Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

The electron attachment effect on the structure and properties of orto-hydroxyaryl Schiff and Mannich bases – hydrogen/proton transfer processes

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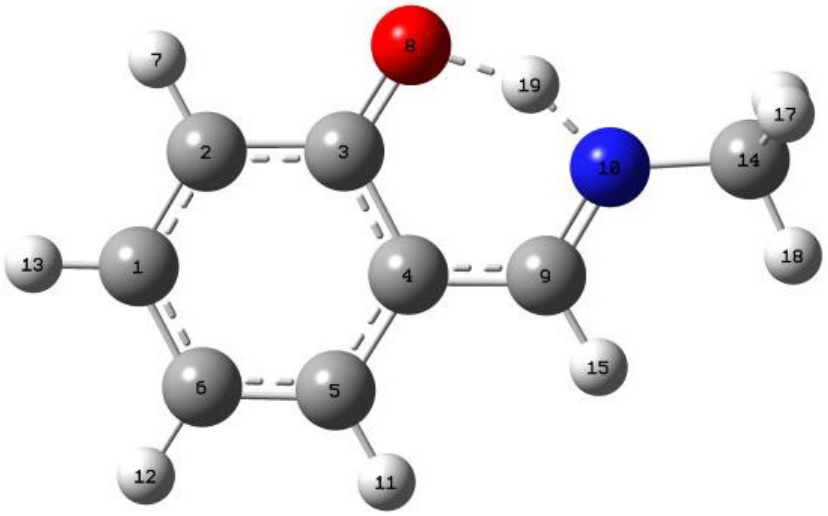
Supporting Information

Table 1S. Coordinates of the transition state of the Schiff base for the reaction of hydrogen transfer within the intramolecular hydrogen bond in molecular and anionic reaction path. Numbering of atoms are declared in the Figure



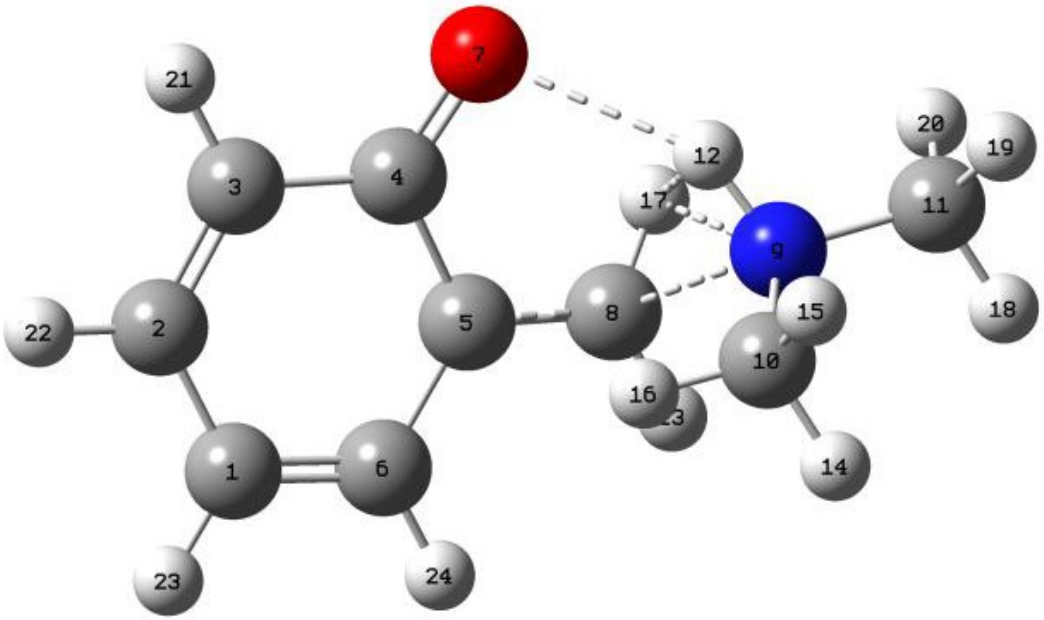
Molecule of the Shiff base

			Coordinates (Angstroms)		
Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	-2.808400	0.255020	0.000000
2	6	0	-1.834882	1.237958	-0.000001
3	6	0	-0.453163	0.888872	-0.000001
4	6	0	-0.126058	-0.520567	-0.000002
5	6	0	-1.151252	-1.498323	-0.000001
6	6	0	-2.481231	-1.124319	0.000001
7	1	0	-2.095606	2.295624	-0.000005
8	8	0	0.487892	1.785124	0.000002
9	6	0	1.254319	-0.882358	0.000001
10	7	0	2.171630	0.045631	0.000001
11	1	0	-0.873288	-2.554392	0.000002
12	1	0	-3.270202	-1.874845	0.000003
13	1	0	-3.859416	0.549249	0.000001
14	6	0	3.592889	-0.233573	-0.000001
15	1	0	1.547800	-1.940480	0.000000
16	1	0	4.063305	0.210302	-0.887887
17	1	0	4.063306	0.210297	0.887887
18	1	0	3.782075	-1.316106	-0.000005
19	1	0	1.584148	1.083692	0.000000

