SUPPORTING INFORMATION

Untangling the Catalytic Importance of Se Oxidation State in Organoselenium-mediated Oxygen-Transfer Reactions: the Conversion of Aniline to Nitrobenzene

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Additional computational details

The Gibbs free energy of each species in condensed phase (water) was estimated as:

$$G = E(M06) + (ZPE + H_{298.15} - TS_{298.15}) + RT \ln\frac{RT}{P} \tag{S1}$$

where the solvation correction is included in E(M06), ZPE is the zero-point energy, H the correction to enthalpy, – TS the correction due to entropy and the rightmost term is added to convert from the gas phase standard state (1atm) to solution standard state (1M). All energies described in the main text are Gibbs free energies calculated according to equation S1.

The energetic span model has been applied as derived by Kozuch and Shaik. Thus, the TOF of the computed catalytic cycles has been obtained according to equation S2:

$$TOF = \frac{k_BT}{h}\frac{1 - e^{\frac{\Delta G_r}{RT}}}{\sum_{i,j=1}^{N} e^{(T_i - I_j + \delta G_{ij})/RT}} = \frac{\Delta}{M} \tag{S2}$$

Notably, in the limit of a single couple of T_i and I_j which dominate in the denominator of equation S2, equation S2 is reduced to the simplified Eyring-like equation S3:

$$TOF = \frac{k_BT}{h}e^{-\frac{\delta E}{RT}} \tag{S3}$$

in which δE is the so-called energetic span of the catalytic cycle and is defined by the energies of the rate determining states, i.e., the TOF determining transition state (TDTS) and TOF determining intermediate (TDI), the two states with the strongest impact on the denominator of equation S2. The identification of these two states has been done according to the concept of degree of TOF control introduced by Kozuch and Shaik, thus associating to each intermediate and to each transition state a quantitative index $X_{TOF,i}$ ($0 < X_{TOF,i} < 1$) according to equations S4:

$$X_{TOF,i} = \left|\frac{1}{TOF}\frac{\partial TOF}{\partial E_i}\right| \tag{S4}$$

The TDI and TDTS have been identified as the species with the degree of TOF control $X_{TOF,i}$ closest to 1. In the case of two species with similar contributions to the TOF, according to the degree of TOF control index (e.g. $X_{TOF,i1} = 0.4$ and $X_{TOF,i2} = 0.6$), the relative contribution has been specified for clarity. All references have been cited in the main text.

The EDA-NOCV was used to identify and characterize the strongest orbital interaction. The NOCV are the eigenvectors of the one-electron deformation density matrix ΔP, and are always coupled in complementary pairs ($\varphi_{\pm k}$) associated to eigenvalues equal in absolute value but with opposed sign ($\pm v_k$). The NOCV can be employed to define a deformation density according to Eq. S5:

$$\Delta\rho = \sum_k \Delta\rho_k = \sum_k v_k\left(|\varphi_k|^2 - |\varphi_{-k}|^2\right) \tag{S5}$$

Thus, the eigenvalue v_k can be interpreted as the fraction of charge which is transferred from one NOCV to the complementary one (φ_{-k} and φ_k) when the orbitals of the two fragments are allowed to mix during bond formation.

Within this formalism, the total orbital interaction can be partitioned into pairwise contributions associated to each different NOCV pair k (Eq. S6)

$$\Delta E_{OI} = \sum_k \Delta E_{OI}^{\ k} \tag{S6}$$

Thus, the strongest orbital interaction can be quantitatively identified. In ADF the meta-hybrid correction employed in M06 functional cannot be further decomposed in the NOCV scheme. Thus, its contribution is listed separately, and all $\Delta E_{OI}^{\ k}$ does not sum up to ΔE_{OI}. In any case, the meta-hybrid contribution accounts for only a couple of kcal mol^{-1} and the EDA-NOCV scheme can be still used to identify the interesting interactions as shown in previous studies.[1]

Table S1 Gibbs free energies (kcal mol^{-1}) for the hydrogen peroxide activation step computed at COSMO-ZORA-M06/TZ2P // ZORA-OPBE/TZ2P with different solvents.

		A	TS1	I	TS2	Pox
benzene	Se(IV)	0.00	19.6	11.9	22.7	-4.6
	Se(VI)	0.00	28.3	22.3	30.5	-2.0
dichloromethane	Se(IV)	0.00	21.5	13.6	23.8	-4.7
	Se(VI)	0.00	30.8	23.5	33.0	-1.8
acetonitrile	Se(IV)	0.00	22.1	14.0	24.1	-4.7
	Se(VI)	0.00	31.6	23.8	33.8	-1.7

Table S2 Activation energies (kcal mol^{-1}) for the acid catalyzed conversion of the N-oxides P1-O, P2-O to P1-OH and P2-OH respectively.

	P1-O to P1-OH	P2-O to P2-OH
Se(IV)	- [a]	1.79
Se(VI)	- [a]	- [a]

[a]No transition state could be located for the analogous process.

Table S3 Activation energies (kcal mol^{-1}) for the direct oxidation of P2-OH to the corresponding N-oxide and competitive selenium-catalyzed dehydration to P-NO.

	P2-OH to N-oxide	P2-OH to P-NO
Se(IV)	28.67	16.64
Se(VI)	26.74	14.43

It can be observed that the direct oxidation of P2-OH to the corresponding N-oxide species occurs with a lower activation energy with respect to the oxidation of P-NO to P-NO_2 (e.g., for Se(IV), a $\Delta\Delta G^{\ddagger}$ of ca. 4 kcal mol^{-1} is computed). However, P-NO formation is strongly favored kinetically due to the very low activation energy of the acid catalyzed dehydration of P-OH2 to P-NO. It is also noteworthy that, as reported in the main text, P2-OH to P-NO acid-catalyzed dehydration, beside occurring with a low activation energy, is also exergonic (-28.89 kcal mol^{-1}). Thus, the formation of P-NO is expected to be irreversible, additionally highlighting the role of P-NO intermediates in the conversion from aniline to nitrobenzene.

Table S4 Activation energies[a] (kcal mol^{-1}) for the direct peroxyselenurane (I) oxidation of aniline to aniline N-oxide.

	$\Delta G^{\ddagger}$	$\Delta G^{\ddagger\prime}$
Se(IV)	44.91	58.83
Se(VI)	31.55	55.47

[a]$\Delta G^{\ddagger}$ is computed with respect to the peroxyselenurane (I), while $\Delta G^{\ddagger\prime}$ with respect to the free seleninic and selenonic acids (considering that I is destabilized with respect to the free reactants).

Table S5 Gibbs free energies (kcal mol-1) for the three catalytic cycles computed at COSMO-ZORA-OPBE/TZ2P // ZORA-OPBE/TZ2P.

		A	TS1	I	TS2	Pox	TSox	P1-O	P1-OH
1st Cycle	Se(IV)	0.00	25.47	21.76	26.63	-3.98	22.48	-13.39	-25.25
	Se(VI)	0.00	35.3	31.00	37.47	-1.65	19.35	-13.39	-25.25
		A	TS1	I	TS2	Pox	TSox	P2-O	P2-OH
2nd Cycle	Se(IV)	0.00	25.47	21.76	26.63	-3.98	23.56	-29.36	-34.09
	Se(VI)	0.00	35.3	31.00	37.47	-1.65	23.86	-29.36	-34.09
		A	TS1	I	TS2	Pox	TSox	P-NO2	
3nd Cycle	Se(IV)	0.00	25.47	21.76	26.63	-3.98	25.19	-64.42	
	Se(VI)	0.00	35.3	31.00	37.47	-1.65	24.07	-64.42	

Table S6 TOF ratio for the three catalytic cycles, TDTS and TDI for each cycle (level of theory COSMO-OPBE // OPBE.

		TDTS	TDI	$\frac{TOF^{Se(VI)}}{TOF^{Se(IV)}}$
1st Cycle	Se(IV)	TS2(53%), TSox(40%)	A(60%), Pox(40%)	$2.1\ 10^{-8}$
	Se(VI)	TS2	A	
2nd Cycle	Se(IV)	TS2(17%), TSox(80%)	A(20%), Pox(80%)	$6.5\ 10^{-8}$
	Se(VI)	TS2	A	
3rd Cycle	Se(IV)	TSox	Pox	$8.4\ 10^{-7}$
	Se(VI)	TS2	A	

When compared to the data presented in the main text, OPBE (Table S2 and Table S3) provides a qualitative analogous description of the reaction mechanisms and of the TOF behavior. However, OPBE predicts a more moderate effect of the increasing energetic span for the three Se(IV) catalytic cycles. Indeed, along the three cycles, the rate determining states shifts from being the H_2O_2 activation stage to the substrate oxidation stage. In the 1st cycle, for the Se(IV) catalyzed process both TS2 and TSox have a strong TDTS percentage, with the H_2O_2 activation contributing moderately more to the catalyst performance. However, moving to the second and to third catalytic cycles, the TDTS for the Se(IV) catalyzed process becomes mostly (80%) or totally the TSox, respectively. The effect is the same as the one observed in the main text: the TOF ratio is reduced along the overall mechanism, due to an increase in the activation energy of the substrate oxidation. However, since the three barriers for the substrate oxidations increase less at the OPBE than at the M06 level of theory ($\Delta\Delta G^‡$ between the last and first oxidation of ca. 2.5 and 6 kcal mol^{-1} respectively), the effect is way less relevant with the OPBE functional. Cautiously, we envision the experimental behavior to be somewhere in-between these two pictures. Nevertheless, the important conclusion is that Se(IV) remains consistently a better catalyst than Se(VI), in line with the control experiments reported in the main text. DLPNO-CCSD(T) calculations further corroborate these conclusions (Table S7)

Table S7 DLPNO-CCSD(T) // OPBE Gibbs free energies of critical steps in the catalytic mechanism.

