Behaviour of Cation-π Interaction in presence of External Electric Field

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RSC advances

Supplementary material

Table S1 Interaction energy (in kcal/mol) for benzene-Na^+ in presence of external electric field at different level of theories.

Field Strength (in au)	B3lyp					MP2				
	cc-pVDZ	cc-pVTZ	Aug-cc-pVDZ	Aug-cc-pVTZ	6311+g (2d,2p)	cc-pVDZ	cc-pVTZ	Aug-cc-pVDZ	Aug-cc-pVTZ	6311+g (2d,2p)
0.03	-57.23	-58.70	-58.66	-58.78	-59.11	-53.54	-55.69	-56.24	-54.88	-55.21
0.0275	-54.51	-55.87	-55.74	-55.94	-56.17	-50.99	-52.58	-53.49	-52.69	-52.52
0.025	-51.83	-53.03	-52.84	-53.09	-53.33	-48.42	-49.93	-50.75	-49.99	-49.84
0.0225	-49.12	-50.26	-49.97	-50.26	-50.47	-45.85	-47.28	-48.01	-47.29	-47.15
0.02	-46.85	-47.40	-47.81	-47.46	-47.59	-43.30	-44.60	-45.25	-44.59	-44.46
0.0175	-43.69	-44.59	-44.20	-44.58	-44.75	-40.72	-41.93	-42.49	-41.88	-41.74
0.015	-41.04	-41.80	-41.33	-41.71	-41.89	-38.13	-39.22	-39.71	-39.17	-39.04
0.0125	-38.31	-38.85	-38.42	-38.85	-38.99	-35.52	-36.48	-36.90	-36.41	-36.25
0.01	-35.57	-35.93	-35.49	-35.93	-36.03	-32.89	-33.76	-34.05	-33.65	-33.48
0.0075	-32.76	-33.00	-32.51	-32.97	-32.94	-29.93	-30.93	-31.16	-30.78	-30.64
0.005	-29.90	-30.01	-29.47	-29.92	-30.00	-27.26	-28.03	-28.18	-27.87	-27.72
0.0025	-27.00	-26.90	-26.36	-26.81	-26.92	-24.54	-25.06	-25.10	-24.88	-24.71
0	-23.95	-23.69	-23.10	-23.58	-23.69	-21.75	-21.93	-21.90	-21.76	-20.97

Table S2 (a) Calculated BSSE values (in kcal/mol) for benzene-Li^+ in presence of external electric field at different level of theories.

Field strength (in au)	B3lyp					MP2				
	ccpvDz	ccpvTZ	Aug-ccpvDz	Aug-ccpvTZ	6311+g (2d,2p)	ccpvDz	ccpvTZ	Aug-ccpvDz	Aug-ccpvTZ	6311+g (2d,2p)
0.03	6.774	3.961	0.737	0.330	0.557	9.587	5.643	2.171	1.077	2.340
0.0275	5.879	3.364	0.649	0.320	0.522	8.665	5.018	2.078	1.005	2.221
0.025	5.095	2.848	0.601	0.311	0.492	7.858	4.469	2.017	0.969	2.130
0.0225	4.413	2.401	0.571	0.302	0.465	7.151	3.988	1.973	0.945	2.055
0.02	3.814	2.015	0.552	0.293	0.442	6.533	3.566	1.939	0.927	1.993
0.0175	3.292	1.684	0.539	0.288	0.427	5.994	3.198	1.911	0.911	1.937
0.015	2.840	1.402	0.529	0.284	0.417	5.525	2.877	1.887	0.895	1.885
0.0125	2.450	1.163	0.521	0.282	0.411	5.119	2.600	1.866	0.880	1.799
0.01	2.118	0.964	0.514	0.279	0.407	4.771	2.361	1.846	0.865	1.788
0.0075	1.840	0.800	0.508	0.276	0.404	4.476	2.157	1.826	0.849	1.741
0.005	1.608	0.670	0.501	0.273	0.402	4.230	1.985	1.806	0.832	1.692
0.0025	1.423	0.569	0.494	0.269	0.401	4.020	1.843	1.786	0.814	0.000
0	1.279	0.496	0.000	0.265	0.400	3.848	1.722	1.764	0.794	1.590
-0.0025	1.171	0.448	0.478	0.260	0.400	3.707	1.626	1.739	0.772	1.531
-0.005	1.097	0.423	0.468	0.255	0.399	3.586	1.548	1.707	0.747	1.467
-0.0075	1.056	0.419	0.457	0.249	0.399	3.476	1.484	1.665	0.717	1.391
-0.01	1.037	0.436	0.466	0.245	0.397	3.353	1.426	1.598	0.679	1.293

