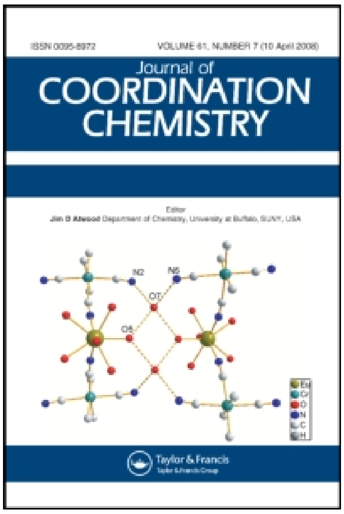

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FOURIER-TRANSFORM RAMAN AND INFRARED SPECTRA AND VIBRATIONAL ASSIGNMENT FOR SOLID GLUTARIMIDE

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The FT-Raman and FT-IR spectra of crystalline glutarimide and its *N*-deuterated derivative have been recorded in the range 4000–100 cm^{-1}. A complete vibrational assignment is given for all internal modes and is supported by normal coordinate analysis based on a general valence force field. The calculated frequencies are in very good agreement with experiment. A close similarity is found for frequencies of the corresponding vibrations of glutarimide and uracils in the solid state. It is concluded that the strength of hydrogen bonding in glutarimide is very similar to that in crystalline pyrimidine nucleic bases.

Keywords: Glutarimide; uracils; heterocycles; vibrational spectra; hydrogen bonding; normal coordinate analysis

INTRODUCTION

This work is part of a wider series of papers[1–9] aimed at studying structure and properties of glutarimide derivatives, which are of pharmacological interest. Glutarimide (2,6-piperidinedione) has been found in a number of antibiotics with the antiviral and fungicidal activity.[10–13] Furthermore, the 2,6-piperidinedione moiety constitutes an important centre in several new

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anticancer drugs which have recently been introduced into experimental chemotherapy.[14–16] In our theoretical studies[7] it was demonstrated that the molecule bears a striking similarity to uracil and thymine with respect to structural features and electron density distribution. Recently, we have studied interactions of glutarimide with a series of metal ions and have shown that the stability constants of complexes formed in aqueous solution[1–4] and the structures of complexes in the solid state[5] are similar to those of the corresponding metal complexes of uracil and thymine. It should be emphasized that both Antineoplaston A10 (the glutarimide anticancer drug) and uracil form very similar types of hydrogen bonding in the crystal.[8] These data support our earlier suggestion[6] that the drugs may mimic nucleic acid bases and they may form competitive hydrogen bonding with biological molecules containing the adenine moiety.

Very recently[9] we have measured the infrared spectra of monomer glutarimide in low-temperature argon and nitrogen matrices. In the present paper the Raman and infrared spectra of a solid glutarimide are reported for the first time. Comparison of the frequencies of the corresponding modes in going from monomer to the crystal provides direct information on the strength of N–H···O hydrogen bonding formed by glutarimide molecules. This may shed some light on a possible mechanism of biological activity of the glutarimide drugs.

Vibrational assignment presented in this work will be important for the further spectroscopic studies on metal complexes with glutarimide.

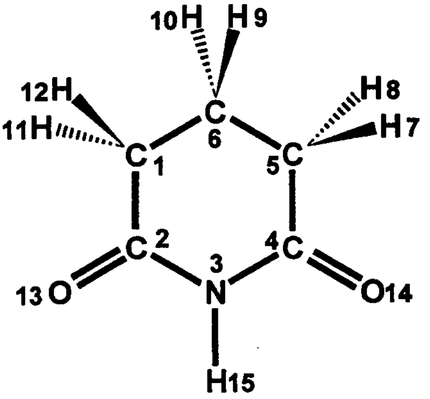
EXPERIMENTAL

Glutarimide was purchased from the Aldrich Chemical Co. The *N*-deuterated derivative was prepared by repeated crystallization from C_2H_5OD (99.5% deuterated) until no bands due to N–H vibrations were detected in the spectra.

