Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Supporting Information

Peroxide Activation by Selenium-doped Graphite

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1. Details of the materials used

D-(+)-Glucose	Anhydrous powder, Product No. A16828 (Alfa Aesar)
Benzeneseleninic acid	Crystal with lumps, Product No. 12635 (Sigma Aldrich)
Graphene Oxide (GO)	Powder, 15-20 sheets, 4-10% edge-oxidized, Product No. 796034 (Sigma Aldrich)
H_2O_2	50% w/w aqueous solution, Product code: H2220 (Rankem)
Glutathione Reduced (GSH)	Product No. 48938 (SRL)
Glutathione Reductase (GR) from baker's yeast	100 unit/mg protein (biuret), ammonium sulphate suspension, Product No. G3664 (Sigma Aldrich)
β-NADPH tetrasodium salt	Product No. 99197 (SRL)
Alkenes and alkanes	Sigma-Aldrich, Alfa Aesar and TCI Chemicals
Solvents (For analysis, in UV-vis, GC, GCMS, HRMS)	Merck, analytical (HPLC) grade
TEMPO	Product No. 0120256 (Spectrochem)
DMPO	Product No. D2362 (TCI Chemicals)

2. FESEM Images (with elemental mapping)

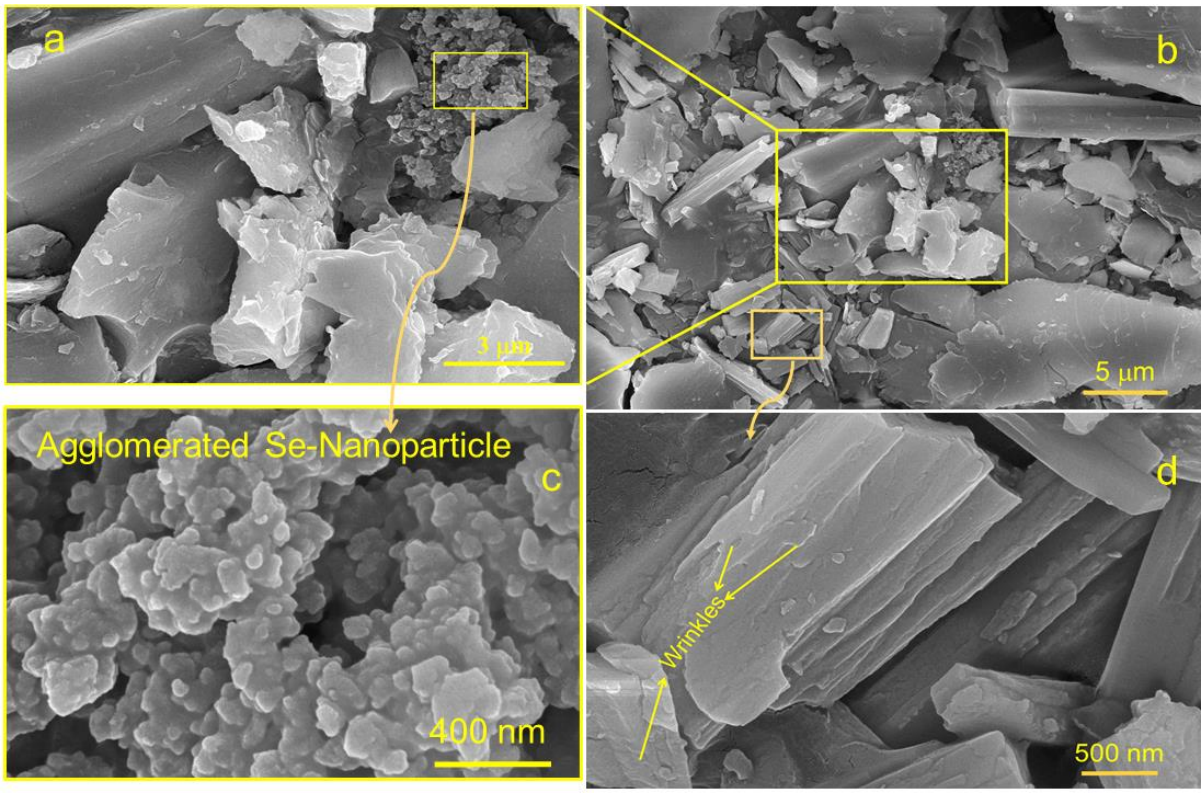


Fig. S1.1 FESEM Images of Se-DG-1 in different resolutions.

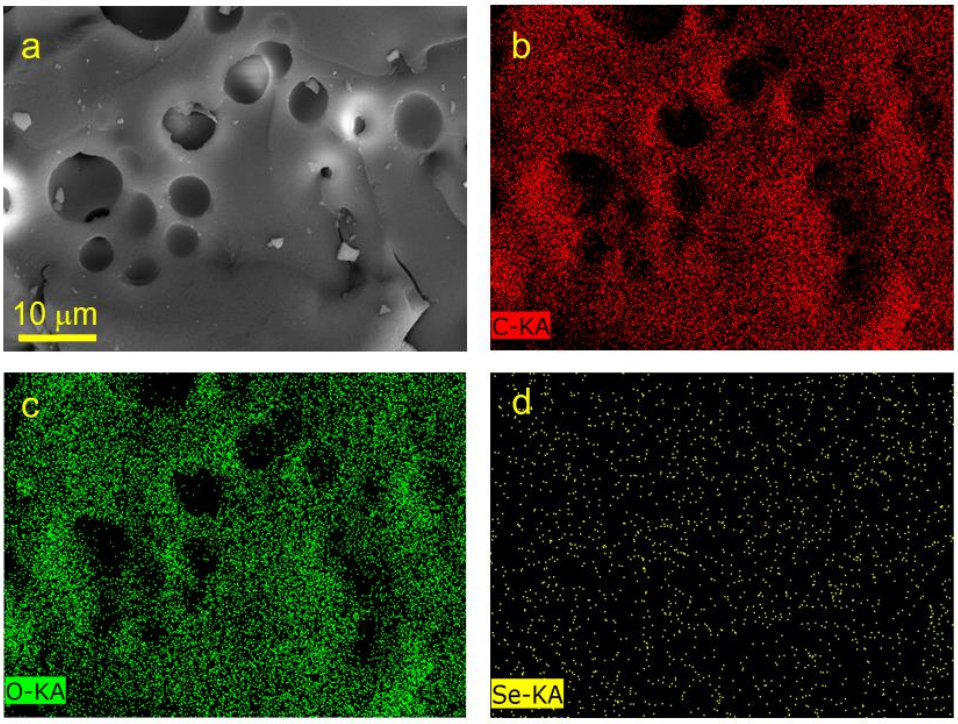


Fig. S1.2 Elemental mapping of C, O and Se in Se-DG-1.

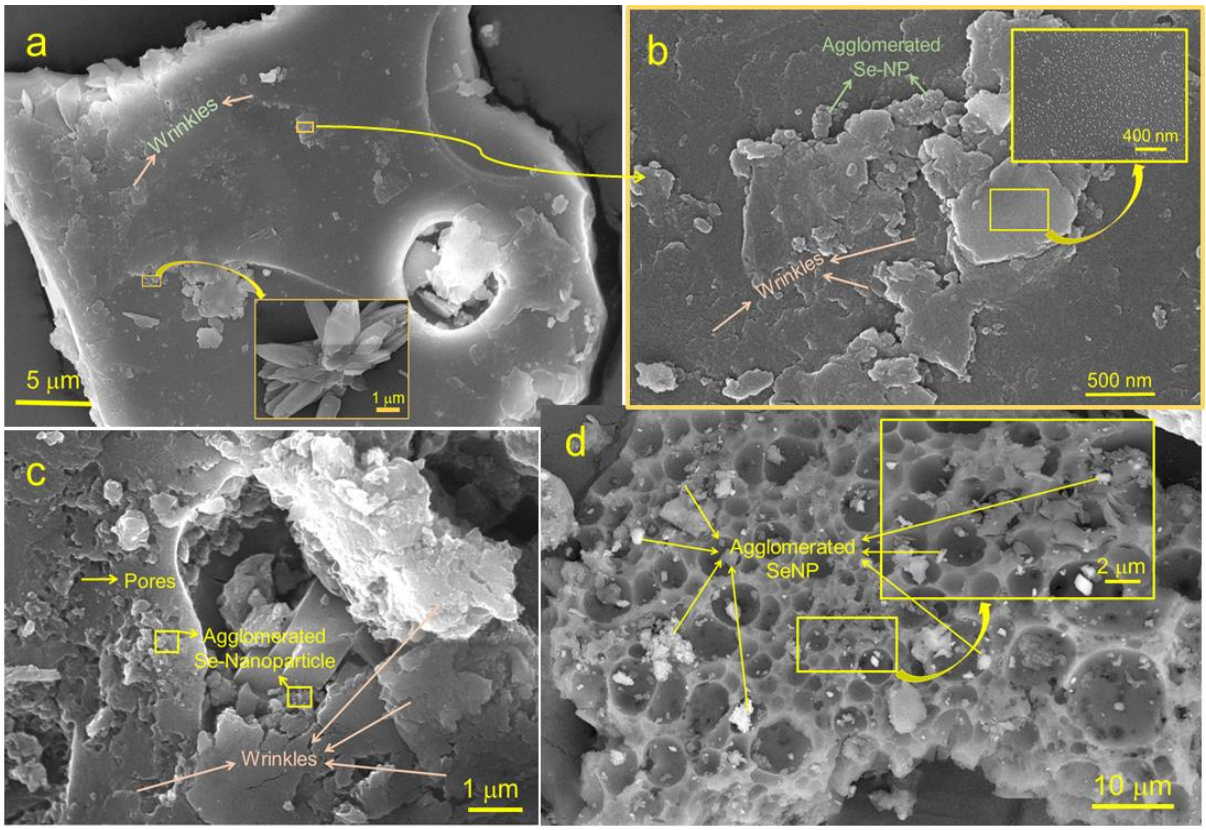


Fig. S2.1 FESEM Images of Se-DG-2 in different resolutions.

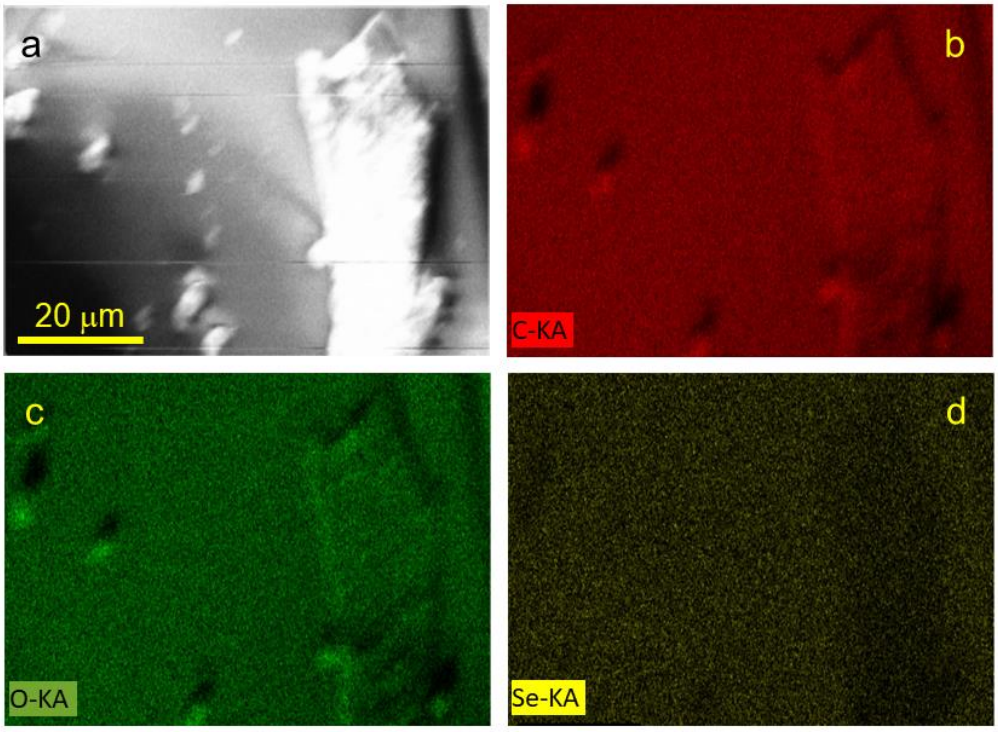


Fig. S2.2 Elemental mapping of C, O and Se in Se-DG-2.

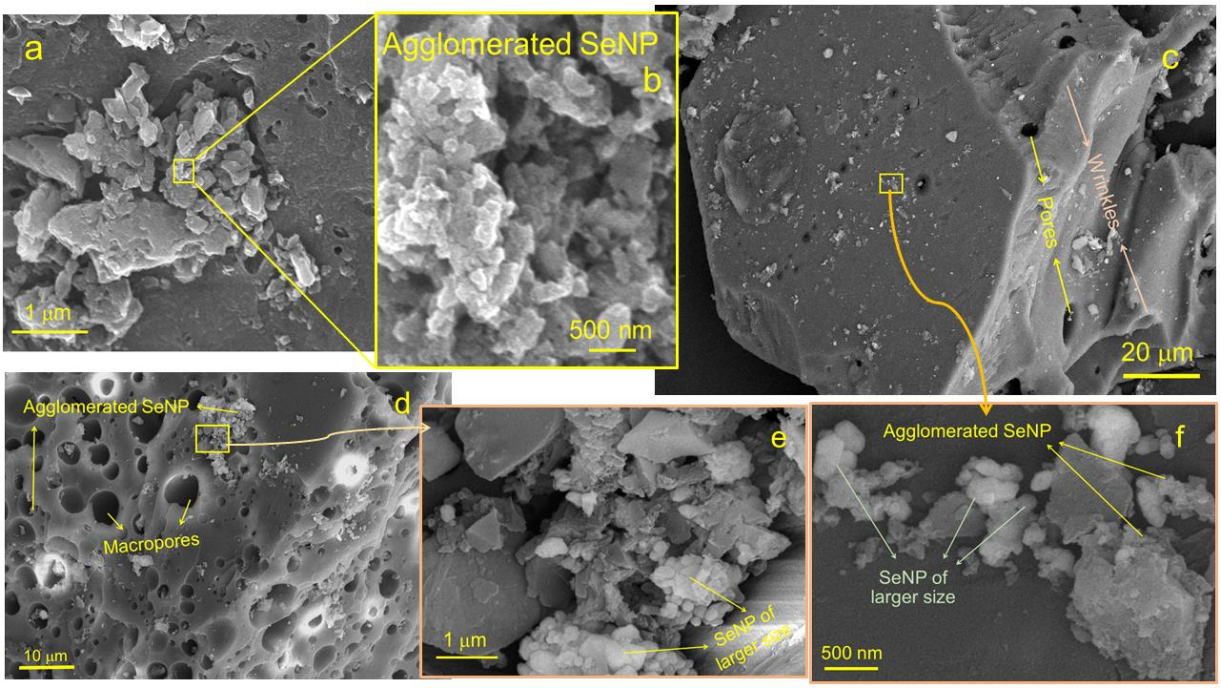


Fig. S3.1 FESEM Images of Se-DG-6 in different resolutions.

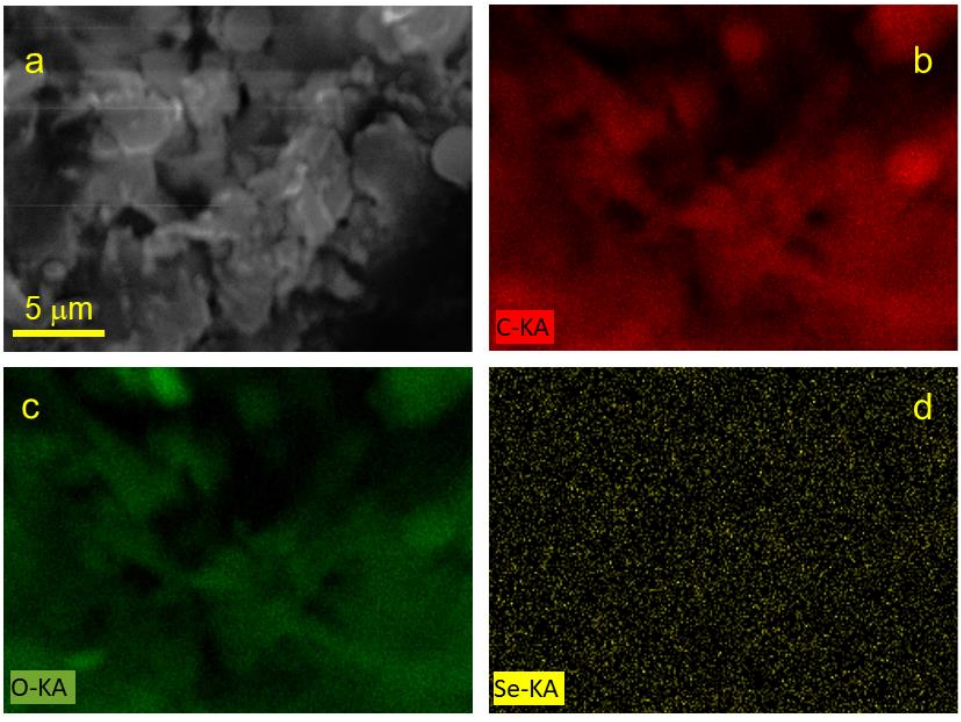


Fig. S3.2 Elemental mapping of C, O and Se in Se-DG-6.

3. HRTEM Images

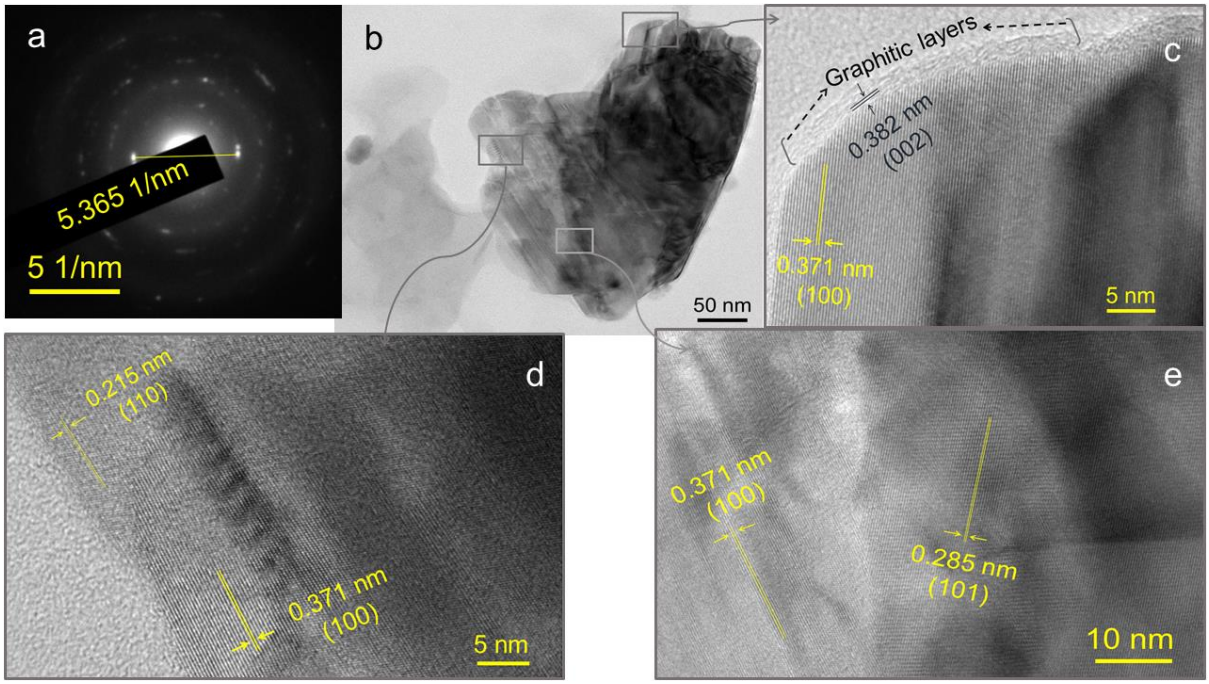


Fig. S4. HRTEM Images of Se-DG-1 in different resolutions.

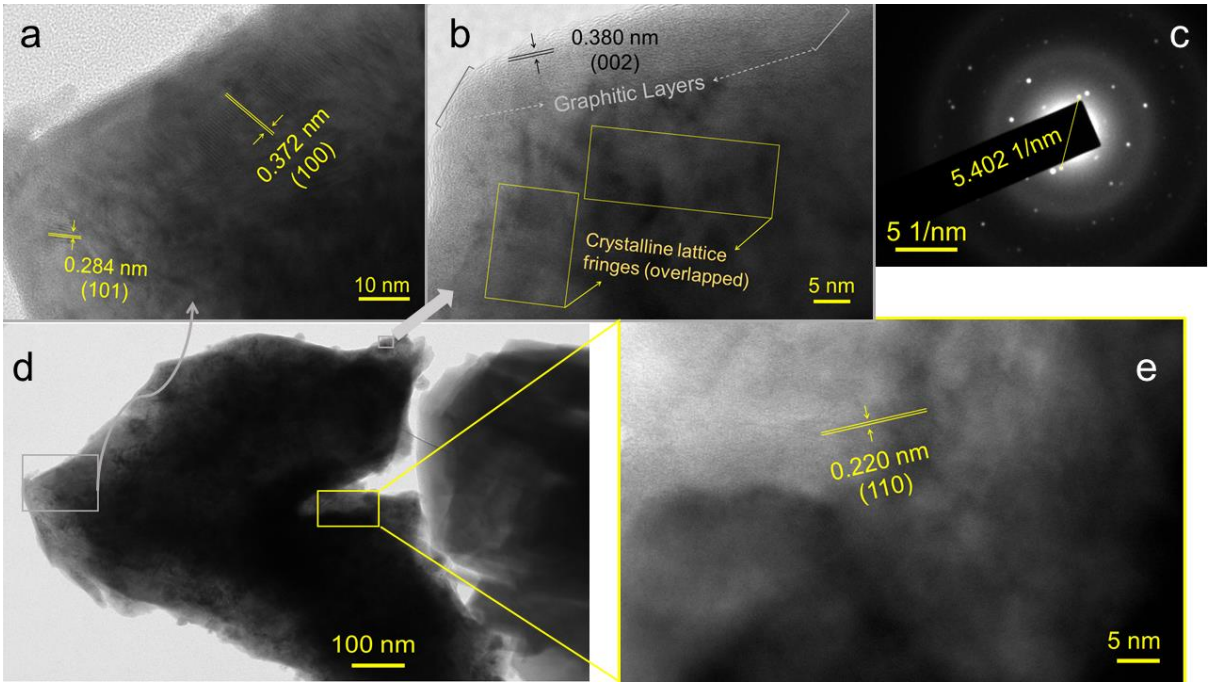


Fig. S5. HRTEM Images of Se-DG-2 in different resolutions.

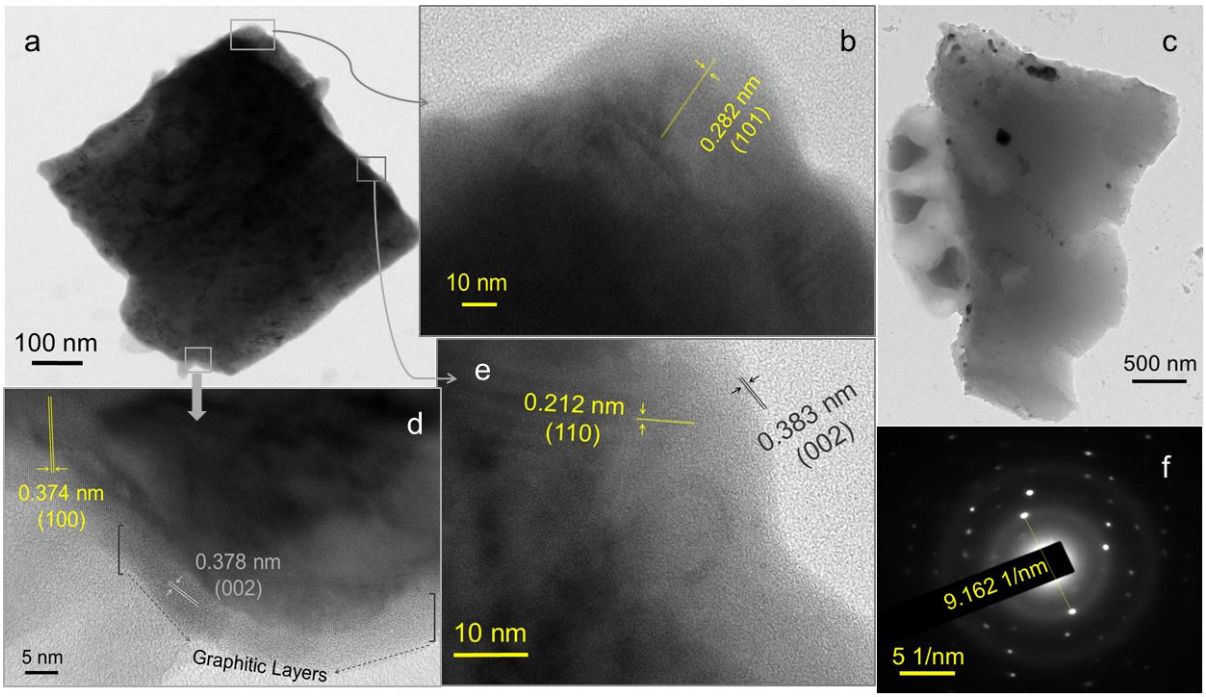


Fig. S6. HRTEM Images of Se-DG-6 in different resolutions.

In the HRTEM images, amorphous lattice fringes of graphitic layers are denoted by black and grey lines while regular lattice fringes of trigonal Se-crystals (t-Se) are denoted by yellow lines.

