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Normal coordinate analysis of 2′-deoxythymidine and 2′-deoxyadenosine

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Abstract. The proposed valence force field allows us to reproduce the vibration modes of 2′-deoxythymidine and 2′-deoxyadenosine. The present calculations are based on the Wilson GF-method and a non-redundant set of symmetrical coordinates. The calculated wavenumbers have been compared to the available Raman and infrared peak positions observed in solid, amorphous or aqueous samples. Moreover, the results obtained with the present force field allow us to assign some of the characteristic vibration modes for the thymidine and adenosine residues involved in DNA double-helical chains.

Key words: 2′-deoxythimidine, 2′-deoxyadenosine, DNA, vibration modes

Introduction

We have recently published the normal coordinate analysis of 5′-dGMP (Ghomi and Taillandier 1985) and 2′-deoxycytidine (2′-dC) (Letellier et al. 1986). The non-redundant force field obtained in these calculations was also able to reproduce the vibrational characteristics of the cytidine (dC) and guanosine (dG) residues involved in DNA double helical chains (Letellier et al. 1986).

New spectroscopic studies on oligonucleotides and polynucleotides show that adenosine (dA) and thymidine (dT) residues may exist in both right- and left-handed conformations (Thomas and Peticolas 1983; Benevides et al. 1984; Thomas and Benevides 1985; Jollès et al. 1985; Adam et al. 1986 a, b). Moreover, some of the characteristic vibration modes of the dT and dA residues are found to be altered by both right → right and right → left conformational transitions. It would therefore be helpful to interpret these experimental phenomena by a normal coordinate treatment.

In this paper, our purpose is to obtain a reliable force field for 2′-deoxythymidine (2′-dT) and 2′-deoxyadenosine (2′-dA) for which recent Raman and infrared data are available. Obviously, the present calculations constitute the first step in the vibration mode analysis of the dT and dA residues encountered in oligonucleotides and polynucleotides.

Calculations

The normal coordinate analysis detailed here has been made using the Wilson GF-method (Wilson et al. 1955). The calculation formalism and the notations have been described in our former papers (Ghomi et al. 1985; Letellier et al. 1986).

To perform the numerical calculations, the original NCTB program (Shimanouchi 1968) has been vectorized in order to improve its run time on a Cray-1s computer. The array processing considerably accelerates the numerical calculations in comparison with the classical scalar computers.

As the out-of-plane modes of the pyrimidine and purine bases, particularly those of the thymine and adenine residues have been studied recently (Letellier et al. 1987 a, b), our attention in this paper was especially focused on the planar modes of the bases. On the basis of these considerations, one expects 78 vibration modes from 2′-dT and 75 from 2′-dA. 99 internal coordinates are numbered in both 2′-dT (32 stretchings + 57 bendings + 10 torsions) and 2′-dA (33 stretchings + 57 bendings + 9 torsions). So, there are 22 redundant coordinates in 2′-dT and 24 in 2′-dA. To preserve the harmonic approximation of the potential field, these redundant coordinates have been removed by a standard $B \cdot \tilde{B}$ matrix-product diagonalization procedure (Gusoni and Zerbi 1968) in order to obtain as many internal co-

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ordinates as the expected vibration modes (normal coordinates). As in the case of 5′-dGMP, the local symmetry of the different molecular sites has been taken into consideration and the redundancies have been resolved in the bases, sugars and C5′-tetrahedral sites separately (Ghomi and Taillandier 1985).

To construct B and G matrices the crystal structure of 2′-dT (Young et al. 1969) and that of 2′-dA (Watson et al. 1965) have been used. Both of the nucleosides are in *anti* position and contain a *C3′-exo* sugar pucker.

The elements of the interatomic interaction matrix, F, have been evaluated by a valence force field approximation. For the thymine-residue, we have used the uracil force constants (Ghomi et al. 1986) as initial values and introduced the methyl-group force field (Susi and Ard 1975) in the C5-position and also the supplementary force constants which taken into account the H → C replacement in the N1-site. Then, the force constants have been slightly refined around their initial values in order to obtain a good agreement for 2′-dT and its N3-deuterated analog wavenumbers (Table 1 a). As far as the adenine-residue is concerned, the stretching and bending force constants; i.e. diagonal terms of the F matrix, are those adopted by Majoube (1985) in his recent normal coordinate analysis. Unfortunately, non-diagonal valence force constants were not available and our preliminary calculations with only Majoube's diagonal force constants gave a very poor agreement with the experimental results especially with those arising from the C8-deuterated analog of 2′-dA.

