

Landolt-Börnstein
Group VII: Biophysics

Volume 1
Nucleic Acids

Subvolume C
Spectroscopic and Kinetic Data. Physical Data I

	Title Page, Contributors, Preface	
3	Spectroscopic and kinetic data	1
3.1	Electronic circular dichroism (CD) spectroscopy of nucleic acids (W.C. JOHNSON)	1
3.1.1	Introduction	1
3.1.2	Methods	1
3.1.3	Comments on the CD data	2
3.1.4	Data	3
3.1.4.1	CD spectra for nucleic acid monomers	3
3.1.4.2	CD spectra for dinucleotides	5
3.1.4.3	CD spectra for homopolynucleotides	9
3.1.4.4	CD spectra for other synthetic polynucleotides	13
3.1.4.5	CD spectra for natural nucleic acids	21
3.1.5	References for 3.1	24
3.2	Melting temperatures of polynucleotide complexes (W. GUSCHLBAUER)	25
3.2.1	Introduction	25
3.2.2	Data	35
3.2.2.1	Melting temperatures of polydeoxyribonucleotide hetero-complexes	35
3.2.2.2	Melting temperatures of polyribonucleotide hetero-complexes	38
3.2.2.3	Melting temperatures of hybrid hetero-complexes	46
3.2.2.4	Melting temperatures of homo-complexes	49
3.2.2.5	pK values of homo-complexes	53
3.2.3	References for 3.2	56
3.3	The classical Raman, resonance Raman, and infrared spectroscopy of nucleic acids (W.L. PETICOLAS)	60
3.3.1	Introduction	60
3.3.2	The theory of the relation between vibrational frequencies and conformation	60
3.3.3	Theory of Raman intensity and Raman hypochromism	61
3.3.4	Characterization of experimentally induced changes in DNA conformation by Raman spectroscopy	61
3.3.5	The use of Raman spectroscopy to solve the conformational code of DNA	64
3.3.6	The resonance Raman effect in nucleic acids	65
3.3.7	Low frequency Raman modes and dynamics of DNA	65
3.3.8	The characterization of the conformations of nucleic acids using infrared spectroscopy	65
3.3.9	Data on Raman spectroscopy of nucleic acids	66
3.3.10	References for 3.3	86

3.4	NMR data on oligonucleotides (C. ALTONA)	88
3.4.1	General remarks	88
3.4.2	Proton NMR spectroscopy of oligomers	88
3.4.3	Structure and conformations of oligomers	90
3.4.4	Organization of the oligonucleotide H-1 NMR tables	92
3.4.5	Data	100
3.4.5.1	Coupling constants of RNA sequences	100
3.4.5.2	Chemical shifts of RNA sequences	108
3.4.5.3	Coupling constants of DNA sequences and RNA-DNA hybrids	129
3.4.5.4	Chemical shifts of DNA sequences and RNA-DNA hybrids	143
3.4.6	References for 3.4	186
3.5	Survey of chemical shift values in tRNA (C.W. HILBERS, J.A.L.I. WALTERS)	191
3.5.1	Introduction	191
3.5.2	Data on H-1, C-13 and N-15 nuclei resonances in tRNAs	192
3.5.3	References for 3.5	200
3.6	Thermodynamics and kinetics of base-pairing (D.H. TURNER, N. SUGIMOTO, S.M. FREIER)	201
3.6.1	Introduction	201
3.6.2	Methods	201
3.6.3	Arrangement of data	202
3.6.4	List of symbols and abbreviations	203
3.6.5	Data	204
3.6.5.1	Thermodynamic parameters for duplex formation by RNA oligonucleotides	204
3.6.5.2	Thermodynamic parameters for oligonucleotides with loops	208
3.6.5.3	Thermodynamic parameters for coil-helix transition in single stranded RNA	210
3.6.5.4	Thermodynamic parameters for duplex formation by DNA oligonucleotides	210
3.6.5.5	Thermodynamic parameters for duplex formation by DNA oligonucleotides containing mismatches	211
3.6.5.6	Thermodynamic parameters for helix initiation and propagation in 1 M NaCl.	213
3.6.5.7	Bimolecular helix initiation for RNA and DNA	214
3.6.5.8	Free energy increments for internal G:U pairs in RNA oligonucleotides	214
3.6.5.9	Free energy parameters for RNA helix termini	215
3.6.5.10	Free energy increments for loops	216
3.6.5.11	Thermodynamic parameters for single mismatches in DNA oligonucleotides	217
3.6.5.12	Kinetic parameters for double helix formation by oligonucleotides	218
3.6.5.13	Kinetics of hairpin loop formation by oligomers	220
3.6.5.14	Kinetic parameters for binding between tRNA and oligonucleotides	221
3.6.5.15	Kinetics of tRNA associations through complementary anticodons	222
3.6.5.16	Kinetics of double helix formation for polynucleotides	223
3.6.5.17	Kinetic parameters for intramolecular conformational changes in RNA	224
3.6.5.18	Kinetic parameters for stacking in single strands	225
3.6.6	References for 3.6	226

