

SUPPORTING INFORMATION

Sequential oxidations of phenylchalcogenides by H₂O₂: insights in the redox behavior of selenium from a DFT analysis

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Table S1 Reaction energies (in kcal mol⁻¹) for the neutral pathway in the gas phase. Level of theory ZORA-OLYP/TZ2P

		ΔE		
		S	Se	Te
1-2	1 + H ₂ O ₂	0.0	0.0	0.0
	RC	-1.9	-1.9	-2.1
	TS	25.3	22.0	14.4
	2 + H ₂ O	-38.7	-28.1	-34.8
2-3	2	0.0	0.0	0.0
	TS	38.8	30.9	31.5
	3	-11.9	-26.7	-30.1
3-4	3 + H ₂ O ₂	0.0	0.0	0.0
	RC	-3.5	-2.8	-2.5
	TS	15.8	14.0	6.8
	4 + H ₂ O	-63.1	-49.4	-52.9
4-5	4 + H ₂ O ₂	0.0	0.0	0.0
	RC	-3.9	-4.5	-6.3
	TS	22.3	27.8	23.5
	5 + H ₂ O	-71.6	-31.5	-25.3

Table S2 Reaction energies (in kcal mol⁻¹) for reaction **2-3** in water. Level of theory COSMO-ZORA-OLYP/TZ2P.

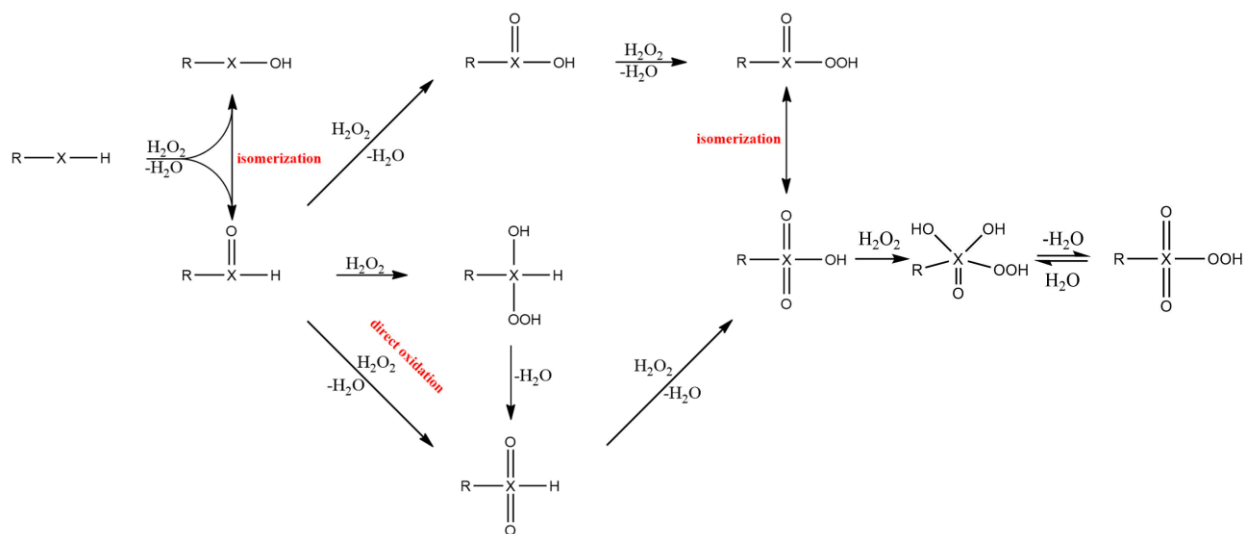
		ΔE		
		S	Se	Te
2-3	2	0.0	0.0	0.0
	TS_23	40.1	32.3	33.7
	3	-	-	-

Table S3 Reaction energies (in kcal mol⁻¹) for the anionic pathway in the gas phase. Level of theory ZORA-OLYP/TZ2P.

		ΔE		
		S	Se	Te
1a-3a	1 + H ₂ O ₂	0.0	0.0	0.0
	RC	-14.5	-14.0	-12.4
	TS	-2.3	-3.8	-4.2
	3 + H ₂ O	-48.7	-38.9	-40.5
3a-4a	3 + H ₂ O ₂	0.0	0.0	0.0
	RC	-16.2	-18.2	-18.4
	TS	-5.1	-6.1	-6.4
	4 + H ₂ O	-71.9	-58.9	-62.6
4a-5a	4 + H ₂ O ₂	0.0	0.0	0.0
	RC	-13.9	-14.9	-15.2
	TS	-2.7	1.7	1.6
	5 + H ₂ O	-87.0	-49.0	-44.3

Table **S4** Reaction energies (in kcal mol⁻¹) for the anionic pathway water. Solvation energies are reported in parentheses. Level of theory COSMO-ZORA-OLYP/TZ2P.

		ΔE					
		S		Se		Te	
1a-3a	1 + H ₂ O ₂	0.0	(-63.7)	0.0	(-62.6)	0.0	(-58.4)
	RC	-1.5	(-51.2)	-1.6	(-50.1)	-1.7	(-47.7)
	TS	5.9	(-56.1)	3.9	(-54.8)	1.9	(-52.2)
	3 + H ₂ O	-48.4	(-63.9)	-42.4	(-66.1)	-47.8	(-65.8)
3a-4a	3 + H ₂ O ₂	0.0	(-64.3)	0.0	(-66.5)	0.0	(-66.2)
	RC	-6.6	(-54.7)	-8.1	(-62.9)	-8.7	(-56.5)
	TS	1.8	(-57.5)	1.4	(-63.2)	0.2	(-59.6)
	4 + H ₂ O	-77.4	(-69.8)	-64.8	(-72.4)	-71.5	(-75.1)
4a-5a	4 + H ₂ O ₂	0.0	(-70.2)	0.0	(-72.9)	0.0	(-75.6)
	RC	-3.6	(-60.0)	-4.9	(-62.9)	-5.0	(-65.4)
	TS	6.3	(-61.3)	11.4	(-63.2)	11.4	(-65.8)
	5 + H ₂ O	-86.1	(-69.3)	-47.7	(-71.6)	-41.8	(-73.2)



Scheme **S1** Mechanistic pathway for the oxidation of a general organochalcogenide (X= S, Se or Te)

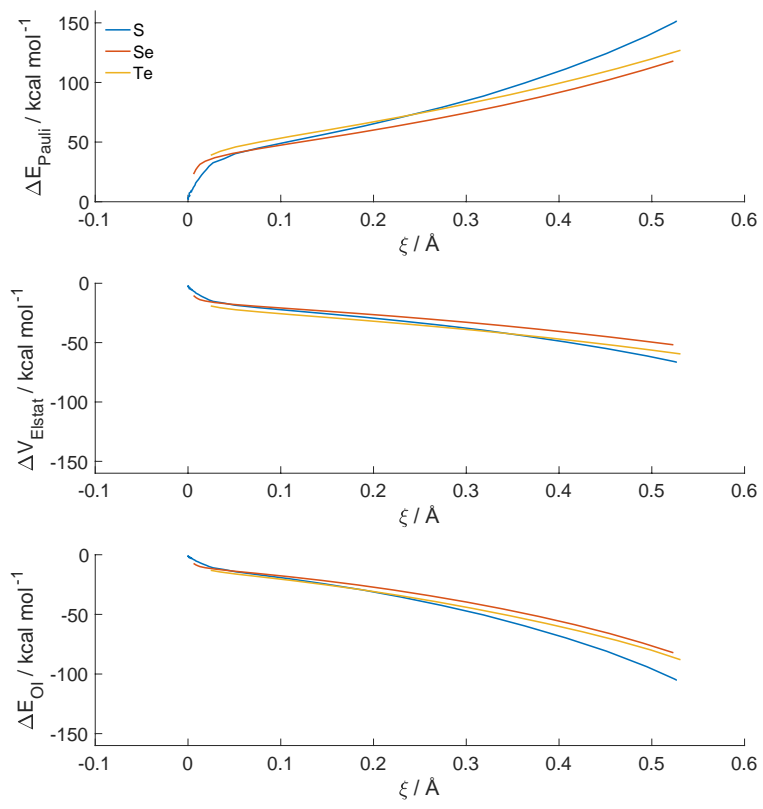


Figure S1 Energy decomposition analysis for reaction (4-5).

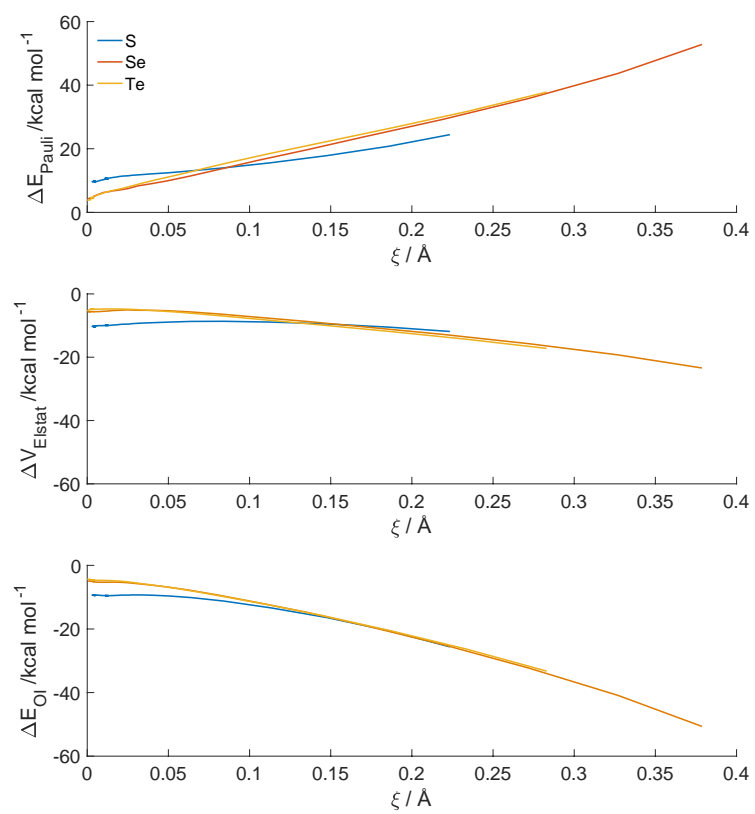


Figure S2 Energy decomposition analysis for reaction (4a-5a).

Table S5 Reaction energies (in kcal mol⁻¹) for the neutral pathway in the gas phase. Level of theory COSMO-ZORA-OLYP/TZ2P.

