.6349574
H	11.6820280	8.9082760	15.5427903
H	14.8879732	10.8710394	12.6886431
H	14.7558789	12.9884839	7.5392239
H	15.6243789	10.6732485	6.3994201
H	20.1615507	7.9462458	6.5163081
H	22.4609188	8.0228148	8.1297015
H	24.0685570	11.0468699	12.0054758
H	22.8034124	12.9005403	13.7553956
H	18.2516119	15.5176016	13.5631264
H	16.3284134	15.9190272	11.6276558

TURBOMOLE (QM) and ChemShell Energies (MM and QM/MM)

	QM/MM	QM	MM
B3LYP/B1	-4168.563485	-4071.114230	-97.449255
B3LYP/B2*	-4169.434871	-4071.985615	-97.449255
PBE0/B2/*	-4167.783248	-4070.333993	-97.449255
B3LYP-D/B2*	-4169.921018	-4072.471762	-97.449255
[A]M06/B2/*	-4169.303006	-5491.655204	-97.449255
[4]B3LYP/B1	-4168.563421	-4071.114166	-97.449255

*B3LYP/B1 geometry

[A]Additional contribution to MM energy and charges: 1419.801453

Figure 7

Compound I, water and $SerO^-$ intermediate (^{360}**IC2**)

C	25.8244605	5.9036589	11.5053814
H	26.9129802	5.7601560	11.3729338
H	25.5660600	5.5575111	12.5235959
O	25.4585625	7.2399565	11.2869639
H	23.9779304	7.5292438	11.5590824
C	19.7159186	14.0614553	7.0769036
H	20.4025603	14.3156905	6.2618028
H	18.9864190	13.3464348	6.6855362
S	20.6988119	13.2697552	8.4081082
C	30.9766976	8.2637406	11.1029828
H	30.9797971	9.2946549	10.7417428
H	31.9430690	8.0262791	11.5577965
C	29.8893099	8.0778001	12.1475602
O	30.0023377	7.2841293	13.0754270
O	28.8387579	8.8534782	11.9338146
H	28.0176440	8.6736680	12.5488253
C	11.8404639	8.2188324	16.4173404
H	12.2759634	8.7211109	17.2824530
O	12.7620513	7.2226197	15.9001415
C	14.0930440	7.3649621	16.0963636
O	14.5880456	8.3311532	16.6611350
C	14.8711079	6.2089271	15.5007902
H	14.1504815	5.4646396	15.1510180
C	15.8011540	5.5909545	16.5577724
H	15.3072885	5.5018509	17.5282837
H	16.1252541	4.6007571	16.2386033
H	16.6982447	6.2058175	16.6561385
C	15.7309038	6.7066647	14.3176239
H	16.4084667	7.4655353	14.7441018
O	16.4918472	5.5921966	13.8673537
H	16.8835199	5.8801708	13.0159889
C	14.9729255	7.3749155	13.1413676
H	14.2854529	8.1005754	13.5874876
C	14.1381469	6.3736600	12.3245885
H	13.5930317	5.6987836	12.9922857
H	13.3963770	6.8846710	11.7042299
H	14.7724072	5.7667110	11.6741949
C	16.0119271	8.1869853	12.3308815
H	16.6015784	8.7422796	13.0770250
O	16.8784916	7.2429303	11.6877018
H	17.7961644	7.6149517	11.6359158
C	15.5167924	9.2607342	11.3157940
H	16.4095479	9.8522390	11.0755007
C	15.0161696	8.6680457	9.9884664
H	14.0561999	8.1526293	10.0931603
H	14.8814760	9.4600530	9.2433335
H	15.7466132	7.9487748	9.6080432
C	14.4281105	10.2288413	11.8465804
H	14.1810013	10.9435971	11.0547630
H	13.5125547	9.6617665	12.0583737
Fe	19.3109789	11.8419860	9.9099940
N	17.7576289	11.9536874	8.6301974
N	20.1266278	10.3311460	8.8164946
N	20.9717678	11.9062290	11.0795272
N	18.5796785	13.4744778	10.8955857
C	16.7007623	12.8336851	8.6603397
C	15.6897743	12.4597427	7.6938880
C	16.1304849	11.3004761	7.1016369
C	17.4305037	11.0172636	7.6841340
C	19.5357168	9.6518908	7.7855264
C	20.4189185	8.6072299	7.2810169
C	21.5636842	8.6466091	8.0459994
C	21.3498496	9.7508832	8.9887435
C	22.1184099	11.1871120	10.9090601
C	23.0937038	11.4800089	11.9499671
C	22.4783227	12.3666039	12.8145776
C	21.1506187	12.6159147	12.2431168
C	19.0110992	13.9324842	12.1126929
C	18.1293225	14.9672668	12.6292896
C	17.1520923	15.1488498	11.6807318
C	17.4298195	14.1809234	10.6323081
C	16.5799916	13.8891770	9.5655778
H	15.6947823	14.5090709	9.4697756
C	18.2629479	9.9586323	7.3048204
H	17.8660269	9.3266510	6.5207659
C	22.2834684	10.2121946	9.9192599
H	23.2362586	9.7072414	9.9151139
C	20.1889118	13.5061573	12.7303000
H	20.3917022	13.9758662	13.6883800
H	19.1977541	9.2172563	11.2892567
O	18.5585740	10.7685137	10.9055963
O	19.3378276	8.2663868	11.5179230
O	26.5810407	8.6432326	13.0284270
H	26.0956262	8.0565430	12.2708127
H	26.2752053	8.2454471	13.8711057
O	22.9631825	7.7279285	11.5328111
H	20.0872290	8.2233089	12.1480156
H	22.5969956	7.8643849	12.4249687
H	25.3048170	5.2414804	10.8128810
H	19.1411092	14.9592862	7.3039724
H	30.8307213	7.5956922	10.2541785
H	10.9692162	7.6689954	16.7732522
H	11.5683065	8.9486379	15.6548572
H	14.6953594	10.8363991	12.7111717
H	14.7369886	12.9691209	7.5496664
H	15.5990469	10.6524997	6.4046673
H	20.1568245	7.9435082	6.4570954
H	22.4579157	8.0237177	8.0665638
H	24.0865086	11.0301771	11.9424600
H	22.8127255	12.8572030	13.7286639
H	18.2470285	15.4500455	13.5994115
H	16.3236329	15.8569508	11.6629983

