

**Effect of Sr^{2+} association on the tautomerization processes of uracil
and its thio- and seleno-derivatives**

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Supplementary Data

Table S1. Energies were calculated with G96LYP functional and with an expanded LAN2DZ basis set for the Sr^{2+} cation, and 6-311+G(3df,2p) basis set for C, O, S, Se, N and H atoms. Zero-Point Vibrational energies were calculated with G96LYP functional and an improved LAN2DZ basis set for the Sr^{2+} cation and with 6-31+G(d,p) basis set for C, O, S, Se, N and H atoms. All values are in hartrees.

	Energy			ZPVE		
	Uracil	2,4-dithiouracil	2,4-diselenouracil	Uracil	2,4-dithiouracil	2,4-diselenouracil
1	-444.7589985	-1090.6806241	-5097.7646022	0.085143	0.080462	0.079407
2a	-444.779712	-1090.7170383	-5097.8036818	0.085697	0.07758	0.075485
2b	-444.7879791	-1090.7238408	-5097.8081268	0.086003	0.07792	0.075604
3a	-444.7759139	-1090.7224526	-5097.8101401	0.085268	0.077841	0.075651
3b	-444.7821756	-1090.7235817	-5097.8103965	0.085646	0.077926	0.075973
4	-444.7748398	-1090.6907804	-5097.7776998	0.085751	0.080811	0.079588
5a	-444.7765029	-	-	0.085716	-	-
5b	-444.7775054	-1090.7160437	-5097.8020021	0.085326	0.07736	0.075378
6a	-444.7465212	-1090.6812594	-5097.7694692	0.08441	0.077153	0.075201
6b	-444.7629515	-1090.6848334	-5097.770446	0.085321	0.077224	0.075312
7	-	-1090.6826945	-5097.7762935	-	0.080079	0.078924
TS1_4	-444.7237049 -444.688676 ^a	-1090.637835 ^a	-	0.083828 0.083934 ^a	0.079312 ^a	-
TS1_2a	-444.7059986	-1090.6466662	-5097.7355497	0.080468	0.07466	0.073076
TS2a_2b	-444.7696482	-1090.7110315	-5097.8012804	0.084182	0.077018	0.075103
TS4_5a	-444.7153288	-	-	0.08079	-	-
TS4_5b	-	-1090.6483424	-5097.7374953	-	0.074814	0.073161
TS5a_5b	-444.7632076	-	-	0.084005	-	-
TS1_7	-	-1090.6724175	-5097.7633306	-	0.080099	0.079158
TS7_4	-	-1090.6782397	-5097.7663707	-	0.08023	0.079061

^a π -type transition state structure.

Figure S1. Bond distances of uracil and uracil-Sr²⁺ complexes **1** and **4** and the corresponding dithio- and dieseleno-derivatives. All bond distances are given in Ångstrom.

