Chlorodifluoroacetyl cyanide, $ClF_2CC(O)CN$: Synthesis, structure and spectroscopic characterization

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SUPPORTING INFORMATION

TABLES

Table S1. Mulliken atomic charges for the molecular and cation-radical forms of $ClF_2CC(O)CN$, calculated with the UB3LYP/6-311+G(3df) approximation.

	Atoms[a]								TAC[b]
	F1	F2	Cl	C1	C2	O	C3	N	
$ClF_2CC(O)CN$	–0.390	–0.350	–0.137	0.782	0.787	–0.616	0.868	–0.945	0
$ClF_2CC(O)CN^{\cdot+}$	–0.169	–0.167	0.127	0.699	0.676	–0.412	1.045	–0.799	+1
Δq[c]	0.221	0.183	0.264	–0.083	–0.111	0.204	0.177	0.146	+1

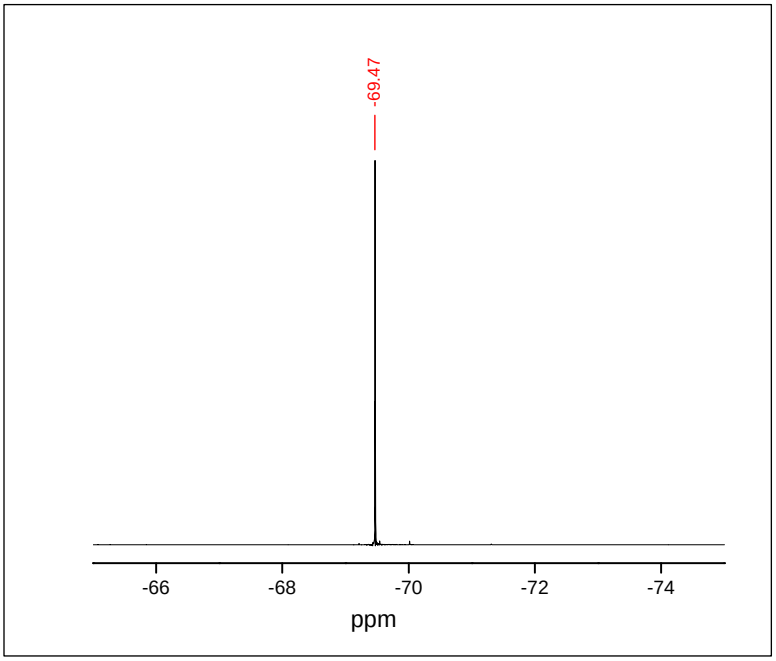
[a]For atom numbering, see Figure 2. [b]Total atomic charge. [c] $\Delta q = q(ClF_2CC(O)CN^{\cdot+}) - q(ClF_2CC(O)CN)$.

Table S2. Total and ionization calculated energies for $ClF_2CC(O)CN$ and its fragments.

Species	Total energy[a] [Hartree]	I_a[a] [eV]
$ClF_2CC(O)CN$	–904.285002	11.15
$ClF_2CC(O)CN^{\cdot+}$	–903.875523	
$ClCF_2^{\cdot}$	–698.029688	8.65
$ClCF_2^{+}$	–697.712164	
$C(O)CN^{\cdot}$	–206.148433	9.12
$C(O)CN^{+}$	–205.813430	
$F_2CC(O)CN^{\cdot}$	–444.016346	9.96
$F_2CC(O)CN^{+}$	–443.650532	
$Cl^{\cdot}$	–460.168406	15.7
Cl^{+}	–459.610460	
$CF_2^{\cdot}$	–237.783724	11.35
CF_2^{+}	–237.366576	

[a]B3LYP/6-311+G(3df)

