

ADDITIONS AND CORRECTIONS

1999, Volume 103

P. Tarakeshwar and Kwang S. Kim*: A Theoretical Investigation of Benzene–AlX₃ and Ethene–AlX₃ (X = H, F, Cl) Interactions

Page 9119: In paragraph 3 of the left column, the first sentence should read as follows:

Earlier theoretical studies on the binding of AlH₃ to NH₃ have obtained a CCSD/DZP ZPVE corrected binding energy of 26.5 kcal/mol.^{12b} However, the study of the interaction of BH₃ with NH₃ has not been reported at the same level of theory.

Page 9120. The last row in Table 3 should read as follows:

TABLE 3: Comparison of the Frequencies of the Stretching and Bending Modes of AlH₃, AlF₃, and AlCl₃ and Their Frequency Shifts in the Complexed States along with the van der Waals Modes at the MP2/6-31+G* Level^a

mode	AlH ₃	C ₂ H ₄ –AlH ₃	C ₆ H ₆ –AlH ₃	AlF ₃	C ₂ H ₄ –AlF ₃	C ₆ H ₆ –AlF ₃	AlCl ₃	C ₂ H ₄ –AlCl ₃	C ₆ H ₆ –AlCl ₃
ϕ_{op}		483[15]	417[1]		370[1]	125[0]		400[20]	104[0]

^a All frequencies are in cm⁻¹. IR intensities (km/mol) are enclosed in brackets adjacent to the frequency shifts. ^b The van der Waals mode definitions are given in ref 45.

Page 9120: In paragraph 2 of the right column, the first two lines should read as follows:

Though the charges on Al exhibit small changes upon complexation in conformers **2**, **4**, and **6**, the changes in the....

Page 9121: In paragraph 1 of the right column, the last sentence should read as follows:

It can also be correlated to the charge transfer from benzene to both AlF₃ (0.10 e) and AlCl₃ (0.13 e) in these conformers.

Page 9122: In paragraph 1 of the left column, the last sentence should read as follows:

What they found was that even in the absence of covalent contributions, Me₃N was very strongly bound to AlCl₃ (binding energy of 49.3 kcal/mol).

Page 9122: In paragraph 1 of the right column, the last but one sentence should read as follows:

This aspect is confirmed by the dominant contributions of the electrostatic energies (ΔE_{es}) to the binding energy.

10.1021/jp993875c

Published on Web 12/01/1999