Supplementary Materials

Theoretical Studies on Selectivity of Dibenzo-18-Crown-6-Ether for Alkaline Earth Divalent Cations

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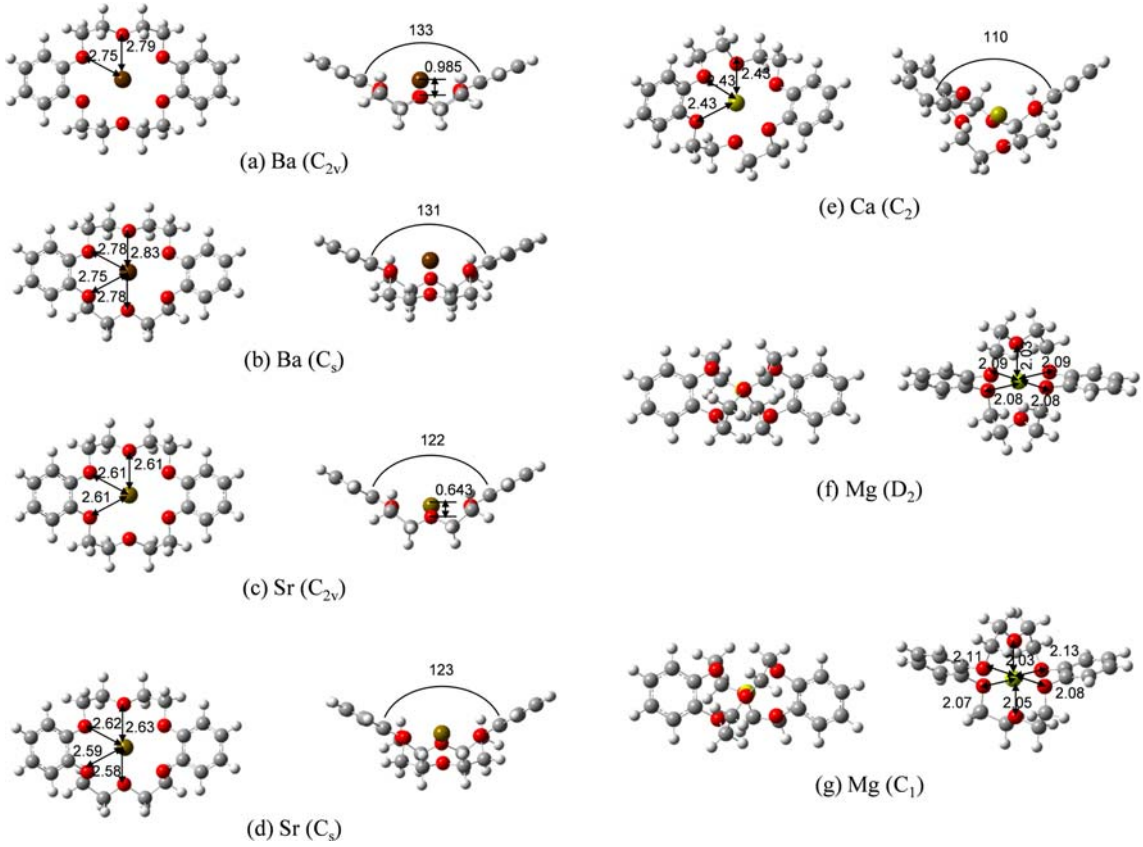

Figure S1. Optimized structures of A^{2+}-DB18C6 at the M06-2X/6-31++G(d, p) level in the gas phase. The angles are in degrees and the distances are in Å.

Table S1. Optimized atomic sphere radii and Calculated hydration free energy of the divalent alkaline earth metal ions

	radius, Å	$-\Delta G_{calc}$[a], kcal/mol	$-\Delta G_{expt}$[b], kcal/mol
Ba^{2+}	1.742	315.15	315.1
Sr^{2+}	1.583	345.98	345.9
Ca^{2+}	1.436	380.90	380.8
Mg^{2+}	1.199	455.80	455.5

[a]IEFPCM calculation with non-electrostatic terms from the SMD model; electrostatic scaling factor, $\alpha = 1.2$. [b]Experimental values from Burgess