H₂O₂				C	3.877624200	0.197126944	1.225659808
E = -0.652819754046 Ha				C	4.683657044	0.442381668	0.113060324
O	0.025860000	0.730350000	-0.314680000	H	2.437160170	-0.223115057	-2.354465157
O	-0.025860000	-0.730350000	-0.314680000	H	1.923389821	-0.365891361	1.930785135
H	-0.749710000	0.927270000	0.235540000	H	4.780729565	0.482909668	-2.041755485
H	0.749710000	-0.927270000	0.235540000	H	4.281582393	0.307746895	2.228533609
H₂O				H	5.719104171	0.743536206	0.245924346
E =				H	0.156334676	-0.487579966	-1.639367842
O	0.000000000	0.000000000	0.000160000	H	-0.115587729	-3.265695895	-0.234001018
H	0.000000000	0.760330000	0.594760000	O	0.137595203	-2.708710200	-1.002095851
H	0.000000000	-0.760330000	0.594760000	O	-0.454422927	-4.630445438	-1.203997666
Sulphur				H	0.409393680	-4.915480505	-1.538460893
1				2			
E = -2.818584561272 Ha				E = -3.018086232681 Ha			
S	0.478804765	-1.463471892	0.000369648	S	0.233449110	-1.134260852	-0.415732403
C	2.053549192	-0.650617872	-0.009795829	H	0.732315384	-1.903072527	-1.461385591
C	3.199106727	-1.457484246	-0.072722684	C	1.918687762	-0.567511963	0.001861569
C	2.201071814	0.741976373	0.042572941	C	2.540619571	-1.063553428	1.143474325
C	4.464973893	-0.877400796	-0.082904276	C	2.525393596	0.411662954	-0.786107698
C	3.472841273	1.311429324	0.030793682	C	3.806215462	-0.585459736	1.487663388
C	4.611468351	0.508857246	-0.031581399	C	3.792210993	0.876606318	-0.437494735
H	3.100941278	-2.539121076	-0.113967195	C	4.433121332	0.378636863	0.698994846
H	1.326597073	1.384900405	0.092398679	H	2.033144069	-1.809180022	1.748443933
H	5.342109897	-1.518137789	-0.131819293	H	2.020118046	0.812360793	-1.662779118
H	3.569213817	2.393831296	0.071155162	H	4.301117020	-0.968521090	-2.376782229
H	5.600711814	0.958022192	-0.040158504	H	4.274706894	1.634905871	-1.049104961
H	-0.276669010	-0.352158145	0.051667914	H	5.417576712	0.749436823	0.972412523
1_RC				O	-0.258812386	-2.069897287	0.635780012
E=-3.47437307 Ha				TS_2-3			
S	0.389727000	-0.801355000	0.034217000	E=-2.956239648417 Ha			
C	2.085671000	-0.275548000	-0.036170000	Nimag=-1495.3 cm ⁻¹			
C	2.778697000	-0.094856000	-1.239492000	S	-0.309981833	1.710224059	0.042208109
C	2.746372000	-0.056409000	1.179909000	C	-1.663818886	0.549941671	0.042375642
C	4.112967000	0.306544000	-1.220068000	C	-2.989829288	0.987407902	0.086154932
C	4.083355000	0.334902000	1.186707000	C	-4.015730102	0.043782301	0.060643420
C	4.773320000	0.521072000	-0.010739000	C	-3.723885263	-1.319175802	-0.000786913
H	2.284688000	-0.270881000	-2.190801000	C	-2.394501552	-1.745126675	-0.050149815
H	2.216378000	-0.185964000	2.119785000	C	-1.358917690	-0.814766020	-0.041924423
H	4.638326000	0.445537000	-2.161765000	H	-3.199936174	2.051251712	0.130204082
H	4.583642000	0.500559000	2.137640000	H	-5.049949935	0.378163625	0.090079324
H	5.814844000	0.830243000	-0.001885000	H	-4.529109684	-2.048838832	-0.017948321
H	0.110119000	-0.636342000	-1.271333000	H	-2.161920647	-2.805496582	-0.107690644
H	0.587717000	-3.432409000	-0.601478000	H	-0.325076909	-1.147501349	-0.099647943
O	0.644746000	-4.333400000	-0.969344000	H	-0.500258344	2.518844089	1.177768524
O	-0.447740000	-4.285141000	-1.939077000	O	-0.942189359	3.231486880	-0.010891298
H	-1.087384000	-4.870899000	-1.502928000	3			
TS_1-2				E=-3.037065050542 Ha			
E=-3.431118436614 Ha				S	0.498128910	-1.735284783	0.390623980
nimag=-519.0 cm ⁻¹				C	1.987104388	-0.805235085	0.168122745
S	0.346925148	-0.862667728	-0.364609282	C	3.169994826	-1.543271471	0.001148135
C	2.020095952	-0.322902076	-0.231373221	C	2.040108803	0.593285159	0.189775063
C	2.833369324	-0.093382084	-1.351394888	C	4.388187993	-0.883097701	-0.129494863
C	2.549760699	-0.184314073	1.061492221	C	3.266242640	1.240354101	0.039496309
C	4.156447670	0.297468274	-1.171526539	C	4.444680221	0.511813687	-0.115262655
				H	3.138891089	-2.629973929	-0.031048835
				H	1.131538196	1.169319843	0.327086286
				H	5.297527024	-1.465773238	-0.255971936
				H	3.295641365	2.327480124	0.052687064
				H	5.396729206	1.023401758	-0.226575200
				O	-0.717244418	-0.593312823	0.269409511
				H	-0.955232010	-0.539223661	-0.669176668

3_RC

E=-3.69538462 Ha

S	0.645207000	-1.046672000	1.081619000
C	2.266877000	-0.486524000	0.650659000
C	3.194418000	-0.367602000	1.699487000
C	2.651561000	-0.146645000	-0.651935000
C	4.483757000	0.086603000	1.440925000
C	3.950230000	0.300096000	-0.896319000
C	4.872693000	0.420815000	0.141721000
H	2.909504000	-0.630834000	2.715833000
H	1.936977000	-0.221710000	-1.464272000
H	5.190714000	0.175020000	2.262583000
H	4.236851000	0.561754000	-1.912490000
H	5.881688000	0.771968000	-0.056208000
O	-0.146239000	-1.174463000	-0.373840000
H	1.362271000	-4.261537000	-1.013563000
O	0.577384000	-3.923966000	-1.476581000
O	-0.411358000	-4.923646000	-1.084372000
H	-0.551389000	-5.366973000	-1.937742000
H	0.002820000	-2.081974000	-0.698151000

TS_3-4

E=-3.664635329170 Ha

Nimag=-430.3 cm⁻¹

S	0.631699079	-1.421450343	0.809834231
C	2.189831117	-0.693785711	0.465948791
C	3.099426787	-0.666011527	1.535067444
C	2.553468496	-0.200202273	-0.793284912
C	4.377211052	-0.154800773	1.332840384
C	3.830502604	0.322002367	-0.972689676
C	4.745569178	0.342575151	0.081742764
H	2.808422418	-1.037125077	2.514522127
H	1.846939400	-0.217804054	-1.615323111
H	5.082088510	-0.134409257	2.159716621
H	4.113987825	0.711231382	-1.947140173
H	5.741426624	0.749817240	-0.069987206
O	-0.393969364	-0.744766117	-0.265464155
H	0.230680938	-3.752566326	0.142380416
O	0.674791366	-3.034279353	-0.345987258
O	0.129721169	-4.622017496	-1.442720898
H	1.040555417	-4.855410720	-1.677132764
H	-0.504328350	-1.459127596	-0.929629218

4

E=-3.275486189307 Ha

S	0.571354475	-1.657207349	-0.923020154
O	0.407079753	-2.875522573	-0.107089251
C	2.012645193	-0.775830819	-0.224827893
C	2.684411245	-1.308414083	0.873921189
C	2.464253477	0.388995675	-0.849668897
C	3.808230498	-0.647691185	1.370933320
C	3.590461837	1.039563838	-0.349391531
C	4.260156022	0.523344668	0.762015509
H	2.327179818	-2.229969419	1.323828524
H	1.941016025	0.788898629	-1.714990018
H	4.335826233	-1.053821468	2.230525031
H	3.946564652	1.948357838	-0.828032139
H	5.140152433	1.031413665	1.148353247
O	-0.601967105	-0.541381871	-0.517604877
H	-0.565766627	-0.384162069	0.442984402

4_RC

E=-3.93448444 Ha

S	1.568759000	-1.837618000	-1.013490000
C	2.741129000	-0.730480000	-0.187453000
C	2.902793000	-0.792865000	1.194388000
C	3.516297000	0.124727000	-0.971087000
C	3.842529000	0.037556000	1.803322000
C	4.453572000	0.950628000	-0.352918000

C	4.614768000	0.908041000	1.032797000
H	2.301144000	-1.485100000	1.775274000
H	3.389395000	0.151567000	-2.050637000
H	3.973507000	0.002115000	2.881976000
H	5.059135000	1.624441000	-0.953543000
H	5.348929000	1.550553000	1.512342000
O	0.379647000	-0.660509000	-1.125183000
H	-0.801211000	-3.448143000	-0.749537000
O	-1.610372000	-3.226399000	-1.249497000
O	-1.520097000	-4.176732000	-2.354532000
H	-2.215598000	-4.804005000	-2.098513000
O	1.137746000	-2.847259000	-0.014570000
H	-0.345403000	-1.080574000	-1.623688000

TS_4-5

E=-3.892798585967 Ha

Nimag=-514.7 cm⁻¹

S	0.641251847	-1.670038017	0.300202152
C	2.208619251	-0.783354668	0.317832886
C	2.951263041	-0.748003950	1.498518824
C	2.697205882	-0.249728708	-0.877851031
C	4.198783342	-0.126130453	1.483800119
C	3.946193295	0.364552175	-0.873436825
C	4.694643433	0.428219920	0.303888760
H	2.554049078	-1.188813703	2.406461499
H	2.116776246	-0.314969422	-1.792747268
H	4.782824853	-0.078053568	2.399076411
H	4.336688865	0.790038232	-1.793895863
H	5.670874733	0.905894497	0.298650638
O	-0.336423845	-0.423876161	-0.060325615
H	0.446855531	-3.490013667	-1.360560666
O	0.112700381	-2.569702155	-1.345430891
O	-0.384946827	-3.674917967	-2.919993794
H	-1.315388764	-3.789129459	-2.672404983
O	0.360772664	-2.181107806	1.637305960
H	-0.962364386	-0.777750987	-0.719006972

5

E=-3.527420782802 Ha

S	0.455578394	-1.390657113	-0.599734623
O	0.549383952	-2.817891372	-0.456605631
C	1.986799421	-0.652929611	-0.043634923
C	2.705001275	-1.265082699	0.986809935
C	2.448856040	0.516897579	-0.649034609
C	3.896153098	-0.687454767	1.418743201
C	3.645166787	1.082167236	-0.209236859
C	4.366333579	0.484240597	0.823519775
H	2.341015921	-2.183541797	1.434652641
H	1.887336828	0.967462605	-1.460096397
H	4.461037562	-1.158926006	2.218580856
H	4.014597581	1.988938677	-0.680900899
H	5.299095444	0.927934139	1.162072200
O	0.050264268	-0.764087079	-1.837620963
O	-0.597162873	-0.918354418	0.553877452
H	-1.038847746	-0.119684350	0.221514506

Selenium

1

E = -2.780213567068 Ha

Se	0.373969000	-1.538444414	-0.003960653
C	2.082288702	-0.652607266	-0.011824729
C	3.226128195	-1.457474502	-0.073755013
C	2.218172841	0.738694428	0.041112599
C	4.491025408	-0.872224514	-0.082857944
C	3.488760893	1.313469247	0.030193675

C	4.630116836	0.514651581	-0.031539584
H	3.137040962	-2.540142797	-0.114947642
H	1.342061362	1.378548107	0.090387578
H	5.371393564	-1.508708721	-0.130601638
H	3.581557238	2.396271395	0.070319429
H	5.617548065	0.968078858	-0.039638616
H	-0.415342066	-0.299488401	0.063122538

I_RC

E=-3.436119 Ha

Se	0.252208172	-0.784334868	0.203970703
C	2.100283832	-0.244041833	0.058370945
C	2.771199818	-0.184656553	-1.166736850
C	2.779463992	0.061076798	1.242054592
C	4.113774634	0.190388553	-1.201208413
C	4.126569854	0.419163994	1.196754347
C	4.797965254	0.489446904	-0.023100976
H	2.259787987	-0.434798184	-2.091356059
H	2.263442351	0.030020742	2.198052780
H	4.626843002	0.238999626	-2.158639275
H	4.646857176	0.653131142	2.122352799
H	5.845760972	0.775409690	-0.056125756
H	-0.092746075	-0.457577605	-1.188686658
H	0.569551482	-3.395234111	-0.795772106
O	0.717363415	-4.255168304	-1.232074085
O	-0.498455697	-4.351243993	-2.037235600
H	-0.964425168	-5.054928998	-1.557442387

TS_1-2

E=-3.397902679558 Ha

nimag=-492.5 cm⁻¹

Se	0.209868934	-0.831191729	-0.314237393
C	2.048828242	-0.275993796	-0.190775028
C	2.850603722	-0.087397909	-1.321860437
C	2.584204259	-0.117305144	1.093270591
C	4.183964145	0.282295556	-1.160307803
C	3.921537306	0.244455667	1.240134134
C	4.722939904	0.447937854	0.116427503
H	2.446560884	-0.231843065	-2.319466185
H	1.965643520	-0.266427314	1.974674563
H	4.804873255	0.435407534	-2.039337350
H	4.334957515	0.370331694	2.237467548
H	5.764907266	0.732465375	0.234735324
H	0.059729352	-0.436472965	-1.721716725
H	-0.129212845	-3.384714732	-0.265589899
O	0.040835765	-2.778658953	-1.020944589
O	-0.458922360	-4.736917069	-1.230238524
H	0.391840197	-4.954985732	-1.639828129

