Table 43A-13-001. Langbeinite-type crystals. Proposed transition schemes [92Art].

Phase	Compound	Transition scheme Space group and transition temperature
I	$(NH_4)_2Cd_2(SO_4)_3$	$P2_13$(92 K) → $P2_1$
	$K_2Co_2(SO_4)_3$	$P2_13$(126 K) → $P2_1$(?) → $P2_12_12_1$
	$K_2Zn_2(SO_4)_3$	$P2_13$(136 K) → $P2_1$(75 K) → $P2_12_12_1$
	$Rb_2Cd_2(SO_4)_3$	$P2_13$(129 K) → $P2_1$(103 K) → P1(68 K) → $P2_12_12_1$
	$Tl_2Cd_2(SO_4)_3$	$P2_13$(128 K) → $P2_1$(120 K) → P1(92 K) → $P2_12_12_1$
II	$K_2Ca_2(SO_4)_3$	$P2_13$(460 K) → $P2_12_12_1$
	$K_2Cd_2(SO_4)_3$	$P2_13$(432 K) → $P2_12_12_1$
	$K_2Mn_2(SO_4)_3$	$P2_13$(190 K) → $P2_12_12_1$
	$Rb_2Ca_2(SO_4)_3$	$P2_13$(183 K) → $P2_12_12_1$
Unknown	$(NH_4)_2Ca_2(SO_4)_3$	$P2_13$(158 K)
	$(NH_4)_2Ni_2(SO_4)_3$	$P2_13$(160 K)
	$(NH_4)_2Mg_2(SO_4)_3$	$P2_13$(160 K)
	$(NH_4)_2Mn_2(SO_4)_3$	$P2_13$(294 K)
	$K_2Mg_2(SO_4)_3$	$P2_13$(64 K) → (55 K) → (51 K)

Table 43A-13-002. Langbeinite-type crystals. Transition temperatures and transition entropies [92Art].

Compound	Θ [K]	ΔS [J K^{-1} mol^{-1}]	Compound	Θ [K]	ΔS [J K^{-1} mol^{-1}]
$K_2Cd_2(SO_4)_3$	432	5.12 [a])	$(NH_4)_2Cd_2(SO_4)_3$	92	8
$K_2Mn_2(SO_4)_3$	191	9.7	$(NH_4)_2Mn_2(SO_4)_3$	294	0.047
$K_2Mg_2(SO_4)_3$	64	3.18	$(NH_4)_2Mg_2(SO_4)_3$	161	0.296

[a]) This result was obtained from differential scanning calorimetry, all other values are from adiabatic calorimetry.

Table 43A-13-003. $(NH_4)_2Cd_2(SO_4)_3$. Atomic coordinates and temperature parameters at RT [75NgH]. U_{ij} [$Å^2$] is defined by Eq. (d) in Introduction.

Atom	Position type	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cd(1)	4b	0.5806(1)	0.5806(1)	0.5806(1)	0.013(1)	0.013(1)	0.013(1)	–0.0008(8)	0.0008(8)	0.0008(8)
Cd(2)	4b	0.8368(1)	0.8386(1)	0.8368(1)	0.013(1)	0.013(1)	0.013(1)	–0.0012(9)	0.0012(9)	0.0012(9)
N(1)	4b	0.065(2)	0.065(2)	0.065(2)	0.022(8)	0.022(8)	0.022(8)	–0.0010(10)	0.0010(10)	0.0010(10)
N(2)	4b	0.301(2)	0.301(2)	0.301(2)	0.028(10)	0.028(10)	0.028(10)	–0.0010(10)	0.0010(10)	0.0010(10)
S	12a	0.6253(2)	0.4745(2)	0.2603(2)	0.0111(9)	0.010(1)	0.009(1)	0.0022(7)	–0.0004(8)	–0.0009(8)
O(1)	12a	0.6588(7)	0.5002(7)	0.3959(6)	0.040(3)	0.046(4)	0.022(3)	–0.001(4)	–0.001(3)	–0.015(3)
O(2)	12a	0.7406(7)	0.4963(7)	0.1834(7)	0.026(3)	0.047(3)	0.032(4)	0.005(3)	0.022(3)	0.008(3)
O(3)	12a	0.5788(6)	0.3423(6)	0.2451(6)	0.033(3)	0.014(3)	0.047(4)	–0.005(3)	–0.020(3)	0.004(3)
O(4)	12a	0.5257(6)	0.5622(6)	0.2152(6)	0.024(3)	0.030(4)	0.047(4)	0.010(3)	–0.012(3)	–0.001(3)

Table 43A-13-004. $(NH_4)_2Cd_2(SO_4)_3$. Interatomic distances and bond angles at RT [75NgH].