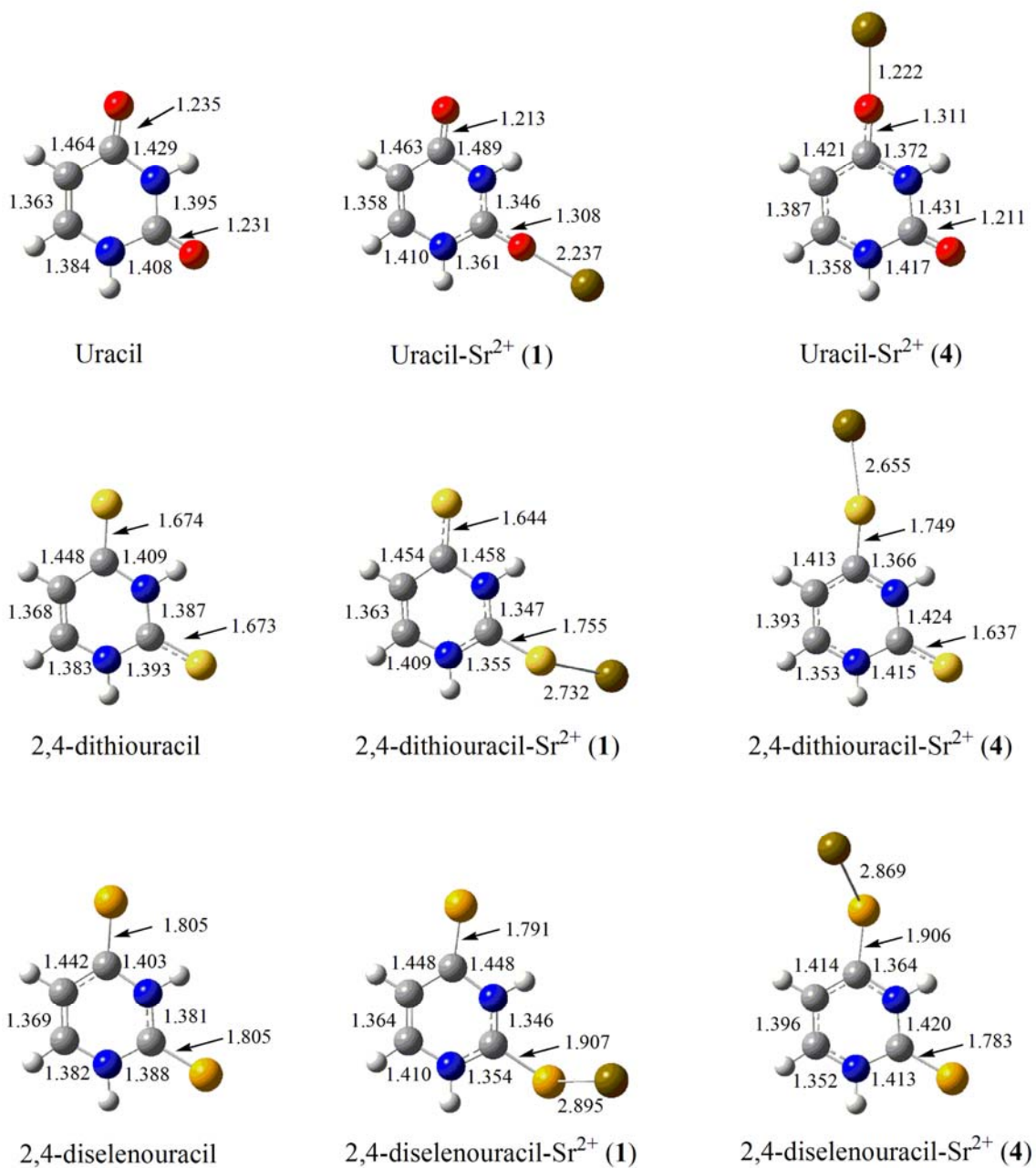
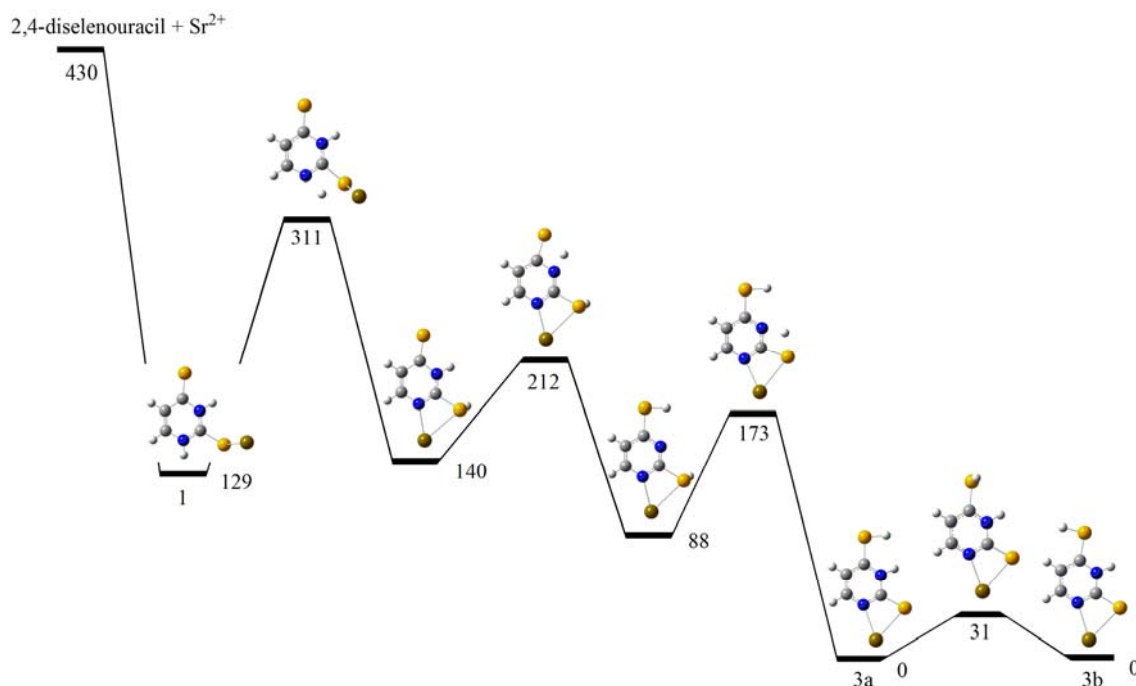


Figure S2. Proposed mechanism connecting complexes **1** and **3b** in the case of 2,4-diselenouracil (energies are in kJ mol^{-1}).**Table S2.** Optimized geometries (Cartesian Coordinates in Å) of Stationary Points of potential energy surfaces connecting the different structures of uracil— Sr^{2+} , 2,4-dithiouracil— Sr^{2+} and 2,4-diselenouracil— Sr^{2+} complexes. These structures were optimized with G96LYP functional and an improved LAN2DZ basis set for the Sr^{2+} cation and 6-31+G (d,p) basis set for C, O, S, Se, N and H atoms.**Uracil— Sr^{2+}**

