

Interaction of Ca²⁺ with Uracil and its Thio Derivatives in the Gas Phase

Cristina Trujillo^a, Al Mokhtar Lamsabhi^a, Otilia M^ó^a, Manuel Yáñez^a and Jean-Yves Salpin^b

Contribution from Departamento de Química, C-9, Universidad Autónoma de Madrid. Cantoblanco, 28049-Madrid (Spain) and Université d'Evry Val d'Essonne – Laboratoire d'Analyse et Modélisation pour la Biologie et l'Environnement (LAMBE).CNRS – UMR 8587 – Bâtiment Maupertuis, Boulevard François Mitterrand, 91025 Evry, France

Supplementary Data (a total of 13 pages)

Table S1. B3LYP/6-311+G(3df,2p) Calculated Total Energies and B3LYP/6-31G(d,p) Zero-Point Vibrational Energies (ZPVE). All values are in hartrees

	Energy				ZPVE			
	Uracil	2-thiouracil	4-thiouracil	2,4-Dithiouracil	Uracil	2-thiouracil	4-thiouracil	2,4-Dithiouracil
1	-1092,03403	-1414,97189	-1414,99144	-1737,92951	0,08653	0,08398	0,08425	0,08167
2a	-1092,06063	-1415,01176	-1415,02393	-1737,97572	0,08701	0,08425	0,08151	0,07882
2b	-1092,06966	-1415,02485	-1415,02925	-1737,98283	0,08734	0,08477	0,08174	0,07910
3a	-1092,05746	-1415,01230	-1415,02608	-1737,98094	0,08664	0,08414	0,08157	0,07900
3b	-1092,06407	-1415,01856	-1415,02753	-1737,98219	0,08703	0,08447	0,08168	0,07909
4	-1092,05027	-1415,00429	-1414,98645	-1737,94119	0,08711	0,08466	0,08438	0,08197
5a	-1092,05763	-1415,01737	-1415,00950	-1737,96974	0,08673	0,08104	0,08403	0,07985
5b	-1092,06006	-1415,02128	-1415,01555	-1737,97549	0,08673	0,08127	0,08415	0,07843
6a	-1092,02317	-1414,99573	-1414,97926	-1737,93183	0,08590	0,08099	0,08404	0,07817
6b	-1092,02317	-1414,99119	-1414,96441	-1737,93554	0,08671	0,08088	0,08334	0,07821
7	-	-	-	-1737,93692	-	-	-	0,08283
TS1_4	-1091,99804	-1414,96324	-1414,96800	-	0,08534	0,08326	0,08334	-
TS1_2a	-1091,98006	-1414,91882	-1414,95265	-1737,89120	0,08179	0,07910	0,07838	0,07713
TS2a_2b	-1092,05108	-1415,00573	-1415,01256	-1737,96977	0,08552	0,08301	0,08073	0,07979
TS4_5a	-1091,98617	-1414,95761	-1414,92208	-1737,89364	0,08206	0,07855	0,07926	0,07733
TS5a_5b	-1092,05051	-1415,01334	-1415,00546	-	0,08552	0,08075	0,08470	-
TS1_7	-	-	-	-1737,92210	-	-	-	0,08288
TS7_4	-	-	-	-1737,92868	-	-	-	0,08302

Table S2. B3LYP/6-31G(d,p) optimized Geometries (Cartesian Coordinates in Å) of the Stationary Points of the potential energy surfaces connecting the different structures of uracil-Ca²⁺, and thiouracils-Ca²⁺ complexes

Uracil								
1			2a					
1	-2.170108	1.305661	0.000000	1	-2.292673	-1.108097	0.000000	
2	-0.768698	1.362295	0.000000	2	-1.045352	-1.671145	0.000000	
3	-2.824697	0.129615	0.000000	3	-2.420962	0.248966	0.000000	
4	-2.664708	2.269541	0.000000	4	-3.134548	-1.791970	0.000000	
5	0.000000	0.256443	0.000000	5	0.086377	-0.914674	0.000000	
6	-2.084923	-1.126521	0.000000	6	-1.227558	1.017927	0.000000	
7	-0.310514	2.264947	0.000000	7	-0.925598	-2.682384	0.000000	
8	-3.906756	0.081826	0.000000	8	-3.385635	0.740491	0.000000	
9	-0.634257	-0.920410	0.000000	9	0.000000	0.454249	0.000000	
10	1.290400	0.341001	0.000000	10	1.232906	-2.374351	0.000000	
11	-2.498615	-2.255205	0.000000	11	-1.374095	2.322698	0.000000	
12	-0.093936	-1.780630	0.000000	12	-0.544047	2.825282	0.000000	
13	3.447034	0.299678	0.000000	13	2.578285	0.351821	0.000000	

2b

1	-2.214743	-1.231800	0.000000
2	-0.955822	-1.758515	0.000000
3	-2.397012	0.124604	0.000000
4	-3.036538	-1.940222	0.000000
5	0.152516	-0.957513	0.000000
6	-1.231755	0.935136	0.000000
7	-0.807915	-2.766275	0.000000
8	-3.393279	0.550615	0.000000
9	0.000000	0.398857	0.000000
10	1.324723	-1.430811	0.000000
11	-1.239635	2.252302	0.000000
12	2.476252	0.561832	0.000000
13	-2.131290	2.642358	0.000000

