

The second paragraph of p. 352 should read:

We can now use Equation (2) to derive the variance of the predicted energies. The predicted energy  $\hat{E}_i$  of structure  $i$  is a linear function of the ECI

$$\hat{E}_i = \sum_{\alpha} X_{i\alpha} J_{\alpha}^* \equiv X_i \cdot J^*$$

where  $J^*$  denotes the vector of the ECI times their respective multiplicities (i.e.  $J_{\alpha}^* = m_{\alpha} J_{\alpha}$ ). The variance of a linear function of a random vector  $J^*$  with known covariance matrix  $V$  is given by:

*etc.*