Table 39A-3-001. $(NH_4)_2BeF_4$. Basic unit cell parameters and thermal expansion coefficients [81Ues].

T [°C]	Unit cell parameters			Lattice volume V [Å^3]	Thermal expansion coefficients [$\cdot 10^{-5}$ K^{-1}]			
	a [Å]	b [Å]	c [Å]		linear α_a	α_b	α_c	volume β
6.0	7.61730(7)	10.52148(10)	5.93188(6)	475.412	8.14	−0.28	2.65	10.51
− 79.0	7.56326(7)	10.54546(10)	5.92632(6)	472.672	8.39	−6.14	−0.40	1.85
− 85.0	7.55951(7)	10.54936(10)	5.92650(6)	472.626	8.14	−6.16	−0.59	1.39
− 91.0	7.55621(7)	10.55386(10)	5.92669(6)	472.637	5.03	−8.53	−0.09	− 3.59
− 93.0	7.55545(7)	10.55536(10)	5.92670(6)	472.657	5.03	−6.16	−0.09	− 1.22
− 95.0	7.55469(7)	10.55626(10)	5.92671(6)	472.651	5.03	−1.42	−0.10	3.51
−101.0	7.55230(7)	10.56048(10)	5.92692(6)	472.707	5.03	−5.64	−0.61	− 1.22
−107.0	7.55006(7)	10.56270(10)	5.92713(6)	472.683	4.75	−2.54	−0.60	1.60
−149.0	7.54282(7)	10.56433(10)	5.92475(6)	472.112	1.19	0.83	2.06	4.08

Table 39A-3-002. $(NH_4)_2BeF_4$. Structure of phase I [81Ono]. Fractional coordinates and temperature parameters at 20(1) °C. The anisotropic temperature parameters b_{ij} are for nonhydrogen atoms and the isotropic B are for hydrogen atoms. b_{ij} and B are defined by Eqs. (b) and (e) in Introduction.

Atom	x	y	z	b_{11} [$\cdot 10^{-4}$], B [Å^2]	b_{22} [$\cdot 10^{-4}$]	b_{33} [$\cdot 10^{-4}$]	b_{12} [$\cdot 10^{-4}$]	b_{13} [$\cdot 10^{-4}$]	b_{23} [$\cdot 10^{-4}$]
N(1)	0.1799(3)	0.0969(2)	0.2500	80(3)	62(2)	167(6)	–1(2)	0	0
N(2)	0.4692(2)	0.8051(2)	0.2500	78(3)	43(2)	137(5)	4(1)	0	0
Be	0.2475(4)	0.4179(3)	0.2500	72(4)	44(2)	121(7)	5(3)	0	0
F(1)	0.0497(2)	0.3932(2)	0.2500	74(2)	140(2)	327(6)	–25(2)	0	0
F(2)	0.2864(2)	0.5624(1)	0.2500	173(3)	45(1)	335(6)	–14(1)	0	0
F(3)	0.3278(2)	0.3589(1)	0.0361(2)	146(2)	112(1)	179(3)	26(1)	14(2)	62(1)
H(1)	0.281(5)	0.129(4)	0.250	3.0(9)					
H(2)	0.109(8)	0.155(5)	0.250	5.5(13)					
H(3)	0.160(4)	0.037(3)	0.141(6)	5.6(9)					
H(4)	0.494(6)	0.736(4)	0.250	3.6(9)					
H(5)	0.541(6)	0.853(5)	0.250	4.5(11)					
H(6)	0.410(5)	0.824(3)	0.130(7)	6.8(10)					

Table 39A-3-003. $(NH_4)_2BeF_4$. Structure of phase I [81Ono]. Interatomic distances and angles in BeF_4 ion at 20(1) °C. Corrected: corrected for thermal vibration.

	Bond lengths [Å]		Bond angles [°]	
	uncorrected	corrected		
Be–F (1)	1.534 (3)	1.550 (3)	F (1)–Be–F (2)	110.83 (20)
Be–F (2)	1.536 (3)	1.548 (3)	F (1)–Be–F (3)	109.15 (13)
Be–F (3)	1.536 (2)	1.548 (2)	F (2)–Be–F (3)	108.37 (13)
average	1.538	1.549	F (3)–Be–F (3)	110.99 (18)
			average	109.84

Table 39A-3-004. $(NH_4)_2BeF_4$. Structure of phase I [81Ono]. Interatomic distances and angles in ammonium ions at 20(1) °C.

