

Biophysical Journal, Volume 96

Supporting Material

Molecular Model of a Cell Plasma Membrane with an Asymmetric Multicomponent Composition: Water Permeation and Ion Effects

Robert Vácha, Max L. Berkowitz, and Pavel Jungwirth

This supplementary file contains interaction parameters of employed potassium (denoted as “oK”) in notation of GROMACS version 3.3.1.

[atomtypes]

name	at.num	mass	charge	ptype	c6	c12
oK	19	39.1000	1.0000	A	1.343697E-03	1.07882507E-06

[nonbond_params]

i	j	func	c6	c12
O	oK	1	1.74327E-03	1.16855e-06
OM	oK	1	1.74327E-03	3.18689e-06
OA	oK	1	1.74327E-03	1.27474e-06
OW	oK	1	1.87524E-03	1.68544e-06
NR5	oK	1	1.80926E-03	1.91215e-06
OS	oK	1	1.74327E-03	1.27474e-06
NR6	oK	1	1.80926E-03	1.91215e-06
NA	oK	1	0.311168E-03	1.50567e-07
CL	oK	1	4.30688E-03	1.07397e-05
OWT3	oK	1	1.82877E-03	1.62088e-06
OD	oK	1	1.74703E-03	9.00436e-07

[pairtypes]

i	j	func	cs6	cs12
O	oK	1	0.00174327	8.94417e-07
OM	oK	1	0.00174327	8.94417e-07
OA	oK	1	0.00174327	8.94417e-07
OW	oK	1	0.00187524	8.94417e-07
N	oK	1	0.00180926	1.35126e-06
NT	oK	1	0.00180926	1.35126e-06
NL	oK	1	0.00180926	1.35126e-06
NR5	oK	1	0.00180926	1.35126e-06
NR5*	oK	1	0.00180926	1.35126e-06
NP	oK	1	0.00180926	1.35126e-06
C	oK	1	0.00177328	1.90792e-06
CH1	oK	1	0.00197797	2.00773e-06
CH2	oK	1	0.00251935	2.77045e-06
CH3	oK	1	0.00303443	3.60755e-06
CR51	oK	1	0.00272554	2.9978e-06
CR61	oK	1	0.00272554	2.9978e-06
CB	oK	1	0.00177328	1.90792e-06
CHE	oK	1	0.00177328	1.90792e-06
H	oK	1	0	0

HO	oK	1	0	0
HW	oK	1	0	0
HS	oK	1	0	0
S	oK	1	0.00366277	3.75629e-06
FE	oK	1	0	0
ZN	oK	1	0	1.0092e-07
NZ	oK	1	0.00180926	1.35126e-06
NE	oK	1	0.00180926	1.35126e-06
P	oK	1	0.00444994	4.89296e-06
OS	oK	1	0.00174327	8.94417e-07
CS1	oK	1	0.00197797	2.00773e-06
NR6	oK	1	0.00180926	1.35126e-06
NR6*	oK	1	0.00180926	1.35126e-06
CS2	oK	1	0.00251935	2.77045e-06
SI	oK	1	0.00444994	4.89296e-06
NA	oK	1	0.000311168	1.50567e-07
CL	oK	1	0.00430688	1.07397e-05
CA	oK	1	0.00116221	7.32988e-07
MG	oK	1	0.000296171	6.06359e-08
F	oK	1	0.00324364	5.21503e-06
CP2	oK	1	0.00251559	3.72821e-06
CP3	oK	1	0.00303071	4.49179e-06
CR5	oK	1	0.00272554	2.9978e-06
CR6	oK	1	0.00272554	2.9978e-06
HCR	oK	1	0.00033741	1.27689e-07
OWT3	oK	1	0.00182877	1.62088e-06
SD	oK	1	0.00376701	4.81601e-06
OD	oK	1	0.00174703	9.00436e-07
CD	oK	1	0.00348732	4.84488e-06