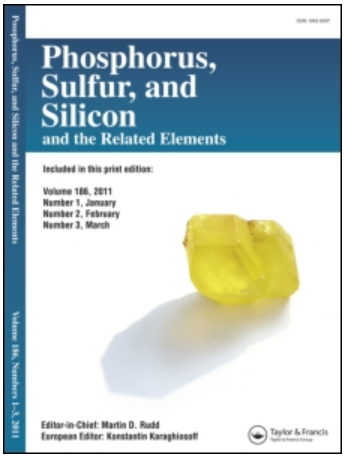


**Phosphorus, Sulfur, and Silicon and the Related Elements**
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**To cite this Article** Fleischer, Holger and Schollmeyer, Dieter(2001) 'Molecular and Crystal Structures of $TeCl_4$-Allylalcohol and -Allylacetate Adducts', Phosphorus, Sulfur, and Silicon and the Related Elements, 169: 1, 271 — 272
**To link to this Article: DOI:** 10.1080/10426500108546640
**URL:** http://dx.doi.org/10.1080/10426500108546640

*Phosphorus, Sulfur and Silicon*, 2001, Vol. 169, pp. 271-272
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# Molecular and Crystal Structures of $TeCl_4$-Allylalcohol and -Allylacetate Adducts

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*(Received August 09, 2000)*



1,2-electrophilic addition of $TeCl_4$ to the C=C bond of allylalcohol is observed, while with allylacetate, 1,3-addition occurs, due to migration of the acetate group. The allylalcohol adduct comprises two different kinds of molecules in the solid state, $Cl_3Te[CH_2CH(Cl)CH_2OH\rightarrow]$ and $Cl_2Te[CH_2CH(Cl)CH_2O\text{-}]$, with dative Te←O and covalent Te-O bonds, five-membered ring structures and Cl-Te···Cl and O-H···O bridges linking the different molecules. In the allylacetate adduct, $Cl_3Te[CH_2CH(CH_2Cl)OC(CH_3)=O\rightarrow]$, a six-membered ring is formed via an intramolecular dative Te←O interaction, the molecules being linked via C-Cl···Te bridges. Multinuclear NMR spectroscopy and $^1H$-$^1H$-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 $TeCl_4$ to allylalcohol forms **1**, a 1:1 adduct of the two pentacyclic compounds $Cl_2Te[-CH_2CH(Cl)CH_2O-]$ (covalent Te–O bond) and $Cl_3Te[-CH_2CH(Cl)CH_2O(H)\rightarrow]$ (dative Te←O). Cl–Te···Cl and O–H···O bridges form links between the different molecules. Reaction of $TeCl_4$ with allylacetate forms $Cl_3Te[CH_2CH(CH_2Cl)OC(CH_3)=O\rightarrow]$, **2**,[1] with a six-membered ring with dative Te←O=C interaction, the molecules being linked via C–Cl···Te bridges.

$^1H$-$^1H$-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).