

Erratum

Some Remarks on the Pariser-Parr-Pople Method

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Wrong formulae were used for the two exchange integrals $K(1s, 2p \sigma)$ and $K(1s, 2p \pi)$ in the calculation whose results were reported in Tables 1, 2 and 3. The corrected results are listed in the following tables.

Table 1. Valence state energy of C (in eV)

| | C ⁺ | C | C ⁻ |
|---------------------------------|----------------|---------------|-----------------|
| Electron configuration | $(sp^2)^3$ | $(sp^2)^3\pi$ | $(sp^2)^3\pi^2$ |
| Orbital exponent of 1s | 5.66 | 5.67 | 5.67 |
| Orbital exponent of 2s | 1.75 | 1.65 | 1.60 |
| Orbital exponent of 2p σ | 1.75 | 1.57 | 1.48 |
| Orbital exponent of 2p π | — | 1.53 | 1.15 |
| Total energy | -1007.98 | -1016.67 | -1012.38 |
| σ -core energy | -1007.98 | -1006.95 | -1005.81 |
| W | — | — 9.72 | — 9.43 |
| $(\pi\pi \pi\pi)$ | — | 16.34 | 12.30 |

Table 2. Valence state energy of pyridine-type N (in eV)

| | N ⁺ | N | N ⁻ |
|---------------------------------|----------------|---------------|-----------------|
| Electron configuration | $(sp^2)^4$ | $(sp^2)^4\pi$ | $(sp^2)^4\pi^2$ |
| Orbital exponent of 1s | 6.65 | 6.66 | 6.66 |
| Orbital exponent of 2s | 2.04 | 1.94 | 1.88 |
| Orbital exponent of 2p σ | 2.07 | 1.87 | 1.71 |
| Orbital exponent of 2p π | — | 1.90 | 1.60 |
| Total energy | -1454.68 | -1465.55 | -1460.38 |
| σ -core energy | -1454.68 | -1453.16 | -1449.77 |
| W | — | — 12.39 | — 13.85 |
| $(\pi\pi \pi\pi)$ | — | 20.22 | 17.08 |

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Table 3. Valence state energy of pyrrole-type N (in eV)

| | N ⁺⁺ | N ⁺ | N |
|-------------------------|---------------------------------|-----------------------------------|--|
| Electron configuration | (sp ²) ³ | (sp ²) ³ π | (sp ²) ³ π ² |
| Orbital exponent of 1s | 6.65 | 6.65 | 6.66 |
| Orbital exponent of 2s | 2.17 | 2.06 | 1.97 |
| Orbital exponent of 2pσ | 2.27 | 2.08 | 1.92 |
| Orbital exponent of 2pπ | — | 2.08 | 1.83 |
| Total energy | -1428.05 | -1454.48 | -1462.10 |
| σ-core energy | -1428.05 | -1426.97 | -1424.26 |
| W | — | -27.51 | -28.64 |
| (ππ ππ) | — | 22.11 | 19.44 |

The usual assumption in the Pariser-Parr-Pople method

$$W(n, 1) = W(n, 2) = -I_n$$

is valid within an error of about 1.7 eV. Thus, the general conclusions reached in the original article remain essentially valid.

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