

Unit cell, SCXRD experimental details and structure refinements data for other examined crystals.

	L2	L4	L5	L6	L7
a (Å)	10.5699(4)	10.564(2)	10.545(3)	10.5605(8)	10.556(1)
V (Å ³)	1180.9(1)	1178.9(8)	1173(1)	1177.8(3)	1176.2(3)
size (μm)	60×55×50	75×55×45	60×60×60	60×70×35	70×50×40
θ_{\max} (MoK α)	32	32	32	31	32
R_{int} (%)	4.35	6.08	9.29	8.37	5.74
indep. refl.	120	125	124	116	125
obs. refl.	96	97	91	85	103
$[F_o > 4\sigma(F_o)]$					
Ref. param.	12	12	13	12	12
$R1_{\text{all}}$ (%)	4.68	4.61	7.98	6.64	3.75
$R1_{\text{obs}}$ (%)	3.45	3.19	5.43	4.29	2.88
$\Delta\rho_{\max}$ (e/Å ³)	0.55	0.53	1.10	1.00	0.46
$\Delta\rho_{\min}$ (e/Å ³)	−1.10	−0.62	−0.81	−1.16	−0.74

	L7_Tl	L8_Tl	L10	L12	L12_Tl
a (Å)	10.6514(6)	10.6480(5)	10.5364(6)	10.5700(3)	10.6477(5)
V (Å ³)	1208.4(2)	1207.3(2)	1169.7(2)	1180.9(1)	1207.2(2)
size (μm)	70×50×40	60×60×50	60×50×50	55×50×40	55×50×40
θ_{\max} (MoK α)	32	32	32	32	32
R_{int} (%)	6.65	4.66	3.69	3.55	3.63
indep. refl.	128	129	125	125	128
obs. refl.	94	101	97	109	112
$[F_o > 4\sigma(F_o)]$					
Ref. param.	14	14	12	12	13
$R1_{\text{all}}$ (%)	5.96	5.39	3.92	2.78	4.18
$R1_{\text{obs}}$ (%)	4.36	4.14	2.76	2.29	3.84
$\Delta\rho_{\max}$ (e/Å ³)	1.12	1.42	0.49	0.56	1.05
$\Delta\rho_{\min}$ (e/Å ³)	−1.08	−1.07	−0.75	−0.67	−1.50

	L19	L19_Tl
a (Å)	10.5699(5)	10.6716(6)
V (Å ³)	1180.9(2)	1215.3(2)
size (μm)	50×60×70	50×60×70
θ_{\max} (MoK α)	32	32
R_{int} (%)	9.34	5.22
indep. refl.	125	128
obs. refl.	89	114
$[F_o > 4\sigma(F_o)]$		
Ref. param.	13	14
$R1_{\text{all}}$ (%)	6.43	3.55
$R1_{\text{obs}}$ (%)	3.64	3.26
$\Delta\rho_{\max}$ (e/Å ³)	0.70	1.33
$\Delta\rho_{\min}$ (e/Å ³)	−0.73	−1.06

Selected bond distances and structural parameters for for other examined crystals.

	L2	L4	L5	L6	L7
n.e ⁻ (A)	4.2	4.2	4.2	4.2	4.2
n.e ⁻ (A')	1.3	1.5	5.7	1.6	2.0
n.e ⁻ (Y')	9.1	9.1	9.1	9.1	9.1
<i>x</i> _{48f} (X)	0.3130(4)	0.3127(4)	0.3134(6)	0.3129(6)	0.3130(3)
<i>x</i> _{32e} (A')	0.522(4)	0.520(3)	0.5107(16)	0.521(5)	0.519(2)
<i>x</i> _{32e} (Y')	0.392(10)	0.392(9)	0.405(2)	0.400(3)	0.398(3)
A-X (×6)	2.720(3)	2.720(3)	2.710(4)	2.718(5)	2.717(3)
A-Y' (×2)	2.41(8)	2.41(8)	2.52(2)	2.48(3)	2.46(3)
<A-O>	2.643	2.643	2.663	2.659	2.653
B-X (×6)	1.983(2)	1.982(2)	1.980(2)	1.982(2)	1.981(1)
A'-X (×3)	2.81(5)	2.80(4)	2.75(2)	2.80(6)	2.79(3)
(×3)	2.69(5)	2.69(4)	2.69(5)	2.69(6)	2.69(3)
A'-Y' (×2)	2.81(12)	2.77(11)	2.71(3)	2.86(7)	2.80(4)
<A'-O>	2.77	2.75	2.72	2.77	2.76
Y'-X (×3)	3.13(9)	3.12(9)	3.00(2)	3.05(3)	3.07(3)
(×3)	3.49(7)	3.49(10)	3.63(3)	3.58(4)	3.55(4)
<Y'-X>	3.31	3.31	3.32	3.32	3.31
X-X (u.)	2.810(6)	2.804(6)	2.810(9)	2.806(9)	2.807(5)
X-X (s.)	2.800(2)	2.800(3)	2.792(4)	2.798(3)	2.797(2)
<X-X>	2.805	2.802	2.801	2.802	2.802
X-B-X (u.)	90.2(2)	90.1(2)	90.4(2)	90.2(3)	90.2(1)
X-B-X (s.)	89.8(2)	89.9(2)	89.6(2)	89.8(3)	89.8(1)
B-X-B	140.8(2)	140.9(2)	140.5(3)	140.8(4)	140.8(2)
B-X-A	104.11(7)	104.08(7)	104.19(9)	104.1(1)	104.12(5)
A-X-A	86.8(1)	86.7(1)	86.9(2)	86.8(2)	86.8(1)
σ ² (B)	0.05	0.01	0.15	0.03	0.05