3a

1	0.006519	-1.741914	0.000000
2	-0.691322	-0.576666	0.000000
3	1.385834	-1.803293	0.000000
4	-0.579581	-2.656007	0.000000
5	0.000000	0.590698	0.000000
6	2.092878	-0.594092	0.000000
7	1.928348	-2.740386	0.000000
8	1.381089	0.573244	0.000000
9	-0.624383	1.691701	0.000000
10	3.398252	-0.603008	0.000000
11	1.838088	1.484901	0.000000
12	-2.748606	0.813025	0.000000
13	3.854553	0.257002	0.000000

3b

1	0.023378	-1.742261	0.000000
2	-0.683950	-0.588878	0.000000
3	1.408374	-1.794512	0.000000
4	-0.552287	-2.663374	0.000000
5	0.000000	0.590832	0.000000
6	2.095881	-0.575847	0.000000
7	1.937839	-2.739633	0.000000
8	1.371934	0.580136	0.000000
9	-0.642133	1.680385	0.000000
10	3.387432	-0.374853	0.000000
11	3.924122	-1.187451	0.000000
12	1.862404	1.475953	0.000000
13	-2.755808	0.793109	0.000000

4

1	-2.265620	1.030117	0.000000
2	-2.713482	-0.242040	0.000000
3	-0.921031	1.325394	0.000000
4	-3.024176	1.806485	0.000000
5	-1.875435	-1.366549	0.000000
6	0.000000	0.253340	0.000000
7	-3.709950	-0.448784	0.000000
8	-0.577717	2.350046	0.000000
9	-0.504540	-1.008808	0.000000
10	-2.253085	-2.505714	0.000000
11	1.287368	0.396988	0.000000
12	0.124619	-1.806758	0.000000
13	3.390582	0.813547	0.000000

5a

1	-2.158394	-1.337449	0.000000
2	-2.309430	0.040568	0.000000
3	-0.919943	-1.890485	0.000000
4	-3.079213	-1.910058	0.000000
5	-1.230472	0.857922	0.000000
6	0.208122	-1.004258	0.000000
7	-3.250579	0.424893	0.000000
8	-0.768610	-2.962912	0.000000
9	0.000000	0.373460	0.000000
10	-1.345572	2.170731	0.000000
11	1.419539	-1.372377	0.000000
12	2.476418	0.644182	0.000000
13	-2.755808	0.793109	0.000000

5b

1	-2.249097	-1.198559	0.000000
2	-2.332604	0.173643	0.000000
3	-1.029879	-1.798985	0.000000
4	-3.191727	-1.734648	0.000000
5	-1.224011	0.945732	0.000000
6	0.130694	-0.964533	0.000000
7	-3.237562	0.641124	0.000000
8	-0.915699	-2.875691	0.000000
9	0.000000	0.430162	0.000000
10	-1.488267	2.234171	0.000000
11	1.318834	-1.412895	0.000000
12	2.598287	0.423359	0.000000
13	-0.703297	2.803262	0.000000

6a

1	-2.313244	0.816715	0.000000
2	-2.721579	-0.457814	0.000000
3	-0.973640	1.211202	0.000000
4	-3.102974	1.563886	0.000000
5	-1.799592	-1.390375	0.000000
6	0.000000	0.215299	0.000000
7	-0.695294	2.257310	0.000000
8	-0.455365	-1.089302	0.000000
9	-2.201598	-2.642746	0.000000
10	1.289348	0.396841	0.000000
11	0.244795	-1.826182	0.000000
12	3.255981	1.250433	0.000000
13	-1.510689	-3.323667	0.000000

6b

1	-2.281415	0.991965	0.000000
2	-2.757529	-0.265451	0.000000
3	-0.924609	1.311420	0.000000
4	-3.030323	1.779512	0.000000
5	-1.872949	-1.232858	0.000000
6	0.000000	0.262553	0.000000
7	-0.589573	2.340547	0.000000
8	-0.522473	-1.008699	0.000000
9	-2.195565	-2.506180	0.000000
10	1.294641	0.380149	0.000000
11	0.099031	-1.813932	0.000000
12	3.366389	0.911786	0.000000
13	-3.165672	-2.613027	0.000000

TS1_4

1	-2.478439	-0.338043	-0.165234
2	-1.536176	-1.389714	-0.107355
3	-2.121922	0.967743	-0.072702
4	-3.491316	-0.654817	-0.389872
5	-0.243785	-1.13847	0.168645
6	-0.713356	1.255015	0.115177
7	-1.778163	-2.294912	-0.509185
8	-2.830861	1.765436	-0.265082
9	0.019145	0.136099	0.798773
10	-0.003601	2.162854	-0.262976
11	-0.260962	0.110003	1.78908
12	2.315056	0.121514	-0.119057
13	0.756652	-1.795124	-0.156903