We have therefore introduced a reasonable set of interaction force constants (Table 1 b) and refined them in order to improve the agreement between the experimental and calculated results. Sugar force constants are those used in our previous calculations on 5′-dGMP and 2′-dC (Ghomi and Taillandier 1985; Letellier et al. 1986).

Cartesian displacements of the vibrating atoms, i.e. elements of the L_x matrix, have been transferred to a DPS 6/96 CII-Honeywell Bull computer connected to a SE-293 BBC plotter in order to draw the molecular deformations during the selected characteristic vibration modes.

Results and discussion

FT-IR and off-resonance Raman spectra of 2′-dT ($\lambda_{\text{exc.}} = 514.5$ nm) in the solid state, have been performed by Mathlouthi et al. (1984) and resonant Raman spectra of 2′-dT and 2′-dA ($\lambda_{\text{exc.}} = 257$ nm) in solution (pH 7) studied by Jollès et al. (1985). The

Table 1 a. Force constants of the thymine-residue. Bond-stretch and stretch-stretch interaction force constants are in mdyne/A. Angular bending, bend-bend interaction and torsion force constants in mdyne/A. Stretch-bend interaction force constants are in mdyne. The notations and symbols are those used by Susi and Ard (1975). (*a*) Values used in our former calculations on uracil and its ^{18}O-derivatives (Ghomi et al. 1986); (*b*) Present work; (*c*) Susi and Ard (1975)

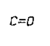
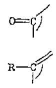
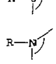
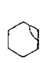
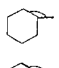
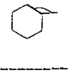
Diagonal force constants					
Bond-stretch F.C.			Angular bending F.C.		
	(a)	(b)		(a)	(b)
C1′-N1		3.96	C1′-N1		1.909
N-H	5.568	5.568	N-H	0.412	0.403
C-H	5.292	5.292	C-H	0.409	0.475
C-N	6.38	6.28	C=O	1.213	1.213
C-C	6.202	6.37			
C=O	11.00	10.70		1.647	1.957
C=C	9.00	9.00		0.621	0.621
Torsion F.C.				0.808	1.008
C5-CH3	0.10				
Non-diagonal force constants					
Str. bend. interactions			Str. Str. interactions		
	(a)	(b)		(a)	(b)
	0.614	0.90	ortho	1.044	1.200
			meta	-0.356	-0.356
			para	0.557	0.557
	0.421	0.421	C=O, C=C	-0.226	-0.226
			C=O, ring	1.391	1.191
	0.177	0.197			
Methyl-group force constants					
	(c)	(b)		(c)	(b)
C5-CH3 st.	4.889 ± 0.178	5.189	C5-CH3	1.014 ± 0.078	1.014
Symm. st.	4.956 ± 0.034	4.956	Symm. bend.	0.569 ± 0.009	0.445
Asymm. str.	4.746 ± 0.032	4.746	Asymm. bend.	0.538 ± 0.009	0.405
			Rocking	0.663 ± 0.021	0.493
C-CH3 Str., Ring str.	0.471 ± 0.115	0.471	C-CH3 Str., Symm. bend	-0.465	-0.465

Table 1 b. Non-diagonal force constants of the adenine-residue. The diagonal force constants are those used by Majoube (1985) in his normal coordinate analysis of the adenine-residue (py): pyrimidic ring; (im): imidazolic ring

Adenine-residue Non-diagonal force constants			
Str.-Str. F.C. (mdyn/A)		Str.-bend. F.C. (mdyn)	
C=C, C-C(py)	0.500	C-N, DCH(py)	0.200
C-C, C=N(py)	0.500	C=N, DCH(py)	0.200
C=N, C-N(py)	0.651	C=C, DR (py)	0.810
C=C, C-N(py)	0.500	C-C, DR (py)	0.448
CC, CN(im, py)	0.600	C=N, DR (py)	0.322
CN, CN(im, py)	0.600	C-N, DR (py)	0.631
C6-N6, ring	0.501	C6-N6, DR(py)	0.431
C8=N7, C2=N3	-0.100	C=N, DCH(im)	0.080
C8=N7, C4=C5	0.100	C-N, DCH(im)	0.400
C2=N3, C4=C5	0.200	C=C, DR(im)	0.530
Bend.-bend. F.C. (mdyn.A)		C=N, DR(im)	0.631
N7CH, N3CH	0.300	C-N, DR(im)	0.531
N7CH, N1CH	-0.1210	C1′N9, DR(im)	0.530
N9CH, N3CH	0.290	CC, DR(im, py)	0.260
N9CH, N1CH	-0.1501	CN, DR(im, py)	1.230

