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New alluaudite-related triple molybdates $Na_{25}Cs_8R_5(MoO_4)_{24}$ (R = Sc, In): synthesis, crystal structures and properties

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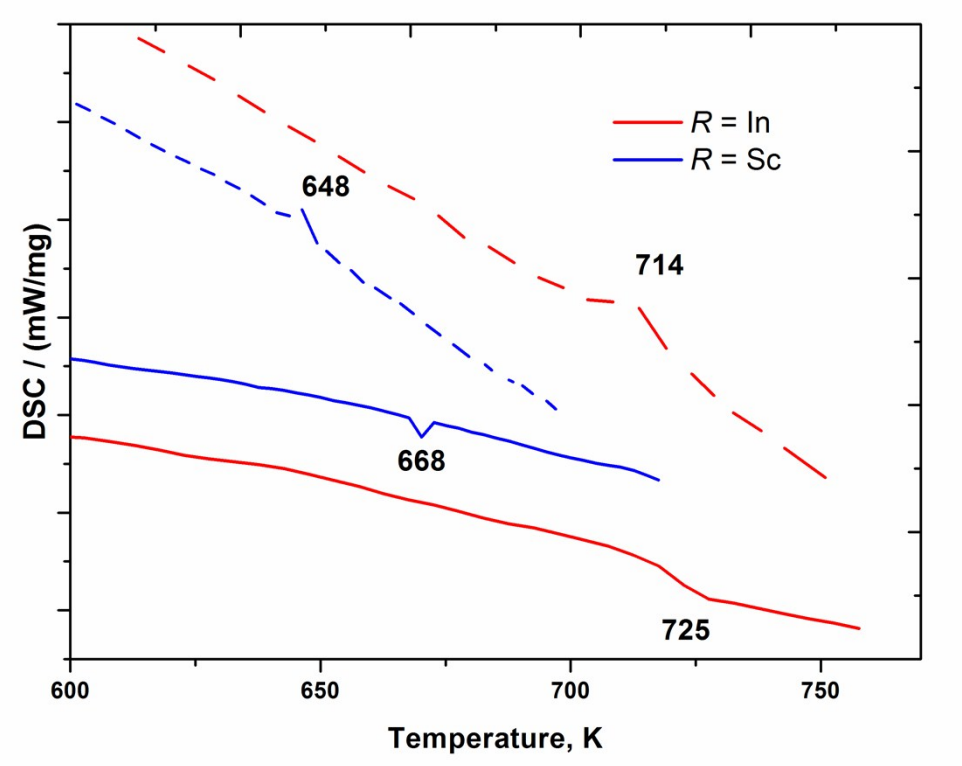

Fig. 1S. The fragments of heating (solid lines) and cooling (dotted thick lines) process in the phase transitions regions of DSC curves for $Na_{25}Cs_8R_5(MoO_4)_{24}$, R = Sc, In.

Table 1S. Atomic coordinates and equivalent isotropic displacement parameters for $Na_{25}Cs_8Sc_5(MoO_4)_{24}$ and $Na_{25}Cs_8In_5(MoO_4)_{24}$

Atom	$Na_{25}Cs_8Sc_5(MoO_4)_{24}$					$Na_{25}Cs_8In_5(MoO_4)_{24}$				
	Occupancy	***x/a***	***y/b***	***z/c***	U_{eq} (Å²)*	**Occupancy**	***x/a***	***y/b***	***z/c***	U_{eq} (Å²)*
Mo(1)		0.60185(4)	0.18473(4)	0.21950(2)	0.0175(1)		0.60400(7)	0.18251(7)	0.22064(3)	0.0154(2)
Mo(2)		0.10938(4)	0.18166(4)	0.27973(2)	0.0153(1)		0.10938(7)	0.17870(6)	0.27938(3)	0.0132(2)
Mo(3)		0.61231(4)	0.24187(5)	0.47128(2)	0.0158(1)		0.61379(6)	0.24036(7)	0.47162(3)	0.0135(2)
Mo(4)		0.38968(4)	0.20063(5)	0.34721(2)	0.0164(1)		0.39066(7)	0.19681(7)	0.34723(3)	0.0141(2)
Mo(5)		0.61247(4)	0.72625(4)	0.39656(2)	0.0153(1)		0.61259(7)	0.72738(7)	0.39640(3)	0.0134(2)
Mo(6)		0.10279(4)	0.26485(4)	0.52728(2)	0.0158(1)		0.10483(6)	0.26558(7)	0.52783(3)	0.0149(2)
Mo(7)		0.88169(4)	0.21549(4)	0.39810(2)	0.0151(1)		0.88315(7)	0.21756(7)	0.39833(3)	0.0152(2)
Mo(8)		0.11154(4)	0.69466(4)	0.35097(2)	0.0155(1)		0.11013(7)	0.69155(7)	0.35032(3)	0.0136(2)
Mo(9)		0.28441(4)	0.56432(4)	0.68396(2)	0.0151(1)		0.28648(6)	0.56513(7)	0.68379(3)	0.0131(2)
Mo(10)		0.28498(4)	0.48102(4)	0.44278(2)	0.0154(1)		0.28655(6)	0.48105(7)	0.44219(3)	0.0135(2)
Mo(11)		0.22201(4)	0.43293(5)	0.18662(2)	0.0192(1)		0.21896(7)	0.43204(7)	0.18606(3)	0.0166(2)
Mo(12)		0.79029(4)	0.47039(4)	0.05627(2)	0.0150(1)		0.79118(6)	0.47094(6)	0.05676(3)	0.0123(2)
Cs(1)		0.48727(3)	0.98108(3)	0.43223(2)	0.0261(1)		0.48585(6)	0.98003(5)	0.43257(3)	0.0265(2)
Cs(2)		0.50603(4)	0.95377(4)	0.28253(2)	0.0369(1)		0.50778(7)	0.95067(6)	0.28367(3)	0.0395(2)
Cs(3)		0.00867(4)	0.95015(4)	0.21580(2)	0.0304(1)		0.00906(6)	0.94734(6)	0.21424(3)	0.0319(2)
Cs(4)		0.00611(4)	0.46959(4)	0.43175(2)	0.0288(1)		0.00767(8)	0.46875(7)	0.43325(4)	0.0442(2)
(*R*, Na)(1)	0.792(2)/0.208	0.83804(9)	0.29014(10)	0.52000(4)	0.0098(2)	0.897(2)/0.103	0.83903(5)	0.29078(5)	0.52070(2)	0.0091(2)
(*R*, Na)(2)	0.538(5)/0.462	0.65527(11)	0.17249(12)	0.34880(5)	0.0114(4)	0.644(3)/0.356	0.65712(7)	0.16977(7)	0.34913(3)	0.0101(3)
