Electronic Supplementary Material (ESI) for

Theoretical Studies Unveiled the Unusual Bonds in Oxygenation Reactions Involving Cobalt(II)-Iodylarene Complexes

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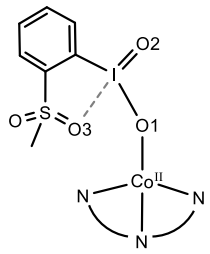
PART I. Computational methodology

The structural information of Co(II)-iodylarene adduct $[Co^{II}Tp^{tBu}(^{s}PhIO_2)]^+$ (**1**) was obtained from the Cambridge Crystallographic Data with the deposition number CCDC-1818934.[1] Thioanisole and 9,10-dihydroanthracene (DHA) were employed as substrates to study the reaction mechanism and oxidation ability of **1** in O-atom transfer reaction and in C−H bond activation. Calculations were carried out with density functional theory (DFT) with the Gaussian16 software (Revision B01).[2] The spin-unrestricted B3LYP-D3(BJ) functional was utilized[2-4] with Grimme's D3 dispersion corrections and the Becke−Johnson damping factor.[5,6] Solvent effects (chloroform, ε = 4.7113) were included in all calculations using the conductor-like polarizable continuum model (CPCM).[7,8] The experimental temperature of 296.15K was adopted in the free energy calculations. Based on the crystal structure, the performance of six DFT functionals were evaluated (B3LYP-B3(BJ), B3LYP, BP86-D3(BJ),[9] PBE0-D3(BJ),[10] TPSSH[11-13] and M062X[14]). All functionals presented similar results and the B3LYP-D3(BJ) functional was selected for the remaining calculations. Considering the balance between computational accuracy and efficiency, we finally chose the following basis set (abbreviation as B1 for clarity) for optimization: Lanl2dz for cobalt, Lanl2dzdp for iodine, the oxygen attached to iodine, hydrogen attached to boron, and electron-rich N, S, B atoms were calculated with the 6-31G** basis set, and the rest atoms use the 6-31G basis set. Single point energy (SPE) calculations were carried out with a higher base set (denoted as B2): Lanl2tz for Co, Lanl2dzdp for I, and 6-31+G** for the rest atoms. Transition states were ascertained by vibrational frequency analysis to possess a single mode along the reaction coordinate with a sole imaginary frequency. Mulliken charges and spin densities were analyzed to gain insights into the electronic properties of the key reaction species.

PART II. Benchmark of DFT functionals: Comparison of the calculated geometry of 1 with the experimental one

Table S1. Comparison of experimental and calculated bond lengths and angles of complex **1** on the ground quartet spin state. All calculations were performed with the B1 basis set.

$[Co^{2+}Tp^{tBu}(^{s}PhIO_2)]$	Experiment	Calculations					
		b3lyp-d3(bj)	b3lyp	bp86-d3(bj)	pbe0-d3(bj)	tpssh	m062x
$Co\text{-}N_{avg}$	2.026[a]	2.061	2.095	2.032	2.062	2.079	2.096
Co-O1	1.925	1.971	2.014	1.915	1.974	2.000	1.985
I-O1	1.814	1.851	1.854	1.914	1.846	1.873	1.819
I-O2	1.780	1.788	1.789	1.815	1.784	1.800	1.766
O3…I	2.662	2.544	2.550	2.523	2.506	2.526	2.514
O1-I-O2	102.20	106.24	106.61	107.49	105.89	106.14	104.30
Co-O1-I	148.34	136.48	136.19	135.14	136.27	135.68	134.90
S=O3…I	116.39	117.83	119.10	117.61	118.58	119.37	118.57



[a] Lengths are in Å units, bond angles are in degree units.

Table S2. Various SCF and free energies of complex **1**. Calculations were done at the UB3LYP-D3(BJ) /B2//B1 level.

	OPT/B1	ΔE	OPT +ZPE	ΔE	SPE/B2	ΔE	SPE+ZPE	ΔE	G	ΔG
^{2}**1**	-2418.194401[a]	19.0	-2417.425961	19.6	-2418.646706	20.2	-2417.878266	20.9	-2417.504441	21.0
^{4}**1**	-2418.224667	0.0	-2417.457219	0.0	-2418.678952	0.0	-2417.911504	0.0	-2417.537832	0.0
^{6}**1**	-2418.172298	32.9	-2417.406916	31.6	-2418.634057	28.2	-2417.868675	26.9	-2417.490879	29.5

[a] Note. Absolute energies are in au units and the relative ones are in kcal mol^{-1} units.

Table S3. Mulliken spin densities and charges of **1**. Calculations were done at the UB3LYP-D3(BJ)/B1 level.

	Charge					Spin density				
	Co	O1	ArI	Tp	O2	Co	O1	ArI	Tp	O2
^{2}**1**	0.66	-0.70	1.63	0.09	-0.68	0.98	0.00	0.00	0.02	0.00
^{4}**1**	0.82	-0.74	1.67	-0.07	-0.68	2.73	0.04	0.02	0.21	0.00
^{6}**1**	0.87	-0.62	1.34	-0.01	-0.58	2.76	1.05	0.41	0.34	0.44

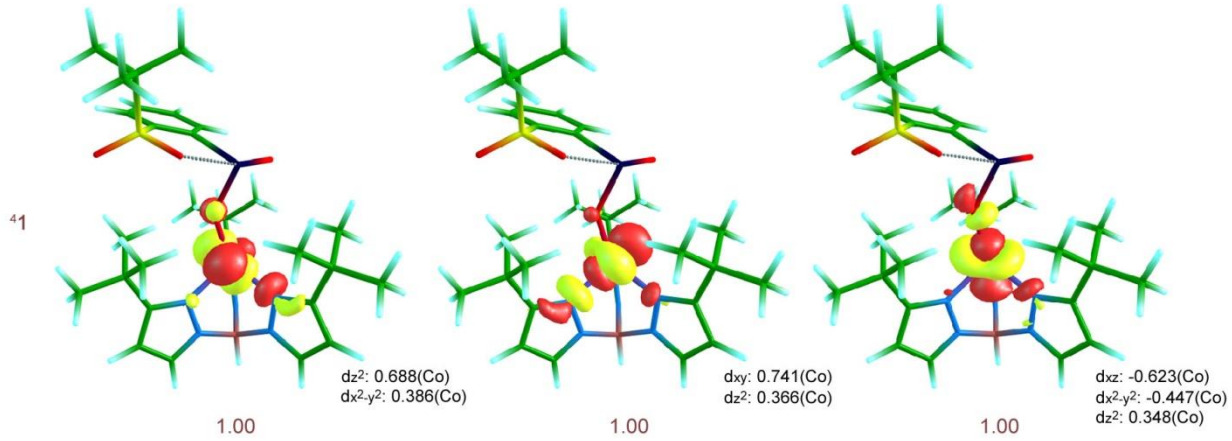


Figure S1. Singly-occupied natural orbitals (SNOs) of ^{4}**1** on the ground quartet spin state. Calculations were done at the UB3LYP-D3(BJ)/B1 level.

PART III. The formation of high-valent metal-oxo complex from 1

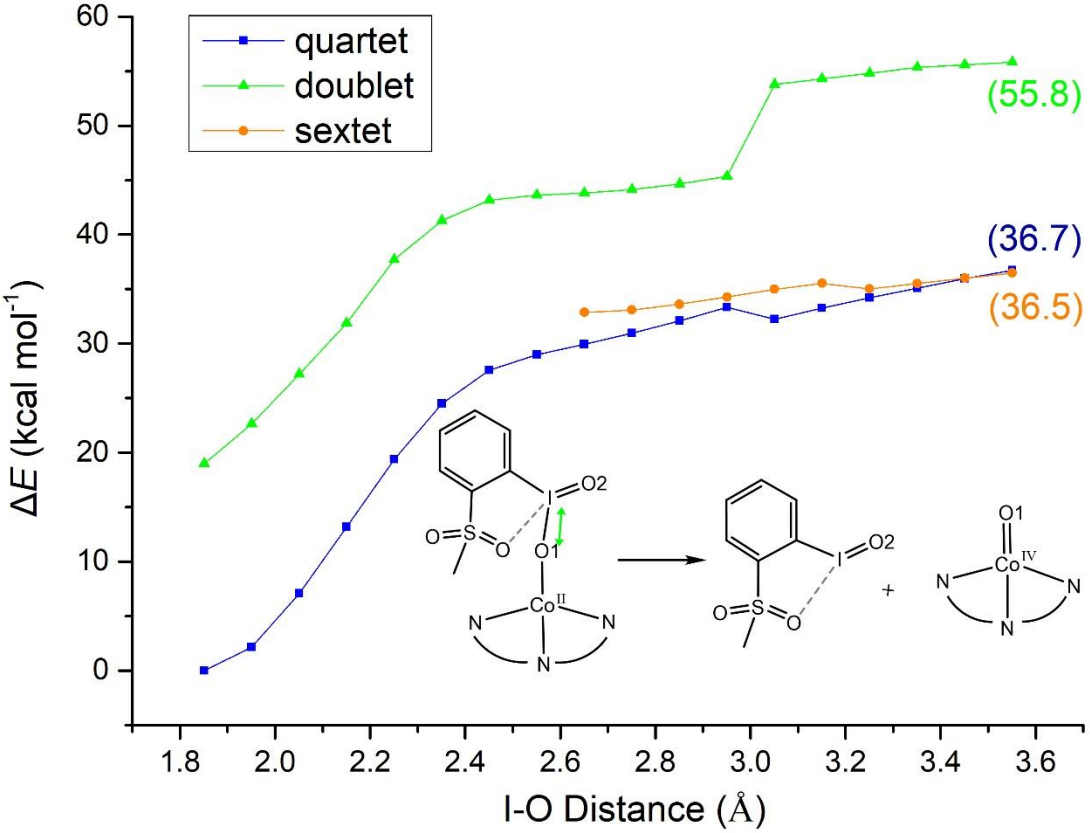


Figure S2. The relaxed scanned energy points during elongation of the I-O distance in the formation of the high-valent cobalt-oxo complex from **1**. Calculations were done at the UB3LYP-D3(BJ)/B1 level.

[Note. Cleavage of the O1-I bond of **1** to form a high-valent cobalt-oxo species is less likely, for the sake of holding a huge barrier of > 35 kcal/mol. For the forming Co(IV)=O species, a spin flip might occurs between the quartet and sextet states due to the small energy gap.]

PART IV. Thioanisole sulfoxidation by 1 via the direct oxygen-atom transfer (DOT) mechanism

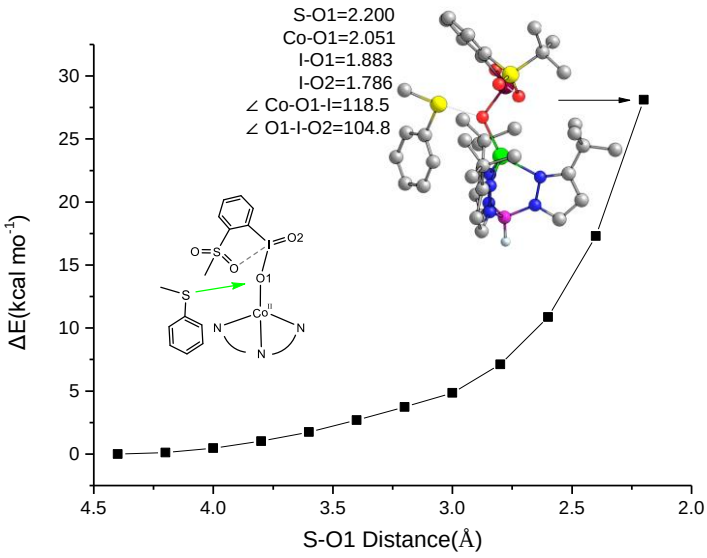


Figure S3. The energy points of relaxed scan along the direct oxygen-atom (O1 atom) transfer from **1** to thioanisole. Calculations were done at the UB3LYP-D3(BJ)/B1 level. Energies are in kcal mol^{-1} and relative to reactant complex.

[Note. The bridged O1 atom is less reactive (with barrier of > 25 kcal mol^{-1}) than the terminal O2 one (with a barrier of 19.3 kcal mol^{-1}), thus the O1 reactivity will not be consider in sulfoxidation.]

Table S4. Various SCF and free energies of key intermediates in thioanisole sulfoxidation by **1**. Calculations were done at the UB3LYP-D3(BJ)/B2//B1.

	OPT/B1	ΔE	OPT +ZPE	ΔE	SPE/B2	ΔE	SPE+ZPE	ΔE	G	ΔG
^{2}RC	-3087.946752[a]	17.8	-3087.046348	18.3	-3088.473690	20.2	-3087.573286	20.7	-3087.135020	21.0
^{4}RC	-3087.975181	0.0	-3087.027621	0.0	-3088.505891	0.0	-3087.606225	0.0	-3087.168445	0.0
^{6}RC	-3087.925751	31.0	-3087.075516	30.1	-3088.462285	27.4	-3087.564156	36.4	-3087.122714	28.7
^{2}TS$_{DOT}$	-3087.906877	42.9	-3087.008117	42.3	-3088. 43768	42.8	-3087.538921	42.2	-3087.099164	43.5
^{4}TS$_{DOT}$	-3087.940442	21.8	-3087.042593	20.7	-3088.473293	20.5	-3087.575444	19.3	-3087.136009	20.4
^{2}PC	-3087.970768	2.8	-3087.070436	3.2	-3088.500010	3.7	-3087.599678	4.1	-3087.163295	3.2
^{4}PC	-3088.005422	-19.0	-3087.105097	-18.6	-3088.536213	-19.0	-3087.635887	-18.6	-3087.198437	-18.8
^{6}PC	-3087.952049	14.5	-3087.053729	13.7	-3088.488865	10.7	-3087.590545	9.8	-3087.149749	11.7

[a] Absolute energies are in au units and the relative ones are in kcal mol^{-1} units.

[Note. The doublet and sextet RCs and PCs are much higher in energy than the ground state quartet ones, thus further geometric and electronic information of the doublet and sextet ones are not presented in the following parts.]

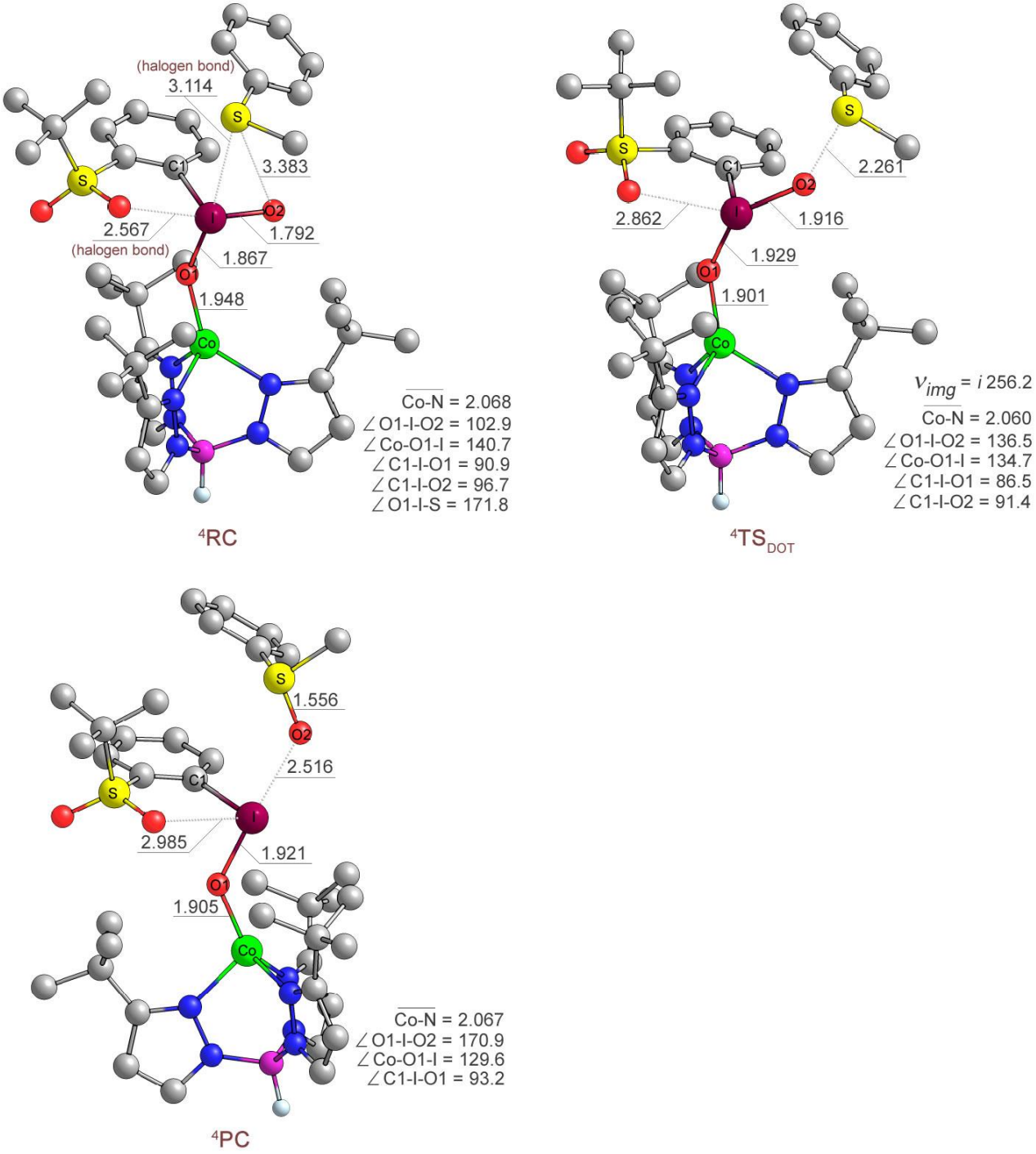


Figure S4. Optimized structures of key intermediates in thioanisole sulfoxidation by **1**. Lengths are in Å units, bond angles are in degree units and imaginary frequencies are in cm^{-1} units. Hydrogen atoms (other than B-H) are omitted for clarity. Calculations were done at the UB3LYP-D3(BJ)/B1.

Table S5. Mulliken spin densities and charges of key intermediates in thioanisole sulfoxidation by **1**. Calculations were done at the UB3LYP-D3(BJ)/B1 level.

	Charge						Spin density					
	Co	O1	ArI	Tp	O2	$PhSCH_3$	Co	O1	ArI	Tp	O2	$PhSCH_3$
^4RC	0.80	-0.79	1.59	-0.07	-0.70	0.17	2.72	0.05	0.01	0.20	0.00	0.00
$^4TS_{DOT}$	0.80	-0.77	1.21	-0.09	-0.61	0.46	2.71	0.08	0.01	0.19	0.00	0.01
^4PC	0.77	-0.78	0.89	-0.09	-0.69	0.90	2.71	0.10	0.01	0.18	0.00	0.00

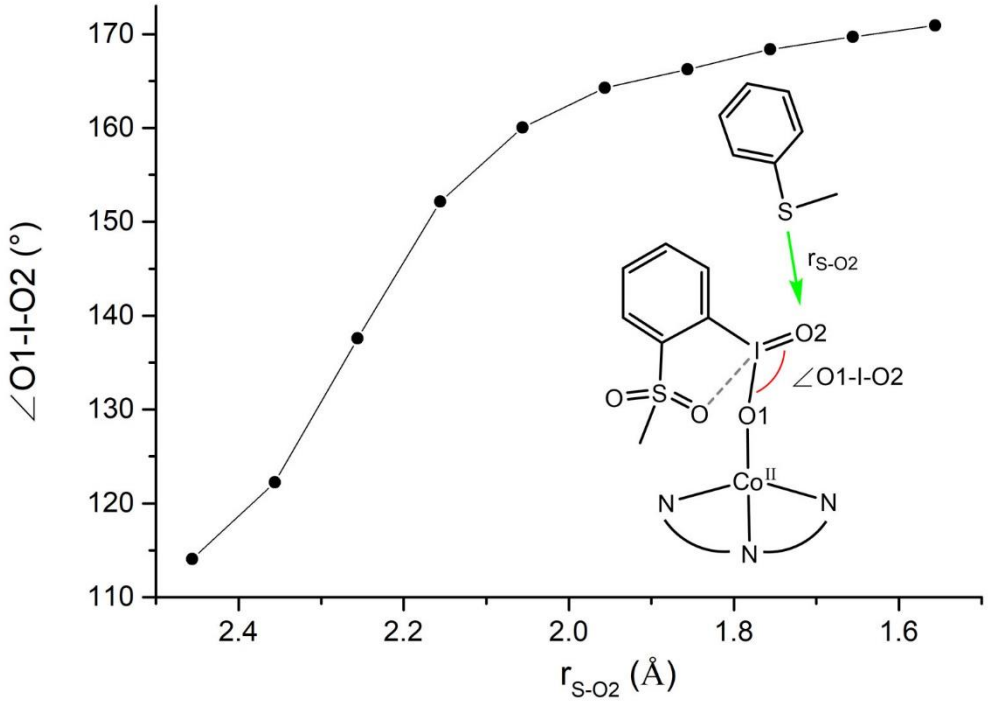


Figure S5. Variation of the ∠O1-I-O2 angle during substrate approaching. Calculations were done at the UB3LYP-D3 (BJ)/B1 level.

[Note. Substrate approaching causes the O1-I-O2 bond gradually becomes collinear, for the sake of gradually forming a 3c-4e bond for the O1-I-O2 moiety.]

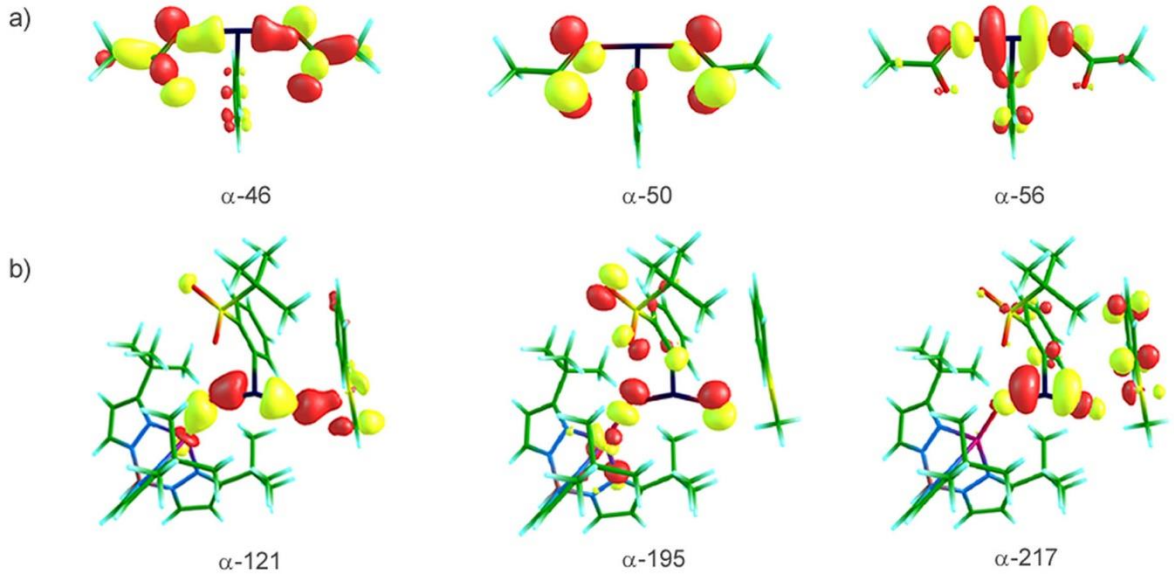


Figure S6. The three representative Pmentel-Rundle molecular orbitals (with orbital numbers) of 3c-4e bonds (a) in PIDA and (b) in the transition state of thioanisole oxidation by **1**.

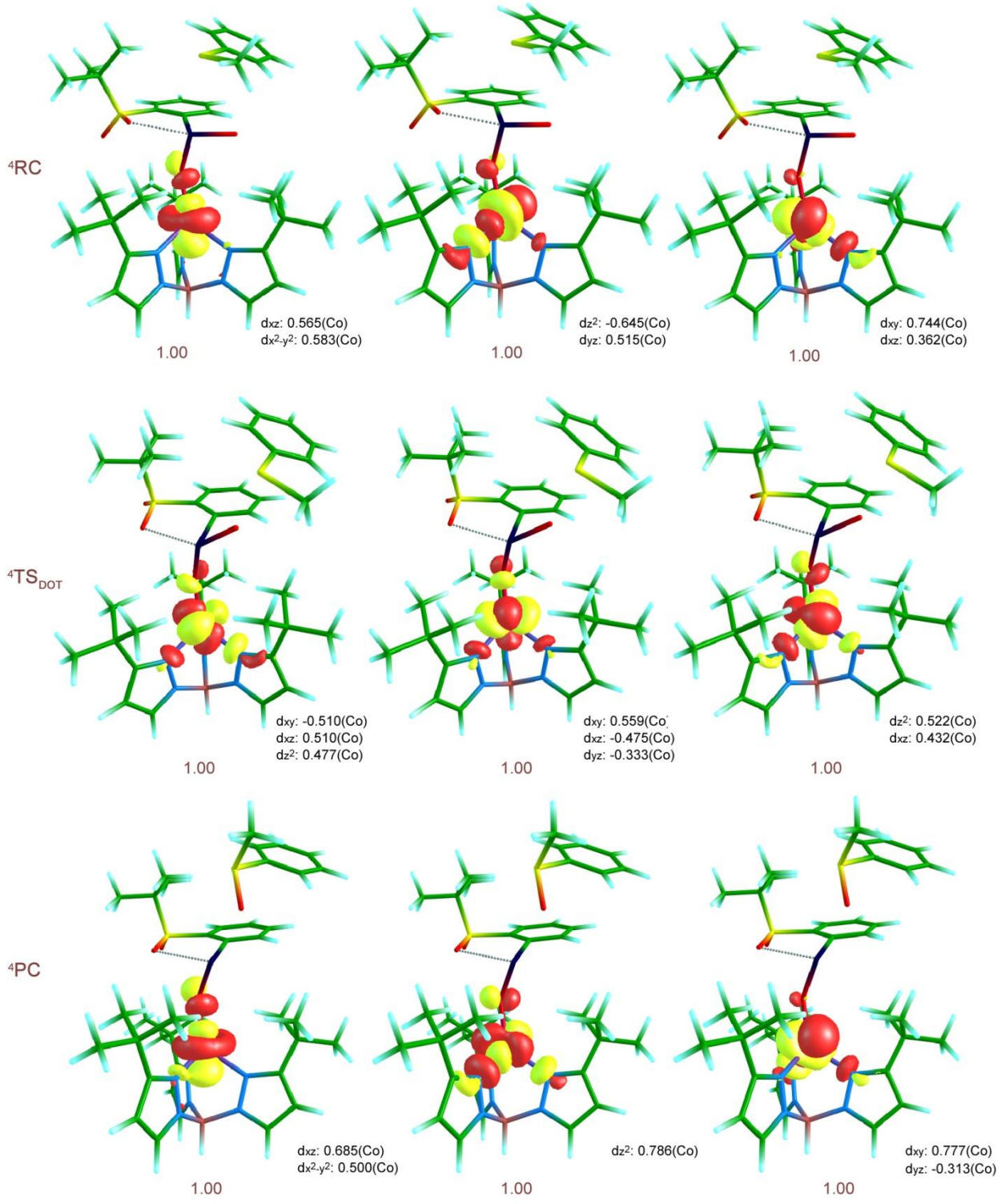


Figure S7. Singly-occupied natural orbitals (SNOs) of the key intermediates in thioanisole sulfoxidation by **1**. Calculations were done at the UB3LYP-D3(BJ)/B1 level.

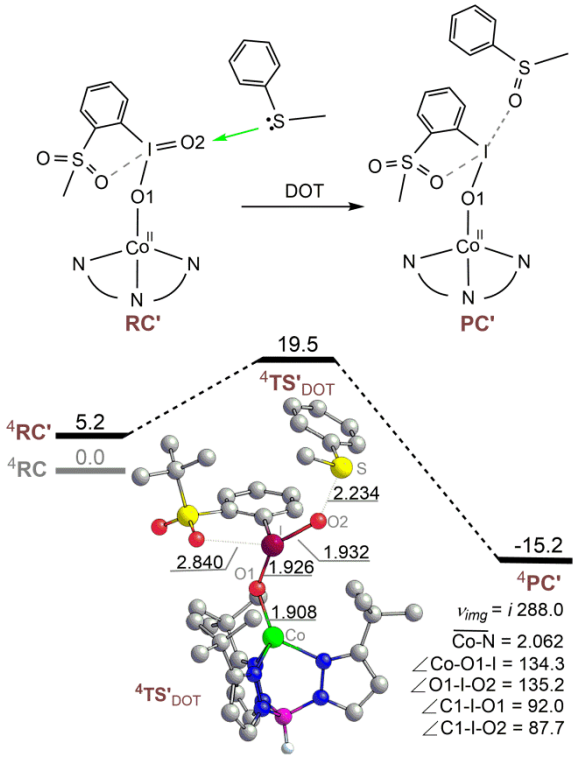


Figure S8. Energy profiles (in kcal mol-1) for sulfoxidation of thioanisole by **1** for the case of non-halogen bond orientation (RC'). Energies were calculated at the UB3LYP-D3(BJ)/B2//B1+ZPE/B1 level in solvent. The geometric information of the transition states is presented. Hydrogen atoms (expect hydrogen of the H-B moiety) are omitted for clarity. Lengths are in Å units, angles are in degree units, and the imaginary frequencies are in cm^{-1} units. The energy of reagent complex (RC) with halogen bond interaction is taken as the reference energy point (0.0 kcal mol^{-1}).

[Note. Although the substrate takes a quite different approaching orientation, the geometry of the transition state keeps nearly the same shape and the activation energy is also close, compared with those of the route in the XB-oriented mode. Further inspection of the variation of the O1-I-O2 angle (Figure S10) reveals that 3c-4e bonding interaction runs also in this non-XB-oriented reaction mode.].

[Note. (1) In reagent complex (RC) with halogen bond, the vacant ligand position of the iodine in the Co-$PhIO_2$ complex is occupied by the sulfur of thioanisole, substrates ligate slightly with the iodine of Co-$PhIO_2$, forming a cis-position to the attacking O2 atom of Co-$PhIO_2$; (2) while in RC without halogen bond, substrates point directly to O2 atom and form a week hydrogen bond between O2 and thioanisole. The vacant ligand position of iodine keeps vacant.]

Table S6. Various SCF and free energies of reaction intermediates in thioanisole sulfoxidation by 1 for the case of non-XB orientation. Calculations were done at the UB3LYP-D3(BJ)/B2//B1.

	OPT/B1	ΔE	OPT +ZPE	ΔE	SPE/B2	ΔE	SPE+ZPE	ΔE	G	ΔG
^{4}RC	-3087.975181[a]	0.0	-3087.075516	0.0	-3088.505891	0.0	-3087.606225	0.0	-3087.168445	0.0
^{4}RC'	-3087.965624	6.0	-3087.066482	5.7	-3088.497008	5.6	-3087.597865	5.2	-3087.161225	4.5
^{4}TS'$_{DOT}$	-3087.940619	21.7	-3087.042648	20.6	-3088.473157	20.5	-3087.575186	19.5	-3087.136414	20.1
^{4}PC'	-3088.000106	-15.6	-3087.099520	-15.1	-3088.530955	-15.7	-3087.630369	-15.2	-3087.193745	-15.9

[a]. Absolute energies are in au units and the relative ones are in kcal mol^{-1} units.

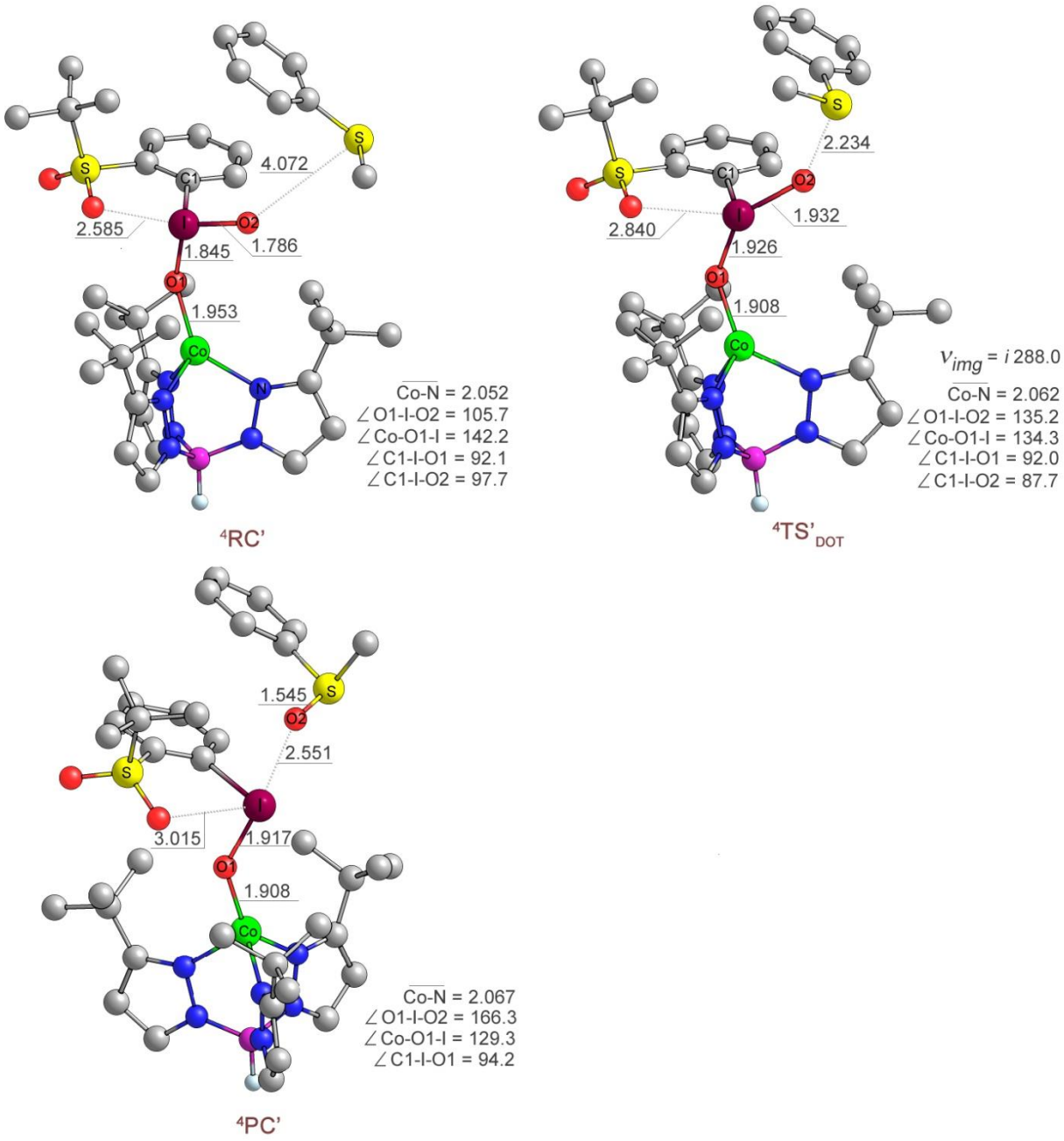


Figure S9. Optimized structures of reaction intermediates in thioanisole sulfoxidation by 1 for the case of non-XB orientation. Lengths are in Å units, bond angles are in degree units and imaginary frequencies are in cm^{-1} units. Hydrogen atoms (other than B-H) are omitted for clarity. Calculations were done at the UB3LYP-D3(BJ)/B1 level.

