Prototropic Tautomerism of Selenouracils. A theoretical study

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Supplementary Information (a total of 14 pages)

Table S1. B3LYP/6-311+G(3df,2p) Calculated Total Energies and B3LYP/6-31G(d,p) Zero-Point Vibrational Energies (ZPVE) of the different tautomeric forms of selenouracils and the transition states associated with the corresponding prototropic tautomerism . All values in hartrees

Stationary Point	**Energy**			**ZPVE**		
	2-Selenouracil	4-Selenouracil	2,4-Diselenouracil	2-Selenouracil	4-Selenouracil	2,4-Diselenouracil
I	-2741.25741	-2741.26056	-5067.54198	0.08481	0.08477	0.08257
IIa	-2741.23837	-2741.23739	-5067.51875	0.08442	0.07976	0.07741
IIb	-2741,22791	-2741,23657	-5067,51783	0,08390	0,07986	0,07746
IIIa	-2741.21932	-2741.22963	-5067.51082	0.08320	0.07934	0.07702
IIIb	-2741,22303	-2741,22963	-5067,51061	0,08363	0,07959	0,07719
IVa	-2741,23721	-2741,23235	-5067,52371	0,07968	0,08393	0,07763
IVb	-2741.23754	-2741.24375	-5067.52390	0.07977	0.08459	0.07722
Va	-2741.22398	-2741.22921	-5067.50824	0.07934	0.08392	0.07692
Vb	-2741,22289	-2741,21353	-5067,50714	0,07912	0,08254	0,07671
VIa	-2741.23713	-2741.23616	-5067.51971	0.07982	0.07994	0.07692
VIb	-2741,22289	-2741,21353	-5067,50714	0,07912	0,08254	0,07671
VIc	-2741.23736	-2741.23691	-5067.51985	0.07987	0.07993	0.07299
VId	-2741,22991	-2741,23616	-5067,51954	0,07954	0,08010	0,07303
TSI_IIa	-2741.18691	-2741.20097	-5067,48301	0.07953	0.07768	0.07537
TSI_IVb	-2741.20127	-2741.18763	-5067.48630	0.07770	0.07941	0.07509
TSI_Va	-2741.19073	-2741.17998	-5067.47616	0.07753	0.07920	0.07509
TSIIa_VIc	-2741.19448	-2741.17673	-5067.47555	0.07770	0.07477	0.07081
TSVIa_IIIa	-2741.18566	-2741.17375	-5067.47249	0.07750	0.07469	0.07086
TSVIc_VIa	-2741.22694	-2741.22185	-5067.50926	0.07912	0.07818	0.07220

Table S2. B3LYP/6-31G(d,p) optimized Geometries (Cartesian Coordinates in Å) of the Stationary Points of the Prototropic Tautomerization Processes of selenouracils

2-Selenouracil

	I				**IIa**		
1	0.225511	1.413443	-0.000506	1	0.178248	1.409684	0.000085
2	-1.568611	1.707941	0.000076	2	1.488113	1.757052	-0.000008
3	-2.507744	0.734579	0.000266	3	2.450474	0.789191	-0.000061
4	-2.090040	-0.661440	-0.000010	4	1.954049	-0.548599	-0.000298
5	-2.823920	-1.637661	-0.000175	5	2.860373	1.536652	0.000111
6	-0.684164	-0.832965	0.000075	6	0.684104	-0.880130	-0.000047
7	0.278863	0.135796	-0.000061	7	-0.273946	0.084888	0.000250
8	0.465568	2.151711	0.000256	8	-0.550678	0.113539	0.000120
9	2.045749	0.192380	0.000046	9	-2.048914	-0.219884	-0.000026

10	-0.359129	-1.793895	0.000063
11	-1.811563	2.764674	0.000120
12	-3.566058	0.955099	0.000781

10	2.364473	-2.374351	0.000385
11	1.709248	2.818598	0.000011
12	3.508450	1.009406	0.000070

IIIa

1	-0.137939	1.561158	-0.000005
2	-1.440767	1.780424	0.000005
3	-2.445127	0.787969	0.000007
4	-1.992735	-0.513004	-0.000002
5	-2.845475	-1.549537	0.000001
6	-0.657935	-0.739803	-0.000019
7	0.315527	0.282973	-0.000026
8	2.047544	-0.209996	0.000005
9	-0.269858	-1.678745	-0.000036
10	-2.389153	-2.403856	0.000066
11	-1.741581	2.826930	0.000011
12	-3.502387	1.012179	0.000036

IVb

1	-0.197175	1.492579	-0.000590
2	-1.551972	1.722516	0.000046
3	-2.511430	0.751486	0.000453
4	-2.120855	-0.641276	0.000037
5	-2.838193	-1.633969	-0.000769
6	-0.706688	-0.796793	0.000934
7	0.171396	0.244200	-0.000244
8	2.013971	-0.218852	0.000017
9	-0.385773	-1.759451	0.001183
10	2.421016	1.183807	-0.001178
11	-1.831406	2.772807	0.000853
12	-3.569097	0.983506	0.000555

Va

1	0.265337	1.404475	-0.000453
2	1.615700	1.698933	0.000065
3	2.522029	0.699011	0.000267
4	2.073931	-0.701810	0.000079
5	2.851604	-1.645901	-0.000254
6	0.671013	-0.915621	0.000201
7	-0.132125	0.088039	-0.000196
8	-2.029148	-0.151738	0.000017
9	-0.415619	2.150083	0.000400
10	-1.893699	-1.605144	0.000662
11	1.870152	2.752921	0.000312
12	3.585688	0.901430	0.000533

