

**Table 39B-9-001.** (NH<sub>4</sub>)<sub>2</sub>Zn(Cl<sub>0.5</sub>Br<sub>0.5</sub>)<sub>4</sub>. Fractional coordinates and isotropic temperature parameters at RT [96Mas]. Atom X means halogen atom to which the atomic scattering factor  $f_X$  was defined as  $(f_{\text{Cl}} + f_{\text{Br}})/2$ .  $B$  is defined by Eq. (e) in Introduction.

Atom	$x$	$y$	$z$	$B [\text{\AA}^2]$
N(1)	0.267(3)	0.105(2)	0.135(2)	5.2(6)
N(2)	0.248(3)	0.820(1)	0.478(2)	3.4(5)
Zn	0.2542(4)	0.4267(2)	0.2299(2)	2.32(5)
X(1)	0.2455(6)	0.4122(3)	−0.0137(3)	4.32(9)
X(2)	0.3115(6)	0.5920(3)	0.3119(4)	5.1(1)
X(3)	−0.0194(6)	0.3725(3)	0.3318(4)	5.0(1)
X(4)	0.4793(7)	0.3192(4)	0.3101(5)	8.0(2)