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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)	ρ (e Å^{-3})	$\nabla^2\rho_{cp}$ (e Å^{-5})	λ	λ_2 (e Å^{-5})	λ_3	ε	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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