Bond lengths [Å]		Bond angles [°]	
N (1)–H (1)	0.84 (4)	H (1)–N (1)–H (2)	108.8 (47)
N (1)–H (2)	0.81 (5)	H (1)–N (1)–H (3)	115.0 (25)
N (1)–H (3)	0.91 (4)	H (2)–N (1)–H (3)	113.6 (35)
average	0.87	H (3)–N (1)–H (3)	90.2 (38)
		average	106.9
N (2)–H (4)	0.74 (4)	H (4)–N (2)–H (5)	117.3 (44)
N (2)–H (5)	0.74 (5)	H (4)–N (2)–H (6)	110.6 (25)
N (2)–H (6)	0.86 (2)	H (5)–N (2)–H (6)	103.6 (32)
average	0.80	H (6)–N (2)–H (6)	110.8 (32)
		average	110.6

Table 39A-3-005. $(NH_4)_2BeF_4$, $(NH_4)_2SO_4$, K_2SeO_4. Structure at RT [81Ono]. Root mean square (r.m.s.) displacements and root mean square amplitudes by thermal motions of BeF_4, SO_4, SeO_4 ions.

	r.m.s displacement [Å] along principal axis			r.m.s amplitude [°] around principal axis		
	≈ *a* axis	≈ *b* axis	*c* axis	≈ *a* axis	≈ *b* axis	*c* axis
BeF_4	0.12_4	0.16_6	0.14_7	7.5_3	6.5_4	7.8_9
SO_4	0.15_2	0.16_3	0.15_4	6.3_2	7.4_3	7.8_7
SeO_4	0.12_2	0.13_4	0.13_0	5.2_6	7.3_3	6.5_8

Table 39A-3-006. $(NH_4)_2BeF_4$, $(NH_4)_2SO_4$, K_2SeO_4. Structure at RT [81Ono]. Root mean square (r.m.s.) displacements along the principal axes of N atoms in $(NH_4)_2SO_4$ and $(NH_4)_2BeF_4$, and of K atoms in K_2SeO_4. The orientation of the principal axis is given in parentheses in degrees such as (θ_a, θ_b, θ_c). For example, θ_a is the angle between its principal axis and the *a* axis.

	axis-1	axis-2	axis-3
$(NH_4)_2SO_4$			
N (1)	0.180 (67, 23, 90)	0.168 (90, 90, 0)	0.158 (23, 67, 90)
N (2)	0.183 (90, 90, 0)	0.181 (18, 72, 90)	0.167 (72, 18, 90)
$(NH_4)_2BeF_4$			
N (1)	0.185 (87, 3, 90)	0.172 (90, 90, 0)	0.154 (3, 87, 90)
N (2)	0.158 (49, 41, 90)	0.156 (90, 90, 0)	0.147 (41, 49, 90)
K_2SeO_4			
K (1)	0.174 (77, 13, 90)	0.168 (90, 90, 0)	0.125 (13, 77, 90)
K (2)	0.162 (90, 90, 0)	0.141 (88, 2, 90)	0.116 (2, 88, 90)

Table 39A-3-007. $(NH_4)_2BeF_4$. Structure of phase I [79Ono]. Fractional coordinates. Anisotropic temperature parameters for nonhydrogen atoms and isotropic temperature parameters for hydrogen atoms at –84 °C. b_{ij} and B are defined by Eqs. (b) and (e) in Introduction.