VIa

1	-0.144659	1.487529	0.000119
2	-1.458520	1.770105	0.000004
3	-2.448382	0.798185	0.000075
4	-1.985384	-0.524747	-0.000099
5	-2.873454	-1.535870	0.000005
6	-0.691191	-0.839984	-0.000015
7	0.165064	0.190816	-0.000009
8	2.027397	-0.162569	0.000027
9	1.859838	-1.616774	-0.000273
10	-2.365583	-2.364290	0.000046
11	-1.718152	2.826077	-0.000034
12	-3.505692	1.030335	0.000410

VIc

1	-0.164131	1.514212	-0.000089
2	-1.484768	1.768831	-0.000048
3	-2.457561	0.780238	0.000188
4	-1.970526	-0.534560	-0.000010
5	-2.837355	-1.563361	0.000024
6	-0.671259	-0.821670	-0.000182
7	0.168111	0.223474	-0.000105
8	2.004610	-0.245535	-0.000005
9	-2.312545	-2.381337	0.000380
10	2.454100	1.146307	0.001419
11	-1.764679	2.819727	-0.000405
12	-3.518588	0.994684	0.000312

TSI_IIa

1	-0.247403	1.404742	-0.000034
2	-1.570374	1.718203	0.000149
3	-2.543564	0.755557	-0.000158
4	-2.043064	-0.575843	-0.000452
5	-2.617146	-1.721553	0.000263
6	-0.710905	-0.836988	-0.000140
7	0.263865	0.098195	-0.000055
8	0.454712	2.134956	0.000486
9	2.037197	-0.178272	0.000007
10	-1.316219	-2.015761	0.000890
11	-1.800051	2.778277	0.000547
12	-3.599002	0.985262	0.000065

TSI_IVb

1	0.059694	1.305431	-0.000596
2	1.356333	1.740442	0.000127
3	2.417272	0.879638	0.000331
4	2.198073	-0.552386	-0.000043
5	3.039443	-1.438800	-0.000116
6	0.809863	-0.907363	-0.000112
7	-0.191663	-0.011296	-0.000285
8	-2.036998	-0.210781	0.000072
9	0.614912	-1.902431	0.001037
10	-1.371285	1.406489	0.000515
11	1.490767	2.817585	0.000355
12	3.440994	1.230447	0.000749

TSI_Va

1	0.360325	1.545944	-0.000025
2	1.742576	1.669238	0.000002
3	2.527751	0.572416	-0.000004
4	1.938235	-0.781355	-0.000002
5	2.598228	-1.809742	-0.000017
6	0.527641	-0.797773	0.000059
7	-0.199010	0.313101	0.000004
8	-0.228740	2.365521	0.000131
9	-1.992634	-0.167046	-0.000007
10	-0.809780	-1.425544	0.000044
11	2.121845	2.684758	0.000027
12	3.607333	0.655168	-0.000058

TSIIa_VIc

1	-0.027849	1.310609	0.000136
2	-1.282073	1.780969	-0.000007
3	-2.360500	0.909064	-0.000105
4	-2.040487	-0.462033	-0.000037
5	-3.042646	-1.352773	0.000191
6	-0.796389	-0.944433	-0.000288
7	0.184642	-0.044590	0.000003
8	2.034960	-0.238776	0.000008
9	-2.639036	-2.237802	0.000145
10	1.346415	1.407511	0.000221
11	-1.406811	2.859437	-0.000103
12	-3.387861	1.247741	-0.000128

TSVIa_IIIa

1	-0.258175	1.670078	-0.000323
2	-1.599759	1.750472	0.000011
3	-2.468507	0.662238	0.000203
4	-1.868635	-0.604923	0.000095
5	-2.616246	-1.716690	-0.000341
6	-0.539177	-0.699618	0.000439
7	0.242328	0.441605	0.000011
8	1.990311	-0.182712	-0.000007
9	-2.039722	-2.497509	-0.000084
10	0.600943	-1.375499	-0.000090
11	-3.545121	0.770213	0.000452
12	-2.007800	2.758951	-0.000033

TSVIc_VIa

1	0.185299	1.502951	-0.009594
2	1.507587	.762066	0.004322
3	2.478942	0.774236	0.009782
4	1.991262	-0.539077	0.000584
5	2.854627	-1.570167	0.004771
6	0.689366	-0.823949	-0.012641
7	-0.151836	0.216532	-0.010981
8	-2.041596	-0.196137	-0.039677
9	2.324667	-2.385448	-0.007557
10	-2.151722	-0.221661	1.422583
11	1.785393	2.813333	0.009206
12	3.540514	0.988189	0.020021

4-Selenouracil

I

1	1.860705	-1.708048	0.000000
2	2.294650	-0.403041	0.000000
3	1.414895	0.629816	0.000000
4	0.000000	0.375612	0.000000
5	-0.338735	-0.968887	0.000000
6	0.515090	-2.062541	0.000000
7	0.133876	-3.220499	0.000000
8	-1.327154	-1.198674	0.000000
9	2.510404	-2.482442	0.000000
10	-1.276056	1.633944	0.000000
11	3.369554	-0.263003	0.000000
12	1.760471	1.653488	0.000000

IIa

1	-2.451059	0.617811	-0.000251
2	-1.623489	1.692502	-0.000202
3	-0.273900	1.503910	0.000340
4	0.167902	0.141350	0.001030
5	-0.620822	-0.900994	0.000659
6	-1.993842	-0.728533	0.000119
7	-2.814925	-1.631033	-0.000331
8	-3.457369	0.728645	-0.000685
9	2.046514	-0.140238	-0.000189
10	1.913491	-1.595657	-0.000338
11	-2.090003	2.672189	-0.000690
12	0.414934	2.338076	0.000195

IIIa

1	2.584155	0.690816	-0.000130
2	1.698927	1.660499	-0.000021
3	0.288236	0.506416	0.000125
4	-0.188896	0.217818	0.000150
5	0.712324	-0.794629	0.000009
6	2.133071	-0.614817	0.000002
7	2.836145	-1.611506	0.000010
8	-2.047107	-0.137509	-0.000043
9	0.425259	-1.765707	0.000088
10	-1.909492	-1.595561	0.000450
11	2.105622	2.672319	0.000057
12	-0.372297	2.363487	0.000092

