No.	ss	$\nu\,(\mathrm{cm}^{-1})$ ds 5°C	ds 95°C	
T7	1377(21)			
				assignment: νPyr/δC6H (Tsuboi et al., 1997)[Thd], νPyr/δC6H/νN1C (Zhu et al., 2008)[Thd]
				structural information: indicator of thymine environment (Movileanu et al., 2002)[poly[d(AT)], polydA·polydT], (Benevides et al., 2005)[poly[d(AT)], polydA·polydT]
				strong hypochromism for ds (Klener et al., 2021)[oligonucleotides], (this work)
		1376(13)	1375(38)	
A7	1378(19)			
				assignment: δC2H/νN1C6/νC6N (Xue et al., 2000)[MeAde]
				structural information: upshift with hydrogen bonding at donor and acceptor sites as well (Fujimoto et al., 1998)[AcAdo, DAcAdo]
				upshift and weak hypochromism for both ds and ts (Klener et al., 2015)[polyA·polyU], hypochromism for ds (this work)
T6	1419(3.7)	–	–	
				assignment: CH_3 umbrella+νC4C5/νC5CH_3 (Zhu et al., 2008)[Thd]
				structural information: upshifts upon H-bonding at N3 (Toyama et al., 1991)[Ado] **upshift in ds (remains for ts) (Klener et al., 2015)[polyA·polyU]**
A6	1425(15)	1422(5.3)	1421(20)	
				assignment: νIm (Fujimoto et al., 1998)[AcAdo, DAcAdo], νC4N9/νN7C8 (Xue et al., 2000)[MeAde]
				structural information: for A-form geometry at 1423 $\mathrm{cm}^{-1}$and for B-form geometry at 1429 cm^{-1} (Tomkova et al., 1994) [poly(AU), polyA·polyU vs poly(d(AU)], 1418 cm^{-1} anti, 1438 cm^{-1} syn (Taillandier et al., 1989)[poly(d(AT))] **hypochromism and slight downshift for ts (Klener et al., 2015)[polyA·polyU], strong hypochromism (this work)**
T6b	–	1449(2.2)	1450(5.3)	
				structural information: **visible only in complexes, similar intensity as T6 visible only in single strand at 1419 cm^{-1}, assigned to uracil (Klener et al., 2015)[polyA·polyU]**
A5	1484(73)	1482(19)	1481(55)	
				assignment: δC2H+νC8N9+δC8H (Fodor et al., 1985)[dAMP], νPur (Fujimoto et al., 1998)[AcAdo, DAcAdo], δC2H/νN1C6/νC6N (Xue et al., 2000)[MeAde]
				structural information: hypochromic for 257 nm (more in alternating dAdT sequence) (Jollès et al., 1985)[poly[d(AT)], polydA·polydT], upshift upon hydrogen bonding at acceptor sites (Fujimoto et al., 1998)[AcAdo, DAcAdo], for A-form geometry at 1480 $\mathrm{cm}^{-1}$and for B-form geometry at 1485 cm^{-1} (Tomkova et al., 1994)[poly(AU), polyA·polyU vs poly(d(AU)]
				downshift for ds (remains for ts) – confirmed A-form marker, hypochromism for ts (Klener et al., 2015)[polyA·polyU], hypochromism for ds (Klener et al., 2021)[oligonucleotides], (this work)
T5	1484(5.0)			
				assignment: νPyr+δC1'H+δ_sC2'H_2 (Zhu et al., 2008)[Thd]
A4	1509(29)	1512(5.2)	1506(26)	
				assignment: νIm (Fujimoto et al., 1998)[AcAdo, DAcAdo], νN7C8/δC8H (Xue et al., 2000)[MeAde]
				structural information: upshift for hydrogen bond at N7 (Fujimoto et al., 1998)[AcAdo, DAcAdo], (Movileanu et al., 2002)[poly[d(AT)], polydA·polydT] **strong hypochromism for ds (remains for ts) (Klener et al., 2015)[polyA·polyU], (Klener et al., 2021)[oligonucleotides] strong hypochromism and upshift for ds (this work)**

Table ?? Assignments of the resonance Raman bands observable in measurements of nucleic acids containing adenine (A) and thymine (T) bases. (Continued, 3 of 4.)

Bibliography

BENEVIDES, J. M.; OVERMAN, S. A.; THOMAS, G. J., 2005. Raman, polarized Raman and ultraviolet resonance Raman spectroscopy of nucleic acids and their complexes. *Journal of Raman Spectroscopy*. **36**(4), 279–299. Available from DOI: 10.1002/jrs.1324.