Raman spectra of the solid compounds were recorded on Bruker 88 FT-Raman spectrophotometer equipped with a Nd-YAG laser (max. power 200 mW and resolution 2 cm^{-1}). IR spectra in the 4000–50 cm^{-1} region were measured on a Bruker ISF-113V FT-IR spectrophotometer. The IR spectra were recorded in KBr pellets and in nujol mulls.

NORMAL COORDINATE CALCULATIONS

The bond lengths and angles used in the normal coordinate analysis were taken from the literature.[17] The conformation of glutarimide is a half-chair



SCHEME 1 Molecular model and atom numbering used in the normal coordinate analysis of glutarimide.

with one carbon atom slightly out of the essentially coplanar system, formed by the remaining five atoms of the glutarimide ring and two oxygen atoms of two carbonyl groups. According to X-ray data only one carbonyl group is involved into the nearly linear N–H···O′ hydrogen bonding with another molecule in the crystal, whereas the second oxygen atom does not participate in hydrogen bonding. To simplify the calculations we used the model corresponding to a single molecule, as shown in Scheme 1, and applied different force constants and bond lengths (1.22 and 1.20 Å) for the carbonyl groups C4O14 and C2O13, respectively. Internal coordinates were defined according to general formulae[18] and following the IUPAC recommendation.[19] To obtain a complete set of the internal coordinates,[18] all 15 bond stretches, 27 valence angle bends, three out-of-plane bends (for atoms O13, O15 and H15) and six torsions for the ring were included in the calculations. This gives a total of 51 internal coordinates for 39 internal modes. The diagonalization of the GF matrix[18] yielded 39 frequencies for all fundamental modes and 12 nulls for all redundant modes which is an additional check of the validity of this procedure. The potential energy was expressed by a simplified general valence force field (SGVFF) since this force field has been shown to be very effective in normal coordinate analysis of structurally related molecules.[20] The procedure for force constant adjustment was the same as that described earlier.[8] Major interaction force constants for the imide group were transferred intact from the scaled *ab initio* force fields for structurally related uracils.[21]

Frequencies computed for glutarimide and its *N*-deuterated derivative are in very good agreement with experiment, and average error is less than

0.5%. Calculations were performed with a modified version of the Schachtschneider program.[22]

RESULTS AND DISCUSSION

The FT-Raman and FT-IR spectra of glutarimide are shown in Figure 1, and the far infrared spectrum is illustrated in Figure 2. The observed and calculated frequencies for glutarimide and its *N*-deuterated derivative are given in Table I along with the potential energy distribution (PED). The complete PED matrix is very complex; therefore only the predominant terms are listed.

Characteristic Frequencies of the $O_{13}C{-}NH_{15}{-}CO_{14}$ Group

The strong band at 3189 cm^{-1} in the infrared spectrum of glutarimide (Figure 1A) is shifted to 2343 cm^{-1} with *N*-deuteration; therefore it is

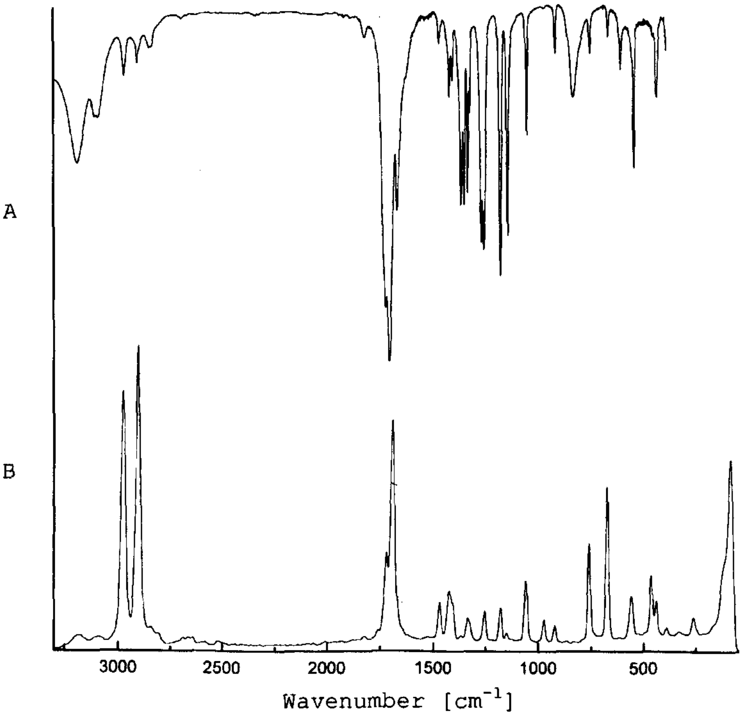


FIGURE 1 A: FT-IR spectrum and B: FT-Raman spectrum of glutarimide.