TS1_2a

1	2.042759	1.577514	0.000077
2	0.657668	1.505197	-0.00006
3	2.819721	0.46092	0.000133
4	2.450909	2.581947	0.00014
5	-0.022211	0.317158	-0.00013
6	2.111427	-0.777892	0.000024
7	0.118019	2.36323	-0.000111
8	3.901262	0.504091	0.000251
9	0.720807	-0.77894	-0.000092
10	2.439727	-1.990657	0.000008
11	-1.311279	0.30946	-0.000205
12	1.044198	-2.015145	-0.000114
13	-3.395073	-0.226728	0.000092

TS2a_2b

1	2.290931	-1.094016	-0.051717
2	1.066126	-1.687236	0.013603
3	2.386611	0.275037	-0.061945
4	3.150015	-1.755747	-0.093454
5	-0.087716	-0.955068	0.057852
6	1.185864	1.013689	0.020024
7	0.974449	-2.702397	0.010055
8	3.341483	0.781966	-0.121959
9	-0.016354	0.412257	0.073991
10	-1.227814	-1.503534	0.063706
11	1.218817	2.344335	-0.062236
12	-2.525368	0.380155	-0.048747
13	1.110838	2.83367	0.770088

TS4_5a

1	1.974507	1.619328	-0.000046
2	2.728996	0.468042	-0.000074
3	0.609875	1.572381	0.000064
4	2.530419	2.550176	-0.000091
5	2.093268	-0.725289	-0.000062
6	-0.057266	0.296198	0.000089
7	3.746078	0.495118	-0.000455
8	0.031814	2.486901	0.000332
9	0.729659	-0.791078	-0.000064
10	-1.342435	0.174405	0.000192
11	2.531121	-1.902784	0.000076
12	-3.445576	-0.199461	-0.000073
13	1.160833	-2.0304	0.000226

TS5a_5b

1	-2.271538	-1.140084	-0.048671
2	-2.295709	0.238065	-0.046887
3	-1.080673	-1.794733	0.011812
4	-3.234504	-1.635928	-0.103614
5	-1.16011	0.96432	0.023041
6	0.116117	-1.010241	0.054114
7	-3.178964	0.740169	-0.119566
8	-1.018121	-2.876141	0.008469
9	0.027286	0.387204	0.068423
10	-1.287825	2.286268	-0.068119
11	1.291792	-1.482965	0.060356
12	2.547228	0.403962	-0.044475
13	-1.288537	2.773769	0.773771

2-thiouracil

1				2a			
1	-2.380114	-1.418694	-0.464023	1	-2.661978	-0.220876	0.000000
2	-1.01523	-1.504332	-0.173921	2	-1.643206	-1.127928	0.000000
3	-3.037787	-0.243104	-0.394989	3	-2.372018	1.111692	0.000000
4	-2.84859	-2.355463	-0.742798	4	-3.670606	-0.620679	0.000000
5	-0.28919	-0.447224	0.222536	5	-0.326109	-0.773488	0.000000
6	-2.337879	0.9715	0.00142	6	-1.001864	1.470258	0.000000
7	-0.556087	-2.408555	-0.215739	7	-1.858419	-2.123490	0.000000
8	-4.095829	-0.171021	-0.617062	8	-3.138192	1.876832	0.000000
9	-0.921366	0.724537	0.301908	9	0.000000	0.560367	0.000000
10	-2.75359	2.093715	0.113231	10	-0.749297	2.761364	0.000000
11	-0.441431	1.530707	0.691885	11	2.520562	0.123899	0.000000
12	3.495569	0.508591	-0.43775	12	0.188990	3.003635	0.000000
13	1.36783	-0.702095	0.727955	13	0.858476	-2.016111	0.000000

2b				3a			
1	2.650764	-0.217923	0.000000	1	0.664009	-1.767751	0.000000
2	1.666439	-1.157041	0.000000	2	-0.330617	-0.839961	0.000000
3	2.332722	1.115209	0.000000	3	2.007155	-1.455493	0.000000
4	3.672041	-0.585259	0.000000	4	0.351582	-2.807840	0.000000
5	0.335231	-0.832620	0.000000	5	0.000000	0.475564	0.000000
6	0.954420	1.434797	0.000000	6	2.349652	-0.096573	0.000000
7	1.912420	-2.145589	0.000000	7	2.785289	-2.208657	0.000000
8	3.105646	1.874643	0.000000	8	1.340138	0.820342	0.000000
9	0.000000	0.489310	0.000000	9	3.605512	0.257448	0.000000

10	0.468487	2.664429	0.000000	10	1.547088	1.818777	0.000000
11	1.149530	3.359738	0.000000	11	-2.784818	-0.518939	0.000000
12	-2.451571	0.230014	0.000000	12	3.807216	1.210203	0.000000
13	-0.866250	-2.046369	0.000000	13	-1.176903	1.719349	0.000000