(*R*, Na)(3)	0.580(5)/0.420	0.33067(10)	0.19562(12)	0.22798(5)	0.0124(4)	0.491(3)/0.509	0.33192(8)	0.19461(8)	0.22819(4)	0.0084(3)
(*R*, Na)(4)	0.242(5)/0.758	0.15663(15)	0.17356(17)	0.14868(7)	0.0166(6)	0.380(3)/0.620	0.15964(11)	0.17153(10)	0.14946(5)	0.0089(4)
(*R*, Na)(5)	0.097(5)/0.903	0.83103(18)	0.1987(2)	0.26752(9)	0.0217(8)	0.020(3)/0.980	0.8315(3)	0.1978(3)	0.26799(13)	0.0135(12)
(*R*, Na)(6)	0.251(4)/0.749	0.33561(17)	0.21187(19)	0.48025(8)	0.0249(6)	0.069(3)/0.931	0.3373(3)	0.2114(3)	0.47994(11)	0.0189(10)
Na(7)		0.15861(19)	0.2370(2)	0.39485(10)	0.0209(6)		0.1588(3)	0.2396(3)	0.39496(15)	0.0170(8)
Na(8)		0.34087(19)	0.7409(2)	0.39466(10)	0.0180(5)		0.3410(3)	0.7420(3)	0.39419(15)	0.0173(9)
Na(9)		0.7636(2)	0.9683(3)	0.43321(12)	0.0336(8)		0.7619(4)	0.9710(4)	0.43425(18)	0.0295(11)
Na(10)		0.7338(2)	0.4917(3)	0.43834(12)	0.0376(8)		0.7363(4)	0.4921(5)	0.43827(18)	0.0337(12)
Na(11)		0.0014(2)	0.9673(3)	0.36827(12)	0.0369(8)		0.0028(4)	0.9684(4)	0.36662(19)	0.0344(12)
Na(12)		0.2315(2)	0.9387(3)	0.31491(10)	0.0251(6)		0.2327(4)	0.9372(4)	0.31381(17)	0.0230(10)
Na(13)		0.50256(2)	0.9727(3)	0.12860(13)	0.0405(9)		0.5030(4)	0.9739(4)	0.1301(2)	0.0393(13)

Na(14)		0.26604(2)	0.4430(3)	0.31504(11)	0.0261(6)		0.2661(3)	0.4418(4)	0.31488(17)	0.0218(9)
Na(15)	0.5	-0.0069(8)	0.0147(9)	0.4899(3)	0.037(2)	0.5	-0.0072(12)	0.0160(12)	0.4887(4)	0.039(4)
Na(16)	0.5	0.5054(7)	0.5180(7)	0.4898(3)	0.033(2)	0.5	0.5043(10)	0.5187(9)	0.4893(4)	0.033(3)
O(1)		0.5989(4)	0.0699(4)	0.1861(2)	0.0315(12)		0.5989(7)	0.0654(6)	0.1872(3)	0.0276(18)
O(2)		0.6570(4)	0.2884(4)	0.1892(2)	0.0263(11)		0.6606(6)	0.2829(6)	0.1906(3)	0.0232(16)
O(3)		0.6631(4)	0.1561(4)	0.2722(2)	0.028(1)		0.6667(7)	0.1539(6)	0.2731(3)	0.0258(17)
O(4)		0.4822(4)	0.2226(4)	0.2337(2)	0.029(1)		0.4882(6)	0.2230(6)	0.2363(3)	0.0272(18)
O(5)		-0.0050(4)	0.2158(4)	0.2619(2)	0.026(1)		-0.0050(6)	0.2151(6)	0.26188(3)	0.0230(17)
O(6)		0.1560(4)	0.2876(4)	0.3116(2)	0.025(1)		0.1573(6)	0.2855(6)	0.3115(3)	0.0199(15)
O(7)		0.1035(4)	0.0662(4)	0.3134(2)	0.030(1)		0.1026(6)	0.0643(6)	0.3129(3)	0.0282(19)
O(8)		0.1787(4)	0.1563(4)	0.2271(2)	0.026(1)		0.1765(6)	0.1513(6)	0.2267(3)	0.0197(16)
O(9)		0.5953(4)	0.3727(4)	0.4545(2)	0.029(1)		0.5975(6)	0.3724(6)	0.4542(3)	0.0273(19)
O(10)		0.5030(4)	0.1866(4)	0.4874(2)	0.026(1)		0.5048(6)	0.1868(6)	0.4872(3)	0.0246(17)
O(11)		0.6590(4)	0.1627(5)	0.4260(2)	0.031(1)		0.6617(6)	0.1592(6)	0.4260(3)	0.0235(17)