4. P-XRD

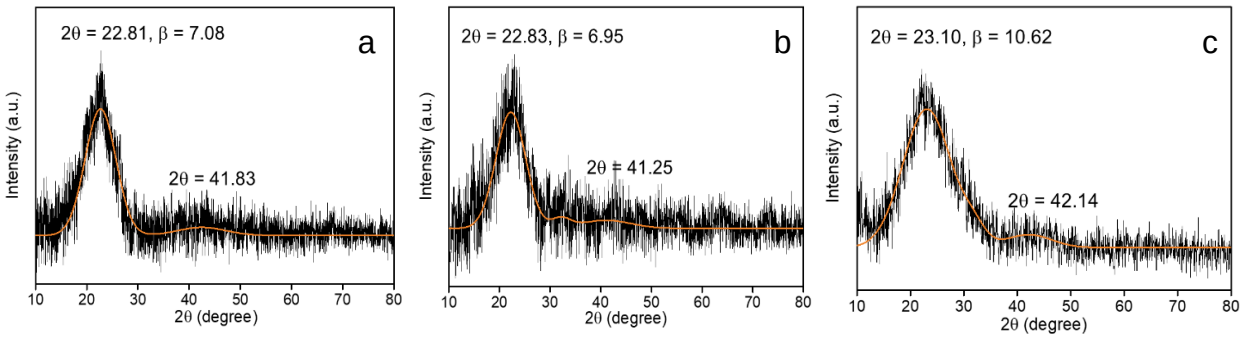


Fig. S7. P-XRD patterns of (a) Se-DG-1, (b) Se-DG-2 and (c) Se-DG-6 ('θ' refers to the diffraction angle and 'β' refers to the FWHM of the corresponding peak). Orange smooth line referred to the peak sums.

5. FT-IR Spectrum

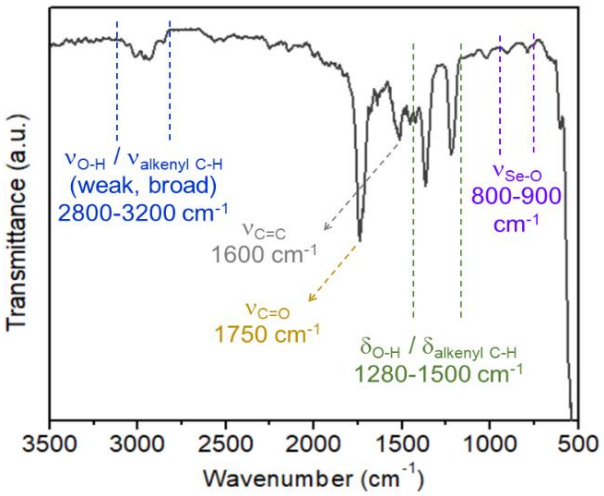


Fig. S8. FT-IR spectrum of Se-DG-6 with the assignment of functional groups. 'ν' denotes the stretching frequency and 'δ' denotes the bending frequency.

6. Raman spectrum

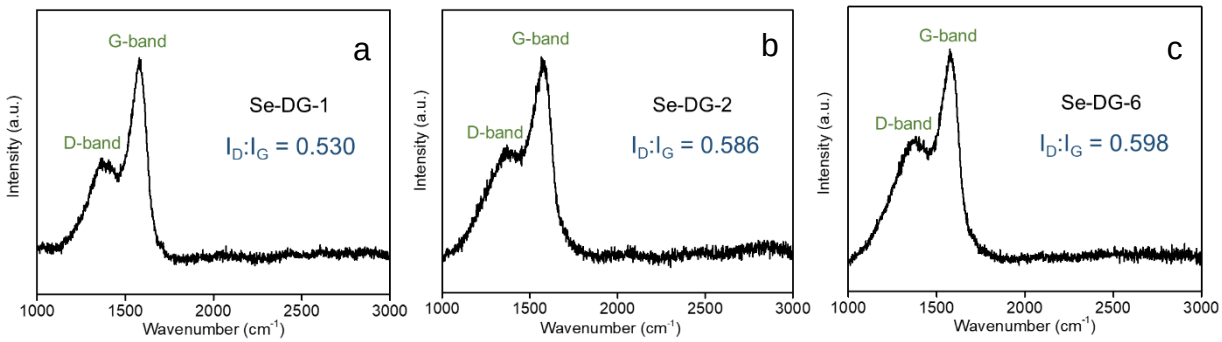


Fig. S9. Raman spectrum of (a) Se-DG-1, (b) Se-DG-2 and (c) Se-DG-6 with I_D:I_G values.

7. BET Surface area analysis

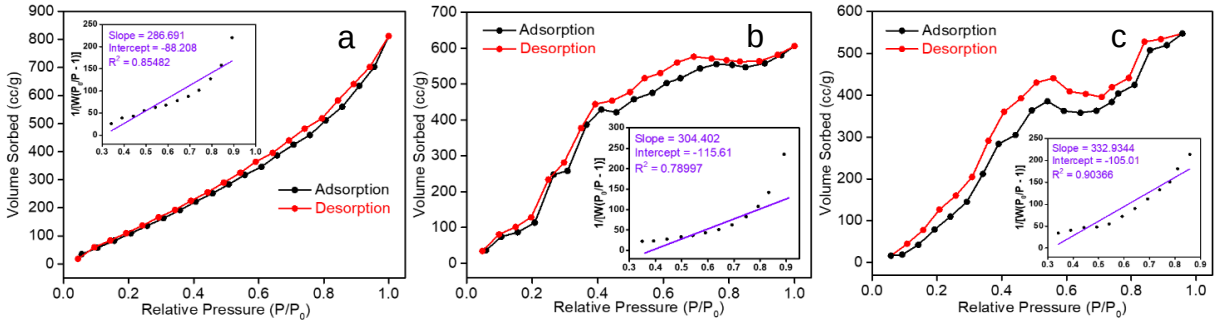


Fig. S10. BET surface area analysis of (a) SE-DG-1, (b) Se-DG-2 and (c) Se-DG-6. Inset: 12 point linear graph.

8. TGA

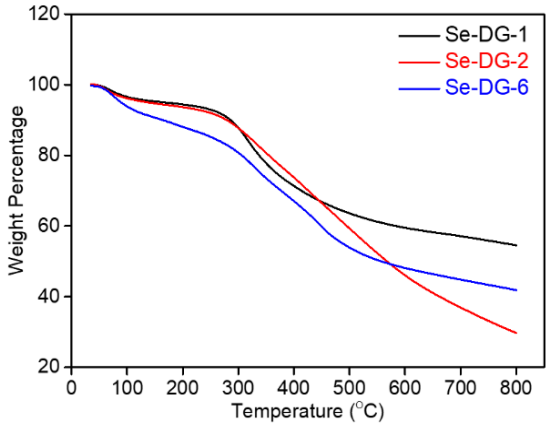


Fig. S11. TGA curves of Se-DG-1, Se-DG-2 and Se-DG-6.

9. XPS

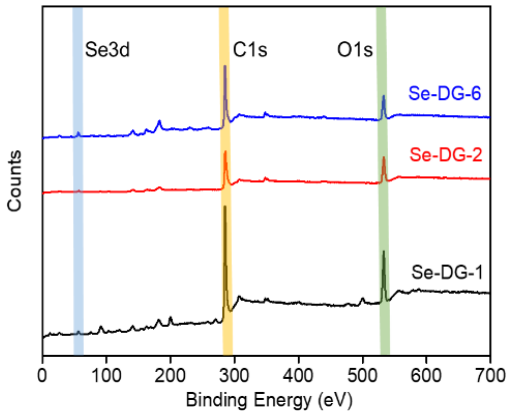


Fig. S12. XPS Survey spectrum of the three Se-DGs.

The atomic percentages of C, O and Se were calculated from the survey spectrum following eqn S1

$$\text{Conc of atom 'X': } \frac{n_x}{\sum_i n_i} = \frac{I_x/S_x}{I_i/S_i} \text{ .....Eqn S1}$$

'n' = the number of atom, 'I' = the area/intensity of photoemission peak, 'S' is sensitivity factor for respective atom.

10. GPx-like activity of Se-doped graphitic materials, measured in UV-vis spectroscopy

10.1. Figures

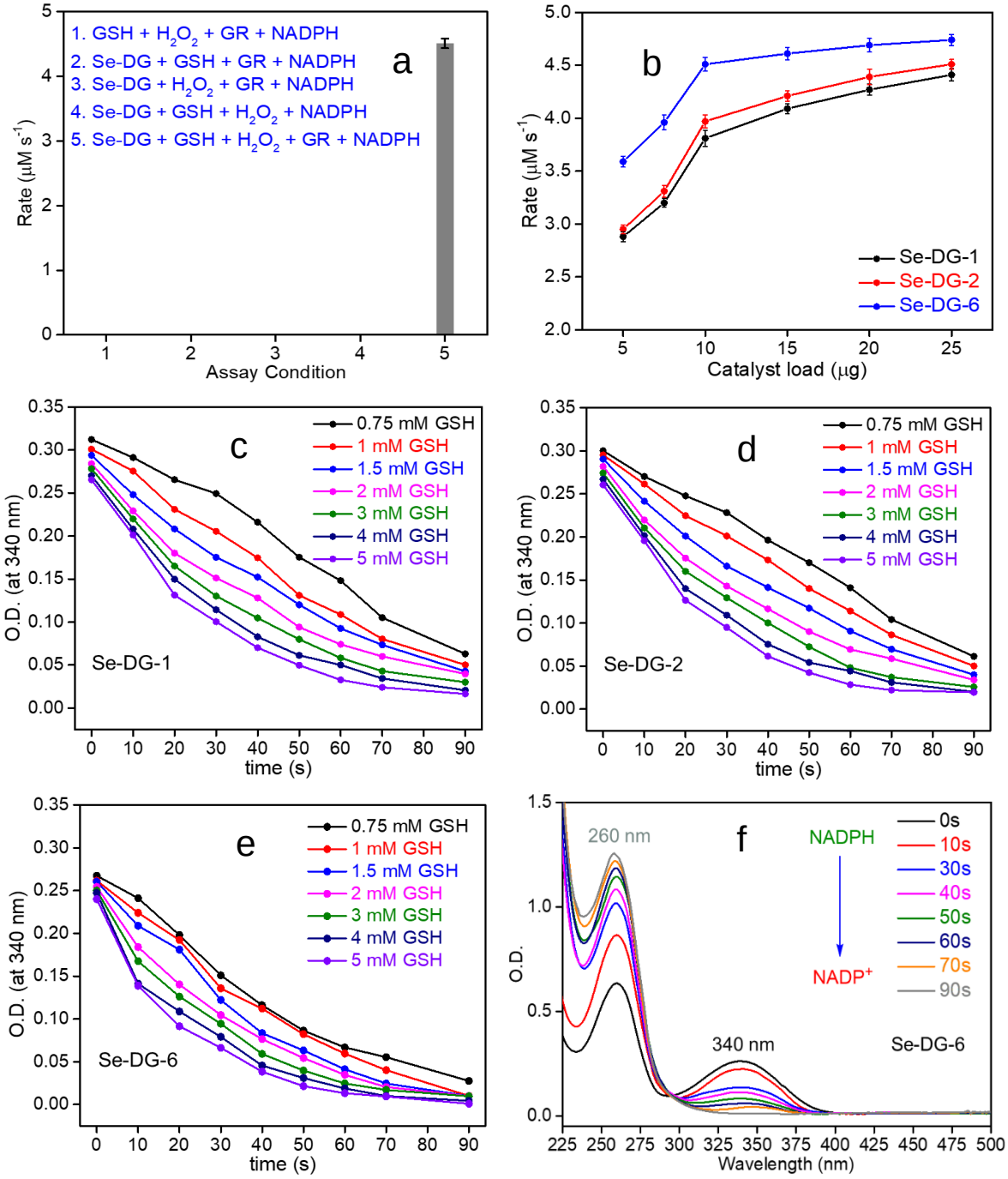


Fig. S13. (a) Bar diagrams of the rate values obtained in absence of any of the components (b) Effect of catalyst-dose (in presence of 4 mM GSH and 100 μM H_2O_2) (c)-(e) Rate determination curves of the degradation of 0.1(M) NADPH in UV-Vis spectroscopy by varying the concentration of GSH from 0.75 mM to 5 mM in presence of 100 μM H_2O_2 and 1.02 Unit GR using 10 μg of Se-DG-1 (a), Se-DG-2 (b) and Se-DG-6 (c) at pH = 7 (maintained by 0.1M phosphate buffer). (f) A representative UV-Vis spectrum for a single batch (10 μg Se-DG-6, 1 mM GSH and 100 μM H_2O_2).

10.2. Tables

Table S1. Initial rates of the NADPH degradation for all the batches of experiments performed to determine GPx-like activity of the three Se-DG materials.

Se-DG dose variation (Fig. S13b)

Assay: 4 mM GSH, 100 μM H_2O_2, 100 μM NADPH, 1.02 U GR, 0.1 M phosphate buffer.

Se-DG dose (μg)	Initial rate (unit: $\mu M.s^{-1}$)		
	Se-DG-1	Se-DG-2	Se-DG-6
5	2.88 ± 0.048	2.95 ± 0.042	3.59 ± 0.051
7.5	3.20 ± 0.041	3.31 ± 0.056	3.96 ± 0.071
10	3.81 ± 0.077	3.97 ± 0.061	4.51 ± 0.065
15	4.09 ± 0.047	4.21 ± 0.048	4.61 ± 0.058
20	4.27 ± 0.052	4.39 ± 0.074	4.69 ± 0.064
25	4.41 ± 0.057	4.51 ± 0.045	4.74 ± 0.053

GSH conc. variation (Fig. 2a)

Assay: 10 μg Se-DG, 100 μM H_2O_2, 100 μM NADPH, 1.02 U GR, 0.1 M phosphate buffer

GSH conc. (mM)	Initial rate (unit: $\mu M.s^{-1}$)		
	Se-DG-1	Se-DG-2	Se-DG-6
0.75	2.72 ± 0.041	2.76 ± 0.071	2.79 ± 0.067
1.0	3.06 ± 0.064	3.10 ± 0.051	3.22 ± 0.046
1.5	3.24 ± 0.043	3.38 ± 0.058	3.74 ± 0.028
2.0	3.41 ± 0.058	3.46 ± 0.072	3.88 ± 0.081
3.0	3.57 ± 0.065	3.68 ± 0.046	4.29 ± 0.072
4.0	3.71 ± 0.047	3.77 ± 0.057	4.51 ± 0.075
5.0	3.80 ± 0.054	3.94 ± 0.063	4.76 ± 0.063

H_2O_2 conc. variation (Fig. 2b)

Assay: 10 μg Se-DG, 4 mM GSH, 100 μM NADPH, 1.02 U GR, 0.1 M phosphate buffer.

H_2O_2 conc. (μM)	Initial rate (unit: $\mu M.s^{-1}$)		
	Se-DG-1	Se-DG-2	Se-DG-6
50	1.26 ± 0.116	1.70 ± 0.128	2.33 ± 0.165
75	2.31 ± 0.131	2.79 ± 0.144	3.59 ± 0.124
100	3.22 ± 0.165	3.88 ± 0.138	4.51 ± 0.141
150	4.09 ± 0.148	4.46 ± 0.152	4.96 ± 0.124
200	4.71 ± 0.133	4.98 ± 0.137	5.22 ± 0.136
250	5.12 ± 0.126	5.23 ± 0.125	5.53 ± 0.155
300	5.43 ± 0.158	5.51 ± 0.134	5.71 ± 0.131

Table S2. Kinetic parameters of GPx like activity of three Se-DGs, calculated from Michaelis-Menten equation.

Catalyst	w.r.t. GSH concentration		w.r.t. H_2O_2 concentration	
	V_{max} ($\mu M\ s^{-1}$)	K_M (μM)	V_{max} ($\mu M\ s^{-1}$)	K_M (μM)
Se-DG-1	4.03 ± 0.042	348.2 ± 21.6	10.08 ± 1.422	239.8 ± 61.0
Se-DG-2	4.16 ± 0.052	365.4 ± 26.3	8.32 ± 0.844	144.8 ± 33.4
Se-DG-6	5.54 ± 0.143	775.3 ± 28.0	7.44 ± 0.547	82.6 ± 17.4

Table S3. Comparison of antioxidant activities of native GPx and nano-enzyme mimics of GPx.

Catalyst		w.r.t. GSH concentration		w.r.t. H_2O_2 concentration	
		V_{max} ($\mu M\ s^{-1}$)	K_M (μM)	V_{max} ($\mu M\ s^{-1}$)	K_M (μM)
GPx[12]		--	10000	--	25
V_2O_5 NW[10a]		14	2220	7.2	110
Mn_3O_4 NP[10b]		1.3	1160	0.93	196
V_2O_5-pDA-MnO_2[11a]		3.2	7200	1.5	160
V-based MOF[11b#]		3.1	3990	1.6	22
GO-Se[12a§]		0.82	720	0.5	40
This work	Se-DG-1	4.03	348.2	10.08	239.8
	Se-DG-2	4.16	365.4	8.32	144.8
	Se-DG-6	5.54	775.3	7.44	82.6

[#]various ligands like halides, -CH_3, -NH_2, -H were used to form various MOFs with V_2O_5. This result was for -Br. [§]the first report of completely metal-free nanomaterial acting as GPx-mimic.

10.3. GPx-activity of Se-DG materials having same molar percentage of Se

Table S4. Calculation of required amount of the catalysts with same molar percentage of Se

	Se-DG-1	Se-DG-2	Se-DG-6
Stoichiometric chemical formula (from XPS)	$C_{81.99}O_{16.76}Se_{1.25}$	$C_{81.81}O_{16.56}Se_{1.63}$	$C_{80.45}O_{16.42}Se_{3.13}$
Corresponding MW	1350.72 amu	1375.37 amu	1477.65 amu
Se amount present in 1 molecule of catalyst	98.70 amu	128.70 amu	247.14 amu
Weight of Se in 10 μg catalyst	--	--	1.67 μg
Required weight of catalyst containing 1.67 μg Se	22.89 μg	17.87 μg	10 μg

From XPS analysis, the amount of Se present in 10 μg (optimal catalyst dose, Fig. S13b) of Se-DG-6 was calculated as 1.67 μg. To keep this amount fixed for Se-DG-1 and Se-DG-2, their required amounts were calculated as 22.89 μg and 17.87 μg respectively. The entire calculation was shown stepwise in Table S4.

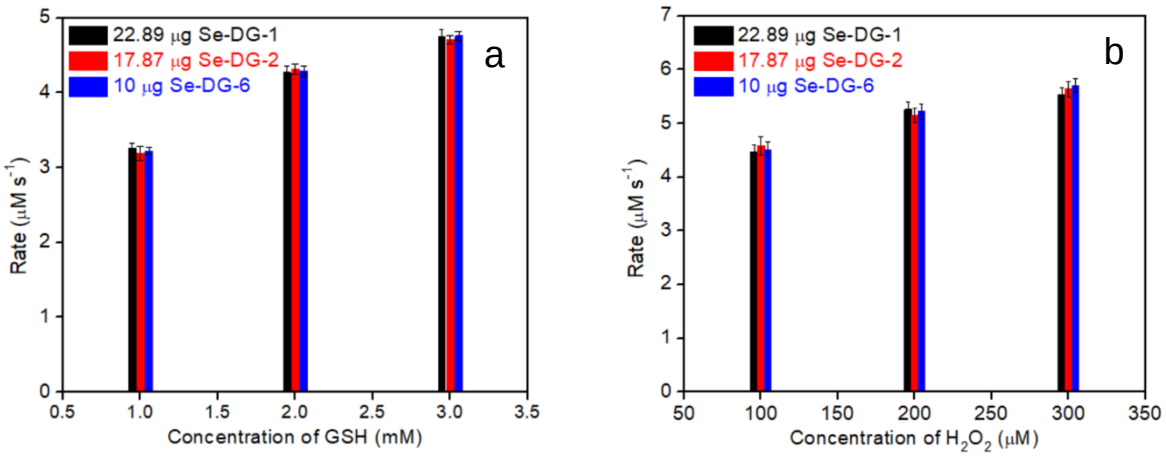


Fig. S14. GPx-like activity of Se-DG-1, Se-DG-2 and Se-DG-6 in their normalized proportion containing equal molar percentage of Se, with respect to the variation of GSH concentration (a) and H_2O_2 concentration (b). The rate values were listed below in Table S5.

Table S5. Initial rates of GPx-like activity of the three Se-DG materials containing equal molar percentage of Se.

GSH conc. Variation (Fig. 14a)

Assay: Se-DG, 100 μM H_2O_2, 100 μM NADPH, 1.02 U GR, 0.1 M phosphate buffer			
GSH conc. (mM)	Initial rate (unit: $\mu M.s^{-1}$)		
	22.89 μg Se-DG-1	17.87 μg Se-DG-2	10 μg Se-DG-6
1.0	3.26 ± 0.071	3.19 ± 0.089	3.22 ± 0.046
3.0	4.27 ± 0.085	4.32 ± 0.070	4.29 ± 0.072
5.0	4.75 ± 0.094	4.71 ± 0.048	4.76 ± 0.063

H_2O_2 conc. variation (Fig. 14b)

Assay: Se-DG, 4 mM GSH, 100 μM NADPH, 1.02 U GR, 0.1 M phosphate buffer			
H_2O_2 conc. (μM)	Initial rate (unit: $\mu M.s^{-1}$)		
	22.89 μg Se-DG-1	17.87 μg Se-DG-2	10 μg Se-DG-6
100	4.47 ± 0.135	4.58 ± 0.168	4.51 ± 0.141
200	5.26 ± 0.139	5.15 ± 0.125	5.22 ± 0.136
300	5.53 ± 0.135	5.64 ± 0.140	5.71 ± 0.131

11. Epoxidation of alkene by H_2O_2 in presence Se-DG materials

11.1. GC Methods

Table S6. GC methods for different alkenes for monitoring the epoxidation reaction.

Inlet			Detector (FID)		
Septum purge flow		3 ml/min	Zero air (carrier gas)		300 ml/min
Split flow		30 ml/min	H_2 (fuel gas)		30 ml/min
Split ratio		30:1	N_2 (make up)		25 ml/min
Substrate	Temp of oven (^oC)		Heating rate (^oC/min)	Hold time (min)	Total run time (min)
	Initial	Final			
Styrene	60	150	10	2	11
	150	300	50	2	16
p-methoxy styrene	60	150	10	2	11
	150	300	20	2	20.5
p-methyl styrene	60	60	-	1	1
	60	140	10	2	11
	140	160	2	2	23
	160	260	5	0	43
p-fluoro styrene	60	120	10	2	8
	120	300	20	1	8
p-nitro styrene	60	80	10	1	3
	80	120	10	1	8
	120	160	20	1	11
	160	300	20	2	20
p-cyano styrene	60	80	5	0	4
	80	120	10	0	8
	120	160	20	1	11
	160	300	20	0	18
cyclopentene, cyclohexene and cyclooctene	60	65	5	0	1
	65	70	1	1	7
	70	100	10	0	10
	100	300	20	0	20
2,3-dimethyl butene	60	70	1	0	10
	70	100	10	0	13
	100	300	20	0	23

11.2. Calibration of the alkenes in GC

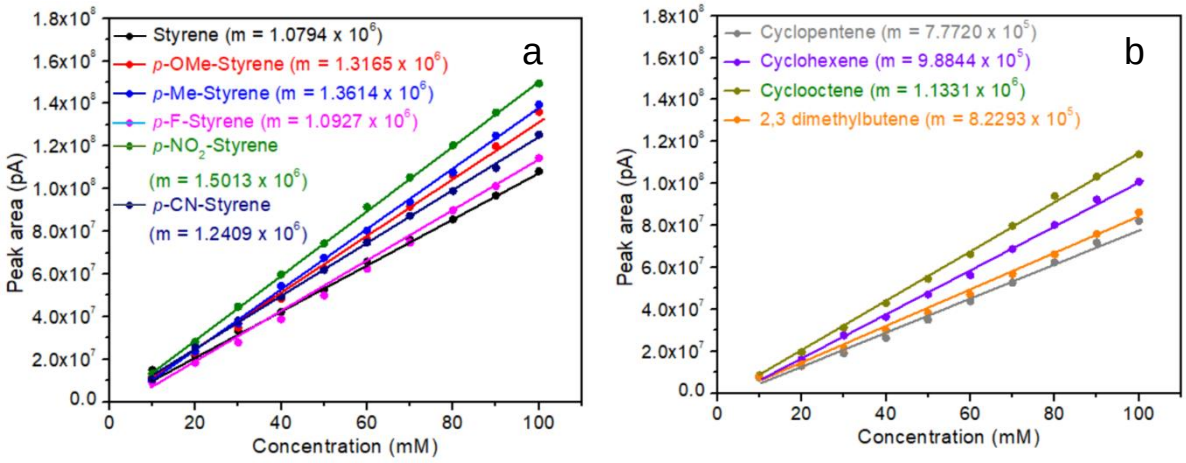


Fig. S15. Linear calibration curves from the GC peak areas (unit: pico Ampere or pA) of known concentrations of the (a) aromatic and (b) aliphatic alkene substrates (within 10 mM to 100 mM conc. range) in the respective GC methods described in Table S6. Slopes (m) of the corresponding curves are mentioned in same colour code.

Table S7. Derived parameters from the linear calibration curves of the alkenes (Fig. S15)

Aromatic alkenes			Aliphatic alkenes		
Alkene	Slope	Linearity (R^2)	Alkene	Slope	Linearity (R^2)
Styrene	1.0794×10^6	0.99972	Cyclopentene	7.7720×10^5	0.99799
p-methoxy-Styrene	1.3165×10^6	0.99895	Cyclohexene	9.8844×10^5	0.99919
p-methyl-Styrene	1.3614×10^6	0.99911	Cyclooctene	1.1331×10^6	0.99886
p-fluoro-Styrene	1.0927×10^6	0.99698	2,3-dimethyl butene	8.2293×10^5	0.99747
p-nitro-styrene	1.5013×10^6	0.99987			
p-cyano-styrene	1.2409×10^6	0.99981			

These slopes were used to calculate the unknown concentration of the solution taken out from the reaction mixture and properly diluted with acetonitrile.

