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Article

Symmetry Breaking Nuclear Quadrupole Coupling Tensor Orientation for CesiumÃƒÂ¢Ã‚Ã‚Ã•133 Nuclei Located in a Mirror Plane

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Abstract

Simultaneous multiple data set fits of all transition peaks of ^{133}Cs nuclei enabled us to obtain accurate cesiumÃƒÂ¢Ã‚Â€Ã‚Â•133 nuclear magnetic resonance (NMR) parameters and Euler angles between the principal axis systems of the chemical shift (CS) and quadrupole coupling (Q) tensors of ^{133}Cs nuclei in Cs_2CrO_4 . Although in a previous study of Cs_2CrO_4 by Power *et al*. (W. P. Power, S. Mooibroek, R. E. Wasylishen, T. S. Cameron, *J. Phys. Chem.* **1994**, *98*, 1552), one central transition was observed for cesium sites 1 and 2 in the ^{133}Cs NMR spectra and one Euler angle between the CS tensors and Q tensors was obtained as 52ÃƒÂ,Ã‚Â° and 7ÃƒÂ,Ã‚Â° for cesium sites 1 and 2, respectively, the present singleÃƒÂ¢Ã‚Â€Ã‚Â•crystal ^{133}Cs NMR measurements found two Euler angles (10(2)ÃƒÂ,Ã‚Â°, 51.9(1)ÃƒÂ,Ã‚Â°, 0ÃƒÂ,Ã‚Â°) for site 1 and two central transition peaks for site 2. Three principal components of the CS tensor for Cs1 are oriented along the crystallographic *a*, *b*, and *c* axes, whereas none of the principal components of the Q tensor for Cs1 are oriented along the crystal axes. The principal component V_{22} of the Q tensor for Cs1 is tilted 10ÃƒÂ,Ã‚Â° from the *b* axis in the *bc* plane, and the other two components are not located in the *ac* plane. Therefore, we have found that the requirement that ÃƒÂ¢Ã‚Â€Ã‚Âœthe quadrupole coupling tensor for a nucleus located in a mirror plane has one principal axis perpendicular to the mirror planeÃƒÂ¢Ã‚Â€Ã‚Â• cannot be applied to Cs1. On the other hand, $\acute{V}_{11}$ and V_{22} for Cs2 are aligned along the *b* axis, and the other components of the CS and Q tensors deviate at an angle of 1.4(1)ÃƒÂ,Ã‚Â° and 10.1(1)ÃƒÂ,Ã‚Â°, respectively, from the *a* and *c* axes in the *ac* plane. A distortionÃƒÂ¢Ã‚Â€Ã‚Â•free powder ^{133}Cs NMR spectrum of Cs_2CrO_4 was measured using a solidÃƒÂ¢Ã‚Â€Ã‚Â•state spin echo technique.

Number of times cited: 1

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