O(12)		0.6910(3)	0.2385(4)	0.5205(2)	0.0238(10)		0.6899(5)	0.2349(6)	0.5214(3)	0.0214(16)
O(13)		0.3260(4)	0.1800(5)	0.3988(2)	0.0302(12)		0.3278(6)	0.1793(6)	0.3993(3)	0.0279(19)
O(14)		0.4004(4)	0.3363(4)	0.3372(2)	0.0336(13)		0.4006(6)	0.3331(7)	0.3355(4)	0.032(2)
O(15)		0.3289(4)	0.1368(2)	0.3002(2)	0.0379(15)		0.3279(6)	0.1299(7)	0.3019(3)	0.032(2)
O(16)		0.5041(4)	0.1393(4)	0.3531(2)	0.0256(11)		0.5047(6)	0.1360(6)	0.3532(3)	0.0200(16)
O(17)		0.5007(4)	0.7775(4)	0.38172(17)	0.0269(11)		0.5009(6)	0.7772(6)	0.3809(3)	0.0247(17)
O(18)		0.6002(4)	0.5959(4)	0.41661(19)	0.0273(11)		0.59823(6)	0.59631(6)	0.41545(3)	0.0253(18)
O(19)		0.6621(4)	0.8112(4)	0.43861(17)	0.0247(11)		0.6607(6)	0.8111(5)	0.4388(2)	0.0182(15)
O(20)		0.6868(4)	0.7267(4)	0.34545(17)	0.0252(11)		0.6875(6)	0.7303(6)	0.3463(3)	0.0230(17)
O(21)		0.1655(4)	0.2730(5)	0.47511(19)	0.0356(13)		0.1672(6)	0.2747(6)	0.4761(3)	0.0273(18)
O(22)		0.0939(4)	0.1336(4)	0.5446(2)	0.0324(13)		0.0955(7)	0.1333(6)	0.5444(3)	0.030(2)
O(23)		0.1615(4)	0.3438(5)	0.5689(2)	0.0287(12)		0.1641(6)	0.3411(7)	0.5700(3)	0.0259(18)
O(24)		-0.0150(4)	0.3201(4)	0.51803(17)	0.0249(10)		-0.0113(5)	0.3212(6)	0.5188(3)	0.0246(17)
O(25)		0.9926(4)	0.2642(4)	0.38213(18)	0.0277(11)		0.9935(5)	0.2670(7)	0.3826(3)	0.0275(18)
O(26)		0.8946(4)	0.0833(4)	0.41351(19)	0.0291(12)		0.8959(7)	0.0828(6)	0.4144(3)	0.030(2)
O(27)		0.8054(4)	0.2236(4)	0.34869(17)	0.0262(11)		0.8068(6)	0.2281(6)	0.3487(3)	0.0215(17)
O(28)		0.8374(3)	0.2946(4)	0.44575(17)	0.0227(10)		0.8375(6)	0.2952(6)	0.4455(2)	0.0237(16)
O(29)		0.0995(4)	0.8261(4)	0.33461(19)	0.0275(11)		0.1001(6)	0.8227(6)	0.3331(3)	0.0258(18)
O(30)		0.1766(4)	0.6218(5)	0.30988(19)	0.0334(13)		0.1730(6)	0.6154(6)	0.3090(3)	0.0269(18)
O(31)		-0.0007(4)	0.6345(4)	0.35555(18)	0.0280(11)		-0.0041(6)	0.6330(6)	0.3570(3)	0.0285(19)

O(32)		0.1716(4)	0.6870(4)	0.40628(18)	0.0269(11)		0.1717(7)	0.6840(6)	0.4043(3)	0.0239(18)
O(33)		0.2203(4)	0.6177(4)	0.73059(17)	0.0245(10)		0.2231(6)	0.6178(6)	0.7306(3)	0.0244(17)
O(34)		0.3597(4)	0.4646(5)	0.7057(2)	0.0351(13)		0.3644(6)	0.4678(6)	0.7051(3)	0.0262(18)
O(35)		0.2036(4)	0.5105(5)	0.64308(19)	0.0324(12)		0.2085(6)	0.5075(7)	0.6433(3)	0.0284(18)
O(36)		0.3633(4)	0.6558(5)	0.6567(2)	0.0324(13)		0.3651(6)	0.6580(6)	0.6563(3)	0.0224(17)
O(37)		0.3526(4)	0.3910(4)	0.4746(2)	0.0332(13)		0.3545(6)	0.3931(6)	0.4746(3)	0.0280(19)
O(38)		0.3695(4)	0.5671(4)	0.4194(2)	0.0304(12)		0.3706(6)	0.5680(6)	0.4182(3)	0.0279(19)