1				2a			
7	1.231557	1.470660	0.005675	7	-1.660961	-1.674962	-0.000140
6	2.631118	1.640764	-0.006296	6	-2.897252	-1.067239	0.000653
1	2.964744	2.678092	-0.011366	1	-3.765824	-1.726766	0.001121
6	3.475703	0.577316	-0.011481	6	-2.978076	0.304252	0.000837
1	4.556594	0.713307	-0.021504	1	-3.932573	0.828277	0.001494
6	2.957140	-0.790677	-0.003096	6	-1.752362	1.036570	-0.000078
8	3.551587	-1.847949	-0.005330	8	-1.855414	2.359812	-0.000516
7	1.468427	-0.821071	0.010385	7	-0.532965	0.429234	-0.000965

1	1.069130	-1.763053	0.018160	6	-0.494758	-0.946197	-0.000618
6	0.644061	0.243293	0.013095	8	0.645143	-1.537419	-0.000783
8	-0.656946	0.109956	0.021775	1	-1.575493	-2.696451	-0.000114
1	0.633090	2.295391	0.011173	1	-0.991845	2.822288	-0.000219
38	-2.882335	-0.120818	-0.005100	38	2.211581	0.182876	0.000292
2b				3a			
7	1.718393	-1.663922	-0.003150	7	-0.099954	0.756987	0.000338
6	2.904290	-0.970346	-0.005544	6	-1.131859	1.654097	0.000158
1	3.817546	-1.567145	-0.010271	1	-0.856627	2.711117	0.000224
6	2.900835	0.408936	-0.002819	6	-2.472638	1.281623	-0.000092
1	3.837828	0.965439	-0.004757	1	-3.281175	2.011141	-0.000237
6	1.630429	1.061277	0.002255	6	-2.775958	-0.094907	-0.000093
8	1.458739	2.382026	0.002760	8	-4.035033	-0.489037	-0.000220
7	0.469814	0.362518	0.005995	7	-1.728830	-0.993133	0.000083
6	0.502034	-1.008739	0.005664	1	-1.882303	-2.008049	0.000046
8	-0.606750	-1.643937	0.008831	6	-0.397828	-0.576178	0.000219
1	1.705351	-2.689154	-0.003422	8	0.548314	-1.436966	0.000197
1	2.302908	2.883175	0.000576	1	-4.196179	-1.457922	-0.000154
38	-2.142698	0.175422	-0.002424	38	2.410032	0.058341	-0.000100
3b				4			
7	-0.107372	0.765256	0.003602	7	3.387360	0.515662	-0.000013
6	-1.139050	1.655139	0.001351	6	2.621269	1.637156	-0.000019
1	-0.869550	2.713980	0.002487	1	3.157166	2.588135	-0.000025
6	-2.484428	1.280102	-0.000991	6	1.235202	1.572655	0.000012
1	-3.279083	2.025590	-0.002579	1	0.636919	2.480140	0.000004
6	-2.774415	-0.098222	-0.000695	6	0.616854	0.293584	0.000029
8	-3.955558	-0.689276	-0.002136	8	-0.679179	0.097547	0.000040
7	-1.724934	-0.987722	0.001043	7	1.436394	-0.806678	0.000022
1	-1.920796	-1.996780	0.000524	1	1.030853	-1.745827	0.000032
6	-0.402841	-0.574719	0.002295	6	2.867331	-0.802682	0.000001
8	0.551456	-1.425235	0.001807	8	3.533700	-1.814058	-0.000018
1	-4.713461	-0.064461	-0.003422	1	4.410385	0.575041	-0.000026
38	2.411744	0.058453	-0.001017	38	-2.891624	-0.114015	-0.000010
5a				5b			
7	-2.907594	0.261193	-0.000807	7	-2.829537	0.362878	-0.000119
6	2.888372	-1.120285	-0.000519	6	-2.893692	-1.029077	0.000170
1	-3.860408	-1.614518	-0.001063	1	-3.897311	-1.455468	0.000243
6	-1.686511	-1.780777	0.000262	6	-1.743869	-1.770414	0.000120
1	-1.626408	-2.868047	0.000549	1	-1.761466	-2.859495	0.000291
6	-0.485171	-0.995618	0.000560	6	-0.488968	-1.063649	-0.000092
8	0.697027	-1.505986	0.000668	8	0.664955	-1.622369	-0.000100
7	-0.543757	0.408755	0.000512	7	-0.474316	0.337770	0.000241
6	-1.749432	0.985786	0.000128	6	-1.623436	1.010909	0.000068
8	-1.956543	2.298506	0.000252	8	-1.534554	2.339311	-0.001381
1	-3.795718	0.773526	-0.000794	1	-3.706350	0.890816	-0.002633
1	-1.128372	2.819716	0.002688	1	-2.388005	2.823463	0.010235
38	2.250090	0.192760	-0.000244	38	2.166755	0.186158	0.000033
6a				6b			
7	3.401757	0.654393	-0.003745	7	3.421406	0.597667	-0.003671
6	2.540902	1.692085	-0.001975	6	2.594083	1.670084	-0.002238