[Note. (1) In reagent complex (RC) with halogen bond, the vacant ligand position of the iodine in the Co-$PhIO_2$ complex is occupied by the sulfur of thioanisole, substrates ligate slightly with the iodine of Co-$PhIO_2$, forming a cis-position to the attacking O2 atom of Co-$PhIO_2$; (2) In RC without halogen bond, substrates point directly to O2 atom and form a week hydrogen bond between O2 and thioanisole. The vacant ligand position of iodine keeps vacant.]

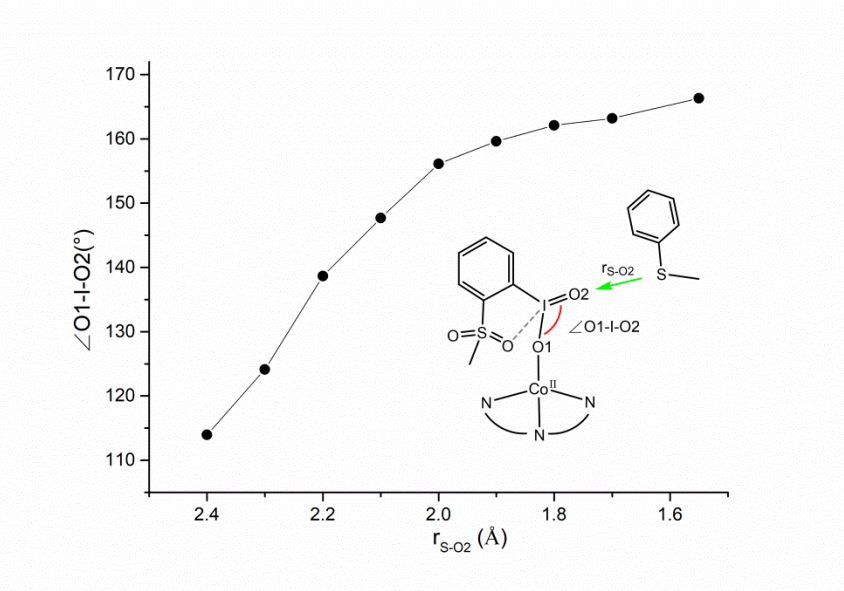


Figure S10. Variation of the O1-I-O2 angle during substrate approaching in thioanisole sulfoxidation by **1** for the case of non-XB orientation. Calculations were done at the UB3LYP-D3(BJ)/B1 level.

[Note. Substrate approaching from the reaction mode of non-XB orientation also causes the O1-I-O2 bond gradually becomes collinear.]

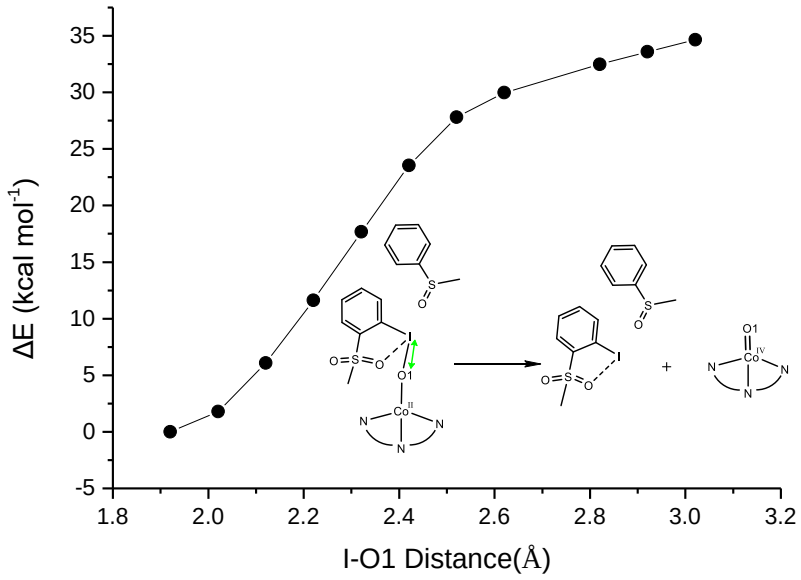


Figure S11. The energy points of relaxed scan for elongation of the I-O1 distance to form a high-valent cobalt-oxo complex. Calculations were done at the UB3LYP-D3(BJ)/B1 level. All energies are in kcal mol^{-1} and relative to the one of reactant complex.

[The new formed cobalt(II)-^{s}PhIO complex can't form high-valent cobalt-oxo species via cleavage of the O-I bond, for the sake of holding a huge activation barrier of > 35 kcal/mol.]

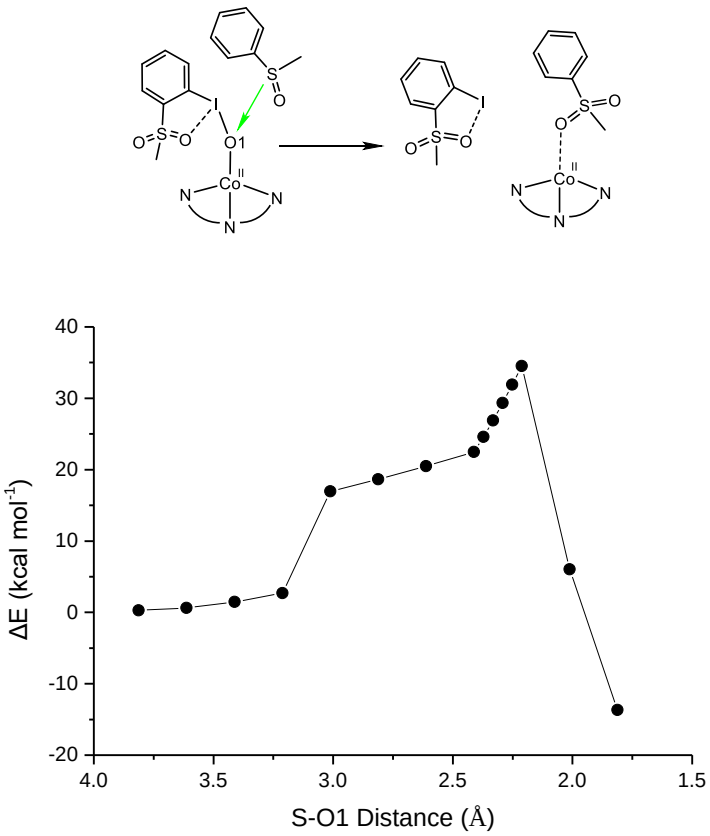


Figure S12. The energy points of relaxed scan in the formation of sulfone from $[Co^{2+}Tp^{tBu}(^{s}PhIO)]^{+}$ and the first oxidized product. Calculations were done at the UB3LYP-D3(BJ)/B1 level. All energies are in kcal mol^{-1} units and are relative to the one of reactant complex.

[Note. The new formed cobalt(II)-^{s}PhIO complex can't react with the oxidized thioanisole (methylsulfinyl)benzene, for the sake of holding a huge activation barrier of > 35 kcal/mol.]

PART V. C-H bond activation of 9, 10-dihydroanthracene (DHA) by 1

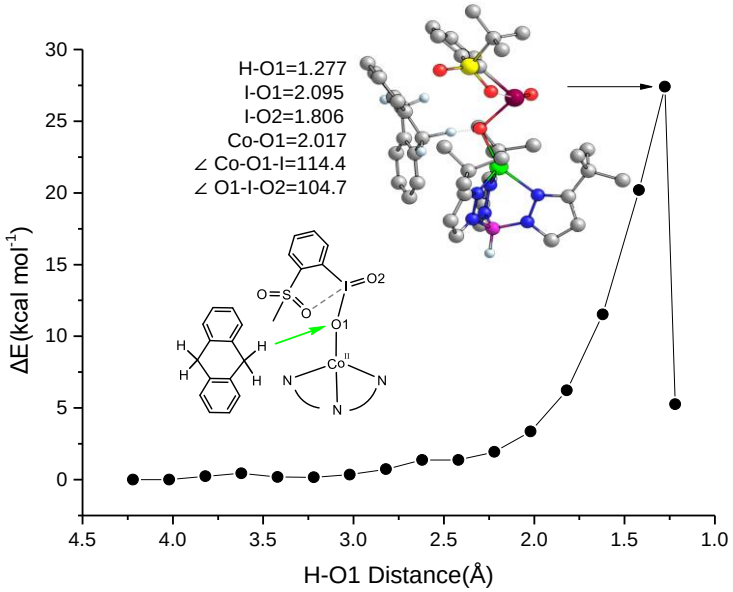


Figure S13. The energy points of relaxed scan in C-H activation of DHA by the O1 atom of **1**. Calculations were done at the UB3LYP-D3(BJ)/B1 level. All energies are in kcal mol^{-1} relative to the reactant complex.

[Note. The bridged O1 atom of **1** holds a much high barrier (> 25 kcal mol^{-1}) in C-H bond activation, thus it's not considered in the following reactivity study.]

Table S7. Various SCF and free energies of key intermediates in C-H bond activation by the O2 atom of **1**. Calculations were done at the UB3LYP-D3(BJ)/B2//B1 level.

	OPT/B1	ΔE	OPT +ZPE	ΔE	SPE/B2	ΔE	SPE+ZPE	ΔE	G	ΔG
$^{2}RC_1$	-2958.889112[a]	22.6	-2957.899297	22.7	-2959.484580	24.3	-2958.494768	24.4	-2957.993386	23.4
$^{4}RC_1$	-2958.925172	0.0	-2957.935535	0.0	-2959.523270	0.0	-2958.533633	0.0	-2958.030603	0.0
$^{6}RC_1$	-2958.871608	33.6	-2957.884775	31.9	-2959.477308	28.8	-2958.490475	27.1	-2957.983793	29.4
$^{2}TS_1$	-2958.847682	48.6	-2957.864541	44.5	-2959.447126	47.8	-2958.463985	43.7	-2957.959265	44.8
$^{4}TS_1$	-2958.882758	26.6	-2957.899583	22.6	-2959.483853	24.7	-2958.500678	20.7	-2957.994492	22.7
$^{2}PC_1$	-2958.932920	-4.9	-2957.950795	-9.6	-2959.541860	-11.7	-2958.559735	-16.4	-2958.044525	-8.7
$^{4}PC_1$	-2959.000332	-47.2	-2958.014197	-49.4	-2959.607692	-53.0	-2958.621556	-55.2	-2958.110144	-49.9
$^{6}PC_1$	-2958.932899	-4.8	-2957.950759	-9.6	-2959.541849	-11.7	-2958.559709	-16.4	-2958.045520	-9.4

a. Absolute energies are in au units and the relative ones are in kcal mol^{-1} units.

[Note. The doublet and sextet RCs and PCs are much higher in energy than the ground state quartet ones, thus further geometric and electronic information of the doublet and sextet ones are not presented in the following parts.]

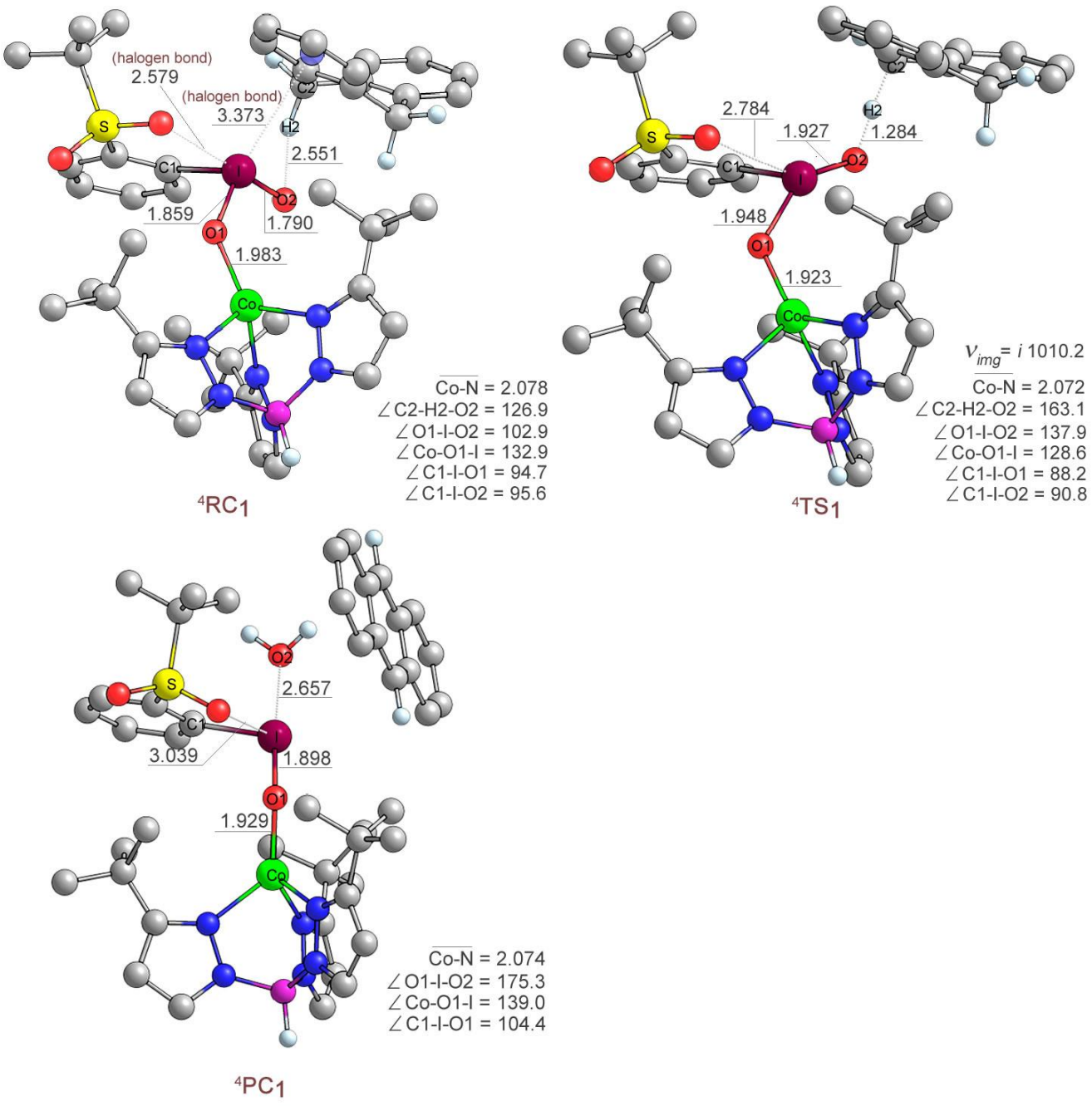


Figure S14. The geometric information of key intermediates in C-H bond activation by the O2 atom of **1**. Lengths are in Å units, bond angles are in degree units and imaginary frequencies are in cm^{-1} units. Some hydrogen atoms are omitted for clarity. Calculations were done at the UB3LYP-D3(BJ)/B1 level.

[Note. (1) In reagent complex (RC) with halogen bond, the vacant ligand position of the iodine in the Co-$PhIO_2$ complex is occupied by the phenyl ring of DHA, substrates ligate slightly with the iodine of Co-$PhIO_2$, forming a cis-position to the attacking O2 atom of Co-$PhIO_2$; (2) while in RC without halogen bond, substrates point directly to O2 atom and form a week hydrogen bond between O2 and the hydrogen of DHA. The vacant ligand position of iodine keeps vacant.]

Table S8. Mulliken spin densities and charges of key intermediates in C-H bond activation by the O2 atom of **1**. Calculations were done at the UB3LYP-D3(BJ)/B1 level.

	Charge						Spin densities					
	Co	ArIO	Tp	O2	H	DHA-H	Co	ArIO	Tp	O2	H	DHA-H
$^4RC_1$	0.80	0.87	-0.08	-0.69	0.20	-0.09	2.74	0.06	0.20	0.00	0.00	0.00
$^4TS_1$	0.77	0.49	-0.09	-0.69	0.36	0.15	2.71	0.21	0.19	-0.02	0.00	-0.10
$^4PC_1$	0.80	0.10	-0.09	-0.72	0.46	0.45	2.71	0.10	0.19	0.00	0.00	0.00

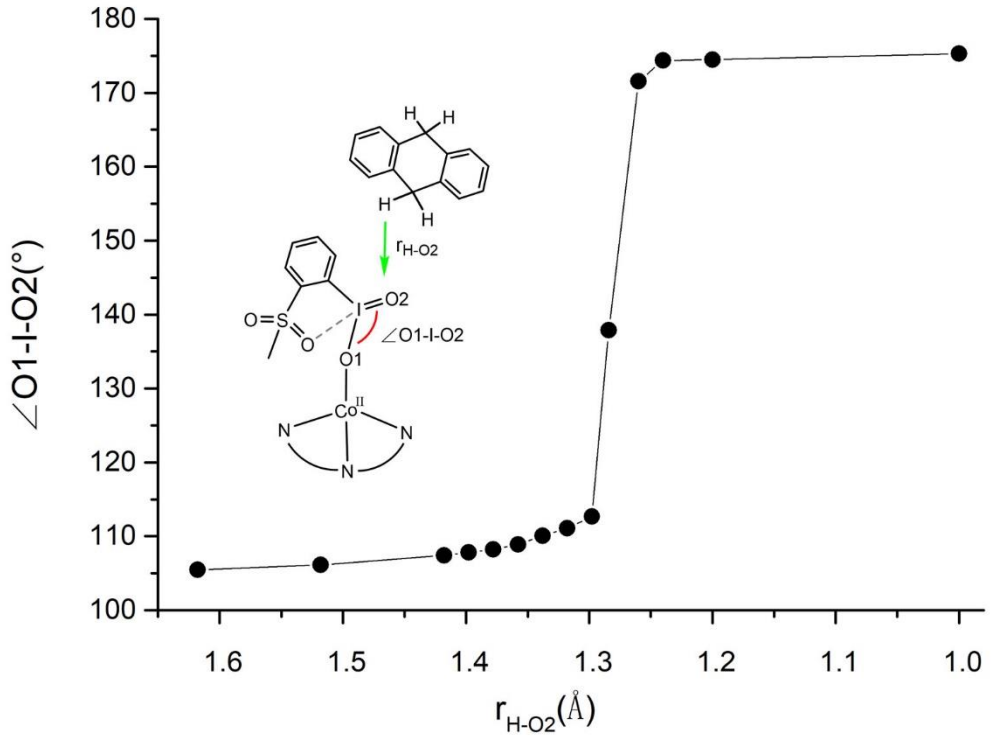


Figure S15. Variation of the ∠O1-I-O2 angle during substrate DHA approaching. Calculations were done at the UB3LYP-D3 (BJ)/B1 level.

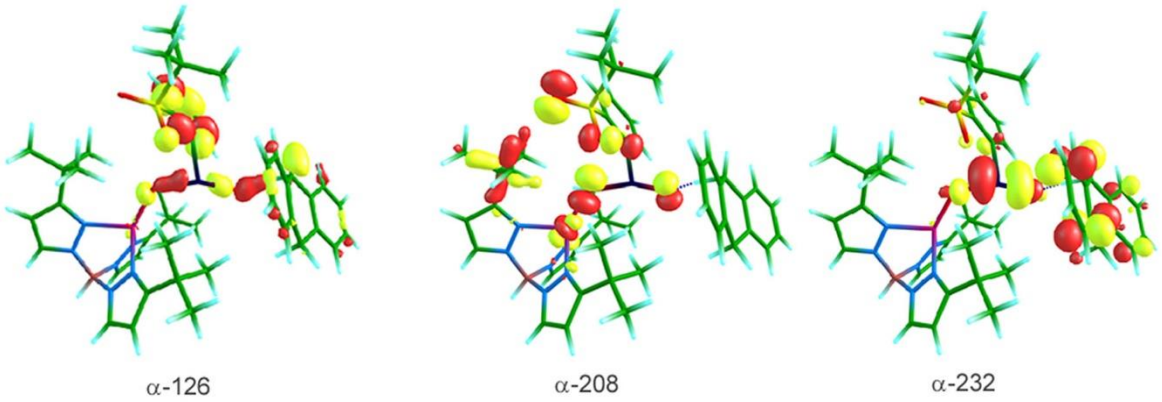


Figure S16. The representative Pmentel-Rundle MOs (with orbital numbers) of 3c-4e bonds in the transition state of the first C-H bond activation of DHA by **1**.

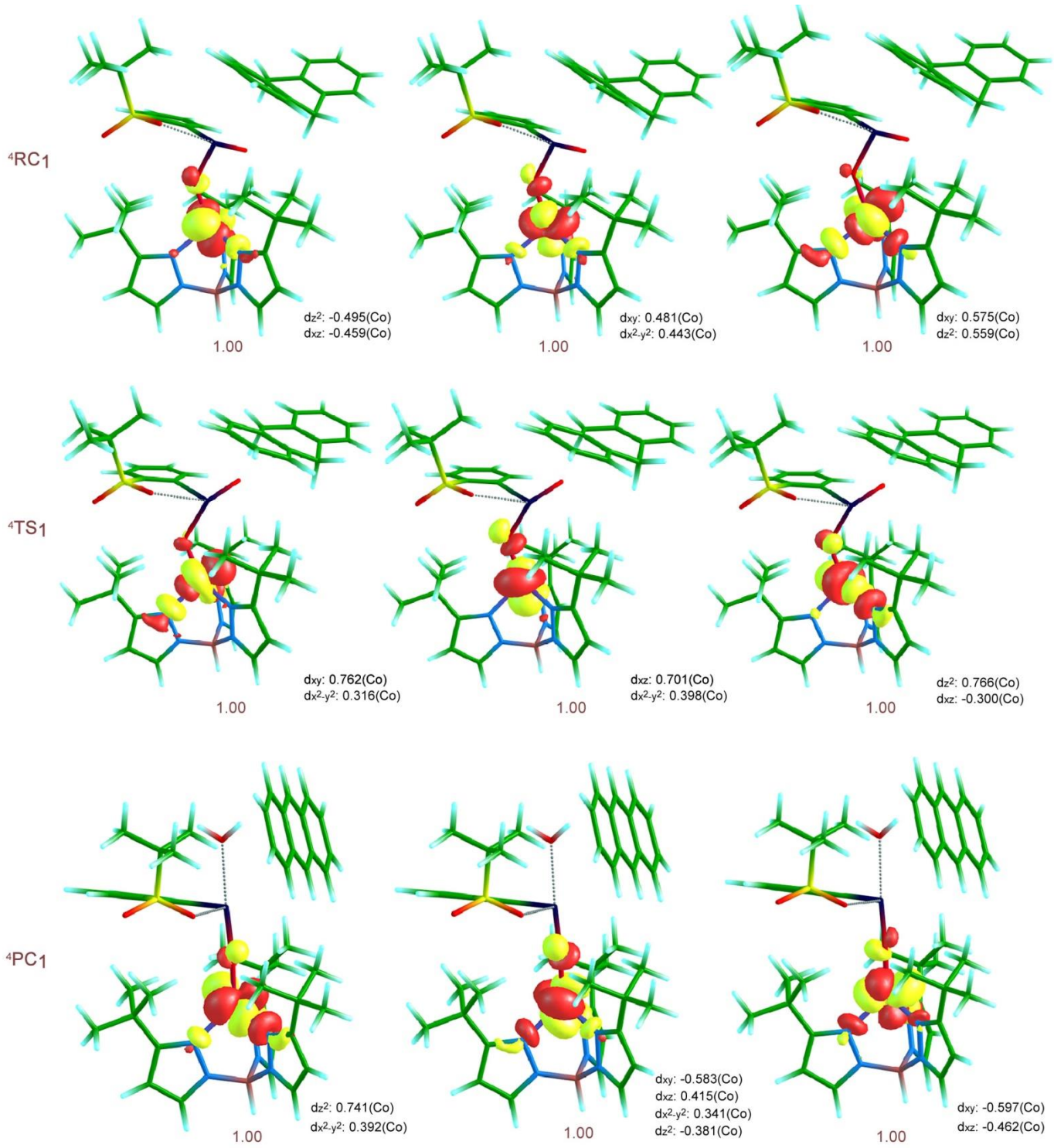
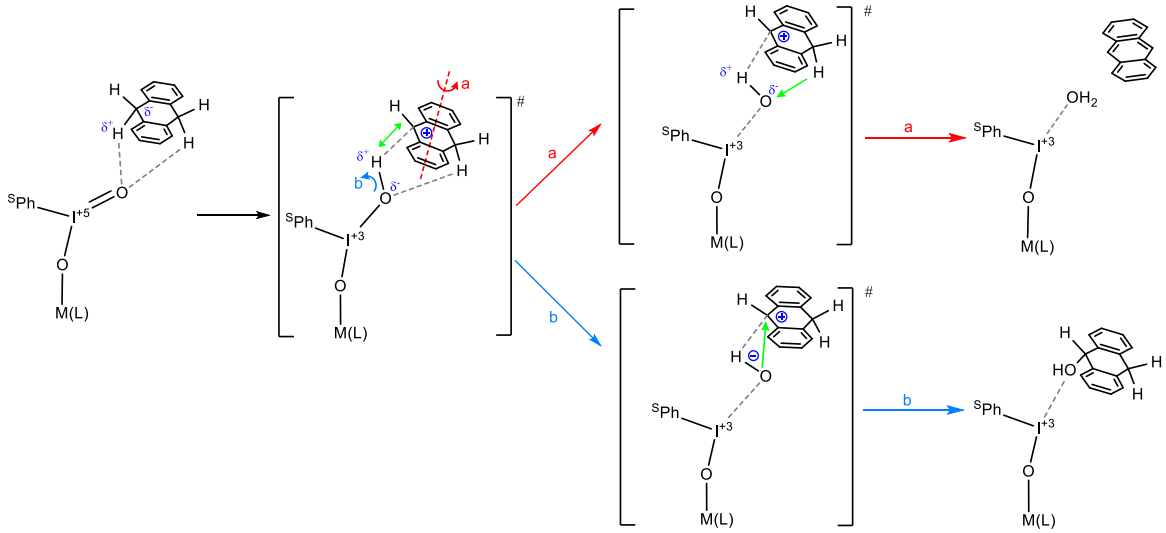


Figure S17. Singly-occupied natural orbitals (SNOs) of key intermediates in C-H bond activation by the O2 atom of **1**. Calculations were done at the UB3LYP-D3(BJ)/B1 level. Positive values represent alpha-electron occupations.



Scheme S1. Schematic plot of the determinant factor controlling the selection between the hydride transfer/proton transfer (HT/PT) pathway to yield anthracene and the hydride transfer/hydroxyl-rebound pathway to yield an alcohol which will be further oxidized to anthraquinone.

[Note. The determinant factor of the selection between the anthracene pathway and the anthraquinone one is the competition between the rotation of DHA-H skeleton and rotation of the OH group, after 2e-oxidation of the DHA-H moiety to form a carbonium species (please see Fig. 1 below). Such kinetical rotation switch was also observed in our previous work (with Prof. Sason Shaik) in ethanol oxidation by Cpd I of P450 (Scheme 2 in ChemBioChem, 2007, 8, 277. The OH group and enol radical rotations of the radical intermediates lead to the formation of gem-diol and formaldehyde complexes) and our work in suicide-inhibition of P450 by cyclopropylamines (Please see Figures 6-7 in Front. in Chem. 2017, 5, 3. DOI: 10.3389/fchem.2017.00003. hydroxylation and dual hydrogen abstraction of cyclopropylalinine to form carbinolamine and imine, respectively.). Such kinetic events need to employ the direct dynamic approach (eg., using the atom-centered density matrix propagation (ADMP) molecular dynamics model, or, using the Born-Oppenheimer molecular (BOMD) dynamics model), which is above of our ability.]

[Note. The hydroxylation pathway will be presented in the following pages just for the theoretical interest, for the sake that no hydroxylated product was observed in experiments.]

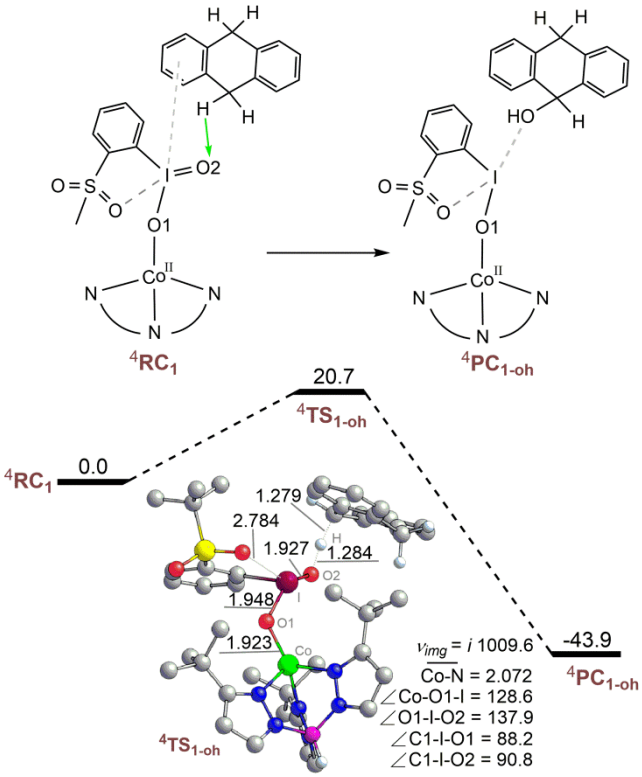


Figure S18. Energy profiles (in kcal mol^{-1}) for hydroxylation of DHA by **1**. Energies were calculated at the UB3LYP-D3(BJ)/B2//B1+ZPE/B1 level in solvent. The geometric information of the transition states is presented. Hydrogen atoms (except hydrogen of the H-B moiety and hydrogen of the methylene group in DHA) are omitted for clarity. Lengths are in Å units, angles are in degree units, and the imaginary frequency is in cm^{-1} units.

Table S9. Various SCF and free energies of key intermediates in hydroxylation of DHA by **1**. Calculations were done at the UB3LYP-D3(BJ)/B2//B1.

	OPT/B1	ΔE	OPT +ZPE	ΔE	SPE/B2	ΔE	SPE+ZPE	ΔE	G	ΔG
$^4RC_1$	-2958.925172[a]	0.0	-2957.935535	0.0	-2959.523270	0.0	-2958.533633	0.0	-2958.030603	0.0
$^4TS_{1\text{-oh}}$	-2958.880762	26.6	-2957.899557	22.6	-2959.483851	24.7	-2958.500647	20.7	-2957.994413	22.7
$^4PC_{1\text{-oh}}$	-2958.985316	-37.7	-2957.995746	-37.8	-2959.5931647	-43.9	-2958.603594	-43.9	-2958.091953	-38.5

a. Absolute energies are in au units and the relative ones are in kcal mol^{-1} units.

