ADDITIONS AND CORRECTIONS

1997, Volume 101A

Pál Jedlovszky and László Turi*: A New Five-Site Pair Potential for Formic Acid in Liquid Simulations

Page 2663. Please note that due to an unfortunate mistake the optimized ϵ_{ii} parameters of a new five-site pair potential for formic acid appeared incorrectly in Table 1. The correct values are collected here in Table 1. We regret the errors.

Nonetheless, we would like to emphasize that the calculations and simulations were performed with the correct parameters. Thus, all the results and conclusions of the paper are unchanged.

TABLE 1: Optimized Parameters and Charges of Formic Acid Monomer

i	q_i (e)	σ_{ii} (Å)	ϵ_{ii} (kJ/mol)
C	0.444 69	3.727	0.376
(C═)O	−0.432 36	2.674	1.214
(C—)O	−0.552 96	3.180	0.392
(C—)H	0.107 32	0.800	0.020
(O—)H	0.433 31	0.994	0.100

10.1021/jp990716k
Published on Web 04/24/1999