FIGURES



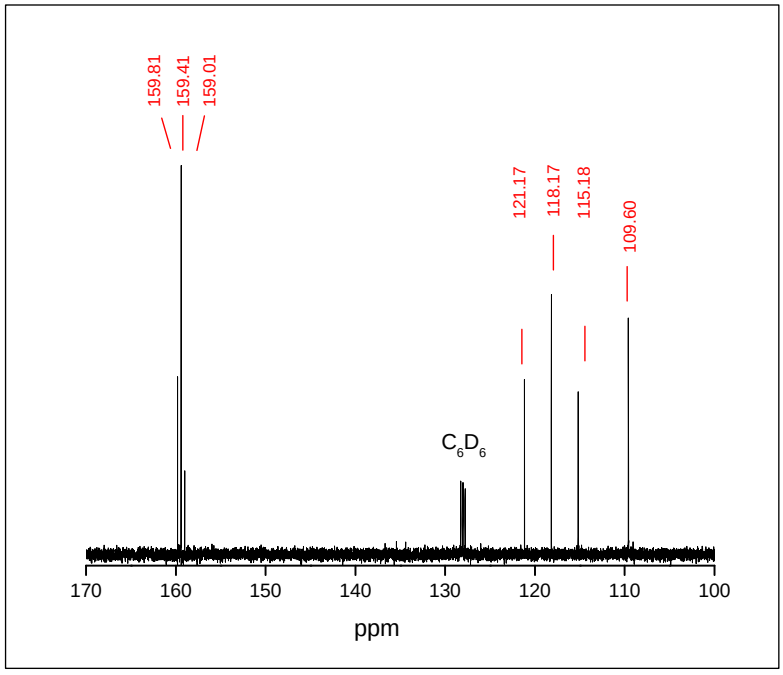


Figure S1. ^{19}F and ^{13}C NMR spectra of $ClF_2CC(O)CN$. C_6D_6 was used as an external lock.

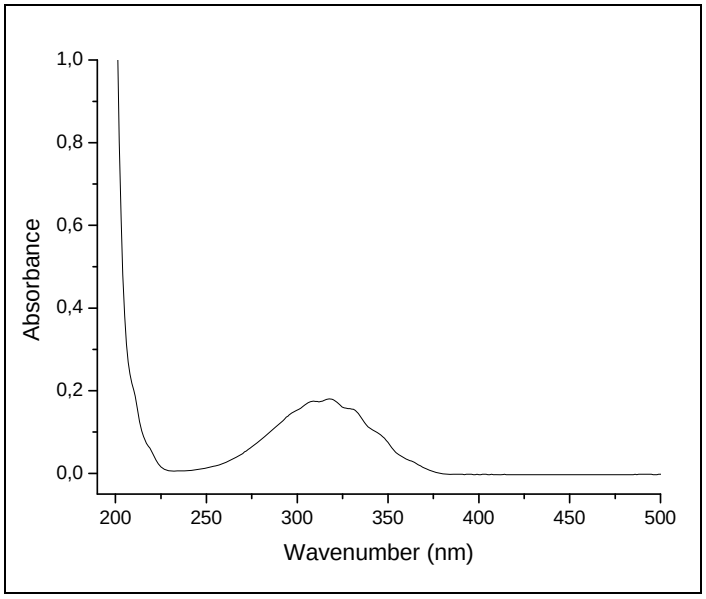


Figure S2. UV-visible spectrum of gaseous $ClF_2CC(O)CN$.

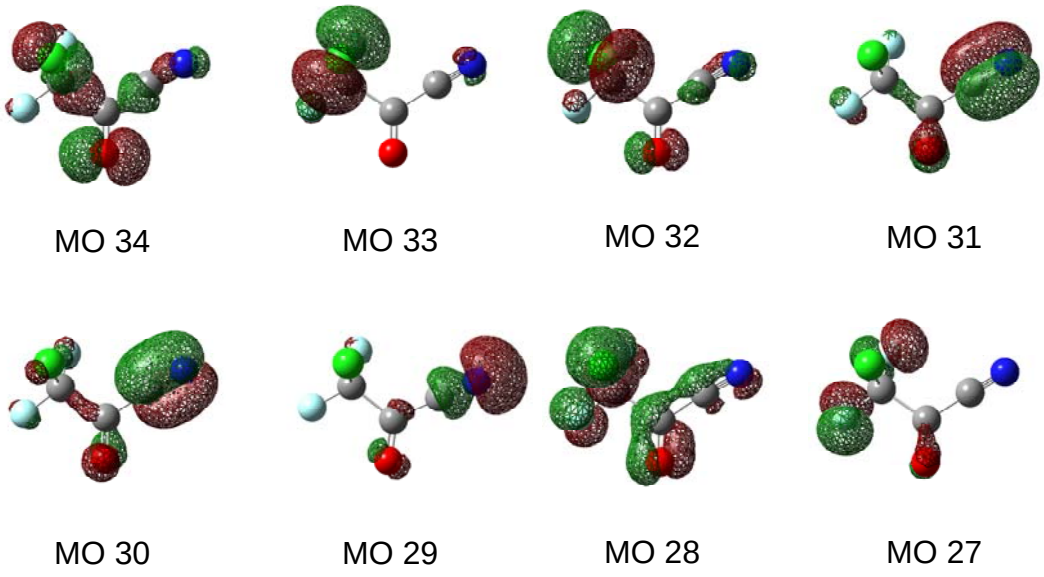


Figure S3. Character of the highest occupied molecular orbitals of $ClF_2CC(O)CN$.