O(39)		0.2198(4)	0.4223(4)	0.39723(16)	0.0238(10)		0.2236(6)	0.4204(6)	0.3975(2)	0.0188(16)
O(40)		0.2056(4)	0.5485(4)	0.48337(16)	0.0209(10)		0.2056(6)	0.5466(6)	0.4829(3)	0.0178(15)
O(41)		0.1475(5)	0.5245(5)	0.2131(3)	0.060(2)		0.1415(9)	0.5233(7)	0.2094(4)	0.058(4)
O(42)		0.1432(4)	0.3549(5)	0.1547(2)	0.0351(14)		0.1417(7)	0.3503(7)	0.1547(3)	0.033(2)
O(43)		0.3029(4)	0.4990(5)	0.14797(19)	0.0328(12)		0.3010(6)	0.4964(6)	0.1475(3)	0.0220(16)
O(44)		0.2863(4)	0.3651(5)	0.23200(18)	0.0342(13)		0.2827(7)	0.3696(6)	0.2324(3)	0.0276(19)
O(45)		0.8735(4)	0.5603(4)	0.0778(2)	0.0315(12)		0.8721(6)	0.5628(6)	0.0770(3)	0.0261(18)
O(46)		0.7231(4)	0.4194(4)	0.10259(16)	0.0212(10)		0.7234(6)	0.4196(6)	0.1035(3)	0.0235(17)
O(47)		0.7120(4)	0.5298(4)	0.01510(17)	0.0210(10)		0.7127(6)	0.5289(6)	0.0155(3)	0.0202(16)
O(48)		0.8637(4)	0.3724(4)	0.02735(18)	0.0244(10)		0.8676(6)	0.3748(6)	0.0286(3)	0.0208(16)

* $U_{eq} = (U_{11} + U_{22} \sin^2\beta + U_{33} + 2U_{13} \cos\beta) / 3\sin^2\beta$.

Table 2S. Selected interatomic distances (Å) in $Na_{25}Cs_8Sc_5(MoO_4)_{24}$ and $Na_{25}Cs_8In_5(MoO_4)_{24}$

$Na_{25}Cs_8Sc_5(MoO_4)_{24}$		$Na_{25}Cs_8In_5(MoO_4)_{24}$	
Mo(1)–tetrahedron		**Mo(1)–tetrahedron**	
Mo(1)–O(1)	1.741(5)	Mo(1)–O(2)	1.725(7)
Mo(1)–O(2)	1.752(5)	Mo(1)–O(4)	1.759(8)
Mo(1)–O(3)	1.773(6)	Mo(1)–O(1)	1.763(7)
Mo(1)–O(4)	1.790(5)	Mo(1)–O(3)	1.781(9)
<Mo(1)–O>	*1.764*	*<Mo(1)–O>*	*1.757*
Mo(2)–tetrahedron		**Mo(2)–tetrahedron**	
Mo(2)–O(5)	1.736(5)	Mo(2)–O(7)	1.736(8)
Mo(2)–O(6)	1.748(5)	Mo(2)–O(5)	1.740(8)
Mo(2)–O(7)	1.752(5)	Mo(2)–O(6)	1.764(7)
Mo(2)–O(8)	1.823(5)	Mo(2)–O(8)	1.815(8)
<Mo(2)–O>	*1.765*	*<Mo(2)–O>*	*1.764*
Mo(3)–tetrahedron		**Mo(3)–tetrahedron**	
Mo(3)–O(9)	1.740(5)	Mo(3)–O(10)	1.729(8)
Mo(3)–O(10)	1.745(5)	Mo(3)–O(9)	1.753(8)
Mo(3)–O(11)	1.764(5)	Mo(3)–O(12)	1.783(8)
Mo(3)–O(12)	1.791(5)	Mo(3)–O(11)	1.793(8)
<Mo(3)–O>	*1.760*	*<Mo(3)–O>*	*1.765*
Mo(4)–tetrahedron		**Mo(4)–tetrahedron**	
Mo(4)–O(13)	1.746(5)	Mo(4)–O(13)	1.749(8)
Mo(4)–O(14)	1.747(5)	Mo(4)–O(14)	1.756(8)
Mo(4)–O(15)	1.785(5)	Mo(4)–O(16)	1.780(8)
Mo(4)–O(16)	1.788(5)	Mo(4)–O(15)	1.782(8)
<Mo(4)–O>	*1.767*	*<Mo(4)–O>*	*1.767*
Mo(5)–tetrahedron		**Mo(5)–tetrahedron**	
Mo(5)–O(17)	1.747(5)	Mo(5)–O(17)	1.744(8)
Mo(5)–O(18)	1.755(5)	Mo(5)–O(19)	1.747(7)
Mo(5)–O(19)	1.758(5)	Mo(5)–O(18)	1.752(8)
Mo(5)–O(20)	1.796(5)	Mo(5)–O(20)	1.781(8)
<Mo(5)–O>	*1.764*	*<Mo(5)–O>*	*1.756*
Mo(6)–tetrahedron		**Mo(6)–tetrahedron**	
Mo(6)–O(21)	1.736(5)	Mo(6)–O(21)	1.727(8)
Mo(6)–O(22)	1.738(5)	Mo(6)–O(22)	1.739(8)
