This copy of the ESI replaces the previous version published on 29.01.2020 to update the data availability statement.

SUPPLEMENTARY INFORMATION

FEMTOSECOND-TO-NANOSECOND DYNAMICS OF FLAVIN MONONUCLEOTIDE MONITORED BY STIMULATED RAMAN SPECTROSCOPY AND SIMULATIONS

Prokopis C. Andrikopoulos,[a*#] Yingliang Liu,[a#] Alessandra Picchiotti,[b] Nils Lenngren,[b] Miroslav Kloz,[b] Aditya S. Chaudhari,[a] Martin Precek,[b] Mateusz Rebarz,[b] Jakob Andreasson,[b, c] Janos Hajdu,[b, d] Bohdan Schneider[a] and Gustavo Fuertes[a*]

[a] Institute of Biotechnology of the Czech Academy of Sciences, BIOCEV, Průmyslová 595, CZ-252 50 Vestec, Czechia

[b] Institute of Physics of the Czech Academy of Sciences, ELI Beamlines, Za Radnicí 835, CZ-252 41 Dolní Břežany, Czechia

[c] Condensed Matter Physics, Department of Physics, Chalmers University of Technology, 412 96 Gothenburg, Sweden

[d] Department of Cell and Molecular Biology, Uppsala University, Husargatan 3 (Box 596), SE-751 24 Uppsala, Sweden

#: These authors contributed equally

Correspondence to: Gustavo Fuertes e-mail: Gustavo.Fuertes@ibt.cas.cz and Prokopis C. Andrikopoulos e-mail: Prokopios.Andrikopoulos@ibt.cas.cz

DATA AVAILABILITY STATEMENT.

Data for this paper, including transient absorption spectra (Fig. 3 and Fig. S1) and transient femtosecond-stimulated Raman spectra (Fig. 6 and Fig S3) are available at Zenodo at https://doi.org/10.5281/zenodo.7599770.

List of Contents

1. Additional TA, FSRS and fluorescence lifetime experiments

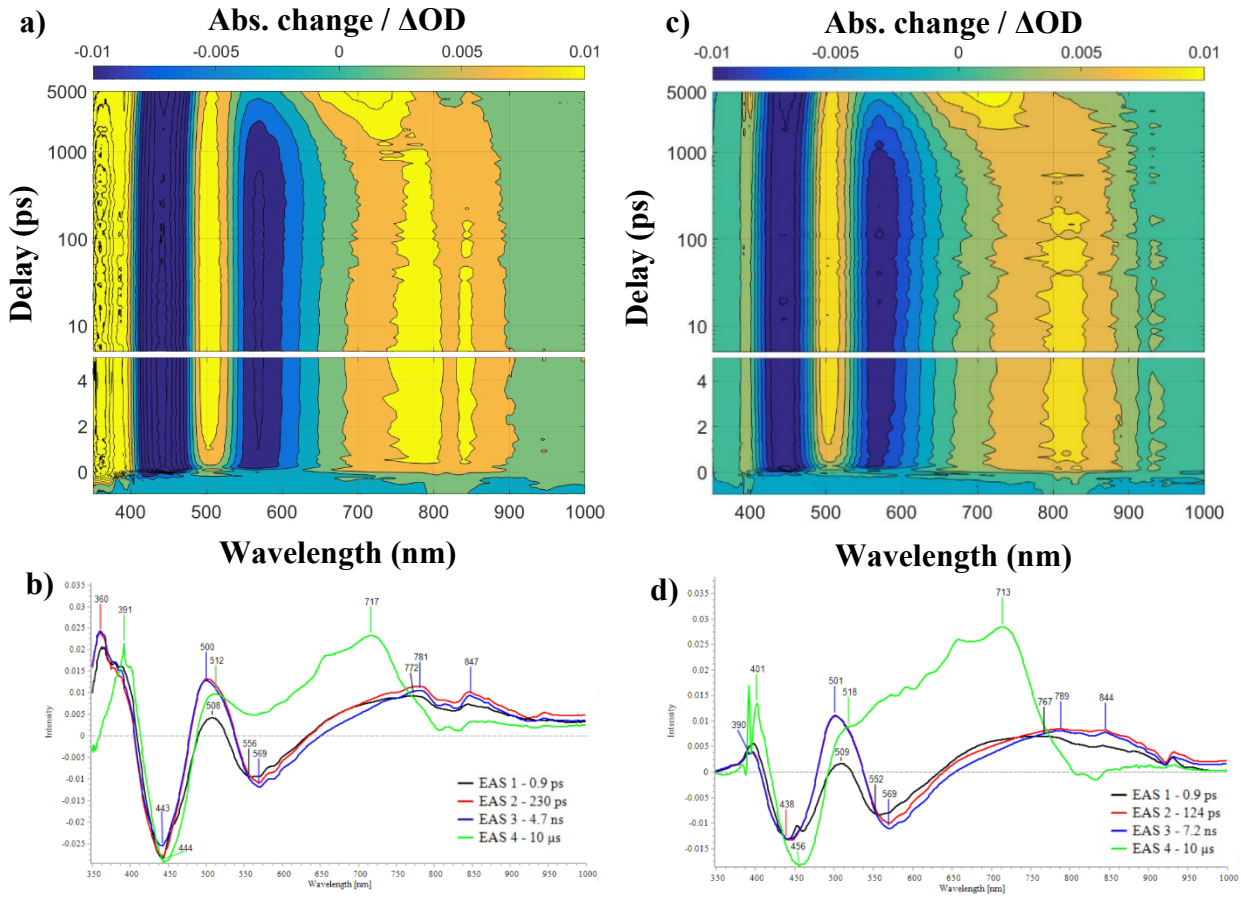
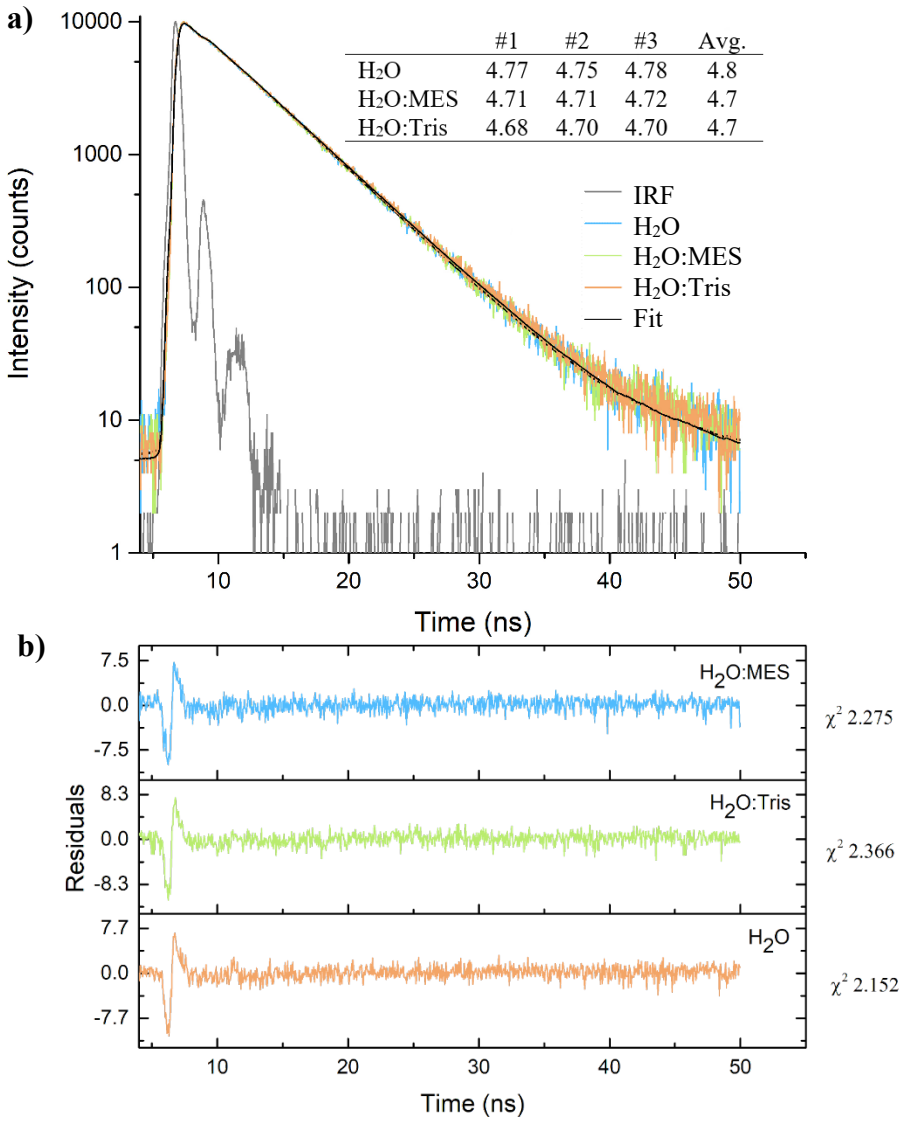