TURBOMOLE (QM) and ChemShell Energies (MM and QM/MM)

	QM/MM	QM	MM
B3LYP/B1	-4168.593721	-4071.125891	-97.467831
B3LYP/B2*	-4169.465544	-4071.997713	-97.467831
PBE0/B2/*	-4167.816517	-4070.348687	-97.467831
B3LYP-D/B2*	-4169.944221	-4072.476391	-97.467831
[A]M06/B2/*	-4169.331522	-5491.669415	-97.467831
[4]B3LYP/B1	-4168.593590	-4071.125760	-97.467831

*B3LYP/B1 geometry

[A]Additional contribution to MM energy and charges: 1419.805724

Figure 7

TS for H^+ transfer from the ultimate proton donor E360 to reprotonate $SerO^-$ (**^{360}TS3)**

C	25.8320900	5.8952623	11.5243370
H	26.9193048	5.7522062	11.3917348
H	25.5699027	5.5511510	12.5408306
O	25.4686907	7.2347262	11.3079311
H	23.9675238	7.5304809	11.5756649
C	19.7148410	14.0614757	7.0776280
H	20.4017372	14.3154112	6.2626400
H	18.9852885	13.3465366	6.6862392
S	20.6973979	13.2701155	8.4092156
C	30.9670197	8.2671220	11.1037865
H	30.9708350	9.2976156	10.7411997
H	31.9317433	8.0310741	11.5634387
C	29.8710835	8.0813415	12.1429574
O	29.9867575	7.2842089	13.0703226
O	28.8218350	8.8501040	11.9249017
H	27.9682493	8.6718364	12.5337469
C	11.8397715	8.2188342	16.4175636
H	12.2751823	8.7214050	17.2825436
O	12.7609355	7.2222191	15.9004965
C	14.0920489	7.3641307	16.0965690
O	14.5873987	8.3302155	16.6611803
C	14.8696369	6.2078228	15.5009613
H	14.1484054	5.4639341	15.1516377
C	15.7998361	5.5897331	16.5576971
H	15.3068672	5.5021855	17.5288175
H	16.1221733	4.5988433	16.2389310
H	16.6978326	6.2035151	16.6546116
C	15.7293562	6.7046226	14.3169912
H	16.4080734	7.4625154	14.7432029
O	16.4885665	5.5890383	13.8664085
H	16.8800034	5.8771456	13.0149701
C	14.9717412	7.3738553	13.1413735
H	14.2849425	8.0999490	13.5878264
C	14.1361353	6.3727205	12.3253319
H	13.5911323	5.6984292	12.9937133
H	13.3942037	6.8835415	11.7049258
H	14.7697577	5.7653226	11.6747755
C	16.0114993	8.1856475	12.3309611
H	16.6014906	8.7401395	13.0774547
O	16.8778273	7.2417654	11.6876102
H	17.7960559	7.6129830	11.6354456
C	15.5166450	9.2595366	11.3159647
H	16.4093999	9.8510404	11.0754451
C	15.0160378	8.6667083	9.9886987
H	14.0559187	8.1515598	10.0933044
H	14.8812346	9.4584890	9.2433148
H	15.7465510	7.9472833	9.6087417
C	14.4282079	10.2278918	11.8467148
H	14.1809076	10.9425462	11.0548073
H	13.5126649	9.6608314	12.0585995
Fe	19.3104987	11.8426420	9.9102070
N	17.7569364	11.9539012	8.6308005
N	20.1259192	10.3319442	8.8161094
N	20.9715256	11.9071681	11.0788619
N	18.5791310	13.4745087	10.8964282
C	16.7003439	12.8338121	8.6604345
C	15.6893869	12.4600774	7.6939273
C	16.1296776	11.3006439	7.1020506
C	17.4295695	11.0170919	7.6847073
C	19.5354246	9.6524789	7.7857301
C	20.4187238	8.6081836	7.2808752
C	21.5639816	8.6481790	8.0452217
C	21.3505696	9.7527548	8.9874845
C	22.1185993	11.1891403	10.9079657
C	23.0931976	11.4812790	11.9494692
C	22.4777045	12.3670660	12.8147650
C	21.1498536	12.6162037	12.2434047
C	19.0097162	13.9323179	12.1134413
C	18.1279784	14.9671693	12.6300627
C	17.1512986	15.1492313	11.6811958
C	17.4291595	14.1811886	10.6327029
C	16.5797131	13.8895722	9.5659836
H	15.6945430	14.5096270	9.4698774
C	18.2617671	9.9586731	7.3053857
H	17.8648953	9.3261053	6.5218027
C	22.2842635	10.2153334	9.9167422
H	23.2386073	9.7131041	9.9104553
C	20.1876999	13.5052152	12.7311043
H	20.3899285	13.9738688	13.6896742
H	19.1950493	9.2164781	11.2890058
O	18.5583500	10.7691559	10.9060677
O	19.3367405	8.2652741	11.5157728
O	26.5869555	8.6309970	12.9817210
H	26.0755277	7.9992548	12.2100349
H	26.3128914	8.2438516	13.8382206
O	22.9587696	7.7233710	11.5407397
H	20.0824326	8.2235276	12.1504504
H	22.5909522	7.8675555	12.4316042
H	25.3101246	5.2408077	10.8262627
H	19.1403331	14.9595496	7.3044994
H	30.8257651	7.5982576	10.2548260
H	10.9682952	7.6693252	16.7734222
H	11.5679583	8.9485846	15.6549047
H	14.6957247	10.8354232	12.7112418
H	14.7366445	12.9695402	7.5497190
H	15.5982810	10.6527080	6.4050117
H	20.1565934	7.9441580	6.4572102
H	22.4586326	8.0258812	8.0655028
H	24.0863954	11.0323240	11.9414736
H	22.8119658	12.8568443	13.7293431
H	18.2456751	15.4498965	13.6002114
H	16.3227294	15.8571993	11.6632828

