ADDITIONS AND CORRECTIONS

2000, Volume 104B

Lin Zhu and Karl Seff*: Cation Crowding in Zeolites. Reinvestigation of the Crystal Structure of Dehydrated Potassium-Exchanged Zeolite X

Page 8948. Tables 2 and 3 were in error and should be replaced by the following. (A wrong unit-cell constant (0.324% too short) was used for least-squares refinements and for the calculation of bond lengths and angles. The reported unit-cell constant, $a = 25.083(5)$ Å, is correct.)

The following bond lengths and interatomic distances in the abstract and the text have changed (insignificantly) by less than 1.6 of their respective esds as follows:

Page 8946, abstract, line 8. 3.86(5) and 3.86(5).

Page 8949, column 1, paragraph 2, lines 2−13. 2.683(9), 2.475(14), 2.936(18), 2.509(23), 2.96(3), 2.64(4), and 2.87(15), respectively.

Page 8949, column 2, paragraph 1, lines 3−9. 3.86(5), 3.86(5), 4.55(8), and 4.16(8), respectively.

Page 8950, column 2, paragraph 3, lines 4 and 6. 2.663(8), 2.923(17), and 3.372(8), respectively.

We are grateful to Werner H. Baur for finding this error.

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TABLE 2: Positional,[a] Thermal,[b] and Occupancy Parameters

atom	Wyc. pos.	cation site	*x*	*y*	*z*	U_{11}[c] or U_{iso}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}	occupancy[d] varied	occupancy[d] fixed
Si,Al	192(i)		−555(1)	1243(1)	352(1)	19(1)	19(1)	17(1)	−3(1)	2(1)	−4(1)		192
O(1)	96(g)		−1105(2)	1105(2)	0	31(3)	31(3)	39(5)	5(2)	−8(2)	−8(2)		96
O(2)	96(g)		−45(2)	−45(2)	1398(3)	25(3)	25(3)	35(5)	10(3)	7(3)	7(3)		96
O(3)	96(g)		−707(2)	−707(2)	381(3)	46(3)	46(3)	37(5)	21(4)	−5(3)	−5(3)		96
O(4)	96(g)		1771(3)	1771(3)	3176(3)	44(4)	44(4)	26(3)	31(4)	2(3)	2(3)		96
K(Ia)	16(c)	I	0	0	0	10(4)							6
K(Ib)	32(e)	ca. I	96(6)	96(6)	96(6)	45(6)							4
K(I′a)	32(e)	I′	609(11)	609(11)	609(11)	45(21)							4
K(I′b)	32(e)	I′	794(9)	794(9)	794(9)	30							4
K(I′c)	96(g)	ca. I′	762(45)	674(19)	674(19)	30							4
K(II)	32(e)	II	2451(1)	2451(1)	2451(1)	32(2)	32(2)	32(2)	13(2)	13(2)	13(2)	28.4(4)	
K(III)	96(g)	III	1250	1250	4078(8)	182(23)	182(23)	31(13)	−52(24)	0	0	12.2(9)	
K(III′a)	96(g)	III′	586(15)	586(15)	4216(11)	47(13)						10.7(18)	
K(III′b)	96(g)	III′	792(14)	792(14)	4222(10)	48(12)						12.8(21)	
												$\sum K^+ =$ 90.1(29)	

[a] Position parameters are given × 10^4. [b] Thermal parameters have the units Å^2 × 10^3. Numbers in parentheses are the esds in the units of the least significant digit given for the corresponding parameter. Parameters without esds were fixed in least-squares refinement; the positional and anisotropic thermal paremeters without esds were fixed by symmetry. [c] The anisotropic temperature factor = $\exp[(-2\pi^2a^{-2})(h^2U_{11} + k^2U_{22} + l^2U_{33} + 2hkU_{12} + 2hlU_{13} + 2klU_{23})]$. [d] Occupancy factors are given as the number of atoms or ions per unit cell.