Mo(6)–O(23)	1.759(5)	Mo(6)–O(23)	1.750(8)
Mo(6)–O(24)	1.811(5)	Mo(6)–O(24)	1.790(8)
<Mo(6)–O>	*1.761*	*<Mo(6)–O>*	*1.752*
Mo(7)–tetrahedron		**Mo(7)–tetrahedron**	
Mo(7)–O(25)	1.733(5)	Mo(7)–O(25)	1.727(8)
Mo(7)–O(26)	1.739(5)	Mo(7)–O(26)	1.769(8)
Mo(7)–O(27)	1.776(5)	Mo(7)–O(27)	1.787(8)
Mo(7)–O(28)	1.802(5)	Mo(7)–O(28)	1.788(8)
<Mo(7)–O>	*1.759*	*<Mo(7)–O>*	*1.768*
Mo(8)–tetrahedron		**Mo(8)–tetrahedron**	
Mo(8)–O(29)	1.736(5)	Mo(8)–O(29)	1.731(8)
Mo(8)–O(30)	1.751(5)	Mo(8)–O(30)	1.762(8)
Mo(8)–O(31)	1.752(5)	Mo(8)–O(31)	1.773(8)
Mo(8)–O(32)	1.797(5)	Mo(8)–O(32)	1.775(8)
<Mo(8)–O>	*1.759*	*<Mo(8)–O>*	*1.760*
Mo(9)–tetrahedron		**Mo(9)–tetrahedron**	
Mo(9)–O(33)	1.746(5)	Mo(9)–O(33)	1.742(8)
Mo(9)–O(34)	1.758(6)	Mo(9)–O(34)	1.753(8)

Mo(9)–O(35)	1.765(5)	Mo(9)–O(35)	1.753(9)
Mo(9)–O(36)	1.780(6)	Mo(9)–O(36)	1.791(8)
<Mo(9)–O>	*1.762*	*<Mo(9)–O>*	*1.760*
Mo(10)–tetrahedron		**Mo(10)–tetrahedron**	
Mo(10)–O(37)	1.739(5)	Mo(10)–O(37)	1.733(8)
Mo(10)–O(38)	1.742(5)	Mo(10)–O(39)	1.735(7)
Mo(10)–O(39)	1.758(5)	Mo(10)–O(38)	1.750(8)
Mo(10)–O(40)	1.821(5)	Mo(10)–O(40)	1.826(8)
<Mo(10)–O>	*1.765*	*<Mo(10)–O>*	*1.761*
Mo(11)–tetrahedron		**Mo(11)–tetrahedron**	
Mo(11)–O(41)	1.735(6)	Mo(11)–O(41)	1.717(9)
Mo(11)–O(42)	1.741(6)	Mo(11)–O(42)	1.745(9)
Mo(11)–O(43)	1.791(6)	Mo(11)–O(44)	1.784(9)
Mo(11)–O(44)	1.799(6)	Mo(11)–O(43)	1.789(8)
<Mo(11)–O>	*1.767*	*<Mo(11)–O>*	*1.759*
Mo(12)–tetrahedron		**Mo(12)–tetrahedron**	
Mo(12)–O(45)	1.742(5)	Mo(12)–O(45)	1.721(8)
Mo(12)–O(46)	1.750(5)	Mo(12)–O(46)	1.769(8)
Mo(12)–O(47)	1.777(5)	Mo(12)–O(47)	1.774(8)
Mo(12)–O(48)	1.811(5)	Mo(12)–O(48)	1.808(7)
<Mo(12)–O>	*1.770*	*<Mo(12)–O>*	*1.768*
Cs(1)–polyhedron		**Cs(1)–polyhedron**	
Cs(1)–O(17)	2.960(5)	Cs(1)–O(17)	2.964(8)
Cs(1)–O(16)#1	3.032(5)	Cs(1)–O(15)#1	3.022(7)
Cs(1)–O(10)#1	3.050(5)	Cs(1)–O(9)#1	3.053(8)
Cs(1)–O(10)#2	3.134(5)	Cs(1)–O(9)#2	3.121(8)
Cs(1)–O(46)#3	3.207(5)	Cs(1)–O(46)#3	3.201(9)
Cs(1)–O(47)#3	3.233(5)	Cs(1)–O(47)#3	3.215(8)
Cs(1)–O(19)	3.263(5)	Cs(1)–O(18)	3.251(8)
Cs(1)–O(11)#1	3.331(6)	Cs(1)–O(12)#1	3.347(8)
Cs(1)–O(13)#1	3.513(6)	Cs(1)–O(13)#1	3.482(9)
Cs(1)–O(43)#3	3.737(5)	Cs(1)–O(44)#3	3.775(8)
<Cs(1)–O>	*3.246*	*<Cs(1)–O>*	*3.243*
Cs(2)–polyhedron		**Cs(2)–polyhedron**	
Cs(2)–O(4)#3	2.966(5)	Cs(2)–O(2)#3	2.927(8)
Cs(2)–O(16)#1	3.098(5)	Cs(2)–O(15)#1	3.072(7)
Cs(2)–O(44)#3	3.145(6)	Cs(2)–O(43)#3	3.142(9)
Cs(2)–O(34)#4	3.180(6)	Cs(2)–O(34)#4	3.190(9)
Cs(2)–O(2)#3	3.201(6)	Cs(2)–O(1)#3	3.252(8)
Cs(2)–O(43)#3	3.384(6)	Cs(2)–O(3)#1	3.376(9)