4	Physical data for nucleic acids and their constituents	228
4.1	Energetics of DNA and RNA double helices (M.D. FRANK-KAMENETSKII)	228
4.1.1	Introduction	228
4.1.2	Bending and torsional rigidity of double helices	230
4.1.3	Energetics of the helix-coil transition	232
4.1.4	Energetics of the B-Z transition	236
4.1.5	References for 4.1	239
4.2	Calorimetric studies on DNAs and RNAs (H.H. KLUMP)	241
4.2.1	Introduction	241
4.2.2	Data	243
4.2.2.1	Conformational transitions in helical polynucleotides	243
4.2.2.2	Property diagrams of all double helical polynucleotides	246
4.2.2.3	Energetics of helix/helix transitions	250
4.2.2.4	Thermodynamics of RNA single-strand unfolding	253
4.2.2.5	Molecular forces that stabilize DNA sequences	254
4.2.2.6	Concluding remarks	255
4.2.3	References for 4.2	255
4.3	Solution properties of DNA: sedimentation, scattering of light, X-rays and neutrons, and viscometry (H. EISENBERG)	257
4.3.1	Introduction	257
4.3.2	Methods	258
4.3.2.1	Ultracentrifugation, partial volumes and interaction parameters	258
4.3.2.2	Total intensity light scattering	260
4.3.2.3	Small angle X-ray and neutron scattering	261
4.3.2.4	Viscometry	262
4.3.2.5	Quasielastic light scattering	263
4.3.3	The persistent chain	263
4.3.4	Data on solution properties	265
4.3.4.1	Partial volumes and interaction parameters in multicomponent systems	265
4.3.4.2	Hydration of DNA	265
4.3.4.3	Molecular parameters of aqueous solutions of linear X-DNA (X = Na, Cs, Li, Rb)	268
4.3.4.4	Calculated neutron scattering length increments for linear CsDNA	270
4.3.4.5	Molecular parameters of linear CoIE 1 DNA	271
4.3.4.6	Physical chemical properties of CoIE 1-plasmid DNA in solution	272
4.3.4.7	Molecular size and sedimentation coefficient for PM 2 Hae III uniformly sized NaDNA fragments	273
4.3.4.8	Persistence length and excluded volume parameters for high molar mass linear T7 DNA	273
4.3.4.9	Temperature dependence of DNA apparent volumes	274
4.3.5	References for 4.3	274

4.4	Interaction of DNA and RNA with metal ions (J.J. BUTZOW, G.L. EICHHORN, Y.A. SHIN)	277
4.4.1	Introduction	277
4.4.2	Data on interaction of metal ions with DNA, synthetic polydeoxynucleotides and synthetic polyribonucleotides	282
4.4.2.1	Binding of metal ions	282
4.4.2.1.1	Association constants	282
4.4.2.1.2	Binding characteristics	288
4.4.2.2	Effects of metal ion binding on conformation of DNA	296
4.4.2.2.1	Helix coil transition (melting temperature)	296
4.4.2.2.2	Transition between right- and left-handed helix	320
4.4.2.2.3	Other conformational changes: secondary (except right-left handed), tertiary, quaternary structures	334
4.4.2.2.4	Hydrodynamic property changes	341
4.4.3	Data on interaction of metal ions with RNA	345
4.4.3.1	Binding of metal ions	345
4.4.3.1.1	Types of metal ion binding sites in tRNAs	345
4.4.3.1.2	Details of metal ion binding sites in RNAs	346
4.4.3.1.3	Association constants for metal ion-tRNA interactions	364
4.4.3.2	Effects of metal ion binding on conformation of RNA	368
4.4.3.2.1	Effects on secondary structure	368
4.4.3.2.2	Effects on tertiary structures	376
4.4.3.2.3	Thermal melting effects - tRNAs	390
4.4.4	Data on metal ion catalyzed degradation of RNAs and polyribonucleotides	394
4.4.5	Data on metal ion catalyzed degradation of DNAs and polydeoxynucleotides	411
4.4.6	References for 4.4	434