	A	TS1	I	TS2	Pox	$\Delta G^‡$(TSox1)	$\Delta G^‡$(TSox3)
Se(IV)	0.00	22.9	15.2	24.6	-2.4	24.2	30.4
Se(VI)	0.00	31.4	24.1	34.5	0.4	19.2	26.8

Table S8 DLPNO-CCSD(T) // OPBE activation energies (kcal mol^{-1}) of critical reactive steps in the interconversion mechanism. (see scheme 8 and relative discussion)

	TSa	TSc
	50.06	33.4

Table S9 DLPNO-CCSD(T) // OPBE activation energies (kcal mol^{-1}) for the solvent assisted TS2 and TSox1.

	TS2	TSox1
Se(IV)	24.2	27.1
Se(VI)	32.1	21.7

Table S10 Absolute TOF (s^{-1}) values computed at M06 // OPBE.

1st Cycle	Se(IV)	$2.5 \cdot 10^{-7}$
	Se(VI)	$7.9 \cdot 10^{-13}$
2nd Cycle	Se(IV)	$2.5 \cdot 10^{-9}$
	Se(VI)	$7.9 \cdot 10^{-13}$
3nd Cycle	Se(IV)	$6.4 \cdot 10^{-12}$
	Se(VI)	$7.9 \cdot 10^{-13}$

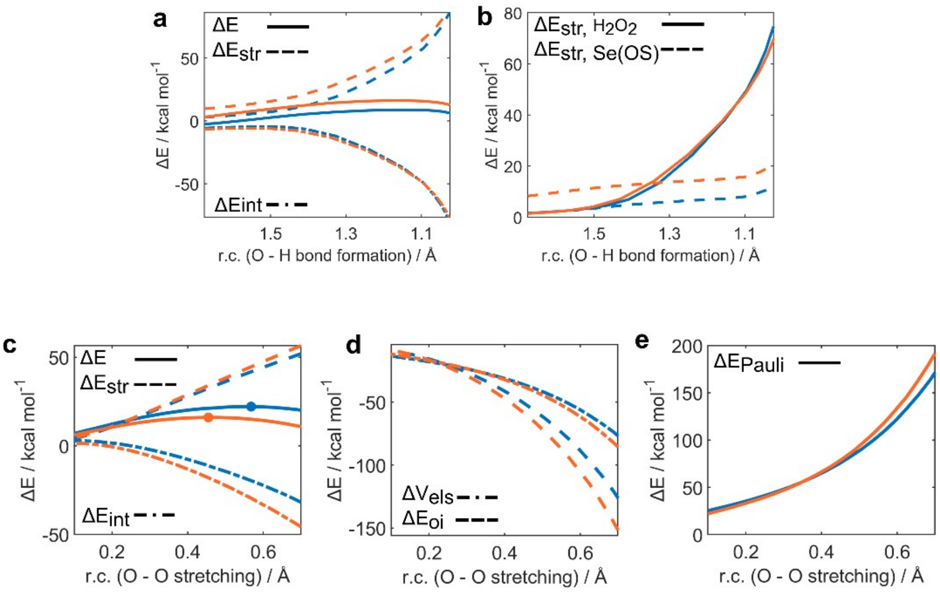

Figure S1 Activation strain and energy decomposition analysis of (**a, b**) H_2O_2 addition to seleninic (blue) and selenonic (orange) acids and (**c–e**) of aniline oxidation to aniline N-oxide (P1-O) by peroxyseleninic (blue) and peroxyselenonic (orange) acids, along the complementary reaction coordinates (r.c.) to Figure 4.

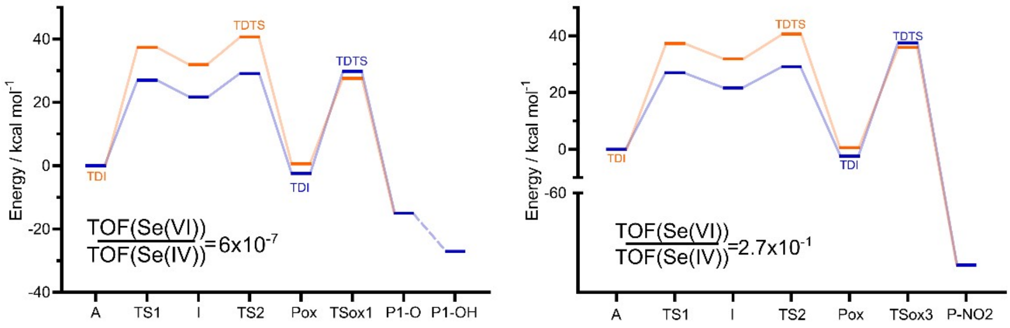

Figure S2 Gibbs free energy profile, and calculated TDI and TDTS for the 1st and 3rd catalytic cycle and relative TOF ratio: Se(IV) mediated process (blue); Se(VI) mediated process (orange). Level of theory: COSMO-OPBE0 // OPBE.

Analogous conclusions can be drawn by calculations carried out at the COSMO-OPBE0//OPBE level of theory. The results are, in this case, closer to COSMO-M06 // OPBE description of the mechanism.

Table S11: Cartesian coordinates (Å), energies (kcal mol^{-1}) and imaginary frequencies (cm^{-1}) of the optimized structures. Level of theory: COSMO-ZORA-M06/TZ2P-ae // ZORA-OPBE/TZ2P.

Main Mechanism

H_2O_2
E= -569.11
Nimag=0

O	-0.017100000	-0.718700000	-0.823300000
O	0.017100000	0.718700000	-0.823300000
H	0.791700000	0.875400000	-0.263300000
H	-0.791700000	-0.875400000	-0.263300000

Aniline
E= -2396.33
Nimag=0

C	-11.181000000	5.302100000	-1.140900000
C	-12.010500000	5.682500000	-0.090000000
C	-10.004300000	4.617800000	-0.850700000
H	-12.935800000	6.220000000	-0.293000000
H	-9.338900000	4.311300000	-1.656700000
C	-11.675700000	5.387400000	1.224400000
C	-9.659600000	4.317500000	0.460000000
H	-12.340800000	5.689400000	2.032900000
H	-8.736500000	3.776800000	0.666300000
C	-10.491500000	4.698200000	1.522900000
H	-11.446800000	5.535900000	-2.169300000
N	-10.183600000	4.344900000	2.829900000
H	-10.601500000	4.930000000	3.537800000
H	-9.202800000	4.188300000	3.007900000

A(Se(IV))
E= -2552.98
Nimag=0

Se	1.180800000	0.219500000	-0.744900000
O	1.584800000	1.730300000	-0.298700000
C	-0.721500000	0.123000000	-0.285900000
C	-1.341200000	1.255300000	0.225500000
C	-1.430600000	-1.050300000	-0.526100000
C	-2.700000000	1.203600000	0.523000000
C	-2.789000000	-1.090400000	-0.228400000
C	-3.420800000	0.034400000	0.296500000
H	-0.754200000	2.158400000	0.384000000
H	-0.934300000	-1.930700000	-0.932700000
H	-3.198300000	2.082600000	0.929000000
H	-3.355600000	-2.002800000	-0.406900000
H	-4.484400000	-0.000500000	0.526200000
O	1.776000000	-0.910000000	0.552600000
H	1.498300000	-0.516200000	1.394200000

A(Se(VI))
E=-2733.96
Nimag=0

Se	1.585300000	-1.505500000	-0.524600000
O	1.656200000	-3.070800000	-0.192400000
C	3.241400000	-0.673300000	-0.001900000
C	4.008500000	-1.283900000	0.981500000
C	3.623400000	0.501200000	-0.636500000
C	5.205000000	-0.677100000	1.348600000
C	4.825600000	1.089300000	-0.257300000
C	5.609900000	0.503700000	0.732500000
H	3.682300000	-2.214200000	1.439000000
H	3.002500000	0.935200000	-1.416100000
H	5.824600000	-1.135500000	2.117000000
H	5.150300000	2.007400000	-0.743000000
H	6.549700000	0.969600000	1.023000000
O	1.114000000	-0.953700000	-1.961400000
O	0.456800000	-0.784100000	0.661100000
H	-0.165000000	-0.289800000	0.102600000

H_2O
E= -423.38
Nimag=0

O	0.000000000	0.000000000	-0.803100000
H	0.000000000	0.756600000	-0.208100000
H	0.000000000	-0.756600000	-0.208100000

TS1 (SeIV)
E=-3107.90
Nimag=-737

Se	0.932700000	-0.096000000	-0.957400000
O	-0.193000000	-1.387500000	-1.137000000
C	0.066300000	1.041800000	0.352200000
C	0.664600000	2.264900000	0.639100000
C	-1.107300000	0.641600000	0.977500000
C	0.073000000	3.100900000	1.580300000
C	-1.686700000	1.485400000	1.920100000
C	-1.099700000	2.710900000	2.220700000
H	1.583600000	2.570100000	0.140700000
H	-1.562700000	-0.313000000	0.724800000
H	0.531600000	4.060400000	1.812900000
H	-2.606900000	1.183400000	2.417500000
H	-1.560300000	3.368000000	2.956200000
O	2.038300000	-0.940000000	0.225600000
H	1.486900000	-1.339500000	0.914000000
O	-0.718300000	0.481400000	-2.417800000
O	-0.193700000	0.436900000	-3.749000000
H	-0.443500000	1.319200000	-4.056100000
H	-0.708300000	-0.731900000	-1.932900000