Fig. S1

Experimental transient absorption spectra, contour plots (**a**, **b**) and not normalized 1st to 4th EAS plots (**c**, **d**) of the H_2O:MES pH=6.0 and H_2O:Tris pH=8.0 samples.



	#1	#2	#3	Avg.
H_2O	4.77	4.75	4.78	4.8
H_2O:MES	4.71	4.71	4.72	4.7
H_2O:Tris	4.68	4.70	4.70	4.7

Fig. S2

a) Experimental fluorescence lifetime spectra and fit, plots for the H_2O (cyan), H_2O:MES (light green) and H_2O:Tris (orange) samples. The fit is shown with a black line and the IRF with grey. Lifetimes for three separate measurements for each sample are included in the inset table (in ns). The average of those corresponds to the values given in **Table 1** in the main text. b) Fit residuals including χ^2 values.

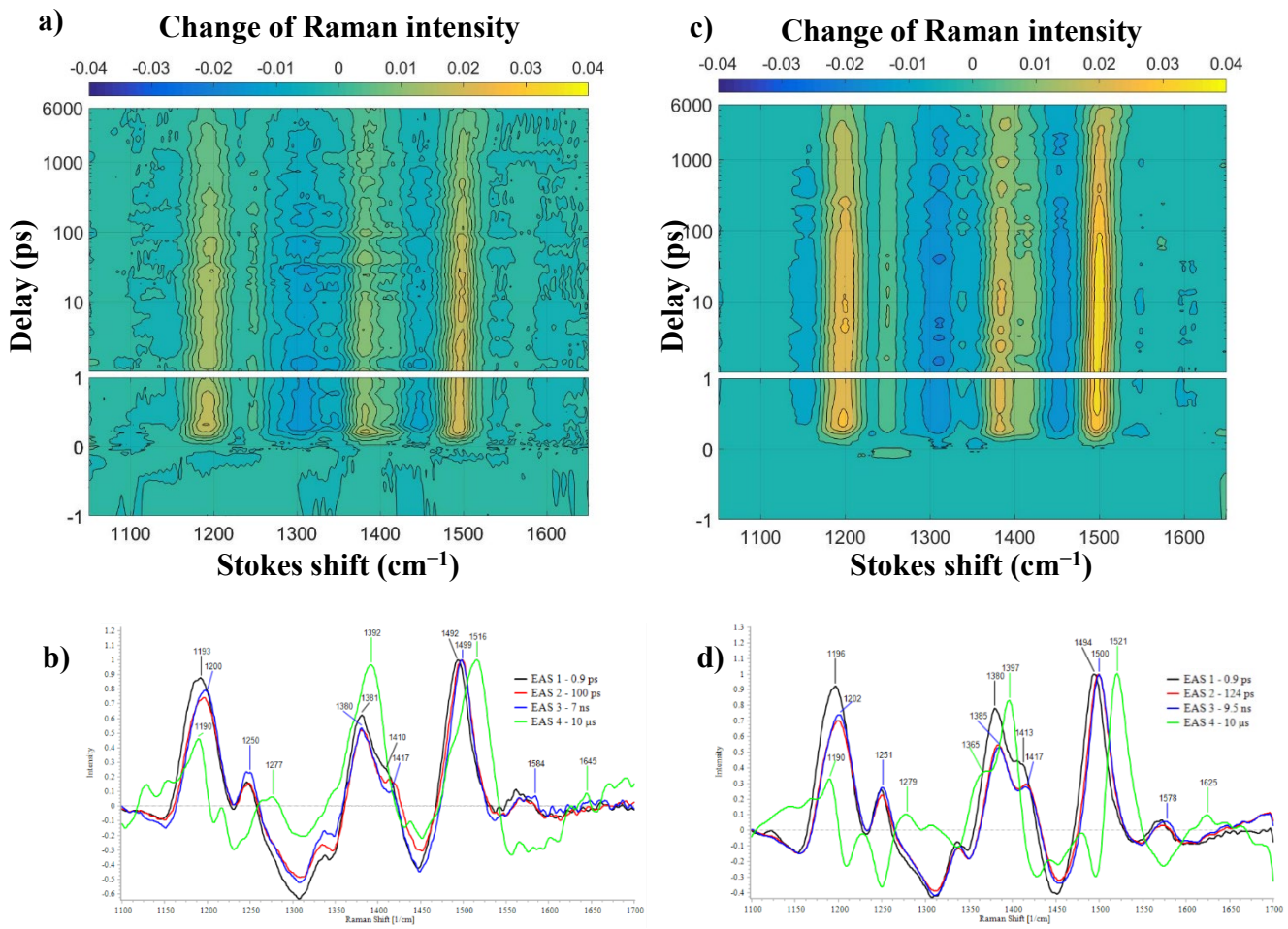


Fig. S3

Experimental stimulated Raman spectra, contour plots (a, b) and their normalized 1st to 4th EAS plots (c, d) of the H_2O:MES and H_2O:Tris samples.

