P. G. Perkins et al.

for γ_{AB} . The philosophical points are possibly less useful and, in some cases positively misleading. There is an urgent need for a workable method for calculating solid-state quantities and our approach is claimed to be a step in the right direction. We welcome any suggestions which improve the generality of the method.

Reference

1. Perkins, P. G., Marwaha, A. K., Stewart, J. J. P., Theor. Chim. Acta (Berl.) 57, 1 (1980)

Received February 1, 1982

Erratum

The Structure of the Active Oxygen Complex of Catalase: Model Calculations

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Theoret. Chim. Acta (Berl.) 60, 379-383 (1981)

Due to the choice of an improper geometry for the structure 3 of Fe(P)(O), the results reported in the Note added in proof are erroneous. We have found that when a more realistic geometry is used for structure 3, this one is more stable than structure 4 by about 20 kcal/mole.

Received April 26, 1982