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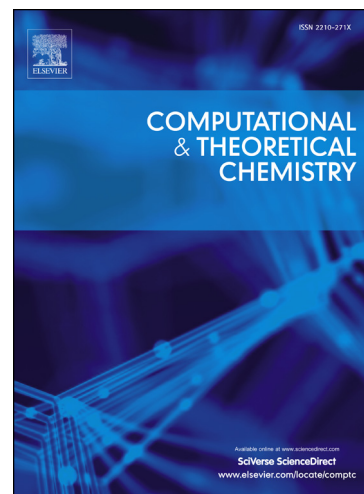
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# More Insight in Multiple Bonding with Valence Bond Theory

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**Title Running Head:**

**Abstract:**

An original procedure is proposed, based on valence bond theory, to calculate accurate dissociation energies for multiply bonded molecules, while always dealing with extremely compact wave functions involving three valence bond structures at most. The procedure consists of dividing the bond-breaking into sequential steps, thus breaking one by one the separate components of the multiple bond. By using the Breathing-Orbital Valence Bond method (P.C. Hiberty, S. Shaik, *Theor. Chem. Acc.* 108 (2002) 255-272), it is ensured that both static and dynamic differential electron correlations are taken into account in each step. The procedure is illustrated for typical examples of multiply bonded molecules, N<sub>2</sub>, C<sub>2</sub> and CO. The so-calculated total dissociation energies are at par with accurate calculations by state-of-the-art standard methods in the same basis set. The procedure also allows one to get some deep insight into the properties of the individual bonds that constitute the multiple bond. A so-called quasi-classical state is defined, in which the electrons of the bond under study have only one spin arrangement pattern,  $\uparrow\uparrow$  thus disabling the exchange of the two spin arrangements that is necessary for a covalent bonding interaction to take place. Taking this quasi-classical state as a non-bonded reference, one may estimate the “*in situ* bonding energy” of an

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