Atom	x	y	z	b_{11} [$\cdot 10^{-4}$], B [Å^2]	b_{22} [$\cdot 10^{-4}$]	b_{33} [$\cdot 10^{-4}$]	b_{12} [$\cdot 10^{-4}$]	b_{13} [$\cdot 10^{-4}$]	b_{23} [$\cdot 10^{-4}$]
N (1)	0.1862 (3)	0.0993 (3)	0.2500	62 (4)	37 (2)	98 (8)	4 (3)	0	00
N (2)	0.4598 (3)	0.8037 (3)	0.2500	62 (4)	31 (2)	101 (8)	8 (3)	0	00
Be	0.2510 (5)	0.4187 (4)	0.2500	52 (5)	27 (3)	69 (10)	2 (3)	0	00
F (1)	0.0540 (3)	0.3812 (2)	0.2500	57 (3)	88 (3)	287 (9)	– 19 (2)	0	00
F (2)	0.2726 (3)	0.5643 (2)	0.2500	123 (4)	31 (2)	306 (9)	– 7 (2)	0	00
F (3)	0.3362 (2)	0.3648 (2)	0.0347 (2)	100 (2)	89 (2)	116 (5)	29 (3)	– 5 (3)	– 45 (3)
H (1)	0.306 (7)	0.127 (5)	0.250	2.4 (1.3)					
H (2)	0.117 (7)	0.168 (5)	0.250	1.6 (1.1)	Bonded to N (1)				
H (3)	0.169 (4)	0.048 (3)	0.141 (6)	1.8 (0.8)					
H (4)	0.480 (7)	0.727 (5)	0.250	2.5 (1.2)					
H (5)	0.556 (7)	0.849 (5)	0.250	2.5 (1.3)	Bonded to N (2)				
H (6)	0.392 (6)	0.824 (4)	0.131 (7)	2.9 (0.9)					

Table 39A-3-008. $(NH_4)_2BeF_4$. Structure of phase I [79Ono]. Root mean square (r.m.s.) displacements and amplitudes of BeF_4 by thermal motion.

	r.m.s displacement [Å] along principal axis			r.m.s amplitude [°] around principal axis		
	≈ *a* axis	≈ *b* axis	*c* axis	≈ *a* axis	≈ *b* axis	*c* axis
T = RT	0.12_4	0.16_6	0.14_7	7.5_3	6.5_4	7.8_9
T = –84 °C	0.10_7	0.13_4	0.12_5	7.8_8	5.0_2	6.2_8

Table 39A-3-009. $(NH_4)_2BeF_4$. Structure [79Ono]. Correspondence of the constituent atoms between phase I and phase III.

phase I	phase III	phase I	phase III
N (1)	N (11), N (12)	H (1)	H (11), H (12)
N (2)	N (21), N (22)	H (2)	H (21), H (22)
Be	Be (1), Be (2)	H (3)	H (31), H (32), H (33), H (34)
F (1)	F (11), F (12)	H (4)	H (41), H (42)
F (2)	F (21), F (22)	H (5)	H (51), H (52)
F (3)	F (31), F (32), F (33), F (34)	H (6)	H (61), H (62), H (63), H (64).

Table 39A-3-010. $(NH_4)_2BeF_4$. Structure of phase III [79Ono]. Fractional coordinates. Anisotropic temperature parameters for nonhydrogen atoms and isotropic temperature parameters for hydrogen atoms at –140 °C. b_{ij} and B are defined by Eqs. (b) and (e) in Introduction. See Fig. 39A-3-003 about the choice of the unit cell and Table 39A-3-009 about the correspondence between the atoms in phases I and III.