1	2.999382	2.684968	-0.004125	1	3.086197	2.646285	-0.004321
6	1.140319	1.558690	0.002209	6	1.192529	1.581185	0.001760
1	0.489096	2.431361	0.003651	1	0.570110	2.474422	0.003018
6	0.601835	0.264367	0.004491	6	0.605980	0.302023	0.004369
8	-0.676495	-0.049118	0.007612	8	-0.681368	0.037655	0.008200
7	1.516145	-0.789145	0.003205	7	1.480054	-0.775041	0.003167
1	1.134999	-1.739243	0.005874	1	1.113947	-1.731532	0.005698
6	2.888256	-0.565145	-0.000961	6	2.849206	-0.595285	-0.000822
8	3.742067	-1.582773	-0.002432	8	3.534084	-1.730922	-0.001698
1	3.345758	-2.478200	-0.000226	1	4.500094	-1.539022	-0.004418
38	-2.893342	-0.121065	-0.001722	38	-2.890871	-0.126591	-0.001760
TS1_4				TS1_2a			
7	-2.132761	-1.307604	-0.123225	7	1.352789	1.522690	0.000153
6	-2.965452	-0.168946	-0.230498	6	2.747114	1.583227	-0.000181
1	-3.994638	-0.388183	-0.519118	1	3.165664	2.590050	-0.000277
6	-2.488518	1.113279	-0.118461	6	3.518305	0.448968	-0.000358
1	-3.114004	1.971801	-0.366220	1	4.606390	0.485286	-0.000466
6	-1.074827	1.274312	0.149231	6	2.798815	-0.791338	-0.000091
8	-0.251318	2.129055	-0.177318	8	3.121955	-2.019724	0.000000
7	-0.461295	0.076517	0.852047	7	1.395284	-0.782311	0.000170
6	-0.814238	-1.176989	0.202627	6	0.655010	0.329024	0.000306
8	0.136173	-1.924606	-0.104958	8	-0.648268	0.333323	0.000506
1	-2.447159	-2.196188	-0.529592	1	0.817900	2.391920	0.000357
38	1.932936	0.033459	-0.086590	38	-2.832530	-0.119706	-0.000115
1	-0.758001	0.073211	1.844418	1	1.704702	-2.029171	0.000408
TS2a_2b				TS4_5a			
7	-1.703637	-1.669941	0.009422	7	3.436397	0.437727	-0.000227
6	-2.899686	-1.002197	-0.060516	6	2.706078	1.614493	-0.000175
1	-3.800248	-1.616534	-0.108732	1	3.288829	2.536038	-0.000351
6	-2.912072	0.380767	-0.067211	6	1.329216	1.598915	0.000081
1	-3.842176	0.943401	-0.132690	1	0.772115	2.533732	0.000132
6	-1.663360	1.054136	0.024687	6	0.626927	0.334209	0.000316
8	-1.616877	2.396518	-0.063841	8	-0.675772	0.240193	0.000562
7	-0.487342	0.378897	0.086834	7	1.391858	-0.784695	0.000349
6	-0.498412	-0.997102	0.064355	6	2.767419	-0.752396	-0.000038
8	0.618056	-1.620927	0.075208	8	3.184636	-1.951088	-0.000155
1	-1.670967	-2.695506	0.003823	1	4.460819	0.441412	-0.000512
1	-1.507450	2.881920	0.779671	38	-2.862168	-0.108458	-0.000125
38	2.157617	0.176465	-0.028281	1	1.794091	-2.045150	0.000252
TS5a_5b				TS1_4 π			
7	3.272060	-0.207804	-0.038766	6	-1.192346	0.485403	1.685620
6	2.821191	-1.507399	-0.026393	7	-0.342755	1.362376	0.948506
1	3.580764	-2.288847	-0.063242	6	-0.406758	1.420272	-0.485490
6	1.465604	-1.749297	0.020372	6	-1.765791	-0.788111	-0.342820
1	1.076130	-2.766041	0.026434	7	-0.727990	0.119448	-1.007658
6	0.587591	-0.616165	0.042605	8	0.004520	2.354547	-1.143848
8	-0.713335	-0.746712	0.050204	8	-2.333819	-1.605403	-1.026987
7	1.078938	0.664062	0.051411	6	-1.841027	-0.563446	1.106438
6	2.388071	0.846761	0.012565	1	-2.501760	-1.207201	1.688916
8	2.904808	2.080525	-0.101917	1	-1.274444	0.717302	2.749911
1	4.273156	-0.005046	-0.123812	1	-0.166257	2.283796	1.371555
38	-2.730183	0.181020	-0.014064	1	-0.888410	0.149733	-2.028449

