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The nature of the chemical bond revisited. An energy partitioning analysis of diatomic molecules E_2 (E = N–Bi, F–I), CO and BF

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In Table 1, the calculated values for the overlaps of the σ orbitals give only the $p(\sigma) - p(\sigma)$ contributions but not the s–s and s–$p(\sigma)$ overlap components of the diatomic molecules. The data for the π overlap give only one π component. There are minor corrections to some calculated E–E bond lengths. The correct values for the complete σ and π overlaps and the calculated bond lengths are as follows:

In Table 2, the N–N bond length which was used for the EDA calculations of CO and BF is 1.109 Å but not 1.105 Å . In Table 3, the calculated E–E bond lengths are 1.435 Å for F_2 (not 1.424 Å), 2.040 Å for Cl_2 (not 2.037 Å), 2.390 Å for Br_2 (not 2.381 Å), and 2.870 Å for I_2 (not 2.860 Å).

Table 1

	N_2	P_2	As_2	Sb_2	Bi_2
Overlap σ	1.58	1.46	1.34	1.26	1.15
Overlap π	0.74	0.61	0.55	0.48	0.47
E–E bond length	1.109 (1.09768)	1.939 (1.8931)	2.170 (2.103)	2.592 (2.48)	2.743 (2.660)

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