SHORT COMMUNICATIONS

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible.*

Acta Cryst. (1982). B**38**, 344

X-ray structure analysis and molecular conformation of *tert*-butyloxycarbonyl-L-prolylproline (Boc-Pro-Pro): errata.

By M. E. KAMWAYA, O. OSTER and H. BRADACZEK, *Institut für Kristallographie, Freie Universität Berlin, Takustrasse* 6, *D*-1000 *Berlin* 33, *Federal Republic of Germany*

(*Received* 6 *November* 1981)

Abstract

Two errors in the paper by Kamwaya, Oster & Bradaczek [*Acta Cryst.* (1981), B**37**, 1564–1568] are corrected: On p. 1565, left column, line 5 from the top should read 'C_s-C$^{\gamma}$-*endo* (C$^{\beta}$-*exo*) for ring I and C_s-C$^{\gamma}$-*exo* (C$^{\beta}$-exo) for ring II.' On p. 1567, right column, line 11 from the top should read 'prolyl residue can, therefore, be regarded as C_s-C$^{\gamma}$-*endo* (C$^{\beta}$-*exo*) for ring I and C_s-C$^{\gamma}$-*exo* (C$^{\beta}$-*exo*) for ring II.'

All relevant information is given in the *Abstract*.

0567-7408/82/010344-01$01.00

Acta Cryst. (1982). B**38**, 344–346

Refinement of the Nd_2O_3 and Nd_2O_2S structures at 4 K.

By M. FAUCHER, *ER* 210, *CNRS*, 92190 *Meudon-Bellevue*, J. PANNETIER, *Institute Laue–Langevin, BP n°* 156, 38042 *Grenoble CEDEX*, Y. CHARREIRE, *ER* 211, *CNRS*, 92190 *Meudon-Bellevue*, and P. CARO, *ER* 210, *CNRS*, 92190 *Meudon-Bellevue, France*

(*Received* 16 *March* 1981; *accepted* 25 *June* 1981)

Abstract

Structural parameters of polycrystalline Nd_2O_3 and Nd_2O_2S were refined at 4 K from neutron powder diffraction data to provide accurate atomic positions for the *ab initio* calculation of crystal-field parameters. The 4 K and 300 K structures of Nd_2O_3 are not significantly different. The parameters of Nd_2O_2S are close to those of Ho_2O_2S and La_2O_2S at room temperature.

1. Introduction

Spectroscopic experiments are often performed at low temperature so that calculation of *ab initio* crystal-field parameters (c.f.p.) requires structural data at the same temperature. However, c.f.p. of Nd^{3+} in Nd_2O_3 (Caro, Derouet, Beaury & Soulié, 1979) were derived from absorption spectra at 4 K and compared (Faucher, Dexpert-Ghys & Caro, 1980) with *ab initio* values based on the room-temperature structure of Boucherle & Schweizer (1975). In the same way, experimental c.f.p. of Nd^{3+} in Nd_2O_2S determined at 1·6 K by Souillat, Rossat-Mignod & Linares (1972) were compared with calculated values utilizing the room-temperature structure of Ce_2O_2S (Zachariasen, 1949).

In the present study, we have redetermined the structural parameters of the two compounds at 4 K from neutron powder diffraction data using both a conventional (integrated intensities) and a profile refinement method (Rietveld, 1969). The results were subsequently used to calculate (presumably) more accurate electrostatic c.f.p. (point charge + dipolar contribution).

2. Experimental and refinement

Polycrystalline Nd_2O_3 (99·99% from Pechiney) was heated for 12 h at 1300 K to eliminate hydroxide and oxycarbonates. Nd_2O_2S was prepared from the oxide by the flux technique proposed by Ozawa, Forest, Jaffe & Ban (1971): a mixture of Nd_2O_3, sulfur and sodium carbonate in the molar ratio 1:3:1 was fired at 1370 K for 2 h in an argon atmosphere. The sample was then washed with water and dried.

0567-7408/82/010344-03$01.00