

Preliminary communication

BIS(2-(2-PYRIDYL)PHENYL)TRITELLURIDE – SYNTHESIS AND CRYSTAL STRUCTURE

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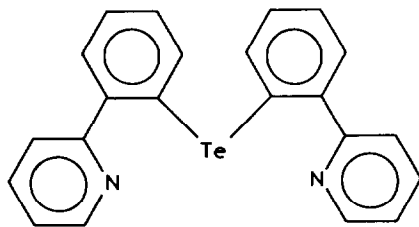
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Summary

The synthesis and molecular structure of bis(2-(2-pyridyl)phenyl)tritelluride are described. There is a short Te...N non-bonded interaction of 2.554(7) Å, which may be responsible for the stability of the molecule. The tritelluride can be converted into the related ditelluride by treatment with copper in refluxing dioxane. The ditelluride may also be prepared by a route not involving the tritelluride.

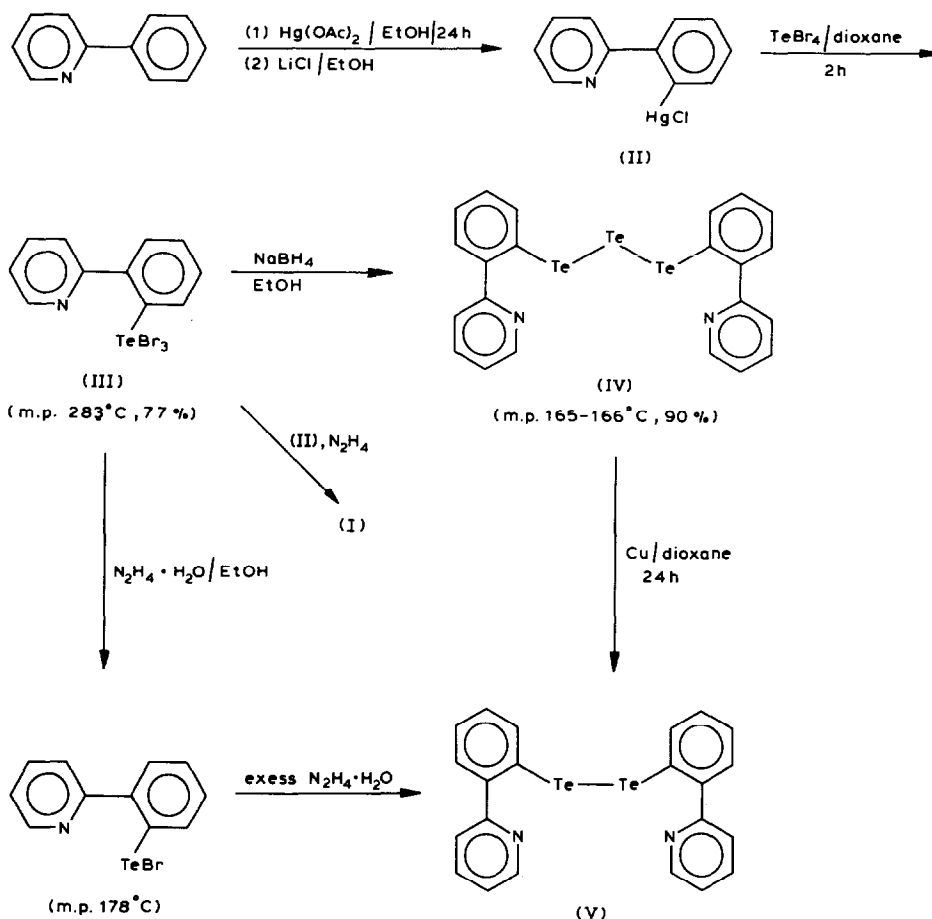
Whilst attempting to prepare the functionalised tellurium-containing ligand (I), we tried, by use of NaBH₄, to reduce an organytellurium tribromide (III) directly to the sodium organytelluride(-1). Instead a novel tritelluride was isolated in good yield (see Scheme 1). The tritelluride was converted into the ditelluride (V) by treatment with copper powder in refluxing dioxane.