TURBOMOLE (QM) and ChemShell Energies (MM and QM/MM)

	QM/MM	QM	MM
B3LYP/B1	-4168.593550	-4071.124950	-97.468600
B3LYP/B2*	-4169.465540	-4071.996939	-97.468600
PBE0/B2/*	-4167.817025	-4070.348425	-97.468600
B3LYP-D/B2*	-4169.944531	-4072.475930	-97.468600
[A]M06/B2/*	-4169.331286	-5491.668832	-97.468600
[4]B3LYP/B1	-4168.593421	-4071.124820	-97.468600

*B3LYP/B1 geometry

[A]Additional contribution to MM energy and charges: 1419.806146

Figure 7
Compound I (^{360}**Cpd I**)

C	25.8867882	5.8294156	11.5638404
H	26.9690571	5.6952042	11.4408010
H	25.5987367	5.5398370	12.5836634
O	25.5134155	7.1750514	11.2775520
H	23.8728720	7.5519482	11.6686773
C	19.7040428	14.0688240	7.0807765
H	20.3943367	14.3225741	6.2686431
H	18.9750876	13.3552059	6.6859867
S	20.6797700	13.2771162	8.4168243
C	31.0109491	8.2581872	11.1076981
H	31.0068231	9.2949537	10.7596393
H	31.9884652	8.0179695	11.5418174
C	29.9141270	8.0464940	12.1676452
O	30.0665079	7.1178907	12.9949661
O	28.9174104	8.8455887	12.0900812
H	27.5771345	8.7454185	12.8524774
C	11.8353706	8.2157225	16.4241782
H	12.2733357	8.7169928	17.2885902
O	12.7523702	7.2148227	15.9072418
C	14.0840676	7.3504259	16.1023746
O	14.5851543	8.3151925	16.6641154
C	14.8551037	6.1880706	15.5089617
H	14.1287930	5.4479809	15.1621281
C	15.7831456	5.5641923	16.5652506
H	15.3005323	5.5061666	17.5437967
H	16.0736880	4.5586131	16.2617069
H	16.6996377	6.1531893	16.6419624
C	15.7146175	6.6763334	14.3213817
H	16.4054565	7.4247983	14.7446311
O	16.4576373	5.5516598	13.8648129
H	16.8543288	5.8404020	13.0163695
C	14.9578744	7.3558553	13.1509037
H	14.2755325	8.0825592	13.6027940
C	14.1154025	6.3623684	12.3324826
H	13.5734880	5.6848242	12.9999221
H	13.3705132	6.8789103	11.7206220
H	14.7433324	5.7577111	11.6738669
C	15.9982441	8.1680842	12.3424764
H	16.5866545	8.7229873	13.0900913
O	16.8669478	7.2238719	11.7011257
H	17.7821479	7.5989355	11.6424741
C	15.5047294	9.2406028	11.3253204
H	16.3983029	9.8301944	11.0829208
C	15.0024403	8.6463569	9.9992891
H	14.0400813	8.1356790	10.1044031
H	14.8711662	9.4368805	9.2519315
H	15.7298145	7.9229060	9.6208831
C	14.4184816	10.2121089	11.8550675
H	14.1694298	10.9239130	11.0611640
H	13.5028029	9.6471796	12.0718473
Fe	19.2902412	11.8398375	9.9012389
N	17.7380471	11.9528278	8.6241605
N	20.1038873	10.3358338	8.7998775
N	20.9531299	11.9097986	11.0634415
N	18.5585534	13.4620754	10.8964538
C	16.6886534	12.8283098	8.6505365
C	15.6735979	12.4569364	7.6856164
C	16.1056494	11.2935799	7.0975786
C	17.4071412	11.0056146	7.6768069
C	19.5178765	9.6522554	7.7824691
C	20.4043976	8.6129836	7.2699204
C	21.5572175	8.6653149	8.0211136
C	21.3468066	9.7723853	8.9609605
C	22.1025040	11.2128401	10.8806919
C	23.0779011	11.4969040	11.9256244
C	22.4581474	12.3626337	12.8062869
C	21.1259357	12.6104757	12.2419078
C	18.9822884	13.9151110	12.1095909
C	18.1028720	14.9530520	12.6280506
C	17.1301318	15.1422854	11.6780545
C	17.4059886	14.1760665	10.6256356
C	16.5660788	13.8914254	9.5600600
H	15.6832037	14.5136304	9.4582084
C	18.2310192	9.9509635	7.3041311
H	17.8312838	9.3081430	6.5305167
C	22.2787337	10.2520591	9.8684147
H	23.2485003	9.7795243	9.8388519
C	20.1651078	13.4868694	12.7333271
H	20.3649150	13.9546198	13.6928097
H	19.1690046	9.2052755	11.2696435
O	18.5468119	10.7557294	10.8940533
O	19.3285875	8.2579974	11.5071109
O	26.5710269	8.7815855	13.0612758
H	25.9946824	7.7899811	11.9211807
H	26.3750264	8.2986118	13.8886166
O	22.9048290	7.7223118	11.5480694
H	20.0521408	8.2455288	12.1666920
H	22.4779691	7.9127608	12.4058079
H	25.3471447	5.1907459	10.8645891
H	19.1301423	14.9674791	7.3068818
H	30.8608226	7.5974739	10.2538911
H	10.9617565	7.6702129	16.7809471
H	11.5650295	8.9457368	15.6612488
H	14.6899510	10.8223544	12.7164450
H	14.7220419	12.9693025	7.5438823
H	15.5715174	10.6477448	6.4006808
H	20.1413153	7.9453352	6.4494938
H	22.4557094	8.0484848	8.0384197
H	24.0729218	11.0521787	11.9107981
H	22.7917305	12.8422875	13.7264614
H	18.2212626	15.4328889	13.5995477
H	16.3035729	15.8525998	11.6601615