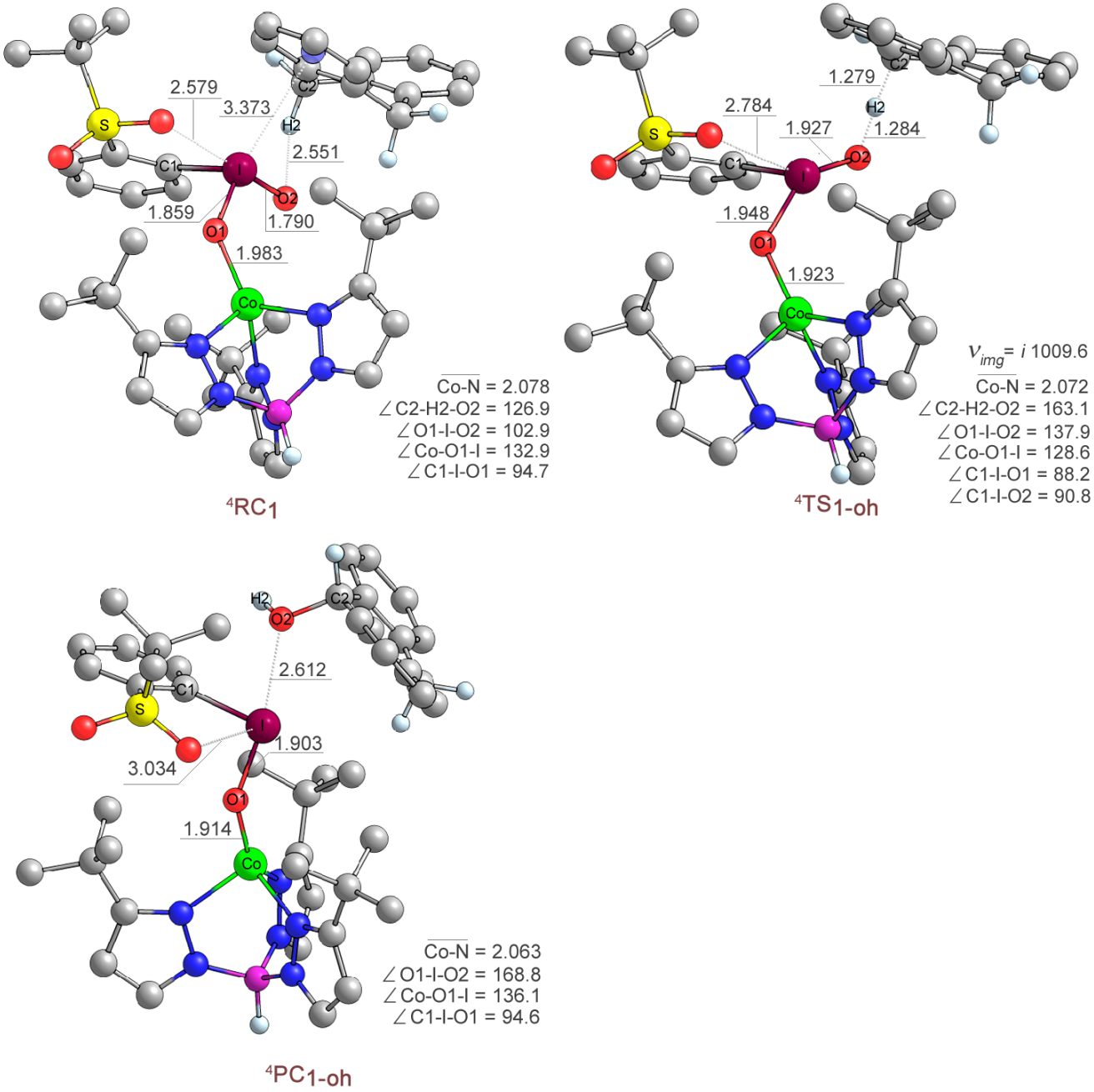


Figure S19. The geometric information of key intermediates in hydroxylation of DHA by **1**. Lengths are in Å units, bond angles are in degree units and the imaginary frequency is in cm^{-1} units. Unimportant hydrogen atoms are omitted for clarity. Calculations were done at the UB3LYP-D3(BJ)/B1 level.

Table S10. Mulliken spin densities and charges of key intermediates in hydroxylation of DHA by **1**. Calculations were done at the UB3LYP-D3(BJ)/B1 level.

	Charge						Spin densities					
	Co	ArIO	Tp	O2	H	DHA-H	Co	ArIO	Tp	O2	H	DHA-H
$^4RC_1$	0.80	0.87	-0.08	-0.69	0.20	-0.09	2.74	0.06	0.20	0.00	0.00	0.00
$^4TS_{1\text{-}oh}$	0.77	0.49	-0.09	-0.69	0.36	0.15	2.71	0.07	0.19	-0.02	0.00	-0.10
$^4PC_{1\text{-}oh}$	0.78	0.10	-0.09	-0.72	0.45	0.46	2.71	0.11	0.19	0.00	0.00	0.00

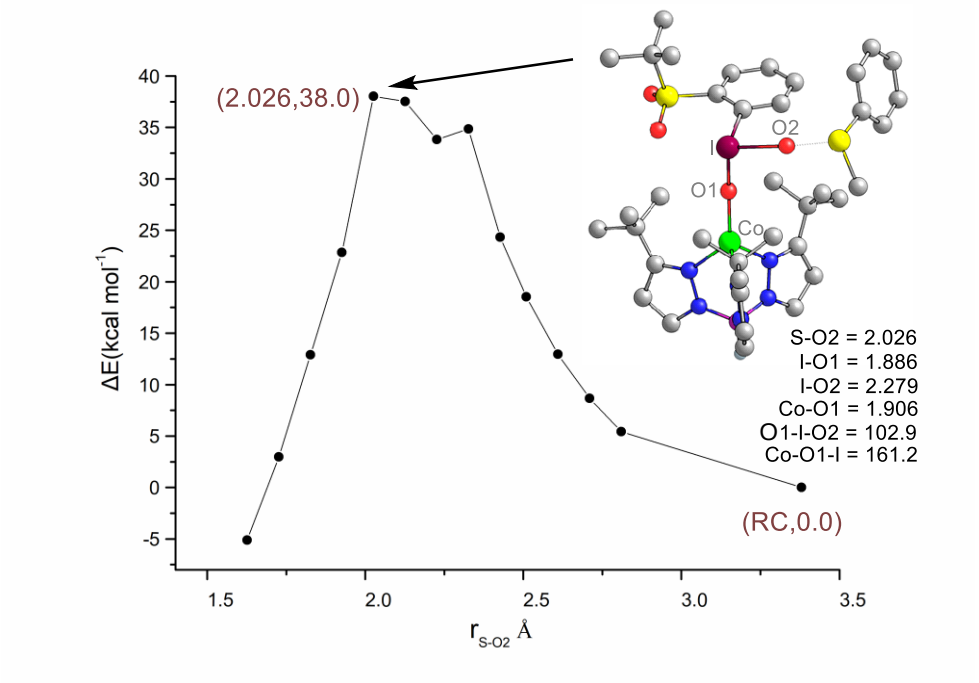


Figure S20. The relaxed scanned energy points along the I-O distance in thioanisole oxidation by 1, with the O1-I-O2 angle fixed from the starting RC state. Geometric information of the maximum pint is presented. Bonds are in Å units, angels are in ° units.

[Note. To evaluate the effect of electron delocalization of the 3c-4e bond in the O1-I-O2 moiety on activation energy, we fixed the O1-I-O2 angle from RC, where the three represented Pmentel-Rundle molecular orbitals were not observed, thus we believe no 3c-4e bond exists. For such non-3c-4e-bond case, the activation energy of thioanisole sulfoxidation by 1 is ca. 38 kcal mol^{-1}.]

PART VI. Thioanisole sulfoxidation by a $^{s}PhIO_2$ molecule

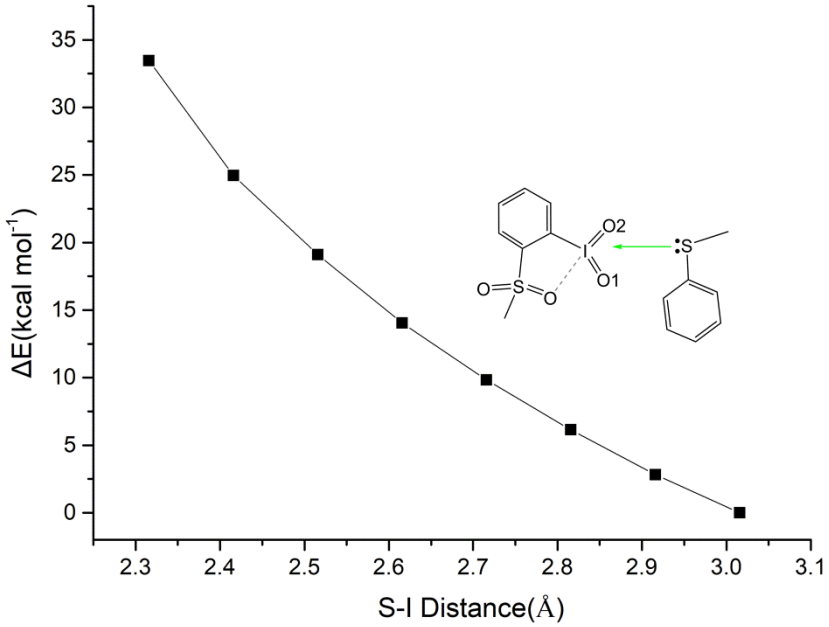


Figure S21. The energy points of relaxed scan along nucleophilic attack of iodine to the sulfur of thioanisole. Calculations were done at the UB3LYP-D3(BJ)/ Lanl2dzdp (I), 6-31G** (O1, O2, S), 6-31G (rest) level.

[a]Note: The proposed process of electrophilic attacking[15,16] of iodine to surfur encounters a barrier of > 30 kcal mol^{-1} and thus this mechanism doesn't likely happen.

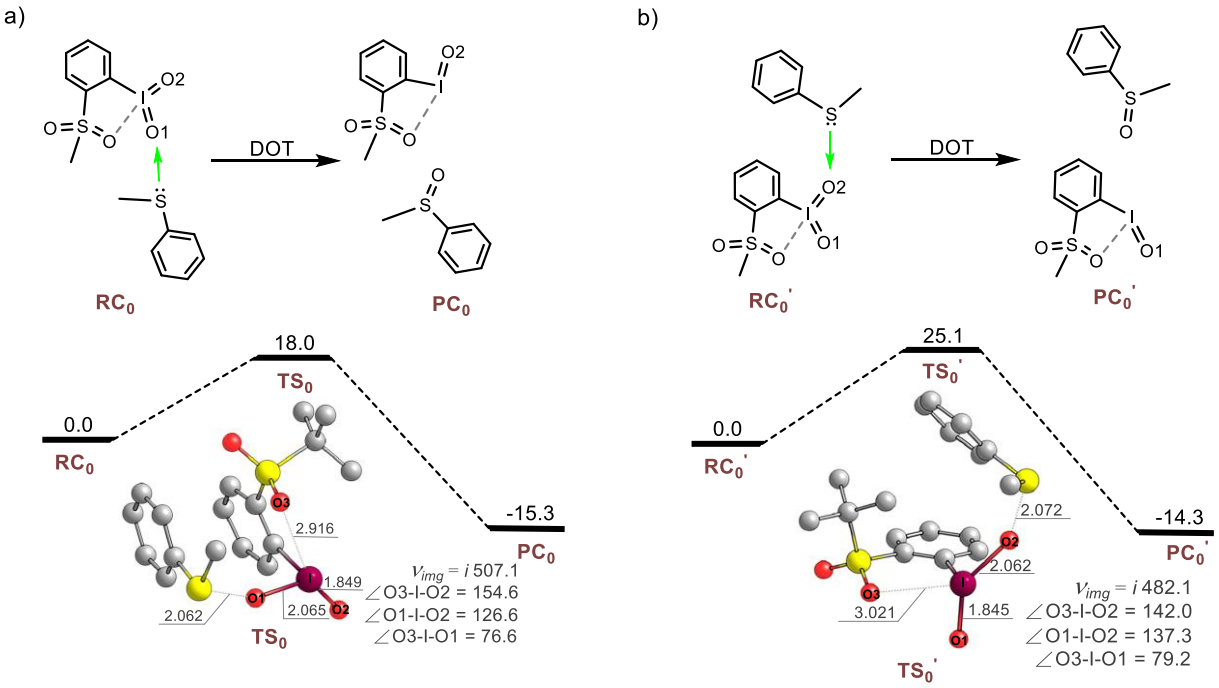


Figure S22. Energy profiles for thioanisole sulfoxidation by (a) the O1 atom, and (b) the O2 atom in $^{s}PhIO_2$ via the direct oxygen-atom transfer mechanism. Calculations were done at the UB3LYP-D3(BJ)/B2'//B1' level. (B1': Lanl2dzdp (I), 6-31G** (O1, O2, S), 6-31G (rest); B2': Lanl2dzdp(I), 6-31+G**(rest)). Energies are in kcal mol^{-1} units, lengths are in Å units, angles are in degree units, and imaginary frequencies are in cm^{-1} units.

Table S11. Various SCF and free energies of key intermediates in thioanisole sulfoxidation by the O1 atom of $^{s}PhIO_2$ molecule. Calculations were done at the UB3LYP-D3(BJ)/B2'//B1' level.

	OPT/B1	ΔE	OPT +ZPE	ΔE	SPE/B2	ΔE	SPE+ZPE	ΔE	G	ΔG
RC_0	-1768.811509[a]	0.0	-1768.459312	0.0	-1769.059850	0.0	-1768.707653	0.0	-1768.517193	0.0
TS_0	-1768.777416	21.4	-1768.426145	20.8	-1769.030245	18.6	-1768.678912	18.0	-1768.481318	22.5
PC_0	-1768.839730	-17.7	-1768.485943	-16.7	-1769.085873	-16.3	-1768.732086	-15.3	-1768.541010	-14.9

a. Absolute energies are in au units and the relative ones are in kcal mol^{-1} units.

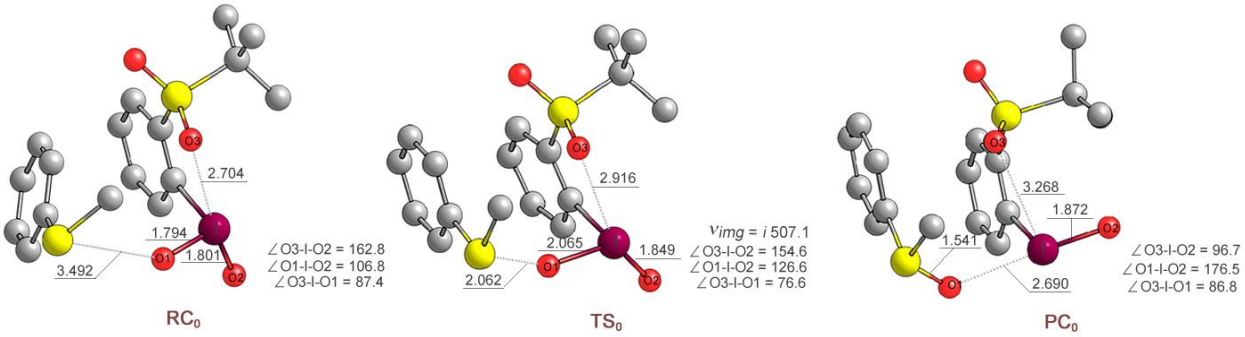


Figure S23. The geometric information of key intermediates in sulfoxide sulfoxidation by the O1 atom of $^{s}PhIO_2$ molecule. Calculations were done at the UB3LYP-D3(BJ)/ B1' level. Lengths are in Å units, angles are in degree units, and imaginary frequencies are in cm^{-1} units.

Table S12. Mulliken spin densities and charges of key intermediates in sulfoxide sulfoxidation by the O1 atom of $^{s}PhIO_2$ molecule. Calculations were done at the UB3LYP-D3(BJ)/ B1' level.

	Charge				Spin density			
	O1	ArI	O2	$PhSCH_3$	O1	ArI	O2	$PhSCH_3$
RC_0	-0.69	1.44	-0.73	-0.02	0.00	0.00	0.00	0.00
TS_0	-0.63	0.99	-0.76	0.40	0.00	0.00	0.00	0.00
PC_0	-0.68	0.67	-0.76	0.77	0.00	0.00	0.00	0.00

Table S13. Various SCF and free energies of key intermediates in thioanisole sulfoxidation by the O2 atom of $^{s}PhIO_2$ molecule. Calculations were done at the UB3LYP-D3(BJ)/B2'//B1' level.

	OPT/B1	ΔE	OPT +ZPE	ΔE	SPE/B2	ΔE	SPE+ZPE	ΔE	G	ΔG
RC_0'	-1768.814107[a]	0.0	-1768.461394	0.0	-1769.063386	0.0	-1768.710673	0.0	-1768.519248	0.0
TS_0'	-1768.768779	28.4	-1768.417057	27.8	-1769.022354	25.7	-1768.670631	25.1	-1768.472307	29.5
PC_0'	-1768.833450	-12.1	-1768.480456	-12.0	-1769.086498	-14.5	-1768.733504	-14.3	-1768.536688	-10.9

a. Absolute energies are in au units and the relative ones are in kcal mol^{-1} units.

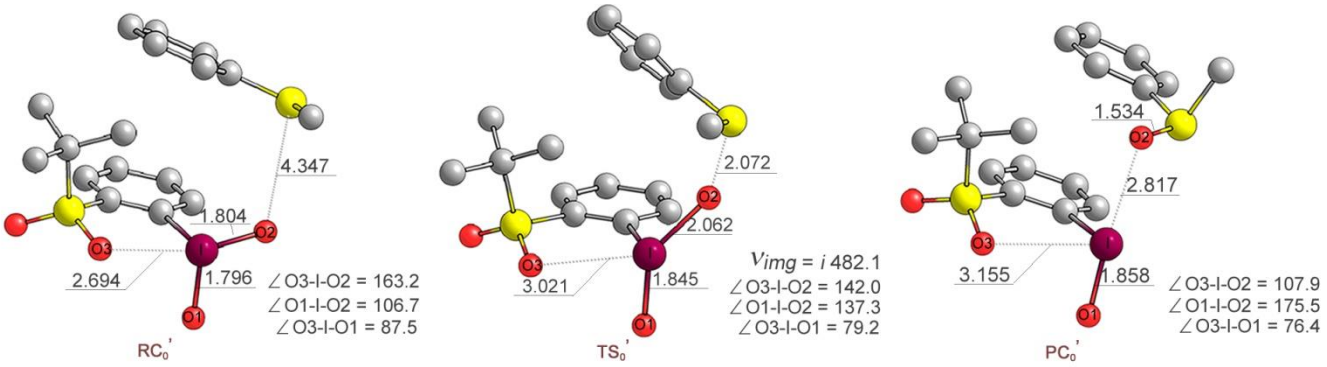


Figure S24. The geometric information of key intermediates in sulfoxide sulfoxidation by the O2 atom of $^{s}PhIO_2$ molecule. Calculations were done at the UB3LYP-D3(BJ)/ B1' level. Lengths are in Å units, angles are in degree units, and imaginary frequencies are in cm^{-1} units.

Table S14. Mulliken spin densities and charges of key intermediates in sulfoxide sulfoxidation by the O2 atom of $^{s}PhIO_2$ molecule. Calculations were done at the UB3LYP-D3(BJ)/ B1' level.

	Charge				Spin density			
	O1	ArI	O2	$PhSCH_3$	O1	ArI	O2	$PhSCH_3$
RC_0'	-0.71	1.43	-0.72	0.00	0.00	0.00	0.00	0.00
TS_0'	-0.74	0.95	-0.76	0.43	0.00	0.00	0.00	0.00
PC_0'	-0.77	0.67	-0.68	0.78	0.00	0.00	0.00	0.00

PART VII. C-H activation of DHA by a $^{s}PhIO_2$ molecule

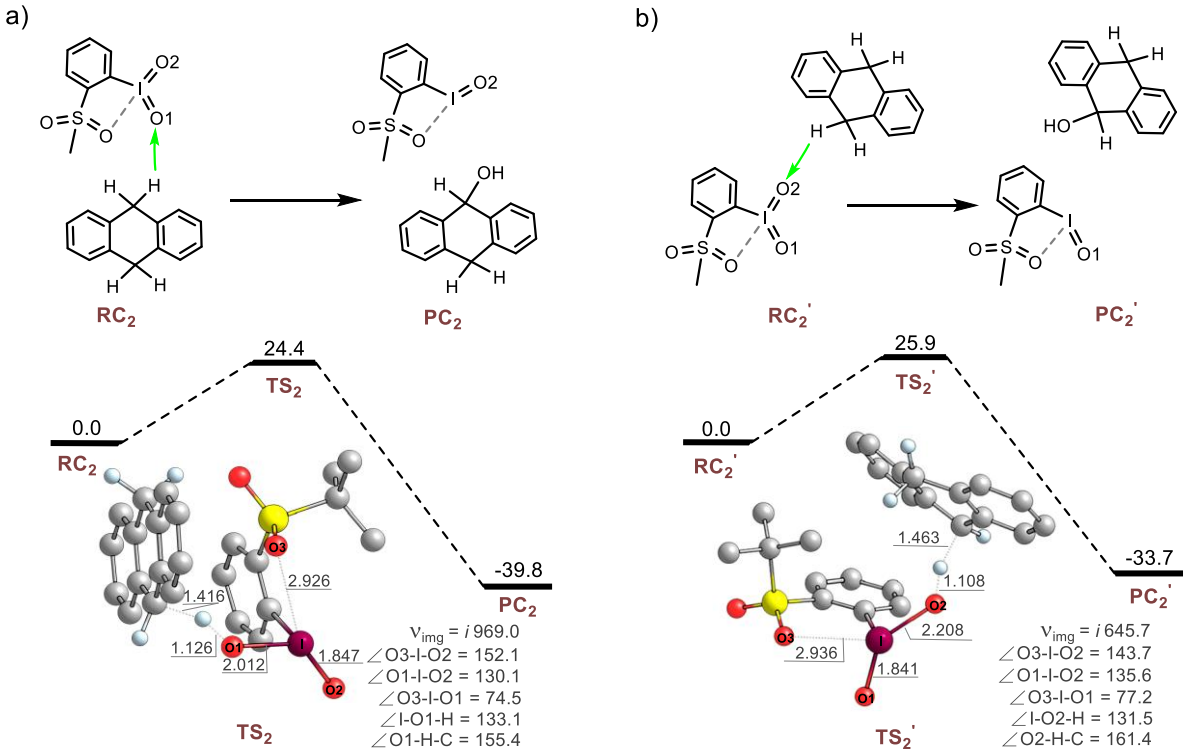


Figure S25. Energy profiles (in kcal mol^{-1}) for C-H activation by the (a) O1 atom and (b) O2 atom of $^{s}PhIO_2$ molecule. a) The **RC_2** is oxidized by O1 and b) the **RC_2'** is oxidized by O2. Calculations were done at the UB3LYP-D3(BJ)/B2'//B1' level. (B1': Lanl2dzdp (I), 6-31G** (S, O1, O2), 6-31G (rest); B2': Lanl2dzdp(I), 6-31+G**(rest)). Lengths are in Å units, angles are in degree units, and imaginary frequencies are in cm^{-1} units.

Table S15. Various SCF and free energies of key intermediates in C-H activation of DHA by the O1 atom of $^{s}PhIO_2$ molecule. Calculations were done at the UB3LYP-D3(BJ)/B2'//B1' level.

	OPT/B1	ΔE	OPT +ZPE	ΔE	SPE/B2	ΔE	SPE+ZPE	ΔE	G	ΔG
RC_2	-1639.771580[a]	0.0	-1639.330354	0.0	-1640.088531	0.0	-1639.647306	0.0	-1639.389802	0.0
TS_2	-1639.720270	32.2	-1639.286044	27.8	-1640.042698	28.8	-1639.608472	24.4	-1639.345196	28.0
PC_2	-1639.822808	-32.1	-1639.380814	-31.7	-1640.152742	-40.3	-1639.7107471	-39.8	-1639.441453	-32.4

a. Absolute energies are in au units and the relative ones are in kcal mol^{-1} units.

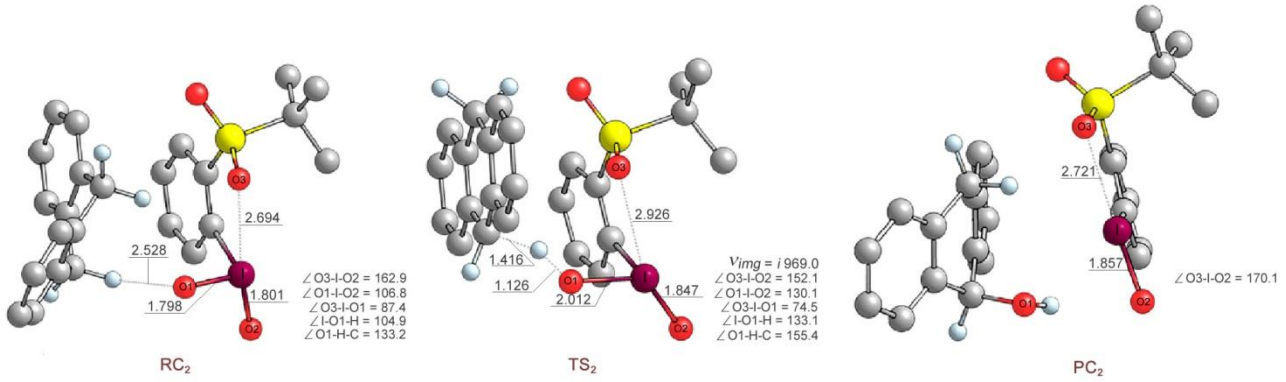


Figure S26. The geometric information of key intermediates in C-H activation of DHA by the O1 of $^{s}PhIO_2$ molecule. Calculations were done at the UB3LYP-D3(BJ)/B1' level. Lengths are in Å units, angles are in degree units, and imaginary frequencies are in cm^{-1} units.

Table S16. Mulliken spin densities and charges of key intermediates in C-H activation of DHA by the O1 of $^{s}PhIO_2$ molecule. Calculations were done at the UB3LYP-D3(BJ)/B1' level.

	Charge				Spin density			
	O1	ArI	O2	DHA	O1	ArI	O2	DHA
RC_2	-0.69	1.44	-0.73	-0.02	0.00	0.00	0.00	0.00
TS_2	-0.75	1.09	-0.73	0. 39	0.00	0.00	0.00	0.00
PC_2	-0.70	0.76	-0.76	0.70	0.00	0.00	0.00	0.00

Table S17. Various SCF and free energies of key intermediates in C-H activation of DHA by the O2 atom of $^{s}PhIO_2$ molecule. Calculations were done at the UB3LYP-D3(BJ)/B2'//B1' level.

	OPT/B1	ΔE	OPT +ZPE	ΔE	SPE/B2	ΔE	SPE+ZPE	ΔE	G	ΔG
RC_2'	-1639.768023[a]	0.0	-1639.326681	0.0	-1640.086149	0.0	-1639.644808	0.0	-1639.387167	0.0
TS_2'	-1639.713969	33.9	-1639.279261	29.8	-1640.038272	29.8	-1639.603563	25.9	-1639.338662	30.4
PC_2'	-1639.812042	-27.6	-1639.369835	-27.1	-1640.140723	-27.1	-1639.698515	-33.7	-1639.430188	-27.0

a. Absolute energies are in au units and the relative ones are in kcal mol^{-1} units.

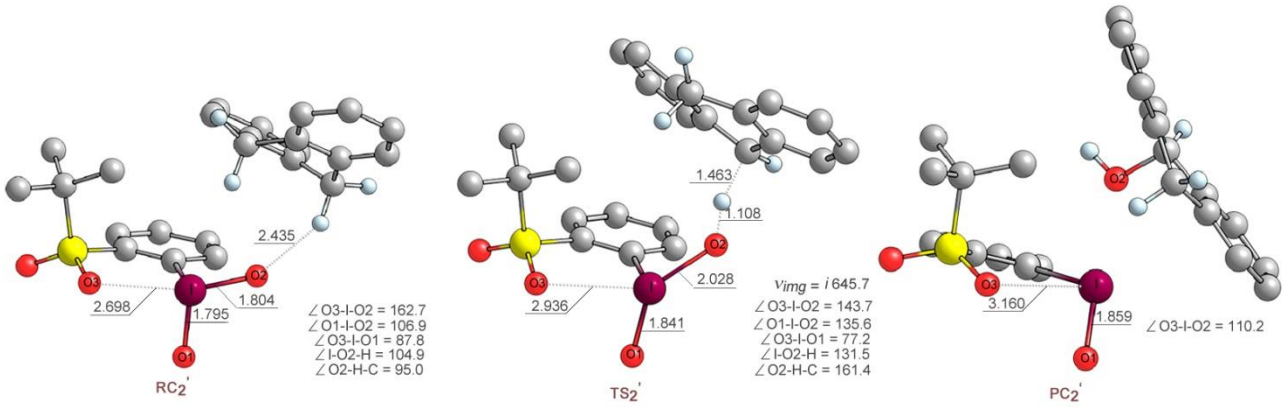


Figure S27. The geometric information of key intermediates in C-H activation of DHA by the O2 of $^{s}PhIO_2$ molecule. Calculations were done at the UB3LYP-D3(BJ)/B1' level. Lengths are in Å units, angles are in degree units, and imaginary frequencies are in cm^{-1} units.

Table S18. Mulliken spin densities and charges of key intermediates in C-H activation of DHA by the O2 of $^{s}PhIO_2$ molecule. Calculations were done at the UB3LYP-D3(BJ)/B1' level.

	Charge				Spin density			
	O1	ArI	O2	DHA	O1	ArI	O2	DHA
RC_2'	-0.71	1.44	-0.72	0.00	0.00	0.00	0.00	0.00
TS_2'	-0.71	1.06	-0.76	0. 42	0.00	0.00	0.00	0.00
PC_2'	-0.75	0.64	-0.70	0.81	0.00	0.00	0.00	0.00

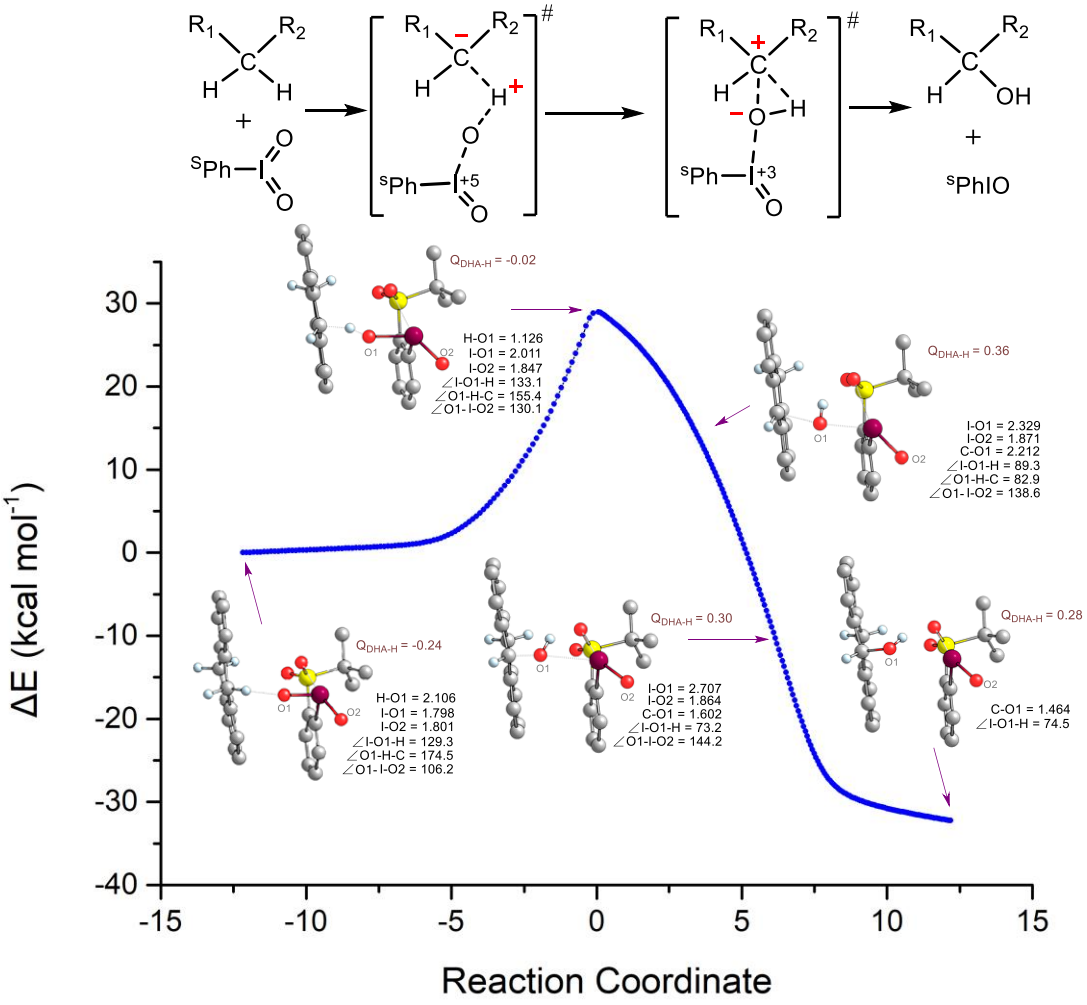


Figure S28. Intrinsic reaction coordinate scan of DHA hydroxylation by $^{s}PhIO_2$ via a hydride transfer/hydroxyl-rebound mechanism, starting from the hydrogen abstraction transition state leading back to reactants or forward to products. Geometric and electronic information of key intermediates were presented. Lengths are in Å units and angles are in degree units. Q denotes the value of Mulliken charge.

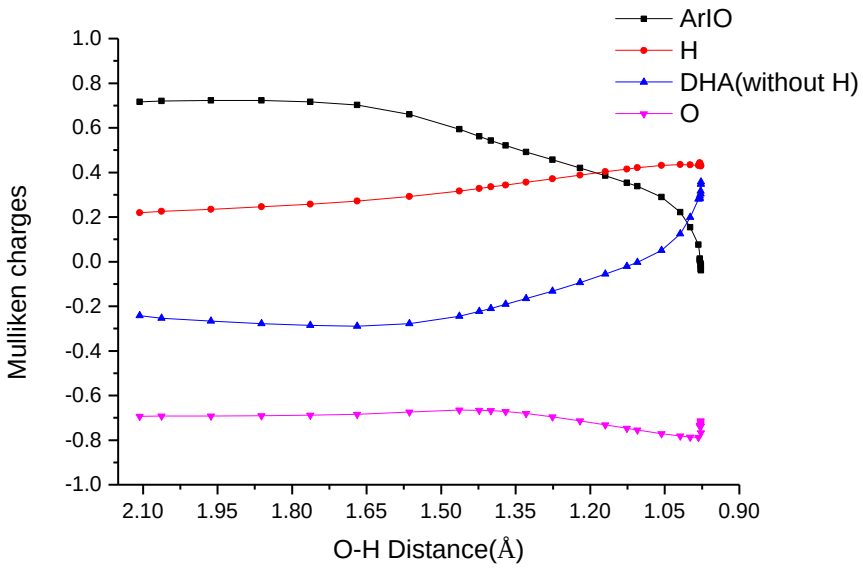


Figure S29. The Variation of Mulliken charges of the critical specie along C-H activation by the O1 of $^{s}PhIO_2$ molecule. Calculations were done at the UB3LYP-D3(BJ)/B1' level.