IVb

1	-2.496710	0.698227	0.000039
2	-1.590201	1.728095	0.000004
3	-0.230529	1.554860	-0.000097
4	0.328514	0.241612	-0.000077
5	-0.645946	-0.755917	-0.000007
6	-1.974620	-0.495962	0.000070
7	-2.743209	-1.592826	-0.000010
8	2.068286	-0.209797	0.000012
9	-0.325382	-1.719950	-0.000094
10	-3.668596	-1.297753	-0.000093
11	-2.024562	2.723343	-0.000001
12	0.442101	2.402264	0.000262

Va

1	-2.402334	0.684340	0.000441
2	-1.521620	1.754256	0.000030
3	-0.189370	1.515677	-0.000341
4	0.317896	0.156034	-0.000407
5	-0.622619	-0.864971	-0.000418
6	-1.881366	-0.575629	-0.000052
7	-2.819093	-1.537382	-0.000141
8	2.075757	-0.207170	0.000120
9	-3.404813	0.811041	0.000895
10	-2.341899	-2.384866	0.001007

VIa

1	2.521415	0.703478	-0.000273
2	1.641747	1.713278	-0.000006
3	0.262954	1.530537	0.000150
4	-0.180337	0.202363	0.000017
5	0.672571	-0.823693	-0.000089
6	1.976333	-0.511762	0.000010
7	2.841899	-1.540666	0.000117
8	-2.041385	-0.163428	-0.000040
9	2.315917	-2.355797	0.000345
10	-1.851263	-1.613054	0.000564

11	-1.968041	2.740721	0.000164	11	2.066195	2.715008	0.000082
12	0.513179	2.338319	-0.000561	12	-0.421019	2.370737	0.000942

VIc

1	-2.501452	0.682289	-0.000085
2	-1.632353	1.703979	-0.000216
3	-0.256131	1.523024	0.000017
4	0.189031	0.192369	0.000785
5	-0.650988	-0.841369	0.000609
6	-1.949391	-0.535760	0.000511
7	-2.786415	-1.587597	-0.000494
8	2.050602	-0.167795	-0.000208
9	1.857461	-1.616974	0.001573
10	-3.688516	-1.230889	-0.001070
11	-2.065108	2.701774	-0.000320
12	0.427167	2.363782	0.000590

TSI_IIa

1	2.452194	0.499734	0.000834
2	1.746560	1.659314	-0.000050
3	0.379219	1.648436	-0.000486
4	-0.237312	0.369862	-0.000038
5	0.483787	-0.770611	-0.000072
6	1.861233	-0.795938	-0.000024
7	2.565411	-1.790272	-0.000613
8	3.464779	0.504295	0.002717
9	-2.010797	-0.155927	0.000117
10	-0.806027	-1.415419	-0.000377
11	2.327704	2.575772	-0.000786
12	-0.192700	2.565152	-0.002363

TSI_IVb

1	1.799547	-1.764489	0.000000
2	2.283818	-0.492786	0.000000
3	1.418776	0.574495	0.000000
4	0.000000	0.388513	0.000000
5	-0.409137	-0.960522	0.000000
6	0.472402	-1.973679	0.000000
7	0.283578	-3.240352	0.000000
8	-1.406607	-1.149125	0.000000
9	-1.247651	1.677441	0.000000
10	1.617857	-3.079161	0.000000
11	1.795849	1.587765	0.000000
12	3.361572	-0.373825	0.000000

TSI_Va

1	-2.493495	0.647391	0.000642
2	-1.600900	1.724324	-0.000227
3	-0.265169	1.510186	-0.000539
4	0.303205	0.165483	0.000356
5	-0.650470	-0.824715	0.002708
6	-1.965480	-0.593324	0.000763
7	-2.567508	-1.725703	-0.001800
8	-3.495769	0.773761	-0.001041
9	2.062810	-0.164682	-0.000203
10	-1.284776	-2.025994	-0.001140
11	0.416214	2.350440	-0.001333
12	-2.053318	2.707864	-0.000753

TSIIa_VIc

1	-2.450426	0.593733	0.001108
2	-1.655831	1.666905	-0.000276
3	-0.282213	1.474007	-0.000472
4	0.185972	0.138682	-0.000201
5	-0.600651	-0.940613	-0.000147
6	-1.911581	-0.672677	0.000365
7	-2.924811	-1.460464	-0.000511
8	2.058384	-0.138300	0.000065
9	1.929183	-1.594595	0.000253
10	-3.458576	-0.197615	-0.000602
11	-2.116840	2.649665	-0.000244
12	0.399127	2.315133	-0.000746

TSVIa_IIIa

1	2.624689	0.667591	-0.001792
2	1.730637	1.666467	-0.000274
3	0.337497	1.518998	0.002202
4	-0.175406	0.215473	0.000215
5	0.705019	-0.784736	-0.001968
6	2.067875	-0.548160	-0.000642
7	2.596306	-1.716047	0.002103
8	-2.030588	-0.120776	-0.000088
9	1.233101	-1.940632	0.001020
10	-1.874141	-1.575649	-0.000680
11	2.152085	2.670040	-0.000841
12	-0.313080	2.384338	0.003988

TSVIc_VIa

1	2.502145	0.708406	0.005181
2	1.623563	1.723221	0.009787
3	0.248046	1.534332	-0.003680
4	-0.189083	0.203405	-0.006878
5	0.667191	-0.820268	-0.011261
6	1.966894	-0.511644	-0.012422
7	2.835078	-1.561281	-0.097871
8	-2.047432	-0.176859	0.003733
9	-1.838508	-1.623620	-0.019548
10	3.081023	-1.882426	0.780039
11	2.047710	2.724802	0.023620
12	-0.440027	2.371849	-0.006375

