Supplement materials

Title: Exploring cation-π Interaction in the complexes with B≡B triple bond: A DFT study

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Supplement Figure S1: Optimized structures of the chosen complexes obtained at B3LYP/6311 ++G(d,p) level of theory.

Figure S1a: Optimized structures of the cation-π complexes.

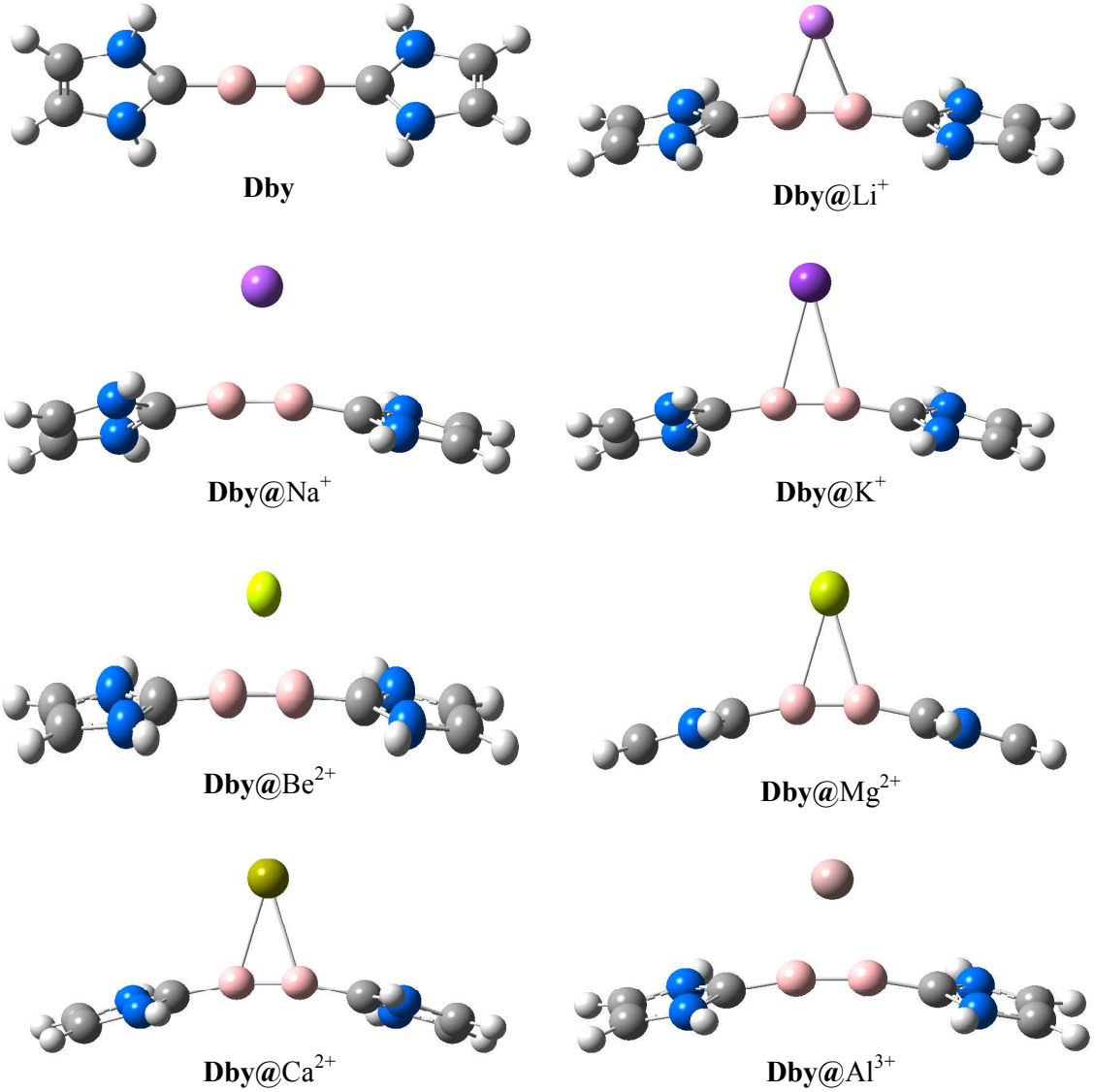
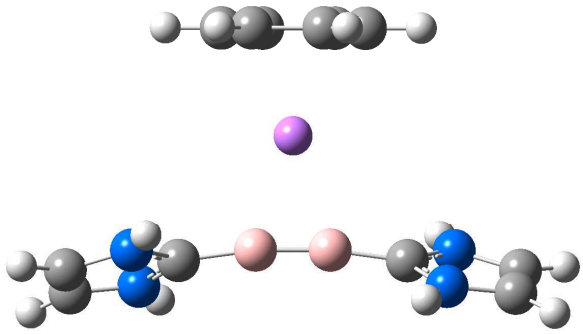
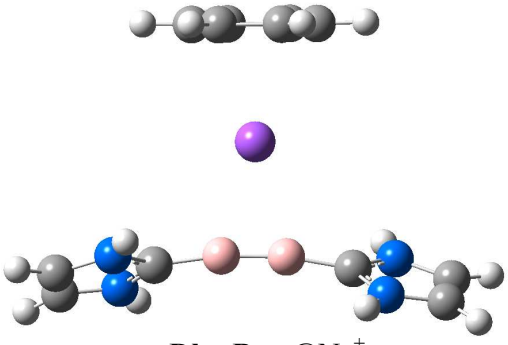