11.3. Optimization of the reaction condition: graphical approach

Optimization of the reaction condition (Table 3) of epoxidation using 1 mmol styrene has been picturized graphically in Fig. S16. From fig. 'a' to 'd', the four parameters were optimized sequentially to get the best reaction condition, presented in Scheme 2 (in the manuscript). Conversion of the alkenes and yield and selectivity of the epoxides were calculated using equation 2, 3 and 4.

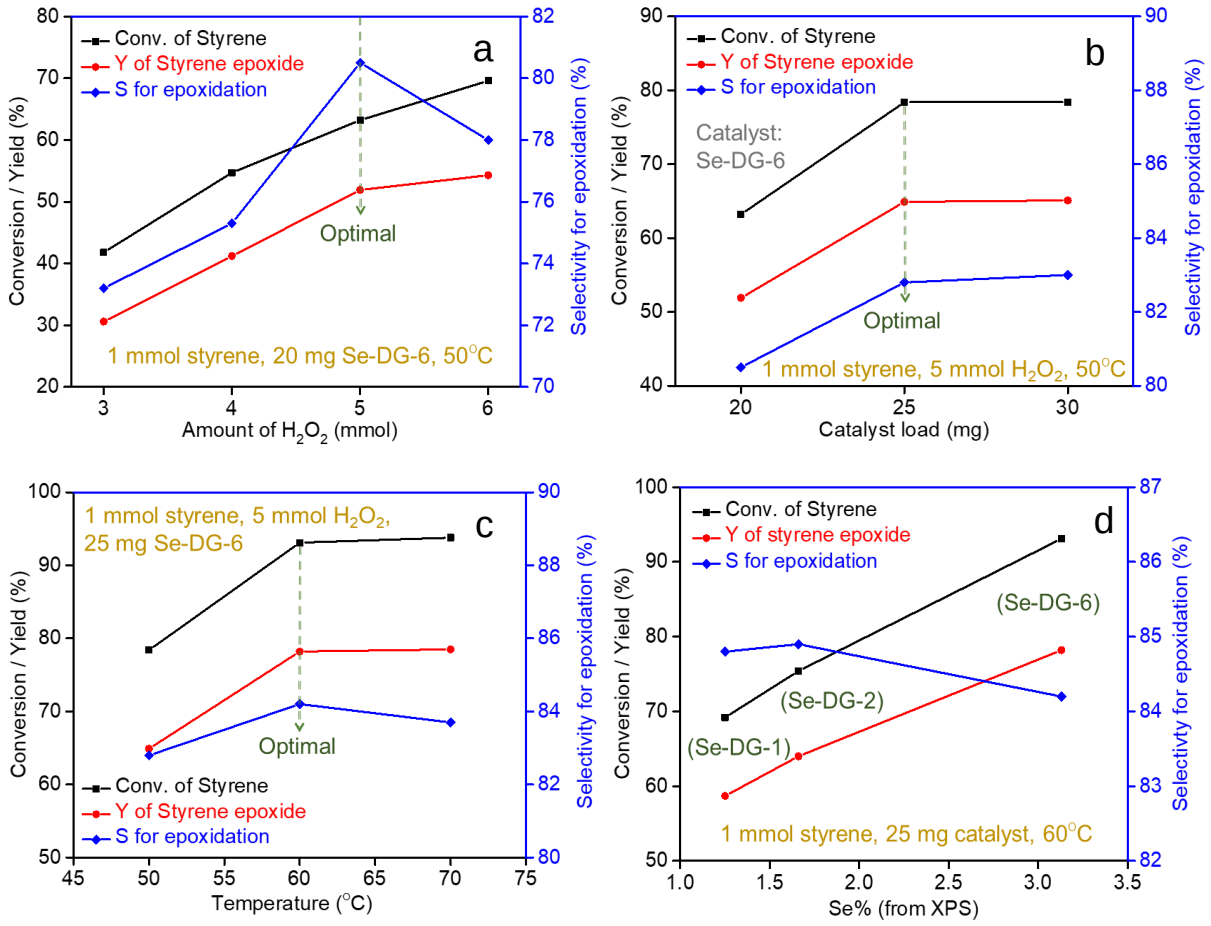


Fig. S16. Optimization of the reaction condition of Se-DG catalysed epoxidation. (a) Effect of H_2O_2 amount on the extent of epoxidation where 5 equiv. H_2O_2 w.r.t. styrene found to be the optimal. 6 equiv. of H_2O_2 resulted in a slight increase in the conversion, but the selectivity towards epoxide decreased due to hydrolysis of the epoxide. (b) Effect of Se-DG-6 load, which showed 25 mg as the optimal. (c) Effect of temperature, where 60 ^oC found to be the optimal. (d) Effect of Se% in the three Se-DG materials on the extent of epoxidation. Conversion and yield% changed linearly with the increase of Se% while selectivity remained almost same. All the reactions were carried out using 1 mmol styrene in 5 ml MeCN.

11.4. GC-MS chromatogram

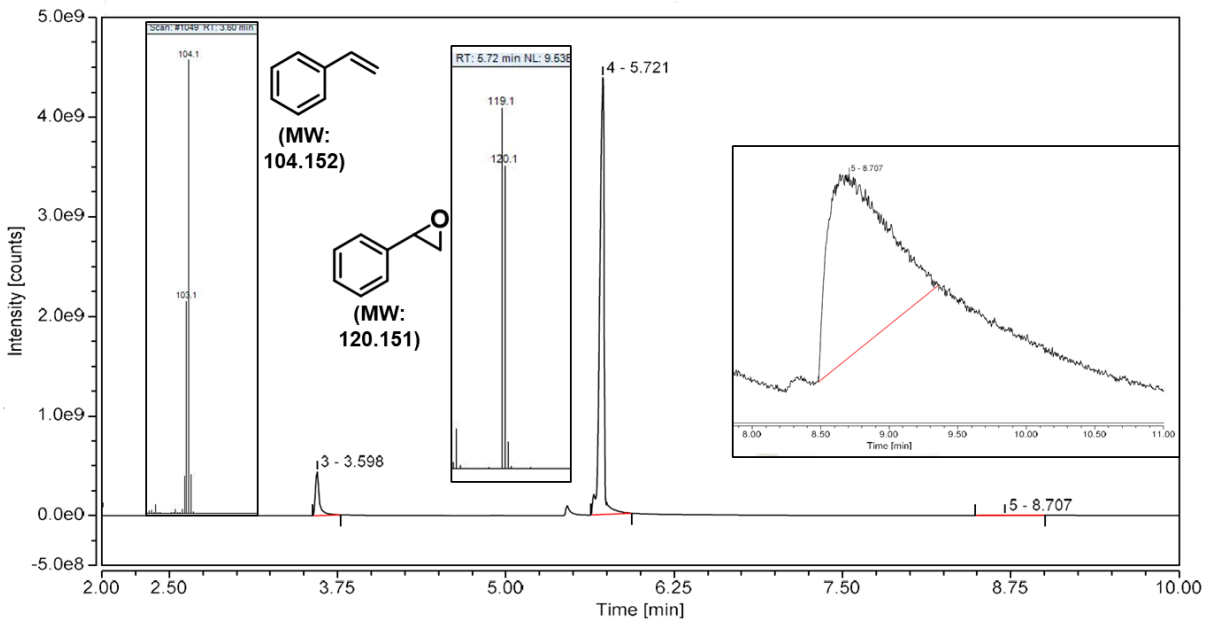


Fig. S17. GC-MS figure for the conversion styrene to styrene epoxide in presence of Se-DG. The peak at retention time (RT) = 3.598 min correspond to styrene and at RT = 5.721 min correspond to styrene epoxide. The small peak of minor product styrene glycol is obtained at RT = 8.707, which is shown in zoomed image in inset. The mass values are also presented in inset.

12. NMR spectrum of the products

Styrene epoxide

^{1}H NMR (400 MHz, CD_3Cl): δ = 7.34-7.37 (m, 2H, Ar), 7.31-7.33 (m, 1H, Ar), 7.28-7.30 (m, 2H, Ar), 3.86-3.87 (dd, 1H), 3.14-3.16 (dd, 1H), 2.80-2.82 (q, 1H). **^{13}C{H} NMR (100 MHz, CD_3Cl)**: δ = 137.72 (Ar), 128.63 (Ar), 128.31 (Ar), 125.62 (Ar), 52.50, 51.33

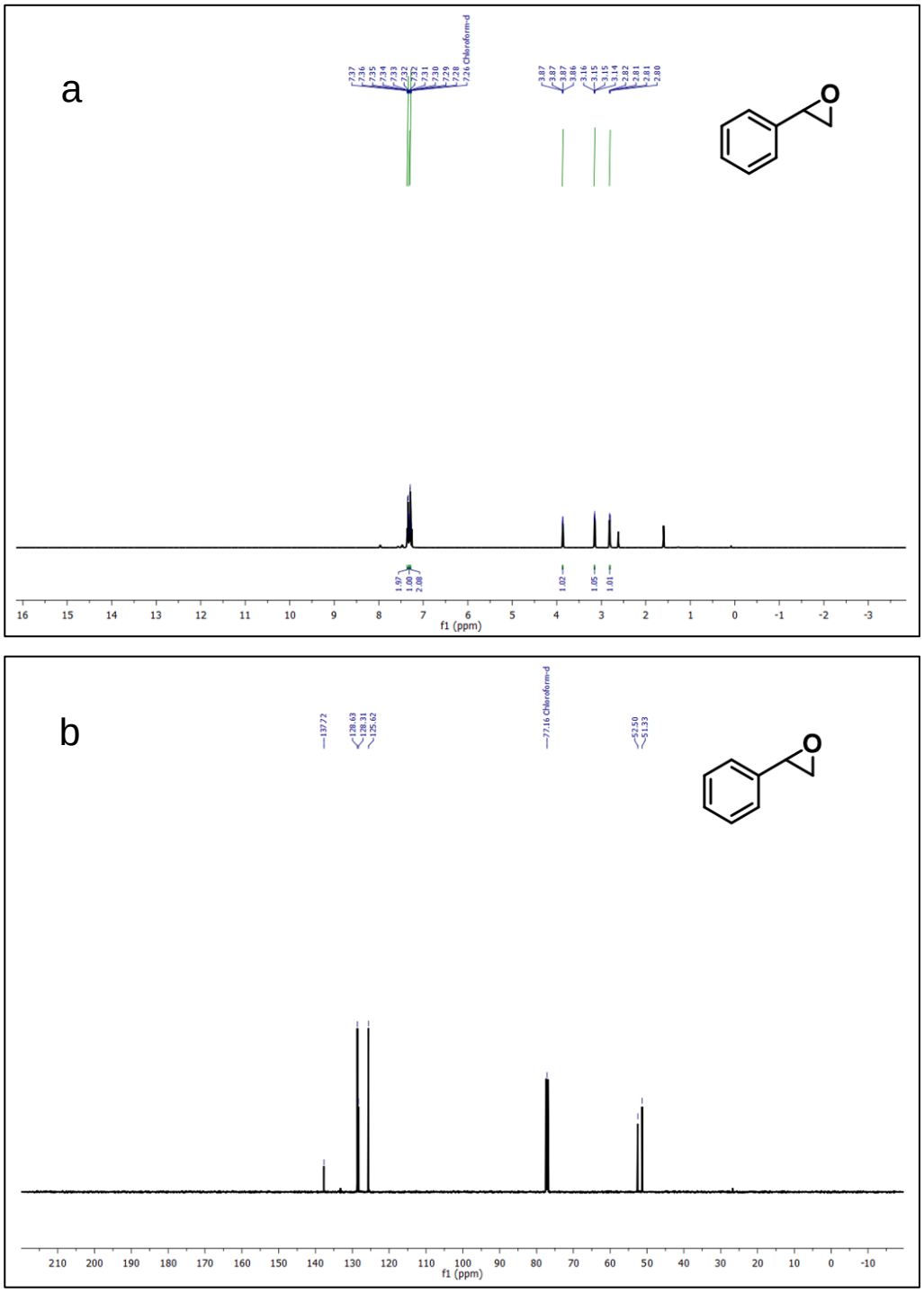


Fig. S18. (a) ^{1}H and (b) ^{13}C NMR spectra of styrene epoxide

Styrene glycol (1-Phenylethane-1,2-diol)

^{1}H NMR (400 MHz, CD_3Cl): δ = 7.34-7.35 (t, 3H, Ar), 7.27-7.30 (m, 1H, Ar), 7.23 (s, 1H, Ar), 4.79-4.82 (dd, 1H), 3.73-3.76 (d, J=12, 1H), 3.63-3.67 (dd, 1H), 2.49 (s, 1H, O-H), 2.03 (s, 1H, O-H). **^{13}C{H} NMR (100 MHz, CD_3Cl)**: δ = 140.64 (Ar), 128.72 (Ar), 128.19 (Ar), 125.62 (Ar), 74.83, 68.25

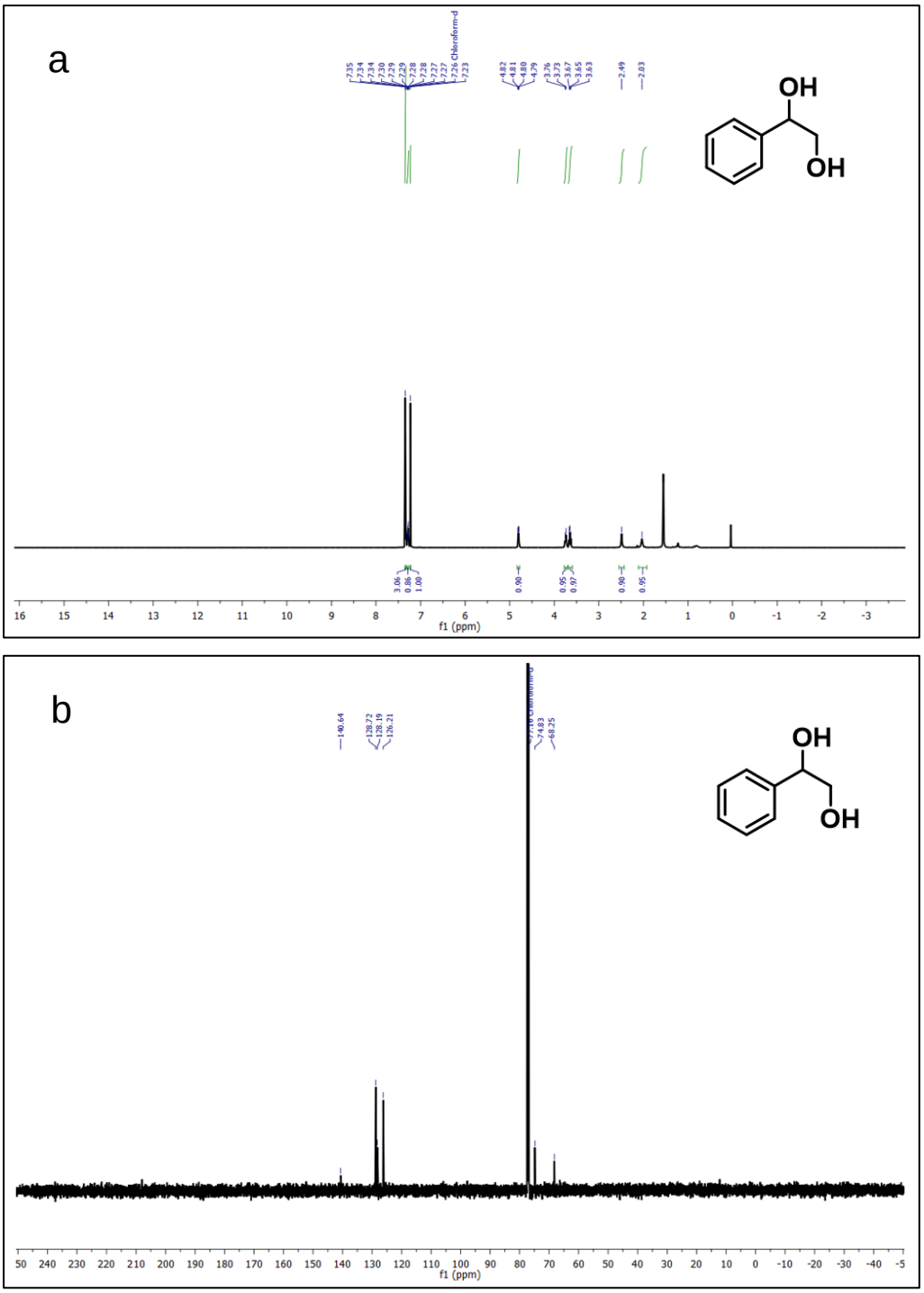
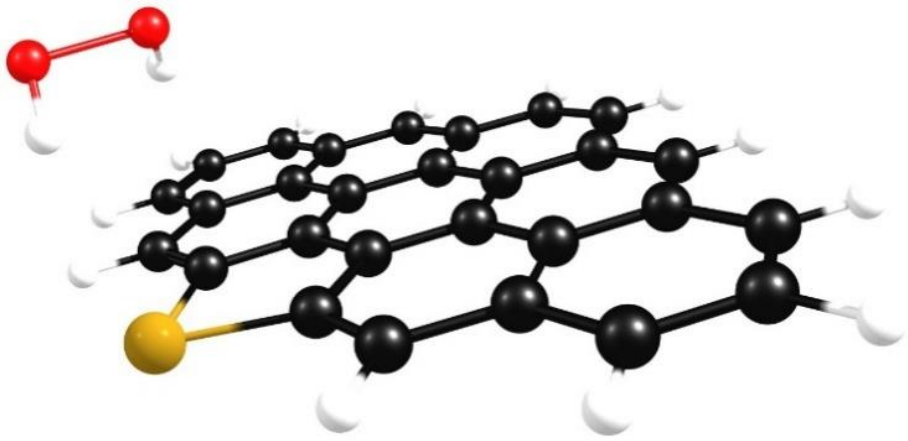


Fig. S19. (a) ^{1}H and (b) ^{13}C NMR spectra of styrene glycol

13. Theoretical results

Table S8. Cartesian coordinates of the optimized geometries in DFT with the relevant energy values. Code: Gaussian. Exchange correlation function: m052x. Basis set: 6-311G(d,p). Solvent: Acetonitrile (SMD). Keywords 'opt=tight' and 'int=ultrafine' were added.

Molecule: 5Se-R-1							
C	-3.777859	-1.451790	0.082021	H	-3.071006	3.128206	-0.445868
C	-2.952654	-0.308897	-0.084151	C	1.072904	-3.168060	0.056127
C	-1.554935	-0.483789	-0.138516	C	3.269230	-2.085285	-0.148576
C	-0.957394	-1.758704	-0.017263	C	-1.280284	1.956117	-0.412553
C	-1.800940	-2.909852	0.149222	C	0.202911	-4.319985	0.222545
C	-3.163392	-2.743066	0.196266	H	0.666318	-5.294206	0.315042
C	-0.740534	0.642114	-0.299095	C	-1.141196	-4.199307	0.266834
C	0.438683	-1.884937	-0.069727	C	2.443339	-3.247112	0.011901
C	1.244782	-0.735311	-0.229367	Se	0.173564	3.208219	-0.615751
C	0.634574	0.517031	-0.356685	H	-5.817132	-2.117027	0.258253
C	1.391297	1.715417	-0.511458	H	-1.763191	-5.076510	0.393964
C	2.748677	1.663783	-0.545688	C	4.669875	-2.145331	-0.189977
C	3.413470	0.381076	-0.426476	C	4.806272	0.264506	-0.460240
C	2.651978	-0.812835	-0.271459	H	5.410463	1.154824	-0.578388
H	-3.804943	-3.606876	0.323999	C	5.415680	-0.983887	-0.343796
H	3.357146	2.551418	-0.658184	H	6.495354	-1.047630	-0.373500
C	-5.166574	-1.261380	0.130758	H	2.928204	-4.211626	0.104884
C	-5.701619	0.015212	0.017229	H	5.164322	-3.104021	-0.099656
H	-6.774905	0.145459	0.056766	O	1.267265	1.798360	2.714017
C	-4.887996	1.135409	-0.145703	O	1.579605	3.177871	2.582143
H	-5.330583	2.119626	-0.230380	H	0.994200	3.454310	1.858040
C	-3.497316	1.002177	-0.200723	H	1.926250	1.376765	2.142761
C	-2.623752	2.146354	-0.365032				

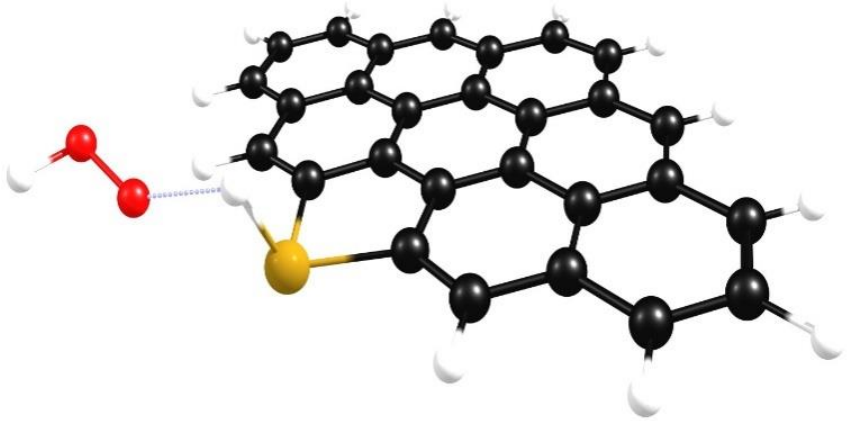


E^0 = -3627.565959 E^0 + ZPE = -3627.231087

ΔG^0 = -3627.283654

Molecule: 5Se-TS-1

C	4.177305	0.448291	0.113655	H	2.176936	-3.757316	-0.188031
C	3.056496	-0.417311	0.022688	C	0.019603	3.481264	0.079178
C	1.766023	0.150805	-0.015519	C	-2.399916	3.059840	-0.033860
C	1.561455	1.547695	0.046719	C	0.806370	-2.115229	-0.162310
C	2.703035	2.414943	0.138145	C	1.186987	4.342082	0.170431
C	3.961604	1.865772	0.170525	H	1.024321	5.411409	0.219102
C	0.662311	-0.701380	-0.108283	C	2.441649	3.843439	0.198586
C	0.258713	2.066696	0.008005	C	-1.273304	3.944404	0.053893
C	-0.845387	1.190270	-0.083887	Se	-0.978475	-2.900929	-0.360834
C	-0.620988	-0.186897	-0.156093	H	6.326060	0.506817	0.214377
C	-1.698588	-1.105282	-0.245983	H	3.291405	4.510929	0.267451
C	-2.985817	-0.695496	-0.255631	C	-3.727029	3.514620	-0.049697
C	-3.251775	0.730232	-0.186995	C	-4.553262	1.236466	-0.196267
C	-2.175082	1.660587	-0.107253	H	-5.388985	0.551212	-0.254861
H	4.827479	2.513301	0.240316	C	-4.777951	2.611237	-0.129938
H	-3.806630	-1.399916	-0.279615	H	-5.794710	2.980387	-0.139725
C	5.454531	-0.131463	0.145011	H	-1.462136	5.010046	0.106571
C	5.601095	-1.510640	0.086894	H	-3.924499	4.577683	0.003354
H	6.593851	-1.939559	0.112006	O	-4.395773	-3.283586	1.039638
C	4.497118	-2.357718	-0.003807	O	-3.041823	-3.678668	0.728129
H	4.637434	-3.429981	-0.048518	H	-1.342063	-3.311865	1.037738
C	3.203484	-1.832763	-0.039089	H	-4.880875	-4.103574	0.909832
C	2.033207	-2.686120	-0.138078				

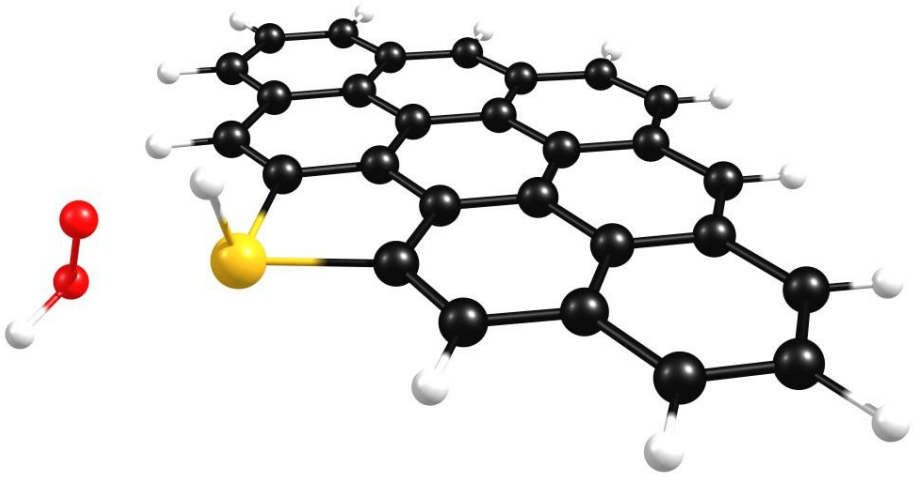


E^0 = -3627.467459 E^0 + ZPE = -3627.137384

ΔG^0 = -3627.187162 ν_{imag} = -613.058

Molecule: 5Se-P-1

C	4.154355	0.524492	-0.033051	H	2.208718	-3.709995	0.070172
C	3.043164	-0.358165	0.001892	C	-0.045389	3.494587	-0.041766
C	1.741967	0.188079	0.006721	C	-2.459061	3.045222	0.010711
C	1.520616	1.582936	-0.023009	C	0.802217	-2.097944	0.077724
C	2.651806	2.468343	-0.058375	C	1.111039	4.373720	-0.079242
C	3.919076	1.939342	-0.062595	H	0.933084	5.441565	-0.100710
C	0.650383	-0.686685	0.045676	C	2.372983	3.894066	-0.087086
C	0.209591	2.080589	-0.014240	C	-1.342603	3.944383	-0.032000
C	-0.884286	1.185700	0.022298	Se	-1.028374	-2.955801	0.035202
C	-0.645691	-0.194022	0.049247	H	6.304103	0.618317	-0.062467
C	-1.716787	-1.126159	0.088143	H	3.214809	4.574584	-0.114311
C	-3.004912	-0.715791	0.101721	C	-3.791168	3.484978	0.026859
C	-3.285666	0.706313	0.080678	C	-4.593581	1.196215	0.096364
C	-2.217938	1.646689	0.037461	H	-5.421002	0.499224	0.128676
H	4.776219	2.601718	-0.088406	C	-4.833703	2.569260	0.069412
H	-3.820332	-1.423653	0.128538	H	-5.854427	2.927325	0.081643
C	5.440993	-0.034569	-0.037051	H	-1.541742	5.009272	-0.050521
C	5.606099	-1.412727	-0.008635	H	-3.998927	4.547272	0.006748
H	6.605468	-1.827062	-0.012393	O	-3.652392	-3.600686	-0.879711
C	4.511730	-2.276497	0.024057	O	-3.036146	-3.605935	0.416698
H	4.666383	-3.347745	0.044652	H	-0.943941	-3.291425	1.464659
C	3.208980	-1.772158	0.029984	H	-3.668175	-4.535656	-1.109817
C	2.044582	-2.639119	0.059566				

