DISPLACEMENTS OF BACKBONE VIBRATIONAL MODES OF A-DNA AND B-DNA

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ABSTRACT We display the displacement vectors or eigenvectors of calculations of the A- and B-DNA backbones. These calculations are based on a refinement scheme that simultaneously fit several backbone modes of A-DNA, B-DNA, and A-RNA. We discuss the role of symmetry operations in mode calculations and the relevance of these displacement vectors to the interpretation of linear dichroism measurements performed on the A- and B-DNA helix.

Linear dichroism data on nucleic acids have been interpreted in terms of structural details of the backbone phosphate oxygen displacements during normal mode vibrations (1, 2). The interpretation of the infrared dichroism has led to structural parameters disagreeing with x-ray scattering data (3).

The structural interpretation of the dichroism data has been criticized by Beetz et al (4). Their criticism notes that a PO_4 moiety, when incorporated into a nonsymmetric structure like a nucleic acid backbone, no longer vibrates in patterns displaying the high symmetry characteristic of the free ion or simple compounds. Furthermore, the mechanical coupling of the PO_4 to the rest of the nucleic acid molecule through the covalent bonds that bind the moiety into the backbone communicates vibrational energy to the rest of the polymer. Hence atoms other than those of the PO_4 group may participate in the vibrational motion excited by the IR photons, and the partial charges on these other atoms contribute to the observed dipole moment of the excited line. This additional contribution bears no simple relation to the PO_4 vibrations, either in magnitude or direction, and so serves to confuse the interpretation of the observed dichroism. We present the numerical results of a normal mode vibration calculation on the backbone of A-DNA and B-DNA. The eigenvectors so obtained show that both criticisms are well founded.

Double helical DNA composed of homopolymer chains—that is, all base pairs identical—and of infinite length possesses a screw-axis operator that is a true symmetry operator. The screw-axis operation rotates the helix and shifts the helix along its axis such that the nth unit cell of two bases and the associated backbone atoms assume the previous positions of the $n + 1$ unit. An additional c_2 operation exists that interchanges the backbones but also interchanges the complementary base pairs and is therefore not a true symmetry operation. The screw-axis operator and its higher powers form an Abelian group if periodic boundary conditions are assumed. No other true symmetry operators exist for the simple homopolymer double helix. Therefore, all the irreducible representations are one-dimensional and characterized by simple phase shifts of the displacement from one unit cell to the next. This is shown in detail by Higgs (5).

The absence of higher symmetry means that the actual displacements for each vibrational

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mode must be determined by the diagonalization of the secular matrix. These displacements are found as eigenvectors of the diagonalization. No further symmetry-related block diagonalization is possible.

Polar moments are associated with these vibrational modes because the atoms have unbalanced charges; the polar moment interacts with electromagnetic fields giving rise to electric dipole IR absorption. This is usually the dominant term for IR absorption. These polar modes also can be analyzed with the help of group theory and must conform to irreducible basis functions. For these Abelian groups this means that both displacement eigenvectors and polar moment vector have the same phase shift, θ, from one unit cell to the other as this is the only symmetry-determined part of the problem. The vectors within a unit cell of the displacement and the vector within a unit cell of the polar moments need not be colinear and would only be colinear by some accident, as, for example, if all effective charges on the various atoms were equal.

The orientation of the polar moment within a unit cell of double helical DNA must be calculated rather than inferred from group theory. This is because no further symmetry information is available to reduce the matrix describing a single unit cell. The polar moments arise from the vibrational modes and have both the same frequency and θ dependence, but the polar moment is not necessarily a simple function of the vibrational displacements.

In Fig. 1 we show the DNA backbone-ribose model we adopted in this investigation. All the hydrogen atoms are assumed to be rigidly attached to their bonded atoms following common usage. The base atoms were neglected assuming relatively little interaction between the backbone and the bases for the relevant modes. More elaborate calculations (6) have confirmed the validity of this approximation.