Anion of the Shiff base

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.835507	0.250518	0.025672
2	6	0	1.829472	1.229950	0.016692
3	6	0	0.465951	0.879042	-0.005904
4	6	0	0.113635	-0.531159	-0.016645
5	6	0	1.158184	-1.494803	-0.009094
6	6	0	2.498027	-1.116020	0.012343
7	1	0	2.081335	2.291632	0.026307
8	8	0	-0.491709	1.793385	-0.014908
9	6	0	-1.265554	-0.885199	-0.030947
10	7	0	-2.200198	0.074315	-0.082045
11	1	0	0.889924	-2.554614	-0.016134
12	1	0	3.281500	-1.876001	0.019092
13	1	0	3.884546	0.552927	0.042148
14	6	0	-3.593880	-0.245715	0.067594
15	1	0	-1.562830	-1.942556	-0.023821
16	1	0	-3.926816	-0.199788	1.126085
17	1	0	-4.212882	0.464425	-0.498465
18	1	0	-3.820447	-1.262721	-0.298806
19	1	0	-1.527313	1.139718	-0.041090

Table 2S. Coordinates of the transition state of the Mannich base for the reaction of hydrogen transfer within the intramolecular hydrogen bond in molecular and anionic reaction path. Numbering of atoms are declared in the Figure



Molecule of the Mannich base

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.626308	-1.262	0.095847
2	6	0	-3.057183	0.045515	0.508311
3	6	0	-2.257038	1.150713	0.388858
4	6	0	-0.906507	1.040697	-0.13904
5	6	0	-0.528284	-0.285231	-0.679155
6	6	0	-1.390059	-1.417412	-0.470472
7	8	0	-0.078001	1.978576	-0.09387
8	6	0	0.675772	-0.379674	-1.351435
9	7	0	2.252082	-0.007618	0.246798
10	6	0	2.108942	-0.898696	1.387613
11	6	0	3.61451	0.190054	-0.227101
12	1	0	1.77552	0.881862	0.406596
13	1	0	1.028352	-1.338848	-1.729469
14	1	0	2.548059	-1.876693	1.147787
15	1	0	2.602392	-0.512157	2.296579
16	1	0	1.042782	-1.037996	1.604966
17	1	0	1.124283	0.516186	-1.769403
18	1	0	4.040312	-0.772908	-0.540772
19	1	0	4.277945	0.623018	0.543021
20	1	0	3.606895	0.865573	-1.091342
21	1	0	-2.583977	2.132919	0.729459
22	1	0	-4.053829	0.151496	0.942043
23	1	0	-3.294184	-2.113345	0.220802
24	1	0	-1.058185	-2.398182	-0.817455

Anion of the Mannich base

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.700772	-1.135615	0.120174
2	6	0	-3.036577	0.20493	0.412208
3	6	0	-2.109175	1.233303	0.261301
4	6	0	-0.778667	0.979388	-0.198443
5	6	0	-0.481175	-0.393947	-0.594998
6	6	0	-1.428443	-1.422098	-0.366254
7	8	0	0.149036	1.872868	-0.217924
8	6	0	0.825986	-0.637256	-1.133761
9	7	0	2.077307	-0.005907	0.206679
10	6	0	1.963538	-0.707462	1.479761

11	6	0	3.441276	0.139929	-0.28849
12	1	0	1.558174	0.905007	0.214546
13	1	0	1.129311	-1.671875	-1.311835
14	1	0	2.43127	-1.698246	1.403669
15	1	0	2.459188	-0.14931	2.293721
16	1	0	0.902695	-0.826945	1.725961
17	1	0	1.209953	0.082733	-1.856756
18	1	0	3.894258	-0.847903	-0.445567
19	1	0	4.077003	0.701056	0.421153
20	1	0	3.425395	0.681605	-1.241203
21	1	0	-2.362752	2.260623	0.528215
22	1	0	-4.03853	0.437143	0.781807
23	1	0	-3.43214	-1.932152	0.260655
24	1	0	-1.16322	-2.450361	-0.626717