ADDITIONS AND CORRECTIONS

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F. Pepi, A. Ricci, M. Rosi: Gas-Phase Chemistry of $NH_xCl_y^+$ Ions. 3. Structure, Stability, and Reactivity of Protonated Trichloramine

Page 2088. A transcription error resulted in erroneous N−Cl bond angle of NCl_3 reported in Figure 3 and Table 3. The corrected value is 108.1° instead of 118.1°.

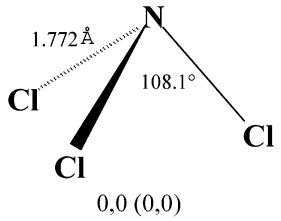

Figure 3. Optimized geometries of the investigated species in their ground states. (Bond lengths in angstroms, angles in degrees). Total energies (kJ/mol), with inclusion of zero point energy, computed at B3LYP (CCSD(T)) level are shown. The energies are relative to the total energy, corrected by the zero point energy, of NCl3: −1435.330851 hartree at B3LYP level and −1433.713664 hartree at CCSD(T) level.

TABLE 3: Optimized Geometries and Energies of NCl_3, $HNCl_3^+$ (I), $HClNCl_2^+$ (II), and $HN(Cl)Cl_2^+$ (III) in Their Singlet Ground States

	NCl_3 $^1A_1$	**I** $^1A_1$	**II** $^1A'$	**III** $^1A'$
r(NCl)	1.772	1.753	1.634	1.635
			2.715	1.688
r(NH)		1.026		1.023
r(ClH)			1.289	
r(ClCl)				2.079
∠(ClNH)		106.3		113.0
∠(ClNCl)	108.1	112.5	115.2	120.1
∠(NClH)			92.1	
∠(NClCl)				117.3
E_{B3LYP}	−1435.336894	−1435.620355	−1.435.602255	−1435.599762
ZPE[b]	0.006043	0.019905	0.013034	0.018368
$E_{CCSD(T)}$	−1433.719707	−1434.007980	−1433.977759	−1433.974459

[a] Bonds lengths in angstroms, angles in degrees, total energies in hartree. [b] Zero point energy.

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