2,4-Diselenouracil

I

1	1.180453	1.638846	-0.000485
2	0.017140	2.369561	0.000059
3	-1.192372	1.754269	0.000213
4	-1.265413	0.318895	0.000047
5	-0.027939	-0.313676	0.000026
6	1.212617	0.265626	-0.000015
7	-0.038069	-1.328742	0.001204
8	2.083078	2.095140	-0.000041
9	-2.775950	-0.641141	-0.000058
10	2.753249	-0.654871	0.000026
11	0.137098	3.446665	0.000433
12	-2.109696	2.325043	0.000860

IIa

1	1.197170	1.607799	-0.000273
2	0.069889	2.357017	0.000063
3	-1.148783	1.741959	0.000209
4	-1.121573	0.313037	-0.000160
5	-0.021147	-0.403758	-0.000535
6	1.195852	0.208031	-0.000215
7	2.114582	2.038773	-0.000563
8	-2.787027	-0.584079	0.000047
9	2.778702	-0.651909	0.000115
10	-2.164914	-1.907146	0.000044
11	0.198652	3.433865	0.000702
12	-2.069739	2.309542	0.000587

IIIa

1	-1.287654	1.733524	-0.000026
2	-0.133866	2.368875	-0.000014
3	1.140929	1.753346	0.000056
4	1.153221	0.376394	0.000065
5	-0.037904	-0.269623	-0.000001
6	-1.288705	0.371807	0.000015
7	2.775543	-0.588687	-0.000030
8	-2.771474	-0.648636	-0.000003
9	-0.095926	-1.282028	-0.000081
10	2.145296	-1.911115	0.000610

IVb

1	1.232321	1.707038	0.000025
2	0.039119	2.381143	0.000013
3	-1.189894	1.774659	-0.000163
4	-1.283465	0.351464	0.000009
5	-0.035232	-0.267756	0.000229
6	1.148937	0.405677	0.000137
7	-2.779743	-0.647288	-0.000009
8	2.714634	-0.664471	-0.000090
9	3.580519	0.511984	0.001199
10	-0.055578	-1.283572	0.000724

11	-0.191345	3.456715	-0.000053	11	0.124476	3.464104	0.000132
12	2.053072	2.335558	0.000129	12	-2.103508	2.354661	-0.000441

Va

1	1.143547	1.647975	-0.000980	1	-1.253985	1.673375	0.000018
2	-0.032948	2.374703	0.000061	2	-0.103888	2.361077	0.000056
3	-1.217729	1.719453	0.000763	3	1.143533	1.748798	-0.000104
4	-1.254028	0.271443	0.000264	4	1.141668	0.347591	-0.000053
5	-0.030962	-0.392264	0.000356	5	0.011088	-0.361527	0.000017
6	1.073077	0.276145	-0.000179	6	-1.126734	0.343115	-0.000014
7	-2.797268	-0.645092	-0.000156	7	2.793123	-0.586087	0.000000
8	2.759816	-0.606904	0.000023	8	-2.778299	-0.588979	-0.000023
9	2.035498	2.121924	-0.000132	9	2.147728	-1.898153	0.000218
10	2.118455	-1.918827	0.001769	10	-2.146121	-1.908848	0.000622
11	0.069715	3.453246	0.000027	11	-0.192749	3.445268	0.000414
12	-2.148594	2.271074	0.001778	12	2.059936	2.327557	0.000014

VIa

VIc

1	-2.501452	0.682289	-0.000085
2	-1.632353	1.703979	-0.000216
3	-0.256131	1.523024	0.000017
4	0.189031	0.192369	0.000785
5	-0.650988	-0.841369	0.000609
6	-1.949391	-0.535760	0.000511
7	-2.786415	-1.587597	-0.000494
8	2.050602	-0.167795	-0.000208
9	1.857461	-1.616974	0.001573
10	-3.688516	-1.230889	-0.001070
11	-2.065108	2.701774	-0.000320
12	0.427167	2.363782	0.000590

TSI_IIa

1	1.186948	1.653077	-0.000265	1	0.868795	-1.732104	0.000000
2	0.091261	2.452049	0.000110	2	-0.401942	-2.227710	0.000000
3	-1.168703	1.916858	0.000236	3	-1.495923	-1.399327	0.000000
4	-1.240151	0.500090	-0.000180	4	-1.339749	0.020141	0.000000
5	-0.118805	-0.258374	-0.000106	5	0.000000	0.438594	0.000000
6	1.137409	0.252926	-0.000120	6	1.050179	-0.401764	0.000000
7	2.119917	2.049152	-0.000836	7	0.152668	1.441993	0.000000
8	-2.650756	-0.688105	-0.000004	8	-2.656656	1.239620	0.000000
9	2.659513	-0.701325	0.000064	9	2.296010	-1.760454	0.000000
10	-1.043957	-1.365652	0.000212	10	-2.498767	-1.804486	0.000000
11	0.280066	3.520210	0.000391	11	-0.494016	-3.308717	0.000000
12	-2.049670	2.542463	0.000522	12	2.879807	-0.106144	0.000000

TSI_IVb

TSI_Va

1	1.170313	1.812560	-0.000622
2	-0.052127	2.472611	0.000109
3	-1.205099	1.765024	-0.000035
4	-1.193214	0.310925	-0.000078
5	0.065882	-0.257682	-0.000213
6	1.187574	0.459764	-0.000121
7	2.037236	2.329792	0.003655
8	-2.678932	-0.690392	0.000058
9	2.620804	-0.712898	0.000030
10	1.027684	-1.381300	-0.000036
11	-0.005101	3.554774	0.000199
12	-2.159673	2.274521	-0.000199