2

E = -2.962897703651 Ha

Se	0.410902342	-1.587061446	-0.805952953
O	0.280556898	-2.982095559	0.071393003
C	2.053089165	-0.682476101	-0.141820348
C	2.758404575	-1.287475625	0.890612546
C	2.503547938	0.486557001	-0.750665889
C	3.939284012	-0.691982976	1.339079326
C	3.683506212	1.075225423	-0.292890979
C	4.399564757	0.486329888	0.750766115
H	2.383168207	-2.208745269	1.328900660
H	1.952748454	0.943780508	-1.570616270
H	4.499638150	-1.152566907	2.149186027
H	4.044207925	1.990510683	-0.755807815
H	5.320547095	0.944952149	1.101522982
H	-0.459301728	-0.572798769	-0.060897404

TS_2-3

E=-2.913602921477 Ha

Nimag=-1340.6 cm⁻¹

Se	-0.184484367	1.760456992	0.001899629
C	-1.661836449	0.485285861	0.022151387
C	-2.973934504	0.950500138	0.069077437
C	-4.017425258	0.024300218	0.055091925
C	-3.747499038	-1.343756440	-0.001256385
C	-2.426915686	-1.794110914	-0.052993750
C	-1.374388861	-0.879470792	-0.049658601
H	-3.162918486	2.019598952	0.108599117
H	-5.045918498	0.375817023	0.088837357
H	-4.565181777	-2.059735769	-0.009866343
H	-2.213271056	-2.858910677	-0.103546330
H	-0.347194256	-1.234335811	-0.102021331
H	-0.470801551	2.575553263	1.246509283
O	-0.979762619	3.368983650	-0.021379096

3

E=-3.005492434296 Ha

Se	0.406377456	-1.819273685	0.464004844
C	2.031133400	-0.816568502	0.192709487
C	3.211941373	-1.546411823	0.009422696
C	2.065181352	0.579613770	0.215235306
C	4.424108186	-0.874680950	-0.139490785
C	3.282417750	1.239538250	0.045054679
C	4.464892829	0.520153691	-0.127567457
H	3.194133716	-2.633727973	-0.025586921
H	1.151544810	1.145622380	0.364344839
H	5.337746424	-1.447668863	-0.279034170
H	3.302929972	2.326912458	0.056816765
H	5.410055612	1.041073796	-0.254612478
O	-0.854305039	-0.518890074	0.219522271
H	-1.045859840	-0.525210477	-0.730001075

3_RC

E=-3.662832 Ha

Se	0.428621920	-0.854966254	1.127875139
C	2.243315122	-0.391048552	0.665920896
C	3.196075047	-0.399114014	1.692932210
C	2.616278544	-0.023382811	-0.629765226
C	4.512192496	-0.029295678	1.421466476
C	3.940671966	0.328333237	-0.891781864
C	4.892576922	0.331921348	0.128009249
H	2.921368809	-0.698079838	2.702501405
H	1.877490041	-0.008851280	-1.424490040
H	5.244779184	-0.035771061	2.225253508
H	4.224884401	0.611059024	-1.902999138
H	5.921262357	0.612147576	-0.082243936
O	-0.303755624	-1.094106428	-0.519833463
H	1.447576454	-4.149517981	-1.051926932
O	0.603788932	-3.935278537	-1.483532300
O	-0.229575980	-5.026991248	-0.988481247
H	-0.354169971	-5.530556120	-1.810067467
H	-0.129414620	-2.022791383	-0.751483270

TS_3-4

E=-3.635998994650 Ha

Nimag=-395.2 cm⁻¹

Se	0.546818248	-1.448001295	0.922772874
C	2.248997467	-0.666579277	0.522867730
C	3.166964365	-0.607472157	1.577978562
C	2.585128321	-0.209672053	-0.753075118
C	4.440218353	-0.093014325	1.344106301
C	3.858269626	0.313930885	-0.966518265
C	4.786882648	0.370390986	0.074313344
H	2.898182346	-0.952818247	2.573781488
H	1.866138694	-0.255169593	-1.563562590

H	5.157270044	-0.046737657	2.159529572
H	4.125993800	0.675602222	-1.956023288
H	5.778338610	0.778177284	-0.103140556
O	-0.493810784	-0.704934507	-0.333501253
H	0.171897606	-3.848677813	0.094731740
O	0.622157401	-3.103597825	-0.346548773
O	0.126733058	-4.668435845	-1.513172172
H	1.049482815	-4.870494225	-1.729469468
H	-0.586153531	-1.446515783	-0.965687178

4

E=-3.222157904542 Ha

Se	0.510335929	-1.720918756	-1.003650083
O	0.349622208	-3.007927285	-0.005550616
C	2.070412654	-0.760831449	-0.246160084
C	2.725339047	-1.299730009	0.857356110
C	2.517582733	0.409991329	-0.858703675
C	3.843107956	-0.639392799	1.369585044
C	3.637652879	1.060901636	-0.341391983
C	4.297944922	0.536824429	0.771628804
H	2.359023675	-2.221287153	1.301854518
H	2.000345792	0.821909249	-1.722524657
H	4.361447246	-1.047642873	2.233906755
H	3.993617351	1.976510311	-0.807164787
H	5.171747281	1.045481329	1.171074494
O	-0.771158952	-0.485723212	-0.525993652
H	-0.745424721	-0.421588748	0.443669810

4_RC

E=-3.882172 Ha

Se	1.569964184	-1.876969630	-1.231510426
C	2.810700685	-0.704727854	-0.261512948
C	2.892570532	-0.796173190	1.124153946
C	3.622805810	0.162637236	-0.990083136
C	3.801307935	0.019486527	1.797687854
C	4.528396091	0.974058137	-0.305699033
C	4.615267298	0.902128606	1.085101433
H	2.256304837	-1.496151058	1.658208087
H	3.554826656	0.217760570	-2.074340443
H	3.874564065	-0.035987826	2.880986117
H	5.164908001	1.659444938	-0.859478628
H	5.323244332	1.533892120	1.615571529
O	0.272182693	-0.574641102	-1.321081478
H	-0.785395904	-3.399978400	-0.661113539
O	-1.666796489	-3.279359632	-1.077411249
O	-1.539558019	-4.144891939	-2.247457098
H	-2.082797303	-4.898139450	-1.965193690
O	1.050798203	-2.953375050	-0.095295481
H	-0.526624608	-1.049068002	-1.616080818

TS_4-5

E=-3.830715949178 Ha

Nimag=-713.6 cm⁻¹

Se	0.538261101	-1.812789493	0.472955483
C	2.257744365	-0.861744649	0.367062082
C	2.958812348	-0.630043798	1.546230581
C	2.739126964	-0.489366285	-0.885609703
C	4.185224217	0.029635314	1.461779062
C	3.969279883	0.165212869	-0.947763714
C	4.686756482	0.424963497	0.220969887
H	2.555822515	-0.953231438	2.500745977
H	2.178109523	-0.704982380	-1.789843310
H	4.748053816	0.230606761	2.369682901
H	4.365882481	0.467627724	-1.913369146
H	5.645516795	0.933788121	0.163483074
O	-0.539960704	-0.367194821	0.286889369
H	0.336973651	-3.464220463	-1.598029340
O	0.045812807	-2.537780859	-1.376725547
O	-0.096090246	-3.483300422	-3.143029062

H	-1.062459260	-3.564414020	-3.114641730
O	0.386214962	-2.333432299	2.009437754
H	-1.178581700	-0.626233359	-0.400024620

5

E=-3.410197731545 Ha

Se	0.394116452	-1.430293628	-0.610670235
O	0.443240640	-3.020434426	-0.345819729
C	2.067513513	-0.628073149	-0.008627176
C	2.791317922	-1.272357723	0.990042777
C	2.490529697	0.555161749	-0.605984211
C	3.987510150	-0.691968708	1.411546109
C	3.691505976	1.117009094	-0.172013409
C	4.434039144	0.497317565	0.833777426
H	2.437980756	-2.204528458	1.418439878
H	1.906727664	1.017687151	-1.395103757
H	4.571237900	-1.175984253	2.190029815
H	4.045946950	2.038568938	-0.626154766
H	5.368922775	0.941079486	1.165992844
O	-0.043408024	-0.801616570	-2.039285680
O	-0.768467334	-0.754807570	0.601886019
H	-1.348104650	-0.177727877	0.074849756

Tellurium

1

E = -2.743343449954Ha

Te	0.226049552	-1.642575091	0.010903251
C	2.118533568	-0.663516395	-0.009235255
C	3.269845171	-1.457382532	-0.074551577
C	2.245076165	0.729032224	0.042858902
C	4.531256695	-0.862867721	-0.085327845
C	3.511208782	1.314668987	0.030749536
C	4.658656027	0.524799149	-0.032556897
H	3.197031024	-2.541390763	-0.118099484
H	1.366558798	1.365062051	0.093490078
H	5.416687996	-1.492310917	-0.135581235
H	3.595637463	2.398252378	0.071929050
H	5.642543870	0.986133682	-0.040768033
H	-0.634364112	-0.217282050	0.052199509

1_RC

E=-3.39950205 Ha

Te	0.152013469	-0.916011490	0.497305114
C	2.176987914	-0.272149902	0.229765003
C	2.847476359	-0.469921353	-0.981840804
C	2.845702326	0.314187158	1.308564587
C	4.175665887	-0.063641944	-1.113220965
C	4.181645115	0.697904759	1.174775992
C	4.847058814	0.515090584	-0.035951573
H	2.347102066	-0.941515941	-1.821958776
H	2.331173821	0.483932512	2.249837978
H	4.688149384	-0.213139073	-2.060566987
H	4.695459905	1.150402304	2.019581657
H	5.884805972	0.821128075	-0.140532823
H	-0.421273270	-0.047688943	-0.807182071
H	0.367491345	-3.333865767	-1.237520280
O	0.601239049	-4.039791385	-1.870394622
O	-0.724964955	-4.568708223	-2.180601101
H	-0.680288202	-5.420558372	-1.716882329

TS_1-2

E= -3.373245524200Ha

nimag=-342.3 cm⁻¹

Te	0.146183693	-1.005984863	-0.129754843
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C	2.156374232	-0.284106185	-0.066497979
C	2.949967301	-0.205795602	-1.216592602
C	2.691314412	0.063660662	1.180102746
C	4.266112081	0.243040742	-1.116560286
C	4.011317772	0.503847946	1.269786880
C	4.799871752	0.597061181	0.123132286
H	2.554420377	-0.492849964	-2.186475556
H	2.087198212	0.007493059	2.082466238
H	4.877030617	0.310186931	-2.013468918
H	4.420066564	0.777768288	2.239254644
H	5.827611166	0.942789202	0.195178704
H	-0.029185693	-0.571369602	-1.725572480
H	-0.117748603	-3.658224172	-0.266740772
O	-0.103485240	-3.011863337	-0.994944000
O	-0.754855805	-4.850187363	-1.528015628
H	-0.039033778	-4.954481649	-2.172890833

2

E = -2.936725056994Ha

Te	0.292417950	-1.652704017	-0.892512197
O	0.241236153	-3.155154991	0.141216057
C	2.088893888	-0.663421792	-0.174982317
C	2.783237488	-1.269598468	0.868489374
C	2.556079533	0.510927970	-0.765246408
C	3.957465733	-0.678340498	1.339413563
C	3.729956310	1.096437959	-0.287251273
C	4.428570069	0.502403632	0.764699291
H	2.406537245	-2.192301090	1.303975255
H	2.021988369	0.979284711	-1.590003199
H	4.503821992	-1.143495770	2.156630267
H	4.098565452	2.013835251	-0.739966097
H	5.343509991	0.959178677	1.133566350
H	-0.682416172	-0.544898574	-0.005219667