FODOR, S. P. A.; RAVA, R. P.; HAYS, T. R.; SPIRO, T. G., 1985. Ultraviolet Resonance Raman Spectroscopy of the Nucleotides with 266-, 240-, 218-, and 200-nm Pulsed Laser Excitation. *Journal of the American Chemical Society*. **107**(6), 1520–1529. Available from DOI: 10.1021/ja00292a012.

FUJIMOTO, N.; TOYAMA, A.; TAKEUCHI, H., 1998. Effects of hydrogen bonding on the UV resonance Raman bands of the adenine ring and its C8-deuterated analog. *Journal of Molecular Structure*. **447**(1-2), 61–69. Available from DOI: 10.1016/s0022-2860(98)00301-9.

JOLLÈS, B.; LAIGLE, A.; CHINSKY, L.; TURPIN, P. Y., 1985. The poly dA strand of poly dA · poly dT adopts an A-form in solution: a UV resonance Raman study. *Nucleic Acids Research*. **13**(6), 2075–2085. Available from DOI: 10.1093/nar/13.6.2075.

KLENER, Jakub; ŠTĚPÁNEK, Josef, 2015. UV resonance Raman study of PolyA and PolyU complexes: Mg^{2+}-induced formation of PolyU·PolyA·PolyU triplexes. *Vibrational Spectroscopy*. **81**(5), 32–39. Available from DOI: 10.1016/j.vibspec.2015.09.003.

KLENER, Jakub; ŠTĚPÁNEK, Josef, 2021. Full UV resonance Raman analysis of temperature effects on the structural arrangement of DNA segments. *Journal of Raman Spectroscopy*. **52**(3), 678–689. ISSN 0377-0486. Available from DOI: 10.1002/jrs.6057.

MOVILEANU, L; BENEVIDES, JM; THOMAS, GJ, 2002. Determination of base and backbone contributions to the thermodynamics of premelting and melting transitions in B DNA. *Nucleic Acids Research*. **30**(17), 3767–3777. ISSN 0305-1048. Available from DOI: 10.1093/nar/gkf471.

TAILLANDIER, E.; LIQUIER, J.; GHOMI, M., 1989. Conformational transitions of nucleic acids studied by IR and Raman spectroscopies. *Journal of Molecular Structure*. **214**, 185–211. Available from DOI: 10.1016/0022-2860(89)80014-6.

TOMKOVA, A.; CHINSKY, L.; MISKOVSKY, P.; TURPIN, P. Y., 1994. A–Z conformational transition in poly(rA−rU) and structure marker bands in UV resonance Raman spectroscopy. *Journal of Molecular Structure*. **318**, 65–77. Available from DOI: 10.1016/0022-2860(93)07895-4.
comment: UV RR spectra of poly(rArU) (A→Z form), poly(dAdU) and poly(rA)·poly(rU) in H_2O, markers of A-form (adenosine C3'-endo/anti), B-form (adenosine C2'-endo/anti), Z-form (adenosine C3'-endo/syn).

TOYAMA, A.; TAKEUCHI, H.; HARADA, I., 1991. Ultraviolet resonance Raman spectra of adenine, uracil and thymine derivatives in several solvents. Correlation between band frequencies and hydrogen-bonding states of the nucleic acid bases. *Journal of Molecular Structure*. **242**, 87–98. Available from DOI: 10.1016/0022-2860(91)87129-6.

TSUBOI, M.; KOMATSU, M.; HOSHI, J.; KAWASHIMA, E.; SEKINE, T.; ISHIDO, Y.; RUSSELL, M. P.; BENEVIDES, J. M.; THOMAS, G. J., 1997. Raman and infrared spectra of (2'S)- 2'-H-2 thymidine: Vibrational coupling between deoxyribosyl and thymine moieties and structural implications. *Journal of the American Chemical Society*. **119**(8), 2025–2032. Available from DOI: 10.1021/ja962676t.

XUE, Y.; XIE, D. Q.; YAN, G. S., 2000. Density functional theory studies on molecular structure and IR spectra of 9-methyladenine: A scaled quantum mechanical force field approach. *International Journal of Quantum Chemistry*. **76**(6), 686–699. Available from DOI: 10.1002/(sici)1097-461x(2000)76:6<686::aid-qua2>3.0.co;2-b.
comment: DFT calculation of IR spectra of 9-methyladenine, force field scaled, without solvent.

ZHU, X. M.; WANG, H. G.; ZHENG, X. M.; PHILLIPS, D. L., 2008. Role of Ribose in the Initial Excited State Structural Dynamics of Thymidine in Water Solution: A Resonance Raman and Density Functional Theory Investigation. *Journal of Physical Chemistry B*. **112**(49), 15828–15836. Available from DOI: 10.1021/jp806248b. J. Phys. Chem. B.