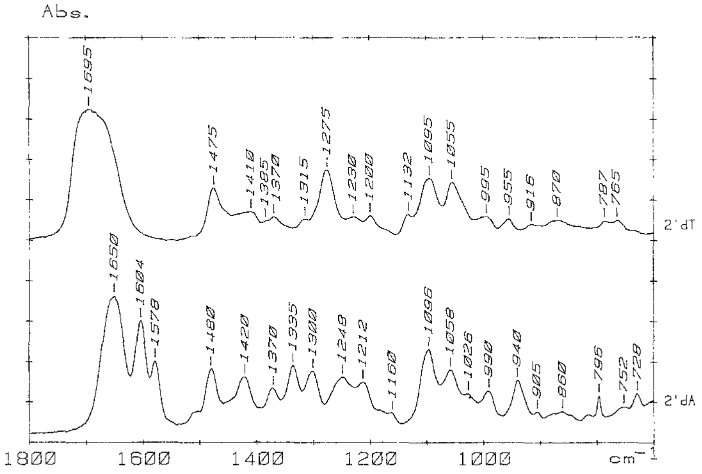


Fig. 1. Infrared absorption spectra of the thin films of amorphous 2′-deoxythymidine (*up*) and 2′-deoxyadenosine (*down*)

infrared spectra of the thin films of amorphous 2′-dT and 2′-dA recorded in our laboratory are shown in Fig. 1 for the spectral region between 1800 and 700 cm^{-1}. The above experimental data together with the 2′-dT infrared spectrum in D_2O (N3-deuterated) and that for the 2′-dA: C8-deuterated derivative (spectra not shown) have been utilized for adjusting the force constants as well as for comparison with the calculated results (Tables 2, 3 and 4).

A. 2′-deoxythymidine and its N3-deuterated analog

Table 2 compares the calculated and experimental wavenumbers for 2′-deoxythymidine between 1800 and 650 cm^{-1}. In Table 4, the comparison was made between the experimental and calculated infrared band-shifts (amorphous sample) upon N3-deuteration.

The majority of the infrared and Raman bands in the 1800–1270 cm^{-1} region originate from the thymidine-residue. It is obvious that because of the crystalline field and Fermi-resonance effects the number of peaks observed in solid samples is larger than that predicted from the normal coordinate calculations on an isolated molecule. So, we have made our assignments on the basis of the experimental results arising from aqueous or amorphous samples. Between 1800 and 1600 cm^{-1}, the vibrational spectra mainly arise from the C=O and C=C bond-stretch modes. They give rise to an intense and non-resolved infrared band situated at 1695 cm^{-1}, not affected by N3-deuteration. The intense infrared band situated around 1475 cm^{-1} (Fig. 2) is that observed in poly d(A–T) · poly d(A–T) spectra for both right- and left-handed conformations (Adam et al. 1986a, b). In contrast, the vibration mode around 1410 cm^{-1} (Fig. 2) shifts from 1425 cm^{-1} to 1401 cm^{-1} in poly d(A–T) · poly d(A–T) infrared spectra upon the $B \rightarrow Z$ transition. The sugar-pucker CH2-scissoring mode situated around 1315 cm^{-1} in 2′-dT (Fig. 2) is found to be altered by the right → right transition of poly d(A–T) · poly d(A–T) showing an infrared band-shift from 1327 cm^{-1} (*B* form) to 1317 cm^{-1} (*A* form). The intense infrared band around 1275 cm^{-1} (Fig. 2) arises from the thymine-residue and is sensitive to N3-deuteration which makes it shift toward higher wavenumbers (Table 4).

The good agreement between the experimental and calculated wavenumbers situated below 1250 cm^{-1}, corresponding mainly to the sugar vibration modes, confirms the validity of the 2′-deoxyribose force field. In Fig. 2 we have illustrated graphically the sugar modes responsible for the two intense infrared bands situated at 1095 and 1055 cm^{-1} (Table 2).

The infrared band at 765 cm^{-1}, also observed in polynucleotide spectra (Adam et al. 1986a, b), has been assigned to the thymine-residue out-of-plane vibrations by our very recent calculations (Letellier et al. 1987a).