Atom or group	Bond	Distance Å	Bonds	Angle deg
SO_4 group	S–O (1)	1.472 (7)	O (1)–S–O (2)	107.5 (4)
	–O (2)	1.454 (8)	–O (3)	110.5 (4)
	–O (3)	1.460 (7)	–O (4)	111.3 (4)
	–O (4)	1.452 (7)	O (2)–S–O (3)	110.9 (4)
			–O (4)	108.1 (4)
			O (3)–S–O (4)	108.5 (4)
NH_4(I) group and environment	N (1)–O (1) 11 × 3	2.97 (1)		
	–O (2) 4 × 3	3.22 (1)		
	–O (2) 6 × 3	3.37 (1)		
	–O (3) 4 × 3	3.36 (1)		
	–O (4) 4 × 3	3.22 (1)		
NH_4(II) group and environment	N (2)–O (2) 6 × 3	3.18 (1)		
	–O (3) × 3	2.97 (1)		
	–O (4) 6 × 3	3.06 (1)		
Cd (1) environment	Cd (1)–O (1) × 3	2.239 (7)	O (1)–Cd (1)–O (1) 2	97.3 (3)
	–O (2) 5 × 3	2.281 (8)	–O (2) 5	80.5 (3)
			–O (2) 10	88.6 (3)
			–O (2) 9	174.0 (3)
			O (2) 5–Cd (1)–O (2) 9	93.9 (3)
Cd (2) environment	Cd (2)–O (3) 5 × 3	2.261 (7)	O (3) 5–Cd (2)–O (3) 9	97.7 (2)
	–O (4) 4 × 3	2.283 (6)	–O (4) 4	89.4 (2)
			–O (4) 8	86.9 (2)
			–O (4) 12	170.9 (2)
			O (4) 4–Cd (2)–O (4) 8	85.3 (2)

Table 43A-13-005. $(NH_4)_2Cd_2(SO_4)_3$. Transition heat and entropy [73Fra, 62Ste].

ΔQ_m [J mol^{-1}]	ΔS_m [J K^{-1} mol^{-1}]	Ref.
907	9.91	73Fra
903(8)	9.87	62Ste

Table 43A-13-006. $(NH_4)_2Cd_2(SO_4)_3$. Raman mode frequencies [cm^{-1}] for $X(ZZ)Y$ geometry [88Gal]. s: shoulder, b: broad line.

300 K	92 K	91 K	81 K	13 K
		9	14	17.4
		11.5		
	24.3(53)	–	–	30.6
		36.6(37)	39.0(05)	39.0(9)
	–	–	–	43.3(12)
51.2(159)	48.8(100)	49.0(5)	–	–
		–	50.0(54)	49.9(16)
		56.9(71)	57.9(88)	53.0(7)
		62.5(5)	63.4(53)	63.3(38)
		68.5(45)	68.9(52)	68.2(28)
		–	–	73.7(19)
75.6(20)	78.0(156)	78.0(71s)	78.6(8s)	78.6(32)
	84.9(131)	83.6(146)	85.3(185)	84.7(198)
		–	–	96.3(66)
103.0(15)	100.0(168)	98.7(87)	100.0(100)	99.9(94)
	108.7(148)	109.1(108)	110.0(134)	108.5(167)
		–	–	112.1(8s)
		123.1(79)	124.3(92)	124.0(86)
	132.8(52)	136.5(53)	137.1(58)	136.5(3)
142.6(s)	–	–	–	142.6(23)
				143.8(28)
				148.7(22)
	155.4(63)	–	–	–
	174.3(52b)	167.0(65)	168.2(75)	167.6(77)
		187.7(75)	187.1(90)	186.5(102)
		–	–	202.0(5)
207.3(168)	–	–	–	–
		212.0(142)	210.0(178)	212.1(155)
	216.1(222)	–	–	–
		220.6(151)	221.2(198)	221.8(215)
		–	234.6(93)	237.0(92)
			–	245.0(s)
			–	267.0(2)
			290.2(27)	293.8(23)
			316.4(29)	318.2(21)
			–	337.1(15)
			350.0	–

Table 43A-13-007. $(NH_4)_2Cd_2(SO_4)_3$, $(ND_4)_2Cd_2(SO_4)_3$. Lines in Raman spectra [cm^{-1}] [79Rab].