Atom	x	y	z	b_{11} [$\cdot 10^{-4}$], B [Å^2]	b_{22} [$\cdot 10^{-4}$]	b_{33} [$\cdot 10^{-4}$]	b_{12} [$\cdot 10^{-4}$]	b_{13} [$\cdot 10^{-4}$]	b_{23} [$\cdot 10^{-4}$]
N (11)	0.0962 (2)	0.0999 (3)	0.2658 (6)	15 (2)	23 (3)	83 (9)	9 (2)	– 6 (3)	– 4 (4)
N (21)	0.2294 (2)	0.8020 (4)	0.2584 (6)	16 (2)	50 (4)	73 (9)	6 (2)	– 4 (3)	– 9 (5)
Be (1)	0.1289 (3)	0.4182 (5)	0.2580 (8)	9 (2)	29 (4)	48 (12)	– 8 (3)	– 1 (4)	– 2 (7)
F (11)	0.0279 (2)	0.3778 (3)	0.2264 (4)	14 (1)	50 (3)	135 (7)	– 6 (1)	– 0 (2)	– 4 (4)
F (21)	0.1326 (2)	0.5649 (2)	0.2954 (4)	18 (1)	19 (2)	108 (6)	3 (1)	– 4 (2)	– 9 (3)
F (31)	0.1743 (2)	0.3841 (2)	0.0351 (4)	19 (1)	31 (2)	70 (6)	7 (1)	16 (2)	– 2 (3)
F (33)	0.1632 (2)	0.3503 (2)	0.4648 (4)	12 (1)	43 (2)	78 (6)	– 0 (1)	– 7 (2)	17 (3)
N (12)	0.3426 (2)	0.3968 (4)	0.2528 (5)	6 (3)	41 (3)	51 (8)	8 (2)	– 0 (3)	7 (5)
N (22)	0.4755 (2)	0.6979 (3)	0.2391 (5)	5 (1)	2 (2)	53 (8)	3 (1)	– 5 (3)	– 3 (4)
Be (2)	0.3738 (3)	0.0813 (5)	0.2570 (8)	11 (2)	8 (4)	80 (13)	– 11 (3)	4 (4)	– 12 (6)
F (12)	0.2795 (2)	0.1271 (3)	0.2836 (4)	7 (1)	46 (2)	130 (7)	4 (1)	6 (2)	1 (4)
F (22)	0.3816 (2)	0.9345 (2)	0.2198 (4)	18 (1)	19 (2)	104 (6)	0 (1)	4 (2)	3 (3)
F (32)	0.4278 (1)	0.1153 (2)	0.4771 (4)	13 (1)	40 (2)	60 (6)	– 4 (1)	2 (2)	– 8 (3)
F (34)	0.4176 (2)	0.1466 (2)	0.0467 (4)	11 (1)	33 (2)	75 (6)	– 5 (1)	– 10 (2)	15 (3)
H (11)	0.153 (4)	0.119 (7)	0.287 (11)	2.3 (1.7)					
H (21)	0.047 (5)	0.161 (7)	0.303 (13)	3.1 (1.8)	Bonded to N (11)				
H (31)	0.096 (4)	0.072 (7)	0.101 (12)	2.5 (1.7)					
H (33)	0.086 (4)	0.031 (6)	0.369 (11)	1.8 (1.6)					
H (41)	0.242 (4)	0.722 (7)	0.241 (11)	2.5 (1.8)					
H (51)	0.286 (4)	0.848 (6)	0.194 (11)	1.7 (1.5)	Bonded to N (21)				
H (61)	0.178 (4)	0.818 (7)	0.137 (12)	2.8 (1.7)					
H (63)	0.212 (4)	0.829 (7)	0.383 (11)	2.2 (1.6)					
H (12)	0.406 (4)	0.382 (6)	0.273 (11)	1.6 (1.6)					
H (22)	0.309 (5)	0.328 (8)	0.244 (13)	2.8 (1.8)	Bonded to N (12)				
H (32)	0.338 (4)	0.421 (7)	0.107 (11)	2.0 (1.6)					
H (34)	0.327 (4)	0.468 (7)	0.332 (13)	2.9 (1.8)					
H (42)	0.481 (4)	0.776 (7)	0.250 (11)	2.3 (1.8)					
H (52)	0.525 (5)	0.637 (8)	0.229 (14)	3.6 (2.1)	Bonded to N (22)				
H (62)	0.437 (4)	0.682 (7)	0.176 (12)	2.1 (1.9)					
H (64)	0.459 (4)	0.680 (6)	0.382 (11)	1.3 (1.6)					

Table 39A-3-011. $(NH_4)_2BeF_4$. Structure of phase III [79Ono]. Interatomic distances [Å] and bond angles [°] of two independent BeF_4 ions. $T = -140$ °C.

Interatomic distance [Å]		Bond angle [°]	
Be(1)–F(11)	1.595(6)	F(11)–Be(1)–F(21)	108.30(34)
–F(21)	1.554(6)	F(11)– –F(31)	105.49(32)
–F(31)	1.528(5)	F(11)– –F(33)	107.39(34)
–F(33)	1.507(6)	F(21)– –F(31)	109.75(34)
⟨Be(1)–F⟩	1.546	F(21)– –F(33)	109.84(33)
		F(31)– –F(33)	115.73(37)
Be(2)–F(12)	1.513(6)	F(12)–Be(2)–F(22)	113.52(34)
–F(22)	1.559(6)	F(12)– –F(32)	109.21(33)
–F(32)	1.576(6)	F(12)– –F(34)	109.97(33)
–F(34)	1.565(6)	F(22)– –F(32)	107.53(32)
⟨Be(2)–F⟩	1.553	F(22)– –F(34)	106.77(32)
		F(32)– –F(34)	109.77(33)

Table 39A-3-012. $(NH_4)_2BeF_4$. Structure of phase III [79Ono]. Interatomic distances and angles of ammonium ions. $T = -140$ °C.