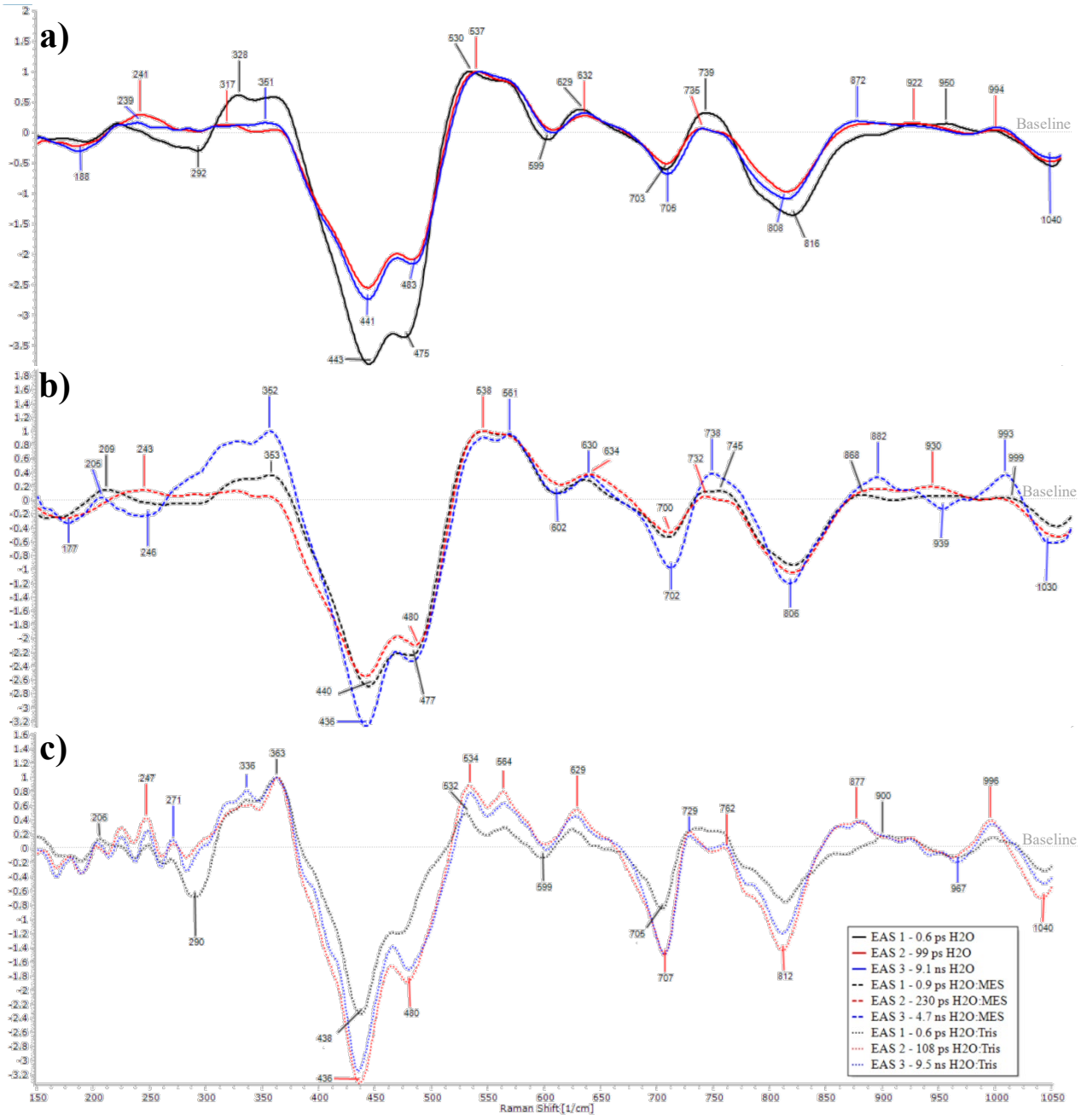


Fig. S4

Components 1, 2 and 3 of the fits of the experimental stimulated data: water (a) – solid lines, MES – dashed lines (b) and Tris – dotted lines (c) in the low-frequency region.

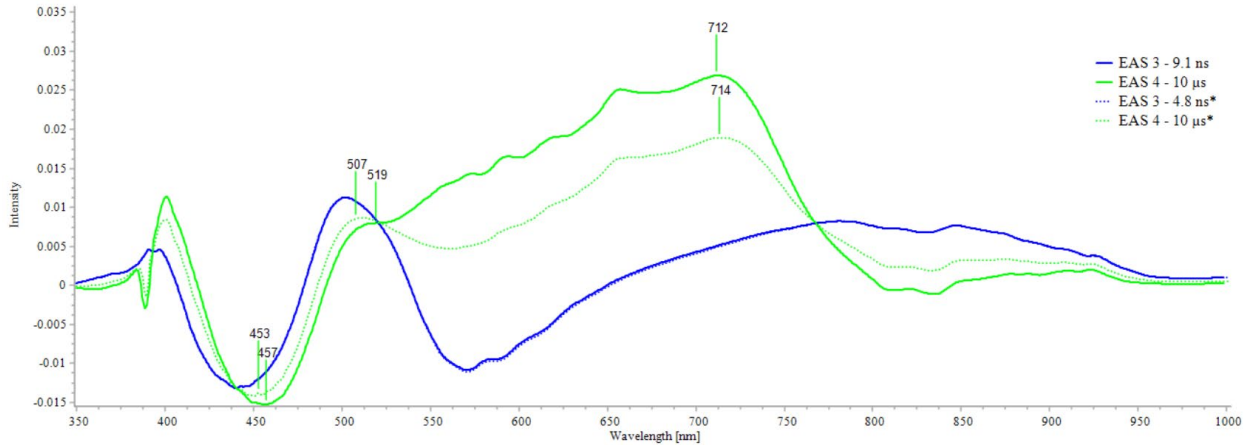


Fig. S5a

Comparison of the 3rd and 4th experimental transient absorption EAS using two different fits for the H_2O sample. The unfixed 3rd EAS (9.1 ns) is shown with a solid blue line, and the one fitted to the fluorescence lifetime of FMN (4.8 ns) with a dashed blue line displaying perfect overlap. In both cases the long component, shown in green, is fixed to the phosphorescence lifetime of FMN (10 µs). The fluorescence lifetime fit produces no difference in the 3rd EAS, while it affects mostly the intensity of the 4th.