TS_2-3

E=-2.886468489537 Ha

Nimag=-1278.0 cm⁻¹

Te	-0.025447251	1.806186613	-0.026413130
C	-1.653669550	0.403718621	0.002960838
C	-2.959151791	0.892286406	0.062075308
C	-4.024720816	-0.008798862	0.054158043
C	-3.786476435	-1.382393746	-0.008537199
C	-2.477055419	-1.861663249	-0.070977463
C	-1.404563065	-0.969486378	-0.072007328
H	-3.133404121	1.964362953	0.107889949
H	-5.044657333	0.366181638	0.098120469
H	-4.620252556	-2.079825868	-0.012803109
H	-2.287772997	-2.931116316	-0.124464679
H	-0.388540429	-1.354690378	-0.131514416
H	-0.428126644	2.739885808	1.332089872
O	-0.984081866	3.499359867	-0.040604472

3

E=-2.984718254073Ha

Te	0.239287521	-1.745114540	0.857032829
C	2.059729831	-0.748207197	0.365719951
C	3.188707842	-1.503971136	0.026505441
C	2.151151196	0.648028779	0.421134467
C	4.403232522	-0.867296041	-0.235840121
C	3.358691704	1.277995530	0.124684644
C	4.489302954	0.523488732	-0.194505171
H	3.125821068	-2.586705776	-0.046693485
H	1.283865291	1.244267156	0.689091657
H	5.276824007	-1.462164445	-0.492261275
H	3.419274072	2.363374286	0.159047524
H	5.431950125	1.018880124	-0.412846863
O	-1.015500259	-0.573227168	-0.173264645
H	-1.030039872	-0.918866306	-1.076986952

3_RC

E=-3.64157092 Ha

Te	0.399047356	-1.027727816	1.243544528
C	2.370473138	-0.386335314	0.732044221
C	3.334704164	-0.302593265	1.743828382
C	2.704838008	-0.027863206	-0.576728436
C	4.622497835	0.141884106	1.445703988
C	3.999763599	0.404265390	-0.867255034
C	4.961749154	0.493927655	0.138774853
H	3.097617919	-0.585021939	-2.767923055
H	1.961639270	-0.082998725	-1.366360242
H	5.363519047	0.205425206	2.239367947
H	4.252698537	0.678430523	-1.889163245
H	5.967401824	0.835057609	-0.092616240
O	-0.321022559	-1.221198531	-0.597592530
H	1.075680153	-4.498155266	-0.705286219
O	0.523213425	-4.160339682	-1.429742510
O	-0.616187344	-5.068680374	-1.335915417
H	-0.495661136	-5.575969093	-2.155676452
H	-0.148006392	-2.138397278	-0.867496650

TS_3-4

E=-3.626646894443 Ha

Nimag=-162.6 cm⁻¹

Te	0.463308653	-1.576114597	1.238474161
C	2.327029998	-0.740924996	0.668775715
C	3.206898387	-0.349298826	1.684534705
C	2.687337038	-0.598424274	-0.674730316
C	4.457339978	0.171681847	1.352508988
C	3.931530993	-0.057884962	-0.994190607
C	4.819076190	0.321964413	0.014171794
H	2.926317282	-0.436257380	-2.731790230
H	2.012682974	-0.904530065	-1.467334432
H	5.141123264	0.472102391	2.142446439
H	4.210422838	0.059125230	-2.038547477
H	5.789432679	0.738197399	-0.243638223
O	-0.702391034	-0.740280388	-0.100093708
H	0.208632993	-3.969563127	0.036909089
O	0.523229673	-3.166720246	-0.405046814
O	0.192754322	-4.189815666	-1.983325766
H	1.129332303	-4.211933302	-2.232244881
H	-0.774320057	-1.428054194	-0.788118937

4

E=-3.206808658600Ha

Te	0.469815945	-1.785938322	-1.099716866
O	0.328180305	-3.142610090	0.093371324
C	2.175807783	-0.738575388	-0.280365816
C	2.811041932	-1.271535972	0.841293874
C	2.644310807	0.433538130	-0.879120182
C	3.920043243	-0.614432379	1.376231085
C	3.754107989	1.084460013	-0.339120160
C	4.390182613	0.560307566	0.787348580
H	2.435219648	-2.188628378	1.288531131
H	2.152070939	0.852122308	-1.754863603
H	4.418234723	-1.022250959	2.252698724
H	4.120920520	1.999554573	-0.797798646
H	5.255889571	1.068102009	1.205317382
O	-0.906564887	-0.468059482	-0.517733275
H	-0.952578652	-0.504043514	0.451832974

4_RC

E=-3.86974381 Ha

Te	2.308028097	-2.285696479	-2.103727681
C	3.042374921	-0.909740366	-0.610172742
C	2.960503338	-1.259885386	0.737491306
C	3.612724798	0.304100021	-1.001757206
C	3.444308053	-0.376594913	1.703584188
C	4.092453593	1.182216540	-0.029687725

C	4.007945953	0.841104732	1.320987043
H	2.517716977	-2.209420455	1.026202326
H	3.678013410	0.581928969	-2.051872735
H	3.379263393	-0.640853859	2.756388598
H	4.530287346	2.131746561	-0.327688289
H	4.383676518	1.526348306	2.076732389
O	0.755297564	-1.219314829	-2.683825395
H	-0.161538945	-3.105723112	-0.569264305
O	-0.938083486	-2.510206414	-0.431692810
O	-2.015148590	-3.278868951	-1.048514024
H	-2.484904311	-3.580697351	-0.254446951
O	1.580912364	-3.567004780	-1.025461426
H	0.042838007	-1.363493236	-2.027823563

TS_4-5

E=-3.822205531589 Ha

Nimag=-578.3 cm⁻¹

Te	0.427121316	-1.982984871	0.661722370
C	2.286271015	-0.933471304	0.410522970
C	2.999410701	-0.579756185	1.555834346
C	2.751083496	-0.641508349	-0.872494082
C	4.205598675	0.104851868	1.405468870
C	3.960132260	0.042914009	-1.003100595
C	4.682820677	0.414579231	0.131236240
H	2.620738843	-0.829915574	2.542543266
H	2.191461462	-0.934803808	-1.756029710
H	4.771463221	0.393792607	2.287593826
H	4.335192751	0.282150551	-1.994880168

H	5.624984196	0.945481167	0.021321796
O	-0.810527996	-0.479175040	0.422660693
H	0.470345131	-3.396079612	-1.694345939
O	-0.032046589	-2.625972642	-1.334968660
O	0.077562087	-3.123578622	-3.301420923
H	-0.861346046	-3.362121773	-3.360243089
O	0.312973213	-2.285098646	2.447050092
H	-1.165337309	-0.540602546	-0.479708762

5

E=-3.385065933847Ha

Te	0.359933279	-1.503801925	-0.647016197
O	0.376442647	-3.253797486	-0.233367762
C	2.192266624	-0.617566422	0.010016994
C	2.955687873	-1.294104979	0.959678742
C	2.585030598	0.603382048	-0.535892125
C	4.151169217	-0.712092786	1.383346348
C	3.784668442	1.167099252	-0.100648202
C	4.561511531	0.512717409	0.856246939
H	2.634399597	-2.252796768	1.355454253
H	1.981357132	1.102322516	-1.288143969
H	4.761460290	-1.221860080	2.124306481
H	4.110926981	2.117760578	-0.514356648
H	5.495073464	0.958373516	1.189855522
O	-0.116284475	-0.881830509	-2.271080058
O	-0.884137091	-0.639934148	0.607424543
H	-1.576691849	-0.227625436	0.063798916

Table S6 Reaction energies (in kcal mol⁻¹) for the anionic pathway in the gas phase. Level of theory COSMO-ZORA-OLYP/TZ2P.

Sulphur

1a

E = -2.729529436735 Ha

C	-0.231854987	-0.000003271	-3.641024045
C	-1.380431278	-0.352154339	-2.872302878
C	0.916719991	0.352152081	-2.872302858
H	-2.283739466	-0.630203767	-3.410988591
H	1.820028028	0.630202042	-3.410988565
C	-1.378574840	-0.351235522	-1.481182111
C	0.914863026	0.351235070	-1.481182077
H	-2.289368220	-0.631050323	-0.948547241
H	1.825655711	0.631052144	-0.948547198
C	-0.231856005	0.000000070	-0.756491049
H	-0.231856208	0.000000742	0.331871791
S	-0.231857246	0.000003930	-5.371923858

1a_RC

E= -3.40547422 Ha

O	2.267109000	0.014276000	0.611405000
H	1.307094000	0.268394000	0.648003000
S	-0.888300000	-0.217630000	0.087706000
O	2.161252000	-1.152606000	-0.288111000
H	1.180581000	-1.139294000	-0.443542000
C	-1.366563000	0.830011000	-1.224340000
C	-0.437043000	1.478606000	-2.077292000

C	-2.736392000	1.081568000	-1.495529000
C	-0.848684000	2.310075000	-3.115289000
C	-3.143114000	1.913780000	-2.534510000
C	-2.206106000	2.542035000	-3.361709000
H	0.623904000	1.316777000	-1.909360000
H	-3.480729000	0.602238000	-0.864062000
H	-0.095180000	2.785876000	-3.743545000
H	-4.208647000	2.074719000	-2.701758000
H	-2.524050000	3.192658000	-4.173875000

TS_1a-3a

E= -3.385945871463 Ha

nimag=-178.8 cm⁻¹

O	3.132650352	-0.208327213	0.326337564
H	3.211081937	-1.158177236	0.487042356
S	-1.072198076	-0.361065524	-0.044181857
O	1.391425231	-0.352842865	0.003930046
H	1.161680735	0.216872957	0.749819949
C	-1.481572917	0.750095041	-1.323509659
C	-0.498529123	1.414842213	-2.097529067
C	-2.834566098	1.024667392	-1.647730277
C	-0.851420092	2.292691727	-3.118215315
C	-3.177857798	1.904261513	-2.670722662
C	-2.192333818	2.553325023	-3.421387276
H	0.545406109	1.218528093	-1.874772401
H	-3.617371775	0.531190164	-1.076049719
H	-0.062574865	2.782488834	-3.689699630

H	-4.231609971	2.085895768	-2.884348712
H	-2.461728449	3.241620975	-4.219982048

3a

E=-2.945059505986 Ha

S	0.158076283	-0.579685415	0.054856913
O	1.060586741	0.166241146	-0.960852344
C	0.488557570	-2.285387446	0.019269895

C	-0.218710023	-3.181390950	0.868558186
C	1.464923545	-2.846594726	-0.847401854
C	0.036373868	-4.543285480	0.848336841
C	1.707709620	-4.215524265	-0.854211466
C	1.005840288	-5.091312154	-0.014078822
H	-0.975254164	-2.786345440	1.547122487
H	2.011274020	-2.171687932	-1.500369332
H	-0.526893032	-5.198534121	1.514601480
H	2.464669095	-4.614126963	-1.532268278
H	1.202424262	-6.161094661	-0.026366195

3a_RC

E=-3.62373471 Ha

O	0.829509000	-0.158730000	1.847906000
H	0.183038000	-0.511339000	1.139248000
S	-0.472327000	-0.794813000	-1.463576000
O	2.017623000	-0.992071000	1.632109000
H	2.372197000	-0.582611000	0.827244000
C	-1.164388000	0.672622000	-2.109443000
C	-0.940267000	1.025377000	-3.464111000
C	-1.966064000	1.537434000	-1.328714000
C	-1.487685000	2.181557000	-4.001489000
C	-2.507922000	2.693343000	-1.882542000
C	-2.281655000	3.036990000	-3.220162000
H	-0.328031000	0.377973000	-4.091330000
H	-2.144167000	1.274156000	-0.290504000
H	-1.295307000	2.424754000	-5.046762000
H	-3.120522000	3.342480000	-1.255985000
H	-2.708225000	3.942810000	-3.644977000
O	-0.907273000	-0.943025000	0.037951000

TS_3a-4a

E=-3.605933819583 Ha
Nimag=-124.3 cm⁻¹

O	2.570902740	0.034881256	1.503978175
H	2.839294807	-0.888247012	1.613429185
S	-0.968469753	-0.932268968	-0.982026202
O	1.461712644	-0.296818209	0.301917057
H	0.666156539	-0.171500496	0.839672700
C	-1.331664312	0.579636170	-1.806336873
C	-0.525796443	1.017454110	-2.881769364
C	-2.438501481	1.371951650	-1.434756347
C	-0.824206906	2.191439205	-3.558726756
C	-2.725736175	2.548714829	-2.121708441
C	-1.930200266	2.974593623	-3.190010118
H	0.343791628	0.430398984	-3.172470753
H	-3.053629584	1.036056091	-0.604794156
H	-0.184791239	2.510148614	-4.381736468
H	-3.585707349	3.146138199	-1.817567899
H	-2.158322932	3.895955814	-3.721379470
O	-1.993291729	-1.139150722	0.148046430