Distance [Å]		Angle [°]	
N (11)–H (11)	0.89 (6)	H (11)–N (11)–H (21)	122.5 (62)
–H (21)	1.01 (7)	H (11)– –H (31)	101.9 (55)
–H (31)	1.01 (7)	H (11)– –H (33)	103.9 (56)
–H (33)	0.96 (7)	H (21)– –H (31)	112.6 (57)
⟨N (11)–H⟩	0.97	H (21)– –H (33)	172.8 (56)
		H (31)– –H (33)	113.2 (58)
N (21)–H (41)	0.87 (7)	H (41)–N (21)–H (51)	103.5 (56)
–H (51)	1.04 (6)	H (41)– –H (61)	102.6 (60)
–H (61)	1.07 (7)	H (41)– –H (63)	120.3 (66)
–H (63)	0.84 (7)	H (51)– –H (61)	105.9 (52)
⟨N (21)–H⟩	0.96	H (51)– –H (63)	115.4 (59)
		H (61)– –H (63)	107.7 (58)
N (12)–H (12)	0.97 (6)	H (12)–N (12)–H (22)	116.3 (61)
–H (22)	0.89 (8)	H (12)– –H (32)	104.1 (52)
–H (32)	0.90 (7)	H (12)– –H (34)	108.1 (53)
–H (34)	0.91 (8)	H (22)– –H (32)	97.0 (64)
⟨N (12)–H⟩	0.92	H (22)– –H (34)	123.8 (63)
		H (32)– –H (34)	104.1 (65)
N (22)–H (42)	0.83 (7)	H (42)–N (22)–H (52)	124.2 (64)
–H (52)	0.98 (8)	H (42)– –H (62)	111.0 (72)
–H (62)	0.71 (7)	H (42)– –H (64)	99.2 (60)
–H (64)	0.90 (6)	H (52)– –H (62)	116.1 (72)
⟨N (22)–H⟩	0.86	H (52)– –H (64)	97.6 (61)
		H (64)– –H (64)	103.1 (69)

Table 39A-3-013. $(NH_4)_2BeF_4$. Structure of phase III [79Ono]. Interatomic distances and angles related with hydrogen bonds. $T = -140$ °C.

X	Y	X–Y	H–Y	∢X–H···Y
N (11) – H (11)···F (12)		2.785 Å	1.92 Å	166°
N (11) – H (31)···F (21)		2.822	1.84	162
N (11) – H (33)···F (31)		2.783	1.83	171
N (21) – H (51)···F (22)		2.690	1.72	153
N (21) – H (61)···F (33)		2.816	1.75	174
N (12) – H (12)···F (11)		2.809	1.85	170
N (12) – H (32)···F (22)		2.848	1.99	158
N (12) – H (34)···F (32)		2.809	1.91	168
N (22) – H (52)···F (21)		2.760	1.80	165
N (22) – H (62)···F (34)		2.796	2.09	173

Table 39A-3-014. $(NH_4)_2BeF_4$. Structure [79Ono]. Root mean square thermal displacements [Å] in direction of principal axes. The orientation of the principal axis relative to the crystallographic axes is given in parentheses in degrees such as (θ_a, θ_b, θ_c). For example, θ_a is the angle between its principal axis and the *a* axis.

Temperature	RT	−84 °C	−140 °C	
Atom (*i*)			Atom (*i*1)	Atom (*i*2)
N (1) or	0.154 (3, 87, 90)	0.133 (16, 74, 90)	0.142 (32, 63, 74)	0.081 (12, 79, 85)
N (11), N (12)	0.185 (87, 3, 90)	0.146 (74, 16, 90)	0.103 (62, 28, 88)	0.153 (80, 11, 86)
	0.172 (90, 90, 0)	0.131 (90, 90, 0)	0.119 (77, 81, 16)	0.094 (85, 87, 6)
N (2) or	0.147 (41, 49, 90)	0.139 (40, 50, 90)	0.136 (17, 77, 79)	0.077 (22, 79, 71)
N (21), N (22)	0.158 (49, 41, 90)	0.127 (50, 40, 90)	0.170 (76, 14, 86)	0.027 (78, 12, 89)
	0.156 (90, 90, 0)	0.134 (90, 90, 0)	0.112 (80, 82, 12)	0.099 (72, 85, 19)
Be or	0.143 (27, 63, 90)	0.124 (33, 57, 90)	0.097 (31, 66, 71)	0.126 (53, 69, 45)
Be (1), Be (2)	0.159 (63, 27, 90)	0.121 (57, 33, 90)	0.133 (64, 26, 90)	0.048 (66, 25, 83)
	0.147 (90, 90, 0)	0.111 (90, 90, 0)	0.091 (73, 82, 19)	0.113 (47, 77, 46)

Table 39A-3-015. $(NH_4)_2BeF_4$. Transition heat and transition entropy per mol [58Hos, 73Str].