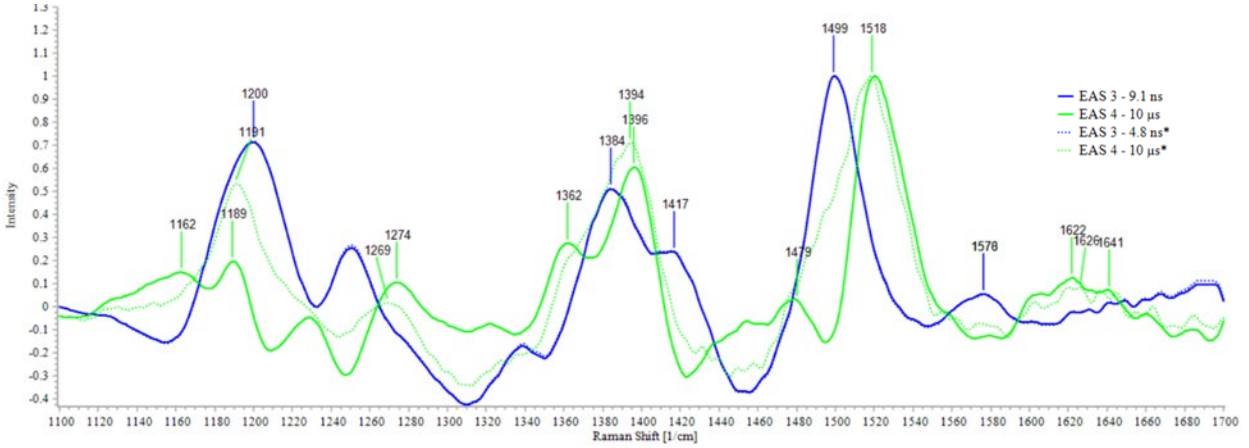


Fig. S5b

Comparison of the 3rd and 4th Raman EAS using two different fits in the high frequency region for the H_2O sample. The not-fixed 3rd EAS (9.1 ns) is shown with a solid blue line, and the one fitted to the fluorescence lifetime of FMN (4.8 ns) with a dashed blue line displaying perfect overlap. In both cases the long component, shown in green, is fixed to the phosphorescence lifetime of FMN (10 µs). The fluorescence lifetime fit is identical within experimental errors with the 3rd EAS, while it affects the 4th. Among other differences in the 4th EAS of the fluorescence lifetime fit (dashed green line), the peak at ~1191 cm^{-1} appears more intense, while bands at 1479 and 1518 cm^{-1} are merged.

2. Molecular Dynamics, Ground State Optimisations

Molecular Dynamics: The conformational space of the ribityl-phosphate moiety was sampled with molecular dynamics. Well within the short MD run of 100 ps at 300 K, the molecule quite rapidly formed a stable geometry with intramolecular hydrogen bonding between the phosphate and ribityl hydrogens and the isoalloxazine ring heteroatoms (**Fig. S6**). This configuration for FMN was reported previously, albeit at a different FMN protonation state (ref. 16, main text).

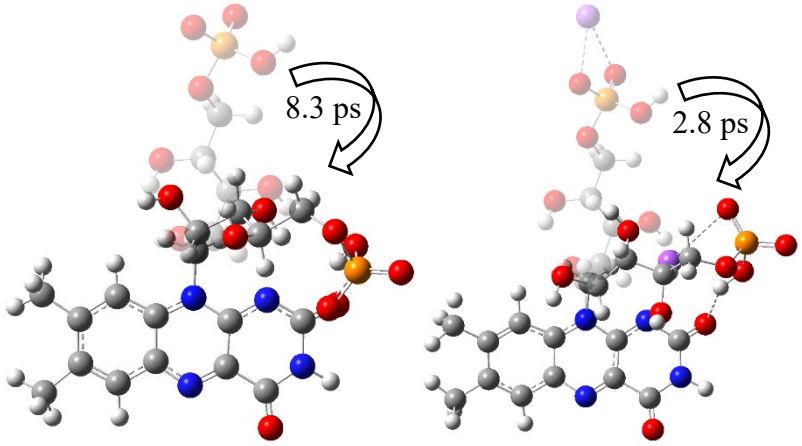


Fig. S6
Structures and folding of the ribityl-phosphate moiety during the MD simulations. The ribityl-phosphate moiety folded within 8.3 ps during the ground-state run of **2** (left). For the run on the excited state S_1 manifold the model of **2** balanced with Na^+, folded even faster at 2.8 ps (right).

Ground State Optimisations: Snapshots from the ground-state MD run were subsequently optimised. The additional intramolecular hydrogen bond yielded an energy gain of ~16 kcal·mol^{-1} when comparing the energy of the pre-MD to the final structure, while an induced folding of the sugar-phosphate moiety towards the isoalloxazine non-polar region resulted in a structure 11 kcal·mol^{-1} higher in energy. Using the most stable structure obtained, several additional models were devised to reflect the conditions of the samples studied experimentally (**Fig. S7**). FMN models with implicit water solvation are designated as **1**, **2** and **3** according to their total charge (0, −1 and −2) respectively. In addition to the above models, micro-solvation was employed, where four explicit molecules of solvent were added in proximity to the polar atoms of the isoalloxazine ring combined with the implicit continuum, yielding the equivalent models **1'**, **2'**, and **3'**, which broadly correspond to the riboflavin model devised in ref. 12. Finally model **2''**, was de with a Na+ counterion to balance the negative phosphate charge (**Fig. 3**).

It can be seen from **Fig. S7** that the number of intramolecular hydrogen bonds depends on the protonation state of the phosphate group, while the $O_{14'}$-H···N_1 bond is present in all models. In the neutral models **1**, **1'**, two additional intramolecular hydrogen bonds are present (O_{16}-H···$O_{14'}$ and O_{17}-H···$O_{2'}$), while in the negative charged or cation balanced models the latter H-bond is absent. Models **3** and **3'** resemble the initial pre-MD structure, since no protons are present to form H-bonds with the isoalloxazine atoms. For the microsolvated models, the additional four hydrogen bonds from equivalent number of water molecules are also drawn (grey dashed lines). The biggest effect of the micro-solvation to the ground-state structures is a lengthening of the C=O bonds by ~0.01 Å while the N_3-H bond is elongated by 0.03 Å. To recapitulate, models **1**–**3** and **1'**–**3'** approximate the samples at different pH conditions with and without buffer (**1**, **1'**: pH < 0.7, **2**, **2'**, **2''**: 0.7 < pH < 6.2, and **3**, **3'**: 6.2 < pH < 10.7). Both models **2'** and **2''**, with their different description of the phosphate moiety, are the default for comparison with the results of the aqueous unbuffered sample with pH measured at 5.9.