B. 2′-deoxyadenosine and its C8-deuterated analog

In Table 3, a comparison has been made between the experimental and calculated wavenumbers of 2′-dA in the 1800–700 cm^{-1} spectral region. In Table 4 the calculated wavenumber-shifts are compared to the infrared band displacements upon C8-deuteration in the adenine residue.

On the basis of the calculated results, the infrared bands situated at 1650, 1604, 1578 and 1510 cm^{-1} involve mainly the pyrimidic ring vibrations (Fig. 3). The last one gives rise to an intense Raman peak observed in the *A* and *B* forms of poly d(A–T) · poly d(A–T) (Thomas and Benevides

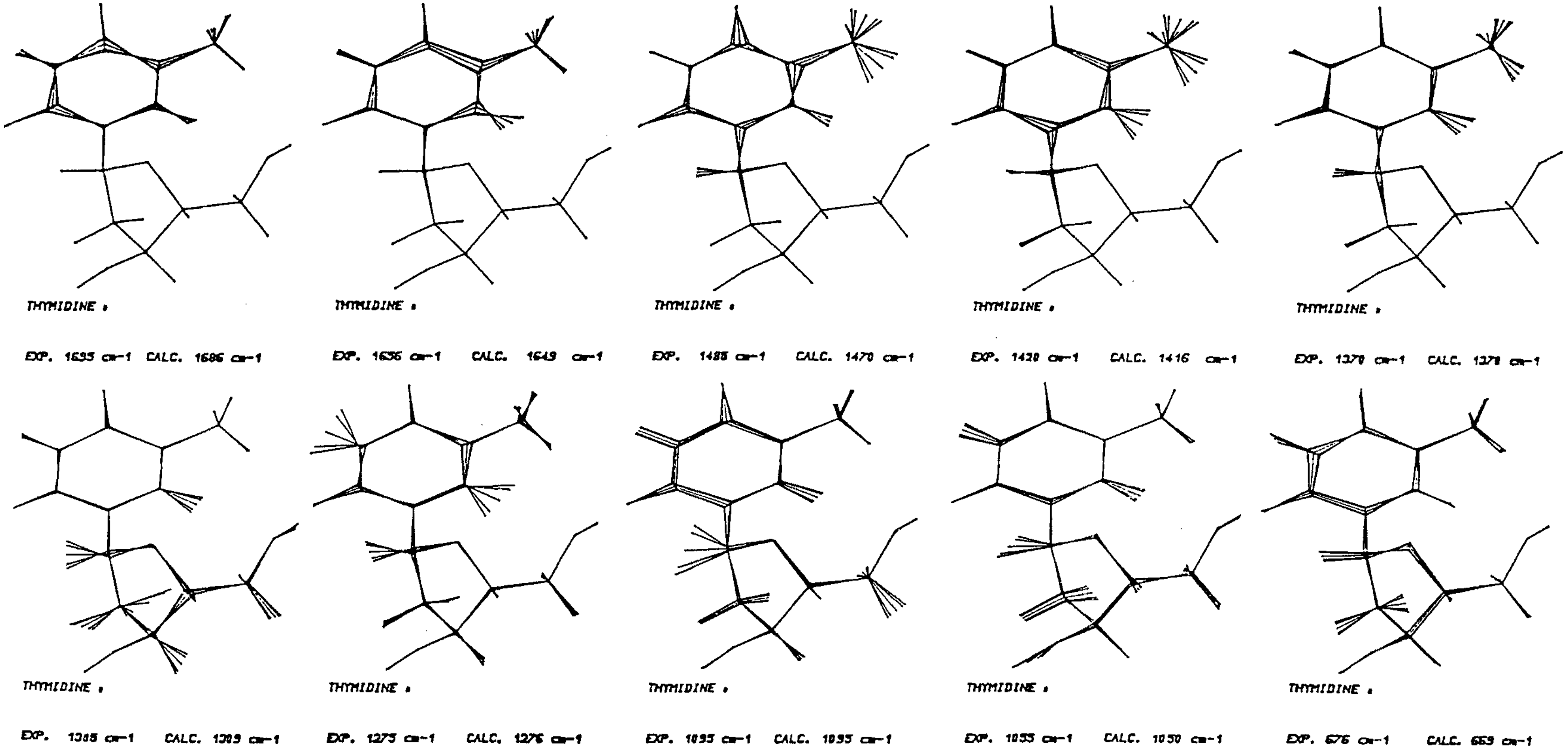


Fig. 2. Representation of the characteristic vibration modes of 2′-deoxythymidine. Experimental wavenumbers arising from the Raman or infrared spectra are also reported. See also Table 2