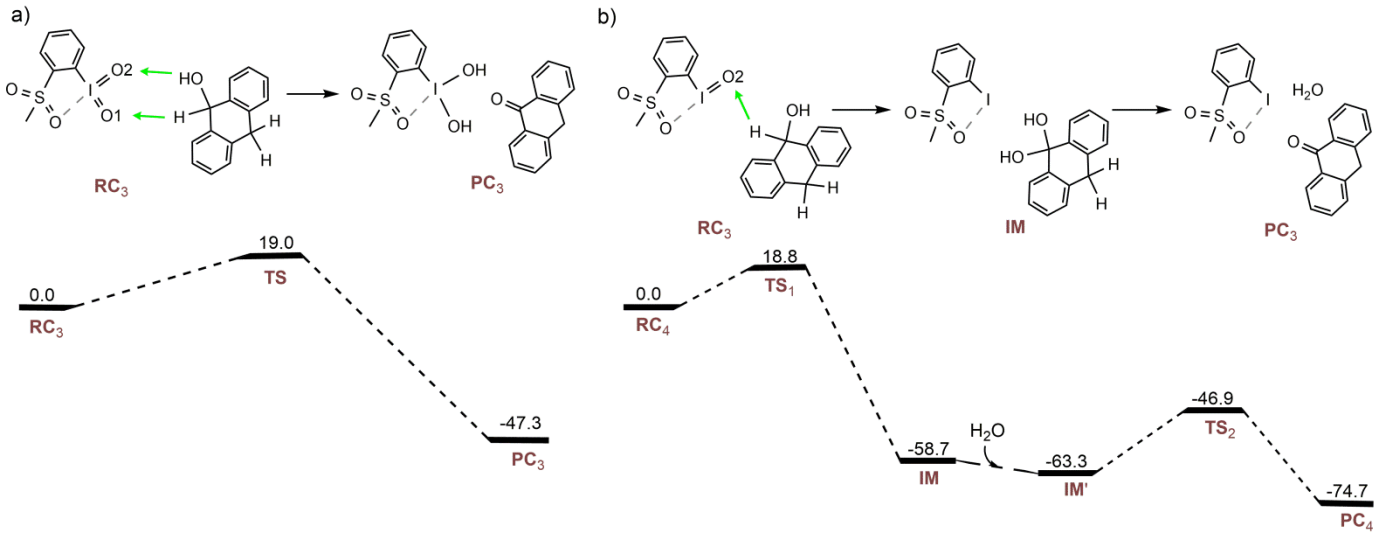


Figure S30. Energy profiles (in kcal mol^{-1}) for formation of ketone product from DHA-OH oxidized by the (a) O1 atom and (b) O2 atom of $^{s}PhIO_2$. Calculations were done at the UB3LYP-D3(BJ)/B2'//B1' level. (B1": Lanl2dzdp (I), 6-31G** (S, O1, O2), 6-31G (rest); B2': Lanl2dzdp(I), 6-31+G**(rest)).

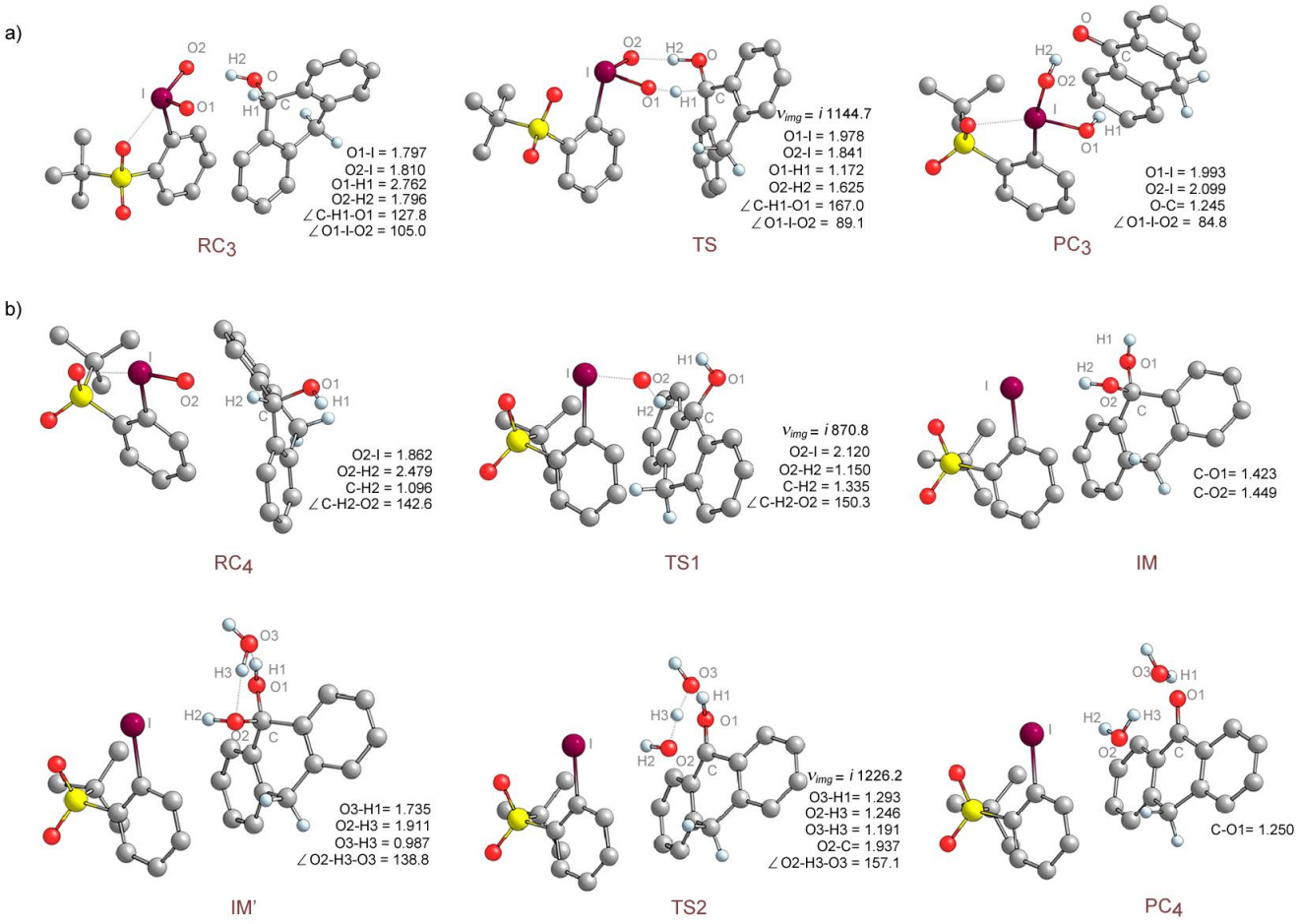


Figure S31. The geometric information of formation of ketone product from DHA-OH oxidized by the (a) O1 atom and (b) O2 atom of $^{s}PhIO_2$. Calculations were done at the UB3LYP-D3(BJ)/B1' level. Lengths are in Å units, angles are in degree units, and imaginary frequencies are in cm^{-1} units.

PART VIII. Thioanisole sulfoxidation by a ^{s}PhIO molecule

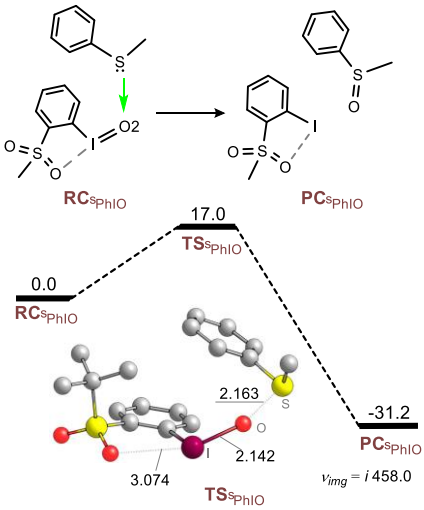


Figure S32. Energy profile (in kcal mol^{-1}) for thioanisole sulfoxidation by the ^{s}PhIO molecule. Calculations were done at the UB3LYP-D3(BJ)/B2'//B1' level. (B1'': Lanl2dzdp (I), 6-31G** (S, O1, O2), 6-31G (rest); B2': Lanl2dzdp(I), 6-31+G**(rest)). Lengths are in Å units, angles are in degree units, and imaginary frequencies are in cm^{-1} units.

Table S19. Various SCF and free energies of key intermediates in thioanisole sulfoxidation by the ^{s}PhIO molecule. Calculations were done at the Calculations were done at the UB3LYP-D3(BJ)/B1' level.

	OPT/B1	ΔE	OPT +ZPE	ΔE	SPE/B2	ΔE	SPE+ZPE	ΔE	G	ΔG
RC_{sPhIO}	-1693.664315[a]	0.0	-1693.314470	0.0	-1693.907187	0.0	-1693.557342	0.0	-1693.370617	0.0
TS_{sPhIO}	-1693.633606	19.3	-1693.285013	18.5	-1693.878784	17.8	-1693.530192	17.0	-1693.339396	19.6
PC_{sPhIO}	-1693.718866	-34.2	-1693.368474	-33.9	-1693.957459	-31.5	-1693.607067	-31.2	-1693.427116	-35.5

a. Absolute energies are in au units and the relative ones are in kcal mol^{-1} units.

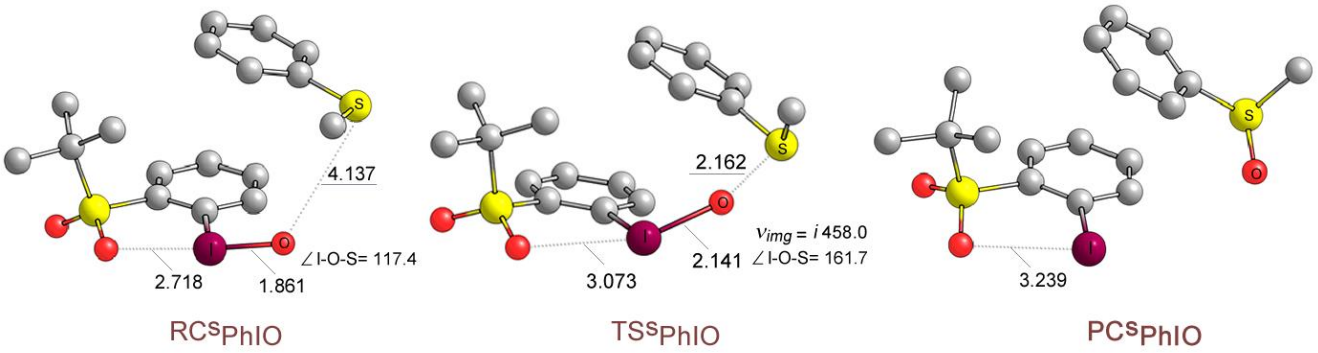


Figure S33. The geometric information of key intermediates in thioanisole sulfoxidation by the ^{s}PhIO molecule. Calculations were done at the UB3LYP-D3(BJ)/B1' level. Lengths are in Å units, angles are in degree units, and imaginary frequencies are in cm^{-1} units.

Table S20. Mulliken spin densities and charges of key intermediates in thioanisole sulfoxidation by the ^{s}PhIO molecule. Calculations were done at the Calculations were done at the UB3LYP-D3(BJ)/B1' level.

	Charge			Spin density		
	O	ArI	PhSCH3	O	ArI	PhSCH3
RC_{sPhIO}	-0.74	0.77	-0.02	0.00	0.00	0.00
TS_{sPhIO}	-0.61	0.31	0.30	0.00	0.00	0.00
PC_{sPhIO}	-0.70	-0.03	-0.72	0.00	0.00	0.00

PART IX. C-H activation of DHA by a ^{s}PhIO molecule

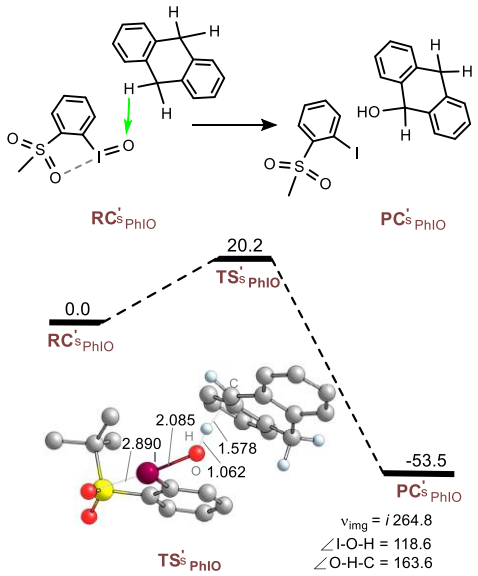


Figure S34. Energy profiles (in kcal mol^{-1}) for C-H activation by the ^{s}PhIO molecule. Calculations were done at the UB3LYP-D3(BJ)/B2'//B1' level. (B1'': Lanl2dzdp (I), 6-31G** (S, O1, O2), 6-31G (rest); B2': Lanl2dzdp(I), 6-31+G**(rest)). Lengths are in Å units, angles are in degree units, and imaginary frequencies are in cm^{-1} units.

Table S21. Various SCF and free energies of key intermediates in C-H activation by the ^{s}PhIO molecule. Calculations were done at the Calculations were done at the UB3LYP-D3(BJ)/B1' level.

	OPT/B1	ΔE	OPT +ZPE	ΔE	SPE/B2	ΔE	SPE+ZPE	ΔE	G	ΔG
RC'_{sPhIO}	-1564.617814[a]	0.0	-1564.179597	0.0	-1564.929408	0.0	-1564.491191	0.0	-1564.240129	0.0
TS'_{sPhIO}	-1564.578122	24.9	-1564.145036	21.7	-1564.892094	23.4	-1564.459008	20.2	-1564.202789	23.4
PC'_{sPhIO}	-1564.699584	-51.3	-1564.259146	-49.9	-1565.016816	-54.8	-1564.576378	-53.5	-1564.319106	-49.6

a. Absolute energies are in au units and the relative ones are in kcal mol^{-1} units.

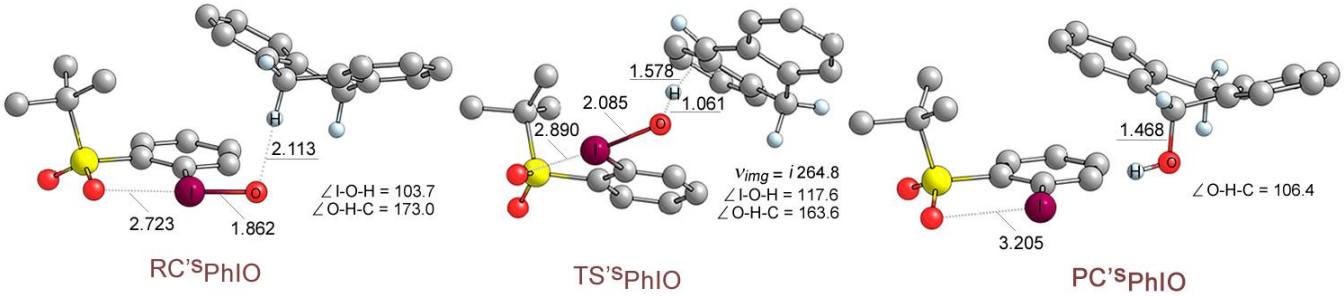


Figure S35. The geometric information of key intermediates in C-H activation by the ^{s}PhIO molecule. Calculations were done at the UB3LYP-D3(BJ)/B1' level. Lengths are in Å units, angles are in degree units, and imaginary frequencies are in cm^{-1} units.

Table S22. Mulliken spin densities and charges of key intermediates in C-H activation by the ^{s}PhIO molecule. Calculations were done at the Calculations were done at the UB3LYP-D3(BJ)/B1' level.

	Charge			Spin density		
	O	ArI	DHA	O	ArI	DHA
RC'_{sPhIO}	-0.74	0.76	-0.02	0.00	0.00	0.00
TS'_{sPhIO}	-0.71	0.52	0.20	0.00	0.00	0.00
PC'_{sPhIO}	-0.70	-0.03	0.73	0.00	0.00	0.00

PART X. Cartesian coordinates

1. The formation of the different spin states of the complex 1

^{2}1

Co	-0.121145000	-0.205922000	-0.187700000	H	-0.171948000	1.553723000	-4.243793000
N	-0.337438000	-0.175853000	1.878250000	H	1.084057000	0.584536000	-3.448348000
N	0.847526000	0.169819000	2.465288000	C	1.816634000	3.258199000	-3.597421000
N	1.325268000	-1.493459000	0.028664000	H	1.309747000	3.451791000	-4.548738000
N	2.280658000	-1.142036000	0.929883000	H	2.678011000	2.609865000	-3.790080000
N	1.241546000	1.262340000	-0.469357000	H	2.181988000	4.215585000	-3.213441000
N	2.115063000	1.316019000	0.581541000	O	-1.612800000	1.027457000	-0.584658000
B	2.159219000	0.212491000	1.658845000	I	-3.373627000	0.939300000	-1.113009000
H	3.087811000	0.391468000	2.389934000	O	-3.834511000	2.657823000	-0.965561000
C	-1.249249000	-0.328550000	2.870995000	C	-3.219400000	0.949069000	-3.272263000
C	-0.624702000	-0.060462000	4.109014000	C	-3.217124000	2.213829000	-3.852429000
H	-1.075813000	-0.095124000	5.085201000	H	-3.332266000	3.094183000	-3.230326000
C	0.696330000	0.244429000	3.808504000	C	-3.054136000	2.319738000	-5.241848000
H	1.526533000	0.494187000	4.448534000	H	-3.040596000	3.300197000	-5.702032000
C	-2.707967000	-0.677917000	2.643451000	C	-2.897711000	1.172467000	-6.026457000
C	-2.860322000	-1.644937000	1.452441000	H	-2.756455000	1.260857000	-7.096426000
H	-2.343028000	-2.589204000	1.650883000	C	-2.928045000	-0.098312000	-5.437639000
H	-2.445399000	-1.237484000	0.530725000	H	-2.804945000	-0.990898000	-6.038668000
H	-3.918788000	-1.863246000	1.273634000	C	-3.101715000	-0.206616000	-4.054917000
C	-3.493919000	0.638875000	2.400197000	S	-3.185764000	-1.823204000	-3.296453000
H	-3.000126000	1.256508000	1.644459000	O	-2.881533000	-1.528450000	-1.839861000
H	-4.524630000	0.423710000	2.094561000	O	-2.323125000	-2.769105000	-4.045535000
H	-3.530857000	1.236727000	3.316753000	C	-4.955885000	-2.409652000	-3.381919000
C	-3.288509000	-1.369804000	3.898725000	C	-4.952687000	-3.756669000	-2.633328000
H	-4.336260000	-1.633717000	3.719718000	H	-4.294239000	-4.481271000	-3.118468000
H	-3.254284000	-0.712509000	4.772735000	H	-5.972681000	-4.152077000	-2.649242000
H	-2.736717000	-2.286425000	4.131396000	H	-4.645520000	-3.632718000	-1.591696000
C	1.660622000	-2.697143000	-0.499480000	C	-5.321061000	-2.576498000	-4.864116000
C	2.864481000	-3.118262000	0.105380000	H	-5.330451000	-1.618901000	-5.392430000
H	3.403243000	-4.028171000	-0.091879000	H	-6.329566000	-2.997426000	-4.918706000
C	3.220763000	-2.110650000	0.997666000	H	-4.637697000	-3.262325000	-5.370427000
H	4.067279000	-2.019534000	1.658148000	C	-5.843873000	-1.374117000	-2.681303000
C	0.850584000	-3.385208000	-1.580658000	H	-5.574340000	-1.258539000	-1.627618000
C	0.568797000	-2.383252000	-2.722730000	H	-6.876293000	-1.734685000	-2.715421000
H	1.498564000	-1.931993000	-3.083686000	H	-5.821020000	-0.402387000	-3.183865000
H	-0.101856000	-1.583282000	-2.394173000	**^{4}1**			
H	0.065271000	-2.885153000	-3.551245000	Co	-0.064194000	-0.010174000	0.054580000
C	-0.483833000	-3.923445000	-1.002700000	N	-0.077387000	0.032506000	2.124216000
H	-1.111171000	-3.121287000	-0.606506000	N	1.207574000	0.021140000	2.592439000
H	-1.050745000	-4.424486000	-1.794914000	N	1.331490000	-1.521786000	-0.081861000
H	-0.290402000	-4.644285000	-0.200959000	N	2.378168000	-1.265459000	0.762465000
C	1.656599000	-4.572722000	-2.151870000	N	1.351018000	1.464606000	-0.152631000
H	1.079381000	-5.055879000	-2.946387000	N	2.382126000	1.248246000	0.721246000
H	1.862851000	-5.321923000	-1.380195000	B	2.427483000	0.006245000	1.643596000
H	2.609817000	-4.238030000	-2.574689000	H	3.436224000	0.015396000	2.284267000
C	1.544214000	2.281734000	-1.311454000	C	-0.905605000	-0.000154000	3.196783000
C	2.628799000	3.004520000	-0.763191000	C	-0.123881000	-0.028912000	4.370634000
H	3.112040000	3.868095000	-1.185216000	H	-0.477080000	-0.055909000	5.386490000
C	2.958046000	2.363067000	0.423241000	C	1.200597000	-0.015381000	3.945229000
H	3.728396000	2.570937000	1.147595000	H	2.120590000	-0.029062000	4.506358000
C	0.824112000	2.590101000	-2.614180000	C	-2.417468000	0.015208000	3.069209000
C	-0.334523000	3.583216000	-2.332838000	C	-2.886914000	-1.182518000	2.206221000
H	0.052378000	4.501221000	-1.877702000	H	-2.631859000	-2.130566000	2.691628000
H	-1.071149000	3.146157000	-1.656431000	H	-2.412503000	-1.187603000	1.221222000
H	-0.830008000	3.851519000	-3.272852000	H	-3.974867000	-1.147691000	2.075869000
C	0.281015000	1.307977000	-3.277656000	C	-2.864649000	1.356381000	2.435039000
H	-0.488059000	0.840426000	-2.662580000	H	-2.393762000	1.531185000	1.464960000

H	-3.952175000	1.365920000	2.298625000	H	-5.708446000	-4.104145000	-2.315876000
H	-2.594835000	2.193129000	3.088478000	C	-5.423055000	-3.081654000	-5.651989000
C	-3.064529000	-0.108522000	4.465736000	H	-5.226201000	-2.141388000	-6.173331000
H	-4.154768000	-0.103247000	4.366085000	H	-6.422592000	-3.419085000	-5.943267000
H	-2.779255000	0.729256000	5.110499000	H	-4.702177000	-3.836395000	-5.976126000
H	-2.771208000	-1.041981000	4.957569000	C	-6.306436000	-1.746438000	-3.669817000
C	1.609852000	-2.666754000	-0.751411000	H	-6.284172000	-1.624951000	-2.583668000
C	2.864893000	-3.146223000	-0.315899000	H	-7.335592000	-1.978057000	-3.960848000
H	3.371359000	-4.034841000	-0.649452000	H	-6.030461000	-0.801912000	-4.148142000
C	3.314128000	-2.234929000	0.633923000	**^{6}1**			
H	4.221620000	-2.212806000	1.215032000	Co	0.049739000	0.107148000	-0.139933000
C	0.670511000	-3.280855000	-1.774279000	N	-0.045095000	-0.107579000	1.861801000
C	0.393821000	-2.274720000	-2.920679000	N	1.188942000	-0.148581000	2.447725000
H	1.329774000	-1.981146000	-3.409384000	N	1.502445000	-1.356884000	-0.334122000
H	-0.106542000	-1.377561000	-2.550694000	N	2.506873000	-1.191882000	0.577182000
H	-0.260670000	-2.739843000	-3.664936000	N	1.450461000	1.628946000	-0.026857000
C	-0.658030000	-3.682496000	-1.083912000	N	2.459972000	1.311041000	0.838183000
H	-1.169522000	-2.809646000	-0.674092000	B	2.484379000	-0.033663000	1.597631000
H	-1.325738000	-4.150037000	-1.813933000	H	3.442762000	-0.089108000	2.308805000
H	-0.466640000	-4.396366000	-0.274637000	C	-0.981569000	-0.239952000	2.837171000
C	1.317554000	-4.546834000	-2.377190000	C	-0.317112000	-0.368973000	4.071259000
H	0.637954000	-4.984395000	-3.115397000	H	-0.764519000	-0.491750000	5.041850000
H	1.512802000	-5.300544000	-1.606603000	C	1.046637000	-0.306364000	3.781006000
H	2.262024000	-4.311223000	-2.880003000	H	1.905298000	-0.363523000	4.429945000
C	1.669070000	2.542391000	-0.908210000	C	-2.472156000	-0.224962000	2.548119000
C	2.928739000	3.026653000	-0.494639000	C	-2.831291000	-1.334346000	1.528258000
H	3.462553000	3.872105000	-0.891647000	H	-2.536306000	-2.318881000	1.905831000
C	3.343666000	2.181310000	0.528987000	H	-2.339376000	-1.185669000	0.563704000
H	4.245637000	2.179625000	1.118905000	H	-3.912113000	-1.344104000	1.351315000
C	0.766191000	3.073968000	-2.004923000	C	-2.883574000	1.164636000	1.994462000
C	-0.534636000	3.635731000	-1.380617000	H	-2.344885000	1.415747000	1.075159000
H	-0.304915000	4.439441000	-0.672374000	H	-3.959094000	1.176878000	1.782676000
H	-1.097865000	2.859498000	-0.858010000	H	-2.670255000	1.951220000	2.725794000
H	-1.179389000	4.045541000	-2.166883000	C	-3.254340000	-0.484808000	3.853941000
C	0.426893000	1.940540000	-3.004259000	H	-4.328739000	-0.477551000	3.644985000
H	-0.181554000	1.159738000	-2.540515000	H	-3.048488000	0.288691000	4.601172000
H	-0.140967000	2.347715000	-3.846970000	H	-2.996566000	-1.459499000	4.281444000
H	1.340000000	1.479248000	-3.395501000	C	1.780074000	-2.461130000	-1.066486000
C	1.488335000	4.206339000	-2.766540000	C	2.999467000	-3.006201000	-0.607332000
H	0.837503000	4.584823000	-3.561322000	H	3.498794000	-3.884190000	-0.977877000
H	2.416239000	3.848228000	-3.225481000	C	3.422063000	-2.178742000	0.428389000
H	1.730037000	5.041838000	-2.101042000	H	4.295332000	-2.227938000	1.058214000
O	-1.615949000	-0.495146000	-1.059537000	C	0.875357000	-2.963889000	-2.176698000
I	-3.352396000	0.107039000	-1.277282000	C	0.820279000	-1.924276000	-3.325069000
O	-3.309373000	1.871217000	-0.991846000	H	1.824420000	-1.729691000	-3.718345000
C	-3.212349000	0.207457000	-3.424157000	H	0.385452000	-0.982491000	-2.982108000
C	-2.947046000	1.475858000	-3.929547000	H	0.200583000	-2.311220000	-4.140969000
H	-2.943180000	2.333304000	-3.265010000	C	-0.550280000	-3.210078000	-1.625002000
C	-2.659909000	1.609321000	-5.296359000	H	-1.015508000	-2.275334000	-1.301206000
H	-2.453084000	2.591858000	-5.703008000	H	-1.181757000	-3.651401000	-2.401084000
C	-2.616294000	0.482335000	-6.122796000	H	-0.525652000	-3.899437000	-0.773593000
H	-2.366421000	0.586659000	-7.171342000	C	1.429335000	-4.293894000	-2.731603000
C	-2.895035000	-0.789275000	-5.604705000	H	0.771366000	-4.658565000	-3.527014000
H	-2.850620000	-1.663582000	-6.241922000	H	1.478657000	-5.061452000	-1.951506000
C	-3.219778000	-0.922049000	-4.251031000	H	2.431642000	-4.162600000	-3.153736000
S	-3.661444000	-2.526593000	-3.588470000	C	1.697790000	2.866588000	-0.518908000
O	-3.716434000	-2.274261000	-2.093864000	C	2.900726000	3.340894000	0.048976000
O	-2.734179000	-3.560289000	-4.113677000	H	3.375406000	4.288897000	-0.133490000
C	-5.412056000	-2.906485000	-4.127044000	C	3.346405000	2.332833000	0.897730000
C	-5.758149000	-4.221290000	-3.401115000	H	4.218365000	2.277419000	1.528834000
H	-5.092398000	-5.032550000	-3.706363000	C	0.778154000	3.566690000	-1.504131000
H	-6.782063000	-4.494307000	-3.673536000	C	-0.633112000	3.716978000	-0.882970000

H	-0.583221000	4.258339000	0.068346000
H	-1.093778000	2.742387000	-0.708827000
H	-1.283561000	4.271390000	-1.567216000
C	0.689014000	2.755191000	-2.821825000
H	0.268425000	1.762628000	-2.645973000
H	0.043173000	3.282902000	-3.533798000
H	1.680984000	2.645000000	-3.274256000
C	1.333661000	4.972568000	-1.818931000
H	0.667743000	5.477916000	-2.525719000
H	2.329108000	4.914235000	-2.272378000
H	1.399360000	5.587027000	-0.914409000
O	-0.995674000	0.206126000	-1.478970000
I	-3.585025000	0.604857000	-1.842007000
O	-3.215332000	2.320816000	-2.330016000
C	-2.942153000	-0.330202000	-3.649694000
C	-2.172768000	0.463648000	-4.495538000
H	-1.964630000	1.495167000	-4.237789000
C	-1.663686000	-0.107727000	-5.669142000
H	-1.059790000	0.498110000	-6.333636000
C	-1.911219000	-1.451620000	-5.973081000
H	-1.496476000	-1.890839000	-6.871747000
C	-2.685032000	-2.239740000	-5.114100000
H	-2.859243000	-3.286155000	-5.331991000
C	-3.214569000	-1.668737000	-3.951139000
S	-4.213069000	-2.655276000	-2.844772000
O	-4.253661000	-1.796828000	-1.586534000
O	-3.660923000	-4.028345000	-2.751573000
C	-5.952737000	-2.716467000	-3.524090000
C	-6.762528000	-3.473860000	-2.454690000
H	-6.382253000	-4.488120000	-2.310049000
H	-7.797501000	-3.540217000	-2.803557000
H	-6.753688000	-2.946067000	-1.497692000
C	-5.908195000	-3.481364000	-4.854835000
H	-5.349300000	-2.936925000	-5.620700000
H	-6.936961000	-3.593878000	-5.210486000
H	-5.479564000	-4.478841000	-4.731401000
C	-6.445364000	-1.274522000	-3.703034000
H	-6.472361000	-0.735060000	-2.752687000
H	-7.467347000	-1.314052000	-4.092105000
H	-5.839517000	-0.718508000	-4.424790000

2.Thioanisole sulfoxidation by complex 1 via the direct oxygen-atom transfer mechanism.