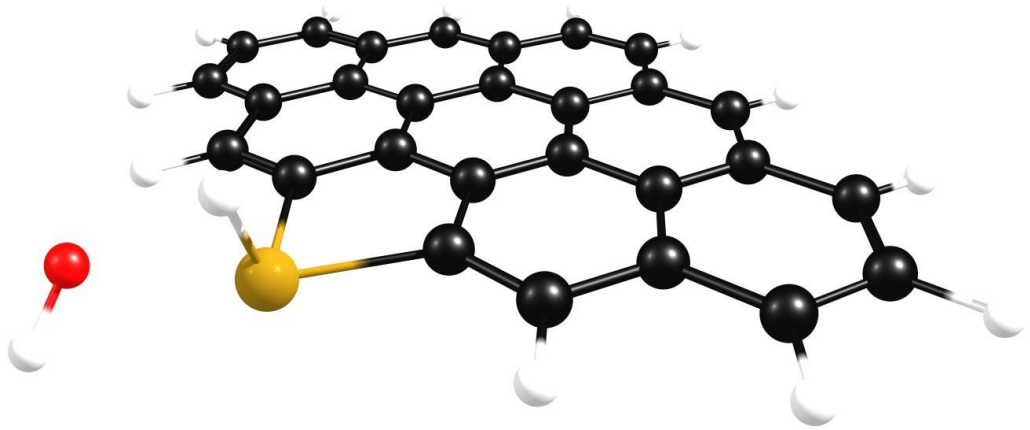


E^0 = -3627.480847 E^0 + ZPE = -3627.148027

ΔG^0 = -3627.197960

Molecule: 5Se-R-2

C	3.856628	1.223646	0.006828	C	2.451390	-2.310960	-0.010046
C	2.953877	0.127971	0.002548	H	2.837492	-3.323680	-0.021088
C	1.566954	0.390104	0.003113	C	-0.867907	3.253767	0.006118
C	1.060796	1.708817	0.002462	C	-3.135215	2.313397	-0.002406
C	1.982363	2.811473	0.010570	C	1.121549	-2.045824	0.003071
C	3.332090	2.558462	0.011402	C	0.079868	4.355278	0.013934
C	0.682421	-0.695440	0.001297	H	-0.316177	5.363008	0.017644
C	-0.325238	1.923030	0.003287	C	1.413896	4.148370	0.014891
C	-1.208689	0.819123	-0.006528	C	-2.230056	3.425231	0.004775
C	-0.688619	-0.482027	-0.005244	Se	-0.514534	-3.272426	-0.077274
C	-1.545447	-1.615577	-0.015678	H	5.939447	1.765163	0.008205
C	-2.890663	-1.478565	-0.022137	H	2.096696	4.988771	0.020376
C	-3.460366	-0.146216	-0.014873	C	-4.529637	2.468039	-0.002951
C	-2.609693	0.994914	-0.007247	C	-4.841632	0.062214	-0.014973
H	4.032692	3.385135	0.016059	H	-5.507445	-0.791049	-0.019620
H	-3.531576	-2.347992	-0.026559	C	-5.360594	1.356189	-0.009229
C	5.231753	0.945925	0.005279	H	-6.433340	1.495645	-0.009277
C	5.680637	-0.367776	-0.000606	H	-2.645208	4.426015	0.008376
H	6.744507	-0.564866	-0.002314	H	-4.952007	3.464768	0.001555
C	4.790198	-1.441116	-0.004757	O	-2.346459	-4.258389	0.233468
H	5.165345	-2.456580	-0.009791	H	-0.349313	-3.576812	1.345430
C	3.410570	-1.220355	-0.003062	H	-2.342728	-4.990488	-0.388447

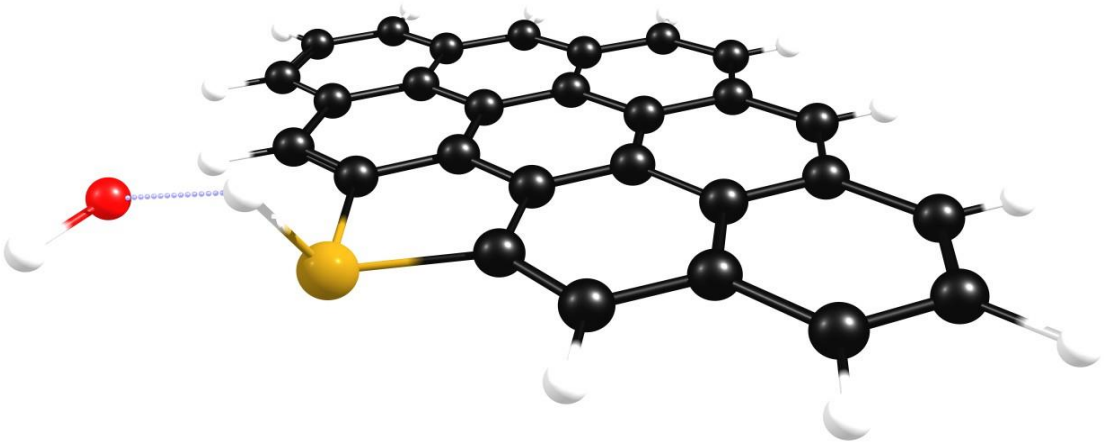


E^0 = -3552.334221 E^0 + ZPE = -3552.004994

ΔG^0 = -3552.052330

Molecule: 5Se-TS-2

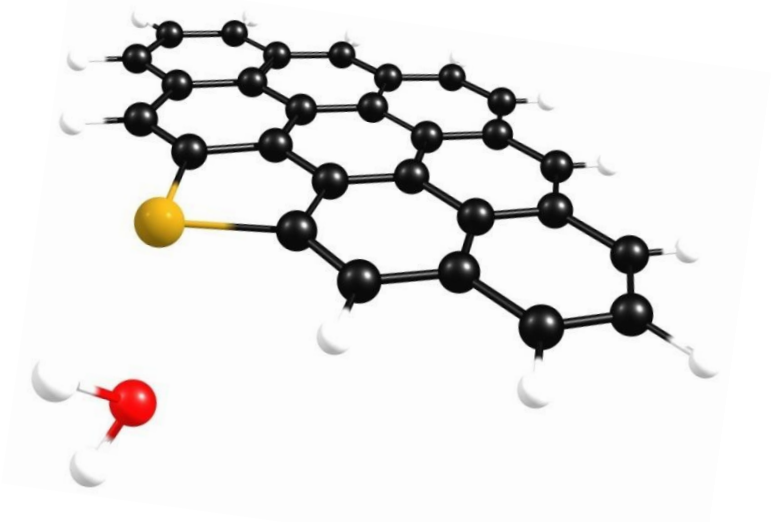
C	3.844093	1.232928	0.052703	C	2.461478	-2.309658	-0.077589
C	2.947207	0.134252	0.000458	H	2.843242	-3.322052	-0.100672
C	1.560748	0.394293	-0.020655	C	-0.891224	3.245002	0.025093
C	1.046983	1.710163	0.002280	C	-3.153983	2.287464	-0.013827
C	1.963448	2.815067	0.057994	C	1.136073	-2.033637	-0.087782
C	3.313963	2.565834	0.079328	C	0.051770	4.349784	0.073299
C	0.677837	-0.688394	-0.068839	H	-0.348250	5.355597	0.098240
C	-0.340149	1.918773	-0.008709	C	1.386941	4.148664	0.087725
C	-1.218614	0.812842	-0.055810	C	-2.255270	3.405124	0.020190
C	-0.690720	-0.481716	-0.088148	Se	-0.431952	-3.219791	-0.195568
C	-1.535625	-1.622788	-0.111481	H	5.924454	1.779443	0.114632
C	-2.881308	-1.506771	-0.094355	H	2.064942	4.992043	0.125621
C	-3.460810	-0.177183	-0.068427	C	-4.549476	2.431376	-0.004904
C	-2.620368	0.973054	-0.049455	C	-4.843210	0.022228	-0.054199
H	4.011743	3.393761	0.120525	H	-5.503644	-0.835073	-0.065738
H	-3.510125	-2.385914	-0.067775	C	-5.371065	1.312647	-0.025659
C	5.219785	0.958592	0.075381	H	-6.444832	1.443474	-0.016632
C	5.674537	-0.352693	0.048107	H	-2.678043	4.402341	0.047575
H	6.738915	-0.545369	0.065830	H	-4.980111	3.424183	0.021304
C	4.789919	-1.429482	-0.001750	O	-2.432147	-4.282499	0.811114
H	5.168863	-2.443106	-0.022016	H	-0.716253	-3.715781	1.179903
C	3.410410	-1.212288	-0.025579	H	-2.467581	-5.231516	0.667287



E^0 = -3552.320919 E^0 + ZPE = -3551.994916

ΔG^0 = -3552.042355 ν_{imag} = -930.791

Molecule: 5Se-P-2							
C	3.981936	0.891264	-0.002795	C	2.273615	-2.508261	0.003412
C	2.985291	-0.119660	0.002176	H	2.563883	-3.550748	0.002402
C	1.628941	0.264533	-0.002176	C	-0.547189	3.331643	0.000445
C	1.239118	1.622640	0.004886	C	-2.889809	2.591193	0.001184
C	2.254894	2.639002	-0.003982	C	0.971547	-2.119220	0.003556
C	3.577039	2.267329	-0.004038	C	0.494729	4.344752	-0.002979
C	0.646281	-0.731466	0.006237	H	0.189862	5.383820	-0.002479
C	-0.122589	1.958923	-0.004191	C	1.805501	4.020728	-0.003507
C	-1.100851	0.938818	0.006287	C	-1.889943	3.619798	-0.000150
C	-0.696270	-0.400917	0.001398	Se	-0.661378	-3.144885	0.003879
C	-1.633103	-1.476974	0.004373	H	6.104504	1.245055	-0.005743
C	-2.966266	-1.213901	0.003063	H	2.559819	4.797726	-0.006220
C	-3.419022	0.161885	0.002842	C	-4.265239	2.865475	0.000281
C	-2.479633	1.232324	0.000440	C	-4.778145	0.491602	0.001631
H	4.348058	3.028828	-0.007904	H	-5.515529	-0.301105	0.001963
H	-3.701173	-2.006867	0.003421	C	-5.185219	1.824813	0.000618
C	5.326425	0.492411	-0.003416	H	-6.242931	2.052928	-0.101000
C	5.655216	-0.857083	-0.001860	H	-2.216595	4.652905	0.000832
H	6.697289	-1.148278	-0.002498	H	-4.602846	3.893862	-0.000282
C	4.673771	-1.846947	0.000510	O	-3.575820	-4.374066	-0.018797
H	4.957027	-2.891714	0.001105	H	-3.604251	-4.972536	0.733580
C	3.317891	-1.504707	0.001215	H	-3.597190	-4.945244	-0.792335

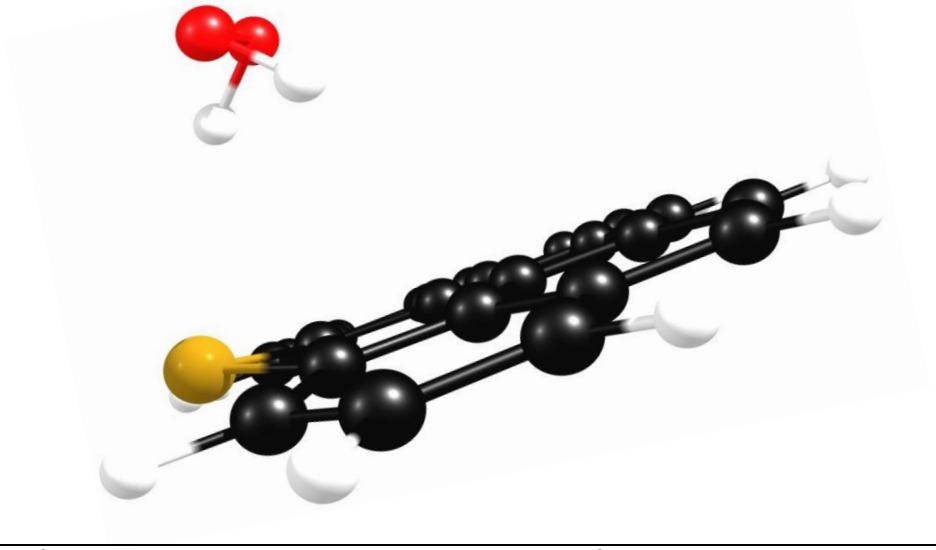


E^0 = -3552.430818 E^0 + ZPE = -3552.100675

ΔG^0 = -3552.151934

Molecule: 6Se-R-1

C	2.810213	2.948488	-0.345021	H	-5.347550	2.386641	0.366386
C	1.557114	3.371527	-0.096428	C	-3.258509	2.738076	0.285877
C	0.461064	2.446566	-0.042117	H	-3.334637	3.809164	0.423109
C	0.665860	1.051831	-0.201384	C	-5.376609	-0.278272	0.022436
C	2.032910	0.597245	-0.433538	C	-5.255632	-1.653908	-0.163311
C	3.080861	1.553851	-0.532999	C	-4.006957	-2.234376	-0.302379
C	-0.822604	2.975529	0.140951	C	4.404289	1.156094	-0.800481
C	-0.485326	0.200731	-0.180335	C	4.718689	-0.169334	-0.982947
C	-1.781956	0.766746	-0.044385	H	5.733690	-0.473454	-1.198941
C	-1.941241	2.173148	0.131872	C	3.711284	-1.131439	-0.874100
C	-2.958175	-0.045181	-0.075242	H	3.947923	-2.181071	-0.992944
C	-2.850357	-1.442180	-0.258417	H	5.167228	1.921047	-0.863817
C	-1.547995	-2.007055	-0.375190	H	-3.906806	-3.302856	-0.443684
C	-0.433572	-1.232860	-0.316005	H	-6.143710	-2.270716	-0.197292
C	2.412402	-0.754702	-0.590472	H	-6.353802	0.174420	0.132067
H	-0.931783	4.045462	0.268777	Se	1.209409	-2.188425	-0.275929
H	3.637742	3.643195	-0.407963	H	3.518438	-0.277992	1.900252
H	1.338226	4.421507	0.048237	O	3.336285	-0.969908	2.553528
H	-1.459324	-3.080950	-0.489668	O	1.949684	-0.801110	2.812989
C	-4.246687	0.536547	0.068048	H	1.544260	-1.405385	2.168164
C	-4.358657	1.960528	0.255028				

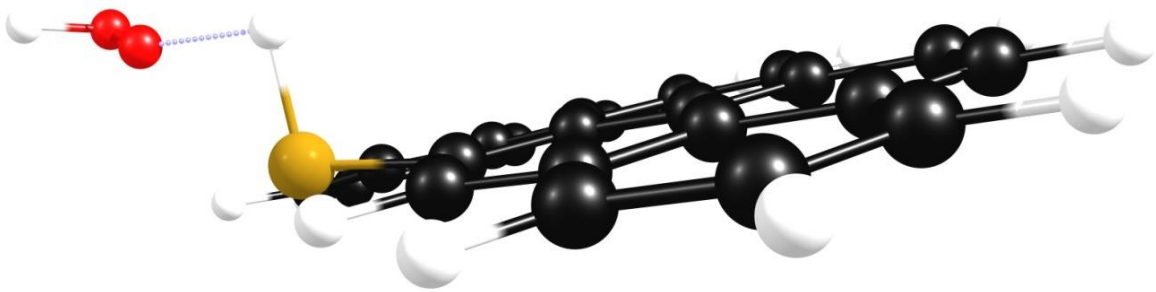


E^0 = -3475.077603 E^0 + ZPE = -3474.766609

ΔG^0 = -3474.817235

Molecule: 6Se-TS-1

C	2.171494	3.567652	0.047647	H	-5.787242	1.641336	-0.517804
C	0.867247	3.773770	-0.215092	C	-3.784958	2.337446	-0.509615
C	-0.063040	2.681642	-0.224252	H	-4.039616	3.369910	-0.711960
C	0.367509	1.348840	-0.003261	C	-5.367383	-0.962435	0.007941
C	1.788977	1.126222	0.226936	C	-5.019978	-2.284080	0.281287
C	2.665380	2.243710	0.283564	C	-3.690899	-2.641156	0.424676
C	-1.418166	2.982194	-0.419939	C	4.036563	2.075247	0.554357
C	-0.628252	0.325883	0.044233	C	4.575058	0.829089	0.759826
C	-1.999936	0.661476	-0.096118	H	5.629081	0.706472	0.966395
C	-2.390212	2.009369	-0.349573	C	3.744415	-0.292930	0.675674
C	-3.022434	-0.329191	0.022067	H	4.151028	-1.289408	0.765904
C	-2.685061	-1.673765	0.294991	H	4.660598	2.958803	0.592048
C	-1.304067	-2.008666	0.409055	H	-3.411884	-3.665968	0.632555
C	-0.342602	-1.064004	0.263353	H	-5.794124	-3.033044	0.379376
C	2.402783	-0.130122	0.414308	H	-6.407901	-0.685706	-0.104735
H	-1.702304	4.011577	-0.600208	Se	1.439796	-1.770750	0.239029
H	2.875523	4.388846	0.081949	H	1.660553	-1.934240	-1.231738
H	0.482871	4.768245	-0.399766	O	3.309562	-2.649741	-1.168424
H	-1.035377	-3.043482	0.586285	O	4.702741	-2.426942	-1.480852
C	-4.390970	0.022771	-0.124504	H	5.038493	-3.324131	-1.561109
C	-4.740000	1.392665	-0.402560				

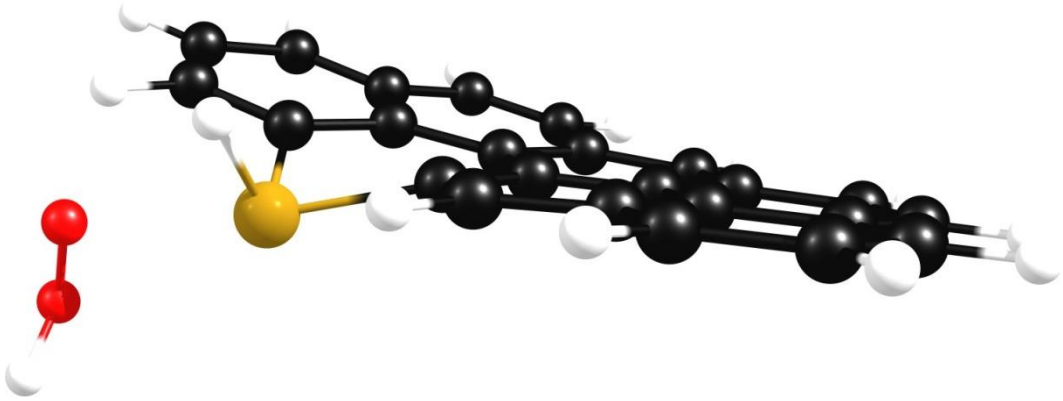


E^0 = -3474.982666 E^0 + ZPE = -3474.676279

ΔG^0 = -3474.724678 ν_{imag} = -394.444

Molecule: 6Se-P-1

C	-2.177696	3.566898	0.064587	H	5.774441	1.652341	-0.353616
C	-0.891022	3.776723	-0.271956	C	3.774626	2.346776	-0.457995
C	0.039170	2.685917	-0.304166	H	4.041149	3.375067	-0.666711
C	-0.392123	1.352480	-0.093097	C	5.331339	-0.945195	0.198646
C	-1.806678	1.115978	0.172607	C	4.965479	-2.262235	0.472732
C	-2.660282	2.242438	0.326468	C	3.629851	-2.618012	0.546454
C	1.399249	2.988434	-0.475079	C	-3.999439	2.090875	0.732688
C	0.604831	0.334532	-0.023540	C	-4.523849	0.848712	0.980232
C	1.977450	0.676081	-0.099892	H	-5.547473	0.732453	1.308420
C	2.373438	2.021369	-0.356126	C	-3.735433	-0.284777	0.748968
C	2.989338	-0.313928	0.080869	H	-4.150757	-1.276698	0.838671
C	2.630131	-1.654455	0.350844	H	-4.603294	2.981783	0.846540
C	1.241546	-1.988659	0.365932	H	3.341735	-3.641526	0.749340
C	0.285628	-1.047421	0.171693	H	5.731803	-3.010819	0.623032
C	-2.428167	-0.148262	0.344707	H	6.377090	-0.671842	0.137803
H	1.684351	4.017824	-0.654506	Se	-1.511043	-1.761249	-0.219958
H	-2.878212	4.387881	0.146809	H	-1.471313	-2.576509	1.002383
H	-0.517660	4.772478	-0.472193	O	-3.380930	-2.87356	-0.273232
H	0.967934	-3.030921	0.498133	O	-4.082382	-2.386867	-1.427127
C	4.363444	0.037142	0.000329	H	-3.950319	-3.095995	-2.064440
C	4.722929	1.403698	-0.285611				

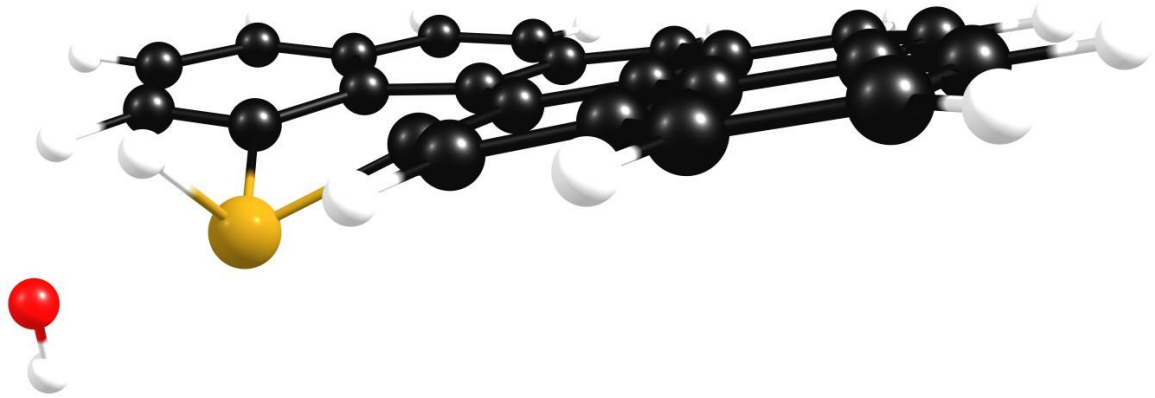


E^0 = -3474.987333 E^0 + ZPE = -3474.678422

ΔG^0 = -3474.726393

Molecule: 6Se-R-2

C	-2.637198	3.249345	0.081774	C	4.434396	1.711027	-0.153349
C	-1.366855	3.587311	-0.210238	H	5.461686	2.051663	-0.179254
C	-0.342008	2.585431	-0.261923	C	3.413066	2.576074	-0.319639
C	-0.658223	1.211273	-0.119105	H	3.595966	3.630829	-0.481232
C	-2.052105	0.837986	0.095372	C	5.231028	-0.594394	0.266173
C	-3.005886	1.877057	0.274885	C	4.972497	-1.946913	0.484075
C	0.990510	3.011720	-0.381055	C	3.670975	-2.418194	0.503162
C	0.421603	0.281783	-0.061159	C	-4.335683	1.590609	0.637613
C	1.759885	0.744178	-0.081245	C	-4.754000	0.296716	0.812367
C	2.042850	2.128108	-0.273295	H	-5.770153	0.075429	1.108367
C	2.847718	-0.162388	0.094836	C	-3.863329	-0.750546	0.546959
C	2.597078	-1.537898	0.307605	H	-4.187215	-1.780305	0.573824
C	1.241794	-1.988928	0.266228	H	-5.018343	2.419043	0.776822
C	0.212453	-1.127974	0.074045	H	3.467239	-3.469227	0.663273
C	-2.563864	-0.483467	0.184187	H	5.795900	-2.632096	0.634885
H	1.188958	4.068747	-0.509915	H	6.250461	-0.230592	0.248290
H	-3.410701	4.359000	0.177527	Se	-1.503753	-1.988501	-0.430991
H	-1.079899	4.620090	-0.359449	H	-1.415287	-2.853316	0.745844
H	1.053603	-3.055129	0.352222	O	-3.228196	-3.252105	-0.586196
C	4.187641	0.308197	0.071191	H	-3.645095	-3.136291	-1.444754