Attribution	$(NH_4)_2Cd_2(SO_4)_3$								$(ND_4)_2Cd_2(SO_4)_3$				
	Cubic phase I (T = –170 °C)				Monoclinic phase II (T = –185 °C)				Cubic phase I (T = –170 °C)				Monoclinic phase II (T = –180 °C)
	Z(*XX*)*Y*	*Z*(*YZ*)*Y*	*Z*(*XZ*)*Y*	*Z*(*YX*)*Y*	*Z*(*XX*)*Y*	*Z*(*XZ*)*Y*	*Z*(*YX*)*Y*	*Z*(*YZ*)*Y*	*Z*(*XX*)*Y*	*Z*(*YZ*)*Y*	*Z*(*XZ*)*Y*	*Z*(*YX*)*Y*	*Z*(*XX*)*Y*
	A + E	F, *x*	F, *y*	F, *z*	A	A	B	B	A + E	F, *x*	F, *y*	F, *z*	A
Lattice vibrations	22								23				26
					38								36
													43
									48				49
	50	49		51	51					50		52	58
					65?								67
	77				79				78			78	76
	85			86					85	85			82
													91
													95
		100	99		98						98	96	
	101			102					101	100			102
	107				109				a.t.				106
													118
					122								122
													125 a.t.?
	131				133				132				131
	154								154				152?
		158			a.t.					159	161	158	160
	171?				168				186?				
	180				180?				180?				178?
					195 a.t.								200 a.t.
	214				210				214				210
					230 a.t.								230
									241?				258?
					313?				283?				
	437				434				436				436
	442	441	440	441	445					441	432	441	

(continued)

Table 43A-13-007 (continued)

Attribution	$(NH_4)_2Cd_2(SO_4)_3$								$(ND_4)_2Cd_2(SO_4)_3$				
	Cubic phase I (T = –170 °C)				Monoclinic phase II (T = –185 °C)				Cubic phase I (T = –170 °C)				Monoclinic phase II (T = –180 °C)
	$Z(XX)Y$	$Z(YZ)Y$	$Z(XZ)Y$	$Z(YX)Y$	$Z(XX)Y$	$Z(XZ)Y$	$Z(YX)Y$	$Z(YZ)Y$	$Z(XX)Y$	$Z(YZ)Y$	$Z(XZ)Y$	$Z(YX)Y$	$Z(XX)Y$
	A + E	F, x	F, y	F, z	A	A	B	B	A + E	F, x	F, y	F, z	A
$\nu_2(SO_4^{2-})$	464	466	466	464	462				464				463
										465	467	466	468
	474				472				473				473
	598	600		599	596				598	599	598	600	598
		605?	604?										609
		613	613	613					612	613	613	613	
	619				615				619				615
$\nu_4(SO_4^{2-})$		621	621	621						620	620	620	619
	638	640	639	638	641				637	638	638	638	634
	646 a.t.	645	646	647						645	645	645	641
					1002	1002	1001	1002					1003
$\nu_1(SO_4^{2-})$	1018	1018	1018	1018	1013	1013	1013	1013	1018	1018	1018	1018	1011
					1022	1022	1023	1023					1021
													1032
												1055	1050 a.t.
								1059?	1060	1061	1060		
					1068								1069
	1075	1076	1076	1076	1075	1071	1071	1070	1088	1089	1090	1089	1085
$\nu_3(SO_4^{2-})$					1085	1085	1083	1083					
	1102				1102								
	1114				1109		1107	1108			1107		1106

(continued)

Table 43A-13-007 (continued)

