Should electronic delocalization be associated with aromaticity? The case of c-P6•T6^{6+}.

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ABSTRACT

Recently Peeks, M. and collaborators have proposed a new index (ID_{opp}) to estimate electronic delocalization. [1] In particular, they have studied the nanoring c-P6•T6^{6+}, [1] a system that has caused controversy among the scientific community. [2-4] According to Peeks, ID_{opp} suggests that the nanoring c-P6•T6^{6+} is aromatic, however we show that ID_{opp} is an unreliable index to estimate aromaticity. We use of the model shown in Figure 1, where we disconnect the porphyrins. In our model the ID_{opp} index has to be zero, however this does not happen despite disconnections. All our analysis is based on Density Functional Theory.

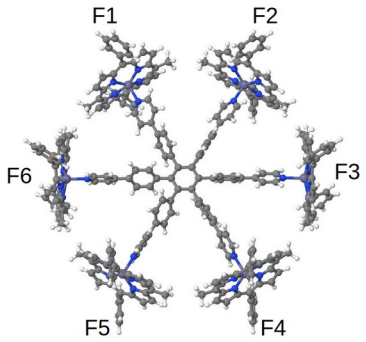

Figure 1: Fragments defined in the nanoring c-P6•T6^{6+}.

References

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