3b

1	0.747241	1.734247	0.000135
2	-0.287645	0.859740	0.000170
3	2.080412	1.361140	0.000298
4	0.486898	2.788908	0.000684
5	-0.017479	-0.476645	0.000000
6	2.349757	-0.012091	-0.000125
7	2.875972	2.096567	0.000757
8	1.297297	-0.875522	-0.000384
9	3.510505	-0.611596	-0.000267
10	4.278818	-0.013109	0.000150
11	-2.759124	0.644821	-0.000257
12	1.502503	-1.876037	-0.000681
13	-1.254556	-1.658089	0.000376

4

1	-2.383728	0.470387	0.000000
2	-2.305315	-0.873599	0.000000
3	-1.254645	1.260093	0.000000
4	-3.383778	0.892315	0.000000
5	-1.111709	-1.601722	0.000000
6	0.000000	0.611408	0.000000
7	-3.152476	-1.436808	0.000000
8	-1.325500	2.338260	0.000000
9	0.009037	-0.746963	0.000000
10	1.141167	1.227139	0.000000
11	0.900079	-1.234372	0.000000
12	2.927761	2.407678	0.000000
13	-1.009278	-3.226695	0.000000

5a

1	0.184023	-2.567330	0.000000
2	1.291611	-1.753493	0.000000
3	-1.058871	-2.018545	0.000000
4	0.376999	-3.634695	0.000000
5	1.194945	-0.397627	0.000000
6	-1.155937	-0.592956	0.000000
7	2.211693	-2.187834	0.000000
8	-1.958376	-2.621447	0.000000
9	0.000000	0.194837	0.000000
10	-2.259946	0.035565	0.000000
11	-1.621609	2.182486	0.000000
12	2.728953	0.449749	0.000000
13	2.191952	1.683094	0.000000

5b

1	-0.020465	-2.588947	0.000000
2	1.152176	-1.861636	0.000000
3	-1.220080	-1.952357	0.000000
4	0.092548	-3.667721	0.000000
5	1.150930	-0.505289	0.000000
6	-1.213306	-0.520761	0.000000
7	2.030983	-2.370397	0.000000
8	-2.159570	-2.491089	0.000000
9	0.000000	0.165686	0.000000
10	-2.257836	0.199733	0.000000
11	-1.376255	2.281044	0.000000
12	2.616879	0.447143	0.000000
13	3.506053	-0.568066	0.000000

6a

1	-2.368187	0.271843	0.000000
2	-2.250554	-1.061985	0.000000
3	-1.281514	1.147425	0.000000
4	-3.384772	0.656918	0.000000
5	-1.039379	-1.582578	0.000000
6	0.000000	0.596486	0.000000
7	-1.421641	2.220941	0.000000
8	0.080619	-0.777665	0.000000
9	1.119370	1.263668	0.000000
10	1.008666	-1.189419	0.000000

6b

1	-2.373614	0.312813	0.000000
2	-2.280553	-1.026285	0.000000
3	-1.275057	1.170826	0.000000
4	-3.383733	0.714441	0.000000
5	-1.075534	-1.560644	0.000000
6	0.000000	0.599736	0.000000
7	-1.398542	2.246327	0.000000
8	0.055864	-0.771820	0.000000
9	1.128067	1.249568	0.000000
10	0.974064	-1.208600	0.000000

11	2.651625	2.754987	0.000000	11	2.706317	2.692706	0.000000
12	-0.953691	-3.324363	0.000000	12	-0.829529	-3.287325	0.000000
13	0.393369	-3.429218	0.000000	13	-2.152159	-3.555268	0.000000

TS1_4

1	-2.446453	-0.940705	-0.273462
2	-1.212064	-1.600491	-0.183296
3	-2.559282	0.400376	-0.132937
4	-3.285846	-1.583821	-0.515086
5	-0.070322	-1.003796	0.181324
6	-1.373579	1.183659	0.14462
7	-1.163129	-2.575431	-0.476164
8	-3.506532	0.908981	-0.272956
9	-0.186352	0.366503	0.563437
10	-1.177954	2.373671	0.081715
11	-0.079341	0.458879	1.581193
12	2.118473	1.078737	-0.253897
13	1.473483	-1.685751	0.12056

TS1_2a

1	2.664348	-1.177080	-0.000018
2	1.326125	-1.522220	-0.000005
3	3.073544	0.123513	-0.000017
4	3.354809	-2.013556	-0.000039
5	0.316809	-0.602121	0.000013
6	2.028764	1.089902	0.000014
7	1.073551	-2.506657	-0.000011
8	4.118716	0.405857	-0.000041
9	0.698674	0.665857	0.000028
10	-1.311250	-1.208444	0.000015
11	0.633000	1.931010	0.000096
12	-3.330702	0.606998	-0.000015
13	1.967447	2.345966	-0.000007

TS2a_2b

1	2.391431	-1.163662	-0.105724
2	1.133373	-1.668741	-0.021395
3	2.579526	0.19697	-0.09048
4	3.201458	-1.882737	-0.17776
5	0.015423	-0.881181	0.060728
6	1.428145	0.99709	0.043545
7	0.99466	-2.678424	-0.040707
8	3.562932	0.645598	-0.155185
9	0.187586	0.476443	0.099699
10	1.550377	2.328472	0.018095
11	1.384003	2.783176	0.860419
12	-2.231319	1.069792	-0.098259
13	-1.540847	-1.590028	0.083569