TS1(SeVI)
E=-3279.37
Nimag=-877

Se	0.575279000	-2.032717000	-0.816489000
O	1.852058000	-3.289801000	-0.785716000
C	1.769609000	-0.610549000	-0.297750000
C	2.228956000	-0.567735000	1.009700000
C	2.125633000	0.315675000	-1.265773000
C	3.096037000	0.464443000	1.355155000
C	2.997234000	1.334545000	-0.895523000
C	3.478778000	1.408960000	0.408025000
H	1.922493000	-1.309998000	1.741649000
H	1.734091000	0.250713000	-2.277436000
H	3.471228000	0.525049000	2.374861000
H	3.294731000	2.075734000	-1.634685000
H	4.156734000	2.212444000	0.689075000
O	0.115539000	-2.139321000	-2.367326000
O	-0.314921000	-2.690447000	0.481845000
H	-1.051720000	-1.809089000	0.301919000
O	-1.027531000	-0.697128000	-0.383120000
O	-1.972967000	-0.598556000	-1.445622000
H	-1.535776000	-1.158183000	-2.120942000
H	1.692440000	-3.791005000	-1.600275000

I(SeIV)
E=-2633.91
Nimag=0

Se	0.570500000	-1.894000000	-1.152000000
O	1.838600000	-3.195600000	-0.684600000
C	1.794000000	-0.572500000	-0.454300000
C	2.230600000	-0.647700000	0.862300000
C	2.227400000	0.434400000	-1.309200000
C	3.119300000	0.314600000	1.329200000
C	3.128600000	1.381900000	-0.833400000
C	3.570600000	1.324400000	0.484200000
H	1.882500000	-1.446400000	1.510700000
H	1.868700000	0.489800000	-2.334400000
H	3.463600000	0.270100000	2.361000000
H	3.478700000	2.171300000	-1.495900000
H	4.269900000	2.071600000	0.855400000
O	-0.381100000	-2.393800000	0.277800000
H	-1.076900000	-1.710800000	0.276600000
O	-0.728600000	-0.363100000	-1.289600000
O	-1.790500000	-0.874100000	-2.114200000
H	-1.623000000	-0.400700000	-2.941500000
H	1.466700000	-4.031200000	-0.998700000

I(SeVI)
E= -3290.22
Nimag=0

Se	0.819600000	-2.140100000	-1.232200000
O	2.143500000	-3.332500000	-0.891800000
C	1.856900000	-0.677700000	-0.496200000
C	2.182200000	-0.664300000	0.851200000
C	2.243300000	0.322300000	-1.376100000
C	2.923500000	0.409700000	1.334600000
C	2.997600000	1.378500000	-0.874400000
C	3.331700000	1.425200000	0.475400000
H	1.874700000	-1.469200000	1.512700000
H	1.968700000	0.275100000	-2.426400000
H	3.187400000	0.444400000	2.390000000
H	3.320800000	2.169800000	-1.548200000
H	3.916600000	2.258200000	0.860700000
O	0.800200000	-2.268100000	-2.834000000
O	-0.116300000	-3.018200000	0.004800000
H	-0.881400000	-2.399900000	0.152800000
O	-0.733500000	-0.955400000	-1.406400000
O	-1.541200000	-0.890000000	-0.209600000
H	-2.403300000	-1.111700000	-0.594500000
H	1.816400000	-3.878800000	-0.164400000

TS2(SeIV)
E= -3106.29
Nimag=-871

Se	0.416900000	-1.782900000	-1.122900000
O	1.966300000	-3.353300000	-1.114200000
C	1.731600000	-0.542900000	-0.442400000
C	1.943900000	-0.439200000	0.925000000
C	2.431300000	0.236700000	-1.356200000
C	2.885100000	0.475900000	1.385600000
C	3.371400000	1.145400000	-0.882100000
C	3.596500000	1.264600000	0.486300000
H	1.385100000	-1.068300000	1.613100000
H	2.258600000	0.139600000	-2.427000000
H	3.062900000	0.570500000	2.455400000
H	3.931200000	1.758900000	-1.585700000
H	4.334100000	1.975900000	0.853700000
O	0.111900000	-2.846900000	0.192800000
H	1.019400000	-3.436800000	-0.216300000
O	-0.894700000	-0.504700000	-0.666200000
O	-2.127300000	-0.991300000	-1.218500000
H	-2.251800000	-0.366300000	-1.949000000
H	1.775400000	-3.955300000	-1.844300000

TS2(SeVI)
E= -3278.17
Nimag=959

Se	0.779000000	-2.071500000	-1.304300000
O	2.402300000	-3.364300000	-0.918900000
C	1.827700000	-0.643700000	-0.522900000
C	2.103900000	-0.636600000	0.834800000
C	2.251000000	0.348600000	-1.393700000
C	2.845300000	0.427500000	1.338500000
C	2.996200000	1.399200000	-0.867000000
C	3.290100000	1.438700000	0.492300000
H	1.756500000	-1.433200000	1.485500000
H	2.011900000	0.304500000	-2.453100000
H	3.075300000	0.460700000	2.401700000
H	3.345100000	2.189700000	-1.528700000
H	3.871500000	2.265300000	0.896300000
O	0.862800000	-2.268200000	-2.897100000
O	0.243200000	-3.246800000	-0.173500000
H	1.306700000	-3.701200000	-0.329500000
O	-0.836500000	-1.166400000	-1.351800000
O	-1.254800000	-0.808100000	-0.040800000
H	-1.700200000	-1.623900000	0.241200000
H	2.509000000	-3.836600000	-1.755400000

Pox(SeIV)
E= -2703.16
Nimag=0

Se	1.136500000	0.069400000	-0.599600000
O	1.618100000	1.543600000	-0.106400000
C	-0.769600000	0.052600000	-0.222300000
C	-1.367300000	1.190800000	0.301200000
C	-1.507900000	-1.084200000	-0.536800000
C	-2.739700000	1.183200000	0.528100000
C	-2.879100000	-1.080600000	-0.305000000
C	-3.492200000	0.051300000	0.226400000
H	-0.755500000	2.062300000	0.524300000
H	-1.025100000	-1.970400000	-0.947200000
H	-3.223500000	2.066200000	0.942400000
H	-3.469900000	-1.964400000	-0.539400000
H	-4.566200000	0.051000000	0.404500000
O	1.691200000	-1.116300000	0.757400000
O	1.333800000	-0.636000000	2.040400000
H	2.007400000	0.049100000	2.185800000

Pox(SeVI)
E= -2881.28
Nimag=0

Se	1.186800000	-0.082100000	0.076700000
O	-0.078500000	-0.808300000	0.753200000
C	1.130800000	1.803900000	0.470800000
C	-0.031500000	2.338000000	1.010400000
C	2.262200000	2.565300000	0.204600000
C	-0.054400000	3.700400000	1.292000000
C	2.216400000	3.924600000	0.492900000
C	1.062800000	4.488300000	1.032200000
H	-0.888900000	1.702000000	1.212300000
H	3.157300000	2.106600000	-0.207300000
H	-0.952000000	4.144600000	1.718000000
H	3.089400000	4.544000000	0.296400000
H	1.036100000	5.553500000	1.255000000
O	0.930200000	-0.147700000	-1.761000000
O	-0.393500000	0.253100000	-2.070400000
H	-0.882400000	-0.576300000	-1.937700000
O	2.683600000	-0.643200000	0.211600000

TSox1(SeIV)
E=-5085.02
Nimag=

C	-9.669200000	5.562000000	-1.544400000
C	-11.021000000	5.734700000	-1.258600000
C	-8.803000000	5.121100000	-0.547900000
H	-11.705700000	6.069400000	-2.035200000
H	-7.746700000	4.976700000	-0.765500000
C	-11.510300000	5.474000000	0.012700000
C	-9.278000000	4.858200000	0.728700000
H	-12.571500000	5.584100000	0.227500000
H	-8.602200000	4.501600000	1.504000000
C	-10.632600000	5.045700000	1.011100000
H	-9.292500000	5.764500000	-2.544700000
N	-11.123600000	4.756300000	2.296400000
H	-11.956900000	5.269000000	2.561000000
H	-10.430300000	4.778900000	3.032500000
Se	-14.129000000	1.665600000	2.912500000
O	-14.230600000	3.051300000	1.983600000
C	-14.403400000	2.406000000	4.726300000
C	-15.277900000	3.471800000	4.905100000
C	-13.767700000	1.814300000	5.812000000
C	-15.509800000	3.958900000	6.189300000
C	-14.001900000	2.307200000	7.093000000
C	-14.873100000	3.377000000	7.282200000
H	-15.758700000	3.927900000	4.041200000
H	-13.074000000	0.990100000	5.653800000
H	-16.190000000	4.797100000	6.336700000
H	-13.498800000	1.855600000	7.947200000
H	-15.056200000	3.758600000	8.285500000
O	-12.470500000	1.290300000	2.956900000
O	-11.651800000	3.096600000	2.612900000
H	-12.567100000	3.213800000	2.211700000

