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Erratum

Erratum to "Electronic structure and spectra of ruthenium diimine complexes by density functional theory and INDO/S. Comparison of the two methods" [J. Organomet. Chem. 635 (2001) 187–196]☆

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There was a misprint in the Results and Discussion section of the above-mentioned article. The coefficient '2' is missing in the formula (line 17 on page 191) for the contribution of the ath AO to the ith MO in the modified Mulliken population analysis (MMPA). The equation should be:

$$\mathbf{c}_{ia^2} + \sum_{b \neq a} 2\mathbf{c}_{ia}\mathbf{c}_{ib}\mathbf{S}_{ab}\frac{\mathbf{c}_{ia^2}}{\mathbf{c}_{ia^2} + \mathbf{c}_{ib^2}}.$$

The correct formula has been applied in calculations, and the results in the paper (Table 2) are not affected by this error.

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