TURBOMOLE (QM) and ChemShell Energies (MM and QM/MM)

	QM/MM	QM	MM
B3LYP/B1	-4168.604108	-4071.134275	-97.469833
B3LYP/B2*	-4169.473824	-4072.003991	-97.469833
PBE0/B2/*	-4167.823472	-4070.353639	-97.469833
B3LYP-D/B2*	-4169.952022	-4072.482189	-97.469833
[A]M06/B2/*	-4169.340784	-5491.684074	-97.469833
[4]B3LYP/B1	-4168.603951	-4071.134118	-97.469833

*B3LYP/B1 geometry

[A]Additional contribution to MM energy and charges: 1419.813124

Cpd I formation via E244 pathway
Figure 8

Compound 0 (^{244}**Cpd 0**)

C	21.0604577	1.0401663	14.7742525
H	21.8279657	0.6847346	15.4778113
H	21.4383491	0.8431239	13.7687959
C	19.8555869	0.1474202	14.9499182
O	19.7870121	-0.9127369	14.3067645
O	18.8758171	0.4318347	15.7904366
H	18.8967631	1.3500737	16.2166012
C	19.9095624	13.8381916	6.9609498
H	20.5661295	14.0208713	6.1041491
H	19.1567445	13.1039392	6.6605577
S	20.9228688	13.1485068	8.3316401
C	11.9622076	8.2658287	16.4125826
H	12.4741207	8.7535780	17.2434885
O	12.8294406	7.2636645	15.8158847
C	14.1646401	7.3853427	15.9307177
O	14.7159288	8.3487529	16.4448738
C	14.8942035	6.2110636	15.3079889
H	14.1534069	5.5611017	14.8315987
C	15.6436012	5.4153012	16.3948106
H	16.0722077	4.5099668	15.9590018
H	16.4570284	6.0101330	16.8207170
H	14.9674979	5.1242262	17.2072711
C	15.8706327	6.7453238	14.2378574
H	16.6033747	7.3719513	14.7685601
O	16.5393424	5.6085747	13.6882759
H	16.9268355	5.8981949	12.8461185
C	15.2052594	7.6134998	13.1317742
H	14.4432253	8.2141210	13.6360980
C	14.4798430	6.7589810	12.0800699
H	15.1756559	6.2252245	11.4271826
H	13.8504977	6.0094015	12.5695364
H	13.8303203	7.3693918	11.4478332
C	16.2453942	8.6291583	12.6128059
H	16.6093946	9.1505373	13.5127395
O	17.3504229	7.8669854	12.0725076
H	18.0551002	8.4917929	11.7511846
C	15.8043731	9.7604652	11.6338488
H	16.6778025	10.4176579	11.5687576
C	15.5423870	9.3289326	10.1888328
H	15.4490717	10.2141454	9.5539082
H	16.3965740	8.7599140	9.8188162
H	14.6311504	8.7336408	10.0704454
C	14.5787507	10.5813944	12.0913480
H	14.2862071	11.2496311	11.2759282
H	13.7272438	9.9125100	12.2640691
Fe	19.6497678	11.8218926	9.8665365
N	18.0358868	11.8789415	8.6501361
N	20.4345269	10.2440205	8.8646248
N	21.2530144	11.8073720	11.1328593
N	18.8576936	13.4204718	10.8905415
C	16.9647843	12.7367114	8.6909667
C	15.9538175	12.3415341	7.7224835
C	16.4310218	11.2152502	7.1010031
C	17.7507294	10.9609547	7.6726788
C	19.8698383	9.6202832	7.7889531
C	20.7407104	8.5493057	7.3025835
C	21.8403761	8.5219444	8.1342553
C	21.6229885	9.6109282	9.0993988
C	22.3872265	11.0456676	11.0086946
C	23.3764956	11.4121028	12.0152841
C	22.7817854	12.3668765	12.8210308
C	21.4463166	12.5936063	12.2441463
C	19.2988207	13.8858138	12.1031862
C	18.3864436	14.8949851	12.6353429
C	17.4116225	15.0758924	11.6862730
C	17.6966377	14.1095251	10.6295638
C	16.8399315	13.8088657	9.5733157
H	15.9452749	14.4156755	9.4784858
C	18.6230244	9.9574045	7.2527509
H	18.2722310	9.3743143	6.4086807
C	22.5267653	10.0088470	10.0886665
H	23.4405646	9.4300514	10.1804861
C	20.4903621	13.5016816	12.7133550
H	20.7017973	13.9976950	13.6563963
H	20.0707487	9.7590791	11.9984704
O	18.6988120	10.7005740	10.9970494
O	19.3954949	9.4646810	11.3551884
O	19.5541399	6.5480658	13.4429525
H	20.1323663	7.3418124	13.5343314
H	18.7433074	6.9038071	13.0121389
O	18.5146336	2.8237068	16.9302611
H	18.6823380	2.9818010	17.8843731
H	18.7092123	3.6932573	16.4973044
O	19.4040617	5.2510710	15.8766841
H	19.3524357	6.0668063	16.4293541
H	19.2502516	5.6045287	14.9661339
H	20.9388272	2.1138544	14.9173133
H	19.3650184	14.7661518	7.1353861
H	11.1267888	7.7167387	16.8469119
H	11.6432993	9.0112489	15.6840822
H	14.7467194	11.2327372	12.9490225
H	14.9956565	12.8391686	7.5729712
H	15.9054432	10.5571256	6.4091175
H	20.5083949	7.9318154	6.4349421
H	22.7244400	7.8853727	8.1699459
H	24.3966979	11.0289003	11.9950458
H	23.1386337	12.9237524	13.6874111
H	18.4647653	15.3268083	13.6330708
H	16.5256910	15.7102544	11.7141434