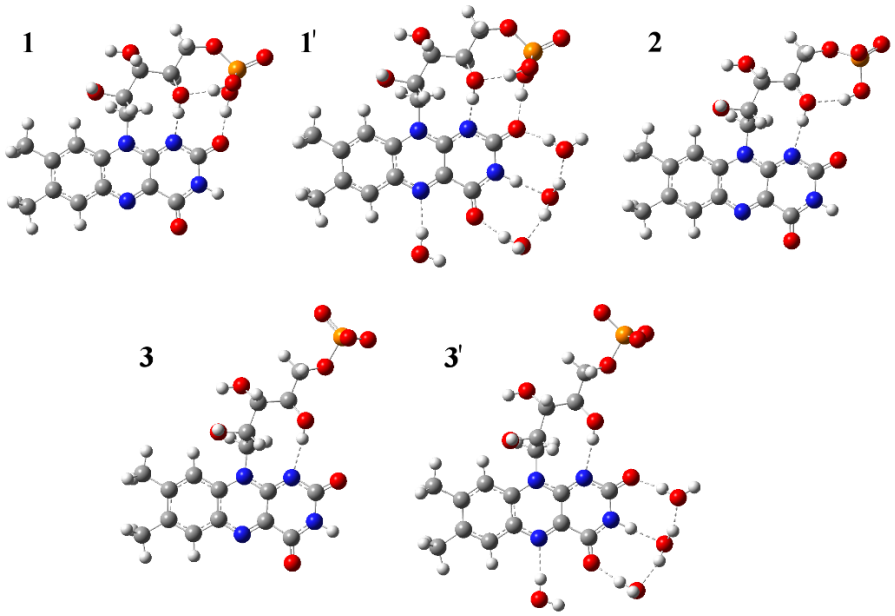


Fig. S7
Structural models of FMN optimised in the water polarisable continuum (PCM) with B3LYP-D/def2-TZVP. The Neutral model **1** is shown on the top left corner, and the micro-solvated equivalent **1'** on the top middle part. The negatively charged model **2** with a deprotonated phosphate oxygen is shown on the top right corner. Model **3** with a total charge of -2 and its microsolvated equivalent (**3'**) is shown on bottom left and right corner, respectively. Dashed lines show the hydrogen bonding network. Atoms are coloured as follows, C: grey, H: white, N: blue, O: red, Na: violet.

3. Canonical orbitals, triplet spin densities and excited-state tables.

a) Singlet–Singlet Excitations: All percentage contributions and participating orbitals are included in **Table 1** of the main text. The neutral **1'** $S_0 \rightarrow S_1$ excitation involves an 88.5% contribution from HOMO (139) to LUMO (140), assigned as a ππ* excitation (**Fig. S8**). Similarly, the $S_0 \rightarrow S_2$ excitation of **1'** involves the HOMO−1 (138) (85.4%), also assigned as ππ*. If the charge in the phosphate moiety is unbalanced (**2'**), then HOMO 139 containing phosphate oxygen lone pairs is found to be dominant in the $S_0 \rightarrow S_1$ transition (52.9%), which is then described as nπ* (**Fig. S9a**). The $S_0 \rightarrow S_2$ is still assigned as ππ* with minimal contribution from the phosphate moiety (**Fig. S9a**, orbital 135, 82.6% contribution). In **2''**, the MO 140 containing phosphate oxygen lone pairs, does not participate in the $S_0 \rightarrow S_1$ and does so only by 2.8% in the $S_0 \rightarrow S_2$ transition, while MO 142 with limited lobes extending from the phosphate moiety, participates in both excitations by 6.0% and 84.8%, respectively (**Fig. S9b**). Therefore the $S_0 \rightarrow S_1$ transition can be described as ππ* by the contributing HOMO (144, 92.2%). Finally, in **3'** both the $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$ excitations are ππ* due to MOs 136 (89.1%) and 131 (86.9%), respectively (**Fig. S10**).

b) Triplet–Triplet Excitations The orbitals involved in the 830-nm T–T transition of **2'** are shown in **Fig. S11a** along with their coefficients. More dominant are the MOs 128 (0.48) and 135 (0.6) which involve lone pairs from both the isoalloxazine ring and the phosphate indicating a nπ* transition. The spin density in the triplet of **2'** is located both in the phosphate and isoalloxazine moieties (**Fig. S11a**, right). The orbitals involved predominantly in the 775 nm T–T transition of **2''** (**Fig. S11b**) are 140 (0.78) and 141 (0.58) localized mostly in the ribityl and phosphate moieties, determining also T_{775} as an nπ* state. From the spin density surface it is surmised that the triplet unpaired electrons are localized only in the isoalloxazine ring.

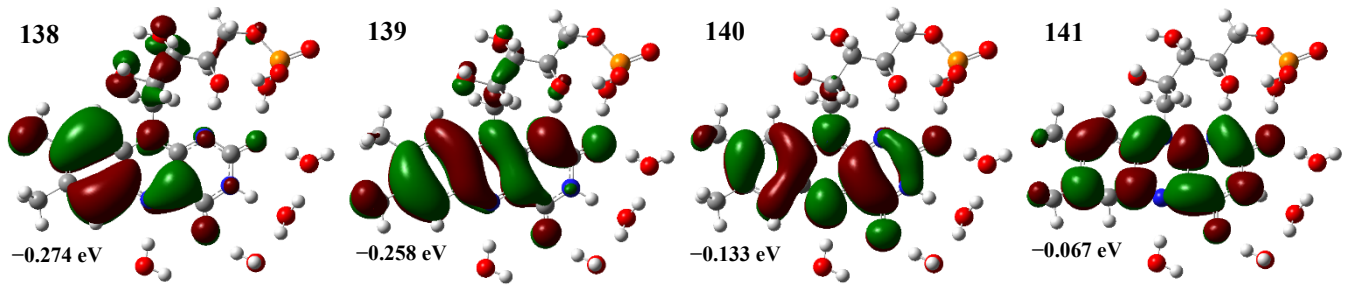


Fig. S8

Canonical orbitals involved in the $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$ vertical excitations of model **1'** together with their assignments, orbital energies and coefficients. The HOMO is MO 139 and LUMO 140.

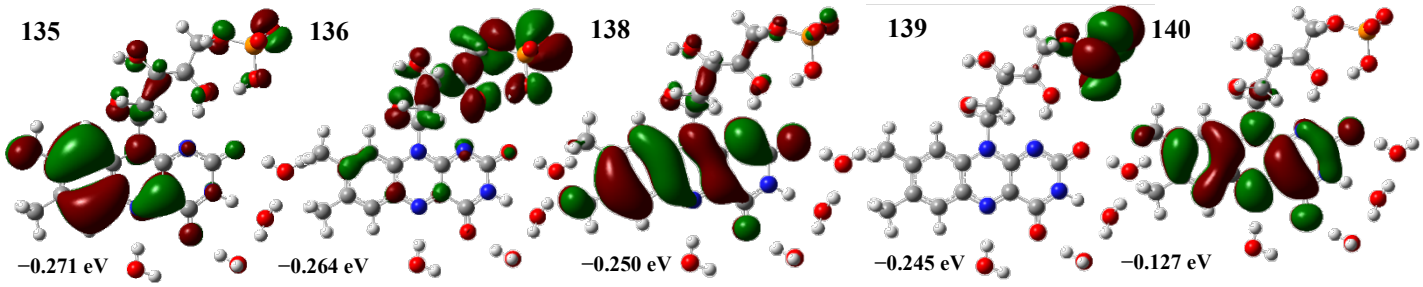


Fig. S9a

Canonical orbitals involved in the $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$ vertical excitations of model **2'** together with their assignments, orbital energies and coefficients. The HOMO is MO 139 and LUMO 140.