4a

E=-3.197528379950 Ha

S	0.077432245	-0.389096575	0.037728131
O	0.379602704	0.021298717	-1.382064673
C	0.389079433	-2.264324092	-0.022074292
C	-0.281056016	-3.119869862	0.855068757
C	1.372782402	-2.791709786	-0.861306094
C	0.027795500	-4.481367511	0.898226267

C	1.687129608	-4.152300187	-0.824024944
C	1.018315778	-5.003044259	0.060827768
H	-1.066015316	-2.706692260	1.486221461
H	1.871193533	-2.123835242	-1.561846063
H	-0.510242290	-5.142778162	-1.578811502
H	2.448974801	-4.555826610	-1.492578674
H	1.261317680	-6.064151992	0.092379237
O	-1.383578228	-0.328366024	0.408092443

4a_RC

E=-3.87244276 Ha

O	2.952845000	-0.761859000	1.579265000
H	3.286840000	-0.561511000	0.690532000
S	0.058820000	0.315080000	-1.005262000
O	-0.127653000	-0.495809000	0.275784000
O	1.986776000	-1.817344000	1.266696000
H	1.202367000	-1.284184000	0.922930000
O	-0.906202000	-0.064509000	-2.091534000
C	-0.592881000	1.993583000	-0.452624000
C	-0.059977000	2.615163000	0.679132000
C	-1.551258000	2.661530000	-1.213306000
C	-0.485098000	3.892080000	1.048946000
C	-1.983188000	3.937989000	-0.843914000
C	-1.448534000	4.559452000	0.286582000
H	0.676530000	2.087948000	1.282386000
H	-1.960192000	2.154418000	-2.084711000
H	-0.071709000	4.366886000	1.938595000
H	-2.740678000	4.450315000	-1.437561000
H	-1.781017000	5.555421000	0.574571000

TS_4a-5a

E=-3.854588192889 Ha
Nimag=-136.4 cm⁻¹

O	2.020291896	-0.310519824	0.167628656
H	1.706919483	-0.877741677	-0.551031525
S	-0.588673459	-0.059590935	0.132069980
O	-1.307899017	-0.472749257	1.376127325
O	3.653233498	-0.680747724	-0.042707638
H	3.723489700	-1.144510950	0.803336058
O	-1.191839595	-0.525346255	-1.158928152
C	-0.842460876	1.791051741	0.085687235
C	-0.830783307	2.525233365	1.272631367
C	-0.959205443	2.454433437	-1.135817405
C	-0.938834242	3.916230982	1.238290035
C	-1.069396483	3.845929609	-1.171293081
C	-1.056600726	4.581865342	0.015522328
H	-0.752521641	1.997084145	2.219459387
H	-0.978291223	1.867991679	-2.050739478
H	-0.935951673	4.484234029	2.168142585
H	-1.168549724	4.358594587	-2.127726803
H	-1.139095949	5.666982905	-0.011594009

5

E=-3.474114245460 Ha

S	-0.175224766	0.004237785	-0.000790817
O	-0.555287781	-0.898959253	-1.098324288
O	-0.553648255	-0.469858189	1.339652496
O	-0.479294789	1.423936750	-0.250499683
C	1.656132637	-0.026127882	0.003258418
C	2.367676413	0.194316759	1.186785639
C	2.366120054	-0.228884960	-1.184348530
C	3.762823998	0.219562039	1.182035018
C	3.761303590	-0.204036163	-1.190366139
C	4.468098785	0.022104634	-0.007181283
H	1.813444573	0.333713642	2.110168204
H	1.810612785	-0.417304680	-2.098211708
H	4.303433809	0.389308634	2.112642124
H	4.300741480	-0.366920978	-2.122882431
H	5.556652434	0.038721169	-0.010829613

Selenium

1a

E = -2.699207671002 Ha

C	-0.231841018	-0.000052472	-3.616961428
C	-1.380134529	-0.351936502	-2.861353372
C	0.916445339	0.351855665	-2.861353557
H	-2.283558830	-0.630120217	-3.399105926
H	1.819892782	0.629959947	-3.399108359
C	-1.379442390	-0.351475588	-1.468786998
C	0.915737118	0.351452225	-1.468787474
H	-2.289518895	-0.631331413	-0.935675193
H	1.825808788	0.631325492	-0.935676588
C	-0.231866292	0.000033039	-0.746968635
H	-0.231887605	0.000103154	0.341443671
Se	-0.231905963	0.000185524	-5.511274822

1a_RC

E = -3.37431729 Ha

O	2.359776000	0.027815000	0.603404000
H	1.394897000	0.247361000	0.686978000
Se	-0.943370000	-0.315950000	0.198764000
O	2.264014000	-1.133899000	-0.303818000
H	1.278927000	-1.165391000	-0.422413000
C	-1.430669000	0.837485000	-1.239079000
C	-0.477196000	1.464445000	-2.072203000
C	-2.789717000	1.105406000	-1.518927000
C	-0.861727000	2.303698000	-3.116054000
C	-3.171084000	1.945080000	-2.563313000
C	-2.212253000	2.556532000	-3.377157000
H	0.578782000	1.285413000	-1.891797000
H	-3.551058000	0.639423000	-0.898009000
H	-0.093493000	2.767372000	-3.735099000
H	-4.231285000	2.124209000	-2.744091000
H	-2.509415000	3.212484000	-4.192994000

TS_1a-3a

E = -3.358110058333 Ha

nimag = -173.0 cm⁻¹

O	3.224077844	-0.170801538	0.384982075
H	3.355793767	-1.086127138	0.667261585
Se	-1.112769424	-0.514888605	-0.004784187
O	1.557621160	-0.429552546	0.022929286
H	1.215947278	0.165352222	0.706418916
C	-1.546490245	0.736577723	-1.373070860
C	-0.546952107	1.373881520	-2.140226879
C	-2.889182939	1.058206208	-1.671614810
C	-0.877309929	2.280852886	-3.144688908
C	-3.213151780	1.965773612	-2.678293715
C	-2.211842985	2.590248186	-3.428440739
H	0.493223675	1.140802846	-1.933364914
H	-3.683603991	0.584814444	-1.099144227
H	-0.078179119	2.753010229	-3.716438933
H	-4.261549213	2.188510458	-2.878452000
H	-2.465150609	3.299406354	-4.214070398

3a

E = -2.899032455911 Ha

Se	0.114491293	-0.437105622	0.066917570
O	1.178316596	0.253650814	-1.089908454
C	0.466840268	-2.321284083	0.046821472
C	-0.229155168	-3.219759220	0.886719786
C	1.443611385	-2.850891340	-0.824330292
C	0.037912920	-4.583266553	0.853903378
C	1.703855790	-4.217817778	-0.849631069
C	1.009568863	-5.106059023	-0.016839025
H	-0.988264936	-2.841240915	1.572523969

H	1.977937072	-2.155436684	-1.468264921
H	-0.515469620	-5.252884270	1.513742821
H	2.463346619	-4.602703600	-1.532246767
H	1.216586994	-6.173930136	-0.042210960

3a_RC

E = -3.58078768 Ha

O	0.809778000	-0.157223000	1.916653000
H	0.162886000	-0.535380000	1.203669000
Se	-0.395068000	-0.937648000	-1.492824000
O	2.022179000	-0.958760000	1.706453000
H	2.346511000	-0.566885000	0.880483000
C	-1.155870000	0.683583000	-2.188595000
C	-0.970503000	1.046600000	-3.537675000
C	-1.921332000	1.529554000	-1.366172000
C	-1.529844000	2.215776000	-4.043047000
C	-2.477257000	2.698269000	-1.881170000
C	-2.291198000	3.057933000	-3.220571000
H	-0.382678000	0.407437000	-4.196604000
H	-2.063508000	1.245165000	-0.326678000
H	-1.371909000	2.475832000	-5.089795000
H	-3.065513000	3.341383000	-1.226255000
H	-2.727403000	3.972305000	-3.616918000
O	-0.910736000	-0.991032000	0.163909000

TS_3a-4a

E = -3.561617526417 Ha

Nimag = -139.3 cm⁻¹

O	2.768354888	0.093093496	1.157144685
H	2.715959346	-0.498723643	1.921302633
Se	-1.149337581	-1.189281812	-0.907140478
O	1.560837801	-0.636612620	0.323304250
H	0.854646892	0.015074553	0.460373877
C	-1.413391296	0.520046860	-1.784775331
C	-0.507431174	1.000834994	-2.748035300
C	-2.543145026	1.294054703	-1.471771977
C	-0.732255613	2.218176627	-3.383672232
C	-2.759846718	2.513004002	-2.111744786
C	-1.862286284	2.988012805	-3.073655824
H	0.382938970	0.423405078	-2.992688750
H	-3.232791834	0.912207144	-0.722061330
H	-0.017430308	2.576314972	-4.124206965
H	-3.641080537	3.102496400	-1.857139262
H	-2.034414998	3.940592540	-3.570450456
O	-2.461208137	-1.321669620	0.170071371

4a

E = -3.130690814599 Ha

Se	0.099763155	-0.243899208	0.015855793
O	0.114503851	0.074044665	-1.630688955
C	0.470946585	-2.283899886	0.000376687
C	-0.252297533	-3.124755141	0.844141369
C	1.458656290	-2.822480830	-0.823976995
C	0.010906069	-4.497657970	0.869408039
C	1.728316179	-4.193928120	-0.802158712
C	1.006112860	-5.035495201	0.048883255
H	-1.040289545	-2.689972818	1.457970718
H	1.999869297	-2.167767367	-1.506170255
H	-0.564162686	-5.153214793	1.524649983
H	2.495612140	-4.611262016	-1.455291122
H	1.212863915	-6.104549591	0.066367805
O	-1.448068744	-0.247225568	0.664093216

4a_RC

E = -3.80717945 Ha

O	3.019345000	-0.853306000	1.651712000
H	3.466304000	-0.738470000	0.798840000
Se	0.098890000	0.257809000	-1.114791000
O	-0.058800000	-0.601238000	0.342098000

O	2.045145000	-1.889416000	1.298804000
H	1.265722000	-1.339857000	0.941663000
O	-1.099442000	-0.154448000	-2.200694000
C	-0.587038000	2.078660000	-0.488222000
C	-0.064252000	2.682595000	0.655116000
C	-1.561467000	2.733126000	-1.237306000
C	-0.516983000	3.944508000	1.048638000
C	-2.017989000	3.994290000	-0.844275000
C	-1.493617000	4.604331000	0.297656000
H	0.678124000	2.157332000	1.253257000
H	-1.968085000	2.229110000	-2.112488000
H	-0.114668000	4.411221000	1.947426000
H	-2.787406000	4.501701000	-1.426272000
H	-1.847990000	5.586700000	0.605346000

TS_4a-5a

E= -3.780861681707 Ha

Nimag=-136.1 cm⁻¹

O	1.820703197	-0.383073919	0.112215087
H	1.776918177	-1.017148234	-0.618472315
Se	-0.550746406	-0.185316459	0.083085996
O	-1.336237383	-0.605196549	1.485102362
O	3.653256214	-0.574320127	0.044704472
H	3.661898650	-0.908018657	0.952509585
O	-1.332552986	-0.641740825	-1.314493241
C	-0.779973056	1.826029956	0.063580473
C	-0.748986564	2.537186273	1.260282218
C	-0.944894216	2.487375559	-1.150000501
C	-0.884386817	3.927218060	1.241430004
C	-1.082409696	3.877491911	-1.166385958
C	-1.049338034	4.599616158	0.028404982
H	-0.639023617	2.001515943	2.199911184
H	-0.983506553	1.908971390	-2.069818949
H	-0.864859698	4.486769660	2.175747094
H	-1.218085538	4.398142180	-2.113527180
H	-1.153944457	5.682922879	0.014781552