Attribution	$(NH_4)_2Cd_2(SO_4)_3$								$(ND_4)_2Cd_2(SO_4)_3$				
	Cubic phase I (T = –170 °C)				Monoclinic phase II (T = –185 °C)				Cubic phase I (T = –170 °C)				Monoclinic phase II (T = –180 °C)
	$Z(XX)Y$	$Z(YZ)Y$	$Z(XZ)Y$	$Z(YX)Y$	$Z(XX)Y$	$Z(XZ)Y$	$Z(YX)Y$	$Z(YZ)Y$	$Z(XX)Y$	$Z(YZ)Y$	$Z(XZ)Y$	$Z(YX)Y$	$Z(XX)Y$
	A + E	F, x	F, y	F, z	A	A	B	B	A + E	F, x	F, y	F, z	A
$\nu_2(ND_4^+)$		1119	1116		1115	1116			1119				
								1130		1126		1126	1133
					1131	1132	1136	1141?					
	1145	1149	1148	1145	1150	1148		1152	1147	1152	1147	1149	1152
$\nu_4(ND_4^+)$										1178	1177	1176	
	1195	1194	1193	1194	1196	1191	1196	1196	1198	1203	1206	1199	1206
					a.t.	1203?	1215?						
										1222	1218	1224	
										1235	1237	1235	

a.t.: asymmetric tail; ?: presence of line doubtful in view of very low intensity.

Table 43A-13-008. $(NH_4)_2Cd_2(SO_4)_3$. Raman mode frequencies [cm^{-1}] of *XY*, *ZX*, *ZY* polarization conditions [88Gal]. s: shoulder, b: broad line.

XY		*ZX*			*ZY*	
105 K	81 K	105 K	81 K	13 K	105 K	81 K
			14.2			
	326.8(3)		39.6(4)	40.2(1)		39(3)
			–	43.8(16)		–
50(8b)	51.0(19)	49.3(3b)	50.0(60)	50.0(18)	51(31b)	50(27)
	58.7(25)		57.3(73)	57.3(s)		
				59.7(50)		63.4(32)
	64.0(28s)		62.7(55)	64.6(32)		68.2(33)
	68.2(39)		69.5(5s)	71.0(42)		76.8(30)
	77.4(24)	81(4)	84.1(10)	85.3(95)		84.1(36)
	86.5(37b)		90.8(69)	91.4(42)		85.9(4)
99(18b)	100(38b)	100.5(73)	100.5(135)	98.7(104)	99(71)	99.3(75)
	109.7(5)		110.0(85)	108.5(9)		112.1(4)
			115.2(86)	114.6(62)		
		118.2(4)		117.6(3)		
	128.0(5)			126.2(77)		126.1(39)
	137.0(3)	135.3(3)	137.1(81)	135.3(52)		136.5(33)
				141.6(58)		
	154.8(33)			151.8(33)		
166.4(1b)	167(4)	163.9(45b)		163.4(38b)		169.7(45)
			170(87)	168.2(69)		180.0(4)
			180(7)	179.2(74)		
			201(6b)	197.5(4b)		
			213.3(85)	211.5(73)		
	221.8(41)		223(107)	221.9(105)		
				236.5(6)		
	257.8(31b)			248(85)		
			280.3(8)	273.7(44)	280(24b)	
			292.5(5)	296.2(34b)		
			321.8(48)	320.6(32b)		
				364.5(24b)		

*) See the footnote of Table 43A-13-009.

Table 43A-13-009. $(NH_4)_2Cd_2(SO_4)_3$, $(ND_4)_2Cd_2(SO_4)_3$, $Tl_2Cd_2(SO_4)_3$, $Rb_2Cd_2(SO_4)_3$, $K_2Mn_2(SO_4)_3$. Raman peaks in the region of external vibrations [cm^{-1}] [83Lat2]. X' and Y' are [110] and [$\bar{1}$ 10] axes, respectively.

A + *E*					*E*				*F*, x					*F*, *y*					*F*, *z*			
Z(*XX*)*Y*					*Z*(*Y*′*X*′)*Y*′				*Z*(*YZ*)*Y*					*Z*(*XZ*)*Y*					*Z*(*YX*)*Y*			
TCS	ACS	DACS	RCS	KMS	TCS	ACS	DACS	RCS	TCS	ACS	DACS	RCS	KMS	TCS	ACS	DACS	RCS	KMS	TCS	ACS	DACS	RCS
18	22	22	18		17	24	a.t.	18														
												a.t.					a.t.					
												47	46				48					47
35	53	55	49	69	35	53	55	49	33	53	54			33	52	53		51	33	52	53	
a.t.					45				42					41					42			
									51					51					51			
75	78	79	71		74			76		80	82	72			80	79	76			78	78	72
	a.t.	a.t.	79	90		86	87	a.t.														
										98	98		98		98	96				97	95	
90	107	104	106	109	90	101	103	106				105					106	102				104
								124					122									
111	a.t.	a.t.	130																			
136	147	146	149	147	133	148	149	149										132				
										157	155	155	156		159	157	161	168		158	157	153
					208	211	207															
206	210	212	209	211						210	211	209			210	212	209			208	209	208
													230					230				