^{4}RC			
Co	0.001499000	0.229914000	0.125128000
N	-0.107712000	-0.555397000	2.021069000
N	1.144559000	-0.787253000	2.516941000
N	1.412002000	-1.107323000	-0.557103000
N	2.401127000	-1.264911000	0.374964000
N	1.442515000	1.652386000	0.638501000
N	2.432276000	1.049438000	1.367926000
B	2.415104000	-0.461820000	1.698128000
H	3.387190000	-0.747566000	2.332642000
C	-1.003452000	-0.949400000	2.957812000
C	-0.297155000	-1.436907000	4.078250000
H	-0.713980000	-1.824558000	4.991233000
C	1.052067000	-1.317404000	3.758774000
H	1.934538000	-1.570847000	4.323207000
C	-2.503168000	-0.892374000	2.733513000
C	-2.878798000	-1.848849000	1.573455000
H	-2.571531000	-2.873529000	1.810121000
H	-2.402084000	-1.546999000	0.638945000
H	-3.960962000	-1.837169000	1.411483000
C	-2.941835000	0.553094000	2.393333000
H	-2.438411000	0.918710000	1.494736000
H	-4.022845000	0.582649000	2.216258000
H	-2.704386000	1.237900000	3.214423000
C	-3.240276000	-1.341075000	4.013472000
H	-4.321560000	-1.292045000	3.849242000
H	-2.993383000	-0.695202000	4.863160000
H	-2.984411000	-2.373087000	4.275824000
C	1.717894000	-1.885451000	-1.622390000
C	2.932990000	-2.554303000	-1.354948000
H	3.448602000	-3.246582000	-1.997095000
C	3.329771000	-2.133624000	-0.089910000
H	4.196574000	-2.388987000	0.497539000
C	0.843668000	-1.976875000	-2.860548000
C	0.636697000	-0.568551000	-3.472317000
H	1.599659000	-0.095383000	-3.694290000
H	0.070586000	0.078129000	-2.798627000
H	0.070298000	-0.654209000	-4.405720000
C	-0.527322000	-2.594879000	-2.489539000
H	-1.063470000	-1.966890000	-1.775685000
H	-1.146685000	-2.691217000	-3.387420000
H	-0.398743000	-3.592110000	-2.054604000
C	1.529293000	-2.876772000	-3.911551000
H	0.898950000	-2.937711000	-4.804726000
H	1.676039000	-3.893303000	-3.530814000
H	2.503573000	-2.472822000	-4.208038000
C	1.772340000	2.959245000	0.503159000
C	2.998549000	3.187859000	1.165223000
H	3.530578000	4.119526000	1.244204000
C	3.379435000	1.960035000	1.694269000
H	4.245949000	1.678767000	2.270123000
C	0.921779000	3.954814000	-0.264767000
C	-0.480625000	4.063159000	0.383620000
H	-0.395049000	4.412812000	1.418581000
H	-1.000826000	3.103835000	0.386920000
H	-1.097838000	4.772208000	-0.177405000
C	0.813764000	3.513189000	-1.746293000
H	0.300155000	2.556584000	-1.852548000
H	0.241562000	4.254438000	-2.314064000
H	1.812874000	3.429611000	-2.188766000
C	1.586919000	5.348577000	-0.217685000
H	0.968989000	6.066067000	-0.767125000
H	2.579651000	5.331007000	-0.680101000
H	1.689787000	5.706400000	0.812441000
O	-1.586585000	0.178102000	-1.001418000
I	-3.049021000	1.232752000	-1.484139000
O	-2.277968000	2.741267000	-2.068295000
C	-3.165267000	0.252083000	-3.399924000
C	-2.515386000	0.933003000	-4.423456000
H	-2.104901000	1.918019000	-4.237912000
C	-2.405966000	0.324573000	-5.680793000
H	-1.921526000	0.858671000	-6.488662000
C	-2.902009000	-0.966593000	-5.884107000
H	-2.791150000	-1.447715000	-6.848072000
C	-3.535004000	-1.653313000	-4.841446000
H	-3.880876000	-2.667420000	-4.992182000
C	-3.696633000	-1.026803000	-3.599463000
S	-4.497637000	-1.895121000	-2.247355000
O	-4.469618000	-0.875589000	-1.127533000
O	-3.832838000	-3.206294000	-2.031676000
C	-6.300763000	-2.170856000	-2.663019000
C	-6.913837000	-2.685845000	-1.345268000
H	-6.452470000	-3.626060000	-1.031808000
H	-7.978654000	-2.866571000	-1.520924000
H	-6.813370000	-1.951074000	-0.543447000
C	-6.402562000	-3.225189000	-3.774496000
H	-6.061451000	-2.838129000	-4.737461000
H	-7.457768000	-3.495078000	-3.883192000
H	-5.843618000	-4.130400000	-3.525112000
C	-6.899393000	-0.825622000	-3.087316000
H	-6.818306000	-0.079076000	-2.294729000
H	-7.960611000	-0.977326000	-3.307884000
H	-6.419794000	-0.442607000	-3.991939000
S	-5.630330000	2.637839000	-2.514046000
C	-5.076559000	2.994315000	-4.176443000
C	-4.056031000	3.914827000	-4.458581000
H	-3.586412000	4.480586000	-3.666286000
C	-3.621353000	4.080265000	-5.778762000
H	-2.833195000	4.793935000	-5.992673000
C	-4.187504000	3.327501000	-6.813529000
H	-3.841308000	3.456343000	-7.832905000
C	-5.210637000	2.414568000	-6.528337000
H	-5.664506000	1.836291000	-7.325489000
C	-5.662868000	2.253298000	-5.216730000
H	-6.472182000	1.565045000	-5.002091000
C	-5.234750000	4.171260000	-1.601470000
H	-5.680080000	5.029791000	-2.106447000
H	-4.154604000	4.296496000	-1.509747000
H	-5.677150000	4.063419000	-0.608850000
^{4}TS$_{DOT}$			
Co	-0.070922000	-0.026605000	0.243186000
N	0.030731000	-0.628609000	2.199715000
N	1.327164000	-0.679859000	2.626831000
N	1.439346000	-1.273838000	-0.405497000
N	2.501652000	-1.225054000	0.454351000
N	1.206435000	1.572222000	0.540374000

N	2.318247000	1.169563000	1.225770000	H	-2.295946000	2.273189000	-3.623679000
B	2.503681000	-0.298407000	1.693026000	C	-2.174871000	0.972620000	-5.345368000
H	3.538839000	-0.407349000	2.281215000	H	-1.717933000	1.726612000	-5.973280000
C	-0.765360000	-0.990742000	3.231550000	C	-2.441943000	-0.302640000	-5.852136000
C	0.051973000	-1.282829000	4.345912000	H	-2.182436000	-0.549812000	-6.874248000
H	-0.268193000	-1.604197000	5.321599000	C	-3.052399000	-1.263655000	-5.042450000
C	1.361328000	-1.073487000	3.922405000	H	-3.268714000	-2.252960000	-5.425526000
H	2.296320000	-1.178353000	4.448194000	C	-3.379282000	-0.956418000	-3.713562000
C	-2.280063000	-1.033717000	3.120595000	S	-4.246331000	-2.221176000	-2.775108000
C	-2.706523000	-1.937449000	1.937716000	O	-4.025017000	-1.912158000	-1.324737000
H	-2.315999000	-2.952723000	2.067945000	O	-3.830368000	-3.545318000	-3.314134000
H	-2.351523000	-1.555078000	0.978322000	C	-6.063671000	-1.973256000	-3.127578000
H	-3.799854000	-1.994292000	1.890724000	C	-6.769819000	-3.102677000	-2.353031000
C	-2.833836000	0.400551000	2.913937000	H	-6.460551000	-4.085738000	-2.716399000
H	-2.437140000	0.863081000	2.004381000	H	-7.848327000	-2.998766000	-2.506823000
H	-3.926497000	0.369915000	2.833315000	H	-6.565876000	-3.037338000	-1.280980000
H	-2.566741000	1.046287000	3.757440000	C	-6.293914000	-2.096230000	-4.640441000
C	-2.877429000	-1.604746000	4.425281000	H	-5.818715000	-1.281059000	-5.193078000
H	-3.968484000	-1.641873000	4.343725000	H	-7.371531000	-2.044400000	-4.825952000
H	-2.622314000	-0.980260000	5.288226000	H	-5.928466000	-3.052374000	-5.023907000
H	-2.514478000	-2.620924000	4.612602000	C	-6.463973000	-0.589547000	-2.599484000
C	1.748654000	-2.135763000	-1.401579000	H	-6.288229000	-0.504149000	-1.523930000
C	3.044128000	-2.648688000	-1.163720000	H	-7.534039000	-0.447344000	-2.781195000
H	3.583145000	-3.357631000	-1.767486000	H	-5.930770000	0.209972000	-3.120562000
C	3.482071000	-2.049131000	0.012527000	S	-5.270822000	3.946714000	-2.481907000
H	4.409106000	-2.151822000	0.552745000	C	-5.008935000	3.579523000	-4.193386000
C	0.804318000	-2.442224000	-2.551777000	C	-4.030720000	4.199286000	-4.988172000
C	0.483619000	-1.140650000	-3.330268000	H	-3.394598000	4.976463000	-4.585671000
H	1.402829000	-0.678300000	-3.707760000	C	-3.875068000	3.806043000	-6.321100000
H	-0.041354000	-0.424188000	-2.695597000	H	-3.123288000	4.291387000	-6.933601000
H	-0.162668000	-1.371346000	-4.184070000	C	-4.672704000	2.790871000	-6.861909000
C	-0.507338000	-3.064048000	-2.009894000	H	-4.538243000	2.485070000	-7.893072000
H	-1.050035000	-2.356234000	-1.379233000	C	-5.649085000	2.175098000	-6.067745000
H	-1.162679000	-3.340034000	-2.842915000	H	-6.277402000	1.394246000	-6.481383000
H	-0.293920000	-3.968573000	-1.428822000	C	-5.826367000	2.571571000	-4.742133000
C	1.473212000	-3.446871000	-3.514536000	H	-6.598740000	2.111371000	-4.136125000
H	0.792148000	-3.664617000	-4.343656000	C	-4.202521000	5.378950000	-2.166470000
H	1.703577000	-4.390529000	-3.007979000	H	-4.475655000	6.215985000	-2.811606000
H	2.401372000	-3.041835000	-3.932921000	H	-3.156998000	5.100330000	-2.305621000
C	1.335731000	2.892787000	0.278361000	H	-4.363251000	5.654517000	-1.123062000
C	2.564999000	3.340198000	0.809809000	**^{4}PC**			
H	2.967504000	4.337364000	0.770164000	Co	0.104129000	-0.069970000	0.224612000
C	3.151602000	2.223389000	1.398005000	N	0.079097000	-0.385211000	2.266174000
H	4.089291000	2.112292000	1.917631000	N	1.351243000	-0.521700000	2.746595000
C	0.261678000	3.685562000	-0.444731000	N	1.459203000	-1.592145000	-0.132461000
C	-1.009527000	3.755385000	0.441027000	N	2.514729000	-1.511912000	0.733886000
H	-0.795188000	4.292333000	1.371415000	N	1.580330000	1.372352000	0.326528000
H	-1.373428000	2.759381000	0.708007000	N	2.601948000	0.970923000	1.139007000
H	-1.812904000	4.275129000	-0.089965000	B	2.592060000	-0.417903000	1.823867000
C	-0.063338000	3.026015000	-1.807397000	H	3.587979000	-0.557229000	2.471056000
H	-0.408362000	1.995922000	-1.693306000	C	-0.775328000	-0.546252000	3.303016000
H	-0.851240000	3.595442000	-2.312322000	C	-0.023426000	-0.790611000	4.473169000
H	0.823588000	3.014154000	-2.449933000	H	-0.401142000	-0.961686000	5.466041000
C	0.757178000	5.124803000	-0.703871000	C	1.310577000	-0.767553000	4.077964000
H	-0.019055000	5.691042000	-1.229358000	H	2.215600000	-0.908166000	4.646085000
H	1.660636000	5.126754000	-1.322992000	C	-2.282992000	-0.450766000	3.143825000
H	0.978300000	5.644026000	0.234555000	C	-2.772276000	-1.458355000	2.073129000
O	-1.589766000	-0.184407000	-0.888305000	H	-2.518405000	-2.482151000	2.368989000
I	-3.214897000	0.826087000	-1.128071000	H	-2.327926000	-1.271566000	1.092494000
O	-3.675608000	2.635483000	-1.560708000	H	-3.861964000	-1.391687000	1.973225000
C	-3.071036000	0.312202000	-3.205882000	C	-2.674186000	0.995531000	2.742983000
C	-2.490345000	1.285654000	-4.018356000	H	-2.157217000	1.320632000	1.834426000

H	-3.755220000	1.060765000	2.573805000
H	-2.406063000	1.702175000	3.535882000
C	-2.970594000	-0.784459000	4.485853000
H	-4.057011000	-0.716679000	4.368409000
H	-2.669664000	-0.084955000	5.273051000
H	-2.725486000	-1.800784000	4.811831000
C	1.679054000	-2.640180000	-0.959052000
C	2.912064000	-3.237027000	-0.609402000
H	3.373628000	-4.092193000	-1.071321000
C	3.404166000	-2.496801000	0.460140000
H	4.309523000	-2.605074000	1.035002000
C	0.684954000	-3.073154000	-2.022118000
C	0.408128000	-1.918390000	-3.018104000
H	1.335002000	-1.597115000	-3.507440000
H	-0.046093000	-1.062805000	-2.513442000
H	-0.294314000	-2.261624000	-3.785297000
C	-0.638990000	-3.496825000	-1.335563000
H	-1.110765000	-2.646174000	-0.839054000
H	-1.340180000	-3.870552000	-2.087176000
H	-0.452722000	-4.288148000	-0.600009000
C	1.253950000	-4.277502000	-2.802449000
H	0.534961000	-4.586011000	-3.568160000
H	1.433000000	-5.132424000	-2.141001000
H	2.195743000	-4.021562000	-3.300992000
C	1.896023000	2.591895000	-0.164277000
C	3.153009000	2.975799000	0.351871000
H	3.687512000	3.888679000	0.154753000
C	3.563010000	1.924771000	1.167085000
H	4.459554000	1.794740000	1.750987000
C	0.971803000	3.352545000	-1.096267000
C	-0.291966000	3.795200000	-0.314278000
H	-0.022039000	4.483526000	0.493952000
H	-0.805553000	2.937275000	0.129288000
H	-0.993485000	4.305342000	-0.984650000
C	0.570231000	2.455961000	-2.292741000
H	-0.023342000	1.593914000	-1.976642000
H	-0.027832000	3.034597000	-3.004367000
H	1.459007000	2.085084000	-2.814387000
C	1.690575000	4.607550000	-1.635850000
H	1.021540000	5.153355000	-2.309237000
H	2.592457000	4.336075000	-2.194999000
H	1.976929000	5.282880000	-0.822715000
O	-1.439296000	-0.234591000	-0.879466000
I	-2.960851000	0.926745000	-1.036319000
O	-4.690998000	2.721710000	-1.371951000
C	-2.969910000	0.821993000	-3.161320000
C	-2.613452000	2.007032000	-3.816007000
H	-2.476783000	2.916379000	-3.247921000
C	-2.432318000	2.014766000	-5.202137000
H	-2.172595000	2.940859000	-5.699066000
C	-2.565977000	0.830339000	-5.929448000
H	-2.392008000	0.820488000	-6.998486000
C	-2.920674000	-0.352716000	-5.276816000
H	-3.004323000	-1.276077000	-5.834714000
C	-3.158333000	-0.364241000	-3.892759000
S	-3.729502000	-1.950799000	-3.224750000
O	-3.665398000	-1.888892000	-1.737648000
O	-2.978996000	-3.013442000	-3.954239000
C	-5.539665000	-2.093735000	-3.679655000
C	-5.988329000	-3.418088000	-3.030058000
H	-5.432716000	-4.266736000	-3.437743000
H	-7.050659000	-3.561787000	-3.250619000
H	-5.858020000	-3.393760000	-1.945675000
C	-5.692799000	-2.144198000	-5.205127000
H	-5.430434000	-1.192253000	-5.673999000
H	-6.743537000	-2.350120000	-5.434121000
H	-5.086304000	-2.941796000	-5.641576000
C	-6.266470000	-0.889055000	-3.074230000
H	-6.115521000	-0.826455000	-1.993531000
H	-7.339417000	-0.992028000	-3.266072000
H	-5.933681000	0.043220000	-3.534839000
S	-6.001898000	2.598466000	-2.201050000
C	-5.642228000	3.335346000	-3.802912000
C	-4.844756000	4.483816000	-3.885809000
H	-4.466999000	4.953806000	-2.984612000
C	-4.519173000	4.994095000	-5.144281000
H	-3.903287000	5.882765000	-5.222641000
C	-4.982698000	4.354315000	-6.303455000
H	-4.722325000	4.750854000	-7.278334000
C	-5.774045000	3.204277000	-6.208092000
H	-6.126166000	2.708085000	-7.105006000
C	-6.106649000	2.685414000	-4.951210000
H	-6.713351000	1.790223000	-4.871830000
C	-7.071102000	3.890961000	-1.502708000
H	-7.973021000	3.965410000	-2.114428000
H	-6.532262000	4.840370000	-1.494304000
H	-7.328770000	3.591310000	-0.485449000

^{4}RC'

Co	-0.546560000	0.837009000	0.170543000
N	-1.457701000	1.255885000	1.951826000
N	-0.533038000	1.310265000	2.957207000
N	0.635506000	-0.684948000	0.889791000
N	1.199978000	-0.314141000	2.080577000
N	0.920891000	2.255812000	0.428893000
N	1.471211000	2.151453000	1.675864000
B	0.977282000	1.091304000	2.691049000
H	1.586805000	1.190578000	3.714079000
C	-2.676062000	1.494464000	2.492530000
C	-2.517732000	1.708139000	3.878077000
H	-3.290146000	1.922164000	4.595826000
C	-1.153887000	1.583857000	4.128561000
H	-0.596703000	1.670718000	5.046977000
C	-3.949389000	1.494666000	1.665575000
C	-4.166313000	0.091475000	1.043310000
H	-4.271245000	-0.663927000	1.829292000
H	-3.330026000	-0.201621000	0.404458000
H	-5.082163000	0.087366000	0.440839000
C	-3.852853000	2.565057000	0.549790000
H	-2.985594000	2.398796000	-0.096467000
H	-4.758368000	2.547427000	-0.067501000
H	-3.748421000	3.567342000	0.978185000
C	-5.157597000	1.832937000	2.564840000
H	-6.072711000	1.837128000	1.964021000
H	-5.046583000	2.820647000	3.024742000
H	-5.277358000	1.090280000	3.360511000
C	1.098600000	-1.918914000	0.576397000
C	1.978083000	-2.339322000	1.598430000
H	2.510146000	-3.272675000	1.653990000
C	2.016093000	-1.299980000	2.521989000
H	2.561751000	-1.198835000	3.445937000
C	0.674679000	-2.674851000	-0.671072000
C	0.989852000	-1.844828000	-1.941043000
H	2.058361000	-1.608855000	-1.995958000

H	0.423468000	-0.912268000	-1.962213000	H	-4.929880000	1.651962000	-6.381878000
H	0.718144000	-2.420563000	-2.832808000	C	-3.789120000	0.404629000	-7.724567000
C	-0.842645000	-2.980375000	-0.601812000	H	-4.623075000	-0.243700000	-7.969902000
H	-1.432940000	-2.061689000	-0.598372000	C	-2.533330000	0.192962000	-8.309424000
H	-1.144852000	-3.575573000	-1.469168000	H	-2.388273000	-0.623732000	-9.008542000
H	-1.077711000	-3.552957000	0.302550000	C	-1.462007000	1.032645000	-8.001445000
C	1.446970000	-4.009855000	-0.751936000	H	-0.493231000	0.862366000	-8.460032000
H	1.143953000	-4.550749000	-1.654215000	C	-0.813188000	4.331133000	-5.564361000
H	1.232110000	-4.647070000	0.112579000	H	-1.229880000	3.875754000	-4.664270000
H	2.528615000	-3.842814000	-0.800537000	H	-1.560637000	4.958302000	-6.055233000
C	1.580496000	3.229722000	-0.238300000	H	0.045806000	4.948923000	-5.293056000
C	2.579666000	3.756807000	0.608363000	**^{4}TS'$_{DOT}$**			
H	3.276008000	4.544868000	0.380719000	Co	-0.431189000	0.784684000	0.196896000
C	2.477147000	3.049182000	1.802542000	N	-1.231856000	1.260249000	2.024960000
H	3.043342000	3.124829000	2.716499000	N	-0.269280000	1.270728000	2.994884000
C	1.190196000	3.656064000	-1.640789000	N	0.700772000	-0.790610000	0.908605000
C	-0.206983000	4.325740000	-1.579308000	N	1.336939000	-0.448127000	2.069254000
H	-0.183225000	5.195371000	-0.913396000	N	1.142069000	2.116447000	0.397986000
H	-0.962177000	3.626037000	-1.212064000	N	1.724640000	1.997539000	1.628022000
H	-0.512793000	4.657459000	-2.575775000	B	1.216009000	0.971819000	2.671696000
C	1.157668000	2.432022000	-2.588218000	H	1.870285000	1.048247000	3.669512000
H	0.376610000	1.723680000	-2.305429000	C	-2.419572000	1.532230000	2.613161000
H	0.945027000	2.757964000	-3.611772000	C	-2.203130000	1.723786000	3.995070000
H	2.121443000	1.911811000	-2.583059000	H	-2.940781000	1.955381000	4.743414000
C	2.214949000	4.675798000	-2.181221000	C	-0.836269000	1.549370000	4.192765000
H	1.929462000	4.981668000	-3.193050000	H	-0.242495000	1.604113000	5.090577000
H	3.219931000	4.242266000	-2.226120000	C	-3.719604000	1.589297000	1.830975000
H	2.251817000	5.573359000	-1.554861000	C	-3.988480000	0.219328000	1.158514000
O	-1.634342000	0.169543000	-1.307859000	H	-4.035452000	-0.575207000	1.911448000
I	-2.808145000	0.721703000	-2.620443000	H	-3.213050000	-0.033778000	0.432142000
O	-2.155296000	2.268364000	-3.231180000	H	-4.946520000	0.247170000	0.627508000
C	-1.903611000	-0.569503000	-4.081918000	C	-3.629632000	2.693805000	0.748475000
C	-0.838447000	-0.001195000	-4.769906000	H	-2.793663000	2.506602000	0.068247000
H	-0.607193000	1.051364000	-4.659182000	H	-4.554518000	2.721223000	0.161182000
C	-0.071493000	-0.817345000	-5.613097000	H	-3.475738000	3.678327000	1.202886000
H	0.758934000	-0.381336000	-6.154447000	C	-4.887487000	1.922276000	2.783358000
C	-0.370568000	-2.175909000	-5.748305000	H	-5.822085000	1.969857000	2.215174000
H	0.234598000	-2.804747000	-6.389425000	H	-4.737565000	2.889368000	3.275534000
C	-1.450901000	-2.736523000	-5.054635000	H	-4.998171000	1.153284000	3.555317000
H	-1.675288000	-3.792421000	-5.141790000	C	1.047229000	-2.062198000	0.603375000
C	-2.227882000	-1.924239000	-4.222949000	C	1.927570000	-2.539012000	1.600793000
S	-3.596471000	-2.638172000	-3.317899000	H	2.383256000	-3.512255000	1.654334000
O	-3.882776000	-1.599749000	-2.249272000	C	2.084747000	-1.491339000	2.502456000
O	-3.241880000	-4.020415000	-2.909387000	H	2.669060000	-1.420762000	3.405438000
C	-5.081299000	-2.679692000	-4.448625000	C	0.520928000	-2.785260000	-0.623857000
C	-6.194330000	-3.336799000	-3.611020000	C	0.903909000	-2.003668000	-1.906299000
H	-5.930337000	-4.358158000	-3.326800000	H	1.989724000	-1.870833000	-1.971620000
H	-7.099982000	-3.370194000	-4.224193000	H	0.423653000	-1.023430000	-1.926882000
H	-6.410351000	-2.757545000	-2.709288000	H	0.569954000	-2.558758000	-2.789591000
C	-4.719603000	-3.521881000	-5.680735000	C	-1.019943000	-2.915075000	-0.533806000
H	-3.953644000	-3.039019000	-6.293637000	H	-1.499255000	-1.932957000	-0.544804000
H	-5.620871000	-3.625478000	-6.292831000	H	-1.400820000	-3.482373000	-1.388507000
H	-4.384128000	-4.523724000	-5.400197000	H	-1.309918000	-3.441193000	0.382971000
C	-5.421158000	-1.232350000	-4.821775000	C	1.140004000	-4.197556000	-0.696834000
H	-5.686338000	-0.641441000	-3.940919000	H	0.759571000	-4.716435000	-1.582689000
H	-6.288664000	-1.246803000	-5.488952000	H	0.876686000	-4.793261000	0.184011000
H	-4.604640000	-0.746719000	-5.362218000	H	2.232268000	-4.151395000	-0.770708000
S	-0.174445000	3.053415000	-6.701554000	C	1.815292000	3.066060000	-0.289973000
C	-1.627555000	2.093692000	-7.089721000	C	2.856874000	3.561267000	0.524597000
C	-2.886843000	2.309611000	-6.507871000	H	3.574552000	4.322612000	0.273119000
H	-3.040501000	3.112821000	-5.800826000	C	2.764092000	2.860817000	1.723730000
C	-3.958899000	1.468222000	-6.831091000	H	3.358675000	2.918497000	2.620820000

C	1.407694000	3.491932000	-1.688125000
C	0.035720000	4.211794000	-1.617993000
H	0.117487000	5.128348000	-1.023592000
H	-0.724639000	3.577917000	-1.152120000
H	-0.309652000	4.468751000	-2.623810000
C	1.321003000	2.259143000	-2.620101000
H	0.590582000	1.529449000	-2.262593000
H	1.015138000	2.575959000	-3.622359000
H	2.292534000	1.758278000	-2.689182000
C	2.452412000	4.471547000	-2.264236000
H	2.155177000	4.773762000	-3.273788000
H	3.441533000	4.004691000	-2.323337000
H	2.531312000	5.374736000	-1.650028000
O	-1.526642000	0.267052000	-1.276837000
I	-2.435211000	1.223785000	-2.680114000
O	-1.941472000	2.597760000	-3.945777000
C	-1.822363000	-0.336503000	-4.023500000
C	-0.728358000	-0.022030000	-4.828917000
H	-0.357066000	0.993432000	-4.857898000
C	-0.129772000	-1.026306000	-5.598209000
H	0.720645000	-0.780557000	-6.221390000
C	-0.617917000	-2.335318000	-5.551060000
H	-0.140786000	-3.117977000	-6.128029000
C	-1.729058000	-2.639633000	-4.760369000
H	-2.111727000	-3.651419000	-4.716124000
C	-2.349699000	-1.635509000	-4.002296000
S	-3.830728000	-2.103307000	-3.093135000
O	-4.067082000	-1.022360000	-2.081208000
O	-3.662688000	-3.511426000	-2.640305000
C	-5.248178000	-2.040055000	-4.308883000
C	-6.488493000	-2.421536000	-3.477761000
H	-6.398957000	-3.433196000	-3.074186000
H	-7.362361000	-2.386702000	-4.135659000
H	-6.646597000	-1.720745000	-2.654081000
C	-4.990530000	-3.053450000	-5.432371000
H	-4.132878000	-2.770302000	-6.048693000
H	-5.874022000	-3.075830000	-6.078411000
H	-4.833676000	-4.059441000	-5.035051000
C	-5.341939000	-0.607441000	-4.845374000
H	-5.507748000	0.111556000	-4.038474000
H	-6.190887000	-0.548762000	-5.533855000
H	-4.441590000	-0.334450000	-5.401168000
S	-2.585552000	3.502247000	-5.884253000
C	-2.204022000	2.175394000	-6.991870000
C	-3.106606000	1.154887000	-7.330486000
H	-4.126169000	1.173717000	-6.971343000
C	-2.688171000	0.106371000	-8.155528000
H	-3.388123000	-0.681865000	-8.409781000
C	-1.380318000	0.073839000	-8.651655000
H	-1.060585000	-0.742898000	-9.288505000
C	-0.486659000	1.104350000	-8.328563000
H	0.524811000	1.090646000	-8.718707000
C	-0.890818000	2.152332000	-7.501166000
H	-0.194924000	2.944590000	-7.246067000
C	-4.351728000	3.305675000	-5.537344000
H	-4.545566000	2.362378000	-5.021428000
H	-4.939119000	3.361851000	-6.455479000
H	-4.625938000	4.133167000	-4.880823000

^{4}PC'

Co	-0.402520000	0.699840000	0.279952000
N	-1.215519000	1.466350000	2.016347000
N	-0.283489000	1.487789000	3.014930000
N	0.518323000	-0.893181000	1.228903000
N	1.175992000	-0.467740000	2.350494000
N	1.298831000	1.867147000	0.386433000
N	1.810771000	1.863349000	1.653372000
B	1.173185000	1.017075000	2.783760000
H	1.803662000	1.147927000	3.791387000
C	-2.381384000	1.926528000	2.526886000
C	-2.181644000	2.247862000	3.887347000
H	-2.909084000	2.636642000	4.578272000
C	-0.847286000	1.956346000	4.153722000
H	-0.273937000	2.049483000	5.061559000
C	-3.645254000	2.057728000	1.694396000
C	-4.011238000	0.693243000	1.058271000
H	-4.184892000	-0.057270000	1.837119000
H	-3.223051000	0.320017000	0.399951000
H	-4.930654000	0.794443000	0.469631000
C	-3.433232000	3.125667000	0.589906000
H	-2.574041000	2.889220000	-0.046378000
H	-4.326592000	3.197440000	-0.041181000
H	-3.244400000	4.109357000	1.033142000
C	-4.815418000	2.514017000	2.592955000
H	-5.725823000	2.605625000	1.991777000
H	-4.610927000	3.487860000	3.050470000
H	-5.005130000	1.788220000	3.390752000
C	0.750549000	-2.218733000	1.089229000
C	1.579998000	-2.644027000	2.152004000
H	1.944309000	-3.640164000	2.332836000
C	1.825117000	-1.511428000	2.920824000
H	2.406191000	-1.381775000	3.819356000
C	0.143897000	-3.047959000	-0.028874000
C	0.568356000	-2.492731000	-1.412396000
H	1.659163000	-2.508669000	-1.519416000
H	0.211706000	-1.470416000	-1.555368000
H	0.128601000	-3.111026000	-2.202711000
C	-1.400709000	-3.016763000	0.093081000
H	-1.785303000	-2.006289000	-0.058907000
H	-1.844021000	-3.656773000	-0.675575000
H	-1.714221000	-3.379867000	1.078830000
C	0.628039000	-4.509119000	0.089067000
H	0.189516000	-5.103254000	-0.719127000
H	0.322038000	-4.954414000	1.042187000
H	1.718936000	-4.576241000	0.009240000
C	2.117385000	2.614707000	-0.388268000
C	3.175333000	3.102000000	0.409983000
H	3.993825000	3.726363000	0.096819000
C	2.945011000	2.602552000	1.688270000
H	3.505655000	2.718983000	2.601375000
C	1.853337000	2.844607000	-1.864702000
C	0.594481000	3.734256000	-2.029170000
H	0.761874000	4.721795000	-1.585673000
H	-0.275033000	3.286937000	-1.540079000
H	0.359688000	3.867647000	-3.091671000
C	1.649012000	1.488941000	-2.584727000
H	0.747822000	0.972544000	-2.243630000
H	1.552641000	1.652960000	-3.662859000
H	2.505246000	0.827666000	-2.414071000
C	3.059590000	3.565634000	-2.504086000
H	2.866585000	3.730348000	-3.569239000
H	3.972512000	2.967815000	-2.409885000
H	3.233699000	4.540748000	-2.037144000
O	-1.472410000	0.128200000	-1.193280000
I	-2.426467000	1.181378000	-2.480496000

O	-3.216925000	2.955441000	-4.134739000
C	-1.687014000	0.092819000	-4.148574000
C	-0.831452000	0.807585000	-4.994726000
H	-0.701049000	1.871972000	-4.855507000
C	-0.141938000	0.141729000	-6.012123000
H	0.513233000	0.703008000	-6.665875000
C	-0.283155000	-1.239486000	-6.163968000
H	0.274282000	-1.766332000	-6.928742000
C	-1.148372000	-1.949057000	-5.328381000
H	-1.257021000	-3.020094000	-5.438648000
C	-1.881519000	-1.287807000	-4.329728000
S	-3.056984000	-2.331390000	-3.422890000
O	-3.468647000	-1.631680000	-2.174816000
O	-2.437936000	-3.685710000	-3.342073000
C	-4.583185000	-2.438709000	-4.495303000
C	-5.508229000	-3.424419000	-3.755375000
H	-5.059766000	-4.419185000	-3.697557000
H	-6.446338000	-3.497064000	-4.314572000
H	-5.734223000	-3.075056000	-2.744632000
C	-4.211448000	-2.964074000	-5.887777000
H	-3.587344000	-2.257553000	-6.440827000
H	-5.136846000	-3.110738000	-6.454282000
H	-3.696378000	-3.926474000	-5.826618000
C	-5.186322000	-1.030299000	-4.552390000
H	-5.489246000	-0.685413000	-3.561411000
H	-6.066792000	-1.049992000	-5.202803000
H	-4.468930000	-0.319082000	-4.968518000
S	-3.911182000	3.374168000	-5.453208000
C	-3.197827000	2.420862000	-6.808837000
C	-3.659199000	1.167220000	-7.230318000
H	-4.539834000	0.718034000	-6.793697000
C	-2.983680000	0.493369000	-8.251970000
H	-3.341144000	-0.475682000	-8.581273000
C	-1.856308000	1.068897000	-8.850617000
H	-1.336429000	0.541612000	-9.642366000
C	-1.404288000	2.326687000	-8.434145000
H	-0.538168000	2.778720000	-8.903530000
C	-2.073912000	3.005972000	-7.412520000
H	-1.728273000	3.982500000	-7.089407000
C	-5.596930000	2.702083000	-5.386690000
H	-5.585888000	1.648692000	-5.106253000
H	-6.083953000	2.845212000	-6.353538000
H	-6.123785000	3.272639000	-4.619900000

3. Complex 1 in the C-H bond activation of 9,10-dihydroanthracene

^{4}RC1

Co	-0.399906000	0.249389000	0.017863000	H	1.187337000	1.105522000	-3.413377000
N	-0.449713000	0.511172000	2.076485000	C	1.900123000	3.815596000	-3.197595000
N	0.804268000	0.369818000	2.602392000	H	1.345272000	4.189116000	-4.064393000
N	0.826598000	-1.430084000	0.095855000	H	2.739709000	3.212952000	-3.560838000
N	1.868314000	-1.215970000	0.957466000	H	2.301085000	4.679383000	-2.657048000
N	1.228633000	1.509294000	-0.269881000	O	-1.997959000	-0.214182000	-1.059952000
N	2.182294000	1.259758000	0.681262000	I	-3.554144000	0.712346000	-1.478397000
B	2.041608000	0.118036000	1.715708000	O	-3.031356000	2.422718000	-1.405784000
H	3.021987000	0.071186000	2.398300000	C	-3.312617000	0.510055000	-3.617008000
C	-1.303326000	0.721772000	3.108468000	C	-2.853819000	1.660462000	-4.250697000
C	-0.571023000	0.708743000	4.313527000	H	-2.744834000	2.579850000	-3.686194000
H	-0.954952000	0.846892000	5.309004000	C	-2.496360000	1.593534000	-5.605348000
C	0.752849000	0.484884000	3.949459000	H	-2.146504000	2.486835000	-6.108550000
H	1.644625000	0.403647000	4.549055000	C	-2.558004000	0.377120000	-6.290607000
C	-2.783517000	0.975811000	2.906826000	H	-2.247589000	0.319151000	-7.326530000
C	-3.428046000	-0.208784000	2.145923000	C	-3.015731000	-0.777418000	-5.643203000
H	-3.377044000	-1.123172000	2.746845000	H	-3.038085000	-1.722619000	-6.169808000
H	-2.915924000	-0.412697000	1.202059000	C	-3.429699000	-0.702230000	-4.309014000
H	-4.481742000	0.004967000	1.936974000	S	-4.089001000	-2.157748000	-3.493236000
C	-2.958262000	2.299735000	2.121327000	O	-4.381164000	-1.651870000	-2.094195000
H	-2.470881000	2.269103000	1.144145000	O	-3.157416000	-3.301721000	-3.665573000
H	-4.020202000	2.506160000	1.967054000	C	-5.731728000	-2.601140000	-4.283996000
H	-2.524573000	3.133637000	2.683825000	C	-6.354942000	-3.616436000	-3.305342000
C	-3.487259000	1.120153000	4.273302000	H	-5.725817000	-4.503975000	-3.196565000
H	-4.557122000	1.293954000	4.117431000	H	-7.319438000	-3.927735000	-3.717742000
H	-3.085506000	1.966882000	4.839663000	H	-6.524008000	-3.173763000	-2.321395000
H	-3.373710000	0.212890000	4.876043000	C	-5.459162000	-3.239289000	-5.653500000
C	0.993116000	-2.658858000	-0.451750000	H	-5.093322000	-2.509960000	-6.379994000
C	2.168560000	-3.233608000	0.079610000	H	-6.408475000	-3.631656000	-6.031704000
H	2.577561000	-4.202121000	-0.148439000	H	-4.751261000	-4.067602000	-5.579824000
C	2.689267000	-2.291990000	0.960136000	C	-6.573565000	-1.327574000	-4.399150000
H	3.573070000	-2.315791000	1.576560000	H	-6.738020000	-0.876592000	-3.421913000
C	0.025141000	-3.260466000	-1.452848000	H	-7.547852000	-1.599746000	-4.816919000
C	-0.081527000	-2.349112000	-2.702519000	H	-6.115629000	-0.590559000	-5.064765000
H	0.907422000	-2.197090000	-3.150122000	C	-5.799934000	3.812038000	-2.633575000
H	-0.507187000	-1.375515000	-2.451410000	H	-4.716841000	3.721276000	-2.813610000
H	-0.737427000	-2.817181000	-3.441521000	H	-6.294184000	3.663472000	-3.598728000
C	-1.362609000	-3.437227000	-0.784616000	C	-6.084687000	5.198500000	-2.090762000
H	-1.780840000	-2.474227000	-0.484708000	C	-6.512450000	6.242222000	-2.920912000
H	-2.056003000	-3.899413000	-1.492173000	H	-6.661673000	6.055124000	-3.980322000
H	-1.277643000	-4.079098000	0.099959000	C	-6.749417000	7.517202000	-2.394851000
C	0.537173000	-4.646997000	-1.901131000	H	-7.080324000	8.319244000	-3.046166000
H	-0.165725000	-5.075796000	-2.622430000	C	-6.567538000	7.750654000	-1.026674000
H	0.616809000	-5.336301000	-1.053373000	H	-6.756513000	8.734856000	-0.611224000
H	1.518670000	-4.573948000	-2.382689000	C	-6.150251000	6.708120000	-0.191507000
C	1.725600000	2.447469000	-1.111000000	H	-6.017993000	6.883704000	0.872017000
C	3.019167000	2.807744000	-0.675383000	C	-5.901916000	5.432766000	-0.714606000
H	3.679937000	3.527307000	-1.125841000	C	-5.436024000	4.286549000	0.161628000
C	3.269105000	2.033481000	0.451526000	H	-4.340157000	4.198717000	0.089018000
H	4.135704000	1.977282000	1.089762000	H	-5.666118000	4.486757000	1.212542000
C	0.956699000	2.981405000	-2.303615000	C	-6.037006000	2.967948000	-0.274086000
C	-0.198692000	3.885485000	-1.805979000	C	-6.413765000	1.979680000	0.645330000
H	0.197518000	4.729248000	-1.230105000	H	-6.305844000	2.171379000	1.707851000
H	-0.897308000	3.325068000	-1.181228000	C	-6.944522000	0.756680000	0.211139000
H	-0.757475000	4.284376000	-2.660891000	H	-7.236158000	0.005013000	0.935975000
C	0.393072000	1.808146000	-3.139477000	C	-7.114003000	0.520302000	-1.155727000
H	-0.381504000	1.259450000	-2.598746000	H	-7.543129000	-0.416039000	-1.492838000
H	-0.057112000	2.193282000	-4.059429000	C	-6.743839000	1.505805000	-2.084574000