(I)

Crystals of IV suitable for single crystal X-ray diffraction studies were obtained from benzene/toluene:

Crystal data. C₂₂H₁₆N₂Te₃, *M_r* = 691.2, monoclinic, space group *I2/c*, *a* 14.721(3), *b* 9.290(4), *c* 15.996(10) Å, β 106.39(3)°, *U* 2098.7 Å³, *Z* = 4, *D_c* 2.188 g cm⁻³, *F*(000) = 1272.



SCHEME 1

Cell dimensions and intensities were measured with an Enraf-Nonius CAD-4 diffractometer using monochromated Mo-K_α radiation. 1634 reflections in the range $2 < \theta < 25^\circ$ having $I > 2.5\sigma(I)$ were used in the analysis. The structure was solved by Patterson and Fourier methods and refined by least-squares with SHELX [1], using anisotropic temperature factors for all non-hydrogen atoms. Hydrogen atoms were located from a difference map and included in fixed positions. The calculations were terminated when all shifts were < 0.1 and R and R_w were 0.064 and 0.088, respectively; $w = 1/(\sigma^2(F) + 0.005F^2)$.

A stereoscopic view of the structure of IV drawn with PLUTO [2] is shown in Fig. 1. The compound exhibits two-fold symmetry with the central tellurium atom lying on a crystallographic two fold axis*.

* The atomic coordinates for this structure are available on request from the Director of the Cambridge Crystallographic Data Centre, University Chemical laboratory, Lensfield Road, Cambridge CB2 1EW (Great Britain). Any request should be accompanied by the full literature citation for this communication.

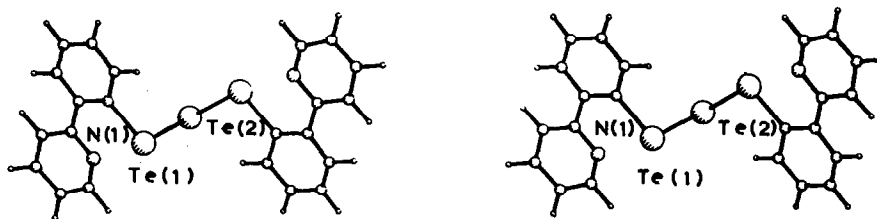


Fig. 1. Stereoscopic view of the molecule. Selected bond lengths (Å) and angles (°): Te(1)–Te(2), 2.776(1); Te(1)–C, 2.130(9); Te(1)···N, 2.554(7); Te(1)–Te(2)–Te(1)', 100.4(1); C–Te(1)–Te(2), 99.1(2); N···Te(1)–Te(2), 170.7(2); N···Te(1)–C, 71.6(3).

Of particular note is the short Te···N non-bonded interaction of 2.554(7) Å, which appears to hold the ligand in an essentially planar geometry; the pyridyl and phenyl rings are, nevertheless, bent very slightly relative to one another to form a shallow V shape, with internal angle 177.2(4)°. The coordination of Te(1), by Te(2), N, and its bonded carbon atom is accurately planar. The torsion angle about the Te(1)–Te(2) bond is 97.3(3)°.

During the course of this work the structure of bis(tris(trimethylsilyl)methyl)tritelluride was reported [3]. The Te–Te bond length found in that compound (2.710(1) Å) is shorter by 0.066 Å than the corresponding length in our structure. This difference may be a manifestation of somewhat stronger Te–C binding involving an aromatic carbon atom (Te–C shorter by 0.083 Å) in our compound.

Apart from the tritelluride ion, [Te₃]²⁻ [4], (Me₃Si)₃C₂Te₃ and the present compound are the only tritellurides reported to date. The bulky (Me₃Si)₃C groups are believed to contribute to the stability of the former compound [3]. The diorganyltritelluride reported here, by contrast, appears to owe its stability to the significant Te···N interaction, suggesting that if the organic ligands have a suitably positioned donor atom, many more successful syntheses of tritellurides should be possible.

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