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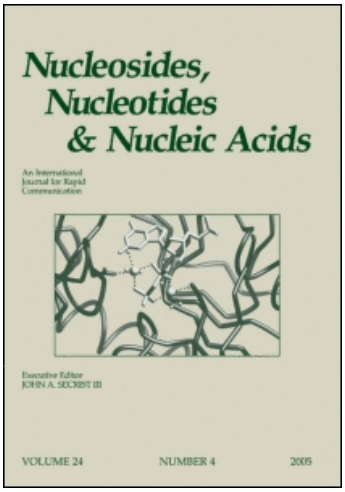

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Vibrational Study of a Nucleoside Analogue with Antiviral Activity, 5-Chloro-2'-deoxyuridine, CDU

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VIBRATIONAL STUDY OF A NUCLEOSIDE ANALOGUE WITH ANTIVIRAL ACTIVITY, 5-CHLORO-2'-DEOXYURIDINE, CDU.

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Abstract: The experimental FTIR and FT-Raman spectra of 5-chloro-2'-deoxyuridine have been assigned on the basis of normal coordinate analyses, in the light of observed and calculated wavenumbers and isotopic shifts. The results indicate that virtually all normal modes of IDU involve some degree of vibrational coupling between the chlorouracil base and the deoxyribose moiety.

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5-Chloro-2'-deoxyuridine, CDU, is principally effective against DNA viruses and its antiviral activity is related to incorporation into DNA in place of the normal component, thymidine. A vibrational analysis of the nucleoside is presented as the basis for an understanding of drug-target interactions.

A comparison was made of the experimental FTIR and FT-Raman spectra of IDU and its deuterated analogue (deuterated at positions N3, O3' and O5') with theoretical frequencies. Calculations were carried out by using a) a specifically designed computer program, Bioviban with a force field transferred from fragments or related molecules[1-3] (overlay technique),[4] and the CDU structure obtained by X ray diffraction[5] and b) the semiempirical molecular orbital method, PM3,[6] in order to evaluate the advantages of both methods for obtaining a reliable assignment of the vibrational spectra.

The FTIR and FT-Raman spectra were recorded on a Bomem DA3 spectrometer (Fig. 1). Some observed and calculated frequencies, and the potential energy distributions (>10%), are shown in Table 1. The results indicate that virtually all normal

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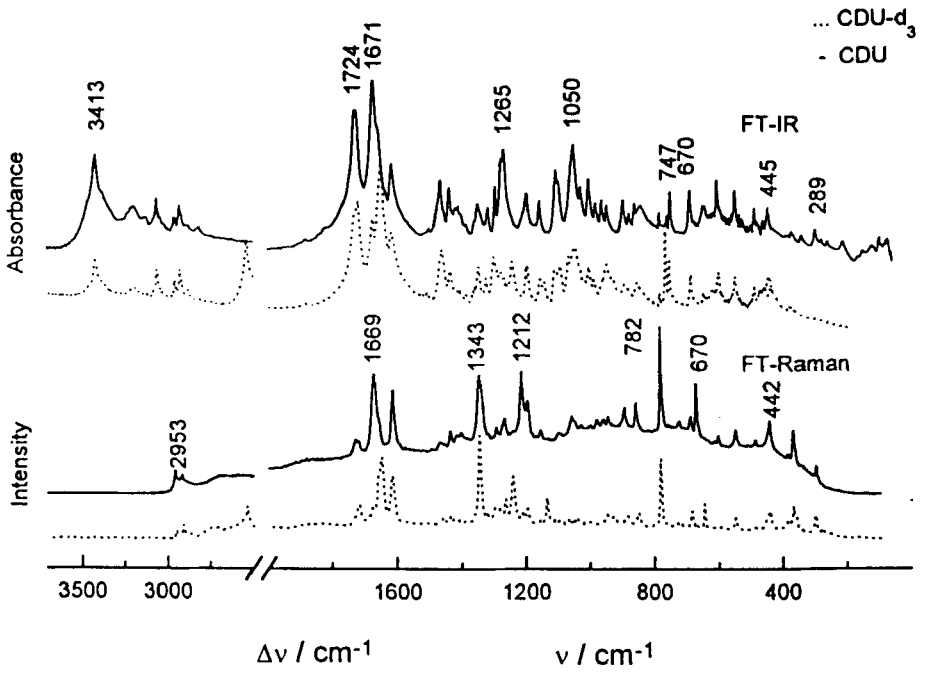

FIG. 1. Spectra of polycrystalline CDU: Mid and far IR and FT-Raman (InGaAs detector at 77 K).

TABLE 1. Assignments for some relevant frequencies of CDU.

Observed wavenumbers		Calculated wavenumbers		Potential energy distribution
FTIR/cm^{-1}	FT-Raman/cm^{-1}	PM3/cm^{-1}	Bioviban/cm^{-1}	PED/%
3413	3400	3360	3102	97νN3H (2291 cm^{-1} 97νN3D)
1724	1727	1945	1826	16νC2O + 12δN1C2N3
1659	1659	1787	1649	19νN1C2 + 17δN3C2O2 - 13δN1C6H
1196	1196	1260	1202	81δC5'O5'H + 4δC4'C5'H
838	658	834	837	54δC2N3H + 5νC5Cl

modes of IDU involve some degree of vibrational coupling between the chlorouracil base and the deoxyribose moiety.

The agreement between calculated and experimental spectra was within 1% for the transferred force field and approximately 10% for PM3.

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