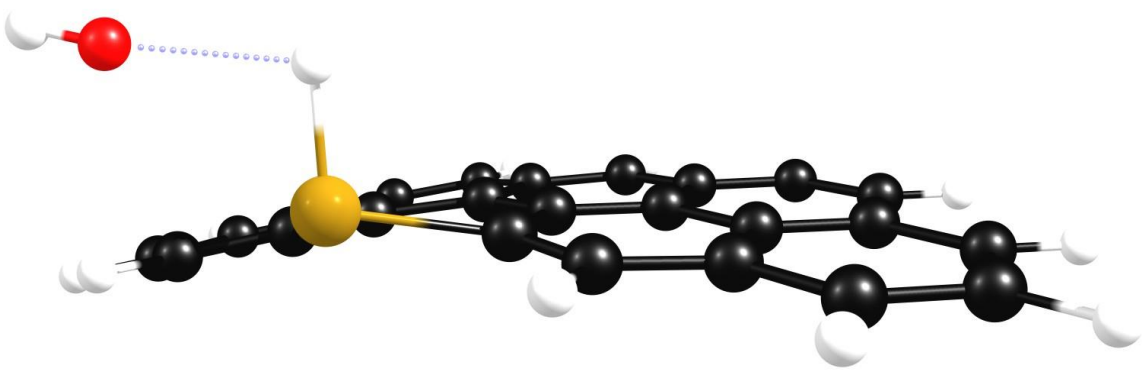


E^0 = -3399.840242 E^0 + ZPE = -3399.535349

ΔG^0 = -3399.580942

Molecule: 6Se-TS-2

C	-2.714207	3.182108	-0.070323	C	4.392896	1.770012	0.249873
C	-1.443756	3.533239	0.206795	H	5.411307	2.131580	0.312037
C	-0.399265	2.549322	0.239604	C	3.348031	2.609798	0.392884
C	-0.687485	1.172183	0.065976	H	3.500745	3.666326	0.572182
C	-2.075664	0.791131	-0.154764	C	5.251252	-0.510710	-0.170937
C	-3.060482	1.807400	-0.280844	C	5.035048	-1.865517	-0.414749
C	0.920854	2.997052	0.391230	C	3.746597	-2.366209	-0.482664
C	0.409769	0.261323	0.013796	C	-4.393699	1.484224	-0.595717
C	1.739909	0.746067	0.083276	C	-4.785854	0.181303	-0.785335
C	1.990460	2.132750	0.299934	H	-5.808667	-0.059657	-1.039039
C	2.854666	-0.133694	-0.069952	C	-3.848915	-0.842443	-0.611531
C	2.649605	-1.511402	-0.310255	H	-4.144017	-1.878711	-0.691769
C	1.308110	-1.997402	-0.333607	H	-5.106967	2.293209	-0.687697
C	0.260232	-1.156299	-0.153594	H	3.570683	-3.418376	-0.665235
C	-2.548196	-0.530968	-0.288964	H	5.879486	-2.527957	-0.548231
H	1.098437	4.054824	0.541510	H	6.260358	-0.122694	-0.115523
H	-3.500929	3.922352	-0.136897	Se	-1.429312	-2.036752	0.082631
H	-1.171223	4.567481	0.371600	H	-1.572648	-2.001094	1.556510
H	1.142961	-3.060489	-0.463356	O	-3.202553	-2.943213	1.631301
C	4.182047	0.366138	0.002048	H	-4.134203	-2.787944	1.800975

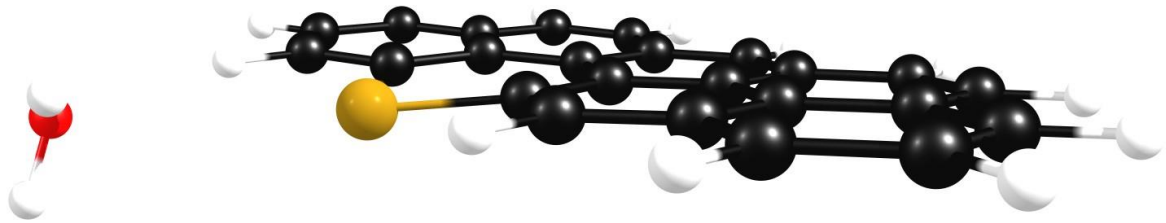


E^0 = -3399.835388 E^0 + ZPE = -3399.533477

ΔG^0 = -3399.580044 ν_{imag} = -476.580

Molecule: 6Se-P-2

C	-2.356689	3.500342	0.062558	C	4.607723	1.450899	-0.071143
C	-1.036584	3.737339	-0.046196	H	5.654844	1.725524	-0.081229
C	-0.092777	2.656986	-0.087762	C	3.641595	2.387978	-0.134971
C	-0.518322	1.303816	-0.043618	H	3.886578	3.440694	-0.196604
C	-1.954341	1.054661	0.036232	C	5.257339	-0.926002	0.100147
C	-2.851425	2.156408	0.110210	C	4.917368	-2.274584	0.187816
C	1.266306	2.990054	-0.142483	C	3.589239	-2.663065	0.191224
C	0.490423	0.286626	-0.035558	C	-4.240356	1.958663	0.215904
C	1.864537	0.652421	-0.043823	C	-4.769171	0.690783	0.246218
C	2.246832	2.024789	-0.113530	H	-5.836554	0.537704	0.329740
C	2.900941	-0.330046	0.023180	C	-3.914059	-0.410225	0.160720
C	2.571167	-1.701413	0.107319	H	-4.315698	-1.415944	0.169754
C	1.194849	-2.063454	0.093728	H	-4.880206	2.829616	0.270408
C	0.213513	-1.127122	0.008644	H	3.319464	-3.709385	0.255205
C	-2.547814	-0.227232	0.053668	H	5.697549	-3.021405	0.252036
H	1.545769	4.035570	-0.185590	H	6.296779	-0.623839	0.095843
H	-3.072323	4.310897	0.111916	Se	-1.545776	-1.825496	-0.145002
H	-0.650301	4.747436	-0.087280	H	-3.771661	-4.253500	0.290526
H	0.939091	-3.115561	0.136851	O	-4.521696	-3.796452	-0.101025
C	4.269293	0.053533	0.017009	H	-4.580891	-4.142249	-0.996267

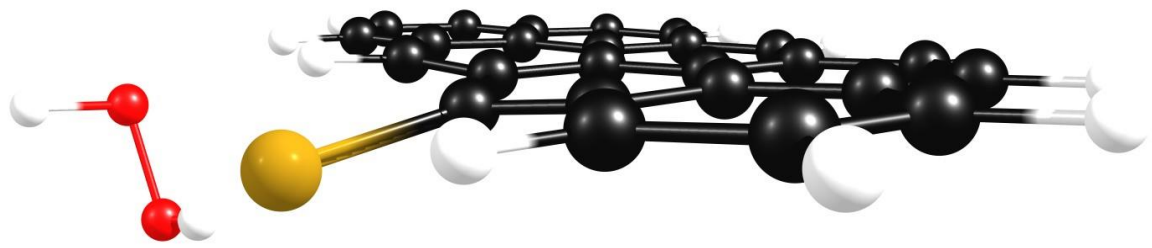


E^0 = -3399.940767 E^0 + ZPE = -3399.635147

ΔG^0 = -3399.685771

Molecule: C=Se-R-1

C	-2.695115	3.652274	-0.176893	H	5.397032	2.154465	0.190825
C	-1.398019	4.016892	-0.091023	C	3.384049	2.808317	0.142664
C	-0.362043	3.028995	0.014092	H	3.636450	3.860637	0.139228
C	-0.715955	1.660378	0.053016	C	5.003908	-0.526971	0.178386
C	-2.089384	1.269354	-0.019019	C	4.659325	-1.878484	0.167780
C	-3.080943	2.269052	-0.151204	C	3.332062	-2.263031	0.139953
C	0.986990	3.399245	0.060349	C	-4.425496	1.897028	-0.257321
C	0.285889	0.674791	0.122521	C	-4.790750	0.564214	-0.229138
C	1.639289	1.064413	0.128561	H	-5.830078	0.282454	-0.321472
C	1.989986	2.446258	0.112907	C	-3.823672	-0.419406	-0.069549
C	2.665232	0.084411	0.147839	H	-4.111363	-1.458866	-0.027887
C	2.319834	-1.287793	0.128059	H	-5.176253	2.669570	-0.364335
C	0.952611	-1.655337	0.121616	H	3.048045	-3.307079	0.147634
C	-0.060264	-0.724075	0.164502	H	5.437402	-2.628616	0.185089
C	-2.469542	-0.097971	0.043148	H	6.046819	-0.236870	0.196459
H	1.247727	4.450148	0.040236	Se	-1.938222	-2.835469	0.665035
H	-3.474062	4.398115	-0.266969	H	-0.010184	-3.926708	1.731930
H	-1.113279	5.060567	-0.111709	O	0.770229	-4.466622	1.962422
H	0.710841	-2.705910	0.067472	C	-1.457582	-1.133170	0.249010
C	4.027515	0.466782	0.167564	O	1.220803	-4.879795	0.678766
C	4.353227	1.869243	0.170685	H	0.884682	-5.779435	0.618384

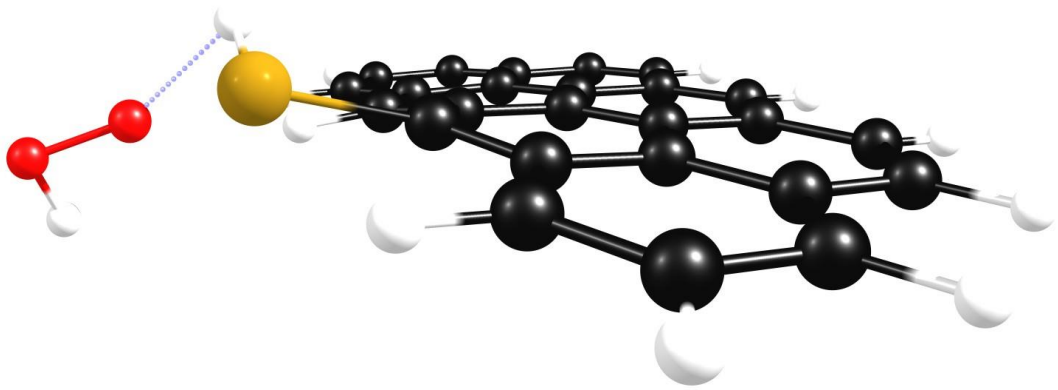


E^0 = -3513.161626 E^0 + ZPE = -3512.842727

ΔG^0 = -3512.893926

Molecule: C=Se-TS-1

C	-2.712913	3.641667	0.052687	H	5.396713	2.200871	-0.189071
C	-1.421922	4.011085	-0.084879	C	3.377281	2.835269	-0.230491
C	-0.371183	3.031453	-0.113371	H	3.620521	3.883530	-0.344357
C	-0.709688	1.659427	-0.022019	C	5.034410	-0.461950	0.158524
C	-2.077588	1.263721	0.101621	C	4.704193	-1.802182	0.347385
C	-3.083954	2.256335	0.155763	C	3.378878	-2.194648	0.405847
C	0.970954	3.408224	-0.206076	C	-4.419992	1.874183	0.303102
C	0.305493	0.686676	-0.001578	C	-4.766289	0.535351	0.382554
C	1.653811	1.086747	-0.037362	H	-5.801494	0.248856	0.501789
C	1.987781	2.464337	-0.164998	C	-3.789163	-0.444466	0.295106
C	2.688421	0.118566	0.069276	H	-4.082201	-1.483961	0.341817
C	2.355002	-1.244022	0.263206	H	-5.183455	2.639618	0.352834
C	0.992345	-1.635316	0.303960	H	3.107558	-3.234097	0.538934
C	-0.024621	-0.714341	0.096550	H	5.489291	-2.538366	0.446966
C	-2.439064	-0.108173	0.156890	H	6.074118	-0.163054	0.119160
H	1.220966	4.458561	-0.290141	Se	-1.848807	-2.864967	-0.274304
H	-3.499437	4.384166	0.084752	H	-0.541199	-3.305675	-0.809092
H	-1.151633	5.055909	-0.163154	O	-0.021701	-4.489596	0.470206
H	0.767968	-2.671742	0.544432	C	-1.402195	-1.108970	0.013781
C	4.045031	0.512951	0.024125	O	0.354831	-5.712558	1.063396
C	4.355747	1.908259	-0.144581	H	0.734429	-5.438977	1.902801

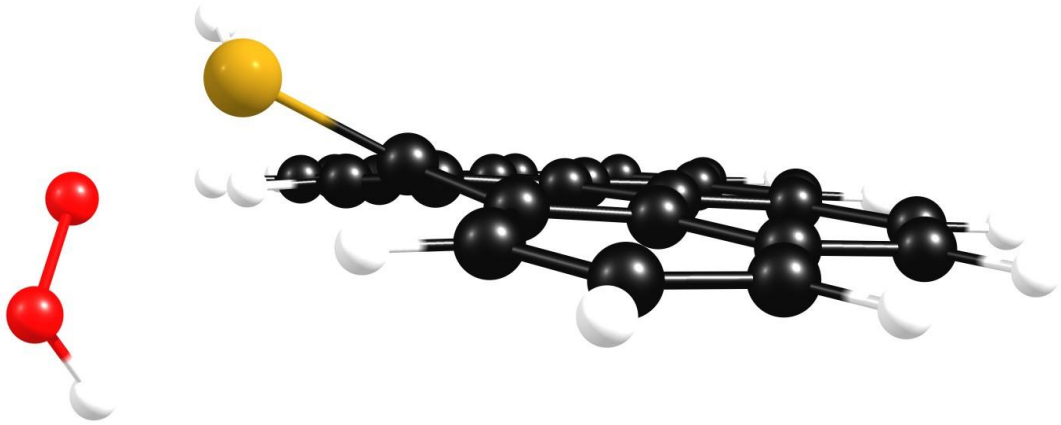


E^0 = -3513.063638 E^0 + ZPE = -3512.749771

ΔG^0 = -3512.798780 ν_{imag} = -133.703

Molecule: C=Se-P-1

C	-2.741507	3.401896	0.175389	H	5.434888	2.416222	-0.130915
C	-1.470733	3.836113	0.017278	C	3.380776	2.934689	-0.167729
C	-0.376059	2.908655	-0.061214	H	3.558928	4.000317	-0.239005
C	-0.642545	1.520431	-0.021182	C	5.235262	-0.267492	0.102998
C	-1.997908	1.058983	0.113482	C	4.978268	-1.631634	0.227757
C	-3.045119	1.998503	0.244091	C	3.677454	-2.108324	0.247027
C	0.947775	3.363558	-0.138836	C	-4.363449	1.550179	0.432035
C	0.432860	0.602630	-0.033450	C	-4.626519	0.198039	0.511398
C	1.758099	1.077651	-0.051372	H	-5.635760	-0.148419	0.689774
C	2.013412	2.479027	-0.126784	C	-3.598001	-0.737664	0.374898
C	2.849227	0.164653	0.016703	H	-3.827199	-1.791093	0.470746
C	2.593080	-1.223907	0.135020	H	-5.158491	2.277645	0.532210
C	1.242160	-1.686346	0.135654	H	3.482761	-3.169089	0.341294
C	0.185496	-0.820980	-0.000998	H	5.804063	-2.325798	0.310334
C	-2.289482	-0.330551	0.132242	H	6.254137	0.097963	0.089841
H	1.137791	4.429316	-0.182320	Se	-1.600744	-2.859852	-0.827539
H	-3.560773	4.105128	0.256060	H	-0.274397	-3.173177	-1.400400
H	-1.247871	4.894516	-0.030434	O	-1.065875	-4.331413	0.429202
H	1.073251	-2.745007	0.281697	C	-1.193022	-1.247245	-0.161745
C	4.183785	0.643502	0.001333	O	-2.083177	-4.457781	1.403509
C	4.411414	2.063822	-0.108221	H	-1.745136	-3.928911	2.138215

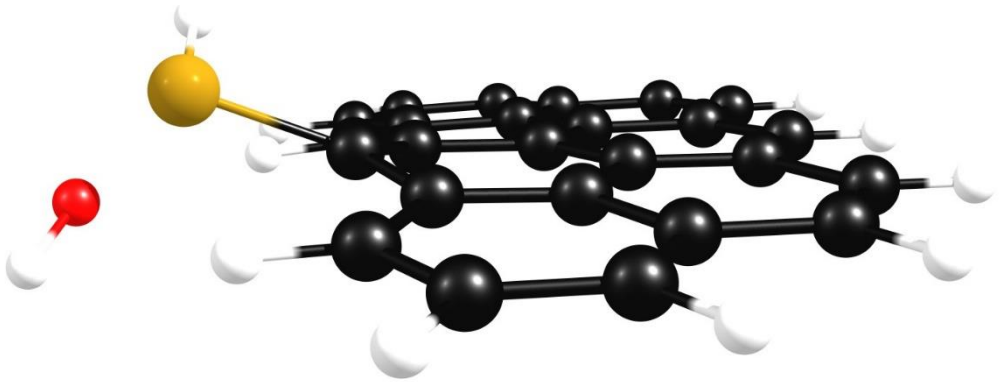


E^0 = -3513.124879 E^0 + ZPE = -3512.809310

ΔG^0 = -3512.857908

Molecule: C=Se-R-2

C	-2.321242	3.794723	0.051416	H	5.653865	1.728846	-0.174388
C	-1.002180	4.049297	-0.100570	C	3.684696	2.509763	-0.226715
C	-0.040790	2.982183	-0.130688	H	4.000507	3.539862	-0.334349
C	-0.489794	1.643055	-0.036514	C	5.109388	-0.895282	0.145377
C	-1.896538	1.372133	0.093900	C	4.675996	-2.208798	0.315811
C	-2.811769	2.447853	0.163632	C	3.324151	-2.510586	0.356390
C	1.330648	3.254852	-0.218158	C	-4.182166	2.189902	0.332138
C	0.455777	0.591012	-0.004792	C	-4.624567	0.887497	0.450166
C	1.833227	0.886383	-0.043654	H	-5.675373	0.685255	0.610920
C	2.270148	2.238298	-0.169852	C	-3.729569	-0.181497	0.379183
C	2.796949	-0.158661	0.054609	H	-4.104731	-1.188796	0.506501
C	2.360698	-1.497396	0.219693	H	-4.874252	3.020249	0.384930
C	0.961492	-1.777417	0.248929	H	2.995181	-3.533858	0.486935
C	0.021758	-0.785883	0.086378	H	5.404442	-3.002505	0.418111
C	-2.368862	0.032686	0.161044	H	6.166895	-0.665808	0.116791
H	1.660283	4.283695	-0.300634	Se	-2.004704	-2.641485	-0.582074
H	-3.039929	4.603592	0.092080	H	-0.750425	-3.102973	-1.204148
H	-0.639514	5.066072	-0.183637	O	-1.655412	-3.964134	0.734644
H	0.659281	-2.797460	0.445866	C	-1.398519	-1.030236	-0.042310
C	4.182964	0.140215	0.017838	H	-2.462889	-4.042405	1.259292
C	4.593089	1.514202	-0.138400				

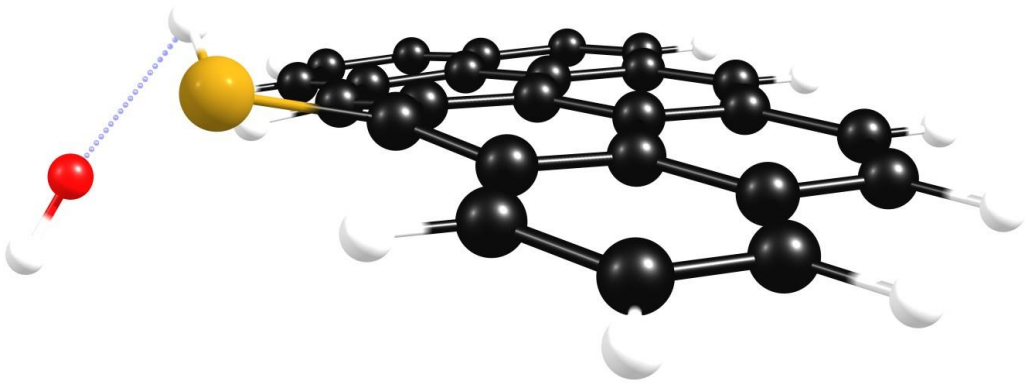


E^0 = -3437.984515 E^0 + ZPE = -3437.673041

ΔG^0 = -3437.719390

Molecule: C=Se-TS-2

C	-2.592643	3.687373	0.151990	H	5.485545	2.093474	-0.156899
C	-1.295327	4.037082	0.006666	C	3.477456	2.773330	-0.209755
C	-0.267608	3.036066	-0.082084	H	3.738376	3.820845	-0.289398
C	-0.633008	1.668378	-0.046847	C	5.065612	-0.562887	0.127577
C	-2.006636	1.294663	0.082156	C	4.708214	-1.902563	0.282331
C	-2.989085	2.305479	0.201034	C	3.376097	-2.274617	0.299446
C	1.083256	3.391799	-0.170873	C	-4.331809	1.945889	0.357324
C	0.362141	0.674956	-0.078080	C	-4.707362	0.611752	0.382628
C	1.717600	1.049197	-0.092658	H	-5.746847	0.342629	0.507594
C	2.079729	2.425935	-0.167456	C	-3.754465	-0.384819	0.229607
C	2.730314	0.058205	0.000041	H	-4.075293	-1.417680	0.231713
C	2.368546	-1.304841	0.149932	H	-5.075657	2.726325	0.454457
C	0.998580	-1.670469	0.137620	H	3.091942	-3.312469	0.416140
C	0.005687	-0.721290	-0.040773	H	5.479580	-2.652611	0.390141
C	-2.399193	-0.070198	0.084031	H	6.110473	-0.279403	0.119432
H	1.353206	4.439841	-0.213109	Se	-1.875779	-2.806379	-0.480650
H	-3.365801	4.440594	0.232795	H	-0.584095	-3.223420	-1.009761
H	-1.000651	5.077814	-0.030463	O	-0.340420	-4.545406	0.727895
H	0.742446	-2.710088	0.336283	C	-1.386921	-1.083139	-0.130617
C	4.095197	0.430566	-0.008019	H	-0.502740	-5.007938	1.553943
C	4.437189	1.824521	-0.135875				

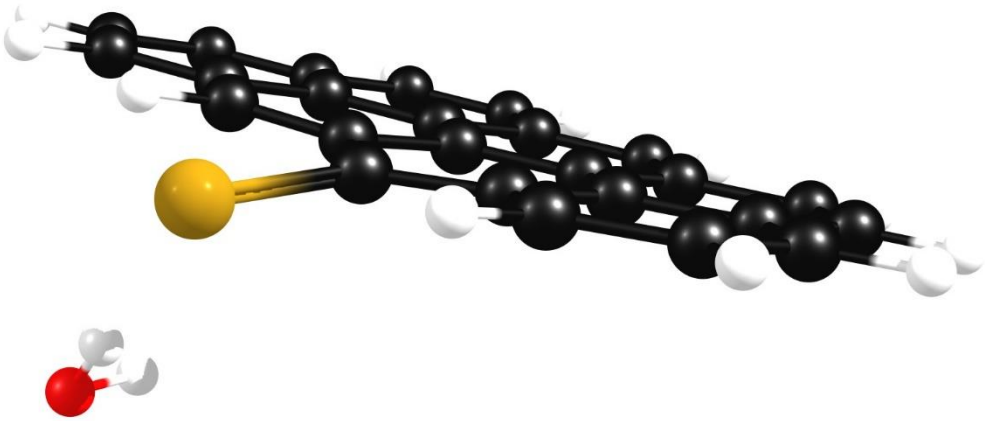


E^0 = -3437.962813 E^0 + ZPE = -3437.653768

ΔG^0 = -3437.701056 ν_{imag} = -199.979

Molecule: C=Se-P-2

C	-2.842704	3.472012	0.194300	H	5.321077	2.344402	0.117475
C	-1.560164	3.885434	0.299173	C	3.276700	2.899622	0.213883
C	-0.477554	2.946438	0.208104	H	3.475560	3.952090	0.370397
C	-0.766364	1.571228	0.030984	C	5.052402	-0.314683	-0.301308
C	-2.120000	1.128095	-0.069255	C	4.773594	-1.666178	-0.517380
C	-3.160684	2.083895	0.000414	C	3.466313	-2.109130	-0.575923
C	0.853994	3.374212	0.279856	C	-4.490722	1.667539	-0.128219
C	0.28054 0	0.638917	-0.086167	C	-4.795026	0.330294	-0.319772
C	1.614371	1.089806	-0.038854	H	-5.823664	0.017241	-0.431860
C	1.900653	2.474289	0.155673	C	-3.780516	-0.615161	-0.358971
C	2.684754	0.171707	-0.190920	H	-4.028709	-1.656687	-0.495521
C	2.404574	-1.199780	-0.409936	H	-5.278105	2.409148	-0.079902
C	1.058842	-1.631311	-0.443544	H	3.240983	-3.154449	-0.742817
C	-0.000700	-0.765349	-0.257023	H	5.587818	-2.366911	-0.639983
C	-2.434621	-0.250707	-0.228282	H	6.079766	0.024331	-0.259255
H	1.065172	4.426725	0.423188	Se	-1.752666	-3.038615	-0.137521
H	-3.661343	4.177850	0.252205	H	1.139488	-2.490606	2.427398
H	-1.321100	4.931137	0.442567	O	0.701169	-3.345936	2.406206
H	0.864562	-2.679190	-0.625026	C	-1.374506	-1.247070	-0.233638
C	4.027973	0.616709	-0.139141	H	0.031585	-3.262322	1.713462
C	4.290218	2.017110	0.074905				