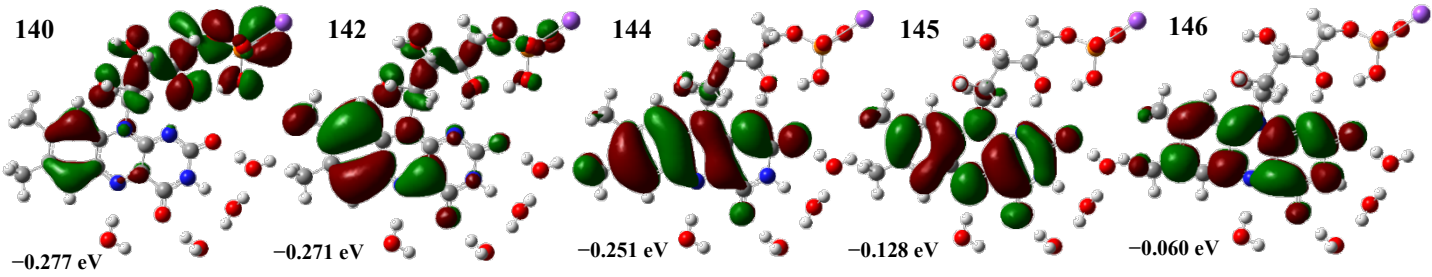


Fig. S9b

Canonical orbitals involved in the $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$ vertical excitations of model **2''** together with their assignments, orbital energies and coefficients. HOMO is 144 and LUMO 145.

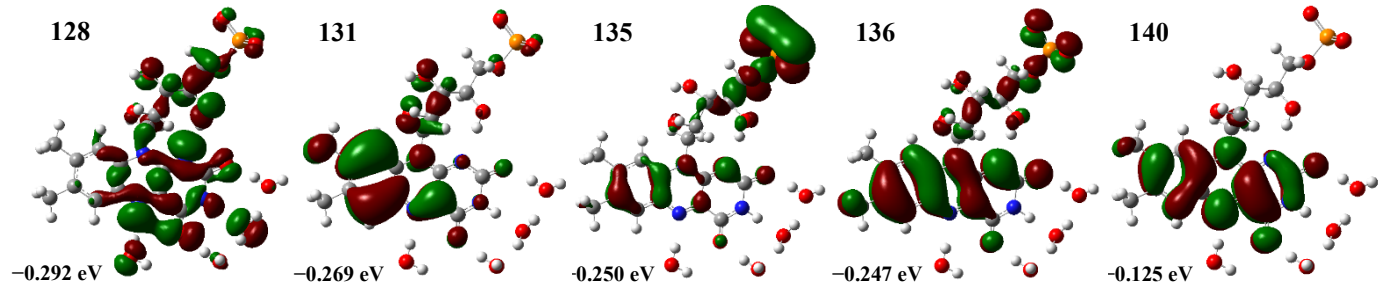


Fig. S10

Canonical orbitals involved in the $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$ vertical excitations for model **3'** together with their assignments, orbital energies and coefficients. The HOMO is MO 139 and LUMO 140.

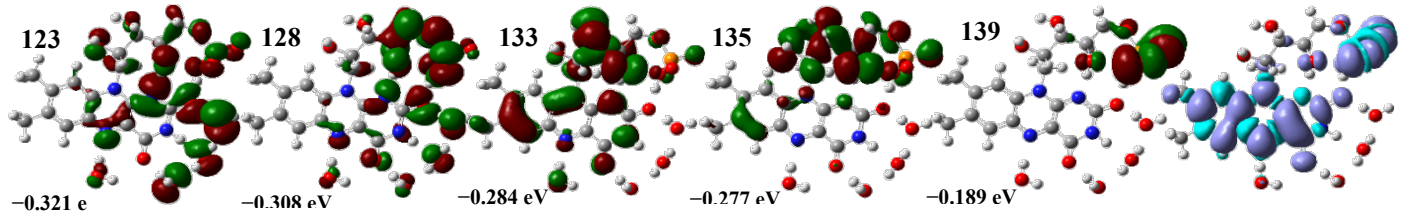


Fig. S11a

Canonical beta orbitals involved in the T_{830} vertical excitation of **2'** with orbital energies. Orbital 139 is the beta LUMO and the coefficients of 123, 128, 133 and 135 are 0.23, 0.48, 0.31 and 0.60 respectively. To the right is the alpha minus beta spin density surface of the T_1 state of **2'**.

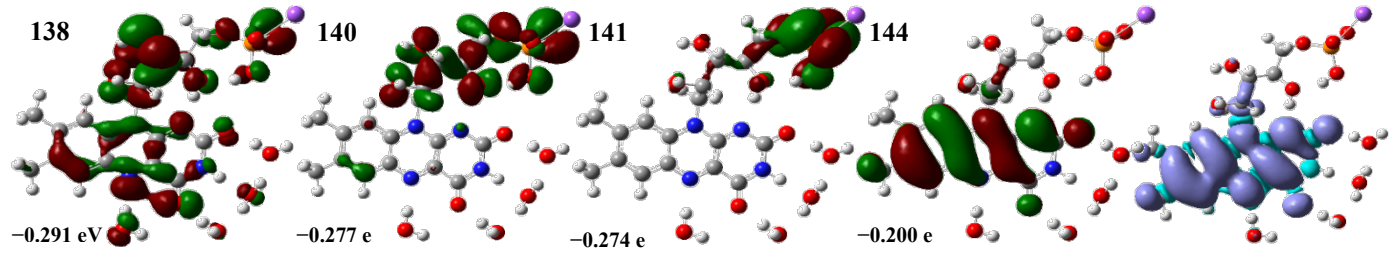


Fig. S11b

Canonical beta orbitals involved in the T_{775} vertical excitation of **2''** with orbital energies. Orbital 144 is the beta LUMO and the coefficients of 138, 140 and 141 are -0.13, 0.78 and 0.58 respectively. To the right is the alpha minus beta spin density surface of the T_1 state of **2''**.