We used the atomic coordinates as given by Arnott et al. (7) in evaluating the matrix, D, that transforms the mass-weighted cartesian coordinates into the internal coordinates. F is the force constant matrix in internal coordinates. The product matrix D^TFD was then diagonal-

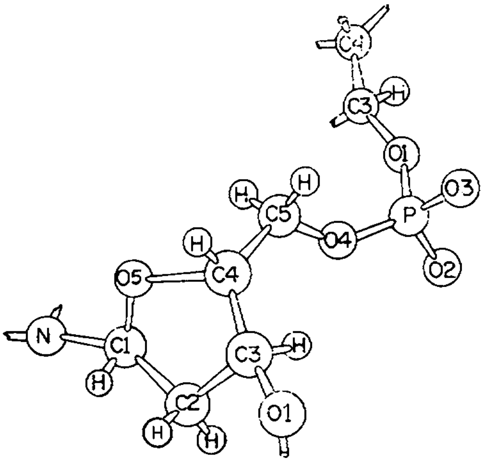

FIGURE 1 Atoms of the DNA backbone chain shown for one full unit and part of a second. Atom N is part of a base unit.

TABLE I
SOME EIGENVECTORS OF A-DNA BACKBONE

ν(Cm^{-1})....	8.0720E+02	8.3195E+02	8.8584E+02	9.7339E+02	9.8939E+02	1.0836E+03	1.1045E+03	1.1227E+03	1.1439E+03	1.1879E+03	1.2099E+03	1.2934E+03
						Eigenvectors						
C1*Δx	1.4450E-02	-1.3569E-02	-4.7680E-02	8.5710E-02	4.6536E-02	2.9552E-02	-2.6547E-02	1.7827E-01	1.0973E-02	1.9759E-02	-2.2492E-03	7.3358E-02
Δy	4.1311E-02	-1.2668E-01	-7.6843E-02	2.3099E-01	-2.9287E-01	-3.8620E-02	1.1512E-01	-5.3830E-01	1.6179E-01	-3.6042E-02	1.4477E-02	-2.1368E-01
Δx	4.7725E-02	2.4406E-01	1.9615E-01	-5.4874E-01	-2.7295E-02	-4.8437E-02	-2.3107E-03	-2.3194E-01	-1.6360E-01	-1.5175E-01	-2.5696E-02	-4.4160E-02
C2	-1.7642E-01	7.2111E-02	1.6288E-01	-4.5538E-02	2.1203E-01	-8.2059E-02	6.9384E-02	-1.9737E-01	5.2046E-02	8.9628E-02	2.4685E-02	-1.2303E-02
	2.8226E-01	1.9750E-02	-1.2214E-01	-7.6247E-02	-3.2003E-01	9.5751E-02	-9.9863E-02	2.2371E-01	-1.5184E-01	-1.1394E-01	-3.4108E-02	4.8621E-02
	2.0951E-02	-1.3494E-01	-2.0509E-01	5.2961E-01	5.9838E-02	4.0264E-02	2.2783E-02	1.4355E-01	1.5397E-01	2.2109E-02	-2.5434E-03	1.9671E-01
C3	2.5650E-01	-1.6160E-01	-3.2576E-01	-2.5245E-01	-2.7193E-01	6.7083E-03	-2.3181E-02	1.6936E-01	1.0816E-01	-1.3864E-01	-1.7903E-02	3.9657E-02
	1.0667E-01	-1.2555E-01	-9.8880E-02	-1.7469E-01	3.6457E-01	-2.3932E-01	1.7478E-01	-2.4614E-01	2.8173E-01	3.7654E-01	1.0659E-01	1.6787E-01
	-4.7128E-02	-3.1282E-01	-5.1229E-02	-3.6055E-02	-1.3467E-02	-6.0409E-02	-7.9411E-02	6.9416E-02	-3.4217E-01	3.6123E-01	7.9349E-02	-6.0039E-01
C4	4.5905E-02	2.7150E-01	4.6207E-01	1.5619E-01	-2.0103E-01	1.7509E-01	-3.4162E-02	-3.7226E-02	3.6409E-02	1.6163E-01	2.0623E-02	1.2694E-01
	-8.1706E-02	1.2041E-01	4.4670E-02	6.6406E-02	4.0217E-01	1.6084E-01	-6.1217E-02	2.6555E-02	4.1104E-02	-5.9149E-01	-1.1830E-01	-2.8743E-01
	-5.4663E-02	-4.4325E-02	-2.1312E-02	2.2528E-01	4.8913E-02	-8.0956E-02	2.1406E-03	-2.9375E-01	-5.0144E-01	-1.7285E-01	-5.6958E-02	4.3812E-01
05	2.1015E-02	-5.1384E-02	-7.9687E-02	1.2020E-02	-5.1795E-02	-3.4547E-02	1.8566E-02	-1.3282E-01	-5.5635E-02	-6.4391E-02	-9.9555E-03	-3.7885E-04
	-1.2545E-01	-4.4046E-02	1.0451E-01	-1.5819E-01	2.3777E-01	-4.9594E-02	-6.9425E-02	4.0855E-01	-2.1261E-01	2.1730E-01	2.0111E-02	2.9228E-01