Cs(2)–O(3)#1	3.388(5)	Cs(2)–O(44)#3	3.378(8)
Cs(2)–O(1)#1	3.389(6)	Cs(2)–O(4)#1	3.406(8)
Cs(2)–O(15)#1	3.431(6)	Cs(2)–O(16)#1	3.424(9)
Cs(2)–O(17)	3.613(5)	Cs(2)–O(17)	3.546(8)
Cs(2)–O(4)#1	3.692(5)	Cs(2)–O(2)#1	3.702(8)
<Cs(2)–O>	*3.317*	*<Cs(2)–O>*	*3.310*
Cs(3)–polyhedron		**Cs(3)–polyhedron**	
Cs(3)–O(5)#5	3.033(5)	Cs(3)–O(6)#5	3.007(8)
Cs(3)–O(31)#5	3.103(5)	Cs(3)–O(31)#5	3.109(8)
Cs(3)–O(33)#4	3.115(5)	Cs(3)–O(33)#4	3.143(9)
Cs(3)–O(41)#5	3.133(6)	Cs(3)–O(7)#5	3.183(8)
Cs(3)–O(6)#5	3.188(5)	Cs(3)–O(41)#5	3.189(10)
Cs(3)–O(7)#1	3.427(6)	Cs(3)–O(30)#5	3.381(9)
Cs(3)–O(30)#5	3.463(6)	Cs(3)–O(5)#1	3.451(9)

Cs(3)–O(35)#4	3.470(6)	Cs(3)–O(8)#1	3.498(7)
Cs(3)–O(8)#1	3.546(5)	Cs(3)–O(35)#4	3.504(9)
Cs(3)–O(5)#1	3.616(5)	Cs(3)–O(25)#3	3.591(9)
Cs(3)–O(25)#3	3.661(5)	Cs(3)–O(6)#1	3.646(8)
<Cs(3)–O>	*3.341*	*<Cs(3)–O>*	*3.337*
Cs(4)–polyhedron		**Cs(4)–polyhedron**	
Cs(4)–O(25)#6	2.968(5)	Cs(4)–O(25)#6	2.936(8)
Cs(4)–O(31)	3.021(5)	Cs(4)–O(24)#7	2.986(8)
Cs(4)–O(24)#7	3.027(5)	Cs(4)–O(31)	3.017(8)
Cs(4)–O(24)	3.126(5)	Cs(4)–O(24)	3.092(8)
Cs(4)–O(39)	3.208(5)	Cs(4)–O(38)	3.252(8)
Cs(4)–O(28)#6	3.263(5)	Cs(4)–O(28)#6	3.255(8)
Cs(4)–O(40)	3.315(5)	Cs(4)–O(40)	3.268(8)
Cs(4)–O(23)#7	3.329(5)	Cs(4)–O(23)#7	3.397(9)
Cs(4)–O(21)	3.565(6)	Cs(4)–O(21)	3.535(9)
Cs(4)–O(35)#7	3.645(5)	Cs(4)–O(32)	3.651(8)
Cs(4)–O(32)	3.670(5)	Cs(4)–O(35)#7	3.753(9)
<Cs(4)–O>	*3.285*	*<Cs(4)–O>*	*3.286*
***M*(1)–octahedron**		***M*(1)–octahedron**	
M(1)–O(24)#8	2.094(5)	*M*(1)–O(24)#8	2.132(7)
M(1)–O(48)#9	2.097(5)	*M*(1)–O(48)#9	2.137(7)
M(1)–O(28)	2.128(5)	*M*(1)–O(40)#2	2.145(7)
M(1)–O(40)#2	2.133(5)	*M*(1)–O(28)	2.161(7)
M(1)–O(32)#2	2.136(5)	*M*(1)–O(32)#2	2.183(7)
M(1)–O(12)	2.161(5)	*M*(1)–O(12)	2.204(7)
<M(1)–O>	*2.125*	*<M(1)–O>*	*2.160*
***M*(2)–octahedron**		***M*(2)–octahedron**	
M(2)–O(16)	2.163(6)	*M*(2)–O(16)	2.180(8)
M(2)–O(36)#2	2.194(6)	*M*(2)–O(3)	2.196(8)
M(2)–O(27)	2.201(5)	*M*(2)–O(36)#2	2.198(8)
M(2)–O(3)	2.208(6)	*M*(2)–O(11)	2.212(8)
M(2)–O(11)	2.217(6)	*M*(2)–O(27)	2.221(8)
M(2)–O(43)#10	2.274(7)	*M*(2)–O(43)#10	2.265(8)
<M(2)–O>	*2.210*	*<M(2)–O>*	*2.212*
***M*(3)–octahedron**		***M*(3)–octahedron**	
M(3)–O(20)#10	2.154(5)	*M*(3)–O(34)#11	2.199(7)
M(3)–O(4)	2.156(6)	*M*(3)–O(20)#10	2.202(7)
M(3)–O(34)#11	2.164(6)	*M*(3)–O(4)	2.230(9)
M(3)–O(8)	2.186(5)	*M*(3)–O(8)	2.244(8)
M(3)–O(15)	2.200(6)	*M*(3)–O(15)	2.270(9)
M(3)–O(44)	2.235(6)	*M*(3)–O(44)	2.313(9)
<M(3)–O>	*2.183*	*<M(3)–O>*	*2.243*
***M*(4)–octahedron**		***M*(4)–octahedron**	
M(4)–O(31)#12	2.243(6)	*M*(4)–O(31)#12	2.240(9)