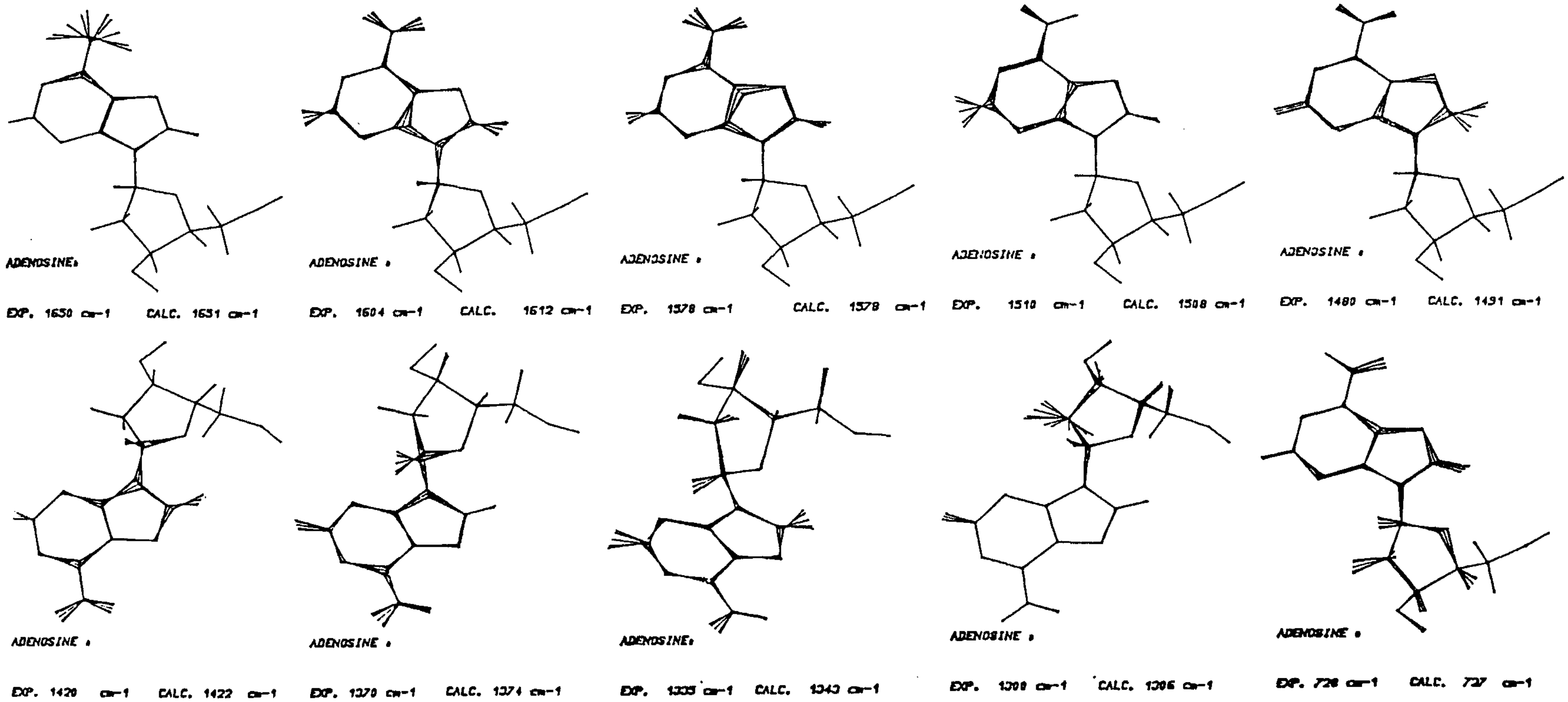


Fig. 3. Representation of the characteristic vibration modes of 2′-deoxyadenosine. Experimental wavenumbers arising from the infrared spectra of amorphous samples are also reported. See also Table 3