Table S2 (b) Calculated BSSE values (in kcal/mol) for benzene-Na^+ in presence of external electric field at different level of theories.

	B3lyp					MP2				
Field strength (in au)	ccpvDz	ccpvTZ	Aug-ccpvDz	Aug-ccpvTZ	6311+g (2d,2p)	ccpvDz	ccpvTZ	Aug-ccpvDz	Aug-ccpvTZ	6311+g (2d,2p)
0.03	7.634	4.011	0.999	0.471	0.915	9.728	4.969	1.757	1.110	1.985
0.0275	6.617	3.390	0.975	0.414	0.870	8.689	4.783	1.694	1.025	1.829
0.025	5.714	2.842	0.95	0.377	0.834	7.772	4.216	1.644	0.995	1.738
0.0225	4.937	2.393	0.933	0.339	0.806	6.965	3.724	1.602	0.97	1.667
0.02	3.832	1.999	0.916	0.314	0.780	6.260	3.298	1.569	0.54	1.607
0.0175	3.649	1.659	0.9	0.304	0.767	5.636	2.928	1.540	0.94	1.554
0.015	3.120	1.374	0.885	0.293	0.753	5.088	2.609	1.515	0.927	1.504
0.0125	2.664	1.151	0.867	0.287	0.730	4.608	2.335	1.490	0.915	1.456
0.01	2.266	0.944	0.851	0.282	0.737	4.189	2.099	1.465	0.904	1.408
0.0075	1.932	0.793	0.829	0.277	0.718	3.824	1.901	1.439	0.891	1.358
0.005	1.660	0.684	0.81	0.274	0.705	3.511	1.735	1.410	0.87	1.307
0.0025	1.429	0.583	0.796	0.270	0.697	3.235	1.596	1.393	0.846	1.255
0	1.232	0.525	0.774	0.267	0.689	2.994	1.532	1.362	0.824	1.229

Table S3 Charge transfer for benzene-Li^+ and benzene-Na^+ in presence of external electric field at different level of theories.

Field strength	B3lyp/ccpvDZ		B3lyp/ccpvTZ		B3lyp/6311+g(2d,2p)	
(in au)	benzene-Li^+	benzene-Na^+	benzene-Li^+	benzene-Na^+	benzene-Li^+	benzene-Na^+
0.03	0.2756	0.1625	0.2746	0.1589	0.2806	0.1620
0.0275	0.2562	0.1442	0.2562	0.1416	0.2628	0.1461
0.025	0.2375	0.1280	0.2387	0.1261	0.2458	0.1318
0.0225	0.2197	0.1133	0.2220	0.1119	0.2294	0.1189
0.02	0.2027	-0.0987	0.2062	0.0991	0.2094	0.1073
0.0175	0.1863	0.0878	0.1910	0.0874	0.1951	0.0966
0.015	0.1706	0.0767	0.1764	0.0767	0.1815	0.0869
0.0125	0.1555	0.0667	0.1627	0.0669	0.1684	0.0780
0.01	0.1409	0.0575	0.1494	0.0579	0.1560	0.0644
0.0075	0.1269	0.0491	0.1365	0.0497	0.1438	0.0630
0.005	0.1133	0.0415	0.1243	0.0423	0.1338	0.0557
0.0025	0.1003	0.0346	0.1125	0.0357	0.1223	0.0489
0	0.0875	0.0284	0.1015	0.0299	0.1109	0.1620
-0.0025	0.0750		0.0901		0.1000	
-0.005	0.0630		0.0792		0.0955	
-0.0075	0.0514		0.0684		0.0781	
-0.01	0.0391		0.0499		0.0665	

Table S4 (a) Thermochemical data for benzene-Li^+ system (in kcal/mol) in presence of external electric field at different level of theories.

