ADDITIONS AND CORRECTIONS

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Timothy I. Morrow and Edward J. Maginn*: Molecular Dynamics Study of the Ionic Liquid 1-n-Butyl-3-methylimidazolium Hexafluorophosphate

Page 12807. Equation 1 reads

$$V_{\mathrm{tot}} = \sum_{\mathrm{bonds}} k_b(r - r_0)^2 + \sum_{\mathrm{angles}} k_\theta(\theta - \theta_0)^2 + \sum_{\mathrm{dihedrals}} k_\chi[1 + \cos(n\chi - \delta)] + \sum_{\mathrm{improper}} k_\psi(\psi - \psi_0)^2 + \sum_{i=1}^{N-1}\sum_{j>i}^{N}\left\{\epsilon_{ij}\left[\left(\frac{r_{\mathrm{min},ij}}{r_{ij}}\right)^{12} - \left(\frac{r_{\mathrm{min},ij}}{r_{ij}}\right)^{6}\right] + \frac{q_i q_j}{r_{ij}}\right\}$$

And should read

$$V_{\mathrm{tot}} = \sum_{\mathrm{bonds}} k_b(r - r_0)^2 + \sum_{\mathrm{angles}} k_\theta(\theta - \theta_0)^2 + \sum_{\mathrm{dihedrals}} k_\chi[1 + \cos(n\chi - \delta)] + \sum_{\mathrm{improper}} k_\psi(\psi - \psi_0)^2 + \sum_{i=1}^{N-1}\sum_{j>i}^{N}\left\{\epsilon_{ij}\left[\left(\frac{r_{\mathrm{min},ij}}{r_{ij}}\right)^{12} - 2\left(\frac{r_{\mathrm{min},ij}}{r_{ij}}\right)^{6}\right] + \frac{q_i q_j}{r_{ij}}\right\}$$

(that is, there is a factor of 2 missing in front of the attractive dispersion term).

Page 12808. The units of Table 2 were incorrectly listed, and several entries were missing. The following is a corrected Table 2.

TABLE 2: Bond, Angle, Dihedral, and Improper Force Constants

force bonds	force constant k_b (kJ mol^{-1} A^{-2})	r_0 (Å)	force bonds	force constant k_b (kJ mol^{-1} Å^{-2})	r_0 (Å)
C_6-N_3	921.1	1.470	$C_7-H_{7,8}$		1.091
C_7-N_1	921.1	1.483	$C_{8,9}-H_{9,10,11,12}$		1.096
$C_{5,4}-N_{1,3}$	1674.7	1.382	$C_{10}-H_{13,14,15}$		1.093
$C_2-N_{1,3}$	1674.7	1.337	C_7-C_8	837.4	1.530
C_4-C_5	1716.6	1.361	C_8-C_9	931.6	1.534
C_2-H_1		1.078	C_9-C_{10}	931.6	1.530
$C_{4,5}-H_{2,3}$		1.078	P−F	1089.8	1.646
$C_6-H_{4,5,6}$		1.089			

angles	k_θ (kJ mol^{-1} rad^{-2})	θ_0 (deg)	angles	k_θ (kJ mol^{-1} rad^{-2})	θ_0 (deg)
$C_8-C_7-N_1$	586.2	112.6	$H_7-C_7-H_8$	148.6	107.2
$C_{5,4}-N_{1,3}-C_2$	544.3	108.3	$H_{7,8}-C_7-C_8$	139.8	111.5
$C_7-N_1-C_{2,5}$	544.3	125.9	$H_{9,10}-C_8-C_7$	139.8	109.5
$C_6-N_3-C_{2,4}$	544.3	125.8	$C_{7,8}-C_{8,9}-C_{9,10}$	244.5	111.6
$H_{4,5,6}-C_6-N_3$	125.6	109.6	$H-C_{8,9}-H$	144.4	106.4
$H_1-C_2-N_{1.3}$	104.7	125.5	$C_{8,9}-C_{9,10}-H$	144.6	109.7
$N_{1,3}-C_{5,4}-C_{4,5}$	544.3	107.2	$H_{9,10}-C_8-C_9$	144.6	109.7
$N_1-C_2-N_3$	544.3	109.1	$H_{11,12}-C_9-C_{10}$	144.6	109.7
$H_{2,3}-C_{4,5}-C_{5,4}$	104.7	130.8	$H_{I3,14,15}-C_{10}-H$	148.6	107.6
$H_{4,5,6}-C_6-H$	148.6	109.3	$N-C_7-H_{8,9}$	125.6	106.8
$N_{1,3}-C_{5,4}-H_{3,2}$	104.7	122.1	F−P − F	812.7	90.0

dihedral	k_χ (kJ mol^{-1})	n	δ (deg)	dihedral	k_χ (kJ mol^{-1})	n	δ (deg)
$C_2-N_{1,3}-C_{5,4}-C_{4,5}$	58.6	2	180	$C_8-C_9-C_{10}-H$	0.67	1	0
$N_1-C_5-C_4-N_3$	58.6	2	180	$H_{2,3}-C_{4,5}-N_{3,1}-C_2$	12.6	2	180
$N_{1,3}-C_2-N_{3,1}-C_{4,5}$	58.6	2	180	$N_{1,3}-C_{5,4}-C_{4,5}-H_{2,3}$	12.6	2	180
$H_1-C_2-N_{1,3}-C_{5,4}$	12.6	2	180	$N_{1,3}-C_2-N_{3,1}-C_{6,7}$	0.0	2	180
$H_2-C_4-C_5-H_3$	8.37	2	180	$H_1-C_2-N_{3,1}-C_{6,7}$	0.0	2	180
$C_{4,5}-C_{5,4}-N_{1,3}-C_{7,6}$	0.0	1	0	$H_{2,3}-C_{4,5}-N_{3,1}-C_{6,7}$	0.0	2	180
$C_{4,5}-N_{3,1}-C_{6,7}-H$	0.0	3	0	$C_2-N_{1,3}-C_{7,6}-H$	0.82	2	180
$C_2-N_{3,1}-C_7-C_8$	0.42	1	180	$N_1-C_7-C_8-H_{9,10}$	0.0	3	0
$C_5-N_1-C_7-C_8$	0.84	1	0	$C_7-C_8-C_9-C_{10}$	0.63	1	0
$N_1-C_7-C_8-C_9$	0.0	1	0	$H_{7,8}-C_7-C_8-H_{9,10}$	0.82	3	0
$H-C_9-C_{10}-H$	0.67	3	0	$H-C_8-C_9-C_{10}$	0.82	3	0
$H_{7,8}-C_7-C_8-C_9$	0.82	2	0	$C_7-C_8-C_9-H_{11,12}$	0.82	2	0

improper	k_ψ (kJ mol^{-1} rad^{-2})	ψ_0 (deg)	improper	k_ψ (kJ mol^{-1} rad^{-2})	ψ_0 (deg)
$H_1-N_1-N_3-C_2$	0.50	0	$H_{2,3}-N_{3,1}-C_{4,5}-C$	0.50	0
$N_{1,3}-C_{4,5}-C_2-C_{6,7}$	0.60	0			

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