Theoret. chim. Acta (Berl.) 17, 163–164 (1970)

Erratum

A CNDO CI Study of the Electronic Structure and Spectrum of Nitrobenzene

B. TINLAND

Theoret. chim. Acta (Berl.) 13, 171—174 (1969)

Received January 12, 1970

An error was found in the atomic coordinates and new computations were performed. Tables 2, 3 and 4 and some results should be corrected as follows:

Table 2. *Atomic coordinates* (Å)

Atom	x	y
O_1	−1.03718	0.
N	0.	0.6232
C_1	0.	2.1132
C_2	−1.22068	2.73516
C_3	−1.19573	4.16495
C_4	0.	4.83464
H_1	−2.14643	2.07072
H_2	−2.12629	4.72309
H_3	0.	5.91464

Table 3. *Singlet transitions*

This work
3.27 (0.)
3.83 (0.)
x 4.68 (0.002)
y 5.12 (0.002)
x 5.84 (0.03)
y 6.67 (0.58)

Table 4. *Valence electrons populations*

	O_1	N	C_1	C_2	C_3	C_4	H_1	H_2	H_3
$1s$							0.94	0.97	0.97
$2s$	1.74	1.14	1.02	1.05	1.03	1.02			
$2p_x$	1.43	1.03	1.02	1.00	1.00	1.00			
$2p_y$	1.78	1.11	0.84	0.99	0.99	1.00			
$2p_z$	1.52	0.98	1.07	0.98	0.99	0.97			
Total	6.47	4.26	3.95	4.02	4.01	3.99			

The computed values for the dipole moment and the ionization potential are now 5.27 Debyes and 11.43 eV, respectively.

I wish to thank Prof. E. Heilbronner and Dr. H. Baumann for bringing this error to my attention.

Dr. B. Tinland
Université de Lyon
Section de Recherches de Mécanique
Ondulatoire Appliquée
43 Boulevard de l'Hippodrome
F-69 Villeurbanne