

LONG RANGE COUPLINGS IN BENZO(b)SELENOPHEN AND BENZO(b)TELLUROPHEN

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The proton magnetic resonance spectra of monobenzoderivatives of five-membered heterocycles exhibit long range couplings as has been previously shown in indane, indole, benzo(b)furan and benzo(b)thiophen (1).

Inter-ring 3,7- and 3,4-couplings with values of 0.65 Hz and 0.14 Hz respectively have been found in benzo(b)selenophen. In benzo(b)tellurophen, a 0.43 Hz inter-ring 3,7- coupling has been observed. We did not see a 2,6- coupling in either case.

The analysis of the PMR spectrum of benzo(b)selenophen was made as follows. H₂ was identified through its coupling with the ⁷⁷Se nucleus (47.7 Hz). H₇ was separated from H₄ by the use of a paramagnetic Eu complex as a "chemical shift reagent" (2), the complexed molecule being 2-hydroxymethyl-benzo(b)selenophen. H₅ and H₆ were then identified from their meta couplings.

The interactions of H₃ with two benzene ring protons are clearly visible in the spectrum. The assignment of these couplings was made through the analysis of the 2- and 3-methylbenzo(b)selenophen spectra: in the latter case, the lines of H₇ are considerably sharpened and, to a lesser extent, the same holds for the H₄ lines. The comparison between 2- and 3-methyl derivatives was necessary due to the fact that, in the benzo(b)selenophen spectrum, the H₂ and H₇ lines are superimposed.

The analysis of the benzo(b)tellurophen spectrum was made in a similar way, using the ¹²⁵Te coupling (101 Hz) and Eu complex with 2-acetyl-benzo(b)tellurophen.

An inter-ring coupling was found in the H₃ lines (0.43 Hz). Frequency sweep decoupling of H₃ sharpened the broad lines of H₇ and so gave the 3,7 assignment of the observed coupling.

We also point out the coupling of H₂ with ⁷⁷Se: its value, 47.7 Hz, is nearly the same as in the selenophen, 48 Hz (3) and it is much greater than most of the values reported in the literature (4-7). The same holds for the coupling of ¹²⁵Te with H₂, 101 Hz (5-7). This point will be discussed in another paper.

The preparation and identification of the compounds studied in this letter has been published separately (8-9).

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CHEMICAL SHIFTS (ppm-ref. TMS) AND COUPLING CONSTANTS (Hz)^(a).

	2	3	4	5	6	7	J ₂₃	J ₃₇	J ₃₄	J ₄₅	J ₄₆	J ₄₇	J ₅₆	J ₅₇	J ₆₇
Se	7.79	7.42	7.69	7.24	7.14	7.77	5.77	0.65	0.14	7.97	1.02	0.48	7.22	1.17	8.27
Te	8.55	7.84	7.71	7.26	7.03	7.82	6.95	0.43	-	7.97	1.07	0.51	7.24	1.08	8.00

(a) The data are obtained from iterative computations done with LEAITR program (QCPE 188). The details of the fitting procedure will be published elsewhere.

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