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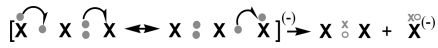
Richard D. Harcourt*: Correction to "Valence Bond Structures for Three-Electron Three-Center and Four-Electron Three-Center Bonding Units: Some Further Examples"†

doi: 10.1021/jp911294x. (a) The entries for Table 4 of the subject paper were calculated using carbon 2pπ AOs. With hydrogen 1s AOs, as described in the paper, the entries are the following.

TABLE 4: Cyclic H_6

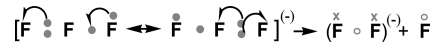
	W(Kekulé)	*W*(Dewar)	energy (au)	*l* in r + *l*y or y + *l*r
1 ↔ **2**	0.446	0.036	−3.1773	
3 ↔ **4**	0.004	0.163	−3.2246	0.8
3	1/6		−3.2026	1.2
4		1/6	−3.2240	0.8

(b) In ref 1, VB studies have been reported for two exit channels for dissociation of X_3^- (X = halogen or hydrogen). With **X** ≡ **R** ≡ **Y**, the $X_3^- \rightarrow X_2 + X^-$ exit channel occurs[1] for X = Cl, Br, I, and H. It is accommodated by



from the ground-state generalized Reactant-like Complex ↔ Product-like Complex (or RC ↔ PC) resonance in the subject paper's Scheme 5.

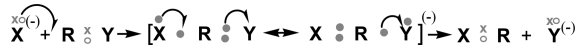
The F_3^- exit channel is primarily[1] $F_3^- \rightarrow F_2^- + F^{\bullet}$. It is accommodated by



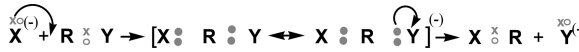
from the excited-state (*) PC ↔ RC resonance in the subject paper's Scheme 5. (Note: RC ≡ (PC)*; PC ≡ (RC)*.)

In ref 2, VB studies of H_3^- with F_3^- are also reported, and their electronic structures are contrasted.

(c) In ref 2, a preference is made for use of



rather than



as a VB formulation for the generalized $\mathbf{X}^{:(-)} + \mathbf{R}{:}\mathbf{Y} \rightarrow \mathbf{X}{:}\mathbf{R} + \mathbf{Y}^{:(-)}$ reaction. These formulations involve one-electron and concerted electron pair delocalizations for Reactants → RC and PC → Products, respectively.

References and Notes

(1) (a) Braida, B.; Hiberty, P. C. *J. Phys. Chem. A* **2008**, *112*, 13045. (b) Braida, B.; Hiberty, P. C. *J. Am. Chem. Soc.* **2004**, *126*, 14890.

(2) Harcourt, R. D. *Int. J. Quantum Chem.* **1996**, *60*, 553. See ref 20d of subject paper for increased-valence revision.

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