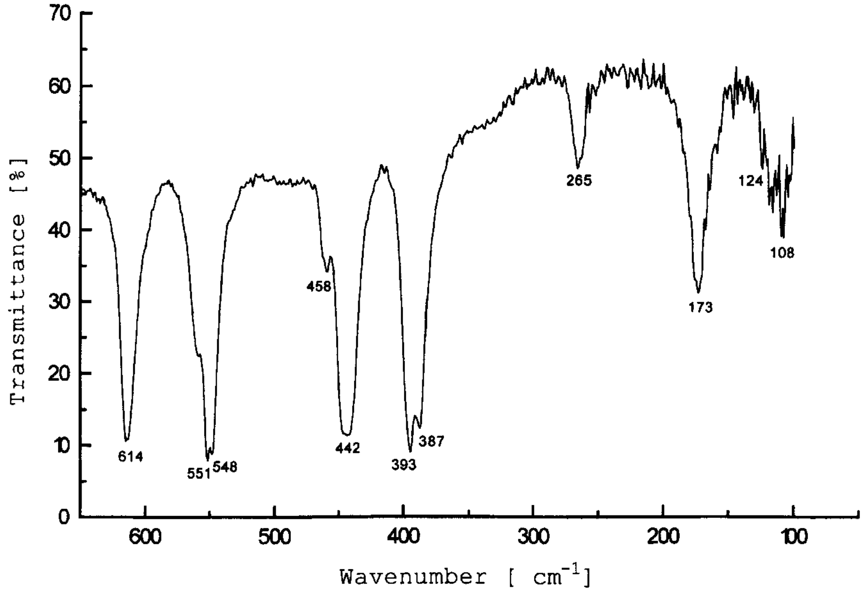


FIGURE 2 Far infrared spectrum of glutarimide.

assigned to the N–H stretching vibration. The corresponding band in the spectra of crystalline uracils was observed at similar wavenumbers, in the range 3200–3110 cm^{-1}.[23–26] The next band, at 3093 cm^{-1}, of a lower intensity in the IR spectrum of glutarimide, is also removed by *N*-deuteration and it can he attributed to a combination tone (involving C=O stretching and NH bending) enhanced in intensity by Fermi resonance with the N–H stretching. Such a characteristic absorption around 3080 cm^{-1} has been found in the spectra of both *cis*- and *trans*-secondary amides.[27] It should be noted that for monomeric glutarimide the N–H stretching mode was observed at 3406 cm^{-1} in an argon matrix.[9] A decrease in the N–H stretching frequency of about 220 cm^{-1} while passing from monomer to the solid state indicates the strength of hydrogen bonding in glutarimide.

The N–H in-plane bending vibration, δ(NH), in solid glutarimide contributes primarily to the weak band at 1409 cm^{-1}. Upon *N*-deuteration this band vanishes and a new strong band appears at 1117 cm^{-1}. Considerable difference in infrared intensity between these two bands is accompanied by a change in the potential energy distributions (PEDs) for the corresponding normal modes. The former is due to the N–H in-plane bending, δ(NH), coupled with a CH_2 deformation, whereas the latter arises from the coupled vibration involving N–D in-plane bending, C–N stretching and C–C

TABLE I Observed and calculated wavenumbers (cm^{-1}) and vibrational assignment for glutarimide and its *N*-deuterated derivative