TSox1(SeVI)
E=-5269.11
Nimag=

C	-12.595700000	5.981700000	-2.897500000
C	-13.792800000	6.069700000	-2.192600000
C	-11.385300000	6.032500000	-2.211800000
H	-14.743200000	6.021200000	-2.720100000
H	-10.445500000	5.956900000	-2.754900000
C	-13.787400000	6.211700000	-0.812800000
C	-11.365400000	6.174400000	-0.832200000
H	-14.726000000	6.260200000	-0.263600000
H	-10.418300000	6.199700000	-0.296400000
C	-12.569500000	6.274200000	-0.131200000
H	-12.606200000	5.867300000	-3.979200000
N	-12.553700000	6.392500000	1.266100000
H	-13.370700000	6.831300000	1.671700000
H	-11.700000000	6.765700000	1.657800000
Se	-13.968800000	2.604500000	3.243100000
O	-14.873600000	3.725200000	2.459200000
C	-14.559400000	2.550500000	5.086700000
C	-14.987300000	3.718000000	5.705900000
C	-14.529200000	1.330800000	5.749200000
C	-15.395700000	3.655400000	7.033800000
C	-14.938000000	1.285200000	7.078700000
C	-15.368900000	2.443200000	7.718700000
H	-15.012200000	4.655500000	5.156700000
H	-14.200900000	0.437100000	5.224600000
H	-15.739600000	4.559000000	7.534500000

H	-14.922200000	0.337100000	7.613500000
H	-15.689900000	2.401200000	8.758100000
O	-12.395700000	3.247600000	3.313400000
O	-12.443300000	4.829800000	2.262500000
H	-13.406300000	4.600300000	2.143100000
O	-13.991600000	1.090000000	2.693800000

TSox2 (SeIV)
E=-5256.91
Nimag=

C	-9.163200000	5.679800000	-1.413600000
C	-10.536300000	5.904200000	-1.462900000
C	-8.587100000	5.172400000	-0.252300000
H	-10.995800000	6.300600000	-2.366000000
H	-7.514500000	4.994200000	-0.209100000
C	-11.330100000	5.627300000	-0.360200000
C	-9.366900000	4.883800000	0.858600000
H	-12.405300000	5.795000000	-0.402800000
H	-8.924500000	4.486000000	1.765900000
C	-10.739700000	5.118300000	0.798700000
H	-8.543200000	5.900100000	-2.280100000
N	-11.584000000	4.795400000	1.879800000
H	-12.474200000	5.290400000	1.850000000
Se	-14.474900000	1.503700000	2.365000000
O	-14.746100000	2.959900000	1.600300000
C	-14.602600000	2.034100000	4.263000000
C	-15.379200000	3.130100000	4.618500000
C	-13.963300000	1.265100000	5.229800000
C	-15.505100000	3.469900000	5.963400000
C	-14.091800000	1.611700000	6.571900000
C	-14.862800000	2.712000000	6.938400000
H	-15.866200000	3.718700000	3.843000000
H	-13.349900000	0.413700000	4.938100000
H	-16.107300000	4.331100000	6.250400000
H	-13.585800000	1.021000000	7.334400000
H	-14.963300000	2.979200000	7.989100000
O	-12.789300000	1.249300000	2.207700000
O	-12.114300000	3.058100000	1.959700000
H	-13.069200000	3.213800000	1.685100000
O	-11.024400000	4.902600000	3.132600000
H	-11.290500000	4.036800000	3.501300000

TSox2 (SeVI)
E= -5439.29
Nimag=

C	-12.498000000	6.014600000	-2.944400000
C	-13.707600000	6.189000000	-2.277800000
C	-11.308600000	5.998600000	-2.221500000
H	-14.643400000	6.202600000	-2.832600000
H	-10.359900000	5.861700000	-2.736700000
C	-13.730600000	6.350700000	-0.900900000
C	-11.313800000	6.150400000	-0.842200000
H	-14.679400000	6.480600000	-0.382200000
H	-10.389300000	6.134400000	-0.274600000
C	-12.530500000	6.330400000	-0.184600000
H	-12.483300000	5.890700000	-4.025100000
N	-12.599300000	6.433100000	1.215500000
H	-13.452100000	6.883700000	1.540500000
Se	-14.050200000	2.594900000	3.264800000
O	-15.008400000	3.676400000	2.499500000
C	-14.567300000	2.538700000	5.127200000
C	-15.031400000	3.694900000	5.741800000
C	-14.461300000	1.329600000	5.801300000
C	-15.398700000	3.631000000	7.081400000
C	-14.830900000	1.284200000	7.142300000
C	-15.296600000	2.430300000	7.779400000
H	-15.117700000	4.622100000	5.181500000
H	-14.107600000	0.444200000	5.279300000
H	-15.770500000	4.524200000	7.580300000
H	-14.757300000	0.345300000	7.688100000
H	-15.586800000	2.387600000	8.827700000
O	-12.487600000	3.314100000	3.285200000
O	-12.588400000	4.770100000	2.217600000
H	-13.564700000	4.599500000	2.132400000
O	-14.003000000	1.079200000	2.726900000
O	-11.506800000	6.998900000	1.835700000
H	-11.322700000	6.328600000	2.518900000

TSox3 (SeIV)
E= -5030.37
Nimag=

C	-9.095300000	-1.425400000	-0.206200000
C	-9.554600000	-0.340200000	-0.955400000
C	-8.989700000	-1.333600000	1.179000000
H	-9.629000000	-0.418300000	-2.038500000
H	-8.631500000	-2.181400000	1.758900000
C	-9.914800000	0.836100000	-0.322500000
C	-9.336500000	-0.155900000	1.825500000
H	-10.278200000	1.695800000	-0.879600000
H	-9.252200000	-0.076000000	2.906400000
C	-9.798700000	0.922500000	1.068900000
H	-8.816300000	-2.349400000	-0.710000000
N	-10.196900000	2.110800000	1.775800000
O	-10.744200000	2.978100000	1.160700000
Se	-7.863500000	2.449300000	5.710200000
O	-8.467100000	0.971600000	5.287200000
C	-9.410700000	3.308100000	6.558100000
C	-10.493000000	2.532200000	6.949500000
C	-9.368300000	4.674600000	6.812800000
C	-11.564100000	3.142800000	7.596100000
C	-10.444200000	5.276700000	7.457200000
C	-11.539700000	4.511200000	7.849000000
H	-10.493800000	1.465400000	6.735400000
H	-8.516100000	5.273600000	6.494500000
H	-12.422400000	2.546200000	7.901800000
H	-10.428200000	6.348100000	7.650600000
H	-12.379300000	4.985400000	8.354400000
O	-7.769800000	3.337400000	4.210600000
O	-9.089600000	2.765700000	3.214900000
H	-9.084300000	1.904200000	3.689600000

TSox3 (SeVI)
E=-5213.74
Nimag=

C	-9.113900000	-2.975700000	0.643500000
C	-10.153900000	-2.336300000	-0.036600000
C	-8.523400000	-2.382900000	1.756300000
H	-10.611000000	-2.810900000	-0.902800000
H	-7.712500000	-2.885100000	2.279200000
C	-10.605500000	-1.102300000	0.391800000
C	-8.968600000	-1.146900000	2.201100000
H	-11.415900000	-0.584000000	-0.114100000

H	-8.513400000	-0.666300000	3.061600000
C	-10.007000000	-0.511900000	1.513100000
H	-8.764200000	-3.947800000	0.299900000
N	-10.464100000	0.742000000	2.024800000
O	-11.295600000	1.344500000	1.413500000
Se	-8.430000000	2.223000000	5.892000000
O	-9.048700000	0.720200000	5.776900000
C	-9.738500000	3.334000000	6.781400000
C	-11.061100000	2.913700000	6.823800000
C	-9.318500000	4.533300000	7.342600000
C	-11.995600000	3.733200000	7.449000000
C	-10.267200000	5.340500000	7.961500000
C	-11.600400000	4.942700000	8.012500000
H	-11.349600000	1.961400000	6.387800000
H	-8.271500000	4.822800000	7.304500000
H	-13.037200000	3.420700000	7.496100000
H	-9.959600000	6.284100000	8.408500000
H	-12.337100000	5.579400000	8.499200000
O	-8.347200000	2.823100000	4.268100000
O	-9.395600000	1.849100000	3.301400000
H	-9.442900000	1.148300000	3.993000000
O	-7.000600000	2.461300000	6.589600000

TSdeh(SeIV)
E=-5299.41
Nimag=

C	-10.752000000	5.720300000	-1.099900000
C	-11.804700000	5.323000000	-0.276800000
C	-9.440600000	5.416900000	-0.745600000
H	-12.831700000	5.552700000	-0.554400000
H	-8.618300000	5.715900000	-1.393500000
C	-11.548100000	4.628400000	0.894300000
C	-9.170900000	4.727500000	0.429700000
H	-12.354000000	4.307100000	1.549000000
H	-8.151700000	4.473700000	0.705100000
C	-10.228900000	4.336300000	1.253300000
H	-10.955700000	6.260000000	-2.023100000
N	-10.062800000	3.529600000	2.422300000
H	-8.831700000	2.475800000	3.435000000
O	-8.815600000	3.243100000	2.628100000
O	-10.540900000	4.764700000	3.724000000
H	-9.785900000	5.368000000	3.661000000
Se	-9.832500000	1.885000000	5.718800000
O	-8.789800000	1.597500000	4.429400000
C	-11.532300000	1.224200000	5.001900000
C	-11.525700000	0.209900000	4.051900000
C	-12.723400000	1.713200000	5.528800000
C	-12.738200000	-0.310000000	3.608400000
C	-13.929900000	1.186800000	5.077800000
C	-13.937500000	0.176700000	4.119900000
H	-10.583100000	-0.154100000	3.649300000
H	-12.714200000	2.513000000	6.266600000
H	-12.744200000	-1.097100000	2.856000000
H	-14.868100000	1.571800000	5.474500000
H	-14.883600000	-0.232500000	3.769700000
O	-10.157000000	3.564300000	5.799900000
H	-10.350200000	4.089000000	4.781000000

