Theoret. chim. Acta (Berl.) 14, 356 (1969)

Erratum

Semi-Empirical All Valence Electrons SCF-MO-CNDO Theory

J. M. SICHEL and M. A. WHITEHEAD

Theoret. chim. Acta (Berl.) **11**, 220–270 (1968)

Received May 9, 1969

Part II

P. 221: In Eq. (1) and in the text after Eq. (3), U_{kk} should be replaced by $\bar{U}_{kk}$ for consistency with Part I. The values used in the calculations were those given for $\bar{U}_{ss}$ and $\bar{U}_{pp}$ in Part I. Eq. 5, part II: $\frac{1}{r_{12}}$.

Part IV

P. 255: Eq. (9) should read:

$$N = 2\sum_i \sum_\kappa \sum_l C^*_{\kappa i} C_{li} S_{\kappa l} = \sum_\kappa \sum_l P_{\kappa l} S_{\kappa l} = \mathrm{tr}\, \boldsymbol{PS}.$$

Part IV

P. 257: The last sentence in Section B should read: "All computed dipole moments are multiplied by the conversion factor 4.80294 from units of (electron × Ångstrom) to Debyes, for comparison with experimental values." The reported values have been calculated correctly.

Part V

P. 267: The equation on this page should read:

$$R''_4(r) = N''_4(0.3r^2 + 0.7r^3)\, e^{-Z'r/3.7a_0}.$$