Glutarimide			*Glutarimide-D*			*Assignment PED* (%)
ν *obsd.* (cm^{-1})		ν *calcd.* (cm^{-1})	ν *obsd.* (cm^{-1})		ν *calcd.* (cm^{-1})	
IR	*Raman*		*IR*	*Raman*		
3189m	3189w	3189	2343m	2345w	2344	ν (N3–H15) (100)
3093^{a}w	3093^{a}w					(1722 + 1410 = 3132)
	2973vs	2976		2973vs	2976	$\nu\,CH_2$ (C1,C5) (99)
2969w		2970	2968w		2970	$\nu\,CH_2$ (C1,C5) (100)
	2925sh	2925	2925sh		2925	$\nu\,CH_2$ (C6) (97)
2908w		2902	2907w		2902	$\nu\,CH_2$ (C1,C5) (97)
	2902vs	2902		2902vs	2902	$\nu\,CH_2$ (C1,C5) (99)
2850w	2844w	2849		2848vw	2849	$\nu\,CH_2$ (C6) (99)
1822^{a}w	1823^{a}w					(1259 + 551 = 1810 or 1180 + 614 = 1794)
1722s	1720m	1723	1718s	1720m	1714	ν(C2–O13) (67) + ν(C4–O14) (17)
1706^{b}vs	1689s	1687	1684s	1689s	1677	ν(C4–O14) (57) + ν(C2–O13) (21)
1668^{b}m			1669^{a}s			
1472w	1473w	1473	1471w	1473w	1473	CH_2 sciss. (C6) (90)
1437sh		1438	1435sh		1430	CH_2 sciss. (C1,C5) (41) + ν(C2–N3) (24)
1423w	1423w	1426	1422w	1419w	1422	CH_2 sciss. (C1,C5) (79)
1409w	1410w	1411	1117s		1112	δ(N3–H15) (55) + CH_2 def. (31)
1394sh		1391			1391	CH_2 def. (40) + ν(C2–N3) (11)
	1380vw	1381		1380vw	1377	ν(C4–N3) (18) + $\nu(C_b-C_c)$ (10)
1353m		1360	1358m		1361	CH_2 def. (63) + $\nu(C_b-C_c)$ (11)
1335m	1336w	1337	1335m	1340w	1337	CH_2 def. (53)
1272s		1269	1268w		1267	CH_2 def. (72) + $\nu(C_b-C_c)$ (10)
1259s	1255w	1255		1259w	1257	CH_2 def. (67) + $\nu(N-C_c)$ (22)
1180s	1182w	1188	1192m	1195w	1188	CH_2 def. (67)
1146s	1150vw	1145	1148w		1151	CH_2 def. (46) + $\nu(C_a-C_b)$ (9)
	1060m	1064	1060w	1062w	1060	$\nu(C_a-C_b)$ (78) + CH_2 def. (13)
1054m		1048	1038s	1043w	1046	CH_2 def. (63)
	973w	975	970vw	967w	973	CH_2 def. (35) + $\nu(C_a-C_b)$ (9)
920w	923w	922	920m	923w	920	$\nu(C_a-C_b)$ (49) + CH_2 def. (10)
	865vw	863	850w	850vw	846	$\nu(C_b-C_c)$ (16) + CH_2 def. (20)
	858vw	858	819w		812	$\delta(C_aC_bC_c)$ (21) + $\nu(C_b-C_c)$ (21)
837m,b	832vw	840	585vw		587	γ(N3 – H15) (62) + CH_2 def. (28)
759w	761m	762	797vw		797	$\nu(C_b-C_c)$ (31) + $\nu(C_a-C_b)$ (17)
673w	674s	677	686m	688m	684	γ(C2 – O13) (26) + γ(C4 – O14) (12)
614m	615vw	617	649vw		649	γ(C4 – O14) (19) + γ(C2 – O13) (15) + CH_2 def. (17)
558sh	561w	565	555sh		557	δ(C2NC4) (25) + $\nu(C_a-C_b)$ (14)
551*m*^{b}		553	546m	545w	547	δ(C4 – O14) (27) + $\nu(C_b-C_c)$(26) + δ(C2 – O13) (23)
548*m*^{b}						
458vw	466m	459	457w	464w	457	$\delta(C_aC_bC_c)$ (36) + δ(C2 – O13) (17) + $\nu(C_a-C_b)$ (14)
442m	443w	448	445m	443w	440	$\delta(C_aC_bC_c)$ (17) + δ(C2C4N) (15) + δ(C2NC4) (14)
393m^{b}	390w	359	391m^{b}	389w	358	δ(C2 – O13) (32) + δ(C4 – O14) (27) + $\nu(N-C_c)$ (37)
387m^{b}		384m^{b}				
265w	263w	271	264w	263w	268	τ(C6 – C1) (55) + τ(N3 – C4) (44)
173w		175	172m		171	τ(C1 – C2) (40) + τ(C4 – C5) (58)
124vw		127		123sh	123	τ(C4 – C5) (32) + τ(C6 – C5) (18) + τ(N3 – C2) (17)