M(4)–O(8)	2.277(6)	*M*(4)–O(8)	2.244(8)
M(4)–O(23)#11	2.297(6)	*M*(4)–O(20)#10	2.270(8)
M(4)–O(20)#10	2.300(6)	*M*(4)–O(42)	2.272(8)
M(4)–O(42)	2.308(6)	*M*(4)–O(23)#11	2.288(8)
M(4)–O(35)#11	2.425(7)	*M*(4)–O(35)#11	2.364(9)
<M(4)–O>	*2.308*	*<M(4)–O>*	*2.280*
***M*(5)–octahedron**		***M*(5)–octahedron**	
M(5)–O(41)#10	2.292(6)	*M*(5)–O(5)#8	2.307(9)
M(5)–O(5)#8	2.313(6)	*M*(5)–O(41)#10	2.325(10)
M(5)–O(27)	2.374(6)	*M*(5)–O(27)	2.374(8)
M(5)–O(3)	2.417(6)	*M*(5)–O(3)	2.379(10)

M(5)–O(30)#10	2.424(6)	*M*(5)–O(30)#10	2.442(9)
M(5)–O(33)#2	2.432(6)	*M*(5)–O(33)#2	2.446(9)
<M(5)–O>	*2.375*	*<M(5)–O>*	*2.379*
***M*(6)–octahedron**		***M*(6)–octahedron**	
M(6)–O(37)	2.284(6)	*M*(6)–O(37)	2.307(8)
M(6)–O(19)#2	2.343(5)	*M*(6)–O(19)#2	2.350(8)
M(6)–O(13)	2.372(6)	*M*(6)–O(13)	2.355(9)
M(6)–O(10)	2.375(6)	*M*(6)–O(10)	2.376(9)
M(6)–O(47)#10	2.401(5)	*M*(6)–O(47)#10	2.408(8)
M(6)–O(21)	2.510(6)	*M*(6)–O(21)	2.513(10)
<M(6)–O>	*2.381*	*<M(6)–O>*	*2.385*
Na(7)–octahedron		**Na(7)–octahedron**	
Na(7)–O(21)	2.346(6)	Na(7)–O(25)#6	2.367(9)
Na(7)–O(25)#6	2.378(6)	Na(7)–O(21)	2.374(9)
Na(7)–O(45)#10	2.410(6)	Na(7)–O(45)#10	2.409(9)
Na(7)–O(13)	2.456(7)	Na(7)–O(39)	2.453(8)
Na(7)–O(6)	2.470(6)	Na(7)–O(6)	2.467(8)
Na(7)–O(39)	2.497(6)	Na(7)–O(13)	2.490(10)
<Na(7)–O>	*2.426*	*<Na(7)–O>*	*2.427*
Na(8)–octahedron		**Na(8)–octahedron**	
Na(8)–O(17)	2.316(6)	Na(8)–O(17)	2.315(9)
Na(8)–O(38)	2.345(6)	Na(8)–O(38)	2.335(9)
Na(8)–O(46)#3	2.431(5)	Na(8)–O(46)#3	2.410(8)
Na(8)–O(2)#3	2.476(6)	Na(8)–O(12)#2	2.480(9)
Na(8)–O(12)#2	2.484(6)	Na(8)–O(2)#3	2.489(9)
Na(8)–O(32)	2.489(6)	Na(8)–O(32)	2.498(10)
<Na(8)–O>	*2.424*	*<Na(8)–O>*	*2.421*
Na(9)–octahedron		**Na(9)–octahedron**	
Na(9)–O(26)#1	2.409(6)	Na(9)–O(26)#1	2.415(10)
Na(9)–O(19)	2.448(6)	Na(9)–O(47)#13	2.432(9)
Na(9)–O(47)#13	2.455(6)	Na(9)–O(19)	2.467(8)
Na(9)–O(22)#2	2.460(7)	Na(9)–O(22)#2	2.469(10)
Na(9)–O(43)#3	2.535(7)	Na(9)–O(43)#3	2.528(10)
Na(9)–O(11)#1	2.869(7)	Na(9)–O(11)#1	2.766(10)
<Na(9)–O>	*2.529*	*<Na(9)–O>*	*2.513*
Na(10)–octahedron		**Na(10)–octahedron**	
Na(10)–O(18)	2.371(6)	Na(10)–O(18)	2.427(10)
Na(10)–O(40)#2	2.451(6)	Na(10)–O(40)#2	2.455(9)
Na(10)–O(35)#2	2.493(6)	Na(10)–O(35)#2	2.466(10)
Na(10)–O(9)	2.499(6)	Na(10)–O(9)	2.503(10)
Na(10)–O(23)#2	2.555(7)	Na(10)–O(23)#2	2.533(10)
Na(10)–O(28)	2.893(6)	Na(10)–O(28)	2.866(10)
<Na(10)–O>	*2.544*	*<Na(10)–O>*	*2.542*
Na(11)–tetragonal pyramid		**Na(11)–tetragonal pyramid**	
Na(11)–O(29)	2.450(6)	Na(11)–O(7)#1	2.407(10)
Na(11)–O(26)#14	2.464(6)	Na(11)–O(29)	2.481(10)