TURBOMOLE (QM) and ChemShell Energies (MM and QM/MM)

	QM/MM	QM	MM
B3LYP/B1	-4129.451203	-4031.940311	-97.510892
B3LYP/B2*	-4130.320423	-4032.809531	-97.510892
PBE0/B2/*	-4128.704350	-4031.193458	-97.510892
B3LYP-D/B2*	-4130.815464	-4033.304571	-97.510892
[A]M06/B2/*	-4130.201962	-5453.983024	-97.510892
[4]B3LYP/B1	-4129.422272	-4031.911380	-97.510892

*B3LYP/B1 geometry
[A]Additional contribution to MM energy and charges: 1421.291955

Figure 8

TS for O-O homolytic cleavage from Cpd 0 (^{244}**TS1**)

C	21.0820084	1.0524846	14.8377640
H	21.8078663	0.6980767	15.5844950
H	21.5020814	0.8211790	13.8570076
C	19.8472118	0.1941383	14.9742519
O	19.7713783	-0.8693646	14.3375480
O	18.8451775	0.5126133	15.7771161
H	18.8764354	1.4349931	16.1918690
C	19.9103035	13.8183398	6.9835269
H	20.5794698	13.9894503	6.1343123
H	19.1567403	13.0877977	6.6757371
S	20.8962284	13.1431544	8.3818357
C	11.9738277	8.2778374	16.3563252
H	12.4774858	8.7523077	17.1999711
O	12.8619412	7.3125534	15.7297346
C	14.1961421	7.4561219	15.8639201
O	14.7153386	8.4055350	16.4346884
C	14.9653466	6.3365597	15.1886397
H	14.2441247	5.6645936	14.7140402
C	15.7804555	5.5467295	16.2299997
H	16.2297722	4.6722835	15.7553575
H	16.5851720	6.1618067	16.6429382
H	15.1455464	5.2080832	17.0573604
C	15.8866659	6.9623845	14.1155982
H	16.5341404	7.6771129	14.6492156
O	16.6895519	5.9240931	13.5628172
H	17.0855555	6.3220832	12.7569838
C	15.1355201	7.7513388	13.0074176
H	14.4363575	8.4096873	13.5283425
C	14.3189438	6.8383388	12.0802898
H	14.9668587	6.1990186	11.4768872
H	13.6596482	6.1882205	12.6637268
H	13.6867484	7.4187126	11.4026055
C	16.1552715	8.6711587	12.2957705
H	16.7348453	9.1529060	13.1010735
O	17.0297126	7.8156748	11.5577482
H	17.9330162	8.2382047	11.4637453
C	15.6356577	9.8479205	11.4082690
H	16.5104024	10.4949212	11.2799055
C	15.2205497	9.4446806	9.9922315
H	15.0423008	10.3376799	9.3902511
H	16.0425686	8.9026862	9.5278129
H	14.3167576	8.8270079	9.9604473
C	14.4706964	10.6747054	11.9882128
H	14.1557165	11.4022397	11.2333969
H	13.6123344	10.0151299	12.1616144
Fe	19.5341174	11.7473475	9.9558474
N	17.9911754	11.8723915	8.6563678
N	20.3339991	10.2098344	8.9207824
N	21.1813251	11.8136462	11.1607137
N	18.8204114	13.4351952	10.9064908
C	16.9339752	12.7527690	8.6860918
C	15.9320359	12.3764989	7.7033639
C	16.3951566	11.2401293	7.0886205
C	17.6965690	10.9605527	7.6786530
C	19.7862248	9.5929331	7.8262583
C	20.6679782	8.5349938	7.3403381
C	21.7562389	8.5033269	8.1838437
C	21.5240180	9.5802834	9.1579420
C	22.2975875	11.0305000	11.0507565
C	23.2932844	11.3900847	12.0532454
C	22.7163286	12.3617833	12.8481001
C	21.3858433	12.6025266	12.2681427
C	19.2506205	13.9018682	12.1230854
C	18.3386129	14.9112791	12.6448675
C	17.3711003	15.0887291	11.6874796
C	17.6617628	14.1216822	10.6349024
C	16.8150961	13.8228340	9.5689360
H	15.9276597	14.4382492	9.4649270
C	18.5571350	9.9408775	7.2717575
H	18.2112682	9.3635473	6.4224669
C	22.4243708	9.9798517	10.1456684
H	23.3309904	9.3930005	10.2456595
C	20.4404329	13.5192484	12.7331927
H	20.6533904	14.0174390	13.6741896
H	19.9285954	9.2531035	11.8779005
O	18.6829412	10.7918898	10.9843948
O	19.5481469	8.4981108	11.3948304
O	19.9986898	6.6194117	13.3076975
H	20.6098813	7.3157444	13.6410790
H	19.6145969	7.1192791	12.5343219
O	18.5150491	2.9395307	16.8736660
H	18.6632485	3.1197506	17.8269575
H	18.7150457	3.7936513	16.4130281
O	19.4231321	5.3232918	15.7119385
H	19.3797293	6.1383457	16.2659134
H	19.2758829	5.6636746	14.7973486
H	20.9771784	2.1316968	14.9490208
H	19.3718070	14.7514122	7.1492493
H	11.1492898	7.7019224	16.7764748
H	11.6401079	9.0389520	15.6510578
H	14.6946330	11.2625651	12.8783475
H	14.9819204	12.8862663	7.5437258
H	15.8672938	10.5810561	6.3993819
H	20.4467068	7.9247937	6.4646891
H	22.6411615	7.8680412	8.2211343
H	24.3044449	10.9835133	12.0353403
H	23.0811487	12.9248950	13.7070984
H	18.4118506	15.3444483	13.6423980
H	16.4862052	15.7248421	11.7071640