1	3.253411	2.473474	0.725346	38	1.636737	-0.569323	0.058324
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2,4-dithiouracil—Sr²⁺

1				2a			
7	1.241378	1.888680	-0.109986	7	-1.297384	2.149252	-0.000023
6	2.612909	1.971618	-0.420229	6	-2.599594	1.724775	-0.000105
1	2.973114	2.969213	-0.668897	1	-3.369382	2.497932	-0.000159
6	3.393630	0.854988	-0.400617	6	-2.867509	0.374159	-0.000090
1	4.453317	0.921681	-0.644149	1	-3.896182	0.014668	-0.000124
6	2.849973	-0.447428	-0.051200	6	-1.760136	-0.529005	0.000013
7	1.431275	-0.375989	0.276093	7	-0.464828	-0.079392	0.000056
1	1.029814	-1.258701	0.602810	6	-0.224588	1.279992	0.000046
6	0.651226	0.721567	0.244410	1	-1.087647	3.152855	-0.000017
1	0.673602	2.737078	-0.100998	16	-2.173067	-2.234813	0.000051
38	-3.325627	-0.413150	-0.226341	16	1.370417	1.935383	0.000103
16	3.625703	-1.895821	0.012933	1	-0.902840	-2.718111	0.000402
16	-1.032643	0.716890	0.738021	38	2.082760	-0.782763	-0.000052
2b				3a			
7	1.404811	2.117794	-0.000107	7	-0.231346	-0.773576	0.001037
6	2.678848	1.618942	-0.000773	6	0.708799	-1.768299	0.000841
1	3.490440	2.348566	-0.000950	1	0.331279	-2.793583	0.001266
6	2.881637	0.252909	-0.000843	6	2.079907	-1.534954	0.000217
1	3.892880	-0.150353	-0.000888	1	2.787380	-2.363471	-0.000010
6	1.727410	-0.583185	-0.000358	6	2.535021	-0.194511	-0.000020
7	0.464193	-0.056284	0.000082	7	1.563711	0.784834	0.000261
6	0.282930	1.306174	0.000331	1	1.825573	1.775713	0.000091
1	1.253189	3.131849	-0.000007	6	0.195095	0.527803	0.000633
16	1.774339	-2.337419	0.000975	16	4.242021	0.148456	-0.000676
16	-1.285321	2.012196	0.000900	16	-0.909511	1.847311	0.000448
1	3.123517	-2.494670	-0.001685	1	4.153449	1.507576	-0.000351
38	-2.055060	-0.727143	-0.000433	38	-2.759403	-0.324146	-0.000433
3b				4			
7	0.232632	-0.783061	0.000576	7	-3.361189	1.041099	-0.121300
6	-0.702157	-1.779871	0.000427	6	-2.477622	2.065237	-0.094395
1	-0.320145	-2.803777	0.000607	1	-2.897210	3.070479	-0.167024
6	-2.077248	-1.555945	0.000099	6	-1.108066	1.835880	0.023286
1	-2.772755	-2.393631	-0.000120	1	-0.405745	2.663471	0.054866
6	-2.537855	-0.219229	0.000073	6	-0.672804	0.494632	0.118405
7	-1.568175	0.765109	0.000290	7	-1.612002	-0.496537	0.087407
1	-1.844296	1.753818	0.000214	1	-1.314522	-1.472658	0.169994
6	-0.202124	0.518596	0.000440	6	-3.021542	-0.330217	-0.033055
16	-4.193411	0.326901	-0.000363	1	-4.365071	1.228537	-0.206045
16	0.897560	1.841404	0.000170	16	0.995584	0.011123	0.320899
1	-4.740914	-0.917106	-0.001028	16	-4.092411	-1.568347	-0.064507
38	2.759917	-0.315469	-0.000233	38	3.605903	-0.231036	-0.100059
5b				6a			
7	-2.792726	0.285969	0.035097	7	-3.200329	1.268394	-0.066502

