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# addenda and errata

## Charge-density analysis of 1-nitroindoline: refinement quality using free *R* factors and restraints. Corrigendum

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The $D_e$ (dissociation energy) values in Table 6 of the article by Zarychta *et al.* [(2011). *Acta Cryst.* B**67**, 250–262] are corrected.

The $D_e$ (dissociation energy) values in the last column of Table 6 of the article by Zarychta *et al.* (2011) were incorrectly given as negative values; they should all be positive. The correct table is given below.

### References

Zarychta, B., Zaleski, J., Kyzioł, J., Daszkiewicz, Z. & Jelsch, C. (2011). *Acta Cryst.* B**67**, 250–262.

**Table 6**
Topological characteristics of the electron density at all the hydrogen BCPs and O2···O2$^{iii}$ short contact in 1-nitroindoline.

$G^{CP}$, $V^{CP}$ and $E^{CP}$ are the kinetic, potential and total electronic energies (Abramov, 1997) at CPs; $D_e$ is the dissociation energy. See Table 5 for a detailed description. Values in italics are from theoretical data.

| Bond | $d$ (Å) | $r_1$ (Å) | $r_2$ (Å) | $\rho$ (e Å$^{-3}$) | $\nabla^2\rho_{cp}$ (e Å$^{-5}$) | $\lambda$ | $\lambda_2$ (e Å$^{-5}$) | $\lambda_3$ | $\varepsilon$ | $G^{CP}$ | $V^{CP}$ (kJ mol$^{-1}$ bohr$^{-3}$) | $E^{CP}$ | $D_e$ (kJ mol$^{-1}$) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| H6···O1 | 2.3057 | 1.3160 | 1.0047 | 0.1007 | 1.53 | 2.28 | −0.37 | −0.37 | 0.00 | 34.60 | −27.50 | 7.10 | 13.75 |
| | *2.3325* | *1.3189* | *1.0402* | *0.0990* | *1.54* | *2.28* | *−0.36* | *−0.38* | *0.04* | *34.60* | *−27.20* | *7.40* | *13.60* |
| H5···O1$^{i}$ | 2.6557 | 1.5091 | 1.1644 | 0.0363 | 0.60 | 0.83 | −0.12 | −0.12 | 0.04 | 12.10 | −7.90 | 4.20 | 3.95 |
| | *2.7912* | *1.5538* | *1.2768* | *0.0291* | *0.51* | *0.67* | *−0.08* | *−0.09* | *0.04* | *10.00* | *−6.30* | *3.70* | *3.15* |
| H6···O1$^{i}$ | 2.8520 | 1.5801 | 1.2841 | 0.0266 | 0.42 | 0.56 | −0.06 | −0.07 | 0.19 | 8.50 | −5.30 | 3.20 | 2.65 |
| | *2.7264* | *1.5348* | *1.2421* | *0.0301* | *0.55* | *0.74* | *−0.09* | *−0.10* | *0.09* | *10.80* | *−6.80* | *4.00* | *3.40* |
| H7*B*···O1$^{ii}$ | 2.4531 | 1.3985 | 1.0856 | 0.0662 | 0.94 | 1.42 | −0.23 | −0.25 | 0.08 | 20.40 | −15.30 | 5.10 | 7.65 |
| | *2.5209* | *1.4065* | *1.1287* | *0.0690* | *0.94* | *1.39* | *−0.23* | *−0.23* | *0.00* | *20.70* | *−15.80* | *4.90* | *7.90* |
| H3···O2$^{iii}$ | 2.4990 | 1.4470 | 1.0638 | 0.0502 | 0.81 | 1.16 | −0.17 | −0.18 | 0.02 | 16.80 | −11.60 | 5.20 | 5.80 |
| | *2.6036* | *1.4614* | *1.1879* | *0.0388* | *0.80* | *1.09* | *−0.14* | *−0.15* | *0.02* | *15.90* | *−10.00* | *5.90* | *5.00* |
| O2···O2$^{iv}$ | 2.8304 | 1.4153 | 1.4151 | 0.0732 | 1.21 | 1.59 | −0.13 | −0.25 | 0.49 | 26.00 | −19.00 | 7.00 | 9.50 |
| | *2.8708* | *1.4355* | *1.4353* | *0.0677* | *1.13* | *1.48* | *−0.13* | *−0.22* | *0.42* | *24.00* | *−17.30* | *6.70* | *8.65* |

Symmetry transformations used to generate equivalent atoms: (i) $1-x, 2-y, -z$; (ii) $1+x, y, z$; (iii) $x, -1+y, -1+z$; (iv) $2-x, 2-y, 1-z$.

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