Table 2. Comparison between the experimental and calculated results for 2′-deoxythymidine. (*a*) The wavenumbers (cm^{-1}) of 2′-dT neutral solution resonant Raman spectrum ($\lambda_{exc.}$ = 257 nm) (Jollès et al. (1985); (*b*) Off-resonance Raman peak positions of the crystalline 2′-dT ($\lambda_{exc.}$ = 514.5 nm) (Mathlouthi et al. 1984); (*c*) FT-IR peak positions of the crystalline 2′-dT ($\lambda_{exc.}$ = 514.5 nm) (Mathlouthi et al. 1984); (*d*) I.R. wavenumbers of the thin films of amorphous 2′-dT (see also Fig. 1). The assignments are based on the internal coordinates for which the potential energy distribution (PED in per cent) is reported

EXPERIMENTAL				CALCULATED	
Raman		IR		FREQ.	ASSIGNMENTS (PED %)
		1715^c	1705^c	1756	C2=O2 (49);C4=O4 (25)
			1695^d		
				1686	C4=O4 (35);C2=O2 (19);C5=C6 (12)
1656^a	1666^b	1665^c		1649	C5=C6 (41);C4=O4 (21)
	1642^b				
1476^a	1486^b	1482^c	1475^d	1470	C4-C5 (24);N1-C2 (13)
	1460^b	1460^c			
	1440^b	1440^c		1443	CH3 - asymmetric deformation (85)
	1408^b	1415^c	1410^d	1416	N1-C6 (24);C1'-N1 (10);C5C6H (9); N1C6H (7)
		1405^c			
	1392^b	1392^c	1385^d	1388	CH3 - symmetric deformation (39); C1'-N1 (8)
1372^a	1368^b	1365^c	1370^d	1370	CH3 - symmetric deformation (19); C2-N3 (10);C5-CH3 (8);N1-C6 (6)
	1326^b	1340^c		1325	HC2'H (19);C4'-O1' (10); C4'-C5' (9);C1'-O1' (9)
		1320^c	1315^d		
				1309	HC2'H (38);C4'-O1' (6);C4'-C5' (6)
		1292^c		1303	C4'-C5' (10);N3-C4 (9);N1C1'H (7); C5C6H (6)
	1282^b	1275^c	1275^d	1276	CN3H (35);C5-CH3 (14);N1C6H (8); C5C6H (6)
		1255^c		1255	C3'-O3' (13);C4'-O1' (8); C1'-O1' (7);HC3'O3' (7)
				1243	C5'O5'H (64);HC5'H (7);C5'-O5' (7)
				1228	HC5'H (52);O5'C5'H (12)
1234^a	1232^b	1225^c	1230^d	1222	CN3H (23);C5-CH3 (23);C2-N3 (6)
	1202^b	1200^c	1200^d	1210	C3'O3'H (30);C2'-C3' (12); C3'-O3' (9);C3'-C4' (8)
				1188	C1'-C2' (11);O1'C4'H (10); C1'-O1' (9);C2'C1'H (7)
	1176^b	1175^c		1184	O3'C3'H (20);C4'-C5' (20); C3'-C4' (14);C2'C3'H (6)
				1157	C4'C5'H (16);C4'-C5' (13); O5'C5'H (10)
	1124^b	1125^c	1132^d	1133	N1-C2 (12);C4'C5'H (10); N3-C4 (10);C4-C5 (8)
	1104^b	1100^c		1113	O1'C4'H (35);O1'C1'H (11); C5'C4'H (10);C1'-C2' (8)
			1095^d	1095	C2-N3 (16);N3-C4 (15);N1-C6 (9) C2'C1'H (11);O1'C1'H (10)
	1068^b	1070^c		1064	O1'C1'H (14);N1C1'H (13); C4'-C5' (9);C3'-O3' (8)
	1054^b		1055^d	1050	C3'O3'H (28);O1'C1'H (12); C2'-C3' (11);C2-N3 (7)
	1028^b	1030^c		1033	C1'C2'H (24);C3'-C4' (10); C3'-O3' (7)
	1020^b			1022	C2'-C3' (16);C3'O3'H (12); O1'C1'H (8)
		1012^c			
	1006^b	1005^c	995^d	993	C3'C4'H (15);C5'C4'H (12); O5'C5'H (11);C5'-O5' (8)
	976^b	975^c		982	CH3 - rockins
	964^b	960^c	955^d	958	C5'-O5' (14);C5'C4'H (11)
				949	O5'C5'H (21);C4'C5'H (20); C3'C4'H (12);C5'-O5' (19) C2'-C3' (9)
				936	C5'-O5' (28);C3'C2'H (16); C1'C2'H (13)
		910^c	916^d	919	C4'C5'H (29);O5'C5'H (26); C4'-O1' (9)
	902^b	900^c			
		883^c		886	C3'-O3' (26);C3'C2'H (14); C5'-O5' (12);C2'-C3' (9)
	874^b	872^c	870^d	885	C5-CH3 (16);C4-C5 (12)
				864	C4'C3'H (37);C2'C3'H (33)
	854^b	852^c		855	C4'C5'H (29);O5'C5'H (20); C4'-O1' (18)
				822	C2=O2 (14);N1-C6 (12); C4-C5 (8);N1-C2 (8)
	794^b	792^c	787^d	773	C1'-N1 (14);C5-CH3 (7); N1C1'O1' (7)
	738^b	734^c		725	C1'-O1' (15);N3C4O4 (8);
				707	C3'C4'O1' (16);C3'C2'H (14); C2'C3'C4' (11)
	676^b	672^c		669	C2N3C4 (10);N3C4C5 (9); C2'C1'O1' (9);C1'O1'C4' (7)