6	-2.657201	1.667147	0.061965	6	-2.135603	2.084932	-0.007363
1	-3.584642	2.239523	0.102895	1	-2.354000	3.156512	-0.033135
6	-1.405659	2.224217	0.031867	6	-0.800959	1.630650	0.084819
1	-1.276635	3.305839	0.048464	1	0.022386	2.339531	0.142004
6	-0.258334	1.359401	-0.022729	6	-0.576588	0.251622	0.116258
7	-0.453901	-0.030634	-0.019456	7	-1.698811	-0.562629	0.057557
6	-1.698825	-0.535826	-0.000418	1	-1.545173	-1.574508	0.089163
1	-3.735684	-0.109119	0.024683	6	-2.984632	-0.050675	-0.031170
16	1.340608	1.988493	-0.071658	16	0.951833	-0.602159	0.250992
16	-1.833175	-2.294876	-0.065431	16	-4.418058	-1.055679	-0.106335
1	-3.160272	-2.407052	0.207102	1	-3.786607	-2.261029	-0.049404
38	2.065390	-0.742212	0.033597	38	3.589571	-0.094069	-0.088837
6b				7			
7	-3.218134	1.266684	-0.073077	7	-2.401275	-1.035856	-0.207919
6	-2.155157	2.090414	-0.012279	6	-3.025056	0.199551	-0.358994
1	-2.380907	3.160374	-0.040726	1	-4.060348	0.160533	-0.701024
6	-0.818610	1.647517	0.084740	6	-2.331732	1.385615	-0.199650
1	-0.000736	2.362490	0.142937	1	-2.798122	2.335244	-0.464601
6	-0.583697	0.268561	0.120936	6	-0.969003	1.336851	0.213429
7	-1.697818	-0.550041	0.060868	7	-0.526738	0.040999	0.732553
1	-1.546937	-1.563665	0.096275	1	-0.439139	0.035628	1.759716
6	-2.987873	-0.049901	-0.033530	6	-1.110447	-1.171142	0.227445
16	0.950635	-0.570879	0.265163	1	-2.881788	-1.879440	-0.540712
16	-4.295708	-1.215860	-0.100356	38	1.930578	-0.099739	-0.169973
1	-5.248527	-0.249243	-0.179965	16	0.245027	2.498996	0.104704
38	3.588999	-0.102057	-0.092873	16	-0.124342	-2.524191	0.110283
TS1 4 π				TS1 2a			
6	-0.313016	0.018623	2.087259	7	1.624664	-1.975678	0.000146
7	0.783460	0.628970	1.426452	6	2.993983	-1.747318	0.000036
6	0.673101	1.233445	0.141616	1	3.618772	-2.641123	0.000003
6	-1.720948	0.254490	0.077347	6	3.498400	-0.467893	-0.000009
7	-0.449674	0.679856	-0.566594	1	4.572071	-0.286598	-0.000149
6	-1.495497	-0.225084	1.438050	6	2.558174	0.608751	0.000035
1	-2.328427	-0.678021	1.977015	7	1.183121	0.297530	-0.000038
1	-0.139951	-0.233814	3.135667	6	0.701113	-0.949602	0.000040
1	1.522149	1.036807	2.012740	1	1.274862	-2.937075	0.000247
1	-0.617541	1.168961	-1.459370	38	-3.041260	0.444918	0.000032
38	0.983532	-1.530944	-0.360332	16	2.667822	2.299805	-0.000019
16	1.822006	2.201438	-0.531424	16	-0.986880	-1.397166	-0.000151
16	-3.135055	0.300517	-0.747205	1	1.042585	1.599074	0.000023
TS2a 2b				TS4 5b			
7	1.493566	2.099976	-0.025835	7	-3.444273	-0.491377	0.000065
6	2.728039	1.529941	-0.127427	6	-2.984252	-1.794590	0.000037
1	3.577414	2.211701	-0.206152	1	-3.747525	-2.573492	0.000024
6	2.851555	0.144074	-0.117323	6	-1.633192	-2.061418	-0.000002
1	3.828211	-0.332336	-0.188072	1	-1.273412	-3.088535	-0.000048
6	1.661731	-0.610780	0.019614	6	-0.700765	-0.962615	-0.000007
7	0.447079	-0.018278	0.093426	7	-1.208043	0.292459	0.000038
6	0.323517	1.356005	0.068283	6	-2.569467	0.560361	0.000020
1	1.402467	3.122607	-0.039310	1	-4.450110	-0.301581	0.000109
38	-2.021203	-0.692013	-0.067423	16	1.009389	-1.307444	-0.000076

16	1.692128	-2.423747	0.014976	16	-2.786483	2.243601	-0.000044
16	-1.218452	2.094857	0.117039	38	3.130311	0.428726	0.000022
1	1.445245	-2.530561	1.351350	1	-1.154982	1.635484	0.000003
TS1 7				TS7 4			
7	1.242218	2.055179	-0.352332	7	-2.785580	0.435096	-0.505094
6	2.552850	1.659568	-0.680327	6	-2.406861	1.724026	-0.721821
1	3.177650	2.438925	-1.116425	1	-3.150361	2.369855	-1.193743
6	2.965051	0.373087	-0.477174	6	-1.134904	2.179217	-0.380093
1	3.974265	0.068959	-0.754082	1	-0.835571	3.203412	-0.595286
6	2.075798	-0.617987	0.096865	6	-0.244131	1.294230	0.263327
7	0.809514	-0.037853	0.541076	7	-0.700872	-0.026500	0.495494
1	0.420989	-0.499012	1.368925	1	-0.389353	-0.448164	1.377419
6	0.365361	1.242537	0.280921	6	-1.989878	-0.547166	0.106398
1	0.930433	3.002433	-0.584340	1	-3.726703	0.129011	-0.774041
38	-2.311007	-0.708100	-0.300006	16	1.364889	1.680695	0.766015
16	2.322168	-2.236346	0.297872	16	-2.438621	-2.104142	0.368137
16	-1.247266	1.725845	0.692329	38	2.219513	-0.769499	-0.328960

