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Erratum: The Structure of Alkali Halide Dimers: A Critical Test of Ionic Models and New Ab Initio Results

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It has come to our attention that some of the *ab initio* results presented are incorrect due to errors in the Cs and C1 basis sets, and a small error in the binding energy of Rb_2F_2. The corrected results are presented below for the species that were affected, modifying the results in Table III of the original paper (see Table I). (Only those values which are different from the results of the original Table III are included.) Note that some of these results are used for comparison with the ionic models in later tables. In addition, some HF data (quoted in Tables V and VI) is affected, and the correct values are given in Table II. All the changes in quoted values are small and none of the conclusions drawn in the article are affected, nor are the comparisons with the ionic models significantly affected. However, the error in the C1 basis is what gave rise to the anomalously short M–Cl bond lengths, and the results presented here lead to longer bonds, in somewhat poorer agreement with the experimental results for Cl containing species.

TABLE I. Corrections to Table III: New MP2 results for monomers and dimers.

System	E_{mon} (h)	r_{mon} (Å)	Δr (Å)	Θ_{XMX}	ΔE_{bind} (kcal/mol)
K_2Cl_2	−42.9886	2.728	0.181	93.4	45.4
Rb_2F_2					48.4
Rb_2Cl_2	−38.8516	2.844	0.192	90.5	43.4
Cs_2F_2	−119.6525	2.440	0.228	78.5	
Cs_2Cl_2	−34.9388	2.984	0.212	86.6	41.0
Cs_2Br_2	−33.3359	3.166	0.219	89.1	39.4
Cs_2I_2	−31.3691	3.421	0.225	91.7	

TABLE II. Corrections to Tables V and VI: New RHF data.

System	Δr (Å)	$\Delta\Theta_{XMX}$
K_2Cl_2	0.193	3.7
Rb_2Cl_2		1.0
Rb_2Br_2	0.219	3.0
Rb_2I_2	0.227	
Cs_2Cl_2	0.237	−2.8
Cs_2Br_2	0.240	−0.7
Cs_2I_2	0.247	1.7