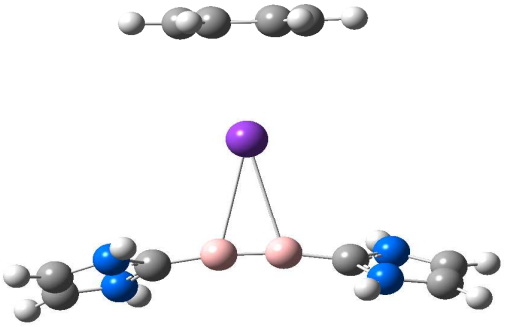
Figure S1b: Optimized structures of the cation-π complexes.



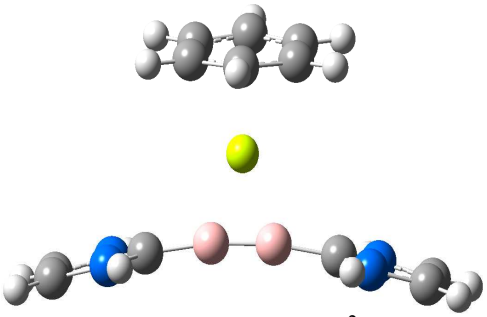
Dby-Ben@Li^{+}



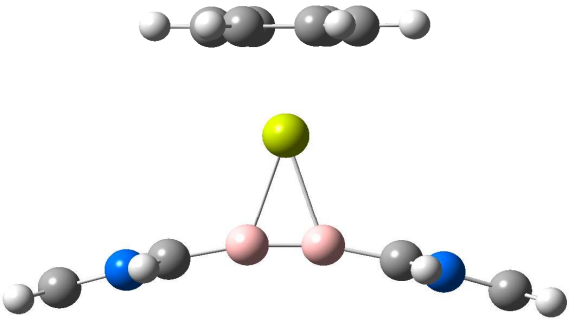
Dby-Ben @Na^{+}



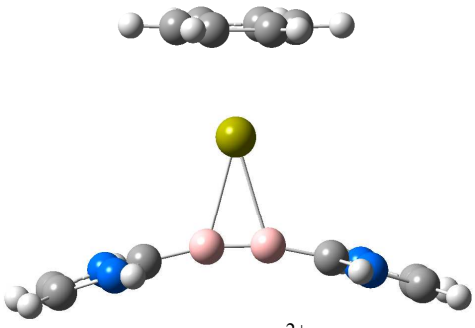
Dby-Ben @K^{+}



Dby-Ben @Be^{2+}



Dby@Mg^{2+}



Dby@Ca^{2+}

Supplement Table S1: BSSE corrections (in $kcalmol^{-1}$) obtained at different level of theories.

System	Level of theories			
	B3LYP/6-311++G(d,p)	B3LYP/6-311++G(2d,2p)	ωB97X-D/ 6-311++G(d,p)	ωB97X-D/6-311++G(2d,2p)
Dby@Li^{+}	0.17	0.20	0.13	0.13
Dby@Na^{+}	0.40	0.51	0.31	0.38
Dby@K^{+}	0.18	0.19	0.15	0.17
Dby@Be^{2+}	0.16	0.19	0.14	0.16
Dby@Mg^{2+}	0.35	0.38	0.28	0.27
Dby@Ca^{2+}	0.16	0.19	0.19	0.22
Dby@Al^{3+}	0.20	0.22	0.17	0.18
Dby-Ben@Li^{+}	0.99	0.77	0.83	0.55
Dby-Ben@Na^{+}	1.11	1.23	0.91	0.92
Dby-Ben@K^{+}	0.55	0.51	0.49	0.44
Dby-Ben @Be^{2+}	1.00	0.76	0.92	0.68
Dby-Ben@Mg^{2+}	1.18	0.96	1.01	0.75
Dby-Ben @Ca^{2+}	0.72	0.61	0.74	0.65

Supplement Table S2: Interaction energy and global hardness (using Koopmans' theorem) obtained at B3LYP/6-311 ++G(d,p) level of theory.

System	Interaction energy (in kcalmol^{-1})	Global hardness (in kcalmol^{-1})
Dby@Li^{+}	−72.1	29.9
Dby@Na^{+}	−56.0	31.1
Dby@K^{+}	−38.2	30.2
Dby@Be^{2+}	−354.8	32.9
Dby@Mg^{2+}	−242.4	27.0
Dby@Ca^{2+}	−160.8	29.6
Dby@Al^{3+}	−645.0	20.7
Dby-Ben@Li^{+}	−87.4	31.0
Dby-Ben@Na^{+}	−67.2	31.4
Dby-Ben@K^{+}	−47.3	30.3
Dby-Ben@Be^{2+}	−408.0	32.2
Dby-Ben@Mg^{2+}	−277.7	34.1
Dby-Ben@Ca^{2+}	−194.9	30.3