TS4_5a

1	1.41478	2.116847	-0.000151
2	2.31162	1.079432	0.000371
3	0.070189	1.880314	-0.000476
4	1.839867	3.114514	-0.000384
5	1.881738	-0.207724	0.000457
6	-0.393287	0.520607	0.000069
7	3.310731	1.266398	0.000257
8	-0.634974	2.700898	-0.00102
9	0.531946	-0.453336	0.000947
10	2.690336	-1.684484	-0.000422
11	-3.653603	-0.517021	-0.000058
12	0.966472	-1.719139	0.000313
13	-1.650112	0.210818	0.000016

TS5a_5b

1	1.561457	2.059599	-0.040377
2	2.02563	0.762937	-0.036963
3	0.222014	2.300019	0.007988
4	2.315216	2.838624	-0.083038
5	1.191436	-0.29857	0.016527
6	-0.658349	1.172919	0.045769
7	3.028187	0.585752	-0.064614
8	-0.181946	3.305396	0.003933
9	-0.118462	-0.120267	0.048185

10	-1.923881	1.234655	0.05605
11	-2.477578	-0.970208	-0.039447
12	1.920302	-1.934031	-0.06486
13	1.806789	-2.160852	1.264013

4-thiouracil

1				2a			
1	-2.404124	0.596976	0.000000	1	0.528654	-2.517606	0.000000
2	-1.166684	1.260503	0.000000	2	-0.752844	-2.045158	0.000000
3	-2.459823	-0.750434	0.000000	3	1.572705	-1.637243	0.000000
4	-3.273957	1.241932	0.000000	4	0.651486	-3.595322	0.000000
5	0.000000	0.590841	0.000000	5	-1.022880	-0.709421	0.000000
6	-1.253064	-1.551462	0.000000	6	1.281105	-0.244294	0.000000
7	-1.142031	2.272265	0.000000	7	-1.548744	-2.680463	0.000000
8	-3.414273	-1.261745	0.000000	8	2.594571	-1.997338	0.000000
9	-0.061399	-0.747472	0.000000	9	0.000000	0.201955	0.000000
10	-1.134208	-3.179006	0.000000	10	2.644160	0.830942	0.000000
11	0.807213	-1.274489	0.000000	11	-1.853877	1.942438	0.000000
12	3.070558	2.162942	0.000000	12	1.941882	1.982070	0.000000
13	1.132232	1.215069	0.000000	13	-2.219476	-0.287373	0.000000

2b				3a			
1	0.405201	-2.552155	0.000000	1	-1.228508	-1.223310	0.000000
2	-0.854606	-2.028473	0.000000	2	-1.207881	0.132779	0.000000
3	1.493643	-1.721996	0.000000	3	-0.084041	-1.999442	0.000000
4	0.481547	-3.634446	0.000000	4	-2.207049	-1.694222	0.000000
5	-1.066196	-0.678849	0.000000	5	0.000000	0.754834	0.000000
6	1.262423	-0.320485	0.000000	6	1.166339	-1.358254	0.000000
7	-1.675539	-2.631168	0.000000	7	-0.148215	-3.080871	0.000000
8	2.493304	-2.137142	0.000000	8	1.158170	0.012807	0.000000
9	0.000000	0.173224	0.000000	9	2.620936	-2.291116	0.000000
10	2.517098	0.879611	0.000000	10	2.021565	0.552607	0.000000
11	3.570220	0.037238	0.000000	11	-2.213224	2.395238	0.000000
12	-1.692093	2.022915	0.000000	12	3.495097	-1.260633	0.000000
13	-2.236178	-0.192362	0.000000	13	0.049168	2.021767	0.000000

3b				4			
1	-1.238877	-1.226092	0.000000	1	-1.887113	1.749876	0.055614
2	-1.213300	0.127799	0.000000	2	-2.839937	0.829061	-0.162774
3	-0.097782	-2.011186	0.000000	3	-0.565993	1.389252	0.253421
4	-2.219537	-1.693156	0.000000	4	-2.21098	2.786097	0.077873
5	0.000000	0.745071	0.000000	5	-2.601023	-0.558038	-0.201648

6	1.154003	-1.375890	0.000000	6	-0.237192	0.022164	0.239739
7	-0.176559	-3.090814	0.000000	7	-3.812233	1.099531	-0.300534
8	1.149974	-0.002701	0.000000	8	0.172852	2.14545	0.473922
9	2.709347	-2.132646	0.000000	9	-1.23536	-0.865817	0.012705
10	2.242162	-3.398079	0.000000	10	1.319217	-0.678262	0.6164
11	2.022133	0.526079	0.000000	11	-1.036258	-1.864927	0.012519
12	-2.204773	2.401023	0.000000	12	3.679654	0.121778	-0.399508
13	0.052116	2.011343	0.000000	13	-3.442365	-1.388969	-0.396038