TSdeh(SeVI)
E= -5483.27
Nimag=

C	-9.290100000	6.596500000	-1.514700000
C	-10.608600000	6.344000000	-1.138900000
C	-8.243400000	5.978200000	-0.837100000
H	-11.429600000	6.820500000	-1.670900000
H	-7.214000000	6.164600000	-1.137900000
C	-10.879200000	5.479200000	-0.091200000
C	-8.501200000	5.116600000	0.221300000
H	-11.900300000	5.266300000	0.214300000
H	-7.688600000	4.620700000	0.742900000
C	-9.824200000	4.870500000	0.595400000
H	-9.079500000	7.270200000	-2.343300000
N	-10.199900000	3.921800000	1.594200000
H	-9.533400000	2.576800000	2.717300000
O	-9.143900000	3.350800000	2.116600000
O	-10.854300000	5.023300000	2.871600000
H	-10.032000000	5.350000000	3.268300000
Se	-10.928300000	2.160900000	4.898200000
O	-10.089200000	1.572300000	3.604800000
C	-12.215700000	0.808900000	5.358600000
C	-13.053200000	0.296500000	4.375300000
C	-12.252800000	0.372900000	6.675300000
C	-13.964400000	-0.689100000	4.736400000
C	-13.171100000	-0.615600000	7.017300000
C	-14.022700000	-1.142800000	6.052000000
H	-12.995100000	0.655300000	3.351100000
H	-11.574100000	0.799600000	7.409400000
H	-14.631300000	-1.105200000	3.983500000
H	-13.217000000	-0.973400000	8.044200000
H	-14.738500000	-1.916000000	6.325600000
O	-11.895500000	3.444300000	4.382400000
H	-11.334900000	4.198800000	3.651800000
O	-10.044100000	2.523500000	6.191400000

TS-P2-O-to-P2-OH (SeIV)
E= -5305.61
Nimag=

N	-9.501300000	3.966000000	3.960500000
H	-9.810600000	5.069000000	4.100600000
O	-8.239300000	3.809000000	4.328400000
H	-7.794100000	4.948400000	4.573800000
Se	-8.539900000	7.223200000	4.523700000
O	-10.008600000	6.421000000	4.332400000
O	-7.398400000	6.006700000	4.903800000
C	-10.429600000	3.041100000	4.628900000
C	-9.945100000	2.049300000	5.467400000
C	-11.793600000	3.217700000	4.423100000
C	-10.850800000	1.200600000	6.097000000
C	-12.686000000	2.369400000	5.064800000
C	-12.217700000	1.357200000	5.898800000
H	-8.875400000	1.960900000	5.626600000
H	-12.152100000	4.006500000	3.767200000
H	-10.479500000	0.416800000	6.754700000
H	-13.755300000	2.502700000	4.912600000
H	-12.921500000	0.695100000	6.399700000
C	-8.055500000	7.595400000	2.660200000
C	-6.713600000	7.613800000	2.295200000
C	-9.055100000	7.928800000	1.753400000
C	-6.371300000	7.958300000	0.990900000
C	-8.701900000	8.273500000	0.452100000
C	-7.363000000	8.289700000	0.072100000
H	-5.944800000	7.338800000	3.014400000
H	-10.100100000	7.897000000	2.054700000
H	-5.324400000	7.963500000	0.691400000

H	-9.477900000	8.526000000	-0.268800000
H	-7.090800000	8.559600000	-0.946900000
O	-9.662300000	3.800400000	2.519600000
H	-9.115100000	3.014200000	2.358900000

P1-O
E= -2557.41
Nimag=0

C	-11.164000000	5.317200000	-1.117500000
C	-12.014200000	5.689000000	-0.079900000
C	-9.995100000	4.612700000	-0.843500000
H	-12.929300000	6.238300000	-0.292900000
H	-9.330300000	4.319700000	-1.653900000
C	-11.698800000	5.358800000	1.233500000
C	-9.672300000	4.278500000	0.467100000
H	-12.365400000	5.630300000	2.050500000
H	-8.769000000	3.713100000	0.690500000
C	-10.527600000	4.661700000	1.489000000
H	-11.414500000	5.575700000	-2.144400000
N	-10.223400000	4.248200000	2.876400000
H	-10.561700000	5.023300000	3.486100000
H	-9.185700000	4.291300000	2.966200000
O	-10.726800000	3.068400000	3.205000000

P1-OH
E= -2570.91
Nimag=0

C	-11.160200000	5.262600000	-1.101200000
C	-12.005800000	5.650600000	-0.064800000
C	-9.974600000	4.605400000	-0.791200000
H	-12.934900000	6.174500000	-0.284000000
H	-9.296600000	4.302200000	-1.587800000
C	-11.673400000	5.386700000	1.255500000
C	-9.631500000	4.327100000	0.526800000
H	-12.344800000	5.697400000	2.055700000
H	-8.698700000	3.822200000	0.757800000
C	-10.483700000	4.713000000	1.564500000
H	-11.420800000	5.475800000	-2.135600000
N	-10.240600000	4.376300000	2.904900000
H	-10.611200000	5.087400000	3.528800000
O	-8.876000000	4.236500000	3.229000000
H	-8.826100000	3.324000000	3.540500000

P2-O
E= -2742.90
Nimag=0

C	-9.216600000	5.594300000	-1.334500000
C	-10.560600000	5.949100000	-1.273900000
C	-8.666700000	4.773400000	-0.353200000
H	-10.995300000	6.585700000	-2.042100000
H	-7.617400000	4.489000000	-0.405500000
C	-11.354700000	5.491900000	-0.227900000
C	-9.452700000	4.302900000	0.691600000
H	-12.404400000	5.775700000	-0.166600000
H	-9.062200000	3.641300000	1.459400000
C	-10.783000000	4.680300000	0.739200000
H	-8.596600000	5.954100000	-2.153400000
N	-11.634400000	4.167000000	1.838500000
H	-12.621000000	4.173800000	1.525900000
O	-11.269300000	3.124800000	2.429900000
O	-11.777500000	5.437800000	2.801400000
H	-11.435600000	5.006100000	3.599200000

P2-OH
E= -2754.16
Nimag=0

C	-11.209800000	5.330200000	-1.154700000
C	-12.042700000	5.657500000	-0.090700000
C	-10.015400000	4.664300000	-0.898200000
H	-12.984200000	6.173700000	-0.271500000
H	-9.350000000	4.401000000	-1.718800000
C	-11.692700000	5.330800000	1.213700000
C	-9.649500000	4.330500000	0.399100000
H	-12.359900000	5.571100000	2.035400000
H	-8.715300000	3.813900000	0.590000000
C	-10.487300000	4.667500000	1.467100000
H	-11.489500000	5.588400000	-2.174000000
N	-10.185100000	4.239200000	2.792700000
H	-8.679900000	3.443900000	3.560600000
O	-8.782700000	4.188700000	2.953000000
O	-10.715600000	5.091800000	3.758600000
H	-10.387500000	5.985900000	3.544200000

P-NO
E= -2347.27
Nimag=0

C	-1.617600000	1.402700000	0.000000000
C	-2.741300000	2.234500000	0.000000000
C	-0.335000000	1.944200000	0.000000000
H	-3.738200000	1.796100000	0.000000000
H	0.534600000	1.289800000	0.000000000
C	-2.587000000	3.609800000	0.000000000
C	-0.173800000	3.323500000	0.000000000
H	-3.440800000	4.284200000	0.000000000
H	0.811800000	3.786400000	0.000000000
C	-1.297800000	4.150600000	0.000000000
H	-1.748200000	0.321600000	0.000000000
N	-1.009400000	5.567100000	0.000000000
O	-1.981300000	6.294900000	0.000000000

P-NO2
E= -2556.71
Nimag=0

C	0.000000000	0.000000000	-1.169200000
C	0.000000000	1.206900000	-1.863400000
C	0.000000000	-1.206900000	-1.863400000
H	0.000000000	2.150300000	-1.321200000
H	0.000000000	-2.150300000	-1.321200000
C	0.000000000	1.214800000	-3.252200000
C	0.000000000	-1.214800000	-3.252200000
H	0.000000000	2.141100000	-3.817700000
H	0.000000000	-2.141100000	-3.817700000
C	0.000000000	0.000000000	-3.926900000
H	0.000000000	0.000000000	-0.080700000
N	0.000000000	0.000000000	-5.406900000
O	0.000000000	1.084500000	-5.969400000
O	0.000000000	-1.084500000	-5.969400000

Direct oxidation via peroxyselenurane

Se(IV)
E= -5478.61

Nimag=-747

C	-1.849933000	-4.557254000	-6.204199000
C	-1.888182000	-5.270132000	-5.008446000
C	-2.285180000	-3.235389000	-6.233084000
H	-1.544261000	-6.301983000	-4.976431000
H	-2.255058000	-2.669932000	-7.162277000
C	-2.358051000	-4.673504000	-3.848346000
C	-2.758867000	-2.626157000	-5.080163000
H	-2.371552000	-5.227444000	-2.911633000
H	-3.091895000	-1.589803000	-5.105230000
C	-2.805076000	-3.349413000	-3.884588000
H	-1.478349000	-5.030147000	-7.110598000
N	-3.246548000	-2.729266000	-2.712111000
H	-3.602662000	-3.347178000	-1.995994000
H	-3.834157000	-1.916606000	-2.839247000
Se	0.783855000	-2.050351000	-0.323532000
O	2.120332000	-2.945324000	0.750388000
C	2.137640000	-0.685735000	-0.574396000
C	2.679973000	-0.019181000	0.516647000
C	2.544700000	-0.395326000	-1.871918000
C	3.640815000	0.962453000	0.298103000
C	3.521387000	0.574210000	-2.077564000
C	4.065488000	1.257457000	-0.994492000
H	2.357908000	-0.273259000	1.522323000
H	2.103736000	-0.914287000	-2.720218000
H	4.066793000	1.494575000	1.147477000
H	3.851684000	0.800036000	-3.090305000
H	4.823494000	2.021792000	-1.157956000
O	-0.025868000	-1.659305000	1.236938000
H	-0.718441000	-1.067302000	0.886821000
O	-0.392851000	-0.818812000	-1.105305000
O	-2.007918000	-1.992987000	-1.618586000
H	-1.288209000	-1.427593000	-2.060674000
H	1.652960000	-3.685867000	1.157627000