TURBOMOLE (QM) and ChemShell Energies (MM and QM/MM)

	QM/MM	QM	MM
B3LYP/B1	-4129.419873	-4031.912938	-97.506936
B3LYP/B2*	-4130.286624	-4032.779689	-97.506936
PBE0/B2/*	-4128.660211	-4031.153276	-97.506936
B3LYP-D/B2*	-4130.774867	-4033.267931	-97.506936
[A]M06/B2/*	-4130.166740	-5453.951380	-97.506936
[4]B3LYP/B1	-4129.416796	-4031.909860	-97.506936

*B3LYP/B1 geometry

[A]Additional contribution to MM energy and charges: 1421.291575

Figure 8

Compound I/OH^- intermediate(^{244}**IC**)

C	21.0371046	0.9589268	14.8602894
H	21.7776407	0.5576157	15.5673879
H	21.4058287	0.7285302	13.8585110
C	19.7722854	0.1559143	15.0385080
O	19.6595660	-0.9299233	14.4399840
O	18.7871239	0.5382578	15.8294876
H	18.8351150	1.4896621	16.2071150
C	19.9299421	13.8452025	6.9361988
H	20.6038509	14.0293703	6.0940839
H	19.1765060	13.1235077	6.6060361
S	20.9117097	13.1422266	8.3225009
C	12.0156136	8.3250455	16.3474883
H	12.5430628	8.8101146	17.1706988
O	12.8865419	7.3601689	15.7010637
C	14.2279296	7.5082163	15.7844598
O	14.7614400	8.4687652	16.3232355
C	14.9643674	6.3705743	15.1054600
H	14.2191010	5.6791450	14.7004829
C	15.8487736	5.6287415	16.1263120
H	16.3143592	4.7654000	15.6476100
H	16.6461474	6.2825528	16.4920532
H	15.2610851	5.2819717	16.9849374
C	15.8253756	6.9280398	13.9455973
H	16.6007224	7.5575781	14.4102440
O	16.4352577	5.8142167	13.3107536
H	16.9054697	6.1917377	12.5392252
C	15.0562860	7.8057255	12.9204313
H	14.4426656	8.4891600	13.5104281
C	14.1227287	6.9786357	12.0268046
H	14.6862920	6.3568527	11.3283941
H	13.5043718	6.3112557	12.6349412
H	13.4456931	7.6150880	11.4480385
C	16.0841109	8.6902029	12.1779723
H	16.6885129	9.1565348	12.9696688
O	16.9310468	7.8397743	11.4081331
H	17.8926392	8.0876733	11.5518768
C	15.5558520	9.8762606	11.3062096
H	16.4283832	10.5247724	11.1711106
C	15.1241391	9.4702304	9.8955416
H	14.9151385	10.3596446	9.2979971
H	15.9489939	8.9422572	9.4202387
H	14.2342102	8.8335080	9.8784314
C	14.3915986	10.6981098	11.8986669
H	14.0479218	11.4123036	11.1432558
H	13.5479131	10.0283949	12.0994275
Fe	19.5060980	11.8208641	9.9677236
N	17.9799148	11.9343489	8.6514236
N	20.2983906	10.2425369	8.9481695
N	21.1519307	11.8776113	11.1633958
N	18.8109608	13.5097241	10.8906681
C	16.9209755	12.8282386	8.6659824
C	15.9223184	12.4490248	7.6810609
C	16.3814121	11.3030325	7.0844107
C	17.6773728	11.0258302	7.6889557
C	19.7508064	9.6194218	7.8437850
C	20.6253377	8.5489011	7.3707778
C	21.6982860	8.5067585	8.2307029
C	21.4602996	9.5956225	9.1946113
C	22.2638602	11.0709929	11.0684424
C	23.2511056	11.4116478	12.0870986
C	22.6697627	12.3745997	12.8834375
C	21.3505690	12.6292054	12.2799793
C	19.2185314	13.9494349	12.1345631
C	18.2988376	14.9483446	12.6595427
C	17.3513987	15.1445821	11.6860384
C	17.6638859	14.1959531	10.6237993
C	16.8123016	13.8923371	9.5445867
H	15.9273778	14.5118072	9.4424130
C	18.5360791	9.9813614	7.2915641
H	18.1859932	9.4084132	6.4406238
C	22.3693905	10.0079479	10.1907883
H	23.2630424	9.4041074	10.3041149
C	20.3835096	13.5352728	12.7577207
H	20.5708398	13.9836001	13.7282447
H	19.8403909	8.9839533	12.2467139
O	18.6617396	10.8683699	10.9949216
O	19.4751599	8.1384992	11.9209405
O	20.3440690	6.4679339	13.7349097
H	21.1295473	6.9561690	14.0303742
H	19.7677558	7.4506803	12.6177763
O	18.5242417	2.9801021	16.8228392
H	18.6926081	3.1524571	17.7727937
H	18.8380939	3.8193175	16.3610810
O	19.5900881	5.2515192	15.8201064
H	19.4274725	6.0265682	16.4030738
H	19.8155358	5.7244178	14.8913811
H	20.9864260	2.0396273	14.9928957
H	19.3938510	14.7773369	7.1145194
H	11.2081909	7.7488858	16.7993455
H	11.6518509	9.0774904	15.6477956
H	14.6240294	11.3015450	12.7761111
H	14.9759861	12.9619678	7.5095638
H	15.8559322	10.6334798	6.4035021
H	20.4069338	7.9379665	6.4949211
H	22.5729339	7.8588186	8.2875482
H	24.2521762	10.9804962	12.0927893
H	23.0165567	12.9068978	13.7691345
H	18.3572554	15.3678638	13.6638621
H	16.4688154	15.7841288	11.6956835

TURBOMOLE (QM) and ChemShell Energies (MM and QM/MM)

