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## Molecular and Crystal Structures of $\text{TeCl}_4$ - Allyl alcohol and -Allylacetate Adducts

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1,2-electrophilic addition of  $\text{TeCl}_4$  to the C=C bond of allyl alcohol is observed, while with allylacetate, 1,3-addition occurs, due to migration of the acetate group. The allyl alcohol adduct comprises two different kinds of molecules in the solid state,  $\text{Cl}_3\text{Te}[\text{CH}_2\text{CH}(\text{Cl})\text{CH}_2\text{OH} \rightarrow]$  and  $\text{Cl}_2\text{Te}[\text{CH}_2\text{CH}(\text{Cl})\text{CH}_2\text{O} \rightarrow]$ , with dative  $\text{Te} \leftarrow \text{O}$  and covalent Te-O bonds, five-membered ring structures and  $\text{Cl} \cdots \text{Te} \cdots \text{Cl}$  and  $\text{O} \cdots \text{H} \cdots \text{O}$  bridges linking the different molecules. In the allylacetate adduct,  $\text{Cl}_3\text{Te}[\text{CH}_2\text{CH}(\text{CH}_2\text{Cl})\text{OC}(\text{CH}_3)=\text{O} \rightarrow]$ , a six-membered ring is formed via an intramolecular dative  $\text{Te} \leftarrow \text{O}$  interaction, the molecules being linked via  $\text{C} \cdots \text{Cl} \cdots \text{Te}$  bridges. Multinuclear NMR spectroscopy and  $^1\text{H}$ - $^1\text{H}$ -NOESY combined with *ab initio* (MP2/LANL2DZP) geometry optimisation show the geometry of the ring structures in solution to be similar to those in the solid state.

**Keywords:** Coordination Chemistry; tellurium; NOESY; crystal structures; *ab initio* calculations

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## RESULTS

The electrophilic addition of  $\text{TeCl}_4$  to allyl alcohol forms **1**, a 1:1 adduct of the two pentacyclic compounds  $\text{Cl}_2\text{Te}[-\text{CH}_2\text{CH}(\text{Cl})\text{CH}_2\text{O}-]$  (covalent  $\text{Te}-\text{O}$  bond) and  $\text{Cl}_3\text{Te}[-\text{CH}_2\text{CH}(\text{Cl})\text{CH}_2\text{O}(\text{H})\rightarrow]$  (dative  $\text{Te}\leftarrow\text{O}$ ).  $\text{Cl}-\text{Te}\cdots\text{Cl}$  and  $\text{O}-\text{H}\cdots\text{O}$  bridges form links between the different molecules. Reaction of  $\text{TeCl}_4$  with allylacetate forms  $\text{Cl}_3\text{Te}[\text{CH}_2\text{CH}(\text{CH}_2\text{Cl})\text{OC}(\text{CH}_3)=\text{O}\rightarrow]$ , **2**,<sup>[1]</sup> with a six-membered ring with dative  $\text{Te}\leftarrow\text{O}=\text{C}$  interaction, the molecules being linked via  $\text{C}-\text{Cl}\cdots\text{Te}$  bridges.

$^1\text{H}-^1\text{H}$ -NOESY show the geometry of the ring structures of **1** and **2** in solution to be similar to those in the solid state. *Ab initio* geometry optimizations show a good agreement in the covalent bond lengths between solid state and isolated molecules, but significant differences between the dative bonds.

## References

- [1] L. Engman *J. Am. Chem. Soc.* **106**, 3977- 3984 (1984).