	-1.2793E-02	2.7863E-01	1.2794E-01	8.8552E-02	4.2638E-02	1.2553E-01	1.2762E-02	2.1625E-01	4.4686E-01	8.8742E-02	2.8641E-02	-1.7455E-01
C5	-9.2321E-02	-2.7727E-02	-1.3983E-01	3.9164E-02	1.2665E-01	-5.3684E-01	1.8811E-01	1.8131E-01	3.6230E-03	-2.6289E-01	-3.0069E-02	-1.2646E-01
	2.5001E-01	3.1117E-01	-2.8622E-02	1.9267E-02	-4.2738E-01	-2.4548E-01	8.4741E-02	6.3979E-02	-9.4487E-04	1.2059E-01	5.5256E-02	4.0253E-02
	3.5664E-02	-2.2376E-02	-1.3719E-02	-5.5105E-02	-2.7268E-02	-3.2796E-02	6.7024E-03	9.4395E-02	4.7406E-02	7.2690E-03	-4.2060E-03	-4.9374E-02
P	5.9447E-02	-2.3924E-01	2.6083E-01	9.4132E-03	-5.5399E-02	1.3482E-02	1.4278E-01	5.3909E-02	-1.3137E-02	-1.2381E-01	4.1161E-01	1.3210E-02
	6.5087E-03	2.6939E-01	-2.4165E-01	-1.2582E-03	5.2995E-02	4.7976E-02	-6.8924E-03	-1.6739E-02	-4.4351E-02	-5.8354E-02	4.9455E-01	5.4285E-03
	2.6217E-01	1.3513E-01	-3.1176E-03	3.1392E-02	3.0172E-02	1.5367E-01	4.6894E-01	5.9223E-02	-1.1627E-01	4.0601E-02	-1.3321E-01	-3.1079E-02
01	-9.8268E-02	5.4142E-02	1.0615E-01	1.1147E-01	5.5571E-02	1.0268E-02	-2.3578E-02	8.8747E-04	-1.5056E-01	8.2772E-02	-4.9386E-03	-1.3286E-01
	-4.3068E-01	-3.1510E-01	2.7270E-01	9.0134E-02	-1.6726E-01	7.2555E-02	-8.4111E-02	9.1140E-02	-3.1326E-02	-7.0302E-02	-4.1061E-02	-6.8375E-02
	-2.5248E-01	-3.6751E-01	1.1018E-01	-2.9041E-01	-1.5152E-01	-1.8082E-03	-2.1724E-03	-1.2795E-02	3.6392E-01	-1.9995E-01	-2.7069E-02	2.5124E-01
02	-7.2974E-02	-2.3780E-02	-4.4887E-02	-4.3608E-02	-1.2532E-02	9.7546E-02	2.2072E-01	1.8604E-02	-1.5452E-02	4.2751E-02	-2.1579E-01	-1.5756E-03
	-1.4158E-01	-1.6350E-02	-4.4760E-02	-4.0544E-02	-2.4704E-02	1.2314E-01	3.3113E-01	3.4543E-02	-3.8317E-02	6.6498E-02	-3.1558E-01	-1.2436E-02
	1.1308E-01	7.0082E-03	6.3286E-02	6.3157E-02	3.0646E-02	-1.3477E-01	-3.7251E-01	-3.6315E-02	2.5741E-02	-6.6036E-02	3.4604E-01	2.3634E-03
03	1.0282E-01	7.4694E-02	2.3507E-02	4.3140E-02	4.3346E-03	-2.1609E-01	-3.4848E-01	-4.4975E-02	6.8867E-02	7.3072E-02	-3.4532E-01	-4.9132E-03
	1.2758E-01	4.0209E-02	1.9699E-02	3.3911E-02	1.0355E-02	-1.7789E-01	-3.3506E-01	-4.8382E-02	6.5412E-02	7.2249E-02	-3.2543E-01	-2.3819E-03
	3.5224E-02	3.2352E-02	1.9280E-03	1.7545E-02	-4.0901E-04	-1.1266E-01	-1.7553E-01	-2.2849E-02	3.7337E-02	3.6155E-02	-1.7003E-01	-7.2049E-04
04	-2.3711E-01	-8.4597E-03	-3.7140E-01	-1.3452E-01	9.7681E-02	5.2015E-01	-2.5471E-01	-1.6970E-01	3.8174E-03	1.3497E-01	-5.2098E-03	4.3663E-02
	4.3299E-01	-2.8871E-01	2.6025E-01	2.3723E-03	1.2694E-01	2.0832E-01	-3.1312E-02	-4.7355E-02	1.2974E-03	7.0858E-03	-4.3951E-02	7.6922E-03
	-2.5223E-01	1.1085E-01	-2.0572E-01	-4.2790E-02	-1.0158E-03	7.4025E-02	-7.0855E-02	-3.7862E-02	7.7723E-03	2.3991E-02	1.7043E-02	1.3157E-02