TSIIa_VIc

1	-1.269575	1.456513	-0.000197
2	-0.195624	2.251374	0.000056
3	1.077452	1.696599	0.000058
4	1.156409	0.290544	0.000000
5	0.086167	-0.509446	0.000148
6	-1.101350	0.092759	-0.000101
7	2.870842	-0.509419	-0.000032
8	-2.831140	-0.595747	0.000013
9	2.329194	-1.867838	0.000366
10	-2.611322	1.180871	-0.000079
11	-0.367098	3.323740	0.000276
12	1.961899	2.321754	0.000349

TSVIa_IIIa

1	-1.282242	1.874813	0.000110
2	-0.080680	2.469669	-0.000042
3	1.141062	1.797644	-0.000248
4	1.091944	0.395662	0.000109
5	-0.099764	-0.201823	0.000896
6	-1.258644	0.545176	0.000294
7	2.669591	-0.638178	-0.000123
8	-2.631750	-0.704827	-0.000160
9	1.953284	-1.914237	0.001734
10	-0.914717	-1.277768	0.000557
11	-0.093899	3.557856	0.000220
12	2.080691	2.336488	-0.000581

TSVIc_VIa

1	-1.223909	1.707079	-0.012785
2	-0.061819	2.381705	0.003974
3	1.175641	1.754652	0.011931
4	1.155561	0.354266	0.001297
5	0.010783	-0.334770	-0.013342
6	-1.119094	0.378367	-0.013294
7	2.786816	-0.611847	0.001203
8	-2.775224	-0.624417	-0.038912
9	2.108906	-1.907597	-0.015480
10	-2.874619	-0.668433	1.423691
11	-0.137839	3.466799	0.008852
12	2.099570	2.322127	0.024490

Table S3. Relative energies (kcal/mol) for the monohydrated and dihydrated clusters of selenouracils.

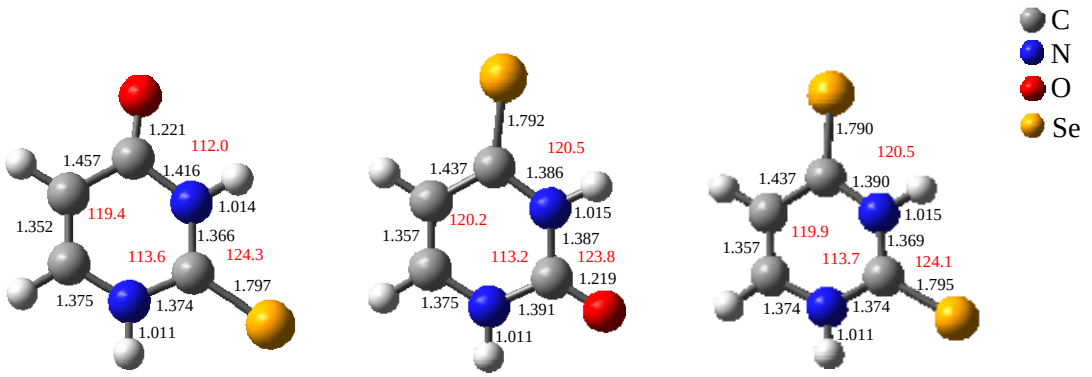
Cluster	2-selenouracil		4-selenouracil		2,4-diselenouracil
	monohydrated	dihydrated	monohydrated	dihydrated	monohydrated
I1	0.0	0.0	0.0	0.0	0.0
I2	1.8	1.5	1.5	4.3	2.1
I3	2.1	3.0	2.2	3.2	2.6

Table S4. Calculated harmonic vibrational frequencies (ν, in cm^{-1}), intensities (in parenthesis in Km/mol) and assignments[a] for the most stable tautomers of selenouracils.

2-selenouracil		4-selenouracil		2,4-selenouracil	
ν (intens.)	assignment	ν (intens.)	assignment	ν (intens.)	assignment
3631 (84)	N1-H stret.	3644 (158)	N1-H stret.	3630 (130)	N1-H stret.
3598 (64)	N3-H stret.	3589 (48)	N3-H stret.	3580 (39)	N3-H stret.
3264 (2.8)	C5-H stret.	3267 (3.3)	C5-H stret.	3270 (5.5)	C5-H stret.
3225 (3.7)	C6-H stret.	3227 (2.6)	C6-H stret.	3231 (3.6)	C6-H stret.
1781 (690)	C4=O stret.	1808 (943)	C4=O stret.	1653 (384)	C5-C6 stret.
1668 (60)	C5-C6 stret.	1663 (393)	C5-C6 stret.	1574 (942)	CNC sym. Stret. + NH sym. bend. ip
1571 (705)	CNC sym. Stret. + NH sym. bend. ip	1506 (59)	N1H bend.ip	1497 (46)	CH bend.ip
1458 (37)	CH bend. ip	1488 (116)	CNC sym. Stret. + N3H bend. ip	1400 (8.0)	NH bend. ip asym.
1407 (47)	CNC asym. stret.	1410 (22)	CH bend.ip	1373 (18)	NCN asym. stret.
1394 (19)	NH bend. ip	1361 (24)	CNC asym. stret.	1282 (60)	C4N3 stret.
1239 (14)	C4-C5 stret.	1264 (14)	C2N1 stret.	1226 (163)	C2N3 stret.
1216 (224)	C4-N stret.	1215 (131)	C4-N stret.	1189 (57)	C=Se asym. stret.
1131 (119)	C=Se stret.	1115 (191)	C=Se stret.	1112 (233)	CH bend.ip
1076 (22)	C6-N1 stret.	1103 (7.4)	CH bend.ip	1079 (69)	CH bend.ip
1005 (9.5)	Ring def. ip	1008 (5.1)	Ring def. ip	990 (20)	Ring def. ip
973 (0.03)	CH bend. op	978 (0.2)	CH bend. op	985 (0.7)	CH bend. op
889 (5.5)	Ring def. ip	915 (15)	Ring def. ip	835 (27)	CH bend. op
822 (55)	CH bend. op	823 (30)	CH bend. op	817 (18)	N3H bend. op
755 (44)	N3H bend. op	770 (49)	Ring def. op	810 (21)	Ring def. ip
732 (52)	NH and CH bend. op	723 (8.2)	N3H bend. op	739 (47)	Ring def. op
701 (1.3)	Ring def. op	719 (51)	Ring def. op	722 (0.05)	Ring def. op
697 (1.9)	Ring def. ip	693 (0.04)	Ring def. ip	674 (0.7)	Ring def. ip
647 (29)	N1H bend. op	581 (49)	N1H bend. op	654 (35)	N1H bend. op
537 (8.9)	Ring def. ip	564 (10)	Ring def. ip	428 (19)	Ring def. op
489 (11)	C=O bend. ip	489 (8.9)	C=O bend. ip	379 (12)	Ring def. ip
422 (13)	Ring def. op	405 (30)	Ring def. op	333 (3.1)	C=Se asym. bend. ip
342 (10)	Ring def. ip	336 (7.7)	Ring def. ip	325 (4.0)	Ring def. ip
217 (5.4)	C=Se bend. ip	222 (3.9)	C=Se bend. ip	165 (0.09)	Ring def. op
177 (1.2)	Ring def. op	171 (0.5)	Ring def. op	156 (0.0)	Ring def. op
157 (0.6)	Ring def. op	152 (0.04)	Ring def. op	134 (1.8)	C=Se sym. bend. ip