Se(VI)
E= -5664.85
Nimag=-545

C	-6.566305000	1.699624000	2.780098000
C	-6.164700000	0.373792000	2.922105000
C	-5.667261000	2.728894000	3.048352000
H	-6.859726000	-0.434574000	2.705408000
H	-5.973452000	3.766355000	2.932037000
C	-4.875623000	0.071043000	3.332203000
C	-4.374579000	2.442473000	3.458551000
H	-4.558349000	-0.966001000	3.426456000
H	-3.667760000	3.247007000	3.653090000
C	-3.980786000	1.109137000	3.612742000
H	-7.577945000	1.930707000	2.453921000
N	-2.670558000	0.811492000	3.989369000
H	-2.527168000	-0.098103000	4.407386000
H	-2.169576000	1.545036000	4.472033000
Se	-0.158527000	-1.149611000	0.160831000
O	0.490514000	-2.861710000	-0.100431000
C	1.632273000	-0.396091000	0.128333000
C	2.652268000	-0.973887000	0.871113000
C	1.843542000	0.718834000	-0.671413000
C	3.920615000	-0.403211000	0.817241000
C	3.122571000	1.263647000	-0.731921000
C	4.157802000	0.708612000	0.014458000
H	2.463265000	-1.856690000	1.474559000
H	1.022219000	1.152115000	-1.235608000
H	4.729819000	-0.840627000	1.399944000
H	3.306144000	2.131397000	-1.363527000
H	5.155036000	1.143129000	-0.031491000
O	-0.961550000	-1.174039000	-1.267795000
O	-0.475391000	-1.786842000	1.797612000
H	-0.802342000	-0.972456000	2.252648000
O	-0.930426000	0.388034000	0.598834000
O	-1.429779000	0.648395000	2.658589000
H	-1.852698000	0.588341000	1.745055000
H	0.241920000	-2.984343000	-1.027991000

Direct oxidation of P2-OH

Se(VI)
E=-5623.03
Nimag=-256

C	-12.613987000	5.971690000	-2.885474000
C	-13.804377000	6.060292000	-2.171095000
C	-11.399818000	6.045606000	-2.211231000
H	-14.760095000	5.985975000	-2.685661000
H	-10.463239000	5.968347000	-2.759753000
C	-13.790459000	6.230685000	-0.793918000
C	-11.363195000	6.213933000	-0.833630000
H	-14.719816000	6.269138000	-0.235067000
H	-10.417850000	6.262388000	-0.305758000
C	-12.564038000	6.320102000	-0.133067000
H	-12.633028000	5.834687000	-3.964651000
N	-12.555368000	6.435346000	1.296634000
Se	-14.000329000	2.581949000	3.221622000
O	-14.944850000	3.658482000	2.431901000
C	-14.561059000	2.541527000	5.073394000
C	-15.019914000	3.708492000	5.671481000
C	-14.486029000	1.336467000	5.758631000
C	-15.413426000	3.659678000	7.004409000
C	-14.881792000	1.305622000	7.092606000
C	-15.342609000	2.462858000	7.712894000
H	-15.080658000	4.633113000	5.103326000
H	-14.134471000	0.442696000	5.249515000
H	-15.780987000	4.562077000	7.489947000
H	-14.832204000	0.369641000	7.646284000
H	-15.653109000	2.432077000	8.755867000
O	-12.444617000	3.293327000	3.265407000
O	-12.549316000	4.819326000	2.224287000
H	-13.528608000	4.635093000	2.154878000
O	-13.952151000	1.059849000	2.698389000
O	-11.369694000	6.920175000	1.779867000
H	-11.243199000	6.332244000	2.549406000
O	-13.629681000	7.142294000	1.806922000
H	-13.595099000	8.011627000	1.367818000

Se(VI)
E=-5440.22
Nimag=-304

C	-9.645059000	5.650163000	-1.699328000
C	-10.998320000	5.810586000	-1.416657000
C	-8.778662000	5.220666000	-0.700075000
H	-11.687757000	6.128271000	-2.196044000
H	-7.720424000	5.084318000	-0.913524000
C	-11.489091000	5.554199000	-0.144599000
C	-9.248758000	4.955845000	0.579690000
H	-12.549112000	5.647632000	0.068741000

H	-8.577475000	4.611695000	1.357837000
C	-10.602899000	5.140059000	0.850510000
H	-9.268632000	5.850039000	-2.700398000
N	-11.131937000	4.824011000	2.152029000
Se	-14.058922000	1.476056000	2.395362000
O	-14.252401000	2.903758000	1.556103000
C	-14.586824000	2.019865000	4.220995000
C	-15.452206000	3.092064000	4.397353000
C	-14.133697000	1.279587000	5.307941000
C	-15.860782000	3.434949000	5.683940000
C	-14.543610000	1.629097000	6.591514000
C	-15.408105000	2.704764000	6.779190000
H	-15.784865000	3.661148000	3.531239000
H	-13.446521000	0.447719000	5.158739000
H	-16.534743000	4.278072000	5.831543000
H	-14.184615000	1.060844000	7.448730000
H	-15.729567000	2.974667000	7.783953000
O	-12.367635000	1.327022000	2.570358000
O	-11.741938000	3.190595000	2.300703000
H	-12.681779000	3.295083000	1.925176000
O	-10.161559000	4.765238000	3.113815000
H	-10.462352000	3.970409000	3.599398000
O	-12.171377000	5.652867000	2.540446000
H	-11.803382000	6.553669000	2.490206000

Alternative H_2O_2 activation mechanisms

TSb Se(IV)
E=-3093.20
Nimag=-387

Se	1.344100000	0.652500000	-0.518200000
O	1.663200000	2.178100000	-0.042200000
C	-0.531800000	0.481700000	-0.039300000
C	-1.123200000	1.563100000	0.610800000
C	-1.282500000	-0.631100000	-0.421100000
C	-2.482000000	1.522300000	0.895400000
C	-2.645400000	-0.650700000	-0.145400000
C	-3.243400000	0.418900000	0.515200000
H	-0.511900000	2.424300000	0.873500000
H	-0.804800000	-1.474500000	-0.910800000
H	-2.951300000	2.360100000	1.408500000
H	-3.241200000	-1.512400000	-0.441500000
H	-4.309700000	0.393900000	0.733800000
O	2.289900000	-0.215700000	1.387800000
H	1.639400000	-0.097000000	2.091600000
O	1.514100000	-1.774300000	-0.239900000
O	2.624600000	-2.191300000	-1.010200000
H	2.184400000	-2.608500000	-1.764400000
H	2.026500000	-1.116300000	0.832100000

TSb Se(VI)
E= -3262.75
Nimag=-634

Se	1.271900000	0.560800000	-0.332500000
O	1.565000000	2.123800000	-0.041600000
C	-0.661400000	0.448400000	-0.057400000
C	-1.239400000	1.298300000	0.873700000
C	-1.388000000	-0.465500000	-0.806100000
C	-2.618100000	1.232300000	1.049500000
C	-2.766700000	-0.505600000	-0.620200000
C	-3.377700000	0.333400000	0.306500000
H	-0.635400000	2.009100000	1.430600000
H	-0.898600000	-1.110000000	-1.529200000
H	-3.096700000	1.893600000	1.769500000
H	-3.362400000	-1.201100000	-1.208600000
H	-4.455700000	0.288000000	0.449400000
O	3.152200000	0.027800000	0.555900000
H	3.317200000	0.725400000	1.204000000
O	1.379600000	-1.380300000	1.025400000
O	1.343500000	-2.540500000	0.241500000
H	1.927700000	-2.325900000	-0.509000000
H	2.434000000	-0.873800000	0.981000000
O	1.596400000	-0.169000000	-1.732200000

TSc Se(IV)
E=-3066.22
Nimag=-890

Se	1.250500000	0.372300000	-0.531900000
O	1.666800000	1.918200000	-0.266100000
C	-0.637900000	0.356500000	-0.035100000
C	-1.153500000	1.508900000	0.548700000
C	-1.447900000	-0.730100000	-0.359100000
C	-2.510800000	1.561500000	0.845100000
C	-2.806500000	-0.656500000	-0.067900000
C	-3.334400000	0.481500000	0.536000000
H	-0.492100000	2.349600000	0.751000000
H	-1.024200000	-1.621300000	-0.813900000
H	-2.928200000	2.453300000	1.309500000
H	-3.454600000	-1.495800000	-0.313700000
H	-4.398400000	0.530200000	0.761800000
O	1.908700000	-0.548700000	1.043200000
H	1.173000000	-0.552300000	1.677900000
O	1.321300000	-2.099800000	0.232900000
O	1.274100000	-3.750400000	-0.812300000
H	1.118400000	-4.318100000	-0.045300000
H	1.922400000	-2.857700000	-0.341800000

