Addendum to “More insight in multiple bonding with valence bond theory” [Comput. Theor. Chem. 1053 (2015) 180–188]

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Addendum

Addendum to “More insight in multiple bonding with valence bond theory” [Comput. Theor. Chem. 1053 (2015) 180–188]

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So as to clarify some inconsistencies between some values reported in the title paper and some former results on the C₂ molecule previously published by some of us, we wish to complete Table 2 in the title paper with footnotes b and c. The conclusions of the paper are unchanged.

Table 2

Properties of the individual bonds of the C₂ molecule, at an MP2-optimized interatomic distance of 1.2139 Å. Energies in kcal/mol.

	$\Delta E (\Psi_{\text{full}} \rightarrow \Psi_{\text{QC}})$	RE ^a	CS factor (%)
σ (outer)	9.7 ^b	0.4	4.4
π_x	92.4	38.7	41.9
π_y	87.4	32.5	37.2
σ (inner)	72.1 ^c	10.9	15.1

^a Defined as in Eq. (5) for the π bonds, and as in Eq. (7) for the σ bond.

^b Owing to the crude GVB-PP level used to describe the three other bonds, this value is not as accurate than the value 14.3 kcal/mol obtained with a multistructure VB method, in Ref. [30b]. This latter value is close to half the experimental vertical $X^1\Sigma_g^+ \rightarrow c^3\Sigma_u^+$ singlet-triplet gap (~28 kcal/mol), as it should. The value derived based on experimental C–H bond dissociation energy differences of HC≡CH vs HC≡C· radical, in Ref. [30a], was gauged as 15–17 kcal/mol.

^c This value cannot be compared with the value 100.4 kcal/mol for the same bond in Ref. [3b], because in this latter case σ (inner) bond is environed by three singlet couplings while in the present case the other bonds are disrupted to triplet coupling.

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