Theoretical eigenvectors (normalized) of backbone vibrations in A-DNA. Vibration amplitudes are expressed in cartesian coordinates as indicated for C1. Refer to Fig. 1 for atom labels and to the text for coordinate designations. The theoretical dioxy vibrations are at 1,210 cm^{-1} (antisymmetric) and 1,105 cm^{-1} (symmetric). A symmetric diester vibration falls at 807 cm^{-1}.

*Atom coordinate vibration amplitude (relative).

TABLE II
SOME EIGENVECTORS OF B-DNA BACKBONE

ν(Cm^{-1})....	7.8903E+02	8.3467E+02	8.8625E+02	9.5978E+02	9.9964E+02	1.0581E+03	1.0944E+03	1.1126E+03	1.1601E+03	1.2008E+03	1.2095E+03	1.2305E+03
						Eigenvectors						
C1*Δx	2.8247E-02	-3.4235E-02	4.1185E-03	1.6064E-02	4.2118E-03	-1.0085E-01	-8.3462E-02	5.3188E-02	5.5689E-02	1.3131E-02	1.4573E-02	8.1501E-02
Δy	-1.1451E-02	-3.4812E-01	1.5599E-01	5.7220E-01	-2.0644E-01	1.0607E-01	-1.5273E-02	3.3443E-02	-1.8789E-01	9.1982E-03	-2.6877E-03	1.1991E-01
Δz	3.9054E-02	-4.0193E-02	6.6518E-02	1.5063E-01	2.0940E-02	-3.9657E-01	-3.3558E-01	2.1127E-01	3.0151E-01	6.9140E-02	6.0839E-02	2.9165E-01
C2	-1.6683E-01	-1.0096E-01	1.3959E-01	2.7866E-02	1.2729E-01	9.5586E-02	1.0280E-01	-6.0414E-02	7.8655E-02	-8.2599E-02	2.3721E-02	-4.6225E-02
	-1.3831E-02	2.9309E-02	1.1706E-02	-3.9285E-01	3.7158E-01	-8.4416E-02	1.1049E-02	-3.1122E-03	2.5883E-01	-6.6746E-02	5.3442E-02	3.7088E-02
	-2.4564E-01	-1.8845E-01	3.2410E-01	2.0542E-01	1.5896E-01	1.9683E-01	1.6266E-01	-9.8573E-02	4.4510E-02	6.7807E-04	-1.3568E-02	-1.8549E-01
C3	-1.7037E-01	9.0041E-02	4.9908E-02	-1.3820E-01	-1.4904E-02	-1.7182E-02	-1.9860E-01	1.2150E-01	-2.9517E-01	6.4220E-01	-1.9448E-01	-2.0811E-02
	1.3072E-01	4.9148E-01	-2.3020E-01	2.2086E-01	-3.1662E-01	-2.0873E-02	-6.5731E-02	2.1752E-02	-9.7200E-02	5.4244E-02	-5.9265E-02	-2.2239E-01
	6.2556E-02	-1.6096E-01	-1.5461E-01	-2.8004E-01	-3.0340E-01	-2.5895E-01	-1.0521E-01	4.6981E-02	-3.8126E-01	-2.7828E-01	1.8997E-02	2.9039E-01
C4	-1.8190E-01	2.5430E-01	-3.5187E-01	2.0794E-01	3.6653E-01	7.8536E-03	-1.2525E-01	1.4719E-01	-6.5673E-02	-2.7811E-01	4.4969E-02	-3.3370E-02
	-2.1856E-02	9.4973E-02	-4.4807E-02	-1.5863E-01	9.3926E-02	3.8778E-01	1.8872E-01	-4.6361E-02	-3.0057E-02	8.3819E-02	8.8325E-02	6.2706E-01
	-1.8874E-02	1.7978E-01	-1.9124E-01	-2.8137E-02	-2.9794E-01	1.8878E-01	7.0376E-02	-6.5200E-02	5.5239E-01	2.3493E-01	1.8375E-02	-9.8578E-02
05	3.7819E-02	-3.7907E-02	2.5305E-02	-5.0565E-02	-4.3325E-02	1.2325E-02	3.6112E-02	-3.4335E-02	-2.5829E-02	1.1836E-03	-1.5757E-02	-7.4551E-02
	6.1729E-03	-2.5673E-01	9.0214E-02	-2.5632E-01	-1.1156E-02	-3.1426E-01	-3.9564E-02	-5.1426E-02	3.8504E-02	-6.3309E-02	-6.2163E-02	-4.4319E-01