a.t.: asymmetry on tail of line.
TCS: $Tl_2Cd_2(SO_4)_3$, ACS: $(NH_4)_2Cd_2(SO_4)_3$, DACS: $(ND_4)_2Cd_2(SO_4)_3$, RCS: $Rb_2Cd_2(SO_4)_3$, KMS: $K_2Mn_2(SO_4)_3$.

Table 43A-13-010. $(NH_4)_2Cd_2(SO_4)_3$, $(ND_4)_2Cd_2(SO_4)_3$, $Tl_2Cd_2(SO_4)_3$, $Rb_2Cd_2(SO_4)_3$, $K_2Mn_2(SO_4)_3$. Correlation of a free SO_4^{2-} ion and internal vibrations of sulfate ions [cm^{-1}] [83Lat2].

T_d Molecule	C_1 Local group	T Factor group	TCS*	ACS*	DACS*	RCS*	KMS*
(ν_1 = 98 cm^{-1})	*A–A*	*A*	1014	1022	1023	1024	1030
		E	1014		1023	1022	1029
		F	1014	1022	1023	1023	1027
(ν_2 = 451 cm^{-1})	*E–A*	*A*	432	437	437	436	447
		F	436	443	545	443	449
		E	437	441	444	442	
		E	453.5	463	463	461	
		F	454	464	467	463	463
		A	459	470	472	467	462
(ν_2 = 1104 cm^{-1})	F_2–*A*	*A*	1073	1083	1090	1090	1103
		E	1073	1112		1088	
		F	1073	1083	1097	1088	1104
		F	1075				
		F	1085				
			1087			1089	
		A	1092	1103		1114	1111
		E	1088	1135		1106	
		F		1117	1143	1127	1136
		F	1107			1144	1139
		F		1143			1155
		A	1118	1195		1145	1120
		E	1119			1137	1146
		F	1123	1196			1122
		F	1124				1223
		F	1187				
			1189		1225	1209	1225
(ν_4 = 613 cm^{-1})	F_2–*A*	*A*	593	602	602	599	604
		E	592			601	
		F		601		601	607
		F	593	609	606	604	610
		F		615			612
		A	612	614	616	621	622
		E	605.5	622		616	
		F	606	621	624	618	625
		F	607			624	629
		F	609				632
			613				
		A	615				
			627	638	642	640	643
		E	628	646		637	
		F	627	641	644	639	
		F	628	645			648
		F	633			645	649
			635				650

Table 43A-13-011. $(NH_4)_2Cd_2(SO_4)_3$. Raman mode frequencies [cm^{-1}] of *XX*, *YY*, *ZZ* polarization conditions [88Gal]. s: shoulder, b: broad line.