5

E= -3.346707202265 Ha

Se	-0.281913953	0.005843783	-0.000724883
O	-0.684385466	-1.010477648	-1.231687765
O	-0.681962617	-0.528205882	1.504174463
O	-0.648042021	1.586613300	-0.279185141
C	1.720156699	-0.017147437	0.001336521
C	2.414563481	0.200008836	1.190154703
C	2.413245884	-0.224908122	-1.189964995
C	3.811003551	0.218310992	1.184721542
C	3.809744050	-0.206242981	-1.192574463
C	4.512291247	0.017621927	-0.006362861
H	1.857124285	0.339804471	2.112232517
H	1.854888881	-0.412619419	-2.102954660
H	4.354108630	0.385509775	2.114070932
H	4.351981460	-0.371097269	-2.122865332
H	5.600780858	0.030794980	-0.009263170

Tellurium

1a

E = -2.671973496621 Ha

C	-0.231861140	0.000018462	-3.591537643
C	-1.379135936	-0.351432549	-2.844613523
C	0.915422844	0.351439657	-2.844613900
H	-2.284500036	-0.630396027	-3.378156818
H	1.820790420	0.630391689	-3.378157423
C	-1.380034635	-0.351468084	-1.450582115
C	0.916322168	0.351469891	-1.450582008
H	-2.289321403	-0.631380420	-0.917011177
H	1.825611089	0.631373383	-0.917010153

C	-0.231856005	-0.000000255	-0.732375399
H	-0.231855156	-0.000004547	0.356107779
Te	-0.231853703	-0.000012344	-5.715076301

1a_RC

E= -3.34459533 Ha

O	2.487085000	0.001236000	0.761408000
H	1.515414000	0.178474000	0.837650000
Te	-1.025139000	-0.529682000	0.268150000
O	2.478570000	-1.042276000	-0.282728000
H	1.502049000	-1.180839000	-0.381940000
C	-1.527392000	0.816401000	-1.304730000
C	-0.550362000	1.402793000	-2.134086000
C	-2.870875000	1.157879000	-1.559931000
C	-0.899311000	2.280648000	-3.160056000
C	-3.219480000	2.035473000	-2.586146000
C	-2.237112000	2.607682000	-3.398945000
H	0.497311000	1.166262000	-1.972034000
H	-3.653112000	0.725971000	-0.940536000
H	-0.114712000	2.713999000	-3.780156000
H	-4.270071000	2.274652000	-2.751710000
H	-2.507731000	3.292811000	-4.200019000

TS_1a-3a

E= -3.331558182171 Ha

nimag=-174.8 cm⁻¹

O	3.326260921	-0.114792216	0.348256869
H	3.533161323	-0.995360910	0.690553595
Te	-1.227469186	-0.621549052	0.195606568
O	1.706386470	-0.481956451	0.066483163
H	1.319869961	0.104893815	0.736483161
C	-1.645973505	0.756907226	-1.369898171
C	-0.610950700	1.338520254	-2.128520923
C	-2.968297530	1.117552516	-1.696671865
C	-0.888626270	2.237102282	-3.158067269
C	-3.243136197	2.015289020	-2.728119023
C	-2.205835338	2.586666904	-3.470264101
H	0.418792585	1.076989141	-1.903142048
H	-3.792246859	0.687697068	-1.131925386
H	-0.063335962	2.668789079	-3.724256218
H	-4.278725676	2.271105550	-2.953023956
H	-2.419392656	3.288212636	-4.274493103

3a

E= -2.874311906285 Ha

Te	0.070133820	-0.245356933	0.091370525
O	1.279108699	0.374999250	-1.215227030
C	0.443472563	-2.353957129	0.076094971
C	-0.239560450	-3.267525920	0.902951301
C	1.420689862	-2.861954337	-0.801534057
C	0.042203800	-4.630279727	0.856775105
C	1.700293900	-4.226086481	-0.845187930
C	1.018062991	-5.128216291	-0.019369915
H	-1.003886500	-2.909947962	1.594033876
H	1.949839262	-2.158387897	-1.442762419
H	-0.502433149	-5.314272722	1.508829430
H	2.462554808	-4.594550645	-1.533303698
H	1.239098469	-6.193191615	-0.055472650

3a_RC

E= -3.55649511 Ha

O	0.789609000	-0.179259000	2.029065000
H	0.159394000	-0.589177000	1.315246000
Te	-0.313811000	-1.131687000	-1.537734000
O	2.040337000	-0.917850000	1.812480000
H	2.334956000	-0.518616000	0.978724000
C	-1.158117000	0.687102000	-2.288217000
C	-1.025160000	1.073717000	-3.633596000
C	-1.876073000	1.526414000	-1.420833000

C	-1.588525000	2.261186000	-4.095763000
C	-2.437899000	2.713988000	-1.887072000
C	-2.301264000	3.094921000	-3.225776000
H	-0.475489000	0.443125000	-4.332518000
H	-1.983091000	1.230515000	-0.379405000
H	-1.471449000	2.539887000	-5.143000000
H	-2.988690000	3.352250000	-1.196142000
H	-2.740281000	4.023008000	-3.586043000
O	-0.885913000	-1.082615000	0.275446000

TS_3a-4a

E= -3.537318678698 Ha

Nimag=-148.9 cm⁻¹

O	2.949951203	-0.010922623	1.371279236
H	2.909474811	-0.665517167	2.083353149
Te	-1.099397579	-1.256701599	-0.869370283
O	1.812046127	-0.705276908	0.450288206
H	1.057210944	-0.117267029	0.626647115
C	-1.419791842	0.609153180	-1.899064524
C	-0.564371454	1.079430845	-2.908807199
C	-2.538480836	1.381743992	-1.551658769
C	-0.823904678	2.285608737	-3.556980697
C	-2.794624954	2.589059678	-2.201047499
C	-1.943273856	3.051395280	-3.209391476
H	0.317542816	0.504921441	-3.190213196
H	-3.196058096	1.015366567	-0.764861305
H	-0.146638359	2.634590935	-4.336219550
H	-3.667687093	3.177323580	-1.917584562
H	-2.144617626	3.993846333	-3.714828754
O	-2.545839338	-1.257372104	0.322220809

4a

E= -3.111872453195 Ha

Te	0.390889723	0.064726139	0.272995338
O	0.659462515	0.408043248	-1.525877958
C	0.610179113	-2.169937557	0.172847903
C	0.284890559	-2.997691904	1.249958136
C	1.090647690	-2.747662132	-1.003691772
C	0.441305368	-4.383804151	1.158422509
C	1.247471966	-4.133051636	-1.103848664
C	0.926707429	-4.955162965	-0.020635965
H	-0.113381731	-2.564526390	2.167678794
H	1.320230202	-2.094295646	-1.845200911
H	0.178898494	-5.020568071	2.003679905
H	1.617212106	-4.575466824	-2.029471152
H	1.049239803	-6.034599568	-0.095477528
O	-1.407060320	0.179988287	0.689209046

4a_RC

E= -3.78893977 Ha

O	2.255160000	-0.221791000	2.490253000
H	2.771433000	-0.961781000	2.134639000
Te	0.459282000	0.279420000	-1.234362000
O	-0.007417000	-0.858376000	0.171132000
O	0.938128000	-0.850825000	2.609188000

H	0.589834000	-0.785415000	1.648323000
O	-0.689084000	-0.049515000	-2.635677000
C	-0.469606000	2.165465000	-0.499020000
C	-0.020366000	2.807683000	0.657772000
C	-1.522061000	2.720189000	-1.227927000
C	-0.618199000	3.997995000	1.080794000
C	-2.124029000	3.908614000	-0.805659000
C	-1.670370000	4.552030000	0.348136000
H	0.786145000	2.376777000	1.248417000
H	-1.869409000	2.200300000	-2.120009000
H	-0.267476000	4.489552000	1.987653000
H	-2.950365000	4.333735000	-1.375325000
H	-2.136915000	5.478824000	0.678088000

TS_4a-5a

E= -3.76219694 Ha

Nimag=-135.8 cm⁻¹

O	1.968898000	-0.474709000	-0.041750000
H	1.925035000	-1.439845000	0.032649000
Te	-0.666663000	-0.373582000	0.115759000
O	-1.443618000	-0.691071000	1.756083000
O	3.711573000	-0.487648000	-0.068764000
H	3.774031000	0.022327000	0.751459000
O	-1.789305000	-0.793141000	-1.283850000
C	-0.798075000	1.834100000	0.070368000
C	-0.850025000	2.547397000	1.268171000
C	-0.846614000	2.516922000	-1.145549000
C	-0.943262000	3.941565000	1.250845000
C	-0.939771000	3.910736000	-1.164249000
C	-0.985131000	4.625818000	0.034426000
H	-0.839818000	2.006254000	2.212094000
H	-0.831669000	1.959257000	-2.079645000
H	-0.989009000	4.494893000	2.188269000
H	-0.982014000	4.439615000	-2.115679000
H	-1.057708000	5.711866000	0.020185000

5

E= -3.320303021669 Ha

Te	-0.419986954	0.007812193	-0.001969984
O	-0.833282619	-1.125993338	-1.374008189
O	-0.832002223	-0.586714708	1.676069230
O	-0.852600339	1.755428994	-0.310329348
C	1.773500528	-0.007575887	0.000459706
C	2.472042864	0.205218041	1.189614083
C	2.470020024	-0.219516008	-1.189956482
C	3.868897618	0.215978086	1.185486720
C	3.866831388	-0.208606256	-1.192273837
C	4.568527223	0.011414856	-0.005394234
H	1.923905218	0.348601170	2.117532249
H	1.919988173	-0.405646425	-2.109105053
H	4.412328074	0.380558454	2.114922144
H	4.408458562	-0.375984768	-2.122240611
H	5.656957431	0.018834901	-0.007698987

Table S7 Reaction energies (in kcal mol⁻¹) for the anionic pathway in water. Level of theory COSMO-ZORA-OLYP/TZ2P.

Sulphur

1a

E = -2.729529436735 Ha

C	-0.231854987	-0.000003271	-3.641024045
C	-1.380431278	-0.352154339	-2.872302878
C	0.916719991	0.352152081	-2.872302858
H	-2.283739466	-0.630203767	-3.410988591

H	1.820028028	0.630202042	-3.410988565
C	-1.378574840	-0.351235522	-1.481182111
C	0.914863026	0.351235070	-1.481182077
H	-2.289368220	-0.631050323	-0.948547241
H	1.825655711	0.631052144	-0.948547198
C	-0.231856005	0.000000070	-0.756491049
H	-0.231856208	0.000000742	0.331871791
S	-0.231857246	0.000003930	-5.371923858

1a_RC

E= -3.48703257 Ha
 O 2.270749000 -0.045995000 0.579404000
 H 1.325890000 0.270744000 0.619661000
 S -0.839549000 -0.146787000 0.133902000
 O 2.089563000 -1.216053000 -0.300370000
 H 1.104102000 -1.161230000 -0.437924000
 C -1.346477000 0.877136000 -1.213612000
 C -0.421862000 1.533266000 -2.055186000
 C -2.717996000 1.073584000 -1.488856000
 C -0.847354000 2.338307000 -3.111876000
 C -3.139034000 1.879868000 -2.545774000
 C -2.208762000 2.520544000 -3.368759000
 H 0.642546000 1.410234000 -1.876415000
 H -3.458984000 0.584188000 -0.861495000
 H -0.105019000 2.827951000 -3.739490000
 H -4.204786000 2.007091000 -2.726390000
 H -2.537894000 3.148637000 -4.192627000

TS_1a-3a

E= -3.47529516 Ha
 nimag=-332.6 cm⁻¹
 O 3.132650352 -0.208327213 0.326337564
 O 2.046047000 0.366320000 1.797461000
 H 2.530382000 -0.456605000 1.963917000
 S -0.262777000 -1.048190000 -1.488415000
 O 1.266918000 -0.185758000 0.355970000
 H 0.396236000 -0.327154000 0.757215000
 C -1.012680000 0.414426000 -2.114026000
 C -0.612346000 0.969733000 -3.349813000
 C -2.046107000 1.073563000 -1.411704000
 C -1.219970000 2.117021000 -3.858195000
 C -2.246416000 2.224202000 -1.920130000
 C -2.240370000 2.755147000 -3.147864000
 H 0.182505000 0.487621000 -3.913197000
 H -2.378445000 0.670610000 -0.458485000
 H -0.891038000 2.516299000 -4.815547000
 H -3.439923000 2.707890000 -1.353921000
 H -2.711516000 3.650976000 -3.544266000