Field strength (in au)	B3lyp/ccpvDZ		B3lyp/ccpvTZ	
	ΔG_{comp}	ΔH_{comp}	ΔG_{comp}	ΔH_{comp}
-0.01	-20	-27	-19	24
-0.0075	-22	-30	-22	-30
-0.005	-25	-33	-25	-33
-0.0025	-27	-36	-27	-36
0	-39	-29	0	0
0.0025	-32	-41	-32	-41
0.005	-35	-43	-35	-43
0.0075	-37	-46	-37	-46
0.01	-40	-49	-39	-48
0.125	-42	-51	-42	-51
0.015	-45	-54	-44	-53
0.0175	-48	-56	-47	-56
0.02	-50	-59	-49	-58
0.0225	-53	-62	-52	-61
0.025	-56	-65	-54	-63
0.0275	-59	-68	-57	-66
0.03	-62	-71	-59	-69

Table S4 (b) Thermochemical data for benzene-Na^+ (in kcal/mol) system in presence of external electric field at different level of theories.

Field strength (in au)	B3lyp/ccpvDZ		B3lyp/ccpvTZ		B3lyp/6311+g(2d,2p)	
	ΔG_{comp}	ΔH_{comp}	ΔG_{comp}	ΔH_{comp}	ΔG_{comp}	ΔH_{comp}
0	-17	-27	-16	-24	-17	-24
0.0025	-20	-28	-19	-27	-20	-27
0.005	-23	-31	-22	-30	-23	-30
0.0075	-26	-34	-25	-33	-26	-33
0.01	-6	-61	-28	-36	-29	-36
0.125	-33	-40	-31	-39	-32	-39
0.015	-36	-44	-35	-43	-34	-42
0.0175	7	-47	8	0	-46	-45
0.02	-42	-50	-41	-49	-40	-48
0.0225	-45	-54	-44	-52	-43	-51
0.025	-49	-57	-47	-55	-46	-54
0.0275	-52	-61	-50	-59	-49	-56
0.03	-56	-64	-54	-62	-52	-59

Table S5 $d_{M\text{-}X}$ distance (in Å) for benzene-Na^+ system in presence of external electric field in different level of theory

Field strength (in au)	B3lyp			MP2		
	Aug-ccpvDz	Aug-ccpvTZ	6311+g(2d,2p)	Aug-ccpvDz	Aug-ccpvTZ	6311+g(2d,2p)
0.03	2.1116	2.0954	2.0934	2.1507	2.1210	2.1260
0.0275	2.1250	2.1091	2.1058	2.1662	2.1409	2.1410
0.025	2.1402	2.1239	2.1219	2.1830	2.1575	2.1574
0.0225	2.1566	2.1418	2.1384	2.2008	2.1757	2.1751
0.02	2.1752	2.1592	2.1553	2.2209	2.1950	2.1946
0.0175	2.1954	2.1726	2.1757	2.2426	2.2165	2.2155
0.015	2.2173	2.2031	2.1976	2.2663	2.2397	2.2385
0.0125	2.2413	2.2251	2.2210	2.2924	2.2649	2.2639
0.01	2.2685	2.2514	2.2400	2.3213	2.2943	2.2931
0.0075	2.2984	2.2812	2.2757	2.3213	2.3267	2.3253
0.005	2.3320	2.3162	2.3108	2.3547	2.3622	2.3617
0.0025	2.3711	2.3552	2.3484	2.3909	2.4045	2.4018
0	2.4188	2.3957	2.3774	2.4861	2.4475	2.4467