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Chem. Mater., 1998, 10(9), 2561-2570, DOI:[10.1021/cm980342s](https://doi.org/10.1021/cm980342s)

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Table of Supporting Information. Possible interatomic distances (Å) involving water molecules.

	Na-LSX	NaK-LSX20	NaK-LSX42	NaK-LSX80(Na)	NaK-LSX80(K)	K-LSX
OW1-O(3)	2.63(1)					2.80(2)
OW1-OW2	2.62(1)					2.70(2)
OW2-O(2)	3.15(2)	3.04(2)	2.98(2)	3.20(2)	3.01(2)	3.06(2)
		3.09(2)	3.02(2)	3.33(2)	2.97(2)	3.07(2)
OW2-O(3)				3.16(2)	3.38(3)	
				3.03(2)	3.39(3)	
OW2-OW2	2.76(2)	2.72(3)	3.13(3)	2.60(3)	3.00(3)	2.94(3)
	2.56(3)	2.67(3)	2.84(3)	2.86(3)	3.05(3)	2.93(3)
	2.77(2)	3.11(3)	2.80(3)	2.95(3)	2.61(4)	2.53(3)
	2.86(2)	3.02(3)				
OW4-O(1)				3.14(8)	2.85(4)	2.87(4)
OW4-O(2)				2.92(5)	3.00(4)	3.17(3)
OW4-OW4						2.77(5)
OW4-OW4B				2.81(6)	3.08(4)	
OW4-OW5	2.99(9)	2.95(23)	3.28(27)	2.60(7)	2.57(9)	3.07(5)
	2.64(7)	2.59(16)	3.38(25)			
OW4-OW6	2.53(4)	2.67(10)	3.06(29)	2.81(14)	3.09(11)	2.89(13)
			2.76(25)		3.16(11)	3.11(12)
OW4-OW7				2.76(13)	2.90(9)	3.16(5)
OW4-OW8	3.14(7)	3.15(18)	2.95(33)		2.44(11)	2.14(6)
	2.94(10)	3.14(20)	3.43(14)		3.42(8)	3.21(6)
		2.38(8)	2.34(22)			
OW4-OW9	2.59(4)	2.70(11)	2.82(21)	3.09(13)	3.38(10)	3.50(5)
	2.82(6)	2.89(14)	2.71(18)	3.37(15)	3.20(9)	3.33(5)
	3.16(4)	3.20(9)	3.33(10)			
OW4-OW10				3.35(12)	2.42(6)	2.16(4)
				2.59(13)	3.26(6)	2.77(5)
OW4B-OW5			3.25(2)		3.24(7)	2.64(5)
OW4B-OW6		2.86(5)	2.84(5)	2.68(9)	2.44(6)	2.60(3)
OW4B-OW8		3.07(6)	3.12(5)	3.22(21)	3.07(9)	3.30(6)
OW4B-OW9			2.72(5)	3.39(12)	2.69(13)	2.77(5)

Table of Supporting Information (continued)

OW5-O(1)	3.10(5) 3.14(4)	3.14(4) 3.10(4)	3.19(3) 3.07(3)	3.25(6) 3.41(6)	3.11(7)	3.19(4)
OW5-O(2)						3.32(4)
OW5-OW5	2.50(4)	2.61(4)	2.62(4)		2.40(14)	3.37(9)
OW5-OW6	2.70(6)	2.89(14)	2.74(7)	2.44(12)	3.41(16)	3.05(12)
OW5-OW7	3.11(7)	3.09(6)	3.13(5)	2.35(10)	3.11(11)	3.38(6)
				3.07(10)	3.08(12)	3.28(5)
OW5-OW8	3.14(7)			2.59(18)		
OW5-OW9	2.92(4)	3.00(4)	3.06(4)	3.43(15)	3.21(9)	3.37(4)
			3.24(4)	3.46(15)	2.63(10)	2.63(6)
OW5-OW10	2.66(5)	2.19(7)	2.25(5)	2.51(13)	3.19(10)	2.95(6)
		2.62(4)	2.44(4)	2.49(12)		2.57(5)
OW6-O(1)				3.32(9)		
OW6-O(4)				2.74(9)		
OW6-OW6		2.63(10)			2.43(11)	3.38(4)
OW6-OW7	2.22(4)	2.17(6)	2.31(5)	3.24(10)	3.45(12)	2.97(9)
		2.52(11)	2.58(7)		3.40(11)	
			3.31(6)		2.05(10)	
OW6-OW8				3.28(25)	3.36(14)	3.25(12)
				2.24(22)		
OW6-OW9	2.66(4)	2.92(8)	2.69(6)	3.26(16)	3.08(16)	2.51(7)
					3.04(13)	3.20(4)
					2.86(10)	
OW6-OW10	2.55(5)	2.35(15)	2.64(8)	2.59(13)	2.75(12)	2.50(13)
	2.68(5)	2.71(15)	2.42(7)	2.82(13)	2.76(12)	2.88(13)
	2.82(5)		3.45(6)	3.00(10)	3.46(8)	3.17(4)
OW7-O(1)	2.75(3)	2.68(3)	2.73(3)	2.84(5)	3.18(7)	2.85(3)
OW7-O(4)	2.88(3)	2.92(3)	2.93(3)	3.18(5)	2.87(6)	2.86(2)
OW7-OW8	2.91(6)	2.41(6)	2.29(4)	3.33(19)	2.58(14)	2.23(5)
	2.28(6)	2.03(8)	2.12(7)	2.72(25)	3.53(10)	3.36(6)
OW7-OW9				2.85(10)		
				3.31(15)		
OW7-OW10				3.29(8)	3.03(8)	3.40(3)
OW8-O(1)	2.97(4)	3.05(6)	2.99(5)	2.78(15)	3.14(8)	2.95(4)

Table of Supporting Information (continued)

OW8-O(4)			3.23(5)	3.17(16)	3.05(8)	3.45(5)
OW8-OW9	2.92(5)	2.75(6)	2.81(6)	2.64(19)	2.72(14)	2.56(5)
	2.93(5)	2.86(8)	2.87(7)	3.47(23)		
OW8-OW10	2.37(6)	2.34(7)	3.28(5)	3.46(25)	3.11(10)	2.83(6)
	3.18(6)	2.91(7)	2.26(5)		2.47(10)	
			2.93(6)			
OW9-OW9	3.02(5)	3.06(6)	3.20(6)	3.51(6)	3.17(17)	3.50(7)
	3.02(5)	3.06(6)	3.20(6)		3.37(15)	2.96(5)
	2.53(4)	2.49(7)	2.59(7)		2.62(16)	
OW9-OW10	2.95(4)	2.85(4)	2.78(4)	2.90(15)	3.39(8)	3.22(4)
				2.64(13)		
OW10-O(1)	2.69(3)	2.76(4)	2.85(3)	3.37(7)	3.05(4)	2.91(3)
OW10-O(4)	2.84(3)	2.98(4)	2.96(3)	3.13(7)	2.90(4)	2.90(3)
OW10-OW10				3.01(11)	3.04(5)	3.45(4)

The distances listed represent possible, not definite, interactions in the range 2.00-3.50 Å. The value in parentheses is the estimated standard deviation.