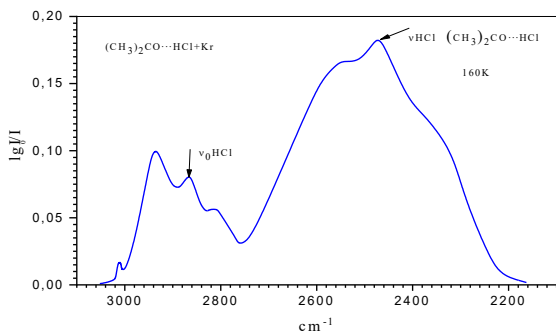
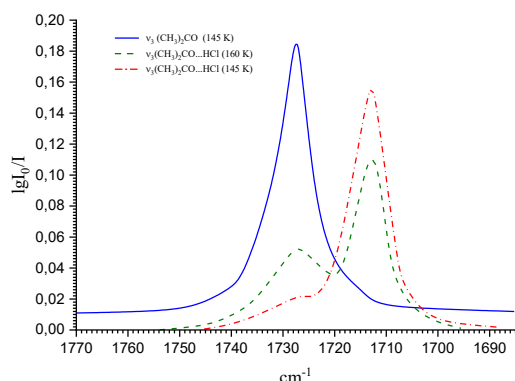


MOTIVATION

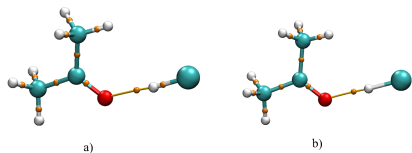
Infrared absorption spectra of free molecules $(\text{CH}_3)_2\text{CO}/\text{HCl}$ and $(\text{CH}_3)_2\text{CO}\cdots\text{HCl}$ complex are recorded in the 4000-900 cm^{-1} region with a Bruker IFS-125 Fourier spectrometer in gas state and with Kr, Xe solutions at different temperatures. In the free acetone and its complex with HCl, the spectral characteristics of the fundamental ranges $Q(\text{C}=\text{O})$, $\nu(\text{C}-\text{C})$, and νHCl are measured. Particular attention is paid to determining the effect of H-Cl and C=O on the bond length, frequency, and intensity in the $(\text{CH}_3)_2\text{CO}\cdots\text{HCl}$ complex. In the calculations, intermolecular interactions, anharmonic potential energy, and dipole moment surfaces are analysed using the DFT method based on the B3LYP/6-311++G(d,p) basis set. The electronic structure and equilibrium geometry of the $(\text{CH}_3)_2\text{CO}\cdots\text{HCl}$ complex are calculated using the Gaussian 09 W package. Topological (QTAIM, NCI and RDG) studies are used to examine interactions (hydrogen bond and Van der Waals interactions) at the crucial locations of connections. Information on the HUMO-LUMO gap and other electronic characteristics is given. A good agreement is observed between experimental and theoretical results.



Absorption spectra of the combination $(\text{CH}_3)_2\text{CO}\cdots\text{HCl}$ $(5+8)\cdot 10^{-5}$ mol/l band of νHCl in the Kr.

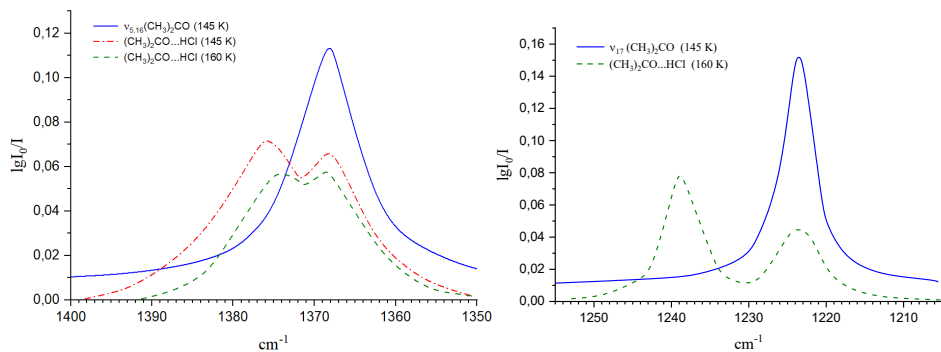


$(\text{CH}_3)_2\text{CO}$ and a combination of $(\text{CH}_3)_2\text{CO}\cdots\text{HCl}$ $(5+8)\cdot 10^{-5}$ mol/l absorption spectra in Kr, at different temperatures. Band for vibration $\nu_3(Q(\text{C}=\text{O}))$.