^{a}Combination bands or ^{b}crystal field splitting.

Abbreviations used: s, strong; m, medium; w, weak; v, very; sh, shoulder; b, broad; ν, stretching; δ, in-plane bending; γ, out-of-plane bending; τ, torsion; def., deformation; $\nu(C_a-C_b) = \nu(C1-C6) + \nu(C6-C5)$; $\nu(C_b-C_c) = \nu(C1-C2) + \nu(C5-C4)$; $\nu(N-C_c) = \nu(N3-C2) + \nu(N3-C4)$; $\delta(C_aC_bC_c) = \delta(C6C1C2) + \delta(C6C5C4)$.

stretching vibrations. It is interesting that the frequency of δ(NH) mode in monomeric glutarimide (1392 and 1398 cm^{-1} in argon and nitrogen matrices, respectively[9]) is very similar to that in the solid state (1409 cm^{-1}). This indicates that the position of the band is only weakly affected by hydrogen bonding and is caused by extensive mixing of the in-plane NH bending vibration with skeletal and CH_2 deformation modes.

It has been shown that the band arising from the N–H out-of-plane (πNH) mode is extremely sensitive to the strength of hydrogen bonding.[23–26] Thus, unequivocal assignment of this "marker band" is indispensable for studying intermolecular interactions. The broad, medium intensity band at 837 cm^{-1} in the infrared spectrum of glutarimide is removed upon *N*-deuteration and can be assigned to the N–H out-of-plane bending vibration. In the IR spectra of crystalline pyrimidine bases the corresponding absorption occurs at very similar wavenumbers, 853 and 865 cm^{-1}, for uracil and 1-methyluracil, respectively.[23] This suggests that the strength of hydrogen bonding formed between glutarimide molecules in the crystal is very similar to that found in crystalline pyrimidine bases.

Anomalous splitting of the carbonyl stretching bands has been observed for both crystalline as well as matrix-isolated pyrimidine bases and it has been attributed to multiple Fermi resonances between the C=O stretching fundamentals and several overtones and combination tones of similar frequencies.[25,26] Moreover, due to intermolecular interaction in the crystal (factor group splitting) infrared and Raman frequencies often do not coincide.[23] In the Raman spectrum of crystalline glutarimide two prominent bands are observed at 1720 and 1689 cm^{-1}. It has been concluded that the lower wavenumber band corresponds to the C4 = O14 stretching vibration (being involved in intermolecular hydrogen bonding in the solid) and the higher wavenumber band is due to the C2–O13 stretching vibration. The coupling between these two vibrations is small, as shown in Table I. In the infrared spectrum of glutarimide some additional bands are also observed in this region. It seems plausible that the splitting of C=O bands has a similar origin as that in the spectra of crystalline pyrimidine bases.[22–26]

The in-plane bending vibrations, δ(CO), are coupled with ring deformation modes and make predominant contributions to the bands at 551/548 cm^{-1} and 393/387 cm^{-1}, as revealed by PED calculations. The corresponding CO in-plane bending modes in solid uracil have been assigned at very similar frequencies, 562 and 423/412 cm^{-1}, respectively.[26]

The CO out-of-plane bending vibrations, γ(CO), in glutarimide contribute significantly to the strong Raman band at 674 cm^{-1}. It is apparent that these modes occur at higher frequencies than the CO in-plane bending modes. Similar effects have also been observed in the vibrational spectra of pyrimidine bases.[22–26]

Torsional modes of the glutarimide ring are assigned to two bands at 266 and 174 cm^{-1} since they are not affected by *N*-deuteration. The assignment of the remaining bands is shown in Table I.

