

Relative Orientation of Quadrupole Tensors from Two-Dimensional Multiple-Quantum MAS NMR [*J. Am. Chem. Soc.* **2001**, *123*, 8135–8136]. Nicholas G. Dowell, Sharon E. Ashbrook, Jamie McManus, and Stephen Wimperis*

Although we appear to have derived mathematical expressions describing the relative orientation of two quadrupole tensors that are correct, our interpretation of the effect of powder averaging on these expressions was incorrect in our recent paper. If the two quadrupolar asymmetries, η_1 and η_2 , are both nonzero then three (not two) Euler angles, α' , β' , and γ' , are required to specify the relative orientation of the two tensors; if either η_1 or η_2 is zero then two (not one) angles, β' and either γ' or α' , are required; if both η_1 and η_2 are zero then only one angle, β' , is required. There are two significant consequences of this error for our paper.

Page 8135, Figure 1c: The simulated cross-peak is correct if, in addition to $\beta' = 24^\circ$ and $\gamma' = 0^\circ$, we also specify that $\alpha' = 0^\circ$.

Page 8136, Figure 3: The simulated cross-correlation peaks are correct if, in addition to the β' and γ' angles given in the figure, we also specify that $\alpha' = 0^\circ$.

Using three Euler angles we are able to obtain a much closer correspondence between the experimental and simulated ^{23}Na triple-quantum MAS NMR cross-peaks of sodium molybdate dihydrate than that shown in Figure 1c. A modified Figure 1c is presented here; the angles $\alpha' = 90^\circ$, $\beta' = 24^\circ$, and $\gamma' = 15^\circ$ are used in the simulation.

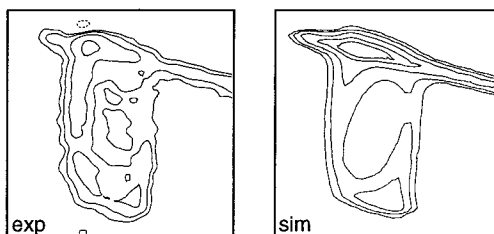


Figure 1.

These corrections do not affect the validity of the novel NMR technique for determining the relative orientation of quadrupole tensors proposed in our paper.

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