	L7_Tl	L8_Tl	L10	L12	L12_Tl
n.e ⁻ (A)	58.9	59.7	4.2	4.2	59.4
n.e ⁻ (A')	-	-	5.0	2.1	-
n.e ⁻ (Y')	4.1	4.8	9.1	9.1	4.7
<i>x</i> _{48f} (X)	0.3107(10)	0.3107(13)	0.3145(3)	0.3130(3)	0.3105(9)
<i>x</i> _{32e} (A')	-	-	0.5134(10)	0.5187(17)	-
<i>x</i> _{32e} (Y')	0.402(9)	0.406(9)	0.4062(13)	0.390(11)	0.404(7)
A-X (×6)	2.759(7)	2.758(10)	2.700(2)	2.720(2)	2.760(7)
A-Y' (×2)	2.52(8)	2.56(8)	2.528(12)	2.40(8)	2.54(7)
<A-O>	2.699	2.709	2.657	2.640	2.705
B-X (×6)	1.991(3)	1.990(4)	1.983(1)	1.9836(9)	1.989(3)
A'-X (×3)	-	-	2.746(11)	2.79(2)	-
(×3)	-	-	2.675(11)	2.69(2)	-
A'-Y' (×2)	-	-	2.77(2)	2.73(12)	-
<A'-O>	-	-	2.725	2.74	-

Y'-X (×3)	3.09(7)	3.05(7)	2.980(11)	3.14(10)	3.07(6)
(×3)	3.66(10)	3.71(10)	3.63(2)	3.46(12)	3.68(8)
<Y'-X>	3.38	3.38	3.305	3.30	3.38
X-X (u.)	2.797(16)	2.80(2)	2.824(5)	2.810(5)	2.793(14)
X-X (s.)	2.834(6)	2.833(7)	2.784(2)	2.800(2)	2.834(5)
<X-X>	2.816	2.817	2.804	2.805	2.814
X-B-X (u.)	89.3(4)	89.2(5)	90.8(1)	90.2(1)	89.2(4)
X-B-X (s.)	90.7(4)	90.8(5)	89.2(1)	89.8(1)	90.8(4)
B-X-B	142.1(6)	142.1(7)	139.9(2)	140.8(2)	142.2(5)
B-X-A	103.7(2)	103.7(2)	104.37(5)	104.12(4)	103.7(2)
A-X-A	86.1(3)	86.1(4)	87.2(1)	86.8(1)	86.0(3)
σ^2 (B)	0.59	0.59	0.71	0.05	0.73

	L19	L19_Tl
n.e ⁻ (A)	4.2	58.2
n.e ⁻ (A')	2.2	-
n.e ⁻ (Y')	9.1	4.9
x_{48f} (X)	0.3130(5)	0.3108(5)
x_{32e} (A')	0.514(3)	-
x_{32e} (Y')	0.396(5)	0.401(6)
A-X (×6)	2.720(3)	2.764(4)
A-Y' (×2)	2.44(4)	2.51(6)
<A-O>	2.650	2.701
B-X (×6)	1.984(2)	1.995(2)
A'-X (×3)	2.77(4)	-
(×3)	2.70(4)	-
A'-Y' (×2)	2.70(7)	-
<A'-O>	2.726	-
Y'-X (×3)	3.09(4)	3.10(5)
(×3)	3.53(6)	3.65(7)
<Y'-X>	3.31	3.38
X-X (u.)	2.810(8)	2.804(8)
X-X (s.)	2.800(3)	2.838(3)
<X-X>	2.805	2.821
X-B-X (u.)	90.2(3)	89.3(2)
X-B-X (s.)	89.8(3)	90.7(2)
B-X-B	140.8(3)	142.1(3)
B-X-A	104.11(8)	103.74(8)
A-X-A	86.8(1)	86.1(1)
σ^2 (B)	0.05	0.5

Notes: u. = unshared edge of the octahedron; s. = shared edge between B and A polyhedral. Bond angle variance (σ^2) was computed according to the formula proposed by Robinson et al. (1971).