	QM/MM	QM	MM
B3LYP/B1	-4129.438711	-4031.937426	-97.501284
B3LYP/B2*	-4130.298485	-4032.797200	-97.501284
PBE0/B2/*	-4128.671352	-4031.170068	-97.501284
B3LYP-D/B2*	-4130.776459	-4033.275175	-97.501284
[A]M06/B2/*	-4130.169804	-5453.945495	-97.501284
[4]B3LYP/B1	-4129.438613	-4031.937328	-97.501284

*B3LYP/B1 geometry

[A]Additional contribution to MM energy and charges: 1421.276976

Figure 8

TS for H^+ transfer from the ultimate proton donor E244 to reprotonate OH^- (**^{244}TS2)**

C	21.0492383	0.9532390	14.8746274
H	21.7848867	0.5482621	15.5842762
H	21.4114714	0.7096763	13.8734311
C	19.7680524	0.1767489	15.0683380
O	19.6377635	-0.9154105	14.4796275
O	18.7964248	0.5865908	15.8569123
H	18.8447758	1.5597907	16.2240663
C	19.9271981	13.8420122	6.9417763
H	20.6031137	14.0242395	6.1008639
H	19.1737548	13.1206996	6.6109659
S	20.9071064	13.1394480	8.3299262
C	12.0200820	8.3225855	16.3487102
H	12.5481160	8.8082386	17.1711539
O	12.8907183	7.3584665	15.7010214
C	14.2326877	7.5081895	15.7790512
O	14.7663941	8.4717374	16.3124267
C	14.9677712	6.3702496	15.0983659
H	14.2204548	5.6784210	14.6974646
C	15.8602838	5.6303901	16.1139295
H	16.3274878	4.7679503	15.6354553
H	16.6594447	6.2844130	16.4749523
H	15.2776799	5.2831427	16.9757740
C	15.8204332	6.9286306	13.9327551
H	16.5984634	7.5574784	14.3938808
O	16.4241608	5.8155849	13.2907221
H	16.8802280	6.1916837	12.5110450
C	15.0463755	7.8081600	12.9121787
H	14.4354768	8.4907765	13.5054181
C	14.1093571	6.9819978	12.0212727
H	14.6690298	6.3599874	11.3199027
H	13.4946537	6.3145823	12.6326493
H	13.4298403	7.6187133	11.4458781
C	16.0688598	8.6952530	12.1672859
H	16.6790976	9.1597653	12.9554365
O	16.9131996	7.8457895	11.3897521
H	17.8670286	8.1051794	11.5206875
C	15.5398287	9.8807024	11.2971756
H	16.4126607	10.5286448	11.1598514
C	15.1039300	9.4740310	9.8879193
H	14.8938322	10.3634242	9.2915398
H	15.9268964	8.9460754	9.4092868
H	14.2142529	8.8371448	9.8732288
C	14.3786452	10.7024224	11.8940270
H	14.0327880	11.4177531	11.1408233
H	13.5355876	10.0328053	12.0966141
Fe	19.5040516	11.8139657	9.9736414
N	17.9781050	11.9276378	8.6582162
N	20.2991026	10.2387209	8.9505750
N	21.1513904	11.8719332	11.1681157
N	18.8086189	13.5015936	10.8967245
C	16.9200038	12.8226596	8.6711283
C	15.9228561	12.4454880	7.6840157
C	16.3820548	11.2995177	7.0872075
C	17.6768294	11.0205587	7.6934875
C	19.7516871	9.6159304	7.8464432
C	20.6267360	8.5465250	7.3722942
C	21.7010950	8.5053724	8.2309694
C	21.4631643	9.5937399	9.1951460
C	22.2650124	11.0678688	11.0709904
C	23.2519725	11.4086925	12.0897136
C	22.6692560	12.3698160	12.8876476
C	21.3495432	12.6232488	12.2851885
C	19.2173849	13.9432686	12.1398215
C	18.2993753	14.9447225	12.6630657
C	17.3525813	15.1416123	11.6889824
C	17.6631604	14.1902056	10.6285368
C	16.8115578	13.8872469	9.5494428
H	15.9277534	14.5081056	9.4462519
C	18.5358825	9.9774009	7.2950694
H	18.1861475	9.4054237	6.4433335
C	22.3725540	10.0068379	10.1906619
H	23.2686729	9.4060186	10.3011327
C	20.3821900	13.5290828	12.7631175
H	20.5700598	13.9781970	13.7331589
H	19.8503478	8.9751781	12.2518001
O	18.6655149	10.8545747	11.0003419
O	19.4724304	8.1394523	11.9126383
O	20.2856630	6.4175415	13.8082947
H	21.0564404	6.9075524	14.1360659
H	19.7012347	7.4592625	12.6103608
O	18.5696016	3.0128302	16.8016055
H	18.7302414	3.1616438	17.7562275
H	18.9346453	3.8731831	16.3517930
O	19.6320578	5.1974108	15.8259850
H	19.4468846	5.9487534	16.4278695
H	19.8913322	5.8084052	14.7392450
H	21.0099080	2.0350845	15.0016306
H	19.3921418	14.7750348	7.1185534
H	11.2132978	7.7461864	16.8014020
H	11.6538617	9.0749331	15.6501959
H	14.6148983	11.3036275	12.7719811
H	14.9777648	12.9601498	7.5108334
H	15.8569797	10.6316561	6.4043286
H	20.4083186	7.9361827	6.4960279
H	22.5765135	7.8583725	8.2866484
H	24.2538995	10.9795255	12.0946464
H	23.0157137	12.9014598	13.7738690
H	18.3586841	15.3658964	13.6666400
H	16.4709345	15.7824580	11.6980461

TURBOMOLE (QM) and ChemShell Energies (MM and QM/MM)

	QM/MM	QM	MM
B3LYP/B1	-4129.437337	-4031.936625	-97.500712
B3LYP/B2*	-4130.297508	-4032.796795	-97.500712
PBE0/B2/*	-4128.670956	-4031.170244	-97.500712
B3LYP-D/B2*	-4130.775538	-4033.274826	-97.500712
[A]M06/B2/*	-4130.168545	-5453.944406	-97.500712
[4]B3LYP/B1	-4129.437236	-4031.936524	-97.500712