Transition heat ΔQ_m [J · mol^{-1}]	Transition entropy ΔS_m [J · K^{-1} · mol^{-1}]	Ref.
1300	7.9	58Hos
1590	9.5	58Hos
836(84)		73Str

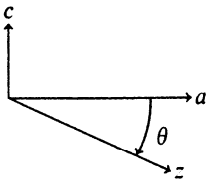
Table 39A-3-016. $(NH_4)_2BeF_4$. Elastic stiffness [$\cdot 10^{10}$ N m^{-2}] [76Ale]. Brillouin scattering. $\lambda = 632.8$ nm.

T [K]	c_{11}	c_{22}	c_{33}	c_{44}	c_{55}	c_{66}	c_{12}	c_{13}	c_{23}
290	3.333	2.377	3.182	0.856	0.672	0.867	1.32	1.60	1.23
280	3.376	2.365	3.215	0.865	0.672	0.876	1.30	1.61	1.22
270	3.412	2.353	3.251	0.875	0.677	0.887	1.29	1.62	1.21
260	3.449	2.340	3.280	0.884	0.661	0.896	1.27	1.63	1.20
250	3.490	2.328	3.309	0.896	0.652	0.909	1.26	1.64	1.19
240	3.527	2.315	3.332	0.907	0.642	0.924	1.25	1.65	1.19
230	3.576	2.317	3.346	0.919	0.631	0.939	1.26	1.66	1.18
220	3.649	2.307	3.353	0.932	0.615	0.958	1.30	1.66	1.17
210	3.740	2.280	3.360	0.948	0.598	0.974	1.33	1.68	1.15
200	3.856	2.250	3.367	0.967	0.581	0.989	1.35	1.70	1.12
190	3.948	2.237	3.377	0.989	0.559	1.002	1.37	1.71	1.12
185	3.967	2.246	3.389	0.989	0.549	1.006	1.38	1.72	1.12
183	3.964	2.246	3.394	1.003	0.547	1.000	1.39	1.71	1.12
182	3.961	2.245	3.394	1.003	0.546	0.999	1.38	1.71	1.12

Table 39A-3-017. $(NH_4)_2BeF_4$. Initial derivatives of ultrasonic velocities with respect to hydrostatic pressure [82Hik]. $T = -60$ °C. $\boldsymbol{k}$: wave vector direction, $\boldsymbol{u}$: polarization (displacement) direction.

	v_{11}	v_{21}	v_{31}	v_{3t}	v_{1t}	v'_{1t}
$\boldsymbol{k}$	[100]	[010]	[001]	[001]	[100]	[100]
$\boldsymbol{u}$				[010]	[001]	[010]
$\frac{1}{v}\left(\frac{dv}{dp}\right)_0$ [$\cdot 10^{-4}$ MPa^{-1}]	1.3	1.6	0.9	1.0	2.1	0.6

Table 39A-3-018. $(ND_4)_2BeF_4$. Quadrupole coupling tensor components of deuteron [69Ale2]. θ: z axis of the electric field gradient tensor rotates gradually in the ac plane with decreasing temperature. The angle of rotation of the z axis is measured from the a axis.



T	$eQ\phi_{xx}/h$	$eQ\phi_{yy}/h$	$eQ\phi_{zz}/h$	θ
°C	kHz			deg
+ 20	±2.7	±1.0	±3.7	0
− 80	±3.6	±0.9	±4.5	10
−110	±5.3	±0.1	±5.4	10
−150	±5.7	±0.2	±5.9	−15

Table 39A-3-019. $(NH_4)_2BeF_4$. ^{9}Be quadrupole coupling tensor ($e^2Q\phi_{ij}/h$ in kHz) in the crystallographic x, y, z frame [80Rut]. $T = 295$ K.

$$\begin{bmatrix} -23 & \pm 14.5 & 0 \\ \pm 14.5 & 5 & 0 \\ 0 & 0 & 18 \end{bmatrix}$$