1985). The 1480 cm^{-1} infrared band has an imidazolic character and is sensitive to C8-deuteration. In polynucleotide infrared spectra this mode is superimposed on that arising from the thymine residue (Table 2, Fig. 2). The vibration mode at 1,420 cm^{-1} is also shifted by C8-deuteration and is found to be altered by both the right → right and right → left-handed conformational transitions (Adam et al. 1986a, b). As in the case of poly d(G–C) · poly d(G–C) (Ghomi et al. 1984) the vibration mode involving mainly the C1′–N9 bond-stretch vibration is taken to be one of the most important infrared markers for detecting the right → left-handed transition of poly d(A–T) · poly d(A–T). The present calculations assign this vibration mode to the 2′-dA infrared band situated at 1,370 cm^{-1} (Fig. 3, Table 3).

Finally, the vibration mode at 1335 cm^{-1} (Raman and infrared spectra) altered by C8-deuteration (Table 4) is found around 1340 cm^{-1} in both right- and left-handed forms of poly d(A–T) · poly d(A–T).

Below 1250 cm^{-1}, the calculated results take account of the infrared modes arising from the sugar vibration modes.

It should be mentioned that the narrow infrared band situated at 796 cm^{-1} is assigned to an adenine-residue out-of-plane vibration mode by our recent calculations (Letellier et al. 1987b).

Conclusion

As shown above, our non-redundant valence force field allows us to assign the most characteristic

Table 3. Comparison between the experimental and calculated results for 2′-deoxyadenosine. (*a*) Resonant Raman peak positions ($\lambda_{\text{exc.}} = 257$ nm) from 2′-dA neutral solutions (Jollès et al. 1984); (*b*) I.R. wavenumbers of the thin films of amorphous 2′-dA (see also Fig. 1). The assignments are based on the internal coordinates for which the potential energy distribution (PED in per cent) is reported