	1.1044E-01	5.7259E-02	-1.4681E-01	-1.9296E-01	2.5426E-02	2.3154E-01	2.2530E-01	-1.4122E-01	-3.7594E-01	-1.0987E-01	-5.6360E-02	-2.2753E-01
C5	2.2452E-01	-1.3806E-01	9.0269E-03	-6.2102E-02	-2.0740E-01	-1.9382E-01	3.0761E-01	-3.3889E-01	9.5611E-02	2.1328E-01	-1.0770E-02	1.1351E-01
	-4.5647E-02	7.9759E-02	2.8126E-02	6.2200E-02	3.0010E-02	2.1374E-02	-1.2864E-01	1.1601E-01	1.1608E-03	-8.9068E-02	-5.1968E-03	-8.9037E-02
	6.5190E-02	3.1018E-01	2.2690E-01	1.7636E-01	3.1470E-01	-3.1700E-01	1.4535E-01	-2.0458E-01	-1.8088E-01	5.7721E-02	-3.7465E-02	8.5453E-02
P	-1.1913E-01	-1.4067E-01	-2.1885E-01	4.3485E-02	5.7824E-02	1.3809E-02	-1.0380E-01	-1.7832E-01	6.6277E-02	-7.8656E-02	-4.7727E-01	8.0260E-02
	1.8909E-01	7.7604E-02	1.4937E-01	-2.6853E-02	-1.8290E-02	-2.1170E-02	2.2517E-01	3.0468E-01	5.4821E-02	-7.2288E-02	-4.0042E-01	4.8117E-02
	-2.2115E-01	2.4678E-01	2.7102E-01	-5.6616E-02	-9.6095E-02	4.7899E-02	-2.0311E-01	-2.2853E-01	1.9141E-02	-1.0492E-01	-1.5936E-01	4.5914E-02
01	1.6816E-01	1.0841E-01	5.6245E-02	1.1620E-01	-2.0626E-01	-3.1323E-02	1.3206E-01	-1.2757E-01	1.6908E-01	-4.1865E-01	1.4923E-01	2.4049E-02
	-7.4469E-02	-3.2091E-02	5.9835E-02	-3.3645E-02	1.3436E-02	-5.9134E-03	-5.2469E-03	-1.1994E-02	-6.9279E-03	4.5463E-02	-1.1105E-02	1.0118E-02
	5.9147E-01	-2.2854E-01	-2.7328E-01	1.6984E-01	3.5353E-01	8.3886E-02	1.9917E-02	1.0995E-01	2.4431E-02	1.8725E-01	-1.7067E-02	-8.1192E-02
02	8.8771E-02	-9.7541E-03	1.9331E-02	-1.0835E-02	2.6808E-02	5.3487E-02	-1.8012E-01	-1.6536E-01	-3.8604E-02	4.2419E-02	2.0658E-01	-2.7306E-02
	1.4506E-01	-1.1274E-02	3.4019E-02	-2.0313E-02	5.4009E-02	1.1269E-01	-3.9568E-01	-3.6764E-01	-8.4504E-02	8.8698E-02	4.4671E-01	-5.8898E-02
	2.2595E-02	-6.2724E-03	-6.1988E-03	7.0779E-03	-1.2315E-02	-1.1581E-02	4.5602E-02	3.5053E-02	1.4027E-02	-1.9868E-02	-3.9820E-02	6.3972E-03
03	-1.8070E-01	5.1328E-02	-7.2289E-03	-1.2915E-03	-5.0817E-02	-1.5770E-01	3.4109E-01	3.1977E-01	-7.1775E-02	1.0902E-01	4.1854E-01	-6.4661E-02
	-6.1112E-02	-4.5598E-03	-5.0892E-03	-5.7900E-03	-1.5228E-02	-1.8388E-02	5.8025E-02	7.0328E-02	-1.1840E-02	1.6748E-02	8.5682E-02	-1.4678E-02
	-1.3684E-01	8.9504E-03	-5.7553E-03	-1.6999E-02	-3.2165E-02	-8.9471E-02	2.0356E-01	2.1413E-01	-5.0652E-02	7.6161E-02	2.5986E-01	-4.1293E-02
04	2.5553E-01	4.9471E-02	3.6193E-01	-1.5923E-01	-6.5097E-02	2.8982E-01	-1.9920E-01	3.2536E-01	-9.3306E-03	-9.6173E-02	2.1348E-02	-5.5320E-02
	-2.9653E-01	-1.6073E-01	-3.4754E-01	7.9336E-02	1.7411E-02	-1.1743E-01	7.6600E-02	-1.6284E-01	1.3355E-02	4.6405E-02	9.6841E-03	2.0084E-02
	-1.8584E-01	-2.6949E-01	-2.0868E-01	-1.0327E-01	-1.2053E-01	2.5246E-01	-1.6630E-01	2.0996E-01	6.2863E-02	-6.5071E-02	3.4210E-02	-6.2670E-02

