Fig. 1. The positions of the U atoms as seen in a projection along the b axis of the unit cell. Uranium atoms belonging to the same hydrolysis complex are joined by dashed lines.

The positions of the uranium atoms as seen in a projection along the b axis are shown in Fig. 1. The uranium atoms occur in pairs with a U—U distance of 4.03 Å. The shortest distance between atoms belonging to different pairs is 7.22 Å. The structure, therefore, seems to be built up from discrete dinuclear complexes.

In the $\text{Th}_2(\text{OH})_2(\text{NO}_3)_6(\text{H}_2\text{O})_6$ complexes found in crystals of $\text{Th}_2(\text{OH})_2(\text{NO}_3)_6 \cdot (\text{H}_2\text{O})_6$, the distance between the Th atoms is 3.99 Å.³ This indicates that the dinuclear U(IV) hydrolysis complexes are very similar to those formed by thorium and the formula for the compound investigated should be written $\text{U}_2(\text{OH})_2(\text{ClO}_4)_6 \cdot (\text{H}_2\text{O})_x$ ($x \approx 13$).

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1. Pocev, S. and Johansson, G. *Acta Chem. Scand.* 27 (1973) 2146.
2. Johansson, G. *Acta Chem. Scand.* 22 (1968) 379.
3. Johansson, G. *Acta Chem. Scand.* 22 (1968) 389.

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Normal Coordinate Analysis of Hexafluoroacetone

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The infrared and Raman spectra of hexafluoroacetone were first reported by Berney.¹ As pointed out by Miller and Kiviat,² his original assignment of the band at 194 cm^{-1} (gas spectrum) as being due to CCC bending is possibly in error. In the present work a harmonic force field was developed for hexafluoroacetone and an alternative assignment of the bands is proposed. This work is part of a larger study on polyfluoro compounds.^{3,4}

Berney¹ concludes that the actual point group of hexafluoroacetone should be C_s instead of C_{2v} , basing his argument mainly on the depolarization ratios of a CF bending and the assumed CO bending vibrations. As Miller and Kiviat point out, however, the intensity of the Raman band at 716 cm^{-1} is too weak to give decisive information on its polarization. They also give evidence indicating that the 320 cm^{-1} band, assigned by Berney to a CO wag, is in fact due to the CCC scissoring mode. This result is in good agreement with the experimental studies of Murto *et al.*,^{5,6} on hexafluoro alcohols. Obviously the full C_{2v} symmetry can be used.

According to Berney, the 194 cm^{-1} band clearly represents a totally symmetric fundamental. Accepting this as a CF_3 rocking band, we are left with one rocking band too many. In our opinion the band at 233 cm^{-1} in the vapour spectrum, the weakest of the rocking bands proposed by Berney, is not a fundamental band; rather, the band at 265 cm^{-1} is the B_1 rocking vibration. This also is a weak band and its depolarization ratio has not been reported. The B_1 CO bending band is probably in the region 450 cm^{-1} –500 cm^{-1} ,^{7,8} being obviously superimposed by other bands. In the present work it is assumed to be at 470 cm^{-1} .

The distribution of the normal modes among the symmetry species is $10A_1 + 4A_2 + 8B_1 + 5B_2$, including two redundancies in the A_1 species and one redundancy in the B_1 species.

The G matrix was calculated by the modified programme written by Schachtschneider⁹ for the Wilson s-vector method. The normal coordinate calculations were carried out on a Univac 1108 computer using a programme written by the author. In the course of the calculations the diagonal and largest off-diagonal elements of the F matrix were first perturbed on order to get the best possible F matrix with a minimum number of parameters. Using the obtained L matrix, a full harmonic force field was developed for each species to fit exactly

Table 1. Potential energy distribution and vibrational assignment of hexafluoroacetone.

	Freq.	PED				Assignment
A_1	1807	49 ν CO,	29 δ CCC,	9 ν CF		ν CO
	1252	50 ν CF,	17 δ CF,	12 ν CO,	9 δ CCC	ν CF
	1200	49 ν CF,	31 δ CF,	19 ν CC		ν CF
	779	28 ν CF,	25 ν CC,	30 δ CF,	8 ν CO	ν CC
	633	30 δ CF,	30 ν CF,	22 δ CCC,	9 ν CO	δ CF
	471	89 δ CF,	5 ν CC			δ CF
	320	60 δ CF,	34 δ CCC			δ CCC
	194	54 δ CF,	31 ν CC,	12 δ CCC		δ CF
A_2	1162	59 ν CF,	16 δ CF,	19 τ CF ₃		ν CF
	533	37 ν CF,	41 δ CF,	21 τ CF ₃		δ CF
	160	6 ν CF,	83 δ CF,	10 τ CF ₃		δ CF
	48	46 δ CF,	52 τ F ₃			τ CF ₃
B_1	1344	62 ν CF,	16 δ CO,	20 δ CF		ν CF
	1275	57 ν CF,	33 δ CF,	10 ν CC		ν CF
	972	49 ν CC,	31 δ CO,	11 ν CF		ν CC
	718	46 δ CF,	31 ν CF,	16 ν CC		δ CF
	528	84 δ CF,	13 ν CF			δ CF
	470	45 δ CO,	31 δ CF,	19 ν CC		δ CO
	265	92 δ CF				δ CF
B_2	1314	52 ν CF,	22 τ CF ₃ ,	22 δ CF		ν CF
	506	39 δ CF,	35 τ CF ₃ ,	17 ν CF,	7 δ CO	δ CF
	368	40 δ CO,	47 δ CF,	12 ν CF		δ CO
	275	62 δ CF,	27 τ CF,	11 δ CO		δ CF
	66	24 τ CF ₃	39 δ CF,	36 δ CO		τ CF ₃

the set of the vapour frequencies given by Berney, with the changes discussed above. The resulting potential energy distributions and the suggested assignments are displayed in Table 1.

1. Berney, C. V. *Spectrochim. Acta* 21 (1965) 1809.
2. Miller, F. A. and Kiviat, F. E. *Spectrochim. Acta Part A* 25 (1969) 1577.
3. Perttilä, M. *Unpublished results*.
4. Cyvin, S. J., Brunvoll, J. and Perttilä, M. *J. Mol. Struct.* 17 (1973) 17.
5. Murto, J., Kivinen, A., Manninen, A. and Perttilä, M. *To be published*.
6. Murto, J., Kivinen, A., Viitala, R. and Hyömäki, J. *Spectrochim. Acta Part A* 29 (1973) 1121.
7. Pace, E. L., Plausch, A. C. and Samuelson, H. V. *Spectrochim. Acta* 22 (1966) 993.
8. Allkins, J. R. and Lippincott, E. R. *Spectrochim. Acta Part A* 25 (1969) 761.
9. Schachtschneider, J. H. *Technical Report Nos. 231-264*, Shell Development Co.

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