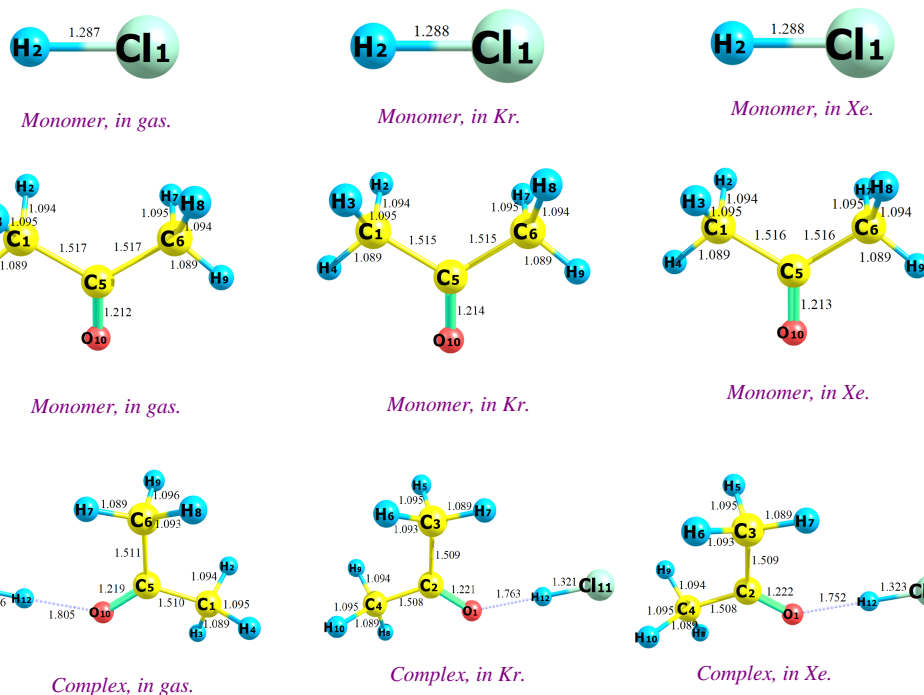


AIM analysis results of the studied complex. The line between acetone and HCl (Gas (a), Kr (b), Xe (b) cases) represents bond paths, and colored dots represent bond critical points.

Complex	Hydrogen bond	ρ (a.u.)	$\nabla^2\rho$ (a.u.)	$G(r)$ (a.u.)	$V(r)$ (a.u.)	$H(r)$ (a.u.)	E_{HB} (kcal/mol)
$(\text{CH}_3)_2\text{CO}\cdots\text{HCl}$	Gas O10-H12	0.035	0.108	0.0268	-0.0265	0.0003	8.31
	Kr O10-H12	0.039	0.115	0.0297	-0.0306	-0.0009	9.6
	Xe O10-H12	0.040	0.117	0.0305	-0.0318	-0.0013	9.97

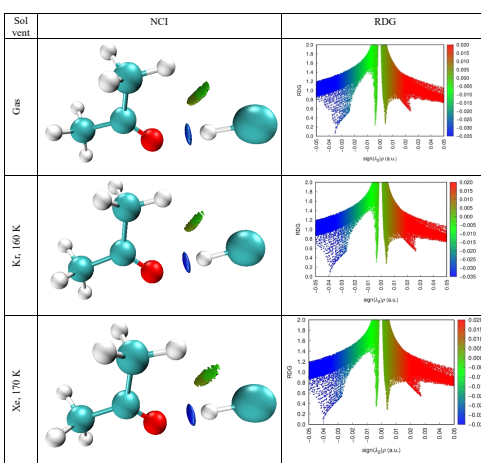


$(\text{CH}_3)_2\text{CO}$ and a combination of $(\text{CH}_3)_2\text{CO}\cdots\text{HCl}$ $(5+8)\cdot 10^{-5}$ mol/l absorption spectra in Kr, at different temperatures. a) Band for vibration $\nu_{5,16}((\text{HCH}))$, b) Band for vibration $\nu_{17}(Q(\text{C}-\text{C}))$.



Optimal geometric structures of free molecules $(\text{CH}_3)_2\text{CO}/\text{HCl}$ and $(\text{CH}_3)_2\text{CO}\cdots\text{HCl}$ complexes.

NCI-RDG analysis



HUMO-LUMO analysis

Molecule	Sol vent	HUMO	E_{HUMO}	LUMO	E_{LUMO}	E_{gap}
HCl	Gas		-8.558		-0.099	-8.459
	Kr		-9.217		-0.068	-9.149
	Xe		-9.218		-0.066	-9.152
$(\text{CH}_3)_2\text{CO}$	Gas		-7.052		-0.781	-6.271
	Kr		-7.091		-0.795	-6.296
	Xe		-7.102		-0.799	-6.303
$(\text{CH}_3)_2\text{CO}\cdots\text{HCl}$	Gas		-7.867		-1.494	-6.373
	Kr		-7.855		-1.447	-6.408
	Xe		-7.855		-1.439	-6.416

CONCLUSION

At ambient temperature, 0.1 cm^{-1} resolution gas-phase spectra of HCl complexes with both normal and completely acetone were recorded. The complexes fell within the 3900–3200 cm^{-1} space. These spectra are contrasted with $(\text{CH}_3)_2\text{CO}\cdots\text{HCl}$ similar spectra. The processes that give rise to the $\nu_1(\text{H}-\text{Cl})$ band shape in these compounds are examined. The analysis is based on high-precision DFT potential energy surfaces estimated for these complexes, which are obtained through variational solutions of one and multidimensional anharmonic vibrational problems. A detailed analysis is conducted on the four bending vibrations and the stretching vibrations of the H-Cl and H-bond of two monomers in perpendicular planes.