TSc Se(VI)
E=-3235.21
Nimag=-716

Se	1.580500000	-1.611300000	-0.601600000
O	1.803400000	-3.173700000	-0.295500000
C	3.218700000	-0.718900000	-0.038500000
C	3.975700000	-1.291900000	0.976900000
C	3.593300000	0.454200000	-0.682500000
C	5.150800000	-0.652600000	1.362400000
C	4.773600000	1.077300000	-0.283300000
C	5.546700000	0.527700000	0.736400000
H	3.662500000	-2.222100000	1.445000000
H	2.986600000	0.858900000	-1.489000000
H	5.761500000	-1.085600000	2.153500000
H	5.090400000	1.993600000	-0.779900000
H	6.469500000	1.019400000	1.041800000
O	1.165700000	-0.920800000	-2.002900000
O	0.507000000	-0.855700000	0.809900000
H	0.161300000	-0.043300000	0.393900000
O	-1.956100000	-2.665000000	-1.418900000
O	-0.734800000	-1.929100000	-0.147100000
H	-1.481100000	-1.711600000	-1.077000000
H	-2.625000000	-2.825000000	-0.734300000

Se(IV) to Se(VI) conversion

TSa

E=-3081.34
Nimag=-851

Se	1.894200000	-2.559700000	-1.734400000
O	2.906600000	-3.439600000	-0.402400000
C	2.209200000	-0.765400000	-1.056500000
C	2.183100000	-0.503800000	0.307500000
C	2.470400000	0.222200000	-1.996900000
C	2.409200000	0.800500000	0.733700000
C	2.699900000	1.521400000	-1.552500000
C	2.668500000	1.808400000	-0.191700000
H	1.987100000	-1.299000000	1.020800000
H	2.486400000	-0.017700000	-3.058100000
H	2.384500000	1.027900000	1.798000000
H	2.905200000	2.308500000	-2.275700000
H	2.850400000	2.825100000	0.152000000
O	0.405900000	-3.039300000	-1.031900000
H	-0.279000000	-2.634800000	-1.877100000
O	1.137200000	-2.317100000	-3.253200000
O	-0.744000000	-2.137100000	-3.007900000
H	-0.773400000	-1.173900000	-2.914800000
H	2.346200000	-4.191900000	-0.155900000

TSb
E= -2649.92
Nimag=-384

Se	1.201100000	-0.641700000	0.212600000
O	1.287900000	0.793200000	-1.427300000
C	-0.711300000	-0.391100000	0.291000000
C	-1.268100000	0.401400000	1.286700000
C	-1.495500000	-1.059700000	-0.642700000
C	-2.650600000	0.533800000	1.335500000
C	-2.878900000	-0.925000000	-0.577900000
C	-3.452500000	-0.128000000	0.407900000
H	-0.624700000	0.898600000	2.008500000
H	-1.041400000	-1.672900000	-1.420000000
H	-3.105200000	1.155500000	2.104800000
H	-3.507300000	-1.440300000	-1.301900000
H	-4.534900000	-0.021800000	0.455000000
O	1.634600000	-0.508200000	1.903600000
O	1.872300000	0.871900000	0.531500000
H	2.190000000	0.701600000	-1.772100000

TSc
E=-4305.11
Nimag=-320

Se	-0.113900000	-0.145500000	3.413300000
O	-0.014200000	1.470200000	3.478400000
C	-1.989900000	-0.591600000	3.553400000
C	-2.882300000	0.454500000	3.737800000
C	-2.401500000	-1.914200000	3.440200000
C	-4.239200000	0.159200000	3.825600000
C	-3.761200000	-2.190800000	3.532300000
C	-4.675400000	-1.158300000	3.724700000
H	-2.515900000	1.476000000	3.808600000
H	-1.684200000	-2.714400000	3.277800000
H	-4.956200000	0.965000000	3.971600000
H	-4.106000000	-3.219600000	3.448100000
H	-5.738300000	-1.383500000	3.792000000
O	0.275900000	-0.810600000	5.073300000
Se	1.801000000	-1.595600000	-0.644400000
O	2.742100000	-1.110200000	0.626700000
C	1.141900000	0.107700000	-1.358500000
C	1.683600000	1.301600000	-0.902600000
C	0.164900000	0.083900000	-2.348500000
C	1.220500000	2.500200000	-1.438000000
C	-0.291500000	1.287200000	-2.876900000
C	0.236000000	2.492900000	-2.421500000
H	2.449200000	1.285900000	-0.130000000
H	-0.254400000	-0.859200000	-2.697200000
H	1.629800000	3.444000000	-1.081000000
H	-1.063300000	1.282800000	-3.644900000
H	-0.123300000	3.432800000	-2.837100000
O	0.370400000	-2.209600000	0.133700000
O	0.289000000	-1.281600000	1.681800000
H	1.278500000	-1.122200000	1.606600000
H	1.235300000	-0.705200000	5.170700000

TSd
E= -4400.03
Nimag=-333

Se	-0.144100000	-0.306600000	3.361000000
O	-0.045800000	1.307800000	3.439900000
C	-2.021300000	-0.718800000	3.584500000
C	-2.905800000	0.332000000	3.781800000
C	-2.438500000	-2.043800000	3.534000000
C	-4.257400000	0.040700000	3.935800000
C	-3.792500000	-2.317500000	3.690600000
C	-4.697800000	-1.278500000	3.891200000
H	-2.536800000	1.354400000	3.808000000
H	-1.728300000	-2.851100000	3.370600000
H	-4.967900000	0.850900000	4.090300000
H	-4.140400000	-3.348000000	3.652500000
H	-5.756700000	-1.500300000	4.011700000
O	0.521000000	-0.949600000	5.069800000
O	-0.087000000	-0.248200000	6.122100000
H	0.468600000	0.547400000	6.180200000
Se	1.213900000	-1.105100000	-1.051400000
O	2.332500000	-0.886200000	0.145000000
C	0.597100000	0.716600000	-1.419300000
C	1.266800000	1.800900000	-0.869500000
C	-0.477100000	0.886400000	-2.286900000
C	0.835600000	3.086600000	-1.183100000
C	-0.900900000	2.175500000	-2.592400000
C	-0.244100000	3.273000000	-2.041400000
H	2.106500000	1.633500000	-0.198600000
H	-0.993400000	0.026500000	-2.712300000
H	1.345900000	3.946400000	-0.752000000
H	-1.746400000	2.322800000	-3.262400000
H	-0.576200000	4.280800000	-2.284800000
O	-0.149700000	-1.777700000	-0.203500000
O	0.045500000	-1.199000000	1.500900000
H	1.024900000	-1.061900000	1.318700000

TS2-SAPE (SeVI)
E= -3712.00
Nimag=-849

Se	0.740277000	-2.066683000	-1.250827000
O	2.493806000	-3.152104000	-1.011834000
C	1.753494000	-0.595697000	-0.482100000
C	2.120419000	-0.619217000	0.852906000
C	2.062675000	0.450100000	-1.336909000
C	2.834465000	0.466612000	1.349896000
C	2.788292000	1.520018000	-0.821105000
C	3.170402000	1.529065000	0.516376000

H	1.859266000	-1.454703000	1.495654000
H	1.746981000	0.436949000	-2.376854000
H	3.129255000	0.476165000	2.397552000
H	3.048096000	2.351669000	-1.473278000
H	3.732729000	2.371959000	0.913499000
O	0.814533000	-2.382425000	-2.833186000
O	0.020442000	-3.055301000	-0.078027000
H	0.681482000	-4.018780000	0.180218000
O	-0.810844000	-1.057822000	-1.469468000
O	-1.253141000	-0.521770000	-0.227552000
H	-1.740086000	-1.278664000	0.136391000
H	2.636117000	-3.364971000	-1.943952000
O	1.536534000	-4.868108000	0.354478000
H	2.140491000	-4.218058000	-0.339405000
H	1.279320000	-5.665671000	-0.120411000

TS2-SAPE(SeIV)
E=-3538.73
Nimag=-769

Se	0.357850000	-1.897109000	-1.132706000
O	2.009454000	-3.346617000	-1.412960000
C	1.707634000	-0.698884000	-0.436458000
C	1.703470000	-0.374378000	0.913057000
C	2.632611000	-0.151433000	-1.318265000
C	2.657087000	0.520677000	1.388697000
C	3.577678000	0.744021000	-0.830409000
C	3.590226000	1.078646000	0.520949000
H	0.970628000	-0.820020000	1.580221000
H	2.633133000	-0.425609000	-2.371175000
H	2.668091000	0.781047000	2.445626000
H	4.311790000	1.175134000	-1.508680000
H	4.335017000	1.776399000	0.899715000
O	-0.178438000	-2.737726000	0.252424000
H	0.571765000	-3.571856000	0.530943000
O	-0.862910000	-0.452740000	-0.902753000
O	-2.087057000	-0.885940000	-1.515230000
H	-2.095546000	-0.326098000	-2.306274000
H	1.703480000	-3.871652000	-2.162053000
O	1.516636000	-4.402932000	0.684907000
H	1.863859000	-4.058918000	-0.340766000
H	1.167631000	-5.296436000	0.608128000

