Molecular Crystals and Liquid Crystals

Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl16

Errata

Version of record first published: 28 Mar 2007.

To cite this article: (1987): Errata, Molecular Crystals and Liquid Crystals, 147:1, 208-208

To link to this article: http://dx.doi.org/10.1080/00268948708084636

Erratum

"The Crystal Structure of Octyl D-Gluconate: A Mesogenic Structure with Monolayer Head-to-Tail Molecular Packing" by Sarama Bhattacharjee, George A. Jeffrey, and John W. Goodby, **Mol. Cryst. and Liq. Cryst. 131**, 244 (1985).

The correct identity of this structure is N-(n-octyl)-D-gluconamide. The remarkable similarity between the DSC properties reported for octyl-D-gluconate[1] and N-(n-octyl)-D-gluconamide[2] prompted a comparison of the two crystal structure analyses.[1,3] This showed the two compounds to be identical. The comparison of the crystal data is shown in Table I.

TABLE I

Comparison of crystal structural data

	Octyl gluconate	Octyl gluconamide
Space group	$P2_1$	$P2_1$
	a = 4.798(1) Å	c = 4.805(1) Å
	b = 32.353(8)	b = 32.425(9)
	c = 5.241(1)	a = 5.252(1)
	β = 94.90(1)°	β = 94.96(1)°

The two sets of atomic coordinates are related by the following origin shifts:

gluconate		gluconamide
x + 1/2	≈	x'
-(y + 2796)	≈	y'
z - 1/2	≈	z'

The correspondence between the two sets of atomic coordinates is then within 0.01 Å ($\sim 2\sigma$). The NH group of the gluconamide was misinterpreted as a carbonyl oxygen in our analysis. The discrepancy was not noted due to the poor quality of our crystals and the ensuing X-ray diffraction data.

This mistake was the consequence of a combination of hospitality and poor handwriting during a lecture tour in the Netherlands by one of the authors (GAJ). We are grateful to Dr. J. Batclaan of Akzo Research, Arnheim, Netherlands for suggesting the possibility of this error.

References

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3. V. Zabel, A. Bahemann, R. Hilgenfeld, W. Saenger, B. Pfannemüller, V. Enkelmann and W. Welte, *Chem. Phys. Lipids*, **39**, 313-327 (1986).