Force Constants

The final set of force constants derived in the normal coordinate analysis of glutarimide is listed in Table II. Obviously, this set is not unique, but is the most concise and is able to reproduce the frequencies of glutarimide and its *N*-deuterated derivative with good accuracy. The calculated values of the carbonyl stretching force constants, 11.06 and 10.27 mdyn Å^{-1}, for *f*(C2O13) and *f*(C4O14), respectively, reflect the corresponding differences in the C=O bond lengths. It should be noted that these values are very similar to those calculated for crystalline uracil and its methyl derivatives (11.0 and

TABLE II Force constants of glutarimide

No.	*Symbol*	*Value*	*No.*	*Symbol*	*Value*
1	*f*(C1C2) = *f*(C4C5)	4.17	26	*f*γ (N3H15)	0.25
2	*f*(C2N3)	4.88	27	*f*τ (C5C6)	0.12
3	*f*(C4N3)	5.47	28	*f*τ (C6C1)	0.13
4	*f*(C1C6) = *f*(C5C6)	3.94	29	*f*τ (C1C2)	0.30
5	*f*(CH^{a})	4.70	30	*f*τ (C2N3)	0.01
6	*f*(CH^{b})	4.54	31	*f*τ (N3C4)	0.01
7	*f*(C2O13)	11.06	32	*f*τ (C4C5)	0.52
8	*f*(C4O14)	10.27	33	*f*(CO,CC)^{o}	0.751
9	*f*(N3H15)	5.61	34	*f*(CO,CN)^{o}	1.181
10	*f*(C2C1C6) = *f*(C4C5C6)	1.61	35	*f*(CC,CN)^{o}	0.401
11	*f*(C1C2N3) = *f*(C5C4N3)	0.55	36	*f*(CC,CC)^{o}	0.101
12	*f*(C2N3C4)	0.52	37	*f*(CN,NC)^{o}	0.394
13	*f*(C1C6C5)	0.64	38	*f*(CC,CN)^{m}	−0.185
14	*f*(CCH^{a})	0.49	39	*f*(CC,CC)^{m}	−0.130
15	*f*(H^{a}CH^{a})	0.43	40	*f*(CC,CC)^{p}	0.164
16	*f*(CCH^{b})	0.61	41	*f*(CC,CN)^{p}	0.164
17	*f*(H^{b}CH^{b})	0.51	42	*f*(CCH,CC)^{p}	0.338
18	*f*(C5C4O14)	1.15	43	*f*(NC,NCO)	−0.443
19	*f*(N3C4O14)	1.46	44	*f*(NC,CNC)	0.425
20	*f*(C1C2O13)	1.54	45	*f*(CC,CCC)	0.417
21	*f*(N3C2O13)	0.87	46	*f*(CC,CCO)	0.225
22	*f*(HN3C2)	0.37	47	*f*(CNC,NCO)	−0.233
23	*f*(HN3C4)	0.48	48	*f*(C4N3,C4N3H)	0.42
24	*f*γ (C2O13)	0.36	49	*f*(C2N3,C2N3H)	−0.07
25	*f*γ (C4O14)	0.22	50	*f*(γN3H,τC2N3)	−0.16

All stretching force constants and stretch–stretch interactions are in units of millidynes per Å, bending in millidyne Å per square radians, stretching-bending interactions in millidynes per radian. Interaction force constant nos 33–47 are those transferred intact from *ab initio* studies.[21] Abbreviations: o, *ortho*; m, *meta*; p, *para* interactions; γ, out-of-plane bending; τ, torsions; H^{a} = H7, H8, H11, H12. H^{b} = H9, H10.

10.0 mdyn Å^{-1}).[22] This force field can be used for the further studies on metal complexes with glutarimide using vibrational spectroscopic methods.

Supplementary Material

A list of the geometrical parameter for glutarimide used in the calculations and a diagram showing the internal coordinates used for the normal mode analysis are available from the author upon request.

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