[a] ip and op stand for “in-plane” and “out-of-plane” respectively

It can be observed, that for the three compounds the N1-H stretching frequency is slightly larger than the N3-H stretching. The C=Se stretch, which is associated with a strong band in the region of 1131 cm^{-1} in 2-selenouracil, appears slightly red shifted in 4-selenouracil, while the C=O stretch is slightly blue-shifted. In 2,4-selenouracil the C=Se stretching as well as the C=Se bending displacements appear coupled as symmetric and antisymmetric combinations. Also the N1C2 and C2N3 stretching displacements appear coupled in the three compounds. The symmetric N1C2N3 stretching couples also with the symmetric combination of the NH bending modes.

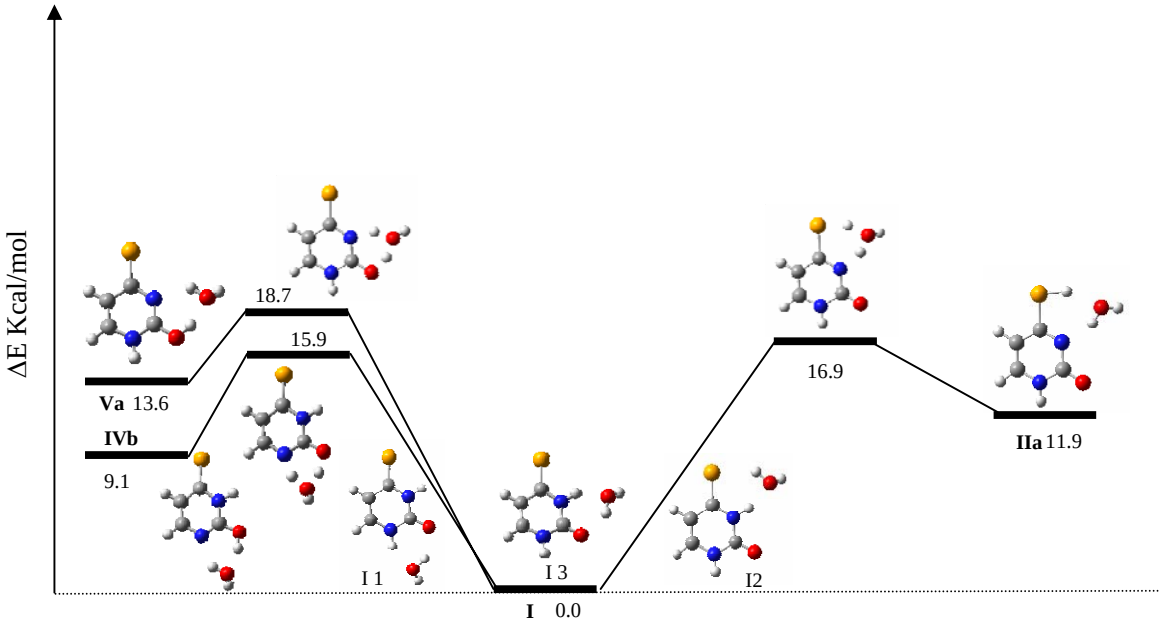


2-Selenouracil 4-Selenouracil 2,4- Diselenouracil

Figure S1. Optimized geometries of the most stable tautomer of 2-selenouracil, 4 selenouracil, and 2,4-diselenouracil. Bond lengths in Å and bond angles in degrees.

