

Table 30A-4-001. CsNO₃. Structure of phase II [84Dea]. $T = 299.5$ K. Fractional coordinates and isotropic temperature parameters. B is defined by Eq. (e) in Introduction.

Atom	x	y	z	B [\AA^2]
Cs(1)	0.4488(2)	0.5610(2)	0.6328(6)	3.6
Cs(2)	0.1079(2)	0.2249(2)	0.0000	3.1
Cs(3)	−0.2289(1)	0.2133(1)	0.6488(6)	3.0
N(1)	0.4365(15)	0.5528(15)	0.1048(22)	2.1
N(2)	0.0906(14)	0.1856(18)	−0.4679(22)	3.2
N(3)	−0.2369(14)	0.2112(17)	0.1299(23)	4.0
O(1)	0.3458(17)	0.5583(20)	0.0243(21)	7.5
O(2)	0.4071(18)	0.4993(17)	0.2403(19)	6.0
O(3)	0.5611(17)	0.6575(16)	0.0549(19)	6.6
O(4)	0.0090(17)	0.1153(14)	−0.3803(17)	4.4
O(5)	0.2110(20)	0.2337(16)	−0.4119(22)	7.0
O(6)	0.0696(21)	0.2490(25)	−0.5950(20)	17.0
O(7)	−0.3186(20)	0.1138(15)	0.2461(20)	7.9
O(8)	−0.1310(16)	0.2926(19)	0.1387(27)	11.0
O(9)	−0.3349(20)	0.2272(16)	0.0312(16)	7.4

Table 30A-4-002. CsNO₃. Structure of phase II [84Dea]. $T = 299.5$ K. Bond lengths [\AA] and angles [$^\circ$] of N atoms.

O(1)–N(1)	1.198(23)	O(2)–N(1)	1.168(20)
O(3)–N(1)	1.325(18)	O(4)–N(2)	1.079(20)
O(5)–N(2)	1.226(20)	O(6)–N(2)	1.291(20)
O(7)–N(3)	1.340(20)	O(8)–N(3)	1.052(17)
O(9)–N(3)	1.398(22)		
O(2)–N(1)–O(1)	117.9(17)	O(3)–N(1)–O(1)	108.8(16)
O(3)–N(1)–O(2)	127.0(17)	O(5)–N(2)–O(4)	114.2(18)
O(6)–N(2)–O(4)	123.9(18)	O(6)–N(2)–O(5)	118.8(19)
O(8)–N(3)–O(7)	130.0(21)	O(9)–N(3)–O(7)	102.7(14)
O(9)–N(3)–O(8)	121.2(21)		