Na(11)–O(7)#1	2.466(6)	Na(11)–O(26)#14	2.490(10)
Na(11)–O(42)#5	2.561(6)	Na(11)–O(42)#5	2.586(10)
Na(11)–O(45)#3	2.615(7)	Na(11)–O(45)#3	2.666(10)
<Na(11)–O>	*2.512*	*<Na(11)–O>*	*2.526*
Na(12)–octahedron		**Na(12)–octahedron**	
Na(12)–O(29)	2.401(6)	Na(12)–O(29)	2.417(9)
Na(12)–O(7)#1	2.413(6)	Na(12)–O(7)#1	2.426(10)
Na(12)–O(46)#3	2.460(6)	Na(12)–O(2)#3	2.456(9)

Na(12)–O(2)#3	2.464(6)	Na(12)–O(46)#3	2.463(10)
Na(12)–O(33)#4	2.524(6)	Na(12)–O(33)#4	2.492(9)
Na(12)–O(15)#1	2.884(7)	Na(12)–O(15)#1	2.791(10)
<Na(12)–O>	*2.524*	*<Na(12)–O>*	*2.508*
Na(13)–tetragonal pyramid		**Na(13)–tetragonal pyramid**	
Na(13)–O(14)#3	2.406(7)	Na(13)–O(3)#1	2.413(10)
Na(13)–O(1)#1	2.458(7)	Na(13)–O(14)#3	2.439(10)
Na(13)–O(18)#3	2.485(6)	Na(13)–O(19)#3	2.470(10)
Na(13)–O(38)#3	2.555(6)	Na(13)–O(39)#3	2.541(10)
Na(13)–O(36)#4	2.664(6)	Na(13)–O(36)#4	2.657(9)
<Na(13)–O>	*2.514*	*<Na(13)–O>*	*2.504*
Na(14)–octahedron		**Na(14)–octahedron**	
Na(14)–O(14)	2.401(6)	Na(14)–O(14)	2.404(10)
Na(14)–O(39)	2.456(6)	Na(14)–O(1)#3	2.451(10)
Na(14)–O(1)#3	2.481(6)	Na(14)–O(39)	2.460(9)
Na(14)–O(6)	2.500(6)	Na(14)–O(6)	2.492(9)
Na(14)–O(30)	2.590(7)	Na(14)–O(44)	2.549(9)
Na(14)–O(44)	2.591(6)	Na(14)–O(30)	2.553(9)
<Na(14)–O>	*2.503*	*<Na(14)–O>*	*2.485*
Na(15)–trigonal prism		**Na(15)–trigonal prism**	
Na(15)–O(22)#15	2.445(13)	Na(15)–O(22)#15	2.443(18)
Na(15)–O(48)#16	2.545(13)	Na(15)–O(48)#16	2.507(18)
Na(15)–O(22)	2.591(12)	Na(15)–O(22)	2.609(17)
Na(15)–O(26)#6	2.728(9)	Na(15)–O(26)#6	2.667(14)
Na(15)–O(48)#10	2.741(13)	Na(15)–O(48)#10	2.690(18)
Na(15)–O(45)#10	2.756(12)	Na(15)–O(45)#10	2.736(18)
<Na(15)–O>	*2.634*	*<Na(15)–O>*	*2.609*
Na(16)–trigonal prism		**Na(16)–trigonal prism**	
Na(16)–O(9)	2.446(11)	Na(16)–O(9)	2.475(16)
Na(16)–O(37)#2	2.515(12)	Na(16)–O(37)#2	2.495(16)
Na(16)–O(9)#2	2.540(11)	Na(16)–O(9)#2	2.560(16)
Na(16)–O(18)	2.669(9)	Na(16)–O(37)	2.661(16)
Na(16)–O(37)	2.712(11)	Na(16)–O(18)	2.680(14)
Na(16)–O(38)	2.841(11)	Na(16)–O(38)	2.839(16)
<Na(16)–O>	*2.621*	*<Na(16)–O>*	*2.618*

Symmetry transformations used to generate equivalent atoms:
#1 $x, y + 1, z$; #2 $-x + 1, -y + 1, -z + 1$; #3 $-x + 1, y + 1/2, -z + 1/2$; #4 $x, -y + 3/2, z - 1/2$;
#5 $-x, y + 1/2, -z + 1/2$; #6 $x - 1, y, z$; #7 $-x, -y + 1, -z + 1$; #8 $x + 1, y, z$;
#9 $x, -y + 1/2, z + 1/2$; #10 $-x + 1, y - 1/2, -z + 1/2$; #11 $x, -y + 1/2, z - 1/2$; #12 $-x, y - 1/2, -z + 1/2$;
#13 $x, -y + 3/2, z + 1/2$; #14 $x - 1, y + 1, z$; #15 $-x, -y, -z + 1$; #16 $x - 1, -y + 1/2, z + 1/2$.