2,4-diselenouracil—Sr²⁺

1				2a			
7	-0.549638	2.149683	-0.522456	7	0.296869	2.516699	-0.015157
6	-1.878862	2.367356	-0.941336	6	-1.010627	2.924600	-0.033970
1	-2.073051	3.338980	-1.393855	1	-1.191403	4.000481	-0.048752
6	-2.818409	1.393732	-0.767824	6	-2.009202	1.975394	-0.028416
1	-3.844192	1.561059	-1.093573	1	-3.055473	2.279512	-0.035726
6	-2.490885	0.125058	-0.150192	6	-1.628138	0.600337	-0.001678
7	-1.107883	0.062392	0.275475	7	-0.312237	0.221425	0.009559
1	-0.865610	-0.777991	0.807587	6	0.668686	1.187701	0.005065
6	-0.166868	1.007289	0.095079	1	1.045634	3.216605	-0.017689
1	0.140267	2.894923	-0.628107	34	-3.057201	-0.648115	0.011570
34	-3.561198	-1.282444	0.133030	34	2.495919	0.774110	0.021436
34	1.593547	0.869296	0.816050	1	-2.195127	-1.845729	0.143668
38	3.401987	-0.995133	-0.464375	38	1.275348	-1.874467	-0.020277
2b				3a			
7	0.389932	2.547570	0.012100	7	0.608527	-1.056859	0.000083
6	-0.900859	3.003496	0.031634	6	-0.364821	-2.019844	0.000092
1	-1.039171	4.085895	0.044554	1	-0.022385	-3.057445	0.000133
6	-1.942988	2.097991	0.030866	6	-1.728064	-1.739782	0.000049
1	-2.972777	2.449882	0.041004	1	-2.459838	-2.546772	0.000041
6	-1.614237	0.712756	0.008290	6	-2.138551	-0.387124	0.000015
7	-0.312883	0.287560	-0.004866	7	-1.131823	0.555749	0.000034
6	0.709795	1.202459	-0.004593	1	-1.364980	1.552962	0.000035
1	1.164274	3.219205	0.012327	6	0.224494	0.255271	0.000042
34	-2.901472	-0.675770	-0.020591	34	-3.965064	0.061415	-0.000035
34	2.507181	0.685770	-0.021091	34	1.467229	1.654003	0.000026
1	-4.090504	0.193735	0.088888	1	-3.749280	1.528863	-0.000133
38	1.113012	-1.900917	0.020595	38	3.163885	-0.761715	-0.000047