TSox1 (SeIV)
E=-5514.25
Nimag=-269

C	-8.778400000	6.534500000	-0.192100000
C	-9.832900000	5.938000000	-0.878500000
C	-8.818400000	6.615500000	1.198000000
H	-9.808900000	5.871400000	-1.964500000
H	-7.997200000	7.078000000	1.742100000
C	-10.922800000	5.425200000	-0.190700000
C	-9.899300000	6.104800000	1.899500000
H	-11.747700000	4.962100000	-0.727300000
H	-9.922400000	6.157000000	2.986800000
C	-10.963000000	5.513500000	1.206900000
H	-7.926500000	6.933900000	-0.738400000
N	-12.044900000	4.978600000	1.903700000
H	-12.937200000	4.831500000	1.388000000
H	-12.181900000	5.348100000	2.834300000
Se	-13.736700000	0.854600000	2.746200000
O	-14.514800000	1.578100000	1.469300000
C	-14.417600000	1.876100000	4.288900000
C	-15.728100000	2.338900000	4.268700000
C	-13.616900000	2.040100000	5.413500000
C	-16.238500000	2.993100000	5.387100000
C	-14.133400000	2.697000000	6.527000000
C	-15.442300000	3.172300000	6.515000000
H	-16.338500000	2.199500000	3.378300000
H	-12.591400000	1.675900000	5.407800000
H	-17.263000000	3.363300000	5.377400000
H	-13.509400000	2.838800000	7.408600000
H	-15.844300000	3.681700000	7.389400000
O	-12.086000000	1.278100000	2.793300000
O	-11.947200000	3.253000000	2.492800000
H	-11.732100000	2.860100000	1.635100000
O	-14.313000000	4.103800000	0.561500000
H	-15.206700000	4.456500000	0.567100000
H	-14.400100000	3.181500000	0.936000000

TSox1(SeVI)
E=-5698.78
Nimag=-231

C	-11.999100000	6.938900000	-2.310600000
C	-12.939300000	5.954700000	-2.603400000
C	-11.779400000	7.309400000	-0.986000000
H	-13.117600000	5.660000000	-3.635700000
H	-11.045000000	8.076300000	-0.747800000
C	-13.658900000	5.341300000	-1.588500000
C	-12.489000000	6.703700000	0.039300000
H	-14.394800000	4.574400000	-1.819200000
H	-12.306000000	6.986600000	1.074600000
C	-13.440100000	5.719300000	-0.257100000
H	-11.437900000	7.415200000	-3.111600000
N	-14.138500000	5.086500000	0.766900000
H	-15.013700000	4.599400000	0.526600000
H	-14.187500000	5.592000000	1.639800000
Se	-14.067200000	0.999000000	2.737800000
O	-15.291500000	1.081500000	1.667000000
C	-14.678800000	1.860400000	4.364300000
C	-16.041600000	1.900000000	4.628200000
C	-13.740900000	2.357400000	5.261100000
C	-16.474800000	2.459500000	5.826800000
C	-14.189200000	2.916300000	6.453400000
C	-15.551700000	2.966900000	6.736200000
H	-16.749400000	1.498700000	3.907300000
H	-12.679900000	2.313000000	5.029100000
H	-17.539800000	2.495500000	6.050000000
H	-13.467400000	3.311900000	7.166000000
H	-15.895400000	3.402200000	7.672900000
O	-12.703300000	1.907600000	2.266100000
O	-13.370900000	3.548700000	1.608500000
H	-13.070200000	3.174800000	0.768100000
O	-16.259100000	3.270400000	0.190100000
H	-17.213300000	3.261000000	0.303000000
H	-15.936200000	2.507000000	0.718400000
O	-13.536100000	-0.474800000	3.113500000

Control Experiments – Experimental Details
General

All commercial materials (aniline, nitrosobenzene, benzeneseleninic acid) were purchased from various commercial sources and used as received, without further purification. *N*-phenylhydroxylamine[1] and benzeneselenonic acid[2,3] were prepared according to the literature. Flash column chromatography purifications were performed with Silica gel 60 (230-400 mesh). Thin layer chromatography was performed with TLC plates Silica gel 60 F_{254}, which was visualised under UV light, or by staining with an ethanolic acid solution of *p*-anisaldehyde followed by heating. ^{1}H and ^{13}C NMR spectra were recorded in $CDCl_3$ using a Mercury 400 spectrometer operating at 400 MHz for ^{1}H and 100 MHz for ^{13}C. ^{1}H NMR signals were referenced to nondeuterated residual solvent signals 7.26 ppm ^{13}C NMR signals were referenced to the central line of the CDCl3 signal (77.0 ppm). Chemical shifts (δ) are given in parts per million (ppm) and coupling constants (J) are given in Hertz (Hz), rounded to the nearest 0.1 Hz. ^{1}H NMR data are reported as follows: chemical shift, integration, multiplicity (s = singlet, d = doublet, t = triplet, ap d = apparent doublet, m = multiplet, dd = doublet of doublet, bs = broad singlet, bd = broad doublet, and so on), coupling constant (J) or line separation (ls).

Reaction of aniline with hydrogen peroxide in the presence of benzeneseleninic acid

Benzeneseleninic acid (57 mg, 0.3 mmol, 0.2 equiv.) and aniline (140 mg, 1.5 mmol, 1.0 equiv.) were treated with 30% hydrogen peroxide (1.5 mL, 15 mmol, 10.0 equiv.) and the mixture was stirred at room temperature for 3 h. Afterwards, the aqueous reaction mixture was extracted with EtOAc (3 x 5 mL). The combined organic phases were washed with brine (10 mL), dried over Na_2SO_4 and concentrated under reduced pressure. *The crude material was purified by flash chromatography to yield nitrobenzene* as a pale yellowish oil (90% isolated yield).

Reaction of aniline with hydrogen peroxide in the presence of benzeneselenonic acid

Benzeneselenonic acid (62 mg, 0.3 mmol, 0.2 equiv.) and aniline (140 mg, 1.5 mmol, 1.0 equiv.) were treated with 30% hydrogen peroxide (1.5 mL, 15 mmol, 10.0 equiv.) and the mixture was stirred at room temperature for 3 h. Afterwards, the aqueous reaction mixture was extracted with EtOAc (3 x 5 mL). The combined organic phases were washed with brine (10 mL), dried over Na_2SO_4 and concentrated under reduced pressure. *The NMR analysis of the crude material highlighted the presence of unreacted aniline (>96%)*.

Reaction of *N*-phenylhydroxylamine with hydrogen peroxide in the presence of benzeneseleninic acid

Benzeneseleninic acid (38 mg, 0.2 mmol, 0.2 equiv.) and *N*-phenylhydroxylamine (109 mg, 1.0 mmol, 1.0 equiv.) were treated with 30% hydrogen peroxide (1.0 mL, 10 mmol, 10.0 equiv.) and the mixture was stirred at room temperature for 3 h. Afterwards, the aqueous reaction mixture was extracted with EtOAc (3 x 5 mL). The combined organic phases were washed with brine (10 mL), dried over Na_2SO_4 and concentrated under reduced pressure. *The crude material (mainly composed by nitrobenzene and diphenyldiazene oxide) was purified by flash chromatography to yield nitrobenzene* as a pale yellowish oil (40 % isolated yield).

Reaction of *N*-phenylhydroxylamine with hydrogen peroxide in the presence of benzeneselenonic acid

Benzeneselenonic acid (41 mg, 0.2 mmol, 0.2 equiv.) and *N*-phenylhydroxylamine (109 mg, 1.0 mmol, 1.0 equiv.) were treated with 30% hydrogen peroxide (1.0 mL, 10 mmol, 10.0 equiv.) and the mixture was stirred at room temperature for 3 h. Afterwards, the aqueous reaction mixture was extracted with EtOAc (3 x 5 mL). The combined organic phases were washed with brine (10 mL), dried over Na_2SO_4 and concentrated under reduced pressure. *The NMR analysis of the crude material highlighted the presence of diphenyldiazene oxide as the main reaction product.*

Reaction of nitrosobenzene with hydrogen peroxide in the presence of benzeneseleninic acid

Benzeneseleninic acid (38 mg, 0.2 mmol, 0.2 equiv.) and nitrosobenzene (107 mg, 1.0 mmol, 1.0 equiv.) were treated with 30% hydrogen peroxide (1.0 mL, 10 mmol, 10.0 equiv.) and the mixture was stirred at room temperature for 3 h. Afterwards, the aqueous reaction mixture was extracted with EtOAc (3 x 5 mL). The combined organic phases were washed with brine (10 mL), dried over Na_2SO_4 and concentrated under reduced pressure. *The crude material was purified by flash chromatography to yield nitrobenzene* as a pale yellowish oil (93% isolated yield).

Reaction of nitrosobenzene with hydrogen peroxide in the presence of benzeneselenonic acid

Benzeneselenonic acid (41 mg, 0.2 mmol, 0.2 equiv.) and nitrosobenzene (107 mg, 1.0 mmol, 1.0 equiv.) were treated with 30% hydrogen peroxide (1.0 mL, 10 mmol, 10.0 equiv.) and the mixture was stirred at room temperature for 3 h. Afterwards, the aqueous reaction mixture was extracted with EtOAc (3 x 5 mL). The combined organic phases were washed with brine (10 mL), dried over Na_2SO_4 and concentrated under reduced pressure. *The NMR analysis of the crude material highlighted the presence of unreacted nitrosobenzene (>96%).*

Nitrobenzene and Diphenyl diazene oxide: NMR Data

Spectroscopic data of nitrobenzene (pale yellowish oil) matched those previously reported in the literature[3,4]. **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm): 7.59 (2H, ap t, ls = 7.8 Hz), 7.74 (1H, ap t, ls =

7.4 Hz), 8.26 (2H, ap d, ls = 8.0 Hz). **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm): 124.1 (CH), 129.9 (CH), 135.2 (CH), 148.8 (C).

Spectroscopic data of diphenyldiazene oxide (yellowish oily solid) matched those previously reported in the literature[3]. **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm): 7.40 (1H, ap t, J = 7.4 Hz), 7.48-7.58 (5H, m), 8.19 (2H, ap.d, J = 7.8 Hz), 8.33 (2H, ap.d, J = 7.5 Hz). **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm): 122.3, 125.5, 128.7, 128.8, 129.6, 131.6, 144.0, 148.3.

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