TABLE 3: Selected Interatomic Distances and Angles

distances (Å)		angles (deg)	
(Si, Al)−O(1)	1.674(4)	O(1)−(Si,Al)−O(2)	111.5(3)
(Si, Al)−O(2)	1.667(3)	O(1)−(Si,Al)−O(3)	109.2(4)
(Si, Al)−O(3)	1.670(4)	O(1)−(Si,Al)−O(4)	108.4(4)
(Si, Al)−O(4)	1.655(3)	O(2)−(Si,Al)−O(3)	107.7(4)
mean (Si, Al)−O	1.667	O(2)−(Si,Al)−O(4)	107.2(4)
K(Ia)−O(3)	2.683(9)	O(3)−(Si,Al)−O(4)	112.9(4)
K(Ib)−O(3)	2.475(14), 2.936(18)	O(3)−K(Ia)−O(3)	88.0(2), 92.0(2)
K(I′a)···K(I′a)	4.55(8),[a] 5.42(4)[b]	O(3)−K(Ib)−O(3)	81.9(6), 86.7(3)
K(I′a)···K(I′b)	3.92(6)[c]	O(3)−K(I′a)−O(3)	93.1(7)
K(I′a)···K(I′c)	4.16(8)[b]	O(3)−K(I′b)−O(3)	76.6(15)
K(Ib)···K(I′b)	3.86(5)[b]	O(2)−K(II)−O(2)	99.6(2)
K(I′b)···K(I′b)	3.32(8)[c]	O(1)−K(III)−O(4)	50.2(2)
K(Ib)···K(I′c)	3.86(5)[b]	O(4)−K(III)−O(4)	78.5(6)
K(I′b)···K(I′c)	3.54(8)[c]	O(1)−K(III′a)−O(1)	114.7(10)
K(I′c)···K(I′c)	3.81(13),[c]3.97(9)[c]	O(1)−K(III′a)−O(4)	57.7(4), 57.7(4)
K(I′a)−O(3)	2.509(24)	O(1)−K(III′b)−O(1)	114.8(10)
K(I′a)−O(2)	3.048(14)	O(1)−K(III′b)−O(4)	57.5(5), 57.5(5)
K(I′b)−O(3)	2.96(3)		
K(I′b)−O(2)	3.335(20)		
K(I′c)−O(3)	2.64(4), 2.87(15)		
K(I′c)−O(2)	3.260(23)		
K(II)−O(2)	2.663(7)		
K(II)−O(4)	3.020(8)		
K(III)−O(4)	2.923(17)		
K(III)−O(1)	3.372(8)		
K(III′a)−O(4)	2.66(3)		
K(III′a)−O(1)	2.94(2), 2.94(2)		
K(III′b)−O(4)	2.63(3)		
K(III′b)−O(1)	2.94(2), 2.94(2)		

[a] Readily avoidable by cation placement. [b] Unavoidable. [c] Avoidable if there are four K(I′a)···K(I′c) contacts per unit cell.

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Shenyan Zhen and Karl Seff*: Crystal Structure of Anhydrous NH_4^+-Exchanged Zeolite X Partially Reacted with $HgCl_2$ Vapor. Cationic Chloromercuric Clusters, Regular Octahedral Hg(II), and Regular Trigonal Hg(II)

Page 10411, Table 1. The *y* coordinate of O(1) should be +0.0014(7), and the *y* coordinate of O(3) should be +0.0675(6).

We are indebted to Werner H. Baur for finding these errors.

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Shenyan Zhen, Donghan Bae, and Karl Seff*: Zn^+ Cations, Probable Tl_4Zn_{12} and Tl_6 Clusters, and Zeolite Desilication (Less Likely Dealumination): Crystallographic Study of the Incomplete Reaction of Zn Vapor with Tl^+-Exchanged Zeolite X

Page 515, lines 2 and 3 of the abstract, and page 516, last paragraph of column 1. $a_0 = 24.950(4)$ Å for crystal 1 and $a_0 = 24.825(3)$ Å for crystal 2.

We are grateful to Werner H. Baur for finding these errors.

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