3b				4			
7	-0.619680	1.074051	0.001952	7	2.605254	1.611090	-0.333058
6	0.336380	2.052401	0.002039	6	1.556549	2.459794	-0.248668
1	-0.024034	3.084100	0.002999	1	1.768194	3.514395	-0.435893
6	1.706408	1.798824	0.001220	6	0.280445	1.996450	0.076025
1	2.417551	2.622748	0.001333	1	-0.544667	2.693386	0.189601
6	2.140914	0.454914	0.000354	6	0.124165	0.617222	0.343642
7	1.147639	-0.505707	0.000471	7	1.224119	-0.182393	0.242134
1	1.400795	-1.499533	-0.000101	1	1.138802	-1.179764	0.460433
6	-0.211693	-0.232184	0.001125	6	2.539712	0.217083	-0.114172
34	3.920067	-0.162326	-0.000868	1	3.537716	1.965192	-0.569128
34	-1.430462	-1.651213	0.000658	34	-1.456478	-0.202271	1.023574
1	4.491912	1.202462	-0.000664	34	3.918734	-0.903356	-0.260629
38	-3.170015	0.732326	-0.001101	38	-3.774411	-0.293318	-0.665516
5b				6a			
7	1.856248	2.035159	0.098889	7	2.564131	1.675358	-0.005156
6	0.877941	3.018497	0.138104	6	1.447379	2.380996	0.235628
1	1.229737	4.048657	0.206232	1	1.566652	3.467703	0.276581
6	-0.445371	2.654630	0.076979	6	0.178861	1.790429	0.443042
1	-1.227051	3.413628	0.100250	1	-0.682860	2.407533	0.690283
6	-0.786473	1.263731	-0.011786	6	0.079913	0.398758	0.383546
7	0.252558	0.318428	-0.009537	7	1.252553	-0.293712	0.130408
6	1.527657	0.710356	0.035692	1	1.202817	-1.316033	0.106195
1	2.840912	2.313002	0.071398	6	2.472132	0.341898	-0.045861
34	-2.542472	0.654758	-0.095063	34	-1.441032	-0.692465	0.756178
34	2.893891	-0.644150	-0.109673	34	4.097827	-0.572945	-0.350221
1	3.705946	-0.132025	1.020664	1	3.507931	-1.934264	-0.305399
38	-1.060578	-1.904271	0.092186	38	-3.887160	0.033026	-0.566977
6b				7			
7	2.575521	1.714013	-0.074425	7	-1.233770	2.344296	-0.308290
6	1.460162	2.429765	0.154883	6	-0.062989	3.072041	-0.492490
1	1.583065	3.516875	0.157147	1	-0.193631	4.082633	-0.881894
6	0.192247	1.853170	0.396606	6	1.178580	2.490118	-0.300374
1	-0.665421	2.481165	0.629851	1	2.084801	3.024528	-0.587369
6	0.089525	0.459709	0.390382	6	1.248825	1.157980	0.191198
7	1.256226	-0.242088	0.150971	7	0.002316	0.627772	0.691710
1	1.206439	-1.265955	0.168705	1	0.006594	0.364387	1.683901
6	2.477236	0.380713	-0.065348	6	-1.252530	1.078390	0.207033
34	-1.430091	-0.608321	0.829878	1	-2.119009	2.730893	-0.654124
34	3.997348	-0.715126	-0.341309	34	2.628870	-0.050992	0.159886
1	4.862916	0.473010	-0.498541	34	-2.626491	-0.134090	0.164031
38	-3.852921	-0.032935	-0.601670	38	0.054980	-1.881719	-0.286575
TS1_2a				TS2a_2b			
7	-0.849558	2.454122	0.179274	7	-0.556020	2.555211	-0.073945
6	-2.223568	2.535988	0.349614	6	0.710688	3.050173	-0.193899
1	-2.622074	3.540351	0.497280	1	0.807318	4.133615	-0.288603
6	-3.003716	1.402391	0.321280	6	1.793659	2.179794	-0.169892
1	-4.083361	1.466116	0.446970	1	2.813231	2.556258	-0.236644
6	-2.349185	0.154812	0.098626	6	1.512695	0.800947	-0.006913

7	-0.948532	0.149235	-0.040681	7	0.243668	0.337178	0.076751
6	-0.197098	1.253425	-0.015294	6	-0.828019	1.199958	0.045397
1	-0.291256	3.311193	0.200168	1	-1.354310	3.199860	-0.095262
34	-2.892133	-1.589965	-0.117740	34	2.947417	-0.513214	0.054775
34	1.678803	1.330270	-0.268457	34	-2.568420	0.548707	0.114165
38	2.856815	-1.279823	0.177577	38	-0.911749	-1.940783	-0.121001
1	-1.081033	-1.157969	-0.257159	1	2.546677	-0.978684	1.406803
TS4 5b				TS1 7			
7	-3.001283	1.324903	0.147874	7	-0.224001	2.475779	0.562286
6	-2.310771	2.522177	0.172399	6	-1.593274	2.643358	0.829256
1	-2.915197	3.426323	0.252781	1	-1.865458	3.583319	1.309143
6	-0.936038	2.532303	0.096905	6	-2.484474	1.642439	0.541634
1	-0.393087	3.475723	0.114728	1	-3.536502	1.750056	0.804447
6	-0.227972	1.282796	-0.004245	6	-2.026837	0.413033	-0.058092
7	-0.957860	0.143738	-0.020484	7	-0.676535	0.507646	-0.535850
6	-2.342022	0.132384	0.044492	1	-0.431338	-0.139731	-1.286761
1	-4.023425	1.326073	0.195574	6	0.257392	1.415132	-0.132416
34	1.656455	1.334177	-0.135588	1	0.442816	3.177978	0.893038
34	-2.905243	-1.622020	-0.056630	34	-2.869060	-1.171217	-0.233770
38	2.987311	-1.219273	0.088069	34	2.091360	1.136433	-0.468616
1	-1.112462	-1.207542	-0.123325	38	1.926821	-1.704124	0.391945
TS7 4							
7	2.245970	1.655711	0.556966				
6	1.371077	2.656560	0.865537				
1	1.797890	3.534418	1.354464				
6	0.008053	2.532629	0.603520				
1	-0.688448	3.307725	0.917492				
6	-0.450348	1.386609	-0.083228				
7	0.519880	0.450905	-0.454909				
1	0.350323	-0.099105	-1.300346				
6	1.883525	0.450566	-0.047711				
1	3.235159	1.749476	0.809905				
34	-2.239570	1.000498	-0.508753				
34	2.947245	-0.975891	-0.284548				
38	-1.710280	-1.742991	0.432832				