XX			*YY*	*ZZ*	Assignments
300 K	105 K	80 K	80 K	80 K	
437.4	438.2	439.6	435.6	434.8	
				446.8	
		454	454	454	$\nu_2(SO_4^{2-})$
462		463	463(s)	462.4	
469.6	467	466		468.4	
		468.4	470	–	
	476	473.8	473.8	473.2	
		481	481	479.2	
600	599.6	598	597.2	596.8	
612		611.2	610	610	
	614	616	617	616	
620	621	621.4	623.2	621.4	$\nu_4(SO_4^{2-})$
636		638.2	638.2	637.6	
	641	643.6	644.2	643.6	
	992.6	–	–	–	
		1003.2	1003.2	1002.2	
		1015.2	1014	1013.6	
1019.2		1018.2	1017.6	1017.2	$\nu_1(SO_4^{2-})$
	1022	1021.2(s)	1021.2(s)	1020.2	
		1024.2(s)	1023.6	1023.8	
		1070	1071.6	1072	
1078.6	1079.6	1078.2	1077.6(s)	1076.8(s)	
		1085.4	1085.4	1085.8	
		1091.4	1096.2	1096.1	
		1103.4	–	–	
1108.6	1106	1108.8	1108	1108	$\nu_3(SO_4^{2-})$
	1118.6	1116		1120	
1134.4		1131.6	1132.8	1132	
	1149.2	1152	1156.2	1154.8	
		1191.6	1195.8	1194.8	
	1200	1204.8	1209	1208	
		1391.4	1394.2	1393	
	1418(s)	1423.8	1415.8	1414	
1427.2	1432(2)	1441.8	1423.6	1424(s)	$\nu_4(NH_4^+)$
			1454.2	–	
1670	1674	1665.2	1673.2	1671.4	
	2849.6(b)			2874.4(b)	$\nu_2(NH_4^+)$
			3032.4		
			3052.8	3051.6(s)	
	3077.6			3071.4	$\nu_1(NH_4^+)$
	3114.8	3124.6	3124.8	3123.4	
	3171.2	3169.6			
		3234.8		3253	$\nu_3(NH_4^+)$
	3284.6	3296			

Table 43A-13-012. $(NH_4)_2Cd_2(SO_4)_3$. Spin-Hamiltonian parameters for Mn^{2+}-doped sample [1]) [86Mis], [2]) [75NgH], [3]) [62Tat].

	[1])	[2])	[3])
$g_{\parallel}$	2.004(1)	1.992(1) (site I) 1.992(1) (site II)	2.000(2)
$g_{\perp}$	2.013(1)		
b_2^0 [GHz]	0.485(2)		−0.4719(4)
b_4^0 [GHz]	0.005(1)	0.0065(3) (site I) 0.0048(3) (site II)	0.0045(30)
b_4^3 [GHz]	−0.03(2)		0.216(107)
A [GHz]	−0.278(3)	0.2910(9)	−0.2829(6)
B [GHz]	−0.246(3)		

Table 43A-13-013. $(NH_4)_2Cd_2(SO_4)_3$. Spin Hamiltonian parameters of Mn^{2+} [75NgH]. A, D and a–F [$\cdot 10^2$ m^{-1}].

Parameter	Site I	Site II
$g_{\parallel}$	1.992 (1)	1.992 (1)
$\lvert A\rvert$	90 (3)	90 (3)
D	−159 (5)	−151 (5)
$(a–F)$	4.0 (1)	4.5 (1)

Table 43A-13-014. $(NH_4)_2Cd_2(SO_4)_3$, $Tl_2Cd_2(SO_4)_3$, $Rb_2Cd_2(SO_4)_3$. Spin-Hamiltonian parameters of Mn^{2+} [90Bab]. The parameters are contained in the Hamiltonian, $\mathbf{H} = g\beta H \cdot S + D(S_z^2 - \frac{35}{12}) - \frac{7}{36}(a-F)(S_z^4 - \frac{95}{14}S_z^2 + \frac{81}{16}) + AS_zI_z + \frac{1}{2}B(S_+I_- + S_-I_+)$. Spectra were recorded by an X-band spectrometer.

Crystal *	g	D [G]	a–F [G]	A [G]
TCS	2.008(1)	147 ± 2	5 ± 2	–95 ± 2
ACS	2.006(1)	168 ± 2	3 ± 2	–100 ± 2
RCS	2.010(1)	183 ± 2	6 ± 3	–94 ± 2

* TCS: $Tl_2Cd_2(SO_4)_3$; ACS: $(NH_4)_2Cd_2(SO_4)_3$;
RCS: $Rb_2Cd_2(SO_4)_3$.

Table 43A-13-015. $(NH_4)_2Cd_2(SO_4)_3$:Tl. Spin-Hamiltonian parameters of paramagnetic centers [87Efi].

	$g_{\parallel}$	$g_{\perp}$		$A_{\parallel}$	$A_{\perp}$
NH_3^+	2.0024	2.0034	^1H	26.2 Oe	24.8 Oe
Cd^+I	1.9968	1.9968	^{14}N	31.3 Oe	12 Oe
Tl^{2+}	1.9940	1.9842	^{111}Cd		12.63 GHz
			^{113}Cd		13.21 GHz
			Tl^{2+}	116.74 GHz	115.90 GHz