Theoretical eigenvectors (normalized) of backbone vibrations in B-DNA. Vibration amplitudes are expressed in cartesian coordinates as indicated for C1. Refer to Fig. 1 for atom labels and to the text for coordinate designations. The theoretical dioxy vibrations are at 1,210 cm^{-1} (antisymmetric) and 1,094 cm^{-1} (symmetric). A symmetric diester vibration falls at 789 cm^{-1}. The line at 835 cm^{-1} has a somewhat better defined antisymmetric diester character than any of the A-DNA lines.

*Atom coordinate vibration amplitude (relative).

ized numerically to obtain the vibrational modes of the backbone-ribose model. Comparisons of the calculated and observed frequencies were shown in an earlier paper (8).

The actual unbalanced charge on each atom will also affect the vibrational modes and this was estimated in previous calculations (8). This effect was found to be small for those modes in the frequency range considered in this paper.

Tables I and II give the maximum displacements of the backbone atoms in x, y, and z directions. The z axis is taken to be the helix axis, and the diad relating the strands of the double helix is along the x axis. Since in the long wavelength limit appropriate to IR absorption all displacements in different cells are in phase, we list in the table only 33 components that correspond to the displacements of the backbone and ribose atoms in one unit cell.

A number of interesting observations can be made about our eigenvalue solutions. The 1,209.9-cm^{-1} line for A-DNA has a large antisymmetric dioxy character, and has total displacements of the $O_2\overline{---}P\overline{---}O_3$ group, which are within 1° of the line connecting the O_2 and O_3 atoms in their unstretched positions. The same is true for the 1,209.5-cm^{-1} line calculated for B-DNA. The lines with symmetric dioxy character have displacements of the O_2PO_3 group lying within 3° of the O_2PO_3 bisector for A-DNA and within 4° of the bisector for B-DNA. The lines with symmetric diester character have displacements that are about 11 and 10° off from the O_1—P—O_4 bisector of A- and B-DNA, respectively. Although the displacements of the atoms in the PO_4 group are not far from those expected from symmetry arguments for an isolated PO_4, all the eigenvectors have considerable displacements over other atoms in the backbone.

The situation is especially unclear for the antisymmetric diester stretch modes. Referring to Table I, where we expect an antisymmetric stretch in the frequency range below 900 cm^{-1}, we see that there are two modes with substantial diester motion at 832 and 886 cm^{-1} but that neither is of markedly antisymmetric character. Furthermore, both modes show equally large or greater ion displacements in the ribose ring than in the backbone oxygens. Substantial displacement of C_1 in the 832 cm^{-1} line suggests that the base atoms may also share substantially in the motion.

Table II shows that this loss of antisymmetric character is not a fluke, but also appears in the B-conformation eigenvectors. The same spread of oscillation amplitude among the atoms of the ribose ring is also observed here, as well as the particular motion of the C_1 atom.

In even the most favorable case among the four lines studied here, that of the antisymmetric dioxy stretch, the characterization is no more than qualitative owing to the large amount of C_3 and C_4 motion in the eigenvector. In the worst case, the characterization is not even qualitative. An interpretation of optical absorption that made quantitative use of the "symmetric" or "antisymmetric" character of these resonances, but had no reference to quantitative experimental information about eigenvectors in these specific molecules, could only be correct by accident.

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