Effect of Ni(II), Cu(II) and Zn(II) association on the keto-enol tautomerism of thymine in the gas phase

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Supporting Information

(A total of six pages)

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Table S1. Total energy (hartrees) and zero point energy (ZPE, hartrees) for the diketo (**R**) and keto-enol (**P**) forms of Thymine-M^{2+} complexes.

	B3LYP/6-311+G(2df,2p)	
	Total Energy	**ZPE**
R	-454.3034294	0.11466
R-Ni^{2+}	-1961.9026335	0.11415
R-Cu^{2+}	-2094.1141515	0.11391
R-Zn^{2+}	-2232.9302219	0.11475
P	-454.2736328	0.11383
P-Ni^{2+}	-1961.9163643	0.11521
P-Cu^{2+}	-2094.0921506	0.11574
P-Zn^{2+} (1)	-2232.9319899	0.11470
P-Zn^{2+} (2)	-2232.9584182	0.11578

Table S2. Cartesian coordinates (Å) for the optimized structures of the diketo (**R**) and keto-enol (**P**) forms of Thymine-M^{2+} complexes.

R

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.118863	-1.241408	0.000000
2	6	0	0.240146	-1.478133	0.000000
3	1	0	0.519892	-2.525487	0.000000
4	6	0	1.156301	-0.487324	0.000000
5	6	0	2.638187	-0.718182	0.000000
6	1	0	2.873236	-1.784687	0.000000
7	1	0	3.106142	-0.261194	-0.875993
8	1	0	3.106140	-0.261201	0.875998
9	6	0	0.672964	0.897583	0.000000
10	8	0	1.381952	1.887119	0.000000
11	7	0	-0.727849	1.030649	0.000000
12	6	0	-1.681075	0.027077	0.000000
13	8	0	-2.878610	0.224069	0.000000
14	1	0	-1.777858	-2.004957	0.000000
15	1	0	-1.086444	1.977214	0.000000

R-Ni^{2+}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.918273	0.257494	0.000359
2	6	0	2.207535	1.370970	-0.000502
3	1	0	2.755666	2.308792	-0.000529
4	6	0	0.793471	1.349169	-0.001610
5	6	0	-0.005477	2.592234	0.000316
6	1	0	0.617744	3.484533	-0.035023
7	1	0	-0.698136	2.616038	-0.851477
8	1	0	-0.636530	2.648728	0.898948
9	6	0	0.149608	0.031832	-0.001566
10	8	0	-1.091756	-0.103186	-0.001700
11	7	0	0.963689	-1.062081	-0.000781
12	6	0	2.364757	-1.065043	0.000356
13	8	0	3.048418	-2.035039	0.001193
14	1	0	3.940180	0.285064	0.000976
15	1	0	0.542825	-1.989638	-0.000732
16	28	0	-2.943148	-0.438949	0.000460

R-Cu^{2+}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.955222	0.038087	0.000006
2	6	0	2.394214	1.233106	-0.000061
3	1	0	3.056254	2.094545	-0.000070
4	6	0	0.986656	1.387842	-0.000118
5	6	0	0.345021	2.710646	0.000037
6	1	0	1.063281	3.528815	-0.002352
7	1	0	-0.323146	2.817778	-0.867986
8	1	0	-0.318515	2.819457	0.871539

9	6	0	0.160739	0.152510	-0.000101
10	8	0	-1.073532	0.211859	-0.000149
11	7	0	0.843226	-1.030256	-0.000030
12	6	0	2.234253	-1.202016	0.000027
13	8	0	2.792429	-2.249615	0.000088
14	1	0	3.972492	-0.067736	0.000047
15	1	0	0.319784	-1.904178	-0.000016
16	29	0	-2.925371	-0.404620	0.000027

R-Zn^{2+}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.625877	0.886074	-0.184286
2	6	0	-1.513675	1.617525	-0.122265
3	1	0	-1.632564	2.687668	-0.262181
4	6	0	-0.275999	1.039635	0.144224
5	6	0	0.974528	1.822415	0.290479
6	1	0	0.879867	2.873962	0.010385
7	1	0	1.419379	1.770122	1.286854
8	1	0	1.793587	1.476292	-0.462939
9	6	0	-0.241876	-0.383864	0.235195
10	8	0	0.859736	-1.056776	0.356853
11	7	0	-1.386509	-1.083249	0.143359
12	6	0	-2.677177	-0.527070	-0.050209
13	8	0	-3.674229	-1.163869	-0.105292
14	1	0	-3.529474	1.327189	-0.351158
15	1	0	-1.358325	-2.099559	0.220267
16	30	0	2.514512	-0.343405	-0.171726