EXPERIMENTAL		CALCULATED	
Raman (a)	IR (b)	FREQ.	ASSIGNMENTS (PED %)
	1650	1651	HN6H (39);C6-N6 (24);C6N6H (22)
1630 (sh)			
	1604	1612	C4-N9 (18);N3-C4 (18);C2=N3 (9)
1584	1578	1578	C5-C6 (31);C4=C5 (12);C5-N7 (6)
	1510	1508	NC2H (26);C2=N3 (15);N1-C2 (14); C5-C6 (12)
1484	1480	1491	NC8H (27);N7=C8 (25);C2=N3 (12); N3-C4 (11)
		1452	N1=C6 (46);C6-N6 (11)
1424	1420	1422	C8-N9 (24);C1'-N9 (15)
	1370	1374	C1'-N9 (26);C6-N6 (11)
		1343	NC8H (13);NC2H (7);C2=N3 (6)
1332	1335		
		1324	C4'-C5' (16);C4'-O1' (14)
	1300	1306	HC2'H (48);C1'C2'H (11)
	1260 (sh)	1264	C1'-O1' (16);C3'-O3' (12)
1248	1248	1244	HC5'H (19);NC2H (10);N9C1'H (9)
		1230	HC5'H (44);NC8H (9)
		1215	NC8H (23);N7=C8 (17)
	1212		
		1206	C3'-C4' (19);O3'C3'H (12); C4'-C5' (9)
		1192	C4'-C5' (17);O3'C3'H (13); C1'-C2' (11);C2'C1'H (10)
	1180 (sh)	1183	N1-C2 (31);C2=N3 (6)
	1160 (sh)	1164	C4'C5'H (21);C2'-C3' (15); C4'-C5' (7)
		1138	C3'-O3' (20);O1'C4'H (12); C4'-C5' (12)
1100 (sh)		1106	O1'C1'H (18);C2'C1'H (17); O1'C4'H (11);C3'-O3' (9)
	1096	1097	O1'C4'H (21);O5'C5'H (19); C4'-C5' (7);O1'C1'H (6)
		1078	C1'-C2' (10);O1'C1'H (7); C2'-C3' (7)
		1067	N1-C2 (17);C6-N6 (15); C2N3C4 (11);N3-C4 (11)
	1058	1061	NC2H (13);C5-N7 (8);C4-N9 (7); C4=C5 (6)
		1053	C5'-O5' (34);C5'O5'H (15)
	1026	1026	O5'C5'H (13);O1'C4'H (10); O1'C1'H (10);C4'-O1' (10)
		1002	C1'-C2' (9);N9C1'H (7); C3'C4'H (6)
		999	C6N6H (46);N1=C6 (15);N3-C4 (7)
	990		
		976	C3'-C4' (27);C3'O3'H (23)
		954	C3'C4'H (22);C5'C4'H (14); C5'-O5' (11)
	940	944	C3'C2'H (25);C5'-O5' (9); C3'C2'H (8)
		931	C5-N7 (29);N7=C8 (7)
		925	C4'C5'H (28);O5'C5'H (17); C5'-O5' (15)
	905	905	C4=C5 (16);C4-N9 (15)
		871	C2'C3'H (37);C4'C3'H (30)
	860	861	C4'C5'H (25);C4'-O1'(20); O5'C5'H (17)
		837	C3'O3'H (32);C3'-O3' (15)
	815	813	C5'O5'H (60);C5'-O5' (9)
	752	775	C1'-N9 (14);C8-N9 (12)
	728	727	C1'-O1' (12);C1'O1'C4' (8); C5-N7 (7);C6-N6 (4);C4=C5 (3) C4-N3 (2);C8=N7 (2);N3=C2 (2) C4-N9 (2)
		714	C3'C4'O1' (13);C2'C3'C4' (11); C3'C4'H (7)
		688	C2N1C6 (15);N3-C4 (13);N3C4C5 (7)

Table 4. Effect of deuteration in N3-site of the thymine residue in 2′-dT and in C8-site of the adenine-residue in 2′-dA. The calculated shift (in cm^{-1}) is reported in parenthesis in front of each characteristic wavenumber. In the same manner the I.R. (amorphous samples) band shifts are indicated. -- non-measurable, ** I.R. bands appearing after deuteration

2'-deoxythymidine		2'-deoxyadenosine	
exp.	cal.	exp.	cal.
1695 (--)	1756 (0)	1650 (0)	1651 (0)
	1686 (-2)	1604 (-1)	1612 (-8)
1475 (0)	1470 (-1)	1578 (-3)	1578 (-5)
1440**	1443 (0)	1510 (--)	1508 (-1)
1410 (-5)	1416 (-1)	1480 (-17)	1491 (-30)
1385 (0)	1388 (-2)	1420**	1452 (-29)
1370 (0)	1370 (-2)	1420 (-15)	1422 (-7)
1315 (--)	1325 (-1)	1370 (-3)	1374 (-1)
	1309 (0)	1335 (-10)	1343 (-13)
1275 (+25)	1276 (+24)	1300 (-2)	1306 (-1)
1230 (+10)	1222 (+16)	1248 (-15)	1244 (-18)
1200 (0)	1210 (+1)	1212 (--)	1215 (-232)
1132 (+18)	1133 (+9)		
1095 (+3)	1095 (+5)	1096 (0)	1097 (0)
1055 (--)	1050 (-7)	940 (-4)	944 (0)
870 (--)	885 (-55)	728 (-5)	727 (-8)

vibration modes of 2′-dT and 2′-dA. It is known that the conformation of both these nucleosides are modified when they are found in the right- and left-handed DNA double-helical chains. Consequently, the vibration modes associated with them will be altered by the conformational changes involved with the right → right or right → left-handed transitions. In order to interpret this kind of spectral evolution the presently proposed force field seems to be quite promising.

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