3a

E= -3.03767596 Ha
 S -0.529895000 -0.940955000 -1.614012000
 C -1.186326000 0.590902000 -2.162851000
 C -1.007580000 0.972834000 -3.514326000
 C -1.890484000 1.464937000 -1.308534000
 C -1.515292000 2.178006000 -3.982044000
 C -2.394976000 2.672887000 -1.793413000
 C -2.216512000 3.044778000 -3.128224000
 H -0.467254000 0.316693000 -4.194859000
 H -2.034642000 1.185364000 -0.269000000
 H -1.364331000 2.448336000 -5.025614000
 H -2.935667000 3.331668000 -1.115587000
 H -2.611764000 3.986285000 -3.500264000
 O -0.870303000 -1.120571000 -0.080153000

3a_RC

E= -3.71094086 Ha
 O 0.681082000 0.067403000 1.578740000
 H 0.108665000 -0.438551000 0.878125000
 S -0.517167000 -0.940779000 -1.623128000
 O 1.834098000 -0.818201000 1.760309000
 H 2.479713000 -0.414908000 1.156569000
 C -1.188132000 0.594516000 -2.163467000
 C -1.009602000 0.971005000 -3.513315000
 C -1.892034000 1.463183000 -1.308956000
 C -1.516304000 2.177768000 -3.981565000
 C -2.395530000 2.671945000 -1.793222000
 C -2.214355000 3.043125000 -3.127134000

H -0.469978000 0.314172000 -4.193190000
 H -2.037584000 1.185274000 -0.269783000
 H -1.365547000 2.448072000 -5.024848000
 H -2.935340000 3.330765000 -1.115314000
 H -2.606863000 3.986207000 -3.498027000
 O -0.876590000 -1.114089000 -0.076932000

TS_3a-4a

E= -3.69752234 Ha
 Nimag=-358.6 cm⁻¹
 O 2.549337000 0.211946000 0.978475000
 H 2.281421000 0.035735000 1.894653000
 S -1.114105000 -1.178562000 -1.116329000
 O 1.308518000 -0.542615000 0.245519000
 H 0.776186000 0.234271000 0.014022000
 C -1.372905000 0.430901000 -1.800561000
 C -0.537054000 0.868612000 -2.850523000
 C -2.394311000 1.283507000 -1.344278000
 C -0.720373000 2.124963000 -3.416413000
 C -2.567809000 2.542012000 -1.922449000
 C -1.737013000 2.974918000 -2.958206000
 H 0.253617000 0.219996000 -3.222729000
 H -3.044526000 0.951452000 -0.540493000
 H -0.067056000 2.445186000 -4.225419000
 H -3.362727000 3.189858000 -1.557750000
 H -1.877062000 3.955416000 -3.405521000
 O -2.212597000 -1.438213000 -0.038237000

4a

E= -3.29956125 Ha
 S 0.087227000 -0.456895000 -0.400968000
 O -1.301823000 -0.454394000 -1.032306000
 C 0.427547000 -2.262657000 -0.187996000
 C -0.424418000 -3.093179000 0.545326000
 C 1.573351000 -2.788585000 -0.784130000
 C -0.125205000 -4.448531000 0.679971000
 C 1.873109000 -4.147819000 -0.649403000
 C 1.024266000 -4.978469000 0.082832000
 H -1.318499000 -2.682516000 1.009183000
 H 2.234610000 -2.138551000 -1.354953000
 H -0.787573000 -5.095908000 1.250970000
 H 2.767575000 -4.554926000 -1.115595000
 H 1.254807000 -6.035639000 0.189620000
 O 0.007759000 0.036005000 1.040910000

4a_RC

E= -3.96806733 Ha
 O 2.378028000 -2.285808000 1.617535000
 H 3.164579000 -2.281645000 1.046345000
 S 0.894513000 0.996766000 -0.542226000
 O 0.150966000 -0.137132000 0.185978000
 O 1.318881000 -2.522143000 0.638660000
 H 0.965245000 -1.596492000 0.490552000
 O 0.812270000 0.784891000 -2.046278000
 C -0.243971000 2.416193000 -0.257081000
 C 0.266278000 3.551124000 0.372441000
 C -1.579805000 2.378643000 -0.665914000
 C -0.560758000 4.655946000 0.597517000
 C -2.403204000 3.480662000 -0.439807000
 C -1.895128000 4.621207000 0.191929000
 H 1.307867000 3.576303000 0.687586000
 H -1.974737000 1.493295000 -1.158303000
 H -0.161549000 5.540755000 1.087965000
 H -3.443708000 3.452972000 -0.756082000
 H -2.539976000 5.479114000 0.365690000

TS_4a-5a

E=-3.95221091 Ha
 Nimag=-319.4 cm⁻¹

O	1.852058000	-0.295631000	-0.068499000
H	1.627215000	-1.235934000	-0.150117000
S	-0.659490000	-0.079178000	0.070288000
O	-1.268644000	-0.510737000	1.378810000
O	3.530655000	-0.540592000	-0.187396000
H	3.718954000	-0.421013000	0.756429000
O	-1.441166000	-0.536047000	-1.134690000
C	-0.844242000	1.749665000	0.063584000
C	-0.847132000	2.453946000	1.269506000
C	-0.885166000	2.434726000	-1.153247000
C	-0.912211000	3.848695000	1.256145000
C	-0.949097000	3.829144000	-1.160546000
C	-0.962383000	4.537747000	0.042843000
H	-0.810772000	1.917818000	2.212854000
H	-0.878428000	1.884738000	-2.089493000
H	-0.925141000	4.396015000	2.195742000
H	-0.990494000	4.361342000	-2.107944000
H	-1.010683000	5.623721000	0.034789000

5

E= -3.57539837 Ha			
S	-0.138292000	0.002237000	-0.000308000
O	-0.568546000	-0.848314000	-1.128140000
O	-0.563141000	-0.521746000	1.313742000
O	-0.498000000	1.426488000	-0.189424000
C	1.666797000	-0.032083000	0.002556000
C	2.365203000	0.206249000	1.190385000
C	2.365102000	-0.243882000	-1.189498000
C	3.759946000	0.230809000	1.182170000
C	3.760385000	-0.218166000	-1.190555000
C	4.460582000	0.019320000	-0.006814000
H	1.824915000	0.365364000	2.117966000
H	1.823729000	-0.433955000	-2.110326000
H	4.298591000	0.412506000	2.108873000
H	4.298924000	-0.387608000	-2.119626000
H	5.547390000	0.036591000	-0.009894000

Selenium

1a

E = -2.78963854985311 Ha			
C	0.000000000	0.000000000	0.799400000
C	0.000000000	-1.204000000	0.064900000
C	0.000000000	1.204000000	0.064900000
H	0.000000000	-2.152800000	0.596100000
H	0.000000000	2.152800000	0.596100000
C	0.000000000	-1.202900000	-1.330800000
C	0.000000000	1.202900000	-1.330800000
H	0.000000000	-2.151600000	-1.864600000
H	0.000000000	2.151600000	-1.864600000
C	0.000000000	0.000000000	-2.042800000
H	0.000000000	0.000000000	-3.129900000
Se	0.000000000	0.000000000	2.721800000

1a_RC

E= -3.45419622 Ha			
O	2.366638000	-0.041234000	0.575011000
H	1.415577000	0.244765000	0.659958000
Se	-0.887134000	-0.235676000	0.245357000
O	2.193432000	-1.214166000	-0.302380000
H	1.202592000	-1.199700000	-0.405912000
C	-1.406489000	0.888196000	-1.230043000
C	-0.460825000	1.528014000	-2.053407000
C	-2.769932000	1.096368000	-1.514645000
C	-0.863645000	2.339489000	-3.115576000
C	-3.168972000	1.908910000	-2.576821000
C	-2.219778000	2.537422000	-3.386960000
H	0.599912000	1.392107000	-1.863002000

H	-3.525910000	0.616836000	-0.897800000
H	-0.108514000	2.820410000	-3.734456000
H	-4.230566000	2.049837000	-2.770741000
H	-2.531259000	3.169905000	-4.214390000

TS_1a-3a

E= -3.44543830 Ha			
nimag=-328.7 cm ⁻¹			
O	2.802381000	-1.465592000	-0.227475000
H	2.962249000	-1.811937000	0.664067000
Se	-0.857026000	0.763376000	0.680121000
O	1.275406000	-0.814140000	0.099053000
H	1.537262000	0.117913000	0.173464000
C	-1.402805000	1.381104000	-1.054029000
C	-0.622491000	2.299028000	-1.783115000
C	-2.608846000	0.938385000	-1.631036000
C	-1.032559000	2.754000000	-3.036859000
C	-3.019232000	1.400518000	-2.882349000
C	-2.234182000	2.310082000	-3.595401000
H	0.311898000	2.661447000	-1.362625000
H	-3.230905000	0.227438000	-1.093331000
H	-0.409288000	3.462954000	-3.578258000
H	-3.957721000	1.043983000	-3.302169000
H	-2.553659000	2.667511000	-4.571057000

3a

E= -2.99514454 Ha			
Se	0.082359000	-0.443804000	0.091544000
O	1.176196000	0.269007000	-1.074917000
C	0.474615000	-2.332787000	0.037114000
C	-0.227644000	-3.212798000	0.882459000
C	1.446786000	-2.853233000	-0.830659000
C	0.039198000	-4.579133000	0.853155000
C	1.707341000	-4.225339000	-0.852947000
C	1.008911000	-5.098692000	-0.015408000
H	-0.984599000	-2.830619000	1.565750000
H	1.991865000	-2.176286000	-1.483534000
H	-0.513087000	-5.245309000	1.513235000
H	2.463862000	-4.613780000	-1.532691000
H	1.213775000	-6.165955000	-0.035904000

3a_RC

E= -3.67073746 Ha			
O	0.670101000	0.075252000	1.614514000
H	0.078398000	-0.475037000	0.920631000
Se	-0.447435000	-1.078156000	-1.641515000
O	1.845102000	-0.779958000	1.816548000
H	2.461420000	-0.414467000	1.160897000
C	-1.185895000	0.610366000	-2.219312000
C	-1.028323000	0.993670000	-3.562708000
C	-1.867379000	1.461104000	-1.339069000
C	-1.542716000	2.208892000	-4.009637000
C	-2.379717000	2.677289000	-1.797013000
C	-2.221803000	3.061046000	-3.130534000
H	-0.502289000	0.346110000	-4.262053000
H	-1.991818000	1.168464000	-0.300529000
H	-1.411618000	2.492919000	-5.051770000
H	-2.905687000	3.329402000	-1.102272000
H	-2.620227000	4.009101000	-3.482341000
O	-0.871578000	-1.159088000	0.071025000

TS_3a-4a

E= -3.65569188 Ha			
Nimag=-338.0 cm ⁻¹			
O	2.580350000	0.165487000	1.127736000
H	2.335054000	-0.061484000	2.039188000
Se	-1.093338000	-1.318251000	-1.087875000
O	1.376184000	-0.611582000	0.378664000
H	0.794151000	0.142327000	0.190462000

C	-1.382083000	0.447965000	-1.836508000
C	-0.542898000	0.902477000	-2.867721000
C	-2.417910000	1.270864000	-1.376747000
C	-0.740444000	2.164542000	-3.423869000
C	-2.608643000	2.534353000	-1.940830000
C	-1.774369000	2.989484000	-2.964508000
H	0.263622000	0.273281000	-3.239913000
H	-3.068033000	0.916835000	-0.581107000
H	-0.084960000	2.505751000	-4.222394000
H	-3.416216000	3.166293000	-1.576308000
H	-1.926208000	3.972955000	-3.401693000
O	-2.366141000	-1.510269000	0.068274000

