

Perspectives on: Ion selectivity

Design principles for K⁺ selectivity in membrane transport

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Please note that Yu et al. (2010. *J. Amer. Chem. Soc.* 132:10847–10856) cited the wrong LJ parameter set used for Na⁺ and K⁺ ions (Andersen, O.S., and B. Roux, personal communication). In their study, Yu et al. (2010) did not use the parameter set from Beglov and Roux (1994. *J. Chem. Phys.* 100:9050–9063), but instead the parameter set from Noskov and Roux (2008. *J. Mol. Biol.* 377:804–818). These two parameter sets yield different K⁺→Na⁺ hydration free energy differences. While the parameters from Beglov and Roux (1994) yield a value of −20.7 kcal/mol, the parameters from Noskov and Roux (2008) yield a value of −18.6 kcal/mol. This consequently modifies two entries in Table I (marked by asterisks below), but has no impact on the published conclusions.

TABLE I
K⁺/Na⁺ selectivity by experiment and calculation

Method	Solvent	ΔΔG (kcal/mol)	Selective for
Experiment	Formamide ^a	−0.9	Na ⁺
	Formamide ^{b,c}	−0.7	Na ⁺
	NMA ^{b,d}	−1.1	Na ⁺
Pairwise Additive	Formamide ^c (CHARMM27)	0.9	K ⁺
	Formamide ^c (OPLS-AA)	1.3	K ⁺
	NMA ^c (CHARMM22/NBFIX)	1.6	K ⁺
	NMA ^{d,g} (CHARMM27)	0.7*	K ⁺
	NMA ^{d,g} (CHARMM27/NBFIX)	2.6*	K ⁺
	Formamide ^c (AMOEBA)	−1.3	Na ⁺
	Formamide ^f (QM/MM)	−2.2	Na ⁺
Polarizable	NMA ^d (Drude)	−0.3	Na ⁺

K⁺/Na⁺ selectivity of bulk liquid formamide and NMA as determined by experimental work, pairwise-additive (nonpolarizable) force field calculations, polarizable force field (AMOEBA and Drude) calculations, and QM/MM (hybrid quantum mechanical and molecular mechanical) calculations. Note that the pairwise-additive force field calculations display positive (K⁺) selectivity, whereas all other determinations display negative (Na⁺) selectivity.

^aMarcus, 1983.

^bCox and Parker, 1973, and Schmid et al., 2000.

^cGrossfield et al., 2003.

^dYu et al., 2010a.

^eNoskov et al., 2004.

^fVarma and Rempe, 2008.

^gNoskov and Roux, 2008.