ERRATA

Corrections to Reviews in Mineralogy Volume 42 –
Molecular Modeling Theory: Applications in the Geosciences

Chapter 14 "Molecular Orbital Modeling and Transition State Theory in Geochemistry "

pages 485-531

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On page 503, with reference to Equations (54), (57) and (58) and the text preceding equation (59), the equations and text should read:

$$l^2 = (\lambda I - H)^{-1} G (\lambda I - H)^{-1} G \tag{54}$$

$$\left(H - \lambda I \right) \Delta \mathbf{x} + G = \mathbf{0} \tag{57}$$

$$G^{\mathsf{T}} \Delta x = \lambda \tag{58}$$

If we express Equation (57) in terms of a diagonal Hessian representation, it rearranges to Equation (53). Substituting into Equation (58), we get

$$\lambda = -\sum_i v_i^{\mathsf{T}} G v_i^{\mathsf{T}} G v_i / (\lambda - b_i) \tag{59}$$