5a

1	-2.659655	-0.282625	0.000000
2	-2.299251	1.040750	0.000000
3	-1.686027	-1.234198	0.000000
4	-3.722978	-0.495432	0.000000
5	-1.000967	1.410542	0.000000
6	-0.317206	-0.830632	0.000000
7	-3.003813	1.776867	0.000000
8	-1.938933	-2.287088	0.000000
9	0.000000	0.533693	0.000000
10	0.919744	-2.011842	0.000000
11	2.536243	0.151055	0.000000
12	-0.846207	2.718750	0.000000
13	0.072490	3.024401	0.000000

5b

1	2.653861	-0.272729	0.000000
2	2.263967	1.055803	0.000000
3	1.713483	-1.253344	0.000000
4	3.722844	-0.454061	0.000000
5	0.952566	1.383260	0.000000
6	0.329599	-0.886244	0.000000
7	2.981847	1.775959	0.000000
8	2.001873	-2.297393	0.000000
9	0.000000	0.465149	0.000000
10	-0.920631	-2.042896	0.000000
11	-2.465070	0.237628	0.000000
12	0.542862	2.639506	0.000000
13	1.237207	3.320910	0.000000

6a

1	-1.779018	1.805079	0.06097
2	-2.826675	0.996801	-0.083711
3	-0.452543	1.358284	0.184209
4	-2.001761	2.869307	0.08767
5	-2.593578	-0.301614	-0.109386
6	-0.215675	-0.006457	0.141779
7	0.349486	2.068704	0.333686
8	-1.326112	-0.813124	-0.012677
9	1.286728	-0.88511	0.328446
10	-1.171437	-1.819529	-0.041461
11	3.702702	0.171283	-0.22438
12	-3.630791	-1.093816	-0.238238
13	-3.457253	-2.049352	-0.232231

6b

1	-1.839403	1.783909	0.068349
2	-2.848781	0.932763	-0.141099
3	-0.508350	1.383495	0.255106
4	-2.104703	2.837913	0.097185
5	-2.549788	-0.351350	-0.162812
6	-0.216831	0.023880	0.219878
7	0.258540	2.117948	0.461641
8	-1.279484	-0.818273	0.001882
9	1.306249	-0.781124	0.528617
10	-1.132057	-1.827194	-0.018086
11	3.678145	0.137036	-0.353526
12	-3.445519	-1.288691	-0.348217
13	-4.336417	-0.902914	-0.450961

TS1_4

1	-2.510205	0.707066	-0.209260
2	-2.330348	-0.657856	-0.115902
3	-1.471281	1.602403	-0.098939
4	-3.515666	1.024348	-0.467746
5	-1.099199	-1.201618	0.140594
6	-0.175868	1.114790	0.186748

TS1_2a

1	-1.483571	2.109285	-0.000203
2	-0.126602	1.833315	-0.000530
3	-2.403307	1.105774	0.000383
4	-1.746623	3.160917	-0.000591
5	0.355587	0.553334	0.000188
6	-1.909740	-0.231010	0.000400

7	-3.071730	-1.291379	-0.412735	7	0.539464	2.597588	-0.000704
8	-1.631877	2.649790	-0.328321	8	-3.465116	1.316538	0.000481
9	-0.129446	-0.264364	0.678236	9	-0.530564	-0.432897	0.000978
10	-0.192398	-0.262890	1.705101	10	-0.867979	-1.697780	-0.000095
11	2.093609	-0.985083	-0.165700	11	3.577248	-0.556558	-0.000095
12	-0.722685	-2.336426	-0.077595	12	1.631666	0.350185	0.000172
13	1.317428	1.837056	-0.038296	13	-2.613230	-1.754675	-0.000395

TS2a_2b

1	-1.575012	2.060334	-0.036680
2	-0.226576	2.214938	0.013324
3	-2.121069	0.793383	-0.047755
4	-2.168675	2.968843	-0.064923
5	0.621101	1.139215	0.042490
6	-1.239815	-0.304612	0.010367
7	0.194813	3.143856	0.013445
8	-3.193533	0.650896	-0.088920
9	0.091119	-0.123496	0.046955
10	-1.853843	-1.992327	-0.063153
11	2.421225	-0.979849	-0.037226
12	1.878009	1.265507	0.048557
13	-1.782718	-2.183452	1.274407

TS4_5a

1	-2.661027	-1.214977	-0.002012
2	-2.995293	0.121517	-0.001585
3	-1.354169	-1.617178	-0.000775
4	-3.490795	-1.912994	-0.003274
5	-2.005900	1.037968	0.000182
6	-0.306045	-0.636287	0.000780
7	-3.965686	0.429355	-0.002369
8	-1.110195	-2.671673	-0.001043
9	-0.692259	0.648100	0.001166
10	3.390858	0.593387	-0.001626
11	-0.690902	1.949944	0.002753
12	-2.024034	2.295355	0.001470
13	1.338024	-1.176855	0.002411

TS5a_5b

1	-2.376057	-1.211749	-0.101048
2	-2.491425	0.158823	-0.062027
3	-1.138015	-1.776459	-0.030497
4	-3.299255	-1.774003	-0.188505
5	-1.403747	0.947284	0.046467
6	0.010728	-0.929869	0.054701
7	-3.403637	0.609231	-0.120217
8	-1.018030	-2.852796	-0.058304
9	-0.176453	0.455503	0.088616
10	1.593858	-1.564522	0.081827
11	2.245091	1.087644	-0.090755
12	-1.628795	2.261553	0.002376
13	-1.534566	2.729084	0.850021