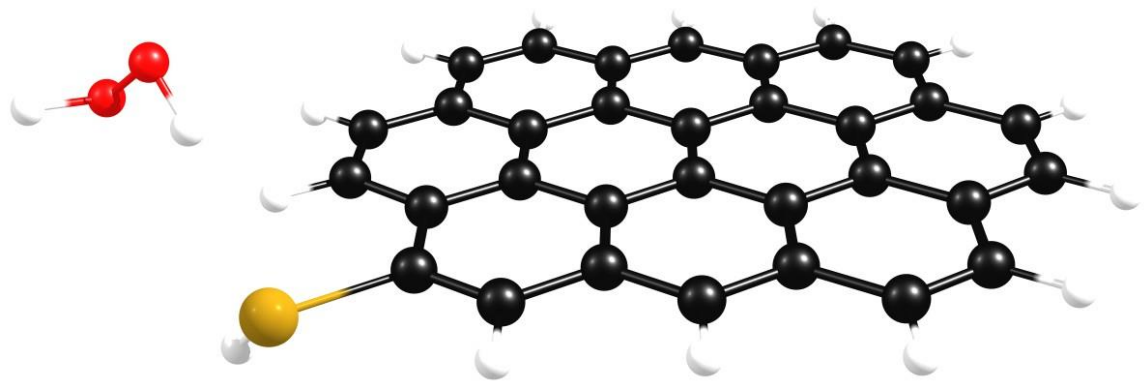


E^0 = -3438.064730 E^0 + ZPE = -3438.751990

ΔG^0 = -3438.801528

Molecule: C-SeH-R-1

C	3.778356	-3.750338	0.198195	H	-5.547861	-0.124797	1.470890
C	2.445128	-3.982715	0.109119	H	-7.441998	1.257842	1.259785
C	1.508007	-2.898936	0.015589	H	4.476808	-4.574755	0.267671
C	2.004950	-1.567624	0.011684	H	2.059980	-4.994390	0.107698
C	3.406485	-1.330287	0.113279	H	-0.247814	-4.130252	-0.079350
C	4.302513	-2.415308	0.200575	H	-2.536126	-3.282682	-0.299795
C	0.132778	-3.116171	-0.078441	H	-5.300532	-0.774214	-1.482029
C	1.110347	-0.481019	-0.068907	H	-4.513562	1.105740	-0.457614
C	-0.274511	-0.716561	-0.170680	C	5.289717	0.234291	0.204137
C	-0.761581	-2.049416	-0.167625	C	5.686141	-2.155819	0.292245
C	-2.174414	-2.262793	-0.278052	C	6.166274	-0.867454	0.293203
C	-3.042682	-1.222761	-0.359471	C	3.492160	2.428229	0.018474
C	-2.582607	0.146035	-0.342897	C	1.217736	3.273917	-0.161211
C	-1.188292	0.375320	-0.254586	C	-1.049590	4.132022	-0.327066
C	1.612510	0.859612	-0.081010	C	0.283562	4.361160	-0.247445
C	-0.686225	1.705415	-0.256110	C	2.592757	3.491838	-0.070733
C	2.997636	1.096256	0.022161	C	4.909762	2.634958	0.115193
C	3.903098	-0.000537	0.106671	C	5.766468	1.587061	0.202658
C	0.716883	1.942907	-0.159005	H	-1.748602	4.956530	-0.387985
Se	-4.917833	-1.673135	-0.387264	H	0.671844	5.371652	-0.245632
C	-1.575224	2.797104	-0.329900	H	2.969784	4.507408	-0.071499
C	-3.445958	1.258431	-0.409154	H	5.280524	3.651987	0.114430
C	-2.956674	2.543695	-0.404462	H	6.833844	1.753774	0.274830
H	-3.640664	3.381465	-0.453599	H	7.230529	-0.681869	0.363832
O	-6.503025	1.467913	1.173339	H	6.369755	-2.992587	0.360073
O	-5.899806	0.551170	2.077501				

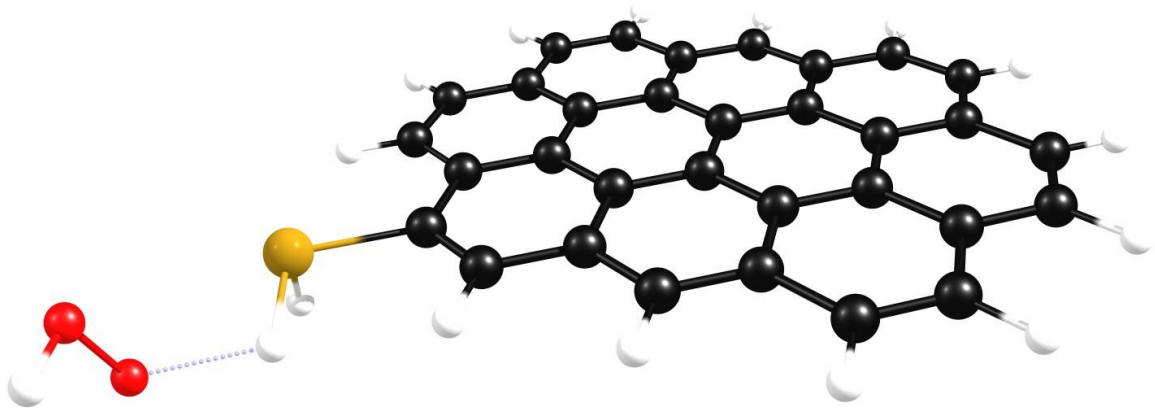


E^0 = -3781.280906 E^0 + ZPE = -3780.898398

ΔG^0 = -3780.954190

Molecule: C-SeH-TS-1

C	-3.021675	-4.184580	0.010855	H	5.391230	-1.602667	0.452549
C	-1.666611	-4.131157	0.016966	H	7.751683	-2.699070	-0.671517
C	-0.974604	-2.873178	0.016668	H	-3.534382	-5.138066	0.011273
C	-1.739180	-1.674811	0.002748	H	-1.077931	-5.039569	0.024123
C	-3.162697	-1.738468	0.004748	H	1.003308	-3.707919	0.036080
C	-3.813790	-2.988879	0.002401	H	3.078233	-2.390095	0.060499
C	0.418646	-2.796232	0.025017	H	5.235642	0.345000	1.334284
C	-1.090768	-0.423276	0.011075	H	4.090024	2.309787	0.012405
C	0.316094	-0.361478	0.009140	C	-5.334384	-0.605080	-0.011397
C	1.071743	-1.563970	0.024586	C	-5.223910	-3.027222	-0.002652
C	2.502697	-1.473074	0.042808	C	-5.963172	-1.867839	-0.009914
C	3.118165	-0.266507	0.046098	C	-4.031486	1.921493	-0.018484
C	2.389455	0.972348	0.019336	C	-1.980050	3.229723	-0.018720
C	0.977999	0.901441	0.013659	C	0.064198	4.545684	-0.020710
C	-1.861625	0.783685	-0.010456	C	-1.290020	4.489187	-0.023772
C	0.211618	2.097355	-0.006135	C	-3.373075	3.152296	-0.022131
C	-3.268841	0.722254	-0.004958	C	-5.463960	1.823814	-0.022291
C	-3.926302	-0.541695	-0.010365	C	-6.084428	0.617730	-0.019876
C	-1.212355	2.032900	-0.003944	H	0.576427	5.499279	-0.025389
Se	5.062914	-0.237622	-0.003379	H	-1.880476	5.396497	-0.032511
C	0.857668	3.350493	-0.008960	H	-3.955228	4.065855	-0.031773
C	3.010373	2.237829	0.009774	H	-6.039832	2.740449	-0.029341
C	2.264808	3.393249	-0.005703	H	-7.165337	0.555286	-0.023129
H	2.759036	4.356164	-0.013251	H	-7.044954	-1.910658	-0.013363
O	7.483380	-1.781196	-0.764441	H	-5.718940	-3.990020	-0.001979
O	7.275274	-1.373218	0.616123				

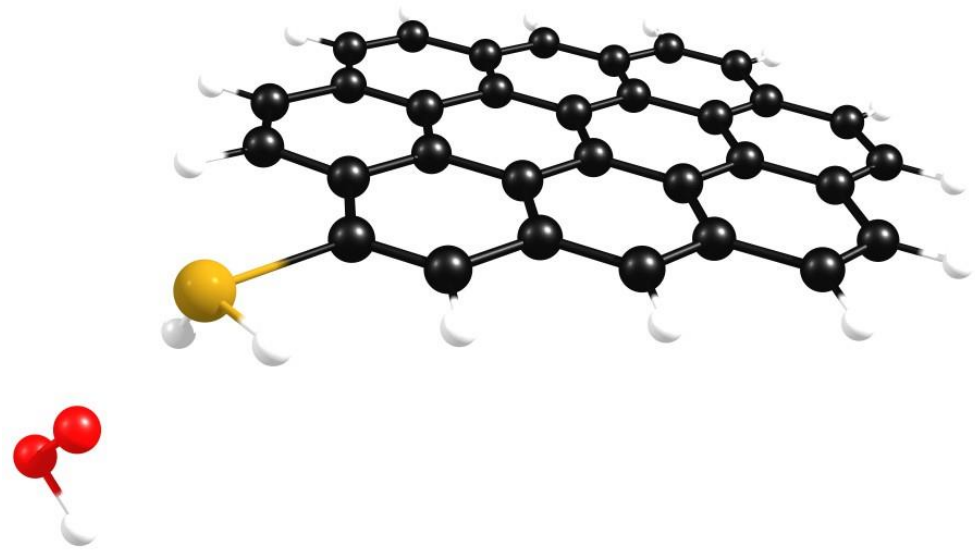


E^0 = -3781.187537 E^0 + ZPE = -3780.809636

ΔG^0 = -3780.863232 ν_{imag} = -636.479

Molecule: C-SeH-P-1

C	-3.262381	-4.078598	-0.007862	H	-3.835851	-4.992864	0.002522
C	-1.928128	-4.109205	-0.066224	H	-1.397302	-5.048049	-0.103722
C	-1.140246	-2.884589	-0.081340	H	0.772788	-3.836836	-0.182619
C	-1.825079	-1.646273	-0.033073	H	2.932927	-2.649850	-0.246348
C	-3.268258	-1.623834	0.029208	H	5.233365	0.149133	0.906296
C	-3.990856	-2.820837	0.041691	H	4.232183	1.977616	-0.289027
C	0.251149	-2.893241	-0.143813	C	-5.352693	-0.351336	0.134653
C	-1.099018	-0.441249	-0.044734	C	-5.404168	-2.769151	0.102517
C	0.305175	-0.467793	-0.104810	C	-6.062206	-1.576228	0.147196
C	0.982572	-1.708568	-0.156488	C	-3.887573	2.097570	0.104158
C	2.435530	-1.690896	-0.212964	C	-1.761737	3.270596	0.026660
C	3.147501	-0.562748	-0.217949	C	0.355869	4.468076	-0.057370
C	2.466848	0.734719	-0.181054	C	-0.977374	4.497521	0.004900
C	1.064694	0.762961	-0.118589	C	-3.152670	3.280963	0.087021
C	-1.801234	0.829781	0.001371	C	-5.342360	2.083080	0.166303
C	0.370786	2.008554	-0.079073	C	-6.027462	0.936230	0.180332
C	-3.206233	0.857297	0.060869	H	0.929546	5.382034	-0.074734
C	-3.956131	-0.377367	0.075244	H	-1.510479	5.435197	0.039052
C	-1.073898	2.032161	-0.015238	H	-3.672355	4.225963	0.120290
Se	5.108542	-0.679129	-0.319204	H	-5.852953	3.033271	0.200762
C	1.085185	3.210279	-0.102847	H	-7.105744	0.937589	0.226386
C	3.157719	1.971785	-0.219143	H	-7.140073	-1.551787	0.192898
C	2.494365	3.161995	-0.179388	H	-5.957678	-3.695429	0.112731
H	3.046376	4.088579	-0.210008	O	7.195568	-0.478349	1.370128
O	6.816690	-1.325824	0.341723	H	7.007067	-1.016879	2.190276
H	4.943559	-2.123874	-0.567619				

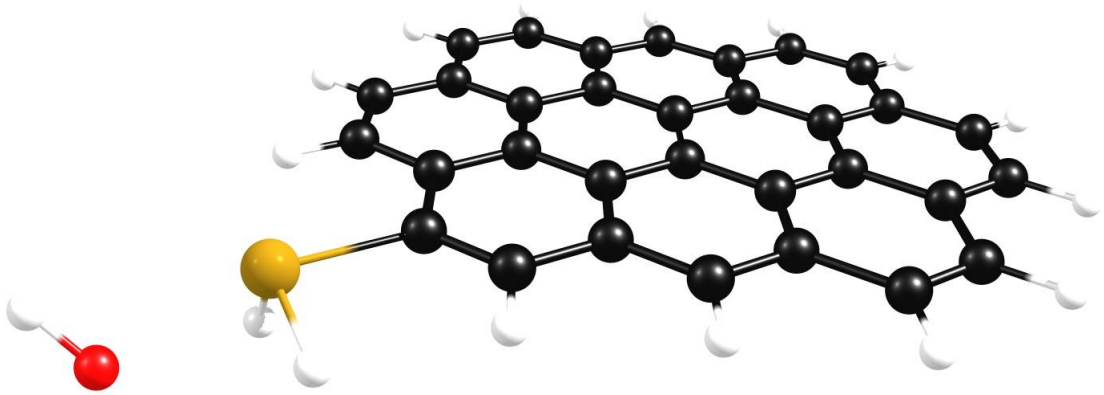


E^0 = -3781.224896 E^0 + ZPE = -3780.842597

ΔG^0 = -3780.897834

Molecule: C-SeH-R-2

C	-3.143822	-4.028174	-0.003437	H	5.223772	-2.179656	0.308412
C	-1.788849	-4.088276	-0.009947	H	-3.734364	-4.935680	-0.001365
C	-0.992911	-2.893259	-0.012240	H	-1.278817	-5.043082	-0.014872
C	-1.654833	-1.635578	-0.001948	H	0.906957	-3.891718	-0.021895
C	-3.078714	-1.579048	-0.003015	H	3.079137	-2.756674	-0.010886
C	-3.833215	-2.770148	0.003168	H	5.449922	-0.145770	1.216505
C	0.402238	-2.933206	-0.016443	H	4.490082	1.842659	-0.016294
C	-0.902546	-0.443724	-0.012812	C	-5.147273	-0.266177	0.014257
C	0.504693	-0.501004	-0.006949	C	-5.241609	-2.688828	0.010905
C	1.159105	-1.761329	-0.016292	C	-5.880783	-1.471320	0.016860
C	2.594591	-1.785615	-0.011742	C	-3.634911	2.141421	0.011967
C	3.326793	-0.644879	-0.002829	C	-1.479979	3.271200	0.003593
C	2.685734	0.644712	-0.010506	C	0.668172	4.409343	-0.004448
C	1.272489	0.700565	-0.011794	C	-0.686050	4.467885	0.000555
C	-1.568995	0.823953	0.005549	C	-2.874644	3.312074	0.009423
C	0.608812	1.956854	-0.002594	C	-5.070526	2.165378	0.019001
C	-2.976580	0.881908	0.001120	C	-5.790665	1.015904	0.021281
C	-3.738761	-0.322157	0.010444	H	1.258896	5.316651	-0.006888
C	-0.815931	2.013816	-0.005814	H	-1.197794	5.421785	0.004040
Se	5.335621	-0.779920	-0.096680	H	-3.377338	4.271653	0.015911
C	1.358222	3.151237	-0.008240	H	-5.566884	3.127458	0.024574
C	3.408392	1.857780	-0.013433	H	-6.872986	1.045274	0.027009
C	2.763883	3.073097	-0.013242	H	-6.962406	-1.423049	0.022661
H	3.338100	3.990810	-0.017180	H	-5.816273	-3.606362	0.013611
O	7.376365	-1.279093	0.282631	H	7.928780	-0.730724	-0.279655

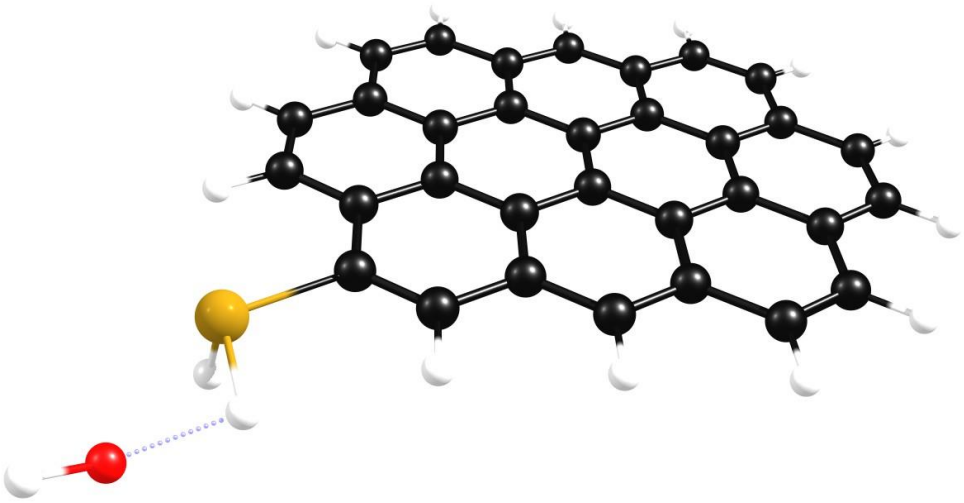


E^0 = -3706.050616 E^0 + ZPE = -3705.674086

ΔG^0 = -3705.724637

Molecule: C-SeH-TS-2

C	3.010930	-4.082855	0.011355	H	-5.516875	-2.019432	-0.152236
C	1.655053	-4.104261	0.020008	H	3.575647	-5.006581	0.012628
C	0.894682	-2.886519	0.019155	H	1.117078	-5.043512	0.030057
C	1.591507	-1.647735	0.001713	H	-1.034079	-3.829398	0.043277
C	3.016350	-1.632509	0.000371	H	-3.176126	-2.630240	0.060161
C	3.735714	-2.845071	-0.001009	H	-5.564712	-0.116276	-1.171812
C	-0.500529	-2.886913	0.030316	H	-4.450134	2.012069	0.044339
C	0.874624	-0.433995	0.010073	C	5.122060	-0.380549	-0.022399
C	-0.533528	-0.450191	0.012396	C	5.145770	-2.805019	-0.008739
C	-1.220621	-1.692720	0.030946	C	5.819899	-1.606638	-0.019442
C	-2.653979	-1.681779	0.046872	C	3.680933	2.069841	-0.031090
C	-3.338020	-0.512777	0.046897	C	1.559992	3.261950	-0.025620
C	-2.679207	0.765690	0.033918	C	-0.553532	4.463099	-0.015849
C	-1.265540	0.773728	0.017708	C	0.801630	4.481373	-0.027156
C	1.577510	0.813503	-0.015855	C	2.955145	3.262077	-0.033900
C	-0.565858	2.010034	-0.003475	C	5.116567	2.052015	-0.038169
C	2.985997	0.830242	-0.014006	C	5.802861	0.882090	-0.034844
C	3.712597	-0.395439	-0.018591	H	-1.117776	5.386976	-0.016591
C	0.859649	2.024622	-0.008060	H	1.341447	5.419618	-0.038632
Se	-5.274859	-0.599372	0.181014	H	3.485590	4.206553	-0.045849
C	-1.279784	3.225793	-0.000298	H	5.640649	2.999209	-0.048063
C	-3.368342	1.995985	0.032010	H	6.885591	0.879989	-0.040190
C	-2.686917	3.190410	0.015728	H	6.902474	-1.590183	-0.024654
H	-3.233569	4.124628	0.016084	H	5.693392	-3.738919	-0.007098
8	-7.331603	-1.863690	-0.580573	H	-8.192234	-2.111254	-0.237110

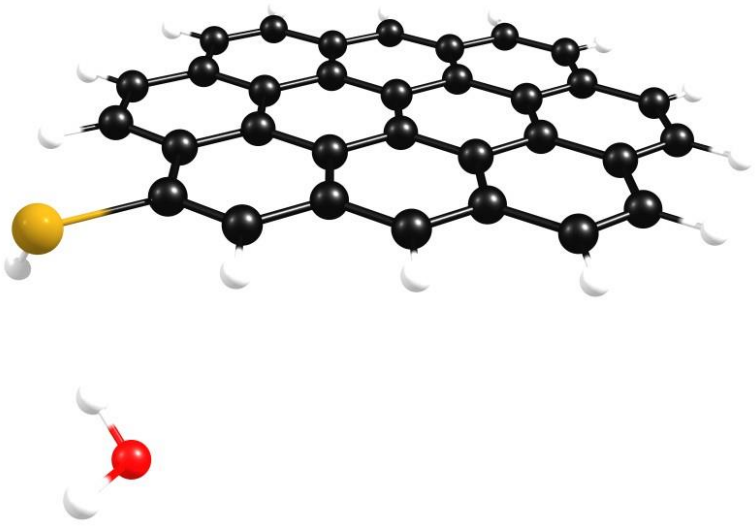


E^0 = -3706.0405867 E^0 + ZPE = -3705.667539

ΔG^0 = -3705.718693 ν_{imag} = -530.506

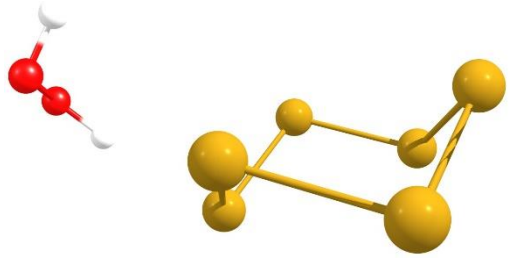
Molecule: C-SeH-P-2

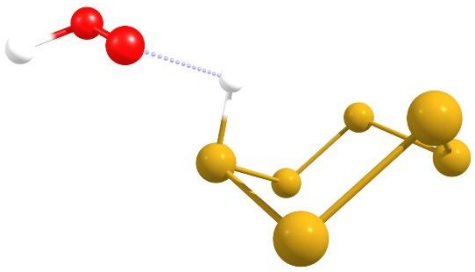
C	-2.770790	-4.122972	-0.115280	H	5.559910	-2.658100	0.830144
C	-1.414034	-4.087636	-0.137780	H	-3.297410	-5.071319	-0.135086
C	-0.702132	-2.838630	-0.113559	H	-0.837371	-5.005671	-0.177268
C	-1.450794	-1.628982	-0.058390	H	1.266649	-3.699665	-0.182694
C	-2.877545	-1.673107	-0.043308	H	3.352183	-2.417304	-0.169983
C	-3.547850	-2.916042	-0.066092	H	5.660621	0.479179	0.901590
C	0.693405	-2.778717	-0.139675	H	4.441991	2.278875	-0.070928
C	-0.782670	-0.384949	-0.040791	C	-5.036325	-0.508140	0.026717
C	0.627121	-0.342473	-0.055749	C	-4.960101	-2.933666	-0.045386
C	1.366157	-1.555010	-0.116559	C	-5.683298	-1.763626	-0.000196
C	2.799618	-1.484232	-0.138454	C	-3.693832	2.002904	0.083615
C	3.454112	-0.293064	-0.116339	C	-1.619738	3.282755	0.094500
C	2.730503	0.959622	-0.062385	C	0.444276	4.571708	0.101654
C	1.313870	0.910379	-0.032436	C	-0.911265	4.533932	0.123085
C	-1.537258	0.833216	0.022494	C	-3.015198	3.224265	0.111767
C	0.560770	2.117947	0.026004	C	-5.129456	1.924519	0.101080
C	-2.947753	0.791798	0.031543	C	-5.768301	0.726924	0.074586
C	-3.625126	-0.464593	0.010710	H	0.971060	5.519826	0.123236
C	-0.867353	2.074034	0.041316	H	-1.490408	5.450383	0.163677
Se	5.376744	-0.344125	-0.280684	H	-3.584781	4.147744	0.151751
C	1.222594	3.365197	0.048737	H	-5.693212	2.850632	0.138613
C	3.361527	2.222515	-0.039849	H	-6.852262	0.680248	0.088891
C	2.630502	3.387648	0.016659	H	-6.767770	-1.792023	0.014181
H	3.139284	4.345676	0.032469	H	-5.470168	-3.891011	-0.065606
O	5.430433	-3.547358	1.188405	H	6.167065	-4.059510	0.839567

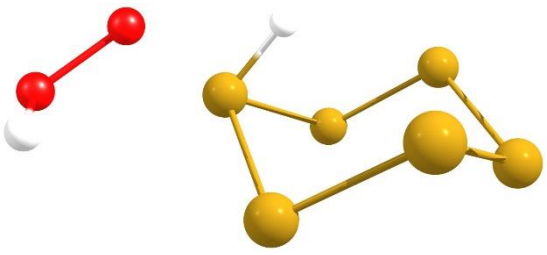


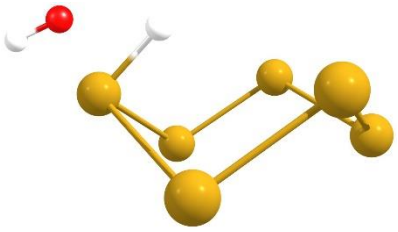
E^0 = -3705.147586 E^0 + ZPE = -3705.769851

