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Erratum

A Remark on the Comparison between the Roothaan Open Shell and Half-Electron Method

P. Čársky and R. Zahradník

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We found a minor error in our computer program which brings about an incorrect evaluation of coulomb J_{mm} integrals in some cases. Two lines in Table 3 should be corrected as follows:

Table 3. Total CNDO/2 energies for systems having a non-degenerate singly occupied molecular orbital. (All entries are in eV.)

Radical	LHP	R	Difference
BH_2	− 134.488	− 134.493	0.005
NO_2	−1317.623	−1317.632	0.009

As the corrected values differ rather little from the original ones, no alternation of the discussion is needed. The same holds about the subsequent Erratum.

Dr. P. Čársky
Dr. R. Zahradník
J. Heyrovský Institute of Physical Chemistry and Electrochemistry
7 Máchova
Prague 2 – Vinohrady
Czechoslovakia