

SUPPLEMENTARY INFORMATION

Characterizing the dark state in thymine and uracil by double reso-nant spectroscopy and quantum computation.

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Table ST1. Vibrational frequencies (cm⁻¹) of the NH stretching modes of thymine

State	Method		NH stretching	
S ₀	Experiment		3505	3455
	MP2	ω	3669	3616
	1D-scan	Δv	-133	-132
	1D-PT2	Δv	-136	-136
	PT2 ^a	Δv	-164	-163
		v	3505	3453
S ₁	CC2	ω	3652	3646
	1D-scan	Δv	-134	-133
		v ^b	3487	3482
T ₁	CC2	ω	3627	3625
	1D-scan	Δv	-135	-132
		v ^b	3461	3462

^afull-dimensional anharmonic calculations, ^b1D-anharmonic model corrected for the anharmonic coupling from the PT2 calculations on the ground state

Table ST2. Vibrational frequencies (cm⁻¹) of the NH stretching modes of uracil

State	Method		NH stretching	
S ₀	Experiment		3503	3453
	MP2	ω	3669	3616
	1D-scan	Δv	-132	-132
	1D-PT2	Δv	-136	-135
	PT2 ^b	Δv	-163	-165
		ν	3506	3451
S ₁	CC2	ω	3657	3651
	1D-scan	Δv	-133	-132
		ν^b	3493	3486
T ₁	CC2	ω	3622	3620
	1D-scan	Δv	-136	-131
		ν^b	3455	3456

^afull-dimensional anharmonic calculations, ^b1D-anharmonic model corrected for the anharmonic coupling from the PT2 calculations on the ground state

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[1] M.J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Scuseria, M.A. Robb, J.R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G.A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H.P. Hratchian, A.F. Izmaylov, J. Bloino, G. Zheng, J.L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J.A.M. Jr., J.E. Peralta, F. Ogliaro, M. Bearpark, J.J. Heyd, E. Brothers, K.N. Kudin, V.N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J.C. Burant, S.S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J.M. Millam, M. Klene, J.E. Knox, J.B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R.E. Stratmann, O. Yazyev, A.J. Austin, R. Cammi, C. Pomelli, J.W. Ochterski, R.L. Martin, K. Morokuma, V.G. Zakrzewski, G.A. Voth, P. Salvador, J.J. Dannenberg, S. Dapprich, A.D. Daniels, Ö. Farkas, J.B. Foresman, J.V. Ortiz, J. Cioslowski, D.J. Fox, in, Gaussian, Inc., Wallingford CT, 2009.