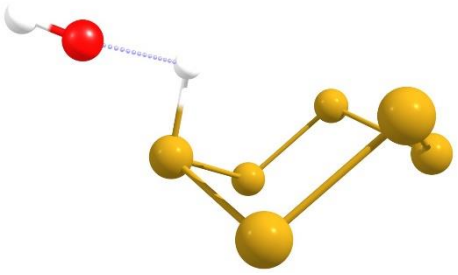
ΔG^0 = -3705.822917

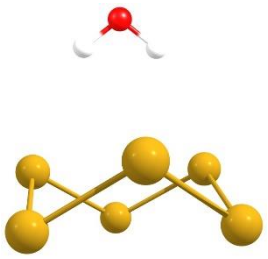
Molecule: t-Se_6-R-1				
Se	-1.384069	1.582217	-1.144817	
Se	0.855714	1.669098	-1.828702	
Se	1.983655	1.346033	0.200943	
Se	-1.655303	-0.728380	-0.833643	
Se	-0.545179	-1.040116	1.213661	
Se	1.693774	-0.958738	0.523217	
O	-4.506375	-0.255279	1.036438	
H	-3.914259	-0.348614	0.271159	
O	-3.661596	-0.673891	2.099857	
H	-3.427627	0.164060	2.520867	
E^0 = -14560.503624			E^0 + ZPE = -14560.469795	
ΔG^0 = -14560.517367				

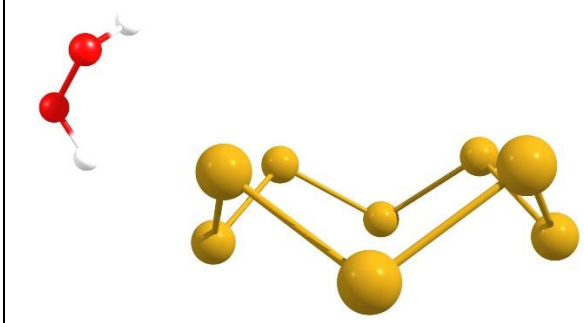
Molecule: t-Se_6-TS-1				
Se	-1.815759	0.611303	-0.227863	
Se	0.037134	2.072182	-0.789081	
Se	1.597970	1.416175	0.816183	
Se	-0.992911	-1.447426	-1.090089	
Se	0.606336	-2.017315	0.503159	
Se	2.392285	-0.606065	-0.051526	
O	-3.817406	0.465997	1.905249	
H	-4.647291	0.495195	1.418207	
O	-3.153568	-0.677041	1.334040	
H	-1.636813	0.212148	1.200897	
E^0 = -14560.405149			E^0 + ZPE = -14560.376652	
ΔG^0 = -14560.421436			ν_{imag} = -1086.6897	

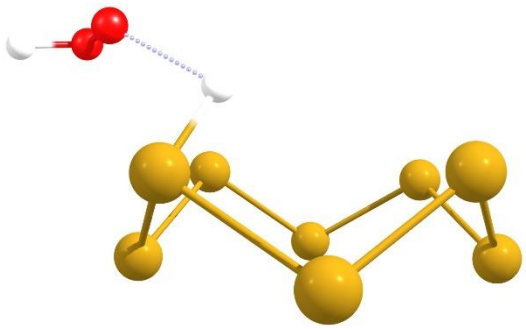
Molecule: t-Se_6-P-1				
Se	-1.723831	0.975278	0.218362	
Se	0.440758	2.124475	-0.671238	
Se	1.994002	1.082500	0.722562	
Se	-1.326580	-1.093030	-0.933903	
Se	0.270065	-2.076480	0.441630	
Se	2.247320	-1.032772	-0.255561	
O	-4.280479	-0.019590	0.484702	
H	-4.230119	-0.953770	0.240494	
O	-3.159740	0.136797	1.340286	
H	-0.907114	0.697139	1.416641	
E^0 = -14560.426608			E^0 + ZPE = -14560.395083	
ΔG^0 = -14560.440033				

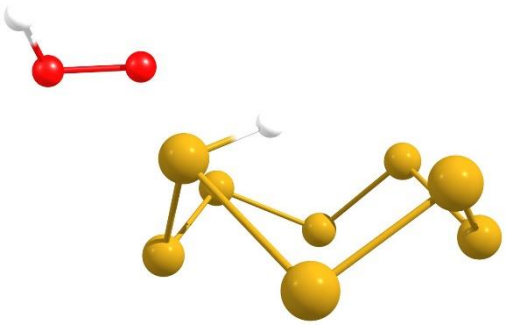
Molecule: t-Se_6-R-2				
Se	-1.983364	-0.838558	0.299696	
Se	-1.445079	1.180079	-0.889063	
Se	0.221209	2.084869	0.449104	
Se	0.199712	-2.159028	-0.690280	
Se	1.799193	-1.167797	0.690976	
Se	2.132408	0.942456	-0.277604	
O	-3.280542	-0.074053	1.465691	
H	-1.030911	-0.606819	1.396657	
H	-4.143412	-0.229478	1.061664	
E^0 = -14485.285579				E^0 + ZPE = -14485.257740
ΔG^0 = -14485.300382				

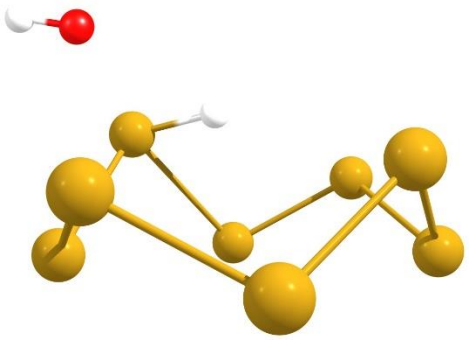
Molecule: t-Se_6-TS-2				
Se	1.828131	-0.974231	0.160567	
Se	-0.185354	-2.119904	-0.632505	
Se	-1.798529	-1.103687	0.712483	
Se	1.506354	1.135752	-0.889103	
Se	-0.155117	2.074483	0.437450	
Se	-2.081951	0.977285	-0.318545	
O	3.116394	0.168631	1.778826	
H	1.528550	-0.523537	1.558509	
H	3.680112	-0.475216	2.219050	
E^0 = -14485.256610				E^0 + ZPE = -14485.232802
ΔG^0 = -14485.275596				ν_{imag} = -1190.9997

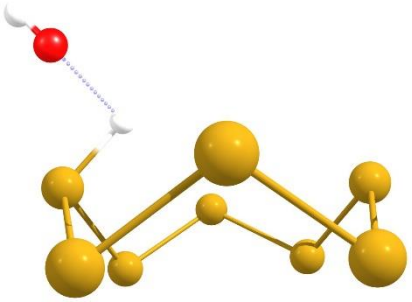
Molecule: t-Se_6-P-2				
Se	1.785611	-1.082007	-1.016912	
Se	-0.257625	-2.053652	-0.399719	
Se	-0.819818	-0.837331	1.526015	
Se	1.069355	0.957002	-1.929079	
Se	0.531173	2.162058	0.008418	
Se	-1.521999	1.200231	0.600484	
O	2.655522	-0.252513	2.410841	
H	2.777031	-0.333247	1.458660	
H	1.697518	-0.260977	2.511657	
E^0 = -14485.372658				E^0 + ZPE = -14485.344215
ΔG^0 = -14485.389531				

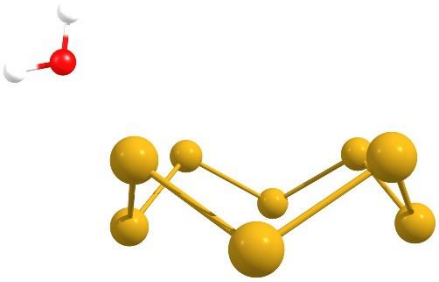
Molecule: t-Se_8-R-1				
Se	1.728730	1.720928	0.246962	
Se	2.215016	-0.184349	-1.023983	
Se	1.486947	-2.002002	0.259096	
Se	-0.203182	2.590904	-0.742766	
Se	-1.931254	1.994433	0.712254	
Se	-2.999882	0.178239	-0.296069	
Se	-0.573944	-2.613491	-0.648426	
Se	-2.179944	-1.715992	0.792744	
O	4.290079	0.476280	1.781264	
H	3.945202	-0.205577	2.373556	
O	5.097214	-0.273208	0.883883	
H	4.511899	-0.353762	0.111683	
E^0 = -19363.483903				E^0 + ZPE = -19363.448260
ΔG^0 = -19363.502360				

Molecule: t-Se_8-TS-1				
Se	-1.917713	-1.697237	0.157882	
Se	-2.261565	0.272728	-1.129981	
Se	-1.492622	1.955178	0.266731	
Se	0.104581	-2.662189	-0.752188	
Se	1.726414	-1.980691	0.759414	
Se	2.891086	-0.255690	-0.313040	
Se	0.535870	2.604281	-0.710547	
Se	2.156427	1.706173	0.712472	
O	-3.033007	-0.507505	1.994480	
H	-1.441665	-0.970477	1.378706	
O	-3.624704	0.798055	1.911137	
H	-4.540892	0.599270	1.691115	
E^0 = -19363.381457				E^0 + ZPE = -19363.351495
ΔG^0 = -19363.403316				ν_{imag} = -958.5955

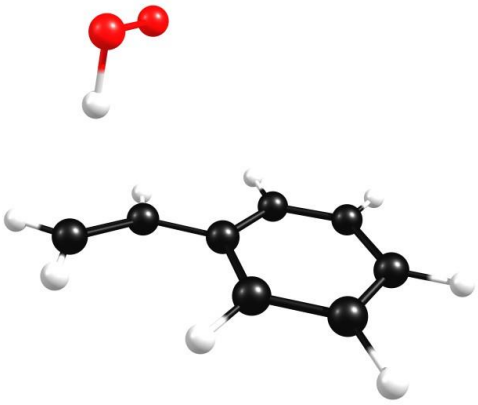
Molecule: t-Se_8-P-1				
Se	1.574586	1.651928	0.479915	
Se	2.231476	-0.007220	-1.130371	
Se	1.884002	-1.944673	0.074167	
Se	-0.420736	2.513557	-0.981559	
Se	-2.104199	1.900734	0.494551	
Se	-2.912725	-0.170843	-0.250447	
Se	-0.232637	-2.701351	-0.581891	
Se	-1.739942	-1.794301	0.960573	
O	2.691659	0.804852	1.896924	
H	0.505703	0.898960	1.168268	
O	4.034121	1.192185	1.644982	
H	4.174008	1.898532	2.288607	
E^0 = -19363.403765				E^0 + ZPE = -19363.370618
ΔG^0 = -19363.422927				

Molecule: t-Se_8-R-2				
Se	0.556145	-2.225985	0.772914	
Se	-1.571033	-2.079159	-0.923547	
Se	-2.756407	-0.603630	0.427166	
Se	2.015786	-1.316097	-0.908396	
Se	2.731378	0.599004	0.160457	
Se	1.317613	2.287516	-0.635548	
Se	-2.296269	1.550911	-0.378366	
Se	-0.481028	2.353641	0.863910	
H	2.299963	-2.749006	2.289653	
O	1.777238	-1.941803	2.202958	
H	-0.068143	-0.967409	1.214622	
E^0 = -19288.263482				E^0 + ZPE = -19288.234105
ΔG^0 = -19288.284303				

Molecule: t-Se_8-TS-2				
Se	2.042922	-1.519457	0.429363	
Se	0.216122	-2.580705	-0.803879	
Se	-1.586060	-2.129037	0.586811	
Se	2.426745	0.424678	-0.892724	
Se	1.508104	2.125265	0.374425	
Se	-0.544526	2.595776	-0.640726	
Se	-2.757072	-0.374777	-0.427278	
Se	-2.128929	1.556293	0.725900	
H	3.297892	-0.795613	2.858328	
O	2.910011	-0.213013	2.197870	
H	1.393638	-0.833560	1.594341	
E^0 = -19288.233609				E^0 + ZPE = -19288.207973
ΔG^0 = -19288.258060				ν_{imag} = -1185.9384

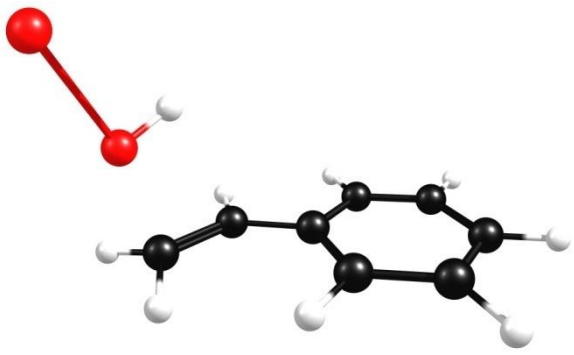
Molecule: t-Se_8-P-2				
Se	-1.667656	-1.863556	-0.495166	
Se	0.236784	-2.638029	0.605084	
Se	2.045830	-1.851286	-0.647771	
Se	-2.373475	-0.008278	0.741888	
Se	-1.682604	1.854146	-0.492738	
Se	0.219334	2.639431	0.604438	
Se	2.844760	0.009146	0.515025	
Se	2.030997	1.862011	-0.650365	
H	-4.779102	-0.014159	-0.310265	
O	-5.648418	-0.028055	-0.726977	
H	-6.268552	0.116696	-0.007379	
E^0 = -19288.350500				E^0 + ZPE = -19288.320562
ΔG^0 = -19288.376090				

Molecule: Styrene-˙OOH-R			
O	-2.591716	1.679954	0.226894
O	-2.743285	0.706570	1.081232
H	-2.388854	-0.098623	0.635969
C	-0.968802	-0.892066	-0.991647
C	-1.749515	-1.837095	-0.457542
H	-1.474919	-2.385090	0.435785
H	-1.308600	-0.379564	-1.885840
C	0.335617	-0.439392	-0.475597
C	0.912971	0.702547	-1.037561
C	1.020253	-1.107281	0.546293
C	2.139031	1.176702	-0.585309
C	2.244131	-0.634040	0.997093
C	2.807639	0.509546	0.434385
H	0.391164	1.221615	-1.832103
H	0.603470	-2.003639	0.985553
H	2.570819	2.063468	-1.029904
H	2.764880	-1.161182	1.785495
H	-2.689447	-2.095683	-0.928039
H	3.763545	0.872973	0.787379



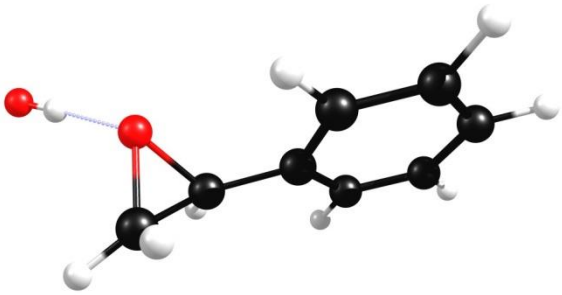
E^0 = -460.638524
E^0 + ZPE = -460.487086
ΔG^0 = -460.526370

Molecule: Styrene-˙OOH-TS			
O	-3.858537	1.197580	-0.995948
O	-2.726764	0.144484	-0.185714
H	-2.231560	-0.089127	-0.986601
C	-0.678940	-1.301492	0.349903
C	-1.770316	-0.901542	1.093981
H	-1.684719	-0.104984	1.817771
H	-0.755956	-2.224363	-0.213135
C	0.552580	-0.553957	0.178825
C	1.555397	-1.092460	-0.643113
C	0.785554	0.685433	0.798677
C	2.754482	-0.421647	-0.834403
C	1.983556	1.353369	0.602810
C	2.972805	0.803947	-0.211956
H	1.381470	-2.044929	-1.128264
H	0.028259	1.128927	1.430287
H	3.517274	-0.851752	-1.469542
H	2.149754	2.307183	1.085655
H	-2.559010	-1.617651	1.269102
H	3.906183	1.330277	-0.360330



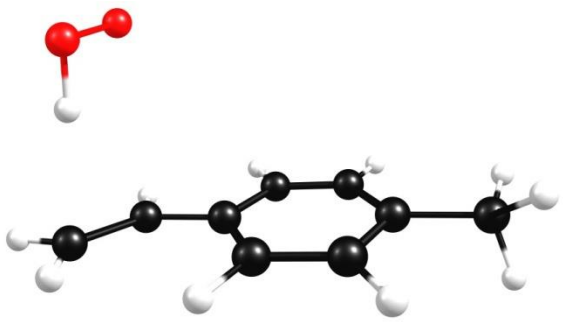
E^0 = -460.558710
E^0 + ZPE = -460.409186
ΔG^0 = -460.446266
ν_{imag} = -973.549

Molecule: Styrene epoxide-˙OH-P			
O	-4.322301	-0.464998	-1.106302
O	-1.936677	0.524810	-0.080085
H	-3.475547	-0.096697	-0.763710
C	-1.010300	-0.411017	0.507373
C	-1.753001	0.535060	1.346697
H	-1.241841	1.413366	1.719525
H	-1.355013	-1.437704	0.483078
C	0.424190	-0.208245	0.177384
C	1.290095	-1.298771	0.214881
C	0.917281	1.053666	-0.154056
C	2.642638	-1.128733	-0.063056
C	2.266957	1.220223	-0.437049
C	3.133158	0.130611	-0.389369
H	0.903652	-2.280172	0.460739
H	0.242883	1.899065	-0.198800
H	3.309654	-1.979892	-0.030977
H	2.643587	2.200310	-0.698203
H	4.183767	0.263160	-0.610939
H	-2.605427	0.183302	1.913557



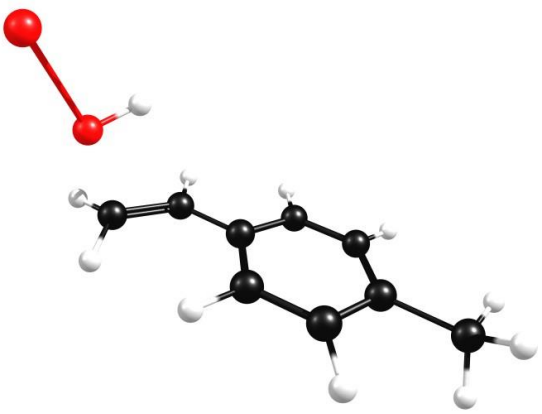
E^0 = -460.676882
E^0 + ZPE = -460.524724
ΔG^0 = -460.562913

Molecule: *p*-Methylstyrene-˙OOH-R			
O	-2.816640	-1.930091	-0.137589
O	-3.028652	-1.055901	-1.081788
H	-2.797626	-0.178801	-0.693942
C	-1.568267	0.972493	0.866736
C	-2.411796	1.736675	0.163554
H	-2.142072	2.185272	-0.784941
H	-1.908279	0.560991	1.811811
C	-0.193534	0.602420	0.491549
C	0.499522	-0.299604	1.300621
C	0.455082	1.112215	-0.640292
C	1.799295	-0.685588	0.992125
C	1.749488	0.723781	-0.944093
C	2.445662	-0.179191	-0.132883
H	0.011945	-0.704517	2.179208
H	-0.048708	1.818869	-1.286440
H	2.316401	-1.388964	1.633140
H	2.235517	1.128265	-1.823872
H	-3.401322	1.948350	0.547875
C	3.860567	-0.567056	-0.461823
H	3.969031	-0.777439	-1.526076
H	4.546442	0.246648	-0.216557
H	4.164899	-1.447603	0.101846



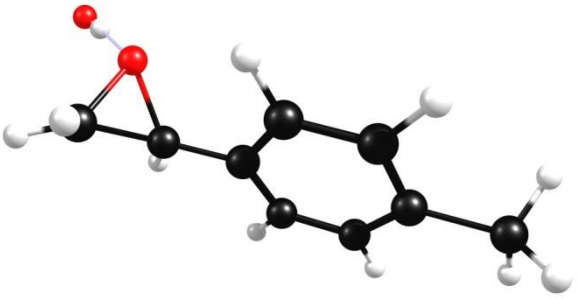
E^0 = -499.959797
E^0 + ZPE = -499.780911
ΔG^0 = -499.822375

Molecule: *p*-Methylstyrene-˙OOH-TS			
O	4.123626	-1.615206	-0.942627
O	3.154874	-0.366500	-0.198543
H	2.691506	-0.118778	-1.013662
C	1.290846	1.353772	0.247507
C	2.347388	0.890725	1.004206
H	2.188890	0.168590	1.791059
H	1.457437	2.216554	-0.387287
C	-0.020288	0.743981	0.159190
C	-0.987709	1.335530	-0.665681
C	-0.372863	-0.421661	0.862825
C	-2.260921	0.794683	-0.774591
C	-1.642600	-0.955948	0.745652
C	-2.610795	-0.357565	-0.070918
H	-0.730498	2.229591	-1.220336
H	0.351438	-0.913373	1.497910
H	-2.992878	1.269833	-1.415660
H	-1.896244	-1.855739	1.293096
H	3.217700	1.521261	1.107078
C	-3.990055	-0.944912	-0.168761
H	-4.518981	-0.838394	0.780666
H	-4.572269	-0.447197	-0.942447
H	-3.942125	-2.010330	-0.397629

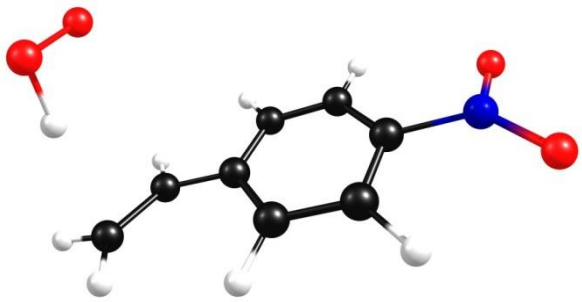


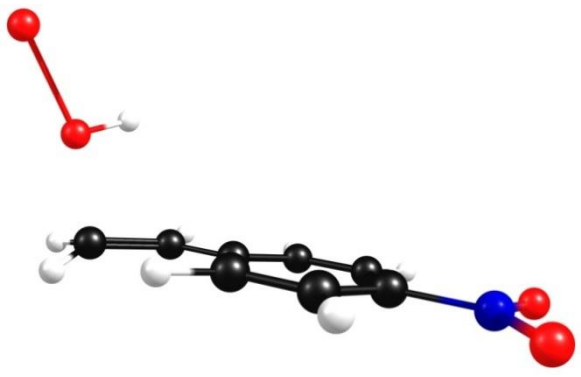
E^0 = -499.880329
E^0 + ZPE = -499.703247
ΔG^0 = -499.742680
ν_{imag} = -960.310

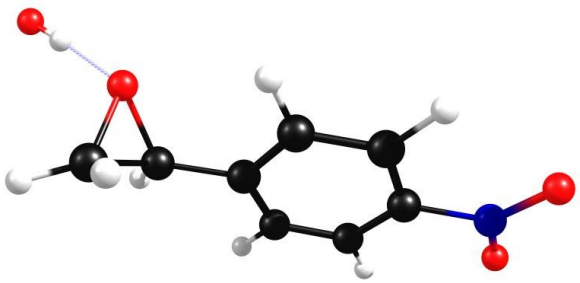
Molecule: *p*-Methylstyrene epoxide-˙OH-P			
O	-4.746725	-0.467749	-1.228246
O	-2.398537	0.555839	-0.157704
H	-3.911647	-0.083914	-0.873319
C	-1.527513	-0.373442	0.522245
C	-2.291246	0.626062	1.275566
H	-1.780585	1.509292	1.637275
H	-1.897686	-1.391642	0.524480
C	-0.073803	-0.223882	0.259196
C	0.753156	-1.339251	0.337372
C	0.485633	1.016032	-0.055409
C	2.123209	-1.217415	0.120061
C	1.849658	1.129447	-0.276131
C	2.691509	0.015836	-0.188566
H	0.325728	-2.307332	0.568758
H	-0.149695	1.888728	-0.137398
H	2.755594	-2.094099	0.185539
H	2.273128	2.095509	-0.523666
H	-3.181654	0.320072	1.809878
C	4.169519	0.158935	-0.431015
H	4.609912	0.866804	0.272949
H	4.677358	-0.797886	-0.319830
H	4.360906	0.535821	-1.436987

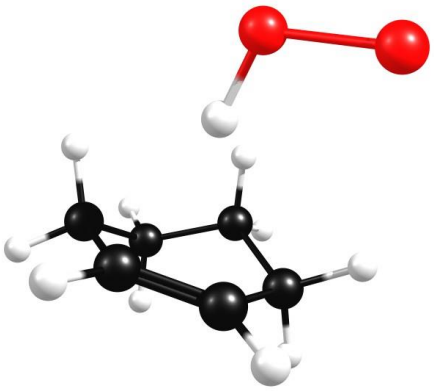


E^0 = -499.997864
E^0 + ZPE = -499.817957
ΔG^0 = -499.857971

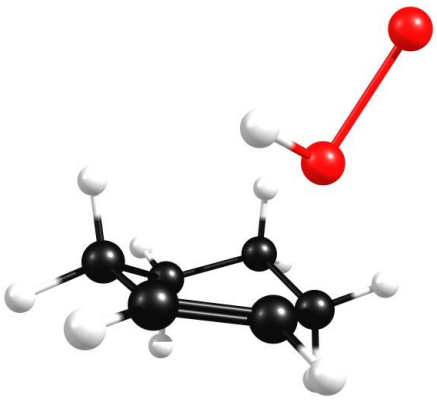
Molecule: *p*-NO_2 styrene-˙OOH-R				
O	-3.245780	-1.954997	-0.494077	
O	-3.452187	-1.030628	-1.390114	
H	-3.330176	-0.172859	-0.923270	
C	-2.316107	0.778306	0.956360	
C	-3.147221	1.617937	0.332478	
H	-2.838074	2.238458	-0.499918	
H	-2.691445	0.179731	1.778970	
C	-0.898428	0.556506	0.621547	
C	-0.233166	-0.508991	1.236013	
C	-0.198220	1.370015	-0.277883	
C	1.098379	-0.773780	0.960259	
C	1.131111	1.120493	-0.565580	
C	1.756366	0.049778	0.060538	
H	-0.767912	-1.137095	1.935911	
H	-0.685473	2.210335	-0.751197	
H	1.613872	-1.596643	1.431429	
H	1.676704	1.745110	-1.256249	
H	-4.174453	1.706973	0.661713	E^0 = -665.177282
N	3.166383	-0.213495	-0.235019	E^0 + ZPE = -665.023036
O	3.733333	0.522221	-1.015760	ΔG^0 = -665.066207
O	3.699133	-1.154237	0.315620	