2,4-dithiouracil

1

1	-1.821080	1.979802	-0.470213
---	-----------	----------	-----------

2a

1	-2.446760	-1.053198	0.000000
---	-----------	-----------	----------

2	-0.460498	1.851383	-0.162987	2	-1.271469	-1.739369	0.000000
3	-2.637553	0.904689	-0.417243	3	-2.424957	0.313065	0.000000
4	-2.142913	2.977356	-0.743465	4	-3.357774	-1.642573	0.000000
5	0.074906	0.688348	0.233976	5	-0.052381	-1.123729	0.000000
6	-2.138835	-0.400604	-0.033790	6	-1.158717	0.955959	0.000000
7	0.137460	2.670848	-0.186690	7	-1.281671	-2.757885	0.000000
8	-3.689655	1.000591	-0.656328	8	-3.347807	0.880982	0.000000
9	-0.737061	-0.370486	0.299148	9	0.000000	0.245373	0.000000
10	-2.963821	-1.804458	0.059301	10	-1.193500	2.695918	0.000000
11	-0.378935	-1.241076	0.681770	11	2.528421	0.349203	0.000000
12	3.657431	-0.820551	-0.459970	12	0.140894	2.891878	0.000000
13	1.741553	0.654684	0.770361	13	1.360694	-2.099110	0.000000

2b

1	-2.555557	-0.806925	0.000000
2	-1.464827	-1.618576	0.000000
3	-2.394297	0.553959	0.000000
4	-3.525206	-1.294439	0.000000
5	-0.183268	-1.136788	0.000000
6	-1.068222	1.051529	0.000000
7	-1.587406	-2.629723	0.000000
8	-3.257274	1.207522	0.000000
9	0.000000	0.214982	0.000000
10	-0.651385	2.740964	0.000000
11	-1.900194	3.250055	0.000000
12	2.498027	0.155529	0.000000
13	1.137097	-2.227807	0.000000

3a

1	-0.994144	-1.544137	0.000000
2	-1.125410	-0.191968	0.000000
3	0.222678	-2.196283	0.000000
4	-1.915771	-2.118683	0.000000
5	0.000000	0.568323	0.000000
6	1.393804	-1.418419	0.000000
7	0.275446	-3.278384	0.000000
8	1.225882	-0.060481	0.000000
9	2.943602	-2.181403	0.000000
10	2.036601	0.555526	0.000000
11	-2.736515	1.679074	0.000000
12	3.697081	-1.058903	0.000000
13	-0.056126	2.283228	0.000000

3b

1	-1.003696	-1.547847	0.000000
2	-1.130685	-0.197237	0.000000
3	0.211183	-2.208429	0.000000
4	-1.927433	-2.119416	0.000000
5	0.000000	0.559544	0.000000
6	1.383416	-1.435316	0.000000
7	0.249878	-3.290345	0.000000
8	1.218831	-0.074996	0.000000
9	3.015095	-2.010004	0.000000
10	2.694668	-3.320692	0.000000
11	2.038635	0.531736	0.000000
12	-2.732685	1.684375	0.000000
13	-0.050375	2.273075	0.000000

4

1	-1.334950	2.069961	-0.009568
2	-2.370809	1.229555	-0.143047
3	-0.048344	1.600871	0.196493
4	-1.563456	3.130133	-0.061758
5	-2.280263	-0.170277	-0.088787
6	0.135305	0.209752	0.285080
7	-3.310738	1.591991	-0.289859
8	0.765882	2.292896	0.351443
9	-0.951646	-0.584755	0.142487
10	1.620673	-0.616961	0.697829
11	-0.840562	-1.593982	0.218694
12	3.998142	-0.164263	-0.467746
13	-3.532378	-1.189990	-0.270266

5a**5b**

1	1.486394	2.213434	-0.000114	1	-1.491751	2.233367	0.001377
2	2.128014	1.000858	-0.000056	2	-2.137259	1.015629	0.001738
3	0.126271	2.246440	-0.000027	3	-0.132511	2.274872	-0.000775
4	2.118991	3.094462	-0.000209	4	-2.127591	3.112005	0.002561
5	1.445728	-0.173806	0.000054	5	-1.445145	-0.148404	0.001078
6	-0.592967	1.013713	0.000077	6	0.595276	1.043833	-0.000955
7	3.145809	0.989494	0.000010	7	-3.152970	1.008404	-0.000460
8	-0.408374	3.188324	-0.000057	8	0.395052	3.220902	-0.000863
9	0.109372	-0.194607	0.000103	9	-0.111267	-0.154836	0.000631
10	2.470979	-1.598190	-0.000019	10	2.303014	1.024621	-0.001548
11	-2.304650	1.025653	0.000087	11	1.886524	-1.670949	0.001851
12	-1.971808	-1.653205	-0.000110	12	-2.224906	-1.716093	-0.003805
13	1.464195	-2.490038	0.001087	13	-3.510232	-1.306322	0.026470