4a

E= -3.23693426 Ha			
Se	0.156730000	-0.314131000	-0.339265000
O	-1.190420000	-0.325634000	-1.372970000
C	0.492297000	-2.283315000	-0.139825000
C	-0.374928000	-3.099544000	0.586101000
C	1.618458000	-2.823472000	-0.760348000
C	-0.115144000	-4.467739000	0.684870000
C	1.878300000	-4.194012000	-0.659135000
C	1.011015000	-5.015806000	0.062429000
H	-1.245599000	-2.671052000	1.077565000
H	2.298957000	-2.185130000	-1.321804000
H	-0.789484000	-5.107810000	1.249840000
H	2.757189000	-4.616249000	-1.141156000
H	1.212173000	-6.081226000	0.143130000
O	-0.416811000	0.083058000	1.204026000

4a_RC

E= -3.90738944 Ha			
O	2.756302000	-2.003802000	1.672886000
H	3.428089000	-2.033797000	0.971322000
Se	0.761393000	0.798926000	-0.830477000
O	0.196896000	-0.254780000	0.402545000
O	1.563360000	-2.432391000	0.943185000
H	1.112959000	-1.546817000	0.727265000
O	0.058100000	0.273278000	-2.269455000
C	-0.348906000	2.403751000	-0.395335000
C	0.172286000	3.352264000	0.485137000
C	-1.611658000	2.573804000	-0.958314000
C	-0.586510000	4.478898000	0.814627000
C	-2.368593000	3.699249000	-0.624688000
C	-1.857067000	4.651272000	0.261309000
H	1.163441000	3.224422000	0.916644000
H	-1.997990000	1.835102000	-1.656188000
H	-0.183775000	5.221279000	1.499772000
H	-3.356252000	3.835254000	-1.059771000
H	-2.446280000	5.528736000	0.516042000

TS_4a-5a

E= -3.88152334 Ha			
Nimag=-300.0 cm ⁻¹			
O	1.769653000	-0.355960000	0.088587000
H	1.755576000	-1.291567000	-0.173303000
Se	-0.579020000	-0.181438000	-0.126550000
O	-1.445392000	-0.709414000	1.206467000
O	3.573977000	-0.439011000	0.287573000
H	3.531034000	-0.386467000	1.254488000
O	-1.363863000	-0.598123000	-1.545118000
C	-0.778659000	1.798271000	-0.044992000
C	-0.512443000	2.453416000	1.156565000
C	-1.137293000	2.500688000	-1.192207000
C	-0.623241000	3.844520000	1.209088000
C	-1.249382000	3.892185000	-1.127939000
C	-0.991725000	4.562567000	0.069065000
H	-0.231497000	1.896657000	2.046195000
H	-1.336858000	1.972440000	-2.119503000

H	-0.422049000	4.364966000	2.142190000
H	-1.538071000	4.449527000	-2.015794000
H	-1.076850000	5.645243000	0.114190000

5

E= -3.45161082 Ha			
Se	-0.224993000	0.001357000	0.000137000
O	-0.715958000	-1.010222000	-1.210026000
O	-0.714664000	-0.509275000	1.492710000
O	-0.669409000	1.569420000	-0.290709000
C	1.738245000	-0.025924000	0.003230000
C	2.415135000	0.195268000	1.200579000
C	2.413472000	-0.226465000	-1.198854000
C	3.811144000	0.214709000	1.188100000
C	3.809478000	-0.204365000	-1.195556000
C	4.506365000	0.016229000	-0.006111000
H	1.871282000	0.343338000	2.127781000
H	1.868720000	-0.403032000	-2.120590000
H	4.352266000	0.383313000	2.115486000
H	4.349470000	-0.362157000	-2.125521000
H	5.593032000	0.031616000	-0.009549000

Tellurium

1a

E = -2.75515269 Ha			
C	-0.231857000	-0.000004000	-3.577699000
C	-1.382348000	-0.353183000	-2.846666000
C	0.918635000	0.353176000	-2.846669000
H	-2.291345000	-0.632622000	-3.373804000
H	1.827631000	0.632608000	-3.373812000
C	-1.382346000	-0.352555000	-1.449955000
C	0.918632000	0.352556000	-1.449958000
H	-2.289106000	-0.630439000	-0.915578000
H	1.825393000	0.630442000	-0.915583000
C	-0.231858000	0.000005000	-0.739758000
H	-0.231857000	0.000009000	0.347476000
Te	-0.231845000	0.000007000	-5.721603000

1a_RC

E= -3.42063841 Ha			
O	2.299363000	0.141722000	0.942071000
H	1.304615000	0.165872000	0.938889000
Te	-0.950663000	-0.774574000	0.014874000
O	2.541816000	-0.887900000	-0.085194000
H	1.606264000	-1.084605000	-0.364352000
C	-1.487672000	0.713316000	-1.433863000
C	-0.542716000	1.268918000	-2.314189000
C	-2.818880000	1.156009000	-1.533730000
C	-0.915072000	2.231285000	-3.255730000
C	-3.189851000	2.116958000	-2.476882000
C	-2.240690000	2.662181000	-3.344471000
H	0.494739000	0.949395000	-2.270339000
H	-3.577050000	0.748747000	-0.869526000
H	-0.161727000	2.643943000	-3.924060000
H	-4.227793000	2.439740000	-2.531004000
H	-2.529551000	3.410477000	-4.078302000

TS_1a-3a

E= -3.41480161 Ha			
nimag=-335.4 cm ⁻¹			
O	3.002257000	-1.389274000	-0.176892000
H	3.186521000	-1.795118000	0.684777000
Te	-0.941984000	0.707895000	0.865562000
O	1.454781000	-0.904928000	0.156358000
H	1.611548000	0.039506000	0.334144000
C	-1.498623000	1.395690000	-1.083298000
C	-0.686741000	2.292727000	-1.800365000

C	-2.699089000	0.971473000	-1.681111000
C	-1.060873000	2.746415000	-3.067040000
C	-3.074288000	1.430058000	-2.945889000
C	-2.257446000	2.319413000	-3.647805000
H	0.246039000	2.643960000	-1.367053000
H	-3.349656000	0.276700000	-1.156121000
H	-0.413048000	3.439793000	-3.599846000
H	-4.009744000	1.086952000	-3.383460000
H	-2.549173000	2.674805000	-4.632960000

3a

E= -2.96994880 Ha

Te	0.034079000	-0.258876000	0.127805000
O	1.256187000	0.401217000	-1.197782000
C	0.458379000	-2.360999000	0.062585000
C	-0.234320000	-3.256452000	0.896315000
C	1.431711000	-2.868331000	-0.810635000
C	0.042593000	-4.622472000	0.855125000
C	1.705976000	-4.237850000	-0.848748000
C	1.015432000	-5.123876000	-0.017999000
H	-0.995994000	-2.892404000	1.584278000
H	1.974606000	-2.185926000	-1.460956000
H	-0.504173000	-5.299975000	1.508310000
H	2.465168000	-4.613601000	-1.532664000
H	1.229935000	-6.189185000	-0.048436000

3a_RC

E= -3.64658029 Ha

O	0.638863000	0.063933000	1.694878000
H	0.058561000	-0.538022000	0.998443000
Te	-0.351324000	-1.258754000	-1.683380000
O	1.854485000	-0.729196000	1.919054000
H	2.436924000	-0.387244000	1.221312000
C	-1.180798000	0.619777000	-2.297643000
C	-1.074346000	1.022466000	-3.639005000
C	-1.822975000	1.465526000	-1.383531000
C	-1.596240000	2.248309000	-4.052052000
C	-2.344120000	2.692304000	-1.802809000
C	-2.233342000	3.092288000	-3.136337000
H	-0.582285000	0.384126000	-4.370817000
H	-1.914076000	1.166299000	-0.342665000
H	-1.503873000	2.545409000	-5.094756000
H	-2.837858000	3.338976000	-1.079834000
H	-2.637103000	4.048362000	-3.459687000
O	-0.831959000	-1.247651000	0.193693000

TS_3a-4a

E= -3.63234741 Ha
Nimag=-315.3 cm⁻¹

O	2.775923000	0.077862000	1.268199000
H	2.545138000	-0.174523000	2.176956000
Te	-1.065135000	-1.405502000	-1.063008000
O	1.618734000	-0.713815000	0.511983000
H	0.985826000	0.005955000	0.342937000
C	-1.401851000	0.530328000	-1.938449000
C	-0.601152000	0.976434000	-3.002054000
C	-2.425504000	1.359298000	-1.461981000
C	-0.821630000	2.229907000	-3.573275000
C	-2.643094000	2.613755000	-2.037648000
C	-1.843772000	3.056364000	-3.094212000
H	0.198519000	0.349907000	-3.393516000
H	-3.052046000	1.021542000	-0.639732000
H	-0.193221000	2.562100000	-4.397179000
H	-3.441779000	3.247699000	-1.657021000
H	-2.014169000	4.032677000	-3.540976000
O	-2.459246000	-1.460605000	0.232736000

4a

E= -3.22244489 Ha

Te	0.224977000	-0.016912000	0.420933000
O	1.156096000	0.565219000	-1.086921000
C	0.556071000	-2.175412000	0.216391000
C	0.373765000	-3.005839000	1.326530000
C	0.928067000	-2.731495000	-1.009653000
C	0.553293000	-4.387434000	1.208783000
C	1.106686000	-4.112139000	-1.128817000
C	0.918765000	-4.941252000	-0.019846000
H	0.092210000	-2.587628000	2.291827000
H	1.083247000	-2.087887000	-1.872961000
H	0.410089000	-5.028819000	2.075705000
H	1.394974000	-4.540925000	-2.086398000
H	1.060035000	-6.015411000	-0.112456000
O	-1.561582000	0.041924000	-0.132530000

4a_RC

E= -3.89318188 Ha

O	1.114582000	-0.137428000	2.852137000
H	1.505464000	-0.978336000	3.142348000
Te	0.961784000	0.653020000	-1.647233000
O	0.689708000	-0.724550000	-0.389136000
O	-0.043878000	-0.608039000	2.094017000
H	0.290299000	-0.561767000	1.128882000
O	-0.250478000	0.205184000	-2.984271000
C	-0.165509000	2.243906000	-0.663830000
C	0.522398000	3.209034000	0.076353000
C	-1.557021000	2.303386000	-0.762245000
C	-0.181542000	4.226824000	0.726552000
C	-2.260639000	3.319337000	-0.111423000
C	-1.573556000	4.280862000	0.634410000
H	1.607943000	3.179542000	0.154398000
H	-2.094926000	1.561860000	-1.348744000
H	0.357294000	4.976156000	1.302150000
H	-3.345080000	3.361801000	-0.187537000
H	-2.122159000	5.072088000	1.139589000

TS_4a-5a

E= -3.86701430 Ha
Nimag=-309.9 cm⁻¹

O	1.844621000	-0.457671000	0.023525000
H	1.879979000	-1.402837000	-0.203573000
Te	-0.620127000	-0.336721000	-0.089706000
O	-1.556726000	-0.815409000	1.436076000
O	3.636460000	-0.386118000	0.159488000
H	3.626415000	-0.304212000	1.125808000
O	-1.695172000	-0.731058000	-1.548229000
C	-0.782862000	1.828870000	-0.020014000
C	-0.622388000	2.495136000	1.196746000
C	-1.025920000	2.541195000	-1.195574000
C	-0.716762000	3.888417000	1.236031000
C	-1.119941000	3.934550000	-1.148711000
C	-0.964995000	4.607177000	0.064879000
H	-0.435716000	1.942670000	2.113938000
H	-1.152562000	2.021036000	-2.141112000
H	-0.597659000	4.409820000	2.182815000
H	-1.315192000	4.492285000	-2.061618000
H	-1.037622000	5.691297000	0.098289000

5

E= -3.42772717 Ha

Te	-0.351017000	0.000221000	-0.005129000
O	-0.892172000	-0.705331000	-1.605766000
O	-0.894289000	-1.016223000	1.420867000
O	-0.891672000	1.741631000	0.194668000
C	1.798509000	-0.006291000	-0.003224000
C	2.476987000	0.335051000	1.167627000
C	2.477273000	-0.343034000	-1.173328000
C	3.873091000	0.338645000	1.158589000
C	3.874221000	-0.335271000	-1.166287000

C	4.569061000	0.004989000	-0.004896000
H	1.942574000	0.593277000	2.077001000
H	1.936176000	-0.609351000	-2.075604000
H	4.413532000	0.602533000	2.063964000
H	4.415443000	-0.596724000	-2.071917000
H	5.655868000	0.009687000	-0.005459000