

ADDITIONS AND CORRECTIONS

1998, Volume 102B

M. Casarin, C. Maccato, and A. Vittadini*: Molecular Chemisorption of TiO₂(110): A Local Point of View

Page 10748. The correct Table 5 is as follows:

TABLE 5: Theoretical CO, H₂O, and H₂S GGA Adsorption Energies (kcal/mol) Decomposed Following Ziegler's Transition State Analysis

	CO	H ₂ O	H ₂ S
ΔE_{Pauli}	45.53	23.12	11.28
ΔE_{elstat}	-31.74	-31.02	-9.99
ΔE_{a_1}	-16.46	-10.87	-6.86
ΔE_{a_2}	-0.08	-0.18	-0.05
ΔE_{b_1}	-3.17	-2.17	-1.66
ΔE_{b_2}	-2.61	-1.58	-1.00
$\Delta E_{\text{prep,mol}}$	0.16	0.35	0.14
$\Delta E_{\text{prep,surf}}$	0.06	1.30	0.16

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Pál Jedlovský and László Turi*: Role of the C-H...O Hydrogen Bonds in Liquids: A Monte Carlo Simulation Study of Liquid Formic Acid Using a Newly Developed Pair-Potential

Page 5430. Please note that due to an unfortunate mistake the optimized ϵ parameters of the 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: Parameters of the Pair Potential of Formic Acid

	O _c	C	H _f	O _h	H _a
σ (Å)	2.674	3.727	0.800	3.180	0.994
ϵ (kJ/mol)	1.214	0.376	0.020	0.392	0.100
q (e)	-0.43236	+0.44469	+0.10732	-0.55296	+0.43331

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