Figure S2

a) Monohydrated species



b) Solvated monohydrated species

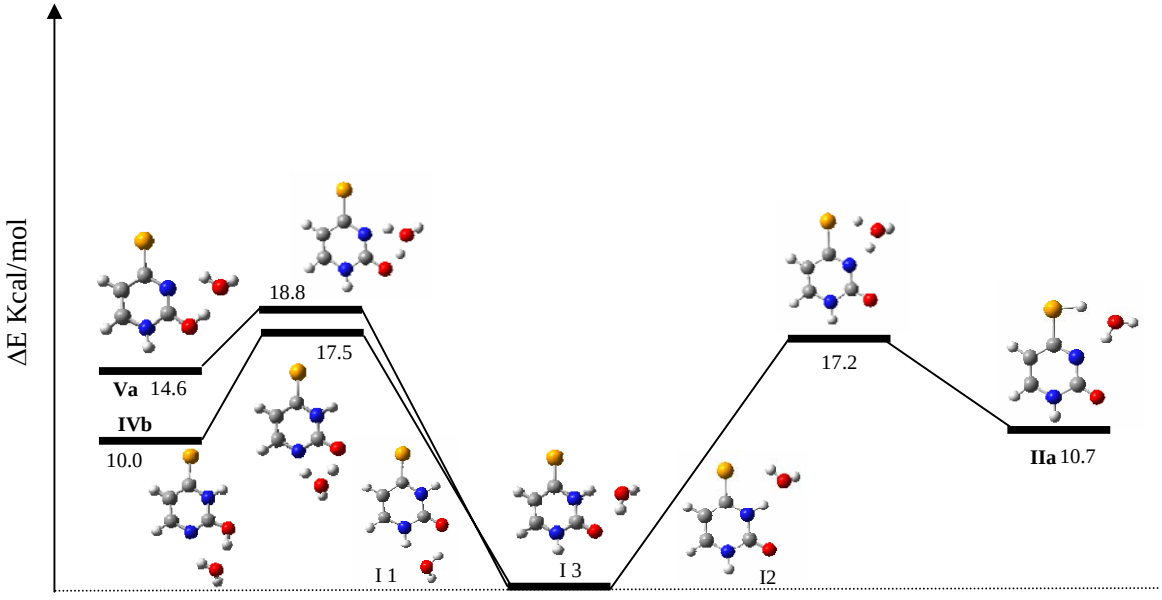
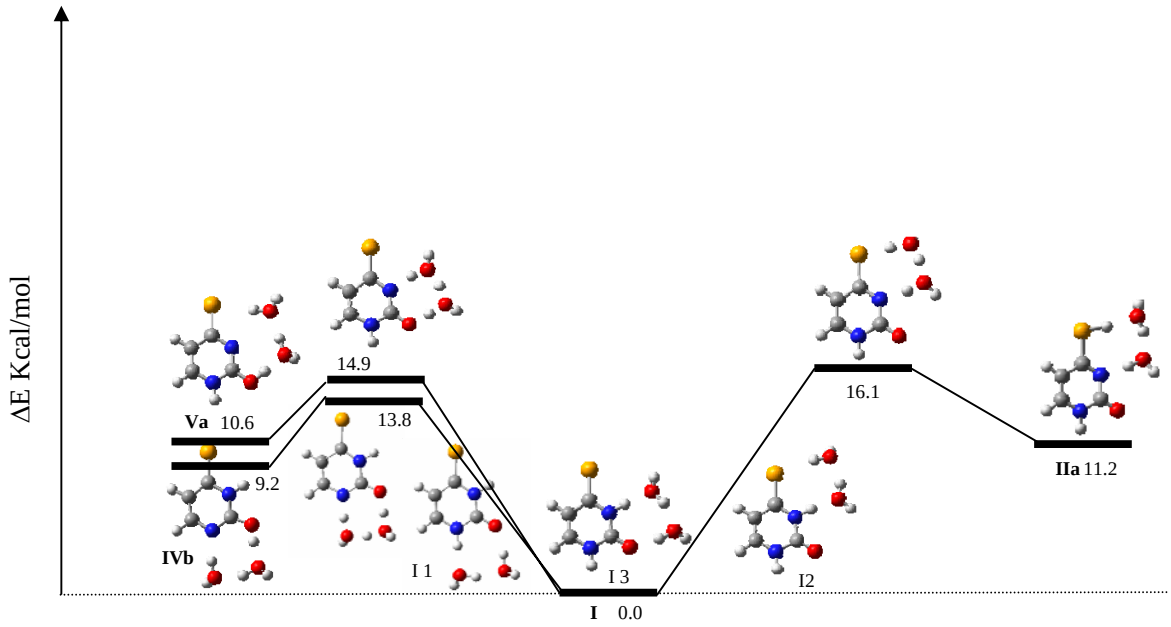


Figure S2 (continued)