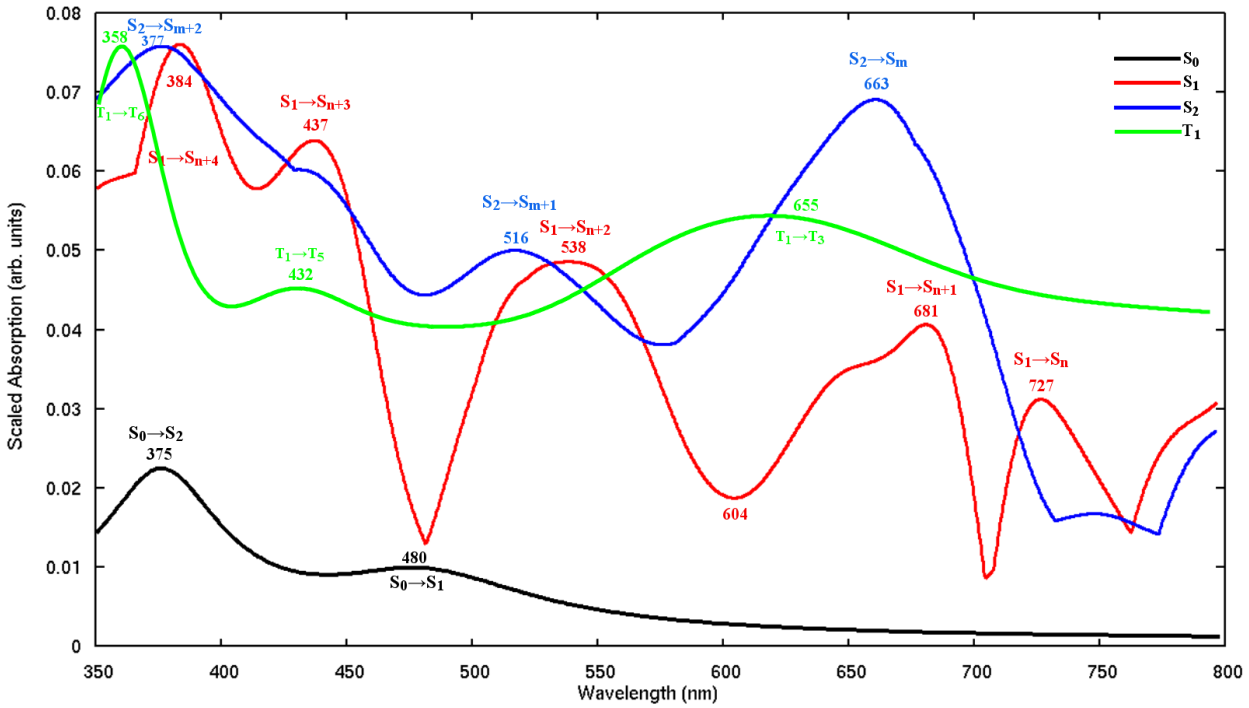


Fig. S12

Calculated absorption spectra of the ground-state (TDDFT) and excited species of **2''**. The spectra of the S_1 and S_2 states are calculated with RT-TDDFT at the B3LYP-D/6-31G*$_{(g)}$ level, the S_0 with TDDFT at the B3LYP-D/6-31G*$_{(g)}$ level and the T_1 spectra with TDDFT at the B3LYP-D/def2-TZVP$_{(aq)}$ level. The S_0 state spectrum is plotted in black, the S_1 in red, the S_2 in blue and the T_1 in light green. The excited state plots are normalized.

Table S1

Energies of all calculated excited states relative to the ground state S_0 in kcal·mol^{-1} (nm in brackets).

	1	**2**	**3**	**1'**	**2'**	**2''**	**3'**
S_1	62.4 [458.2]	55.1 [518.9]	61.6 [464.1]	60.2 [474.9]	59.7 [478.9]	59.8 [478.1]	—
S_2	72.3 [395.5]	61.9 [461.9]	*27.1*[a] [1055.0]	70.8 [403.8]	60.5 [472.6]	71.8 [398.2]	—
T_1	47.1 [607.0]	55.0 [519.8]	31.2 [916.4]	45.2 [632.6]	50.6 [565.1]	44.5 [642.5]	25.2 [1135.0]

a: This optimised structure was excluded from analysis

Table S2

Differences in bond lengths between ground and excited states (in Å). Positive values denote lengthening of the bond in the excited state with respect to the ground state and vice versa. The last two rows display the differences in bond length between the T_1 states of **2'** and **2''** and their respective S_1 states.

	C_6-C_7	**C_{10a}-N_{10}**	**N_5-C_{4a}**	**C_4-C_{4a}**	**N_5···HOH**	**N_1···$HO_{14'}$**
1' S_1	0.050	0.032	0.036	−0.031	−0.097	0.029
1' S_2	0.002	0.013	0.044	−0.017	−0.074	0.002
1' T_1	0.042	0.054	0.036	−0.025	−0.095	0.043
2' S_1	0.043	0.026	0.039	−0.035	−0.093	0.044
2' S_2	0.036	0.023	0.042	−0.036	−0.104	0.012
2' T_1	0.010	0.010	0.054	−0.039	−0.131	−0.072
2'' S_1	0.043	0.027	0.039	−0.034	−0.093	0.055
2'' S_2	0.003	0.013	0.051	−0.021	−0.077	0.001
2'' T_1	0.032	0.047	0.041	−0.027	−0.096	0.059
3 S_1	0.036	0.026	0.043	−0.036	—	—
3 S_2	0.011	0.015	0.053	−0.037	—	—
3 $S_{2(2)}$	0.010	0.014	0.053	−0.038	—	—
3 T_1	0.011	0.015	0.058	−0.040	—	—
Differences in bond lengths between S_1 and T_1 States						
2' T_1	0.033	0.016	-0.015	0.004	0.038	0.116
2'' T_1	0.012	-0.020	-0.002	-0.008	0.003	-0.005

Table S3

Energies in eV and nm of vertical absorptions E^{Vab}, emissions E^{Vem}, 0–0 transitions $E^{0–0}$ and adiabatic energies E^{Ad} for the S_1 state of all calculated species. Scaled ZPVEs (0.9896, ref. 76) were included in the calculation of the 0–0 transitions.

	E^{Vab}		E^{Vem}		$E^{0–0}$		E^{Ad}	
	eV	**nm**	**eV**	**nm**	**eV**	**nm**	**eV**	**nm**
1	2.98	416	2.48	499	2.61	475	2.71	458
2	2.96	418	1.46	851	2.29	542	2.39	519
3	2.95	421	2.46	504	2.56	483	2.67	464
1'	2.90	428	2.37	524	2.53	491	2.61	475
2'	2.86	433	2.36	526	2.51	494	2.59	479
2''	2.88	431	2.40	516	2.51	494	2.59	478
3'	2.86	434	—	—	—	—	—	—

Table S4

Most intense theoretical bands of regions I (~390 nm), II ~, III (~500 nm), IV and V (>600 nm) of the absorption spectrum (values in nm). For **2''** results from the RT-TDDFT calculations are included for the S_1 and S_2 species, while for all models transitions are included for the T_1 state optimisation.

