

**A neutron diffraction study of deuterated semicarbazide hydrochloride. Errata.** By B. K. ROUL and R. N. P. CHOUDHARY, Department of Physics, Indian Institute of Technology, Kharagpur 721 302, India and H. RAJAGOPAL and A. SEQUEIRA, Neutron Physics Division, Bhabha Atomic Research Centre, Trombay, Bombay 400 085, India

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**Abstract**

Details of the hydrogen-bond geometry given in Table 2 of the paper by Roul, Choudhary, Rajagopal & Sequeira [*Acta Cryst.* (1988), C44, 1244–1246] are corrected. Also, the correct bond lengths for Cl—H1, N1—H1 and N3—H4 for SEM.DCl are 2.437 (10), 0.952 (10) and 1.071 (10) Å, respectively.

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In the paper by Roul, Choudhary, Rajagopal & Sequeira (1988) the estimated standard deviations of the bond lengths Cl—H1, N1—H1 and N3—H4 should be (10) and not (1) for the deuterated compound SEM.DCl.

The pairs of lines *a* and *b* referring to the hydrogenated and deuterated compounds in the table of hydrogen-bond geometry were interchanged. Some of the  $X-Y$  and

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$X-H \cdots Y$  values were also incorrectly given. The correct hydrogen-bond geometry is given below in full.

$X-H \cdots Y$	$X-H$ (Å)	$H \cdots Y$ (Å)	$X-Y$ (Å)	$X-H \cdots Y$ (°)
N1—H1…Cl	<i>a</i> 1.003 (10)	2.374 (8)	3.356 (8)	166.0 (5)
	<i>b</i> 0.954 (10)	2.437 (4)	3.365 (7)	164.2 (2.7)
N1—H2…Cl	<i>a</i> 0.987 (10)	2.854 (10)	3.592 (8)	132.2 (6)
	<i>b</i> 0.949 (8)	2.881 (8)	3.458 (9)	120.3 (3.7)
N2—H3…O	<i>a</i> 1.019 (10)	1.942 (11)	2.904 (8)	156.3 (6)
	<i>b</i> 1.028 (6)	1.961 (5)	2.916 (8)	153.4 (5.7)
N3—H4…Cl	<i>a</i> 1.051 (9)	2.104 (4)	3.121 (9)	162.1 (5)
	<i>b</i> 1.071 (10)	2.083 (9)	3.123 (7)	162.3 (3.1)
N3—H5…Cl	<i>a</i> 1.033 (11)	2.069 (10)	3.072 (9)	163.0 (6)
	<i>b</i> 0.988 (3)	2.117 (6)	3.079 (8)	164.0 (4.2)
N3—H6…O	<i>a</i> 1.035 (9)	1.978 (9)	2.839 (7)	138.8 (5)
	<i>b</i> 1.159 (8)	1.952 (7)	2.859 (8)	131.9 (6)

Notes: (a) SEM.HCl, (b) SEM.DCl.

**Reference**

ROUL, B. K., CHOUDHARY, R. N. P., RAJAGOPAL, H. & SEQUEIRA, A. (1988). *Acta Cryst.* C44, 1244–1246.

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