c) Dihydrated species



d) Solvated dihydrated species

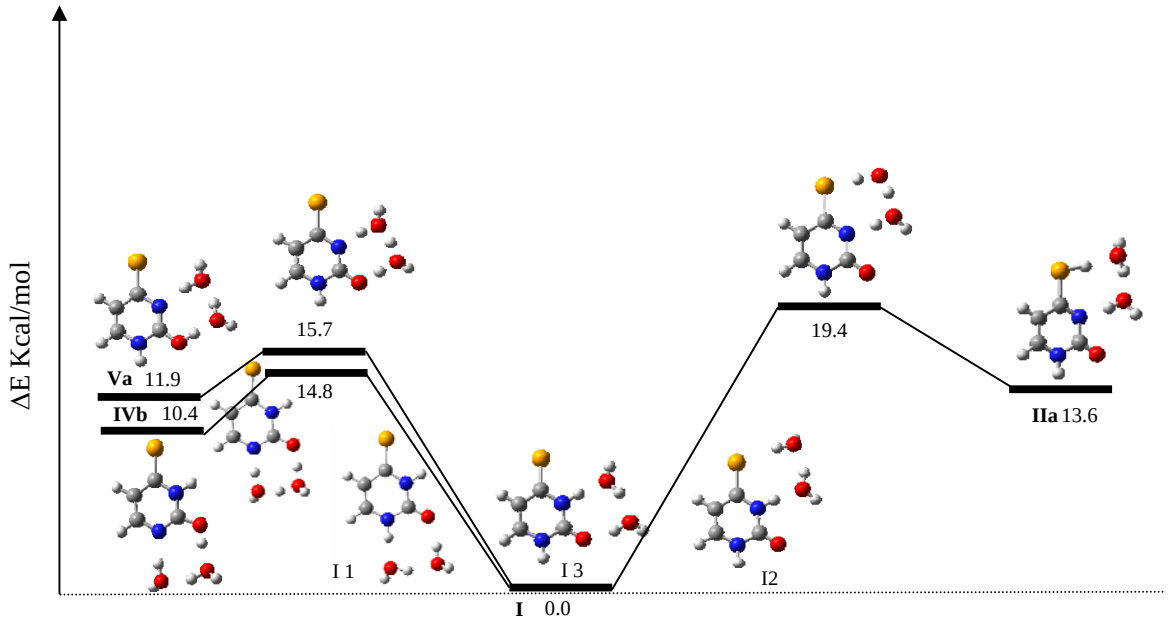
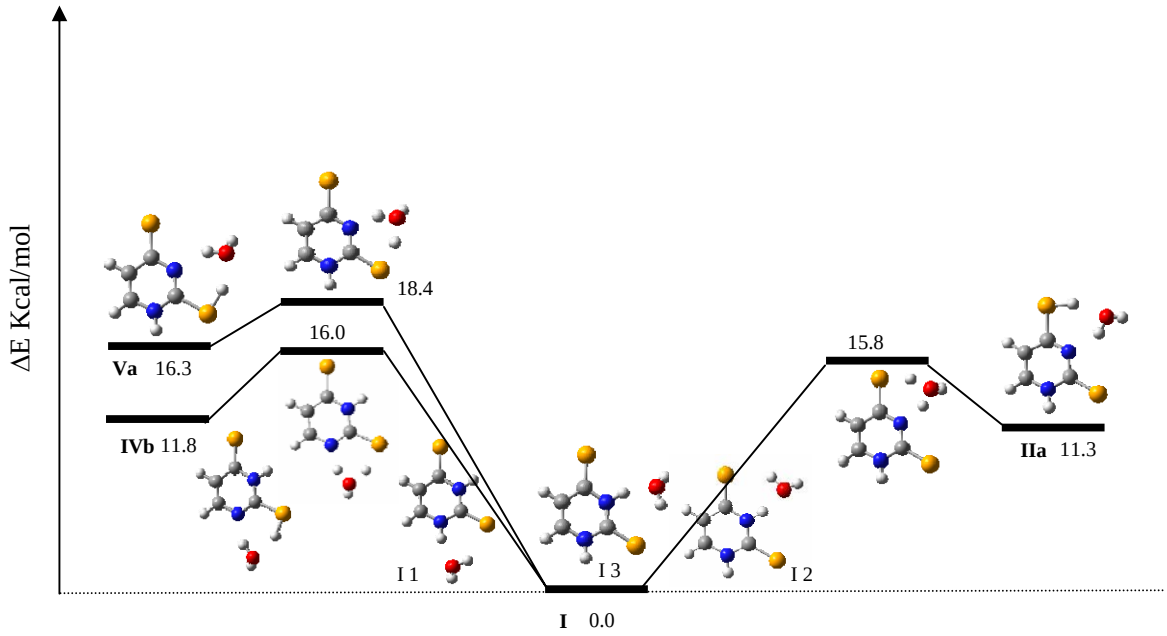


Figure S2. Energy profile for the tautomerization processes of 4-selenouracil

Figure S3

a) Monohydrated species



b) Solvated monohydrated species

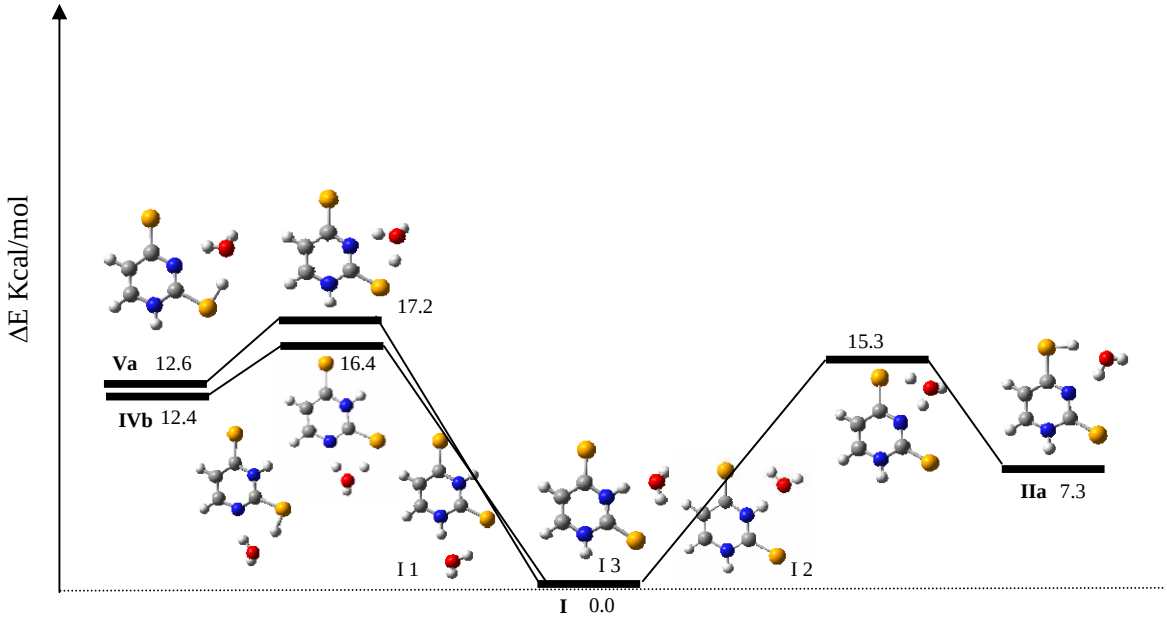


Figure S3. Energy profile for the tautomerization processes of 2,4-diselenouracil