*B3LYP/B1 geometry

[A]Additional contribution to MM energy and charges: 1421.276573

Figure 8

Compound I (^{244}**Cpd I**)

C	21.0143604	0.9290298	14.7437804
H	21.8538371	0.5599325	15.3509713
H	21.2859646	0.7502971	13.7007405
C	19.8105669	0.0401294	15.0617505
O	19.7216010	-1.0190237	14.3482014
O	18.9990022	0.3315670	15.9905930
H	18.4499477	2.1224007	16.5243711
C	19.9308956	13.8429205	6.9657714
H	20.6125570	14.0234339	6.1294689
H	19.1821662	13.1178657	6.6331518
S	20.9101995	13.1509655	8.3596512
C	11.9576218	8.3834824	16.4288223
H	12.4884817	8.8717131	17.2477417
O	12.8157564	7.3941773	15.8006620
C	14.1571076	7.5185366	15.8874585
O	14.7086895	8.4793116	16.4088763
C	14.8766335	6.3588763	15.2270794
H	14.1234668	5.6786330	14.8185384
C	15.7329286	5.6028744	16.2606261
H	16.1738774	4.7157643	15.8019900
H	16.5447120	6.2395151	16.6265109
H	15.1308977	5.2850753	17.1197774
C	15.7585500	6.8935823	14.0725298
H	16.5290424	7.5290734	14.5412551
O	16.3744934	5.7680591	13.4635942
H	16.7760468	6.1087373	12.6382071
C	15.0049901	7.7724226	13.0351157
H	14.4477736	8.5005060	13.6245247
C	14.0144182	6.9710481	12.1806817
H	14.5324349	6.2893664	11.5025228
H	13.3577291	6.3719121	12.8176195
H	13.3763624	7.6260455	11.5782169
C	16.0396887	8.5831648	12.2286713
H	16.7326129	9.0135942	12.9707352
O	16.7531978	7.6393538	11.4286303
H	17.6911170	7.9316642	11.2856575
C	15.5441762	9.7957768	11.3660380
H	16.4299770	10.4285383	11.2339622
C	15.0991815	9.4114656	9.9517646
H	14.8632698	10.3104746	9.3789536
H	15.9206921	8.9091592	9.4441731
H	14.2224751	8.7572802	9.9357071
C	14.3985493	10.6433203	11.9601806
H	14.0636508	11.3544805	11.1983672
H	13.5443509	9.9907668	12.1696771
Fe	19.5314242	11.8312600	9.9837171
N	17.9937645	11.9201950	8.6849909
N	20.3355557	10.2613285	8.9540892
N	21.1852829	11.9003141	11.1700436
N	18.8239504	13.5073350	10.9119756
C	16.9256377	12.8058228	8.7039700
C	15.9267232	12.4185655	7.7223573
C	16.3923439	11.2762123	7.1244843
C	17.6933578	11.0093020	7.7229937
C	19.7815964	9.6252921	7.8599588
C	20.6584588	8.5576416	7.3871714
C	21.7401502	8.5286539	8.2368644
C	21.5064685	9.6242449	9.1929034
C	22.3046231	11.1043972	11.0649693
C	23.2929806	11.4523526	12.0781637
C	22.7073758	12.4120368	12.8789266
C	21.3843358	12.6576922	12.2836577
C	19.2386243	13.9557997	12.1526631
C	18.3114612	14.9450620	12.6825984
C	17.3539846	15.1278301	11.7166044
C	17.6680886	14.1799359	10.6544427
C	16.8108223	13.8685340	9.5808010
H	15.9194005	14.4791296	9.4845997
C	18.5575615	9.9724820	7.3187521
H	18.2049968	9.3950424	6.4720176
C	22.4180204	10.0445339	10.1824539
H	23.3192151	9.4508819	10.2898588
C	20.4127994	13.5588280	12.7659568
H	20.6042698	14.0136274	13.7328229
H	19.3426962	9.1981372	11.4129437
O	18.7271377	10.8555546	11.0357154
O	19.3186123	8.2283519	11.2722223
O	20.0155258	6.4530926	13.4530695
H	20.5478040	7.2042782	13.7874194
H	19.5853171	7.7755564	12.0966385
O	18.2105676	3.0184492	16.8622384
H	18.3595600	2.9927309	17.8326527
H	18.9776403	4.4711507	16.2089835
O	19.5066509	5.2427355	15.8734494
H	19.3206520	6.0216943	16.4423994
H	19.6396684	5.9964883	14.2466445
H	20.9213583	2.0008249	14.9189153
H	19.3931950	14.7750731	7.1390805
H	11.1395898	7.8262123	16.8852653
H	11.6094125	9.1310595	15.7161195
H	14.6421792	11.2534385	12.8299315
H	14.9797262	12.9291436	7.5475054
H	15.8722180	10.6099897	6.4362381
H	20.4349302	7.9364239	6.5198825
H	22.6159473	7.8821589	8.2924523
H	24.3016650	11.0394590	12.0662772
H	23.0577406	12.9531363	13.7578592
H	18.3743919	15.3688791	13.6848386
H	16.4694088	15.7646136	11.7265546

TURBOMOLE (QM) and ChemShell Energies (MM and QM/MM)

	QM/MM	QM	MM
B3LYP/B1	-4129.489361	-4032.006187	-97.483174
B3LYP/B2*	-4130.347529	-4032.864355	-97.483174
PBE0/B2/*	-4128.720315	-4031.237141	-97.483174
B3LYP-D/B2*	-4130.827916	-4033.344742	-97.483174
[A]M06/B2/*	-4130.225168	-5453.989323	-97.483174
[4]B3LYP/B1	-4129.489134	-4032.005960	-97.483174

*B3LYP/B1 geometry

[A]Additional contribution to MM energy and charges: 1421.247329