H	-6.895596000	1.341453000	-3.146349000	C	1.375595000	4.129147000	-2.992086000
C	-6.207173000	2.730902000	-1.655556000	H	0.787112000	4.504295000	-3.835756000
^{4}TS1				H	2.313809000	3.721223000	-3.383416000
Co	-0.533200000	0.067139000	-0.190131000	H	1.610956000	4.977393000	-2.340539000
N	-0.726529000	0.303625000	1.860961000	O	-1.930744000	-0.233104000	-1.477105000
N	0.493970000	0.258075000	2.473327000	I	-3.554227000	0.803419000	-1.771191000
N	0.789697000	-1.516225000	-0.005277000	O	-4.034983000	2.628699000	-2.159072000
N	1.778090000	-1.229929000	0.895383000	C	-3.366622000	0.374867000	-3.865491000
N	0.985391000	1.466901000	-0.324540000	C	-3.022512000	1.465582000	-4.664655000
N	1.919832000	1.271304000	0.653409000	H	-3.040368000	2.462799000	-4.243628000
B	1.808000000	0.106965000	1.667521000	C	-2.632109000	1.247770000	-5.992670000
H	2.743006000	0.128053000	2.412603000	H	-2.360682000	2.094439000	-6.611866000
C	-1.667128000	0.434619000	2.825865000	C	-2.556392000	-0.051933000	-6.500172000
C	-1.026114000	0.469044000	4.082277000	H	-2.213719000	-0.225055000	-7.512886000
H	-1.490654000	0.566162000	5.048051000	C	-2.931378000	-1.137863000	-5.702397000
C	0.335147000	0.354947000	3.814557000	H	-2.877783000	-2.145460000	-6.093733000
H	1.184261000	0.338538000	4.478095000	C	-3.374549000	-0.926233000	-4.389534000
C	-3.142639000	0.573022000	2.501685000	S	-4.011024000	-2.350409000	-3.492223000
C	-3.620959000	-0.624850000	1.643875000	O	-4.279618000	-1.865066000	-2.096357000
H	-3.518694000	-1.560032000	2.204653000	O	-3.091634000	-3.498582000	-3.718335000
H	-3.043265000	-0.732838000	0.722684000	C	-5.672738000	-2.783945000	-4.241537000
H	-4.676428000	-0.496922000	1.378015000	C	-6.195286000	-3.926293000	-3.346177000
C	-3.363262000	1.910799000	1.747995000	H	-5.532469000	-4.794632000	-3.383256000
H	-2.677929000	2.016725000	0.901205000	H	-7.178688000	-4.225426000	-3.721660000
H	-4.394013000	1.973893000	1.387117000	H	-6.303597000	-3.602207000	-2.308317000
H	-3.177125000	2.760695000	2.413878000	C	-5.478624000	-3.258170000	-5.687338000
C	-3.974472000	0.602608000	3.801797000	H	-5.186514000	-2.440909000	-6.350951000
H	-5.036111000	0.707741000	3.554733000	H	-6.437457000	-3.647860000	-6.044115000
H	-3.688752000	1.446767000	4.438019000	H	-4.740528000	-4.061640000	-5.750927000
H	-3.846838000	-0.322798000	4.373268000	C	-6.569218000	-1.545742000	-4.153032000
C	1.040814000	-2.741818000	-0.519591000	H	-6.688802000	-1.232596000	-3.115681000
C	2.222056000	-3.244844000	0.070713000	H	-7.555669000	-1.801686000	-4.552262000
H	2.690192000	-4.194584000	-0.120412000	H	-6.174052000	-0.710277000	-4.739320000
C	2.653641000	-2.261760000	0.954861000	C	-6.456086000	3.361477000	-2.322828000
H	3.508068000	-2.229584000	1.611155000	H	-5.210661000	3.082077000	-2.403767000
C	0.130260000	-3.403678000	-1.536198000	H	-6.779223000	3.120440000	-3.338546000
C	0.048110000	-2.541287000	-2.822037000	C	-6.541704000	4.785576000	-1.968837000
H	1.047181000	-2.388448000	-3.246579000	C	-6.647409000	5.774045000	-2.968614000
H	-0.404199000	-1.567430000	-2.616959000	H	-6.669237000	5.471515000	-4.010939000
H	-0.579307000	-3.047001000	-3.561645000	C	-6.734211000	7.121268000	-2.625660000
C	-1.281777000	-3.577301000	-0.920521000	H	-6.822387000	7.875349000	-3.399624000
H	-1.748421000	-2.607509000	-0.730062000	C	-6.714593000	7.497272000	-1.273651000
H	-1.924572000	-4.119877000	-1.618004000	H	-6.787971000	8.544157000	-1.000311000
H	-1.222788000	-4.136210000	0.020637000	C	-6.604662000	6.523319000	-0.275259000
C	0.689828000	-4.794566000	-1.904583000	H	-6.592890000	6.818645000	0.769214000
H	0.029268000	-5.269310000	-2.637039000	C	-6.509279000	5.167132000	-0.606012000
H	0.748124000	-5.446293000	-1.025710000	C	-6.334729000	4.116729000	0.466994000
H	1.689819000	-4.717891000	-2.346108000	H	-5.262340000	4.065833000	0.725556000
C	1.381944000	2.524027000	-1.070447000	H	-6.840978000	4.427851000	1.387552000
C	2.601477000	3.010785000	-0.551221000	C	-6.785330000	2.730046000	0.067653000
H	3.180462000	3.840278000	-0.917892000	C	-7.097880000	1.765635000	1.030636000
C	2.904807000	2.192754000	0.532702000	H	-7.069983000	2.034859000	2.081825000
H	3.742544000	2.203770000	1.210712000	C	-7.443420000	0.458615000	0.657372000
C	0.569275000	3.048932000	-2.239614000	H	-7.681563000	-0.273862000	1.420482000
C	-0.740790000	3.683735000	-1.707216000	C	-7.488733000	0.103672000	-0.696008000
H	-0.518379000	4.542091000	-1.063754000	H	-7.760205000	-0.904899000	-0.986852000
H	-1.323487000	2.966985000	-1.122929000	C	-7.187995000	1.059493000	-1.669185000
H	-1.364981000	4.024890000	-2.539976000	H	-7.243346000	0.810603000	-2.722869000
C	0.239538000	1.898460000	-3.221767000	C	-6.847721000	2.378142000	-1.302462000
H	-0.409429000	1.146810000	-2.765569000	**^{4}PC1**			
H	-0.277055000	2.300135000	-4.099935000	Co	-0.525055000	0.418286000	-0.103776000
H	1.156420000	1.403425000	-3.559790000	N	-0.534229000	0.305600000	1.969402000

N	0.746129000	0.305263000	2.451283000	I	-3.363165000	1.119574000	-2.179121000
N	0.909503000	-1.064107000	-0.296496000	O	-4.717652000	2.334161000	-4.115957000
N	1.947770000	-0.850957000	0.567035000	C	-2.990177000	-0.190847000	-3.824912000
N	0.895990000	1.942403000	-0.179376000	C	-2.178961000	0.351879000	-4.830836000
N	1.927516000	1.662553000	0.673926000	H	-1.781014000	1.353207000	-4.728122000
B	1.975190000	0.366732000	1.517847000	C	-1.873096000	-0.405829000	-5.967228000
H	2.977723000	0.349582000	2.169298000	H	-1.248708000	0.023253000	-6.741658000
C	-1.371882000	0.190758000	3.027971000	C	-2.349162000	-1.713752000	-6.083697000
C	-0.599109000	0.115050000	4.208150000	H	-2.094735000	-2.314529000	-6.948296000
H	-0.960939000	0.020620000	5.216828000	C	-3.149123000	-2.258803000	-5.074850000
C	0.727774000	0.188848000	3.800041000	H	-3.498572000	-3.280724000	-5.146287000
H	1.642675000	0.166334000	4.369282000	C	-3.495467000	-1.496646000	-3.949355000
C	-2.884617000	0.179771000	2.897823000	S	-4.596886000	-2.316866000	-2.763939000
C	-3.342384000	-0.992968000	1.994784000	O	-4.450856000	-1.622968000	-1.451784000
H	-2.978921000	-1.948250000	2.390139000	O	-4.298667000	-3.775226000	-2.854516000
H	-2.990406000	-0.869744000	0.968516000	C	-6.335512000	-2.040342000	-3.386395000
H	-4.438206000	-1.030767000	1.967722000	C	-7.232853000	-2.701915000	-2.322214000
C	-3.357198000	1.525464000	2.292012000	H	-7.034643000	-3.774305000	-2.248379000
H	-2.988489000	1.640634000	1.269932000	H	-8.275767000	-2.559903000	-2.621718000
H	-4.452552000	1.552663000	2.274230000	H	-7.091684000	-2.239211000	-1.343327000
H	-3.005804000	2.369797000	2.895407000	C	-6.488933000	-2.720798000	-4.752796000
C	-3.521025000	0.014201000	4.295064000	H	-5.866319000	-2.247911000	-5.517473000
H	-4.611625000	0.006490000	4.199440000	H	-7.533670000	-2.622350000	-5.064953000
H	-3.244020000	0.838232000	4.961709000	H	-6.245988000	-3.784721000	-4.698722000
H	-3.214244000	-0.928226000	4.761500000	C	-6.576176000	-0.530538000	-3.464690000
C	1.163588000	-2.209753000	-0.970292000	H	-6.425593000	-0.051937000	-2.496387000
C	2.394853000	-2.735347000	-0.522041000	H	-7.613707000	-0.358810000	-3.762991000
H	2.877769000	-3.636699000	-0.856706000	H	-5.929076000	-0.058071000	-4.207079000
C	2.854622000	-1.848890000	0.446484000	C	-7.614424000	3.335699000	-2.456741000
H	3.749409000	-1.862854000	1.047159000	H	-4.915239000	1.914284000	-4.968788000
C	0.229836000	-2.753123000	-2.032542000	H	-8.324873000	3.528541000	-3.255721000
C	0.222495000	-1.790682000	-3.246343000	C	-6.530479000	4.213721000	-2.277590000
H	1.227712000	-1.697190000	-3.672132000	C	-6.310052000	5.344392000	-3.131379000
H	-0.119431000	-0.792228000	-2.960582000	H	-7.009731000	5.526187000	-3.941153000
H	-0.446715000	-2.173477000	-4.022194000	C	-5.239993000	6.181394000	-2.927209000
C	-1.199902000	-2.896514000	-1.460122000	H	-5.083530000	7.034603000	-3.577925000
H	-1.645085000	-1.928249000	-1.216772000	C	-4.326569000	5.944115000	-1.853872000
H	-1.846283000	-3.391099000	-2.190699000	H	-3.491512000	6.620239000	-1.707615000
H	-1.191542000	-3.507662000	-0.550620000	C	-4.503452000	4.873172000	-1.011518000
C	0.721308000	-4.139280000	-2.501498000	H	-3.815113000	4.692069000	-0.192417000
H	0.041227000	-4.527629000	-3.266602000	C	-5.599383000	3.969932000	-1.193212000
H	0.743303000	-4.852860000	-1.670791000	C	-5.793908000	2.855951000	-0.361942000
H	1.724945000	-4.081792000	-2.936608000	H	-5.565755000	2.691692000	-3.792520000
C	1.185332000	3.111767000	-0.799611000	H	-5.099365000	2.678994000	0.452630000
C	2.429248000	3.581615000	-0.327234000	C	-6.872132000	1.975097000	-0.545623000
H	2.937494000	4.483864000	-0.619091000	C	-7.066377000	0.826019000	0.285418000
C	2.862887000	2.638158000	0.598143000	H	-6.343249000	0.622328000	1.068127000
H	3.758324000	2.597899000	1.196467000	C	-8.147647000	-0.001990000	0.098086000
C	0.263396000	3.750913000	-1.821176000	H	-8.288055000	-0.867411000	0.736245000
C	-1.119286000	4.016475000	-1.179856000	C	-9.098946000	0.269456000	-0.932374000
H	-1.030799000	4.750991000	-0.371692000	H	-9.948814000	-0.392368000	-1.056869000
H	-1.549579000	3.106843000	-0.753391000	C	-8.937361000	1.351875000	-1.763557000
H	-1.814347000	4.408679000	-1.928104000	H	-9.653222000	1.555495000	-2.553622000
C	0.122392000	2.827514000	-3.058002000	C	-7.819712000	2.232956000	-1.609955000
H	-0.279106000	1.846286000	-2.794012000	**^{4}TS1$_{-oh}$**			
H	-0.550833000	3.289387000	-3.789653000	Co	-0.533237000	0.064359000	-0.191541000
H	1.096722000	2.672786000	-3.533728000	N	-0.725474000	0.301049000	1.859781000
C	0.851510000	5.099643000	-2.289933000	N	0.495240000	0.253992000	2.471617000
H	0.174470000	5.562112000	-3.015655000	N	0.788106000	-1.520380000	-0.007462000
H	1.825117000	4.962807000	-2.772315000	N	1.776993000	-1.235438000	0.893082000
H	0.974011000	5.791130000	-1.449753000	N	0.987137000	1.462151000	-0.326502000
O	-2.340707000	0.391930000	-0.755001000	N	1.921633000	1.265583000	0.651180000

B	1.808773000	0.101376000	1.665304000	C	-2.634268000	1.252500000	-5.991461000
H	2.744075000	0.121303000	2.410047000	H	-2.362543000	2.099458000	-6.610134000
C	-1.665497000	0.432816000	2.825157000	C	-2.559546000	-0.046873000	-6.499947000
C	-1.023890000	0.466245000	4.081290000	H	-2.217347000	-0.219467000	-7.512911000
H	-1.487895000	0.563655000	5.047291000	C	-2.934919000	-1.133154000	-5.702829000
C	0.337121000	0.350704000	3.812940000	H	-2.882080000	-2.140489000	-6.094935000
H	1.186510000	0.333195000	4.476097000	C	-3.377500000	-0.922212000	-4.389657000
C	-3.141015000	0.572919000	2.501742000	S	-4.014572000	-2.346630000	-3.493140000
C	-3.621130000	-0.624377000	1.644115000	O	-4.282855000	-1.861952000	-2.096979000
H	-3.519835000	-1.559653000	2.204915000	O	-3.095735000	-3.495102000	-3.719949000
H	-3.043902000	-0.733180000	0.722727000	C	-5.676524000	-2.779093000	-4.242587000
H	-4.676533000	-0.495159000	1.378633000	C	-6.199411000	-3.921757000	-3.347827000
C	-3.360487000	1.911053000	1.748349000	H	-5.536910000	-4.790312000	-3.385447000
H	-2.675428000	2.016319000	0.901257000	H	-7.182950000	-4.220324000	-3.723401000
H	-4.391356000	1.975449000	1.388021000	H	-6.307524000	-3.598217000	-2.309775000
H	-3.173005000	2.760626000	2.414267000	C	-5.482711000	-3.252609000	-5.688666000
C	-3.972170000	0.603331000	3.802273000	H	-5.190383000	-2.435099000	-6.351874000
H	-5.033808000	0.709691000	3.555733000	H	-6.441721000	-3.641760000	-6.045551000
H	-3.685181000	1.447112000	4.438425000	H	-4.744914000	-4.056314000	-5.752758000
H	-3.845311000	-0.322268000	4.373601000	C	-6.572589000	-1.540643000	-4.153380000
C	1.037647000	-2.746177000	-0.522047000	H	-6.692272000	-1.228192000	-3.115834000
C	2.218378000	-3.250741000	0.067973000	H	-7.559050000	-1.795974000	-4.552974000
H	2.685351000	-4.200999000	-0.123420000	H	-6.177030000	-0.704899000	-4.739006000
C	2.651303000	-2.268340000	0.952223000	C	-6.454537000	3.365523000	-2.318543000
H	3.505896000	-2.237301000	1.608355000	H	-5.209244000	3.085846000	-2.399912000
C	0.126229000	-3.406707000	-1.538759000	H	-6.777898000	3.124892000	-3.334291000
C	0.044768000	-2.543740000	-2.824255000	C	-6.539882000	4.789515000	-1.964069000
H	1.043955000	-2.391544000	-3.248754000	C	-6.645318000	5.778317000	-2.963548000
H	-0.406747000	-1.569591000	-2.618812000	H	-6.667142000	5.476107000	-4.005966000
H	-0.583106000	-3.048612000	-3.564040000	C	-6.731850000	7.125452000	-2.620193000
C	-1.285918000	-3.579175000	-0.923004000	H	-6.819815000	7.879787000	-3.393933000
H	-1.751734000	-2.609018000	-0.732362000	C	-6.712235000	7.501035000	-1.268067000
H	-1.929242000	-4.121052000	-1.620546000	H	-6.785402000	8.547851000	-0.994408000
H	-1.227372000	-4.138297000	0.018055000	C	-6.602586000	6.526749000	-0.269971000
C	0.684352000	-4.798017000	-1.907760000	H	-6.590835000	6.821753000	0.774594000
H	0.023244000	-5.271797000	-2.640345000	C	-6.507474000	5.170637000	-0.601125000
H	0.742067000	-5.450157000	-1.029156000	C	-6.333319000	4.119903000	0.471631000
H	1.684380000	-4.722175000	-2.349343000	H	-5.261048000	4.068966000	0.730668000
C	1.384810000	2.518565000	-1.072810000	H	-6.839978000	4.430763000	1.392057000
C	2.605136000	3.003887000	-0.554095000	C	-6.783761000	2.733318000	0.071756000
H	3.185066000	3.832548000	-0.921151000	C	-7.096239000	1.768543000	1.034391000
C	2.907769000	2.185723000	0.529924000	H	-7.068328000	2.037392000	2.085676000
H	3.745750000	2.195808000	1.207648000	C	-7.441721000	0.461630000	0.660676000
C	0.572523000	3.044100000	-2.241960000	H	-7.679815000	-0.271119000	1.423539000
C	-0.736686000	3.680626000	-1.709533000	C	-7.487020000	0.107147000	-0.692816000
H	-0.513174000	4.538793000	-1.066202000	H	-7.758417000	-0.901347000	-0.983997000
H	-1.320251000	2.964676000	-1.125130000	C	-7.186328000	1.063327000	-1.665657000
H	-1.360501000	4.022476000	-2.542297000	H	-7.241687000	0.814834000	-2.719430000
C	0.241171000	1.893723000	-3.223692000	C	-6.846156000	2.381886000	-1.298482000
H	-0.408882000	1.143183000	-2.767204000	**^{4}PC1$_{\text{-oh}}$**			
H	-0.274881000	2.295804000	-4.101992000	Co	-0.691682000	0.184114000	-0.033819000
H	1.157350000	1.397282000	-3.561555000	N	-0.731040000	-0.040804000	2.007309000
C	1.380012000	4.123103000	-2.994919000	N	0.533872000	-0.059472000	2.521930000
H	0.791827000	4.498701000	-3.838595000	N	0.840706000	-1.162106000	-0.355017000
H	2.317654000	3.713916000	-3.386298000	N	1.840589000	-0.976814000	0.559793000
H	1.616530000	4.971263000	-2.343679000	N	0.617091000	1.788510000	0.039679000
O	-1.931933000	-0.232972000	-1.477800000	N	1.651759000	1.509914000	0.889701000
I	-3.554526000	0.805479000	-1.769842000	B	1.774092000	0.146484000	1.620767000
O	-4.033699000	2.631481000	-2.156052000	H	2.766272000	0.134589000	2.287883000
C	-3.368485000	0.378489000	-3.864632000	C	-1.599733000	-0.224258000	3.028088000
C	-3.023983000	1.469573000	-4.663120000	C	-0.862845000	-0.365456000	4.224392000
H	-3.040955000	2.466480000	-4.241328000	H	-1.253651000	-0.523378000	5.214448000

C	0.476367000	-0.254531000	3.860968000	C	-3.404149000	-0.134929000	-3.706835000
H	1.373428000	-0.298048000	4.456836000	C	-2.763648000	0.746103000	-4.588047000
C	-3.103185000	-0.248687000	2.820929000	H	-2.540004000	1.759458000	-4.279869000
C	-3.499883000	-1.454978000	1.930936000	C	-2.382756000	0.306815000	-5.860917000
H	-3.153467000	-2.393548000	2.377541000	H	-1.886129000	0.994161000	-6.535217000
H	-3.081343000	-1.365704000	0.925702000	C	-2.620008000	-1.015555000	-6.242377000
H	-4.591818000	-1.500953000	1.841182000	H	-2.306595000	-1.369647000	-7.216807000
C	-3.552625000	1.067063000	2.140402000	C	-3.255142000	-1.893465000	-5.359928000
H	-3.024001000	1.214343000	1.194248000	H	-3.420429000	-2.925464000	-5.640727000
H	-4.626419000	1.035508000	1.933909000	C	-3.669766000	-1.459527000	-4.091272000
H	-3.344750000	1.932818000	2.778768000	S	-4.508285000	-2.718334000	-3.084215000
C	-3.816715000	-0.372039000	4.183803000	O	-4.379783000	-2.332361000	-1.649679000
H	-4.900932000	-0.364759000	4.031341000	O	-3.960019000	-4.029230000	-3.537523000
H	-3.558703000	0.461641000	4.846017000	C	-6.317901000	-2.663631000	-3.544409000
H	-3.551414000	-1.308893000	4.685461000	C	-6.945816000	-3.830371000	-2.755866000
C	1.224570000	-2.151617000	-1.194739000	H	-6.521157000	-4.790204000	-3.059355000
C	2.501784000	-2.607471000	-0.797406000	H	-8.019795000	-3.841889000	-2.966711000
H	3.084348000	-3.388011000	-1.254534000	H	-6.807073000	-3.701863000	-1.679096000
C	2.853563000	-1.839995000	0.307875000	C	-6.453882000	-2.876145000	-5.058276000
H	3.741383000	-1.850098000	0.918944000	H	-6.028976000	-2.045356000	-5.628171000
C	0.361902000	-2.640069000	-2.344857000	H	-7.520510000	-2.935092000	-5.297794000
C	0.019067000	-1.462032000	-3.290814000	H	-5.982251000	-3.809735000	-5.375650000
H	0.928639000	-0.963611000	-3.643848000	C	-6.887857000	-1.314351000	-3.097251000
H	-0.614512000	-0.729767000	-2.786986000	H	-6.772908000	-1.169185000	-2.020902000
H	-0.530260000	-1.835916000	-4.161359000	H	-7.958064000	-1.303403000	-3.330190000
C	-0.947535000	-3.255922000	-1.792495000	H	-6.425043000	-0.470483000	-3.614496000
H	-1.552017000	-2.502619000	-1.282244000	C	-6.413777000	2.872614000	-2.773324000
H	-1.543460000	-3.666077000	-2.614255000	H	-5.170797000	2.047443000	-4.130098000
H	-0.725421000	-4.069392000	-1.092280000	H	-7.277594000	2.885733000	-3.446199000
C	1.127785000	-3.715375000	-3.144945000	C	-5.665495000	4.174723000	-2.860978000
H	0.504866000	-4.063223000	-3.975348000	C	-5.533479000	4.797775000	-4.114842000
H	1.369318000	-4.580548000	-2.518034000	H	-6.022655000	4.360942000	-4.981674000
H	2.060112000	-3.316467000	-3.560106000	C	-4.796613000	5.974040000	-4.253203000
C	0.821755000	3.025677000	-0.467691000	H	-4.701120000	6.446774000	-5.224214000
C	2.017241000	3.545858000	0.074224000	C	-4.196233000	6.548183000	-3.124081000
H	2.460299000	4.505526000	-0.126956000	H	-3.630451000	7.468735000	-3.216906000
C	2.508289000	2.558427000	0.922546000	C	-4.340504000	5.943102000	-1.874245000
H	3.395366000	2.532911000	1.534090000	H	-3.888180000	6.397516000	-0.998196000
C	-0.142134000	3.678735000	-1.440936000	C	-5.066438000	4.749106000	-1.727430000
C	-1.502827000	3.921724000	-0.744047000	C	-5.182372000	4.105809000	-0.365748000
H	-1.384937000	4.589063000	0.116504000	H	-4.206584000	3.674319000	-0.094241000
H	-1.939039000	2.985067000	-0.386730000	H	-5.366481000	4.880469000	0.388880000
H	-2.203937000	4.381529000	-1.446999000	C	-6.243578000	3.035549000	-0.251619000
C	-0.345560000	2.775669000	-2.681306000	C	-6.644783000	2.588055000	1.018783000
H	-0.805804000	1.820754000	-2.414467000	H	-6.197843000	3.034803000	1.901212000
H	-1.001103000	3.281957000	-3.399304000	C	-7.605131000	1.584793000	1.157319000
H	0.609408000	2.565729000	-3.174033000	H	-7.897989000	1.249715000	2.146355000
C	0.422120000	5.038323000	-1.906377000	C	-8.201017000	1.023691000	0.018499000
H	-0.279809000	5.506843000	-2.604049000	H	-8.957021000	0.253190000	0.119374000
H	1.382877000	4.914875000	-2.417369000	C	-7.823706000	1.474752000	-1.245615000
H	0.564035000	5.718992000	-1.060400000	H	-8.286701000	1.057433000	-2.133388000
O	-2.294795000	-0.296357000	-0.961858000	C	-6.840712000	2.468388000	-1.390198000
I	-3.752632000	0.634971000	-1.753745000				
O	-5.549592000	1.758743000	-3.279924000				

4. Thioanisole sulfoxidation by $^{s}PhIO_2$

RC_0			
I	-6.276369000	-1.115599000	-0.602969000
O	-4.813337000	-1.672909000	0.274234000
O	-6.206895000	0.683714000	-0.640495000
S	-6.756494000	-3.920790000	-2.770229000
C	-5.712612000	-1.350361000	-2.701553000
C	-5.074801000	-0.239631000	-3.251089000
H	-4.931599000	0.645761000	-2.639831000
C	-4.649624000	-0.283856000	-4.585139000
H	-4.145342000	0.574037000	-5.014476000
C	-4.872767000	-1.427414000	-5.360793000
H	-4.538468000	-1.460572000	-6.390749000
C	-5.520378000	-2.536905000	-4.809712000
H	-5.673112000	-3.434536000	-5.396161000
C	-5.941074000	-2.492249000	-3.474961000
O	-6.701938000	-3.698677000	-1.280233000
O	-6.157811000	-5.157566000	-3.342300000
C	-8.553971000	-3.822674000	-3.260111000
C	-9.223225000	-5.012634000	-2.546037000
H	-8.799434000	-5.963674000	-2.879046000
H	-10.289111000	-5.002812000	-2.793700000
H	-9.117966000	-4.934987000	-1.460995000
C	-8.650589000	-3.952351000	-4.786576000
H	-8.191775000	-3.101081000	-5.296826000
H	-9.710029000	-3.975758000	-5.060780000
H	-8.185489000	-4.876755000	-5.138346000
C	-9.105989000	-2.479248000	-2.762196000
H	-9.000845000	-2.377451000	-1.678283000
H	-10.173474000	-2.437826000	-2.999220000
H	-8.623297000	-1.630889000	-3.256628000
S	-2.632799000	-4.325053000	0.911004000
C	-2.492104000	-3.756081000	-0.776254000
C	-3.145254000	-4.387904000	-1.846904000
C	-1.660392000	-2.651704000	-1.033114000
C	-2.966415000	-3.918911000	-3.152242000
C	-1.482882000	-2.191682000	-2.341180000
C	-2.136758000	-2.821735000	-3.407387000
C	-4.341820000	-4.981296000	0.951562000
H	-3.797360000	-5.234627000	-1.675327000
H	-1.171652000	-2.145315000	-0.207624000
H	-3.484986000	-4.415714000	-3.963753000
H	-0.844285000	-1.333371000	-2.523873000
H	-2.009148000	-2.456792000	-4.420405000
H	-4.426849000	-5.928484000	0.414623000
H	-5.021950000	-4.241940000	0.528041000
H	-4.583533000	-5.149457000	2.004115000
TS_0			
I	-6.453256000	-1.035920000	-0.334571000
O	-4.738015000	-1.903222000	0.419322000
O	-6.805244000	0.773897000	-0.472999000
S	-6.656063000	-3.892568000	-2.598817000
C	-5.760872000	-1.248674000	-2.363393000
C	-5.209751000	-0.079644000	-2.891642000
H	-5.245475000	0.827852000	-2.297400000
C	-4.644709000	-0.095422000	-4.171887000
H	-4.211728000	0.812651000	-4.576181000
C	-4.626798000	-1.276879000	-4.921432000
H	-4.169471000	-1.295098000	-5.903424000
C	-5.204416000	-2.439566000	-4.406560000
H	-5.200873000	-3.359798000	-4.976440000
C	-5.785007000	-2.422340000	-3.130661000
O	-6.722406000	-3.837323000	-1.099095000
O	-6.042999000	-5.083805000	-3.252903000
C	-8.404183000	-3.729071000	-3.240800000
C	-9.131596000	-4.980501000	-2.711950000
H	-8.668363000	-5.896170000	-3.088550000
H	-10.168464000	-4.946892000	-3.060898000
H	-9.133773000	-5.004817000	-1.619160000
C	-8.355479000	-3.714905000	-4.775249000
H	-7.838094000	-2.830155000	-5.156444000
H	-9.383718000	-3.691219000	-5.150542000
H	-7.867007000	-4.611158000	-5.165697000
C	-9.023259000	-2.442719000	-2.679063000
H	-9.010897000	-2.435237000	-1.586251000
H	-10.066015000	-2.392430000	-3.008576000
H	-8.512621000	-1.548914000	-3.048651000
S	-3.318468000	-3.388195000	0.595390000
C	-2.910823000	-3.529305000	-1.125626000
C	-3.132402000	-4.682774000	-1.890685000
C	-2.319835000	-2.396746000	-1.719888000
C	-2.736879000	-4.710993000	-3.233104000
C	-1.926641000	-2.437761000	-3.056135000
C	-2.127949000	-3.598046000	-3.817562000
C	-4.399423000	-4.812284000	0.902652000
H	-3.615019000	-5.550854000	-1.463222000
H	-2.187456000	-1.491412000	-1.138524000
H	-2.924395000	-5.603037000	-3.819761000
H	-1.479545000	-1.559838000	-3.509112000
H	-1.826502000	-3.624674000	-4.858908000
H	-3.856285000	-5.753203000	0.792380000
H	-5.258402000	-4.763393000	0.231070000
H	-4.735423000	-4.713200000	1.937033000
PC_0			
I	-7.837564000	-0.399364000	0.159697000
O	-6.010284000	-0.040301000	2.100769000
O	-9.145352000	-0.543977000	-1.172998000
S	-6.044900000	-3.094774000	-1.653821000
C	-6.049051000	-0.292930000	-1.028204000
C	-5.495228000	0.987928000	-1.153456000
H	-5.929482000	1.814736000	-0.604985000
C	-4.386832000	1.201418000	-1.979939000
H	-3.969831000	2.198059000	-2.069491000
C	-3.826123000	0.133608000	-2.683684000
H	-2.965475000	0.289140000	-3.323501000
C	-4.367582000	-1.147306000	-2.554049000
H	-3.924286000	-1.988844000	-3.069966000
C	-5.480876000	-1.367382000	-1.730767000
O	-6.529665000	-3.365357000	-0.266826000
O	-4.890439000	-3.905322000	-2.148134000
C	-7.492740000	-3.310674000	-2.885257000
C	-7.117794000	-4.516855000	-3.761570000
H	-6.202317000	-4.338897000	-4.329267000
H	-7.940305000	-4.682206000	-4.465603000
H	-6.986047000	-5.425389000	-3.168097000
C	-7.636008000	-2.028103000	-3.718673000
H	-7.963253000	-1.193221000	-3.093365000
H	-8.412180000	-2.208356000	-4.470920000
H	-6.712503000	-1.768417000	-4.243999000
C	-8.762221000	-3.580504000	-2.064366000
H	-8.632381000	-4.425201000	-1.384223000

