

**Table 45A-1-001.** ND<sub>4</sub>Al(SO<sub>4</sub>)<sub>2</sub> · 12D<sub>2</sub>O. Crystal structure [67Cro]. Fractional coordinates and anisotropic temperature parameters.  $\beta_{ij}$  [Å<sup>2</sup>] is defined by Eq. (c) in Introduction. The primed deuterium atoms are the half mates of disordered ND<sub>4</sub>. The oxygen atoms in sulfate show disordered feature, the ratio non-primed oxygen: primed oxygen = 1 –  $k$  :  $k$ .

Atom	$x$	$y$	$z$	$\beta_{11} \cdot 10^5$	$\beta_{22} \cdot 10^5$	$\beta_{33} \cdot 10^5$	$\beta_{12} \cdot 10^5$	$\beta_{13} \cdot 10^5$	$\beta_{23} \cdot 10^5$
Al	0	0	0	140(46)	$\beta_{11}$	$\beta_{11}$	–130(100)	$\beta_{12}$	$\beta_{12}$
N	1/2	1/2	1/2	538(33)	$\beta_{11}$	$\beta_{11}$	170(109)	$\beta_{12}$	$\beta_{12}$
D(1)′	0.4479(21)	$x$	$x$	1253(128)	$\beta_{11}$	$\beta_{11}$	–253(390)	$\beta_{12}$	$\beta_{12}$
D(2)′	0.4505(19)	0.5655(16)	0.5134(29)	963(152)	637(147)	1250(204)	224(219)	234(296)	69(339)
S	0.3101(8)	$x$	$x$	249(42)	$\beta_{11}$	$\beta_{11}$	161(108)	$\beta_{12}$	$\beta_{12}$
O <sub>s</sub> (1)	0.2397(6)	$x$	$x$	651(53)	$\beta_{11}$	$\beta_{11}$	–362(100)	$\beta_{12}$	$\beta_{12}$
O <sub>s</sub> (1)′	0.3757(60)	$x$	$x$	4.4(28)					
O <sub>s</sub> (2)	0.3139(6)	0.2649(8)	0.4194(7)	467(49)	673(76)	285(48)	506(100)	87(85)	561(103)
O <sub>s</sub> (2)′	0.2177(38)	0.3775(38)	0.2942(36)	1.0(10)					
O <sub>w</sub> (2)	0.0467(6)	0.1374(5)	0.2993(5)	484(48)	303(38)	432(45)	141(77)	–220(79)	–144(73)
O <sub>w</sub> (2)′	0.0170(5)	–0.0171(5)	0.1505(4)	351(38)	289(36)	156(31)	–18(67)	–94(57)	–4(58)
D(1)	0.1163(6)	0.1681(6)	0.2926(6)	518(48)	699(59)	762(59)	–133(96)	–239(88)	–346(87)
D(2)	–0.0041(6)	0.1952(5)	0.2848(6)	780(58)	490(47)	730(53)	65(102)	–302(98)	–331(78)
D(3)	0.0273(5)	0.0441(5)	0.2027(4)	527(43)	542(43)	307(33)	65(79)	–93(71)	99(67)
D(4)	0.0428(5)	0.9153(5)	0.1856(5)	556(43)	394(38)	407(38)	–31(70)	–168(69)	120(68)
$k = 0.116(22)$									