Molecule: *p*-NO_2 styrene-˙OOH-TS				
O	4.559036	-1.734267	-1.142047	
O	3.703641	-0.481850	-0.307433	
H	3.376272	-0.031854	-1.103527	
C	2.058554	1.325311	0.364954	
C	3.087044	0.684371	1.031936	
H	2.876150	-0.094420	1.749208	
H	2.279814	2.240881	-0.170086	
C	0.701857	0.830775	0.255677	
C	-0.246771	1.619979	-0.416062	
C	0.300871	-0.406232	0.790464	
C	-1.559021	1.204766	-0.541673	
C	-1.006355	-0.834640	0.670054	
C	-1.916698	-0.019538	0.006664	
H	0.057715	2.569311	-0.835725	
H	1.014344	-1.040465	1.296322	
H	-2.290294	1.812000	-1.052653	
H	-1.319396	-1.783873	1.077182	
H	4.010231	1.224762	1.178816	E^0 = -665.097208
N	-3.302238	-0.469081	-0.119022	E^0 + ZPE = -664.945149
O	-3.609776	-1.524852	0.395262	ΔG^0 = -664.986912
O	-4.078659	0.235778	-0.730590	ν_{imag} = -1061.652

Molecule: *p*-NO_2 styrene-epoxide-•OH-P				
O	-5.407403	-0.017837	-1.393102	
O	-3.046105	0.572246	-0.017319	
H	-4.572954	0.215423	-0.927546	
C	-2.212917	-0.525349	0.390557	
C	-2.967375	0.251388	1.381664	
H	-2.441500	0.988231	1.974869	
H	-2.594337	-1.499607	0.111200	
C	-0.751233	-0.331059	0.219116	
C	0.077775	-1.450357	0.162783	
C	-0.205349	0.949726	0.131221	
C	1.449052	-1.300599	0.029497	
C	1.162480	1.116474	-0.003960	
C	1.964204	-0.015747	-0.050296	
H	-0.351290	-2.441833	0.219473	
H	-0.852258	1.815479	0.159139	
H	2.103196	-2.157862	-0.015535	
H	1.598909	2.100961	-0.075782	
H	-3.871178	-0.170457	1.801267	E^0 = -665.215651
N	3.412402	0.152345	-0.199771	E^0 + ZPE = -665.060708
O	4.095804	-0.845561	-0.292713	ΔG^0 = -665.103139
O	3.857051	1.280699	-0.223390	

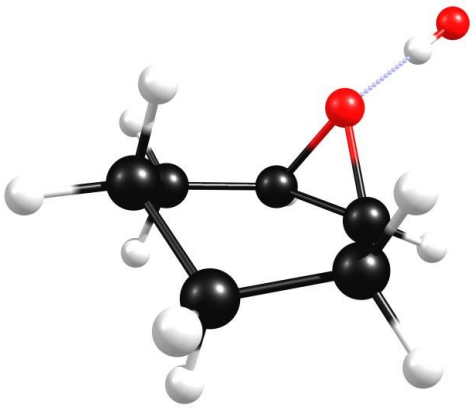
Molecule: Cyclohexene-•OOH-R				
O	2.953011	-0.364453	-0.200796	
O	2.256836	0.616643	-0.705594	
H	1.429663	0.665335	-0.165181	
C	-0.383743	1.071607	0.900281	
C	0.000510	-0.153614	1.276295	
H	0.006692	1.934210	1.431288	
H	0.678107	-0.261503	2.117090	
C	-0.464997	-1.411265	0.593283	
H	0.382919	-2.087621	0.466130	
C	-1.124398	-1.111223	-0.752531	
C	-2.104902	0.052014	-0.613881	
H	-2.838591	-0.193102	0.159420	
C	-1.362246	1.326879	-0.216017	
H	-1.171076	-1.927709	1.251910	
H	-0.828835	1.738941	-1.080058	
H	-2.064913	2.100203	0.100798	E^0 = -385.623083
H	-2.650546	0.212269	-1.544206	E^0 + ZPE = -385.459104
H	-0.354892	-0.842741	-1.483110	ΔG^0 = -385.496686
H	-1.628644	-2.002192	-1.127543	

Molecule: Cyclohexene-˙OOH-TS			
O	-3.246652	0.191406	-0.776862
O	-1.706626	-0.241210	0.023419
H	-1.767304	-1.178593	-0.213722
C	0.493551	-1.310695	0.562275
C	-0.133412	-0.237569	1.159328
H	0.229042	-2.311796	0.881803
H	-0.684394	-0.417935	2.072876
C	0.321515	1.171825	0.906596
H	-0.533994	1.841618	0.994698
C	0.997871	1.312736	-0.455041
C	2.069079	0.237623	-0.628088
H	2.803302	0.331068	0.176999
C	1.444515	-1.158051	-0.579081
H	1.023998	1.443624	1.701195
H	0.901743	-1.356194	-1.512102
H	2.212308	-1.931405	-0.510930
H	2.600468	0.368864	-1.571032
H	0.246277	1.206900	-1.240628
H	1.436065	2.307071	-0.547546

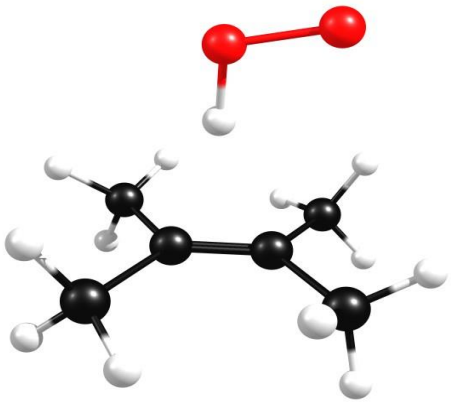


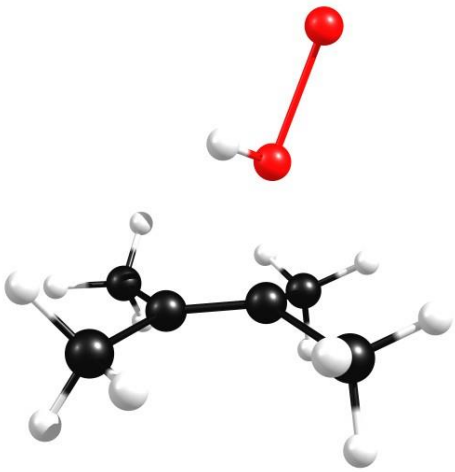
E^0 = -385.540223
E^0 + ZPE = -385.378808
ΔG^0 = -385.413359
ν_{imag} = -754.747

Molecule: Cyclohexene-epoxide-˙OH-P			
8	3.781673	0.015425	-0.360672
8	1.043186	-0.023226	-0.341190
1	2.793408	0.001026	-0.356189
6	0.293918	0.793499	0.595543
6	0.313537	-0.669332	0.725681
1	0.942566	1.365225	1.248314
1	0.960119	-1.104109	1.479496
6	-0.859006	-1.500207	0.286353
1	-1.424396	-1.766404	1.183704
1	-0.490601	-2.429808	-0.152276
6	-0.897815	1.517880	0.016129
1	-1.122284	2.375969	0.650309
1	-0.606391	1.909034	-0.961700
6	-1.765690	-0.748164	-0.688297
1	-2.665365	-1.337477	-0.867468
1	-1.258711	-0.624779	-1.647775
6	-2.130505	0.620011	-0.116885
1	-2.579859	0.477173	0.870131
1	-2.873987	1.114430	-0.742783

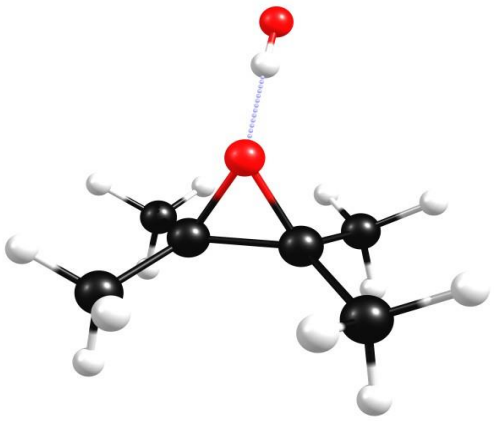


E^0 = -385.665831
E^0 + ZPE = -385.501056
ΔG^0 = -385.536522

Molecule: 2,3 dimethylbutene-˙OOH-R				
O	2.680774	-0.509769	-0.051049	
O	1.717068	-1.375133	0.112141	
H	0.873473	-0.852457	0.074472	
C	-1.097622	-0.243414	-0.022963	
C	-0.373523	0.891045	0.008962	
C	-0.016942	1.622078	1.277965	
H	1.060366	1.576654	1.459904	
H	-0.267645	2.679106	1.156343	
H	-0.536480	1.252048	2.156998	
C	-1.570743	-0.975103	1.210670	
H	-1.515633	-2.052108	1.036923	
H	-0.989441	-0.747716	2.100596	
H	-2.619380	-0.740652	1.414424	
C	-1.541790	-0.907433	-1.302308	
H	-2.605214	-1.148063	-1.226505	
H	-1.397156	-0.290376	-2.184351	
H	-1.018700	-1.857375	-1.448439	E^0 = -386.822068
C	0.116760	1.593104	-1.236097	E^0 + ZPE = -386.640346
H	-0.614703	2.335642	-1.568177	ΔG^0 = -386.679793
H	1.040626	2.128968	-1.014976	
H	0.310309	0.913882	-2.063318	

Molecule: 2,3 dimethylbutene-˙OOH-TS				
O	2.657598	-0.171809	1.037983	
O	0.788119	-0.074104	0.931813	
H	0.839311	-1.023374	1.125564	
C	-1.178492	-0.048923	0.068056	
C	0.203174	0.096048	-0.430297	
C	-1.832958	-1.373562	0.198607	
H	-2.346478	-1.449714	1.158497	
H	-2.609802	-1.442383	-0.574513	
H	-1.161627	-2.218357	0.074885	
C	-1.945283	1.147271	0.499963	
H	-1.383906	1.733655	1.231056	
H	-2.132968	1.804048	-0.355144	
H	-2.897591	0.858015	0.938479	
C	0.723125	-0.973371	-1.366093	
H	0.622190	-1.974719	-0.951278	
H	0.168781	-0.927552	-2.304292	
H	1.776783	-0.786469	-1.562574	E^0 = -386.745821
C	0.602542	1.478912	-0.888585	E^0 + ZPE = -386.564906
H	0.121523	1.696043	-1.842660	ΔG^0 = -386.601254
H	0.322369	2.241863	-0.166156	ν_{imag} = -1111.597
H	1.683029	1.498000	-1.020142	

Molecule: 2,3 dimethylbutene-epoxide-˙OH-P			
O	3.051493	-0.114763	-0.744957
O	0.31627 0	-0.026469	-0.868883
H	2.064475	-0.095397	-0.803355
C	-0.412652	0.754395	0.122983
C	-0.517312	-0.718607	0.105493
C	-1.504025	1.627848	-0.440958
H	-2.238756	1.843439	0.336906
H	-1.073815	2.575188	-0.770048
H	-2.008471	1.168742	-1.285309
C	0.450309	1.479477	1.124589
H	-0.159780	1.780406	1.978041
H	1.281323	0.881316	1.487006
H	0.851678	2.383383	0.662990
C	-1.720238	-1.416192	-0.475758
H	-1.420145	-2.395758	-0.851550
H	-2.465874	-1.569416	0.306541
H	-2.173156	-0.859237	-1.289885
C	0.232683	-1.582146	1.087323
H	1.149380	-1.123158	1.445020
H	-0.407870	-1.798848	1.944002
H	0.486320	-2.529458	0.608331



E^0 = -386.873457

E^0 + ZPE = -386.691862

ΔG^0 = -386.729782

14. Selenium leaching study through ICP-MS

Three reaction mixtures containing Se-DG-1, Se-DG-2 and Se-DG-6 were analysed in ICP-MS after 10 hours of the reaction, followed by catalyst separation through syringe filter. In all the three reaction mixtures, no soluble Se was found (Fig. S20).

TEST REPORT

Issued To,	**Report No.**	**: 100-211225-13**
M/s Sayantan Maity,	Report Date	: 27/12/2021
Department of Chemistry,	Sample Received on	: 25/12/2021
Shiv Nadar University.	Analysis Date	: 25/12/2021 to 27/12/2021
	Report Prepared on	: 27/12/2021
	Sampled By	: Customer

Sample Description : Water
Condition of the sample on receipt : Received in good condition

Page 1 of 1

S. No.	Parameters	Units	Result
	Chemical Analysis		
1.	Se - DG1	µg/L	BLQ (0.001)
2.	Se – DG2	µg/L	BLQ (0.001)
3.	Se – DG6	µg/L	BLQ (0.001)

Fig. S20. ICP-MS data of three reaction mixtures with three Se-DG materials. The detected concentration of Se found 'BLQ' (Below the Limit of Quantification), i.e. below 0.001 parts per billion (ppb or µg/L)

15. Kinetic Results

The kinetic parameters were checked up to 6-hrs, which was the limit time for the autocatalytic growth of the kinetic profile. The Boltzmann fitting (Eqn. 8 in manuscript) was done with fixing the parameters 'y_0' and 'y_{Max}' from the experimental results at t = 0.5 hrs and t = 6 hrs respectively.

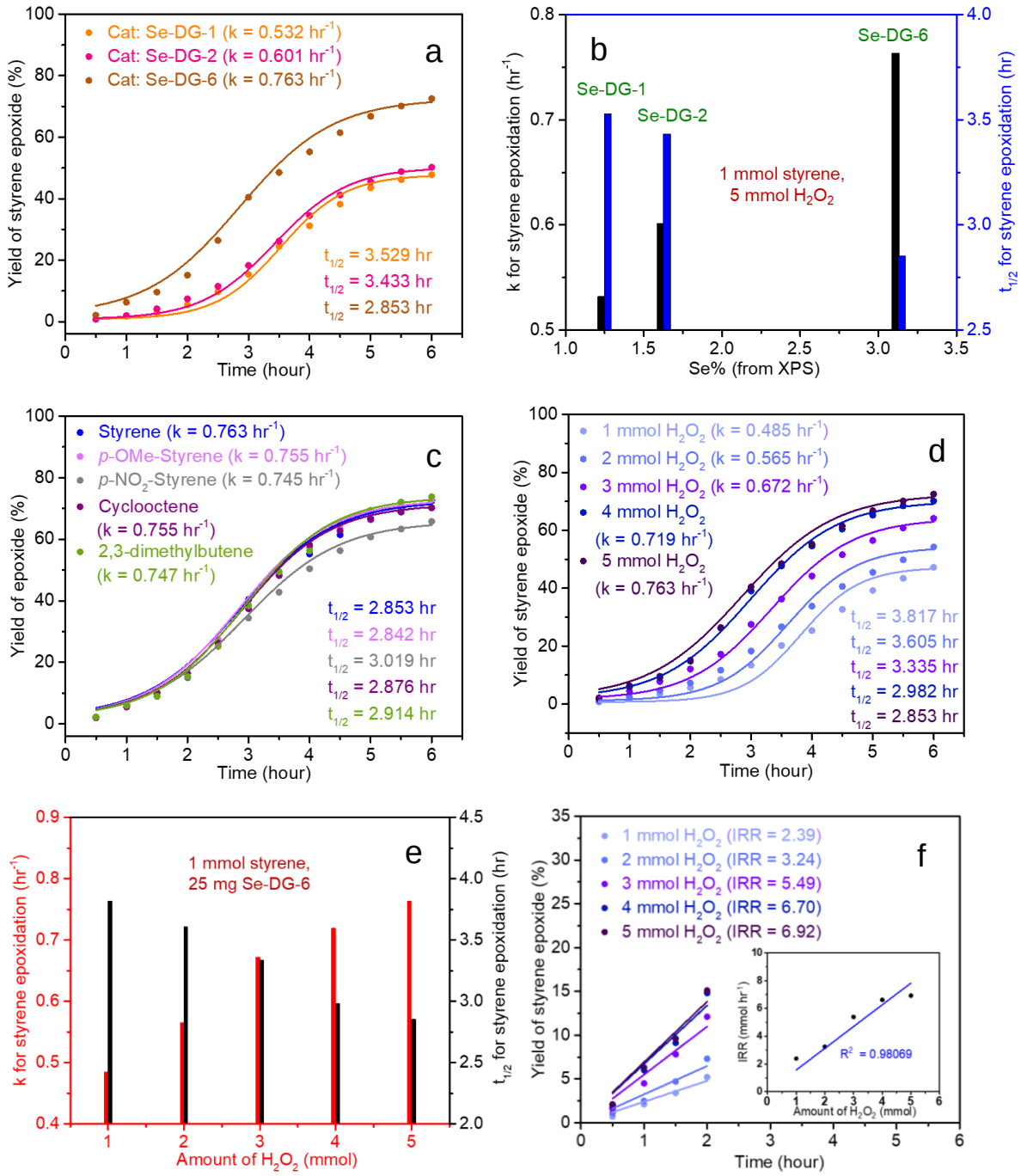


Fig. S21. Kinetic profiles of epoxidation of alkene with H_2O_2 in presence of Se-DG. (a) Faster reaction rate was observed for Se-DG-6 compare to Se-DG-1 and Se-DG-2. (b) Derived 'k' and '$t_{1/2}$' were presented as function of Se% in the Se-DG (Table 10A). The conclusion was,

the extent of Se-load was regulating the reaction kinetics. (c) Kinetic profiles for different alkenes with Se-DG-6. All the kinetic profiles overlapped to each other and the derived kinetic parameters didn't differ to much (Table 10B). (d) Kinetic Profiles for styrene with fixed amount of Se-DG-6) with different concentrations of H_2O_2, showing the elevation of reaction rate with increase of H_2O_2 concentration. (e) Derived 'k' and '$t_{1/2}$' were plotted with [H_2O_2] (Table 10C). (f) Determination of the initial reaction rate (IRR) for styrene epoxidation with different concentrations of H_2O_2 from the induction period of the kinetic profile. Inset of Fig. (f): a linear relationship between IRR and amount of H_2O_2, passing through the origin (0, 0). For (a), (c) and (d), the smooth lines with same colour code represented the non-linear Boltzmann fitting and for (e), the linear fitting. The derived parameters in (a), (c), (d) and (f) were also written in the colour code.

Table S9. IRR of the reactions of epoxidation of styrene with five different concentrations of H_2O_2 using 25 mg Se-DG-6, up to 2 hours (Fig. S21f).

H_2O_2 amount, in 5 ml solution (mmol)	Yield of epoxide after 2 hrs (%)	IRR (mmol hr^{-1})	R^2 of linear graph
1	5.2	2.39	0.98759
2	7.1	3.24	0.98464
3	12.1	5.49	0.98377
4	14.8	6.70	0.98468
5	15.1	6.92	0.98372

16. Recyclability of Se-DG

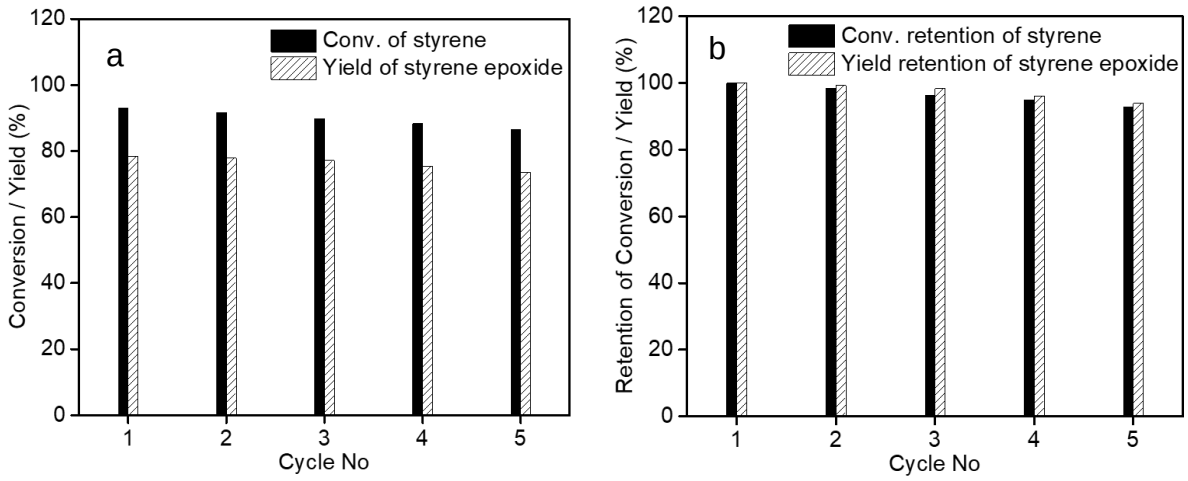


Fig. S22. Recyclability of Se-DG-6 in styrene epoxidation with H_2O_2.

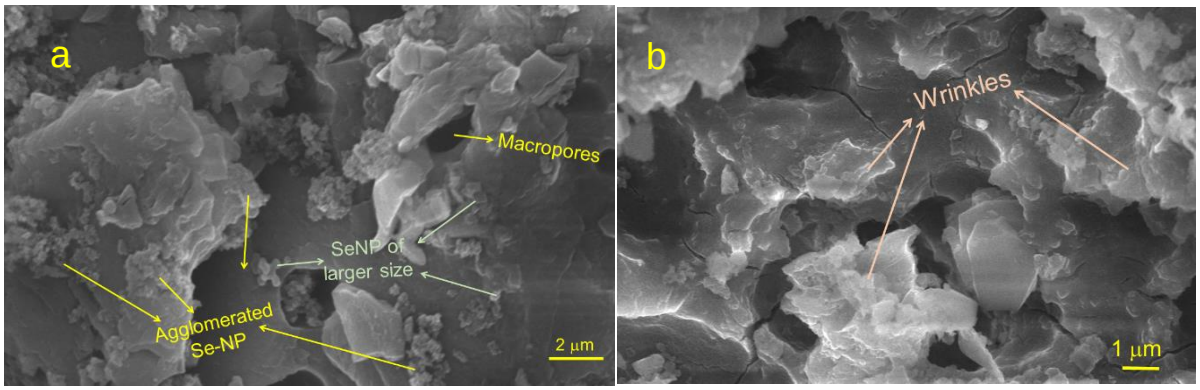


Fig. S23. FESEM images of the recovered Se-DG-6 after 5 cycles.

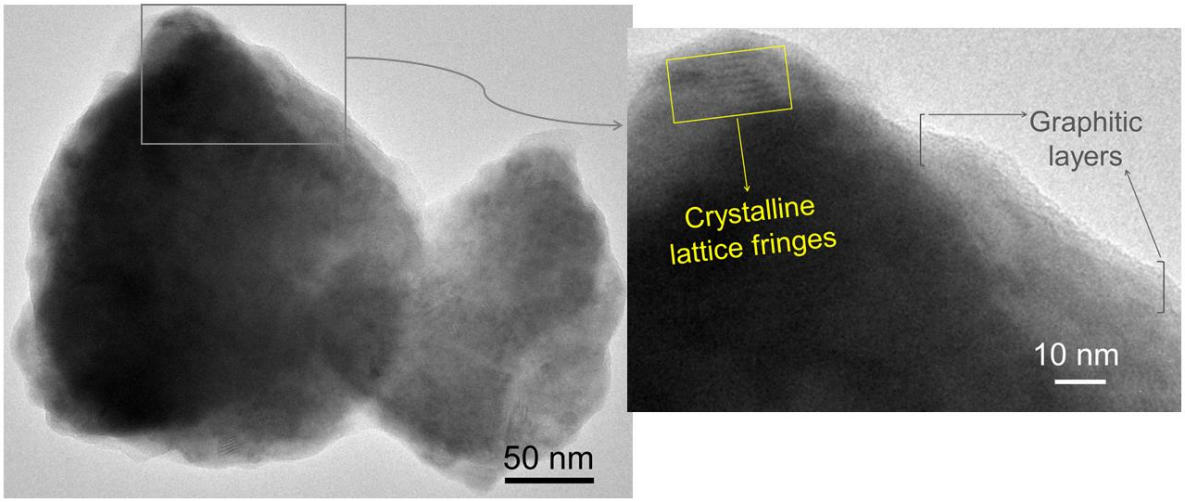


Fig. S24. HRTEM images of the recovered Se-DG-6 after 5 cycles.

17. C-H activation of alkane in presence of alkene

Oxygen gas was purged in a mixture of *p*-Me-styrene, H_2O_2, cyclohexane and Se-DG-6 (scheme 3). After a certain time, a portion of aliquot was taken out, Se-DG was separated through syringe filtration and the mixture was run in HRMS after proper dilution.

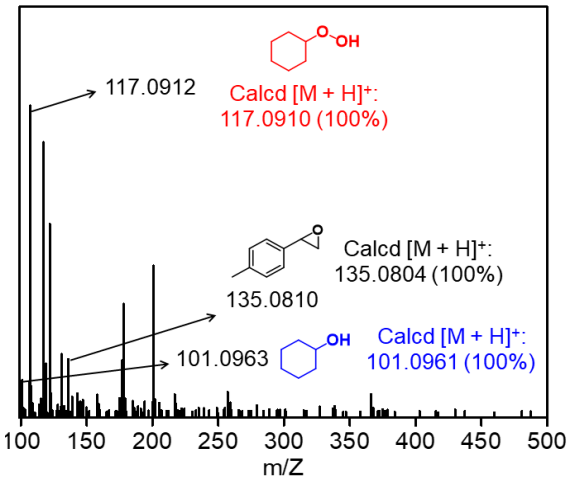


Fig. S25. HRMS data of the reaction mixture (1:1) containing *p*-Me-styrene and cyclohexane showing the formation of cyclohexanol and cyclohexyl hydroperoxide.