H	-9.564686000	-3.825125000	-2.770226000
H	-9.060269000	-2.686952000	-1.508106000
S	-5.183521000	-1.159566000	2.761954000
C	-3.926398000	-1.655180000	1.556493000
C	-3.642913000	-2.983505000	1.221919000
C	-3.187852000	-0.603649000	0.994409000
C	-2.611947000	-3.256981000	0.315459000
C	-2.159263000	-0.886952000	0.094324000
C	-1.868409000	-2.214153000	-0.244604000
C	-6.225648000	-2.652722000	2.802157000
H	-4.221652000	-3.800919000	1.628926000
H	-3.433211000	0.422681000	1.240455000
H	-2.406928000	-4.284074000	0.037133000
H	-1.597302000	-0.074104000	-0.350883000
H	-1.074624000	-2.432515000	-0.950390000
H	-5.700803000	-3.440722000	3.346739000
H	-6.480248000	-2.969900000	1.789540000
H	-7.123240000	-2.370996000	3.357029000

RC_0'

I	-3.121555000	-0.831905000	-0.723526000
O	-1.723079000	-1.850393000	-0.241857000
O	-2.916039000	0.757461000	0.104457000
S	-3.718280000	-2.247850000	-3.940531000
C	-2.465528000	-0.118759000	-2.672311000
C	-1.700264000	1.043562000	-2.633628000
H	-1.547898000	1.554942000	-1.689344000
C	-1.163158000	1.547931000	-3.825178000
H	-0.579689000	2.459516000	-3.799886000
C	-1.391358000	0.891727000	-5.038214000
H	-0.977698000	1.288238000	-5.956972000
C	-2.164376000	-0.273619000	-5.075355000
H	-2.334822000	-0.794928000	-6.009384000
C	-2.707152000	-0.773857000	-3.886028000
O	-3.744959000	-2.743999000	-2.516384000
O	-3.213419000	-3.145584000	-5.013463000
C	-5.452405000	-1.707221000	-4.354046000
C	-6.290684000	-2.999695000	-4.330990000
H	-5.938185000	-3.713552000	-5.079881000
H	-7.327580000	-2.737570000	-4.562901000
H	-6.264435000	-3.472846000	-3.346011000
C	-5.437658000	-1.070068000	-5.750933000
H	-4.839717000	-0.155987000	-5.776997000
H	-6.466375000	-0.806704000	-6.017540000
H	-5.059104000	-1.769228000	-6.500903000
C	-5.908125000	-0.721005000	-3.268926000
H	-5.910384000	-1.188350000	-2.280193000
H	-6.933137000	-0.410369000	-3.493821000
H	-5.286877000	0.178226000	-3.244922000
S	-2.753706000	4.514130000	-2.078262000
C	-3.438424000	3.895639000	-3.602458000
C	-4.527694000	3.012361000	-3.671523000
C	-2.819891000	4.317202000	-4.796178000
C	-4.988961000	2.566041000	-4.915915000
C	-3.276641000	3.853888000	-6.030847000
C	-4.365224000	2.974061000	-6.099043000
C	-3.855891000	3.810413000	-0.802000000
H	-5.019538000	2.670609000	-2.770099000
H	-1.979174000	5.002499000	-4.753208000
H	-5.844933000	1.901348000	-4.955542000
H	-2.784976000	4.184002000	-6.940010000
H	-4.725015000	2.619387000	-7.058628000
H	-3.763266000	2.723347000	-0.746894000
H	-4.892926000	4.108586000	-0.972776000
H	-3.518287000	4.235235000	0.146329000

TS_0'

I	-1.958625000	1.871241000	-3.265102000
O	-0.674182000	1.486664000	-4.532503000
O	-3.189438000	3.454691000	-2.786355000
S	-3.040710000	-1.640039000	-2.982476000
C	-3.675117000	0.870421000	-4.137303000
C	-4.473441000	1.687362000	-4.946203000
H	-4.248726000	2.745042000	-5.009922000
C	-5.568180000	1.145916000	-5.628288000
H	-6.178502000	1.786511000	-6.254769000
C	-5.871423000	-0.214184000	-5.503552000
H	-6.713942000	-0.638911000	-6.036356000
C	-5.080613000	-1.032909000	-4.694332000
H	-5.295216000	-2.090048000	-4.601163000
C	-3.981995000	-0.492102000	-4.007520000
O	-1.648547000	-1.108216000	-2.869033000
O	-3.249437000	-3.003321000	-3.552397000
C	-3.814038000	-1.599197000	-1.286953000
C	-2.982328000	-2.588912000	-0.448718000
H	-3.035345000	-3.599633000	-0.861544000
H	-3.392105000	-2.605570000	0.566198000
H	-1.935075000	-2.280159000	-0.395290000
C	-5.274196000	-2.056521000	-1.409623000
H	-5.867848000	-1.360047000	-2.006404000
H	-5.709761000	-2.086813000	-0.405676000
H	-5.340646000	-3.056144000	-1.846245000
C	-3.706360000	-0.171369000	-0.739576000
H	-2.665648000	0.158446000	-0.686129000
H	-4.125298000	-0.154655000	0.270582000
H	-4.279744000	0.538969000	-1.339154000
S	-4.561797000	4.281158000	-1.472679000
C	-5.678215000	2.939680000	-1.128200000
C	-5.904083000	2.431442000	0.161404000
C	-6.356387000	2.385439000	-2.228567000
C	-6.799651000	1.371325000	0.340222000
C	-7.241405000	1.322574000	-2.040606000
C	-7.465630000	0.810910000	-0.755320000
C	-3.414724000	4.218921000	-0.067206000
H	-5.395548000	2.848944000	1.020868000
H	-6.173011000	2.769831000	-3.222879000
H	-6.970324000	0.982342000	1.338133000
H	-7.744015000	0.889735000	-2.898469000
H	-8.149580000	-0.017731000	-0.610748000
H	-3.020161000	3.206114000	0.034979000
H	-3.891345000	4.545480000	0.858473000
H	-2.600074000	4.901029000	-0.315369000

PC_0'

I	-2.429475000	-0.465362000	-0.865557000
O	-1.192739000	-1.760455000	-0.369823000
O	-4.238387000	1.615230000	-1.443061000
S	-3.630301000	-2.363992000	-3.852049000
C	-2.109504000	-0.103152000	-2.976909000
C	-1.281266000	0.991805000	-3.261424000
H	-0.851860000	1.563271000	-2.446956000
C	-1.013196000	1.359282000	-4.584368000
H	-0.387436000	2.220605000	-4.784267000
C	-1.558591000	0.622143000	-5.636567000
H	-1.357760000	0.900549000	-6.664000000
C	-2.357742000	-0.490566000	-5.364380000
H	-2.749964000	-1.094144000	-6.172608000

C	-2.641549000	-0.855602000	-4.038806000
O	-3.288354000	-2.994271000	-2.544916000
O	-3.409994000	-3.150210000	-5.103843000
C	-5.428891000	-1.870334000	-3.827723000
C	-6.197870000	-3.206253000	-3.808205000
H	-5.978655000	-3.804394000	-4.695964000
H	-7.269397000	-2.982552000	-3.792235000
H	-5.952914000	-3.788927000	-2.916031000
C	-5.727141000	-1.076873000	-5.108528000
H	-5.155732000	-0.146384000	-5.151774000
H	-6.791909000	-0.821620000	-5.114949000
H	-5.509196000	-1.667749000	-6.001812000
C	-5.709387000	-1.049831000	-2.564502000
H	-5.460661000	-1.613922000	-1.662333000
H	-6.779715000	-0.817235000	-2.540689000
H	-5.161199000	-0.105447000	-2.542725000
S	-3.593621000	2.991851000	-1.647866000
C	-3.632711000	3.319554000	-3.427893000
C	-4.473547000	2.556935000	-4.241091000
C	-2.771597000	4.280663000	-3.966519000
C	-4.455448000	2.764683000	-5.623386000
C	-2.765483000	4.487837000	-5.350314000
C	-3.602486000	3.728159000	-6.177319000
C	-4.872069000	4.195937000	-1.147786000
H	-5.113967000	1.807452000	-3.792734000
H	-2.105995000	4.847816000	-3.323549000
H	-5.099502000	2.174434000	-6.266006000
H	-2.101359000	5.229036000	-5.780834000
H	-3.585472000	3.882184000	-7.250598000
H	-5.802033000	3.955609000	-1.667694000
H	-4.536115000	5.203189000	-1.404400000
H	-5.006295000	4.107921000	-0.067732000

5. The C-H bond activation of 9,10-dihydroanthracene by $^{s}PhIO_2$

RC_2			
I	-10.628566000	-2.282406000	0.278425000
O	-9.187786000	-2.534439000	1.324901000
O	-11.215322000	-0.609195000	0.595625000
S	-9.638270000	-4.454484000	-2.388338000
C	-9.683537000	-1.788990000	-1.620322000
C	-9.435103000	-0.428789000	-1.793895000
H	-9.792399000	0.274265000	-1.047965000
C	-8.730674000	-0.002623000	-2.927045000
H	-8.524779000	1.052648000	-3.062789000
C	-8.279448000	-0.931540000	-3.870465000
H	-7.708693000	-0.602194000	-4.728916000
C	-8.542279000	-2.293889000	-3.701116000
H	-8.173774000	-3.020260000	-4.413222000
C	-9.256070000	-2.718368000	-2.574768000
O	-10.006930000	-4.607556000	-0.932821000
O	-8.526803000	-5.272948000	-2.943134000
C	-11.190336000	-4.776356000	-3.371959000
C	-11.527120000	-6.256041000	-3.105262000
H	-10.722909000	-6.913160000	-3.446319000
H	-12.436332000	-6.504071000	-3.661474000
H	-11.709818000	-6.436587000	-2.042960000
C	-10.884676000	-4.524862000	-4.855188000
H	-10.652920000	-3.474307000	-5.050337000
H	-11.774961000	-4.785626000	-5.436216000
H	-10.055103000	-5.146277000	-5.201958000
C	-12.288053000	-3.841604000	-2.844144000
H	-12.472474000	-4.001070000	-1.777824000
H	-13.215403000	-4.064149000	-3.380815000
H	-12.047193000	-2.788724000	-3.018104000
C	-6.284132000	-1.178116000	0.255736000
C	-6.534388000	-3.943203000	-0.293117000
C	-5.874955000	-1.669385000	-1.118527000
C	-5.857053000	-2.158037000	1.331645000
C	-6.004695000	-3.045798000	-1.393240000
C	-5.979989000	-3.534272000	1.056943000
C	-5.356740000	-0.814929000	-2.099170000
C	-5.360481000	-1.741220000	2.571980000
C	-5.622534000	-3.540809000	-2.646059000
C	-5.604488000	-4.469775000	2.027843000
C	-4.974162000	-1.314828000	-3.349742000
C	-4.993594000	-2.680941000	3.543608000
C	-5.110386000	-2.680239000	-3.624541000
C	-5.115846000	-4.048166000	3.270889000
H	-5.875973000	-0.181064000	0.449589000
H	-7.380973000	-1.093291000	0.299153000
H	-7.629284000	-3.854294000	-0.240974000
H	-6.313806000	-4.992681000	-0.509398000
H	-5.249329000	0.243677000	-1.880876000
H	-5.261081000	-0.679222000	2.777863000
H	-5.737463000	-4.599042000	-2.855189000
H	-5.695276000	-5.530146000	1.810205000
H	-4.569706000	-0.643935000	-4.100992000
H	-4.610360000	-2.347579000	4.502696000
H	-4.813747000	-3.074803000	-4.591199000
H	-4.828069000	-4.781599000	4.017293000
TS_2			
I	-10.329116000	-0.876851000	-0.224762000
O	-8.446723000	-0.757684000	0.475082000
O	-11.502908000	0.461817000	-0.717677000
S	-9.203671000	-3.864975000	-1.953802000
C	-9.559325000	-1.097235000	-2.227598000
C	-9.568859000	0.079297000	-2.978636000
H	-10.013028000	0.971773000	-2.551982000
C	-9.024774000	0.080673000	-4.268543000
H	-9.019170000	0.999217000	-4.844245000
C	-8.483090000	-1.090679000	-4.808261000
H	-8.044606000	-1.084542000	-5.798833000
C	-8.513032000	-2.278431000	-4.073789000
H	-8.105987000	-3.194552000	-4.481307000
C	-9.060747000	-2.284584000	-2.784219000
O	-9.229632000	-3.576171000	-0.481932000
O	-8.162875000	-4.780816000	-2.503640000
C	-10.862545000	-4.578937000	-2.437996000
C	-10.935394000	-5.927029000	-1.694257000
H	-10.124804000	-6.592581000	-2.001308000
H	-11.889351000	-6.403037000	-1.942059000
H	-10.889755000	-5.784892000	-0.611247000
C	-10.871633000	-4.775835000	-3.960918000
H	-10.812012000	-3.822760000	-4.493904000
H	-11.814405000	-5.258483000	-4.238122000
H	-10.048381000	-5.417966000	-4.283354000
C	-11.977511000	-3.630197000	-1.981096000
H	-11.948696000	-3.470244000	-0.900366000
H	-12.940223000	-4.088576000	-2.229258000
H	-11.929740000	-2.664065000	-2.492006000
C	-6.158344000	-1.725186000	0.431559000
C	-5.539023000	-4.326622000	-0.810838000
C	-5.814803000	-1.796380000	-0.986632000
C	-6.091379000	-2.931337000	1.252752000
C	-5.532742000	-3.039412000	-1.600503000
C	-5.828832000	-4.191662000	0.665454000
C	-5.803481000	-0.619545000	-1.771473000
C	-6.323931000	-2.854016000	2.644875000
C	-5.225422000	-3.069437000	-2.968588000
C	-5.808964000	-5.333095000	1.480416000
C	-5.500206000	-0.667070000	-3.126431000
C	-6.303305000	-3.995549000	3.439637000
C	-5.206065000	-1.900905000	-3.730790000
C	-6.046752000	-5.246057000	2.853612000
H	-5.887084000	-0.797839000	0.935193000
H	-7.536721000	-1.410075000	0.352348000
H	-6.282323000	-4.995246000	-1.264397000
H	-4.569442000	-4.831564000	-0.939455000
H	-6.048574000	0.325046000	-1.296380000
H	-6.531394000	-1.883634000	3.085932000
H	-5.006763000	-4.024535000	-3.436656000
H	-5.601296000	-6.298961000	1.028485000
H	-5.500809000	0.242518000	-3.716892000
H	-6.485496000	-3.919940000	4.506336000
H	-4.970895000	-1.946587000	-4.788887000
H	-6.030206000	-6.141865000	3.465371000
PC_2			
I	-10.481277000	-2.365899000	0.330855000
O	-7.330886000	-0.770185000	0.521461000
O	-10.781578000	-0.634805000	0.931450000
S	-9.657682000	-4.500444000	-2.428005000
C	-9.711579000	-1.852493000	-1.606900000
C	-9.524410000	-0.481455000	-1.784462000
H	-9.846463000	0.190059000	-0.991556000

C	-8.923309000	-0.018132000	-2.960487000
H	-8.769458000	1.046201000	-3.098173000
C	-8.503471000	-0.920283000	-3.946735000
H	-8.005495000	-0.561925000	-4.838851000
C	-8.716285000	-2.289409000	-3.776689000
H	-8.381126000	-2.997614000	-4.523485000
C	-9.339863000	-2.753593000	-2.609443000
O	-9.922060000	-4.697241000	-0.956517000
O	-8.556542000	-5.274910000	-3.067287000
C	-11.250332000	-4.862342000	-3.327293000
C	-11.541074000	-6.347594000	-3.039390000
H	-10.741096000	-6.989187000	-3.418363000
H	-12.471684000	-6.617258000	-3.548366000
H	-11.666339000	-6.526978000	-1.968646000
C	-11.027260000	-4.612146000	-4.825677000
H	-10.828070000	-3.557733000	-5.035786000
H	-11.941732000	-4.893234000	-5.357809000
H	-10.204097000	-5.217702000	-5.213166000
C	-12.341668000	-3.948536000	-2.750428000
H	-12.466209000	-4.098314000	-1.675244000
H	-13.287775000	-4.194381000	-3.242983000
H	-12.128776000	-2.892313000	-2.938539000
C	-5.927343000	-1.156279000	0.367351000
C	-6.606152000	-3.858396000	-0.306124000
C	-5.664057000	-1.644655000	-1.040296000
C	-5.681891000	-2.241152000	1.388778000
C	-6.012166000	-2.967298000	-1.375435000
C	-6.038966000	-3.564050000	1.066313000
C	-5.113717000	-0.799172000	-2.011959000
C	-5.155887000	-1.946184000	2.651623000
C	-5.792103000	-3.425166000	-2.680323000
C	-5.864457000	-4.572992000	2.021976000
C	-4.901029000	-1.260641000	-3.315742000
C	-4.985601000	-2.957847000	3.603089000
C	-5.239621000	-2.577258000	-3.647240000
C	-5.343763000	-4.273659000	3.286489000
H	-5.293339000	-0.286510000	0.583540000
H	-7.557447000	-0.234775000	-0.257079000
H	-7.692692000	-3.695915000	-0.268510000
H	-6.466045000	-4.912353000	-0.564509000
H	-4.844190000	0.218469000	-1.742929000
H	-4.883312000	-0.922125000	2.889143000
H	-6.072994000	-4.439732000	-2.940047000
H	-6.131656000	-5.595575000	1.772322000
H	-4.469727000	-0.601846000	-4.062176000
H	-4.576518000	-2.722728000	4.579936000
H	-5.073192000	-2.944739000	-4.654770000
H	-5.210779000	-5.064880000	4.017105000

RC_2'

I	-1.903536000	0.096259000	-1.757342000
O	-0.310126000	-0.528080000	-2.298128000
O	-1.622188000	1.751496000	-1.098586000
S	-3.953202000	-1.670131000	-4.086911000
C	-2.732832000	0.784557000	-3.650710000
C	-2.393676000	2.093355000	-3.985468000
H	-1.849947000	2.702024000	-3.271985000
C	-2.769397000	2.597531000	-5.237101000
H	-2.514084000	3.616049000	-5.498891000
C	-3.477898000	1.797006000	-6.139117000
H	-3.759854000	2.189232000	-7.108734000
C	-3.831788000	0.488720000	-5.794531000
H	-4.373940000	-0.140924000	-6.489398000
C	-3.462183000	-0.012269000	-4.540403000
O	-3.032180000	-2.044083000	-2.952253000
O	-3.986608000	-2.519156000	-5.307597000
C	-5.670493000	-1.549636000	-3.372459000
C	-6.044256000	-2.992232000	-2.983478000
H	-6.059620000	-3.647143000	-3.858282000
H	-7.045926000	-2.977425000	-2.542998000
H	-5.347273000	-3.397919000	-2.245515000
C	-6.608834000	-0.991936000	-4.452574000
H	-6.359599000	0.040113000	-4.714548000
H	-7.628716000	-1.000696000	-4.054970000
H	-6.589547000	-1.607708000	-5.355519000
C	-5.602697000	-0.628867000	-2.147476000
H	-4.920412000	-1.018135000	-1.386927000
H	-6.601171000	-0.568249000	-1.703646000
H	-5.303327000	0.384643000	-2.424682000
C	-3.132118000	4.791375000	-1.155337000
C	-4.979848000	2.662495000	-0.735239000
C	-3.749622000	4.632618000	0.220456000
C	-4.128609000	4.474051000	-2.252635000
C	-4.665326000	3.582689000	0.427219000
C	-5.036175000	3.415106000	-2.049758000
C	-3.432445000	5.490165000	1.281380000
C	-4.172678000	5.200128000	-3.449296000
C	-5.247365000	3.408105000	1.688916000
C	-5.961507000	3.095606000	-3.052284000
C	-4.009883000	5.306559000	2.543344000
C	-5.093096000	4.870452000	-4.451027000
C	-4.920037000	4.263011000	2.747911000
C	-5.986825000	3.812068000	-4.254354000
H	-2.727192000	5.800338000	-1.282737000
H	-2.285822000	4.091096000	-1.237114000
H	-4.176761000	1.912473000	-0.795543000
H	-5.913030000	2.118944000	-0.557734000
H	-2.731903000	6.303903000	1.117693000
H	-3.482407000	6.025673000	-3.596646000
H	-5.959037000	2.601635000	1.841229000
H	-6.675730000	2.294728000	-2.885370000
H	-3.755987000	5.976891000	3.358007000
H	-5.114641000	5.438379000	-5.375376000
H	-5.376380000	4.119279000	3.721839000
H	-6.706494000	3.553810000	-5.024156000

TS_2'

I	-1.693934000	0.279515000	-1.720707000
O	-0.249749000	-0.760593000	-2.193805000
O	-1.970393000	2.213335000	-1.175221000
S	-3.729853000	-1.423925000	-4.216333000
C	-2.223570000	0.922065000	-3.721008000
C	-1.696095000	2.156021000	-4.116126000
H	-1.155334000	2.754603000	-3.394355000
C	-1.898466000	2.615881000	-5.421722000
H	-1.478391000	3.568922000	-5.722660000
C	-2.636068000	1.852126000	-6.332199000
H	-2.789435000	2.204352000	-7.345246000
C	-3.175662000	0.626094000	-5.936795000
H	-3.739899000	0.020390000	-6.634713000
C	-2.971985000	0.158276000	-4.629461000
O	-2.953243000	-2.001070000	-3.074711000
O	-3.844729000	-2.202036000	-5.483143000
C	-5.447849000	-1.051452000	-3.597894000
C	-6.049177000	-2.426895000	-3.249804000
H	-6.101394000	-3.071030000	-4.131352000

H	-7.064950000	-2.269120000	-2.873671000
H	-5.465870000	-2.929929000	-2.474249000
C	-6.232184000	-0.365349000	-4.724342000
H	-5.811089000	0.610601000	-4.976205000
H	-7.257661000	-0.202485000	-4.377947000
H	-6.265136000	-0.990053000	-5.620533000
C	-5.328042000	-0.162102000	-2.354263000
H	-4.741734000	-0.649399000	-1.570667000
H	-6.333238000	0.023545000	-1.965535000
H	-4.887947000	0.809898000	-2.588605000
C	-3.681029000	4.086085000	-1.247336000
C	-6.063807000	2.945189000	-0.056617000
C	-3.944308000	4.318942000	0.169350000
C	-4.793766000	3.705137000	-2.113454000
C	-5.115674000	3.789482000	0.766229000
C	-5.987942000	3.192610000	-1.545978000
C	-3.042662000	5.062112000	0.962479000
C	-4.702479000	3.842166000	-3.516399000
C	-5.363089000	4.028266000	2.122720000
C	-7.064410000	2.877127000	-2.382771000
C	-3.297019000	5.284324000	2.313494000
C	-5.771084000	3.496366000	-4.339132000
C	-4.463759000	4.767829000	2.898012000
C	-6.963691000	3.022556000	-3.770143000
H	-2.930789000	4.732964000	-1.701253000
H	-2.844921000	2.886425000	-1.274962000
H	-5.826651000	1.881420000	0.124914000
H	-7.092887000	3.077480000	0.297194000
H	-2.144291000	5.461437000	0.501949000
H	-3.784463000	4.224482000	-3.947701000
H	-6.267236000	3.631335000	2.574848000
H	-7.984949000	2.503890000	-1.944037000
H	-2.597244000	5.859106000	2.910433000
H	-5.683506000	3.602939000	-5.414827000
H	-4.670920000	4.943456000	3.948142000
H	-7.804983000	2.765126000	-4.404191000

PC_2'

I	-2.536120000	1.176110000	-1.001651000
O	-1.658603000	-0.129404000	-0.011593000
O	-3.641821000	3.382326000	-2.545601000
S	-3.663270000	-1.335898000	-3.549637000
C	-1.950240000	0.903391000	-3.065776000
C	-0.985063000	1.821296000	-3.507616000
H	-0.632913000	2.589702000	-2.830258000
C	-0.479956000	1.750170000	-4.810182000
H	0.263702000	2.468319000	-5.136472000
C	-0.921191000	0.746158000	-5.676517000
H	-0.520209000	0.671776000	-6.680439000
C	-1.879973000	-0.172791000	-5.245077000
H	-2.215935000	-0.965119000	-5.901477000
C	-2.409428000	-0.090863000	-3.946677000
O	-3.650514000	-1.577422000	-2.078404000
O	-3.406418000	-2.485192000	-4.468997000
C	-5.320855000	-0.612912000	-4.017351000
C	-6.310848000	-1.785738000	-3.875452000
H	-6.066095000	-2.598080000	-4.563493000
H	-7.313810000	-1.415375000	-4.110810000
H	-6.318256000	-2.174642000	-2.853295000
C	-5.251492000	-0.115564000	-5.468246000
H	-4.565393000	0.728926000	-5.576762000
H	-6.251236000	0.221878000	-5.760960000
H	-4.947108000	-0.913633000	-6.150693000
C	-5.660952000	0.517185000	-3.042837000
H	-5.708385000	0.148652000	-2.016050000
H	-6.640180000	0.927248000	-3.307787000
H	-4.939044000	1.334510000	-3.082426000
C	-4.506870000	4.326692000	-1.803666000
C	-5.913571000	2.580429000	0.106378000
C	-4.046439000	4.233416000	-0.372660000
C	-5.959925000	3.980511000	-2.007715000
C	-4.692471000	3.367363000	0.526879000
C	-6.626240000	3.130926000	-1.106972000
C	-2.891181000	4.923213000	0.025237000
C	-6.632054000	4.458585000	-3.143724000
C	-4.156002000	3.198808000	1.814083000
C	-7.959320000	2.775985000	-1.363114000
C	-2.362610000	4.748255000	1.304918000
C	-7.954112000	4.088752000	-3.399402000
C	-2.996515000	3.875944000	2.200917000
C	-8.619612000	3.242060000	-2.502889000
H	-4.302949000	5.328504000	-2.199527000
H	-3.945850000	3.369153000	-3.469676000
H	-5.601340000	1.545578000	-0.108831000
H	-6.613081000	2.505365000	0.946975000
H	-2.399903000	5.583807000	-0.682488000
H	-6.114059000	5.126216000	-3.827045000
H	-4.649651000	2.528000000	2.510492000
H	-8.477835000	2.125998000	-0.664729000
H	-1.466479000	5.281266000	1.602633000
H	-8.464062000	4.462274000	-4.280681000
H	-2.592951000	3.730566000	3.197062000
H	-9.649545000	2.955286000	-2.686755000

RC_3

O	-5.760698000	0.237838000	0.224653000
C	-5.183951000	-0.797165000	-0.632711000
C	-6.226601000	-2.761067000	1.140565000
C	-6.342934000	-1.643832000	-1.110871000
C	-4.201026000	-1.653980000	0.144847000
C	-6.879992000	-2.592837000	-0.219051000
C	-4.721573000	-2.596847000	1.053014000
C	-6.911652000	-1.475898000	-2.377589000
C	-2.815021000	-1.524796000	-0.006789000
C	-7.984176000	-3.357885000	-0.613089000
C	-3.843142000	-3.377236000	1.814294000
C	-8.015457000	-2.243937000	-2.766999000
C	-1.942443000	-2.313178000	0.751702000
C	-8.553563000	-3.184455000	-1.880974000
C	-2.457146000	-3.235124000	1.669209000
H	-4.676368000	-0.322937000	-1.478981000
H	-5.222260000	1.053928000	0.122745000
H	-6.630703000	-1.997772000	1.823008000
H	-6.481759000	-3.735005000	1.570755000
H	-6.489542000	-0.742471000	-3.058471000
H	-2.425155000	-0.786855000	-0.699704000
H	-8.394654000	-4.095964000	0.069934000
H	-4.244229000	-4.109040000	2.509860000
H	-8.449597000	-2.111338000	-3.752499000
H	-0.869811000	-2.198477000	0.634668000
H	-9.406227000	-3.786710000	-2.177583000
H	-1.785938000	-3.847464000	2.262948000
I	-2.545303000	2.455941000	-0.088709000
O	-2.444023000	1.304081000	-1.464398000
O	-4.312286000	2.594500000	0.278871000
S	0.625871000	1.654849000	1.284607000

C	-2.092742000	1.231639000	1.662004000
C	-3.197342000	0.685480000	2.312855000
H	-4.199899000	0.896312000	1.963414000
C	-2.992370000	-0.192896000	3.384820000
H	-3.848972000	-0.637457000	3.876040000
C	-1.697515000	-0.527938000	3.789877000
H	-1.544908000	-1.230072000	4.600324000
C	-0.590713000	0.026863000	3.140112000
H	0.415867000	-0.243825000	3.434216000
C	-0.794190000	0.920885000	2.082096000
O	0.070089000	2.253201000	0.013057000
O	1.715517000	0.647893000	1.191895000
C	1.180508000	3.083194000	2.348021000
C	2.326661000	3.742703000	1.556857000
H	3.156784000	3.047468000	1.406929000
H	2.691035000	4.596595000	2.136156000
H	1.982611000	4.104010000	0.584562000
C	1.670559000	2.529011000	3.693210000
H	0.857004000	2.081902000	4.270536000
H	2.075867000	3.362328000	4.275811000
H	2.464217000	1.790266000	3.555546000
C	-0.012590000	4.034405000	2.518396000
H	-0.370734000	4.406191000	1.554318000
H	0.318184000	4.895421000	3.107260000
H	-0.839621000	3.561356000	3.055867000
TS			
O	-6.451462000	0.344142000	0.966391000
C	-5.787515000	-0.774987000	0.505002000
C	-4.549597000	-3.144550000	-0.396620000
C	-6.344445000	-1.409272000	-0.711007000
C	-5.284869000	-1.720292000	1.532742000
C	-5.751911000	-2.615212000	-1.152906000
C	-4.663490000	-2.911519000	1.094692000
C	-7.411691000	-0.847973000	-1.429286000
C	-5.410660000	-1.459368000	2.907113000
C	-6.256076000	-3.248924000	-2.291780000
C	-4.174473000	-3.816755000	2.040262000
C	-7.901439000	-1.488050000	-2.570735000
C	-4.918714000	-2.373175000	3.844002000
C	-7.327680000	-2.691513000	-3.002014000
C	-4.294918000	-3.550841000	3.411403000
H	-4.630646000	-0.215717000	0.051523000
H	-5.765463000	1.023812000	1.283231000
H	-4.386763000	-4.204544000	-0.613823000
H	-3.654359000	-2.608244000	-0.761380000
H	-7.848982000	0.078856000	-1.078411000
H	-5.915913000	-0.554363000	3.224091000
H	-5.806620000	-4.178723000	-2.627693000
H	-3.703863000	-4.736151000	1.705178000
H	-8.730734000	-1.053865000	-3.119500000
H	-5.029682000	-2.173070000	4.904708000
H	-7.710846000	-3.192933000	-3.884562000
H	-3.915339000	-4.264137000	4.135403000
I	-3.110065000	2.123373000	0.590244000
O	-3.770950000	0.492302000	-0.314450000
O	-4.614068000	2.109748000	1.652077000
S	0.453925000	1.886556000	0.482777000
C	-1.802172000	0.937514000	1.800112000
C	-2.464840000	0.151690000	2.742644000
H	-3.534862000	0.252933000	2.873039000
C	-1.735517000	-0.773017000	3.498658000
H	-2.258247000	-1.399342000	4.210812000
C	-0.354128000	-0.906023000	3.316300000
H	0.204564000	-1.635911000	3.889410000
C	0.312108000	-0.097117000	2.389920000
H	1.378636000	-0.201022000	2.231614000
C	-0.413763000	0.837471000	1.640333000
O	-0.630044000	2.442064000	-0.407498000
O	1.571669000	1.120222000	-0.130741000
C	1.152252000	3.316420000	1.455188000
C	1.795298000	4.236209000	0.399288000
H	2.597664000	3.723726000	-0.137809000
H	2.221991000	5.101007000	0.916703000
H	1.054476000	4.593521000	-0.320442000
C	2.197577000	2.769194000	2.437803000
H	1.744190000	2.128863000	3.199252000
H	2.661649000	3.619092000	2.948212000
H	2.981296000	2.212174000	1.918230000
C	-0.007676000	4.012514000	2.181316000
H	-0.757913000	4.382846000	1.477800000
H	0.397361000	4.871058000	2.726166000
H	-0.490311000	3.353098000	2.908456000
PC_3			
O	-5.541426000	0.956126000	0.325125000
C	-5.671328000	-0.271248000	0.489373000
C	-5.840607000	-3.221317000	0.796830000
C	-6.611344000	-1.063970000	-0.326186000
C	-4.838195000	-0.984298000	1.489825000
C	-6.698222000	-2.464191000	-0.185759000
C	-4.887373000	-2.389536000	1.615463000
C	-7.418831000	-0.395393000	-1.267813000
C	-3.944584000	-0.233113000	2.282870000
C	-7.602637000	-3.169148000	-0.995646000
C	-4.015388000	-3.016529000	2.521633000
C	-8.310128000	-1.105781000	-2.062792000
C	-3.092654000	-0.868133000	3.178204000
C	-8.401151000	-2.501069000	-1.923815000
C	-3.124863000	-2.268369000	3.291067000
H	-3.325157000	-1.336716000	-0.050125000
H	-4.544654000	1.192959000	-1.439651000
H	-6.492632000	-3.783456000	1.481505000
H	-5.270203000	-3.989263000	0.254947000
H	-7.325994000	0.680675000	-1.352205000
H	-3.940955000	0.842710000	2.162195000
H	-7.674332000	-4.247771000	-0.896372000
H	-4.037910000	-4.097439000	2.615814000
H	-8.929922000	-0.588611000	-2.786340000
H	-2.402201000	-0.291381000	3.782522000
H	-9.093099000	-3.062956000	-2.541909000
H	-2.452877000	-2.770547000	3.978071000
I	-2.126212000	0.640634000	-0.869232000
O	-2.803789000	-1.234116000	-0.869772000
O	-3.806100000	1.046320000	-2.062029000
S	0.539831000	2.378822000	0.760538000
C	-0.480873000	-0.196632000	0.473391000
C	-0.428761000	-1.570776000	0.753512000
H	-1.175550000	-2.222713000	0.321287000
C	0.576586000	-2.106912000	1.567047000
H	0.589042000	-3.173205000	1.767252000
C	1.571393000	-1.283460000	2.107494000
H	2.360412000	-1.701807000	2.721515000
C	1.548126000	0.085232000	1.839906000
H	2.324292000	0.736632000	2.223979000
C	0.517486000	0.612974000	1.044594000

