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J. R. Grover, B.-M. Cheng, W. J. Herron, M. T. Coolbaugh, W. R. Peifer, and James F. Garvey

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
Dept. of Chemistry, Acheson Hall
State University of New York at Buffalo
Buffalo, NY
14214

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Dr. R. DeMarco/Dr. J. Pazik, Chemistry Division
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Intracluster Reactions of Chlorobenzene/Ammonia Mixed Complexs

by

J. R. Grover, B.-M. Cheng, William J. Herron, M. Todd Coolbaugh, William R. Peifer and James F. Garvey*

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Department of Chemistry
University at Buffalo
The State University of New York at Buffalo
Buffalo, NY
14214

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INTRACLUSTER REACTIONS OF CHLOROBENZENE/AMMONIA MIXED COMPLEXES

J. R. Grover*, B.-M. Cheng*,#, W. J. Herron+, M. T. Coolbaugh+, W. R. Peifer+ and J. F Garvey+
**Department of Chemistry, Brookhaven National Laboratory, Upton, NY 11973*
#Synchrotron Radiation Research Center, Taiwan, ROC
+Department of Chemistry, SUNY at Buffalo, Buffalo, NY 14214

The spontaneous disintegration of $(C_6H_5Cl{\bullet}NH_3)^+$ to form $C_6H_5NH_3^+$ has been intensively studied by two-photon techniques at other laboratories. We examined this process using single-photon interactions, and expanded the work to include larger complexes of $C_6H_5Cl + NH_3$ and higher energies. The complexes were prepared by jet expansions of 0.50% C_6H_5Cl in NH_3, using a nozzle 0.010 cm in diameter, the resulting mixtures being analyzed by the method already described[1]. A sharp onset of $C_6H_5NH_3^+$ from $C_6H_5Cl{\bullet}NH_3$ was found at 8.947 ± 0.003 eV, which, when combined with the known heat of formation of $C_6H_5NH_3^+$, gives a dissociation energy $D(C_6H_5Cl{\bullet}NH_3)$ = *ca.* 2 kcal mol^{-1}. Production of $C_6H_5NH_3^+$ from trimers was too weak in the onset region to permit measurement. The ion $C_6H_5NH_2^+$ was also observed, with onsets of 8.849 ± 0.009 and 8.855 ± 0.029 eV from $C_6H_5Cl{\bullet}NH_3$ and $C_6H_5Cl(NH_3)_2$ respectively, clearly below the onset for $C_6H_5NH_3^+$, but far above the thermochemical thresholds near 7.6 eV. For the "parent ions" $(C_6H_5Cl{\bullet}NH_3)^+$, $C_6H_5Cl(NH_3)_2^+$, and $C_6H_5Cl(NH_3)_3^+$ onsets were found at 8.74 ± 0.02, 8.652 ± 0.013, and 8.555 ± 0.012 eV. However, product resolution experiments indicate that in the onset region $(C_6H_5Cl{\bullet}NH_3)^+$ is apparently produced entirely from trimers. This value of the dimer ion onset therefore implies that $D([C_6H_5Cl{\bullet}NH_3]^+) \geq$ *ca.* 9 kcal mol^{-1} (Fig.1). On the other hand, $C_6H_5NH_3^+$ is produced from $C_6H_5Cl{\bullet}NH_3$ at energies >11.5 eV, a process not yet understood.

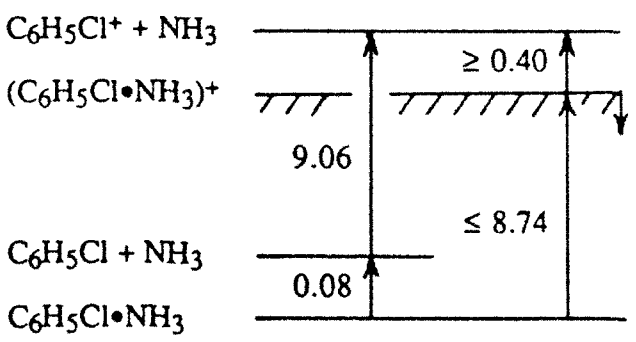

Figure 1. Energy diagram of the system $C_6H_5Cl + NH_3$. The ionization potential for $(C_6H_5Cl{\bullet}NH_3)^+$ is an upper limit if the measured value pertains to a trimer instead of the dimer. (All energies in eV.)

[1] **J. R. Grover, W. J. Herron, M. T. Coolbaugh, W. R. Peifer and J. F. Garvey**, J. Phys. Chem. **95**, 6473-6481 (1991).

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