6a

1	-1.250139	2.060718	0.050507
2	-2.348662	1.321290	-0.086943
3	0.036426	1.521163	0.212637
4	-1.396562	3.138258	0.039405
5	-2.222676	0.000656	-0.065256
6	0.168755	0.140081	0.218382
7	0.887835	2.171859	0.361901
8	-0.990136	-0.587897	0.071766
9	1.606153	-0.827927	0.483833
10	-0.908974	-1.601932	0.085366
11	4.052229	-0.066152	-0.345243
12	-3.699628	-0.904371	-0.223482
13	-3.153891	-2.137835	-0.138820

6b

1	1.294327	2.071343	0.023696
2	2.374246	1.303036	-0.129992
3	-0.000093	1.568474	0.227119
4	1.466929	3.144559	-0.008011
5	2.212105	-0.012898	-0.079099
6	-0.164993	0.189970	0.267343
7	-0.831797	2.241280	0.388730
8	0.969338	-0.566048	0.106755
9	-1.618866	-0.725950	0.617622
10	0.874664	-1.579555	0.152611
11	-4.019360	-0.121284	-0.428565
12	3.554650	-1.107330	-0.245725
13	4.451694	-0.108375	-0.384087

7

1	-0.440694	2.617950	-0.230629
2	-1.489817	1.714448	-0.141741
3	0.866435	2.222007	-0.111169
4	-0.723720	3.629978	-0.500739
5	-1.306463	0.417809	0.200586
6	1.133175	0.861696	0.196469
7	-2.410896	1.996669	-0.475449
8	1.672126	2.911232	-0.338976
9	-0.006290	0.120820	0.717471
10	-0.005930	0.099721	1.743529
11	2.508630	-0.049448	-0.046102
12	-2.349936	-0.862492	-0.029040
13	0.394367	-2.180510	-0.179387

TS1_2a

1	-2.227780	-1.837829	0.001228
2	-0.855205	-1.970478	-0.000125
3	-2.815807	-0.606762	0.001224
4	-2.786916	-2.767053	0.002102
5	-0.012404	-0.895743	-0.000815
6	-1.952998	0.523234	0.000218
7	-0.446853	-2.901251	0.000594
8	-3.893001	-0.497739	0.002210
9	-0.572313	0.305967	-0.000858
10	-2.173965	2.189536	-0.000492
11	1.693862	-1.238066	-0.001201
12	-0.522534	1.602729	-0.001322
13	3.368876	0.894699	0.000963

TS2a_2b**TS4_5b**

1	-1.326520	2.334016	-0.086246	1	2.222251	-1.856620	0.000400
2	0.019853	2.211864	-0.005519	2	2.742950	-0.586944	0.000310
3	-2.118608	1.202926	-0.089830	3	0.870191	-2.055640	0.000121
4	-1.722694	3.343828	-0.136565	4	2.940296	-2.669394	0.000726
5	0.656823	0.996429	0.055441	5	1.929605	0.495151	-0.000110
6	-1.464583	-0.037793	0.012303	6	-0.000279	-0.917092	-0.000259
7	0.602830	3.048817	-0.009779	7	3.750511	-0.448208	0.000449
8	-3.197822	1.275234	-0.140987	8	0.461802	-3.057892	0.000165
9	-0.124332	-0.126380	0.067942	9	0.567118	0.298796	-0.000332
10	-2.392569	-1.574653	-0.009846	10	-1.713043	-1.196455	-0.000404
11	1.662531	-1.813719	-0.093601	11	2.226396	2.154423	-0.000089
12	-2.138916	-1.862782	1.287512	12	-3.462414	0.862181	0.000303
13	2.358485	0.880741	0.077651	13	0.580943	1.626633	-0.000257

TS1_7

1	1.758479	1.974696	-0.505627
2	0.378437	2.066466	-0.279346
3	2.411779	0.801169	-0.334922
4	2.232980	2.887972	-0.845225
5	-0.339755	1.064283	0.236922
6	1.704703	-0.378958	0.106465
7	-0.107041	2.929831	-0.512087
8	3.473150	0.725912	-0.539785
9	0.339707	-0.099006	0.485058
10	0.018412	-0.654235	1.273940
11	-2.357153	-1.415114	-0.459589
12	2.248038	-1.919128	0.209452
13	-2.042581	1.161218	0.500418

TS7_4

1	-1.619479	2.019915	-0.520907
2	-2.243525	0.833418	-0.367027
3	-0.266242	2.172726	-0.266611
4	-2.234731	2.839804	-0.880104
5	-1.634481	-0.328224	0.096256
6	0.453831	1.075450	0.219316
7	-3.236679	0.752167	-0.579119
8	0.225915	3.120101	-0.445151
9	-0.253438	-0.127762	0.411134
10	-0.006988	-0.635141	1.259945
11	2.241088	-1.471146	-0.496160
12	2.141159	1.068837	0.545378
13	-2.371928	-1.770887	0.272782