O	-0.368837000	2.612042000	-0.422787000
O	1.952836000	2.847803000	0.671043000
C	-0.256312000	3.206451000	2.228558000
C	-0.279416000	4.707211000	1.883342000
H	0.732540000	5.098137000	1.749253000
H	-0.751881000	5.242254000	2.713227000
H	-0.857705000	4.895062000	0.975035000
C	0.603522000	2.928424000	3.470094000
H	0.607639000	1.866398000	3.730434000
H	0.175643000	3.480499000	4.313130000
H	1.632836000	3.266288000	3.325249000
C	-1.673216000	2.639616000	2.382543000
H	-2.285886000	2.845425000	1.501729000
H	-2.145317000	3.114032000	3.248720000
H	-1.651709000	1.560927000	2.555552000
RC$_4$			
I	-1.196761000	0.542588000	-0.496126000
O	-7.043973000	-0.548379000	-0.082424000
O	-2.886212000	0.685851000	-1.265201000
S	1.254791000	-1.515432000	1.121228000
C	-1.183824000	-1.589094000	-0.210326000
C	-2.291690000	-2.230012000	-0.758224000
H	-3.050212000	-1.632609000	-1.249643000
C	-2.396967000	-3.622562000	-0.669119000
H	-3.263356000	-4.117015000	-1.090533000
C	-1.384508000	-4.368913000	-0.052936000
H	-1.457740000	-5.448571000	-0.000035000
C	-0.267972000	-3.724738000	0.486884000
H	0.533910000	-4.296303000	0.938146000
C	-0.175732000	-2.325865000	0.422399000
O	1.209508000	-0.113743000	0.566330000
O	2.460315000	-2.350898000	0.862209000
C	0.992013000	-1.386070000	2.960008000
C	2.202977000	-0.589201000	3.481377000
H	3.140564000	-1.114938000	3.282143000
H	2.093139000	-0.474297000	4.564228000
H	2.247702000	0.405064000	3.029823000
C	0.954096000	-2.802606000	3.551193000
H	0.082912000	-3.364004000	3.203022000
H	0.881649000	-2.714367000	4.639966000
H	1.862858000	-3.360747000	3.311893000
C	-0.326726000	-0.638030000	3.190031000
H	-0.305885000	0.360538000	2.746795000
H	-0.479619000	-0.531221000	4.268828000
H	-1.182337000	-1.184226000	2.786688000
C	-5.672591000	-1.026762000	-0.282565000
C	-6.149433000	-3.308149000	1.384139000
C	-5.694462000	-2.399730000	-0.918767000
C	-5.039497000	-1.067968000	1.087733000
C	-5.952982000	-3.519199000	-0.103386000
C	-5.290933000	-2.177482000	1.915448000
C	-5.484990000	-2.569729000	-2.293122000
C	-4.242757000	-0.012914000	1.546604000
C	-6.001023000	-4.793011000	-0.682646000
C	-4.738043000	-2.211434000	3.202075000
C	-5.533229000	-3.846056000	-2.866709000
C	-3.705088000	-0.047311000	2.837094000
C	-5.795276000	-4.958993000	-2.058652000
C	-3.954789000	-1.148125000	3.666433000
H	-5.125044000	-0.320930000	-0.916949000
H	-7.477481000	-0.605278000	-0.950847000
H	-7.207035000	-3.062082000	1.567412000
H	-5.945045000	-4.234118000	1.931348000
H	-5.271680000	-1.701867000	-2.910839000
H	-4.021916000	0.804574000	0.869491000
H	-6.188521000	-5.658710000	-0.054443000
H	-4.919115000	-3.071822000	3.839635000
H	-5.363071000	-3.970881000	-3.930641000
H	-3.087510000	0.772039000	3.189249000
H	-5.828951000	-5.952181000	-2.494024000
H	-3.531203000	-1.184794000	4.664946000
TS1			
I	-0.645706000	-0.247160000	-0.661139000
O	-5.689563000	0.186890000	-1.380373000
O	-3.979137000	-1.113785000	-2.143287000
S	1.569597000	-1.938800000	1.821701000
C	-0.666973000	-2.258281000	0.028361000
C	-1.631297000	-3.084104000	-0.573997000
H	-2.322085000	-2.672214000	-1.300447000
C	-1.707958000	-4.439706000	-0.241589000
H	-2.442747000	-5.067466000	-0.733604000
C	-0.837429000	-4.986233000	0.704622000
H	-0.890935000	-6.037182000	0.962133000
C	0.118252000	-4.171313000	1.308289000
H	0.819042000	-4.584359000	2.021575000
C	0.214546000	-2.806769000	0.979096000
O	2.083641000	-0.853782000	0.938059000
O	2.521012000	-3.007213000	2.253182000
C	0.869460000	-1.179528000	3.376957000
C	2.100907000	-0.678695000	4.156402000
H	2.766769000	-1.503273000	4.420498000
H	1.750328000	-0.201515000	5.077199000
H	2.661265000	0.060739000	3.577270000
C	0.121000000	-2.273255000	4.153689000
H	-0.756312000	-2.630124000	3.607301000
H	-0.221780000	-1.845421000	5.101698000
H	0.772941000	-3.121550000	4.377995000
C	-0.056171000	-0.020143000	2.996273000
H	0.472454000	0.737821000	2.414558000
H	-0.424683000	0.442241000	3.918529000
H	-0.921429000	-0.361389000	2.426083000
C	-5.455624000	-0.992758000	-0.780009000
C	-5.104081000	-3.522065000	0.621957000
C	-6.285595000	-2.150272000	-1.148379000
C	-4.779230000	-1.009901000	0.526918000
C	-6.149105000	-3.369816000	-0.453363000
C	-4.620248000	-2.227284000	1.222638000
C	-7.232100000	-2.025611000	-2.181289000
C	-4.302777000	0.191968000	1.082024000
C	-6.967296000	-4.449072000	-0.811491000
C	-3.970243000	-2.217814000	2.463679000
C	-8.037530000	-3.106781000	-2.529165000
C	-3.670806000	0.188501000	2.321991000
C	-7.903853000	-4.322340000	-1.840801000
C	-3.503121000	-1.021583000	3.013286000
H	-3.209218000	-0.743847000	-1.671043000
H	-4.854424000	-0.077643000	-2.105733000
H	-5.463869000	-4.192628000	1.410148000
H	-4.233185000	-4.027902000	0.177944000
H	-7.322984000	-1.071786000	-2.685751000
H	-4.447245000	1.109924000	0.526086000
H	-6.870664000	-5.389741000	-0.278501000
H	-3.839581000	-3.150551000	3.002946000
H	-8.768100000	-3.008301000	-3.324171000

H	-3.307603000	1.115322000	2.751232000
H	-8.533570000	-5.165943000	-2.102572000
H	-3.013706000	-1.029228000	3.981026000
IM			
I	-0.524498000	-0.687554000	-0.990097000
O	-5.055081000	0.142457000	-0.919525000
O	-3.952635000	-1.674215000	-1.883515000
S	1.639633000	-1.657361000	1.888662000
C	-0.510082000	-2.478580000	0.158060000
C	-1.435574000	-3.451022000	-0.250128000
H	-2.117427000	-3.239001000	-1.062965000
C	-1.500068000	-4.685509000	0.400064000
H	-2.226442000	-5.419658000	0.071267000
C	-0.638226000	-4.968563000	1.461340000
H	-0.678467000	-5.927061000	1.964694000
C	0.284503000	-4.007635000	1.871943000
H	0.974162000	-4.218668000	2.678543000
C	0.354959000	-2.756541000	1.233132000
O	2.138907000	-0.778634000	0.792174000
O	2.619622000	-2.547823000	2.581027000
C	0.844574000	-0.597893000	3.203302000
C	2.015383000	0.166997000	3.850650000
H	2.731629000	-0.518063000	4.310127000
H	1.607077000	0.820620000	4.628147000
H	2.536208000	0.787921000	3.116370000
C	0.151981000	-1.523478000	4.214985000
H	-0.678643000	-2.070397000	3.761490000
H	-0.252634000	-0.904642000	5.022797000
H	0.856865000	-2.236489000	4.650353000
C	-0.148007000	0.363345000	2.540538000
H	0.343279000	0.991936000	1.795076000
H	-0.569100000	1.010340000	3.317783000
H	-0.973673000	-0.169799000	2.065633000
C	-4.925499000	-1.274395000	-0.886804000
C	-5.207765000	-4.009271000	-0.123620000
C	-6.207845000	-2.003413000	-1.265929000
C	-4.460916000	-1.685354000	0.502094000
C	-6.322247000	-3.361380000	-0.917513000
C	-4.585970000	-3.040782000	0.860225000
C	-7.242601000	-1.367953000	-1.958184000
C	-3.885089000	-0.773103000	1.393031000
C	-7.471190000	-4.070113000	-1.288738000
C	-4.127777000	-3.463327000	2.113247000
C	-8.386111000	-2.083162000	-2.330311000
C	-3.434413000	-1.205190000	2.645642000
C	-8.497882000	-3.438189000	-1.999409000
C	-3.550780000	-2.552796000	3.004347000
H	-3.109612000	-1.254434000	-1.620063000
H	-5.075685000	0.382700000	-1.861760000
H	-5.576855000	-4.897625000	0.398078000
H	-4.429946000	-4.357273000	-0.821783000
H	-7.166033000	-0.312512000	-2.192336000
H	-3.802030000	0.267379000	1.106127000
H	-7.565296000	-5.115718000	-1.011613000
H	-4.225033000	-4.508153000	2.390646000
H	-9.185589000	-1.584056000	-2.867238000
H	-3.004273000	-0.492700000	3.340337000
H	-9.384906000	-3.996469000	-2.279730000
H	-3.205627000	-2.890467000	3.975963000
IM'			
I	-0.486455000	-0.678770000	-0.897772000
O	-4.935045000	0.153884000	-0.781765000
O	-3.881191000	-1.686035000	-1.799919000
S	1.687868000	-1.638012000	1.973486000
C	-0.455590000	-2.474515000	0.244004000
C	-1.375869000	-3.452253000	-0.162773000
H	-2.061653000	-3.245279000	-0.973258000
C	-1.430094000	-4.688173000	0.485508000
H	-2.154566000	-5.425130000	0.159033000
C	-0.560434000	-4.968498000	1.541156000
H	-0.591804000	-5.928489000	2.042260000
C	0.357706000	-4.002417000	1.949797000
H	1.052589000	-4.210668000	2.752657000
C	0.415563000	-2.748644000	1.314911000
O	2.172374000	-0.745426000	0.881414000
O	2.681440000	-2.519505000	2.657721000
C	0.880261000	-0.597888000	3.296075000
C	2.040710000	0.182440000	3.943581000
H	2.769188000	-0.493382000	4.397543000
H	1.624569000	0.825684000	4.725553000
H	2.549289000	0.815112000	3.210767000
C	0.206140000	-1.539590000	4.305410000
H	-0.617459000	-2.097488000	3.852377000
H	-0.204759000	-0.931413000	5.118103000
H	0.923905000	-2.243640000	4.734224000
C	-0.129813000	0.350729000	2.641190000
H	0.349470000	0.992485000	1.899143000
H	-0.560463000	0.985450000	3.423260000
H	-0.947132000	-0.192954000	2.163727000
C	-4.869373000	-1.250676000	-0.787139000
C	-5.233454000	-4.013164000	-0.131861000
C	-6.163899000	-1.934736000	-1.207494000
C	-4.411764000	-1.740277000	0.577873000
C	-6.321913000	-3.299927000	-0.905855000
C	-4.580935000	-3.102755000	0.886124000
C	-7.171879000	-1.245320000	-1.888820000
C	-3.805524000	-0.880861000	1.500305000
C	-7.489386000	-3.960350000	-1.307882000
C	-4.135568000	-3.585878000	2.121928000
C	-8.333007000	-1.913594000	-2.291804000
C	-3.365852000	-1.373330000	2.734357000
C	-8.490713000	-3.273927000	-2.003811000
C	-3.526264000	-2.728580000	3.043842000
H	-3.033290000	-1.282101000	-1.522939000
H	-4.960985000	0.440678000	-1.732151000
H	-5.635574000	-4.905627000	0.357682000
H	-4.464981000	-4.364527000	-0.839013000
H	-7.048148000	-0.191980000	-2.105072000
H	-3.692737000	0.166008000	1.249178000
H	-7.617257000	-5.011353000	-1.066697000
H	-4.267862000	-4.636308000	2.361604000
H	-9.110876000	-1.374004000	-2.821424000
H	-2.912149000	-0.701363000	3.454016000
H	-9.392461000	-3.795021000	-2.308095000
H	-3.189398000	-3.113296000	4.000819000
O	-4.735232000	0.319246000	-3.448511000
H	-4.135041000	0.876582000	-3.975389000
H	-4.333921000	-0.567754000	-3.281962000
TS2			
I	-0.433030000	-0.606030000	-0.868770000
O	-5.195768000	0.239216000	-0.844905000
O	-3.829814000	-1.653273000	-1.918410000
S	1.695102000	-1.741365000	1.977370000
C	-0.463834000	-2.443591000	0.203796000

C	-1.400606000	-3.382701000	-0.255641000
H	-2.060212000	-3.131782000	-1.076444000
C	-1.501537000	-4.637106000	0.350674000
H	-2.233173000	-5.346397000	-0.018864000
C	-0.668296000	-4.972997000	1.419504000
H	-0.738602000	-5.946386000	1.889929000
C	0.268333000	-4.047480000	1.877095000
H	0.940731000	-4.302301000	2.685581000
C	0.378508000	-2.778108000	1.281003000
O	2.224878000	-0.842827000	0.912021000
O	2.644425000	-2.685775000	2.640456000
C	0.933925000	-0.701450000	3.326515000
C	2.125776000	0.020679000	3.984382000
H	2.832167000	-0.691941000	4.416498000
H	1.738066000	0.658902000	4.784873000
H	2.652188000	0.652338000	3.263482000
C	0.230589000	-1.639991000	4.318271000
H	-0.609590000	-2.162520000	3.853917000
H	-0.161762000	-1.035195000	5.142528000
H	0.925361000	-2.375077000	4.732469000
C	-0.043663000	0.297494000	2.698715000
H	0.454517000	0.937025000	1.967296000
H	-0.446442000	0.930532000	3.496874000
H	-0.883155000	-0.205616000	2.215030000
C	-5.167268000	-1.064500000	-0.646329000
C	-5.185572000	-3.879909000	-0.035516000
C	-6.274788000	-1.911748000	-1.179093000
C	-4.549023000	-1.530396000	0.625701000
C	-6.299083000	-3.284698000	-0.864347000
C	-4.588307000	-2.901396000	0.947076000
C	-7.300028000	-1.346986000	-1.951361000
C	-3.958636000	-0.612962000	1.507124000
C	-7.349426000	-4.075424000	-1.344808000
C	-4.032871000	-3.332127000	2.157409000
C	-8.340904000	-2.145540000	-2.428465000
C	-3.416320000	-1.053930000	2.715768000
C	-8.364375000	-3.512941000	-2.125878000
C	-3.451566000	-2.416830000	3.039629000
H	-3.035002000	-1.237747000	-1.532286000
H	-5.126400000	0.410045000	-1.974778000
H	-5.533672000	-4.778227000	0.484021000
H	-4.387408000	-4.206459000	-0.721377000
H	-7.275064000	-0.288282000	-2.174354000
H	-3.944416000	0.435762000	1.237742000
H	-7.374643000	-5.132840000	-1.100489000
H	-4.057203000	-4.387374000	2.408319000
H	-9.131437000	-1.705150000	-3.025970000
H	-2.978745000	-0.341976000	3.405800000
H	-9.174880000	-4.136479000	-2.488104000
H	-3.037044000	-2.763155000	3.980369000
O	-4.747725000	0.152089000	-3.184298000
H	-4.214595000	0.809135000	-3.662438000
H	-4.189380000	-0.812814000	-2.765086000
PC_4			
I	-0.529336000	-0.353081000	-0.555150000
O	-5.814065000	0.369639000	-0.914786000
O	-3.543499000	-1.723403000	-2.253741000
S	1.748256000	-1.832349000	2.013067000
C	-0.469338000	-2.326295000	0.238222000
C	-1.395155000	-3.218845000	-0.326660000
H	-2.061170000	-2.884049000	-1.112981000
C	-1.463858000	-4.541521000	0.118968000
H	-2.184169000	-5.215712000	-0.330696000
C	-0.609662000	-4.993163000	1.128002000
H	-0.656584000	-6.018742000	1.474264000
C	0.326581000	-4.118199000	1.676434000
H	1.024971000	-4.464501000	2.426761000
C	0.406174000	-2.781897000	1.242372000
O	2.211915000	-0.781775000	1.062839000
O	2.740841000	-2.845748000	2.483507000
C	1.054107000	-1.008335000	3.535207000
C	2.265842000	-0.330189000	4.203349000
H	3.023132000	-1.063881000	4.489704000
H	1.916082000	0.181942000	5.105496000
H	2.719734000	0.410369000	3.539252000
C	0.453783000	-2.094805000	4.439848000
H	-0.392812000	-2.596989000	3.963857000
H	0.092646000	-1.616875000	5.356491000
H	1.202060000	-2.842615000	4.714023000
C	0.003543000	0.022251000	3.110044000
H	0.432647000	0.781610000	2.453090000
H	-0.377980000	0.516126000	4.010366000
H	-0.841440000	-0.444723000	2.600827000
C	-5.739668000	-0.799245000	-0.478176000
C	-5.100123000	-3.582378000	0.148581000
C	-6.544876000	-1.891798000	-1.061713000
C	-4.885502000	-1.117840000	0.685373000
C	-6.273301000	-3.234181000	-0.729382000
C	-4.608403000	-2.458273000	1.021981000
C	-7.603836000	-1.579816000	-1.934037000
C	-4.362576000	-0.068660000	1.462813000
C	-7.070191000	-4.244755000	-1.285075000
C	-3.810832000	-2.723512000	2.144365000
C	-8.390499000	-2.591511000	-2.476791000
C	-3.583931000	-0.345253000	2.582283000
C	-8.120986000	-3.929629000	-2.149467000
C	-3.309818000	-1.679436000	2.923671000
H	-3.093258000	-1.040301000	-1.732438000
H	-5.582479000	0.320396000	-2.704139000
H	-5.326655000	-4.465395000	0.756052000
H	-4.270866000	-3.873016000	-0.515287000
H	-7.797468000	-0.539845000	-2.167864000
H	-4.588237000	0.950897000	1.173733000
H	-6.863770000	-5.281196000	-1.037158000
H	-3.581018000	-3.751560000	2.403260000
H	-9.208557000	-2.347853000	-3.145275000
H	-3.191481000	0.463788000	3.187701000
H	-8.732676000	-4.723040000	-2.565580000
H	-2.709358000	-1.901551000	3.799060000
O	-5.161593000	0.020221000	-3.548041000
H	-4.773990000	0.779454000	-4.018827000
H	-4.107997000	-1.195536000	-2.872372000

6. Thioanisole sulfoxidation by ^{s}PhIO

RC_{sPhIO}

I	9.239764000	4.050959000	5.866568000
O	9.994614000	3.841725000	7.555385000
O	7.926389000	3.932762000	3.489868000
O	6.240453000	2.269044000	2.464510000
S	7.558920000	2.520342000	3.109457000
C	8.290975000	2.125356000	5.759793000
C	7.642790000	1.599105000	4.636518000
C	7.034412000	0.337423000	4.707861000
H	6.504772000	-0.053751000	3.847824000
C	7.106462000	-0.396368000	5.894340000
H	6.650464000	-1.377183000	5.946932000
C	7.768568000	0.133493000	7.007359000
H	7.836301000	-0.439768000	7.923564000
C	8.357613000	1.401384000	6.947166000
H	8.882428000	1.829356000	7.795908000
C	8.905155000	1.884319000	1.991215000
C	10.249243000	2.104938000	2.699829000
H	11.044980000	1.713797000	2.057855000
H	10.295046000	1.575780000	3.654679000
H	10.439368000	3.166027000	2.874735000
C	8.795637000	2.729717000	0.708262000
H	9.583127000	2.407405000	0.019864000
H	8.935612000	3.792837000	0.920876000
H	7.828032000	2.587005000	0.220494000
C	8.639512000	0.398128000	1.708753000
H	9.392746000	0.047106000	0.995985000
H	7.652294000	0.247691000	1.264256000
H	8.723610000	-0.210059000	2.612758000
S	11.493775000	0.108354000	8.520544000
C	10.983210000	-0.776934000	7.060862000
C	11.147176000	-0.299659000	5.750834000
C	10.369179000	-2.029297000	7.263031000
C	10.710780000	-1.070509000	4.666064000
C	9.923538000	-2.782547000	6.176261000
C	10.092849000	-2.307970000	4.868746000
C	12.286822000	1.619987000	7.865276000
H	11.606380000	0.663668000	5.568601000
H	10.239488000	-2.407077000	8.272437000
H	10.862698000	-0.700828000	3.658087000
H	9.448009000	-3.742207000	6.350611000
H	9.753062000	-2.895710000	4.023018000
H	11.545391000	2.321820000	7.469171000
H	13.049837000	1.370713000	7.124126000
H	12.775898000	2.086431000	8.724507000

TS_{sPhIO}

I	9.228008000	3.529736000	6.084565000
O	10.365895000	2.453967000	7.545844000
O	7.690122000	3.987557000	3.463056000
O	6.146964000	2.331361000	2.246999000
S	7.411033000	2.594416000	2.997398000
C	8.080842000	1.784233000	5.636216000
C	7.403572000	1.515131000	4.436433000
C	6.664290000	0.325816000	4.307606000
H	6.121099000	0.141763000	3.389403000
C	6.621510000	-0.594495000	5.355163000
H	6.052197000	-1.509731000	5.243831000
C	7.313583000	-0.328151000	6.541389000
H	7.299921000	-1.042526000	7.355895000
C	8.036628000	0.858116000	6.683901000
H	8.607342000	1.076898000	7.577977000
C	8.829449000	2.034722000	1.921037000
C	10.138119000	2.187782000	2.705832000
H	10.965467000	1.877156000	2.059276000
H	10.149630000	1.554303000	3.596236000
H	10.305741000	3.223236000	3.009123000
C	8.792768000	2.971371000	0.698414000
H	9.610918000	2.691804000	0.027013000
H	8.928962000	4.014573000	0.995493000
H	7.849093000	2.875845000	0.155228000
C	8.583521000	0.573861000	1.515288000
H	9.378532000	0.272393000	0.825332000
H	7.623645000	0.458010000	1.005937000
H	8.613232000	-0.097157000	2.378273000
S	11.543920000	0.914940000	8.505983000
C	11.080681000	-0.326317000	7.312164000
C	11.085946000	-0.052655000	5.934735000
C	10.617714000	-1.565978000	7.777680000
C	10.656970000	-1.026200000	5.030821000
C	10.161063000	-2.526731000	6.867079000
C	10.185886000	-2.262309000	5.493467000
C	13.112334000	1.547511000	7.825287000
H	11.386618000	0.926946000	5.586987000
H	10.613747000	-1.775574000	8.841827000
H	10.670019000	-0.814704000	3.966823000
H	9.795964000	-3.480642000	7.232365000
H	9.837504000	-3.009495000	4.788769000
H	12.915582000	2.053589000	6.880535000
H	13.834535000	0.738706000	7.696961000
H	13.496811000	2.273728000	8.545133000

PC_{sPhIO}

I	9.351359000	4.092459000	5.197043000
O	10.808069000	1.819183000	8.930075000
O	7.305384000	3.708293000	2.715204000
O	5.854848000	1.626958000	2.369185000
S	7.155683000	2.227442000	2.795932000
C	8.198945000	2.329838000	5.481098000
C	7.405914000	1.688703000	4.510011000
C	6.677533000	0.536591000	4.860251000
H	6.049964000	0.071149000	4.111831000
C	6.739291000	0.016486000	6.151918000
H	6.171556000	-0.871462000	6.403284000
C	7.526697000	0.654785000	7.112991000
H	7.585876000	0.263944000	8.122467000
C	8.249084000	1.804034000	6.782205000
H	8.872830000	2.277629000	7.530045000
C	8.485095000	1.423835000	1.761729000
C	9.844003000	2.017410000	2.145652000
H	10.609178000	1.568631000	1.502842000
H	10.104668000	1.792438000	3.181155000
H	9.860895000	3.099840000	2.003171000
C	8.113101000	1.770651000	0.307131000
H	8.871185000	1.335606000	-0.352128000
H	8.099008000	2.852810000	0.150187000
H	7.137487000	1.359064000	0.038165000
C	8.438461000	-0.092221000	2.005162000
H	9.164611000	-0.567277000	1.336982000
H	7.449629000	-0.501174000	1.782239000
H	8.711382000	-0.347408000	3.032459000
S	10.701380000	0.314043000	8.722613000
C	11.046207000	-0.007187000	6.969897000
C	11.699132000	0.973743000	6.220302000

C	10.603942000	-1.197941000	6.385574000
C	11.942980000	0.743097000	4.863112000
C	10.848719000	-1.420642000	5.025734000
C	11.521328000	-0.453372000	4.267477000
C	12.251729000	-0.408415000	9.378762000
H	11.984692000	1.904732000	6.696521000
H	10.067752000	-1.934668000	6.975336000
H	12.449001000	1.497221000	4.270481000
H	10.509733000	-2.339117000	4.559248000
H	11.703124000	-0.625255000	3.212367000
H	13.099528000	0.125488000	8.942997000
H	12.293320000	-1.469709000	9.122357000
H	12.243077000	-0.283446000	10.463720000

7. The C-H bond activation of 9,10-dihydroanthracene by ^{s}PhIO

RC'$_{sPhIO}$			
I	9.239764000	4.050959000	5.866568000
O	9.994614000	3.841725000	7.555385000
O	7.926389000	3.932762000	3.489868000
O	6.240453000	2.269044000	2.464510000
S	7.558920000	2.520342000	3.109457000
C	8.290975000	2.125356000	5.759793000
C	7.642790000	1.599105000	4.636518000
C	7.034412000	0.337423000	4.707861000
H	6.504772000	-0.053751000	3.847824000
C	7.106462000	-0.396368000	5.894340000
H	6.650464000	-1.377183000	5.946932000
C	7.768568000	0.133493000	7.007359000
H	7.836301000	-0.439768000	7.923564000
C	8.357613000	1.401384000	6.947166000
H	8.882428000	1.829356000	7.795908000
C	8.905155000	1.884319000	1.991215000
C	10.249243000	2.104938000	2.699829000
H	11.044980000	1.713797000	2.057855000
H	10.295046000	1.575780000	3.654679000
H	10.439368000	3.166027000	2.874735000
C	8.795637000	2.729717000	0.708262000
H	9.583127000	2.407405000	0.019864000
H	8.935612000	3.792837000	0.920876000
H	7.828032000	2.587005000	0.220494000
C	8.639512000	0.398128000	1.708753000
H	9.392746000	0.047106000	0.995985000
H	7.652294000	0.247691000	1.264256000
H	8.723610000	-0.210059000	2.612758000
S	11.493775000	0.108354000	8.520544000
C	10.983210000	-0.776934000	7.060862000
C	11.147176000	-0.299659000	5.750834000
C	10.369179000	-2.029297000	7.263031000
C	10.710780000	-1.070509000	4.666064000
C	9.923538000	-2.782547000	6.176261000
C	10.092849000	-2.307970000	4.868746000
C	12.286822000	1.619987000	7.865276000
H	11.606380000	0.663668000	5.568601000
H	10.239488000	-2.407077000	8.272437000
H	10.862698000	-0.700828000	3.658087000
H	9.448009000	-3.742207000	6.350611000
H	9.753062000	-2.895710000	4.023018000
H	11.545391000	2.321820000	7.469171000
H	13.049837000	1.370713000	7.124126000
H	12.775898000	2.086431000	8.724507000
TS'$_{sPhIO}$			
I	9.228008000	3.529736000	6.084565000
O	10.365895000	2.453967000	7.545844000
O	7.690122000	3.987557000	3.463056000
O	6.146964000	2.331361000	2.246999000
S	7.411033000	2.594416000	2.997398000
C	8.080842000	1.784233000	5.636216000
C	7.403572000	1.515131000	4.436433000
C	6.664290000	0.325816000	4.307606000
H	6.121099000	0.141763000	3.389403000
C	6.621510000	-0.594495000	5.355163000
H	6.052197000	-1.509731000	5.243831000
C	7.313583000	-0.328151000	6.541389000
H	7.299921000	-1.042526000	7.355895000
C	8.036628000	0.858116000	6.683901000
H	8.607342000	1.076898000	7.577977000
C	8.829449000	2.034722000	1.921037000
C	10.138119000	2.187782000	2.705832000
H	10.965467000	1.877156000	2.059276000
H	10.149630000	1.554303000	3.596236000
H	10.305741000	3.223236000	3.009123000
C	8.792768000	2.971371000	0.698414000
H	9.610918000	2.691804000	0.027013000
H	8.928962000	4.014573000	0.995493000
H	7.849093000	2.875845000	0.155228000
C	8.583521000	0.573861000	1.515288000
H	9.378532000	0.272393000	0.825332000
H	7.623645000	0.458010000	1.005937000
H	8.613232000	-0.097157000	2.378273000
S	11.543920000	0.914940000	8.505983000
C	11.080681000	-0.326317000	7.312164000
C	11.085946000	-0.052655000	5.934735000
C	10.617714000	-1.565978000	7.777680000
C	10.656970000	-1.026200000	5.030821000
C	10.161063000	-2.526731000	6.867079000
C	10.185886000	-2.262309000	5.493467000
C	13.112334000	1.547511000	7.825287000
H	11.386618000	0.926946000	5.586987000
H	10.613747000	-1.775574000	8.841827000
H	10.670019000	-0.814704000	3.966823000
H	9.795964000	-3.480642000	7.232365000
H	9.837504000	-3.009495000	4.788769000
H	12.915582000	2.053589000	6.880535000
H	13.834535000	0.738706000	7.696961000
H	13.496811000	2.273728000	8.545133000
PC'$_{sPhIO}$			
I	5.824574000	5.299939000	-1.186494000
O	7.600736000	4.424277000	1.910448000
O	3.535664000	4.905287000	-3.395107000
O	1.596594000	3.245357000	-3.184880000
S	3.038293000	3.568300000	-2.960686000
C	4.351731000	3.962484000	-0.428642000
C	3.319120000	3.371320000	-1.181074000
C	2.373048000	2.554917000	-0.535121000
H	1.568005000	2.129794000	-1.119826000
C	2.456345000	2.312478000	0.834994000
H	1.719078000	1.681318000	1.316528000
C	3.492317000	2.887536000	1.573391000
H	3.576675000	2.701387000	2.637713000
C	4.432807000	3.710794000	0.949172000
H	5.241855000	4.134233000	1.530654000
C	4.032715000	2.242882000	-3.820177000
C	5.525339000	2.539555000	-3.639144000
H	6.094773000	1.779279000	-4.184879000
H	5.822888000	2.492704000	-2.589806000
H	5.787872000	3.521654000	-4.037507000
C	3.619046000	2.341208000	-5.301324000
H	4.183582000	1.590969000	-5.864294000
H	3.851399000	3.327835000	-5.711786000
H	2.552015000	2.144613000	-5.428963000
C	3.646814000	0.882751000	-3.219298000
H	4.176562000	0.101311000	-3.774216000
H	2.573274000	0.697807000	-3.308688000
H	3.937685000	0.806462000	-2.168316000
C	6.576778000	1.746943000	3.598596000

C	8.344470000	3.161744000	1.821214000	H	9.210043000	3.313844000	1.164957000
C	7.940861000	2.176290000	4.098323000	H	7.687557000	1.388551000	6.086323000
C	6.589822000	1.382150000	2.129460000	H	5.069348000	-0.132972000	2.283617000
C	8.812916000	2.847831000	3.221620000	H	10.744732000	3.764555000	2.980953000
C	7.466618000	2.062101000	1.262854000	H	8.170842000	2.261813000	-0.762319000
C	8.355231000	1.915289000	5.410986000	H	9.930117000	2.108206000	6.870476000
C	5.743435000	0.393022000	1.614452000	H	5.103449000	-0.693011000	-0.134986000
C	10.079041000	3.247834000	3.665881000	H	11.469953000	3.297094000	5.314255000
C	7.486959000	1.739391000	-0.099795000	H	6.671707000	0.493069000	-1.660818000
C	9.619851000	2.319917000	5.852524000				
C	5.760999000	0.078690000	0.251459000				
C	10.486379000	2.986874000	4.978055000				
C	6.639027000	0.748879000	-0.607917000				
H	6.199112000	0.909713000	4.194684000				
H	5.867738000	2.576999000	3.751801000				
H	7.367939000	4.671542000	0.996245000				

PART XI. References

1.These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via wwwccdccamacuk/data_request/cif

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