P

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.081731	-1.234718	-0.000026
2	6	0	0.282135	-1.484704	0.000004
3	1	0	0.562359	-2.531238	0.000037
4	6	0	1.166795	-0.468647	-0.000009
5	6	0	2.651043	-0.672064	0.000021
6	1	0	3.104855	-0.197868	-0.874241
7	1	0	2.914349	-1.732575	0.000054
8	1	0	3.104829	-0.197799	0.874260
9	6	0	0.651145	0.924114	-0.000056
10	8	0	1.401169	1.884353	0.000023
11	7	0	-0.745160	1.090979	-0.000019
12	6	0	-1.505115	0.055810	-0.000003
13	8	0	-2.846477	0.166457	0.000032
14	1	0	-1.759759	-1.981273	-0.000010
15	1	0	-3.051943	1.113406	0.000041

P-Ni^{2+}

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	7	0	2.304492	0.469818	0.000000
2	6	0	2.244397	-0.886529	0.000000
3	1	0	3.199431	-1.400828	0.000000
4	6	0	1.031027	-1.557635	0.000000
5	6	0	0.898379	-3.045194	0.000000
6	1	0	1.873206	-3.531514	0.000000
7	1	0	0.340484	-3.385667	0.878226
8	1	0	0.340484	-3.385667	-0.878226
9	6	0	-0.095144	-0.695174	0.000000
10	8	0	-1.328226	-1.080762	0.000000
11	7	0	0.000000	0.681403	0.000000
12	6	0	1.192459	1.254659	0.000000
13	8	0	1.440934	2.527431	0.000000
14	1	0	3.208290	0.943704	0.000000
15	1	0	0.674010	3.123465	0.000000
16	28	0	-2.081990	0.627994	0.000000

P-Cu^{2+}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.841715	1.451008	0.000001
2	6	0	2.415125	0.206261	0.000050
3	1	0	3.499460	0.195704	0.000091
4	6	0	1.659113	-0.941841	0.000047
5	6	0	2.215830	-2.335333	0.000015
6	1	0	3.305430	-2.320210	-0.000005
7	1	0	1.882456	-2.887981	0.882330
8	1	0	1.882454	-2.887947	-0.882319
9	6	0	0.271619	-0.685902	0.000053
10	8	0	-0.682102	-1.578113	-0.000204
11	7	0	-0.282706	0.563879	-0.000030
12	6	0	0.506989	1.639141	-0.000044
13	8	0	0.122481	2.876452	-0.000037
14	1	0	2.430346	2.283836	-0.000010
15	1	0	-0.832818	3.048476	-0.000020
16	29	0	-2.103982	-0.317819	0.000046

P-Zn^{2+} (1)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.566349	0.904040	-0.133441
2	6	0	-1.433873	1.643738	-0.086440
3	1	0	-1.560106	2.716838	-0.172635
4	6	0	-0.218333	1.026373	0.089788
5	6	0	1.067065	1.781927	0.216088
6	1	0	0.977295	2.854578	0.021109
7	1	0	1.533314	1.685167	1.203576
8	1	0	1.815385	1.502179	-0.603625

9	6	0	-0.252868	-0.407093	0.149270
10	8	0	0.855440	-1.117967	0.257355
11	7	0	-1.376824	-1.105128	0.089751
12	6	0	-2.514042	-0.457241	-0.024703
13	8	0	-3.672478	-1.040530	-0.055640
14	1	0	-3.476926	1.347211	-0.245031
15	1	0	-3.612564	-2.010745	0.014397
16	30	0	2.485814	-0.364862	-0.119657

P-Zn^{2+} (2)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.020144	1.294213	0.000000
2	6	0	2.454995	-0.008049	0.000000
3	1	0	3.531466	-0.136281	0.000000
4	6	0	1.582662	-1.063022	0.000000
5	6	0	1.993948	-2.505178	0.000000
6	1	0	3.079487	-2.600350	0.000000
7	1	0	1.602835	-3.020604	0.880829
8	1	0	1.602833	-3.020604	-0.880828
9	6	0	0.206250	-0.690251	0.000000
10	8	0	-0.770380	-1.524971	0.000000
11	7	0	-0.193523	0.638919	0.000000
12	6	0	0.715599	1.617752	0.000000
13	8	0	0.461349	2.891825	0.000000
14	1	0	2.693000	2.059852	0.000000
15	1	0	-0.472766	3.154135	0.000000
16	30	0	-2.135723	-0.167014	0.000000