

Supplementary Material

Forsterite

Table A Calculated direction cosines of the eigenvectors of the ^{29}Si shielding tensor (X, Y, Z) with respect to the crystallographic axes (a , b , c) for the $\alpha\text{-Mg}_2\text{SiO}_4$ (forsterite) structure of Hazen³⁷

		X	Y	Z
Si	a	0.1491	0	-0.9888
	b	± 0.9888	0	± 0.1491
	c	0	1	0

Table B Calculated direction cosines of the eigenvectors of the ^{17}O shielding/EFG tensors (X, Y, Z) with respect to the crystallographic axes (a , b , c) for the $\alpha\text{-Mg}_2\text{SiO}_4$ (forsterite) structure of Hazen³⁷

		Shielding			EFG		
		X	Y	Z	X	Y	Z
O1	a	± 0.0063	0	-1	0.0710	0	∓ 0.9975
	b	-1	0	∓ 0.0063	± 0.9975	0	0.0710
	c	0	1	0	0	1	0
O2	a	0	-0.9984	∓ 0.0558	0.8141	0	∓ 0.5807
	b	0	∓ 0.0558	0.9984	± 0.5807	0	0.8141
	c	1	0	0	0	1	0
O3	a	$\mp \mp 0.4149$	$-\pm 0.8959$	$\pm \pm 0.4375$	$\mp \pm 0.8360$	-0.2371	$\pm \pm 0.4949$
	b	$-\pm 0.7978$	$\pm \pm 0.2745$	$-\pm 0.3492$	0.1010	$\mp \pm 0.9529$	$-\pm 0.2858$
	c	-0.4375	$\pm \mp 0.5368$	0.8287	$+\pm 0.5394$	$\mp \mp 0.1889$	0.8206

There are two (O1, O2) and four (O3) possible tensor orientations.

Wadsleyite

Table C Calculated direction cosines of the eigenvectors of the ^{29}Si shielding tensor (X, Y, Z) with respect to the crystallographic axes (a , b , c) for $\beta\text{-Mg}_2\text{SiO}_4$ (wadsleyite)⁴⁴

		X	Y	Z
Si	a	0	1	0
	b	∓ 0.5431	0	-0.8397
	c	0.8397	0	∓ 0.5431

Table D Calculated direction cosines of the eigenvectors of the ^{17}O shielding/EFG tensors (X, Y, Z) with respect to the crystallographic axes (a , b , c) for $\beta\text{-Mg}_2\text{SiO}_4$ (wadsleyite)⁴⁴

		Shielding			EFG		
		X	Y	Z	X	Y	Z
O1	a	0	1	0	1	0	0
	b	1	0	0	0	0	1
	c	0	0	1	0	1	0
O2	a	0	1	0	0	1	0
	b	0	0	1	0	0	1
	c	1	0	0	1	0	0
O3	a	1	0	0	0	1	0
	b	0	-0.7461	∓ 0.6658	± 0.5901	0	-0.8073
	c	0	∓ 0.6658	0.7461	0.8073	0	± 0.5901
O4	a	$-+0.5471$	0.2528	$\mp \pm 0.7980$	$\pm \mp 0.4709$	$+ -0.2097$	-0.8569
	b	0.2796	$+ -0.9537$	$\pm \pm 0.1104$	$\mp \mp 0.3983$	0.9173	$+ -0.0056$
	c	$\mp \mp 0.7890$	$\pm \mp 0.1627$	0.5925	0.7872	$\pm \pm 0.0056$	$\pm \mp 0.5154$

There are one (O1, O2), two (O3) or four (O4) possible tensor orientations.