Model:		**1**	**2**	**3**	**1'**	**2'**	**2''**	**2''***	**3'**
Region	State								
I	S_1	–	–	–	–	–	384, 437	350	–
	S_2	–	–	–	–	–	377	–	–
	T_1	352	359, 388	356	354, 377	363, 383	358	–	359, 387
II	S_1	–	–	–	–	–	480	–	–
	S_2	–	–	–	–	–	481	–	–
III	S_1	–	–	–	–	–	538	548	–
	S_2	–	–	–	–	–	516	–	–
	T_1	445, 562	493, 591	434, 478, 539, 570	440, 555	442, 493, 572	432, 571	–	449, 481, 515, 554
IV	S_1	–	–	–	–	–	604		–
	S_2	–	–	–	–	–	577		–
V	S_1	–	–	–	–	–	681, 727	730, 782	–
	S_2	–	–	–	–	–	663	–	–
	T_1	622, 718	648, 841	–	602, 640, 752	657, 830	598, 616, 655, 708, 739, 775	–	–

*:Vertical $S_0 \rightarrow S_1$ excitation using the S_0 geometry.

Table S5

Spin-orbit coupling terms computed for the ground state, S_1 and S_2 geometries of **2''**. Highlighted in red are the strongest interactions between singlet and triplet states. SOCs are given in cm^{-1} and orbital energies in eV. The dominant active orbitals of each state are given, where n denotes heteroatom lone pairs in the isoalloxazine ring and $n_{(P)}$ in the phosphate moiety.

Singlet / Triplet			**Spin-Orbit Coupling Terms at the S_0 Ground State Geometry**									
			T_1	**T_2**	**T_3**	**T_4**	**T_5**	**T_6**	**T_7**	**T_8**	**T_9**	**T_{10}**
			2.06	2.49	3.09	3.35	3.57	3.58	3.64	3.65	3.75	3.86
			π	π	n	$n_{(P)}$	$n/n_{(P)}$	$n/n_{(P)}$	π	$n_{(P)}$	n	n/π
S_0	-	-	0.6	0.3	15.7	0.7	19.0	23.0	1.3	1.7	1.7	3.8
S_1	π (S_1)	2.88	0.3	0.5	2.1	1.4	6.4	6.7	0.3	2.1	0.7	1.7
S_2	$n_{(P)}$	3.35	0.8	0.2	1.7	0.1	15.2	13.0	11.5	35.7	6.4	10.1
S_3	π (S_2)	3.38	0.7	0.9	6.4	2.3	4.4	7.7	1.3	5.2	1.2	1.8
S_4	n	3.51	7.0	6.6	0.7	3.9	3.4	3.6	3.3	4.9	7.7	5.8
S_5	$n_{(P)}$	3.59	1.6	1.4	2.4	23.3	1.6	2.5	2.9	13.5	3.5	7.7
S_6	$n_{(P)}$	3.66	1.6	1.3	2.0	37.4	10.5	11.1	0.7	2.2	1.9	2.1
S_7	n	3.76	10.4	6.3	3.4	4.0	0.7	3.0	7.6	2.9	18.4	6.3
S_8	n	3.96	1.3	1.0	3.3	13.5	6.7	7.8	1.4	5.1	3.9	1.5
S_9	n	4.13	0.3	0.4	13.2	0.5	1.0	0.9	0.5	0.2	0.6	1.8
S_{10}	$n/n_{(P)}$	4.25	6.8	2.9	5.6	14.8	7.1	8.6	10.8	9.7	13.6	9.7

Singlet / Triplet			**Spin-Orbit Coupling Terms at the S_1 Excited State Geometry**									
			T_1'	**T_2'**	**T_3'**	**T_4'**	**T_5'**	**T_6'**	**T_7'**	**T_8'**	**T_9'**	**T_{10}'**
			1.65	2.23	2.98	3.06	3.26	3.34	3.36	3.48	3.49	3.60
			π	π	n	$n_{(P)}$	$n_{(P)}$	n	$n_{(P)}$	π	n	π
S_{n+2}	$n_{(P)}$	3.06	0.6	0.2	1.5	0.1	18.2	11.9	35.7	7.3	10.6	8.5
S_{n+5}	$n_{(P)}$	3.37	3.4	3.6	2.5	35.0	13.9	3.2	2.8	2.2	1.4	3.1

Singlet / Triplet			**Spin-Orbit Coupling Terms at the S_2 Excited State Geometry**									
			T_1''	**T_2''**	**T_3''**	**T_4''**	**T_5''**	**T_6''**	**T_7''**	**T_8''**	**T_9''**	**T_{10}''**
			1.89	2.06	3.03	3.06	3.27	3.31	3.35	3.49	3.52	3.66
			π	π	n	$n_{(P)}$	$n_{(P)}$	n	n	n	π	$n_{(OH)}$
S_{m+3}	$n_{(P)}$	3.05	0.7	0.3	1.5	0.4	19.2	4.4	38.6	6.9	7.3	12.5
S_{m+5}	$n_{(P)}$	3.36	2.6	1.3	14.9	34.6	14.8	3.4	2.1	1.7	1.3	5.8

4. Computed Raman and pre–resonance Raman spectra

Ground-State Spectra: The predicted ground-state (gs) Raman intensities were identical for models **2'**, **2''** and **3'** but differed from the neutral model **1'**. In the high-frequency region, the ground-state Raman spectra exhibit the strongest peak at ~1330 cm^{-1}. This is assigned to an isoalloxazine ring breathing mode coupled to an adjacent ribityl chain CH out-of-plane bend and is common for all obtained spectra (**Fig. S13a**) and is similar to the 1297, 1312 cm^{-1} bands of the S_1 state of **2'** and **2''**. Similarly the strong gs peak at 1517 cm^{-1} is equivalent to the 1475 cm^{-1} S_1 peak, while the C_2=$O_{2'}$ and C_4=$O_{4'}$ stretching modes are found at 1644 and 1668 cm^{-1}, respectively. The low-frequency region includes features of much less intensity than the high-frequency region. The most intense of those are found at ~740 cm^{-1} due to phosphate and ribityl out-of-plane -OH bending modes and a methyl asymmetric bend at ~1006 cm^{-1}, shown partially in **Fig. S13b**.

Singlet S_2 State Spectra: The Raman spectra of the S_2 excited-state optimised structures **1'**, **2'**, and **3** are shown in **Fig. S14**. It was not possible to locate a minimum on the S_2 potential energy surface for the microsolvated **3'** model so the spectra of **3** without the four explicit water molecules is included in the Figure. The 1594 and 1113 cm^{-1} peaks dominate the spectra of **1'** and **2'**, respectively while the 1468 cm^{-1} peak is intense in the spectrum of **2''**. The peaks are assigned to ring-breathing mode coupled to the solvent, a combination of phosphate P=O stretch and P-OH in-plane bend, and an isoalloxazine breathing mode, respectively.

The spectra of the S_1 state (**Fig. S15**) and the T_1 pre-resonance (**Fig. S17**-**S18**) are discussed in the main text.

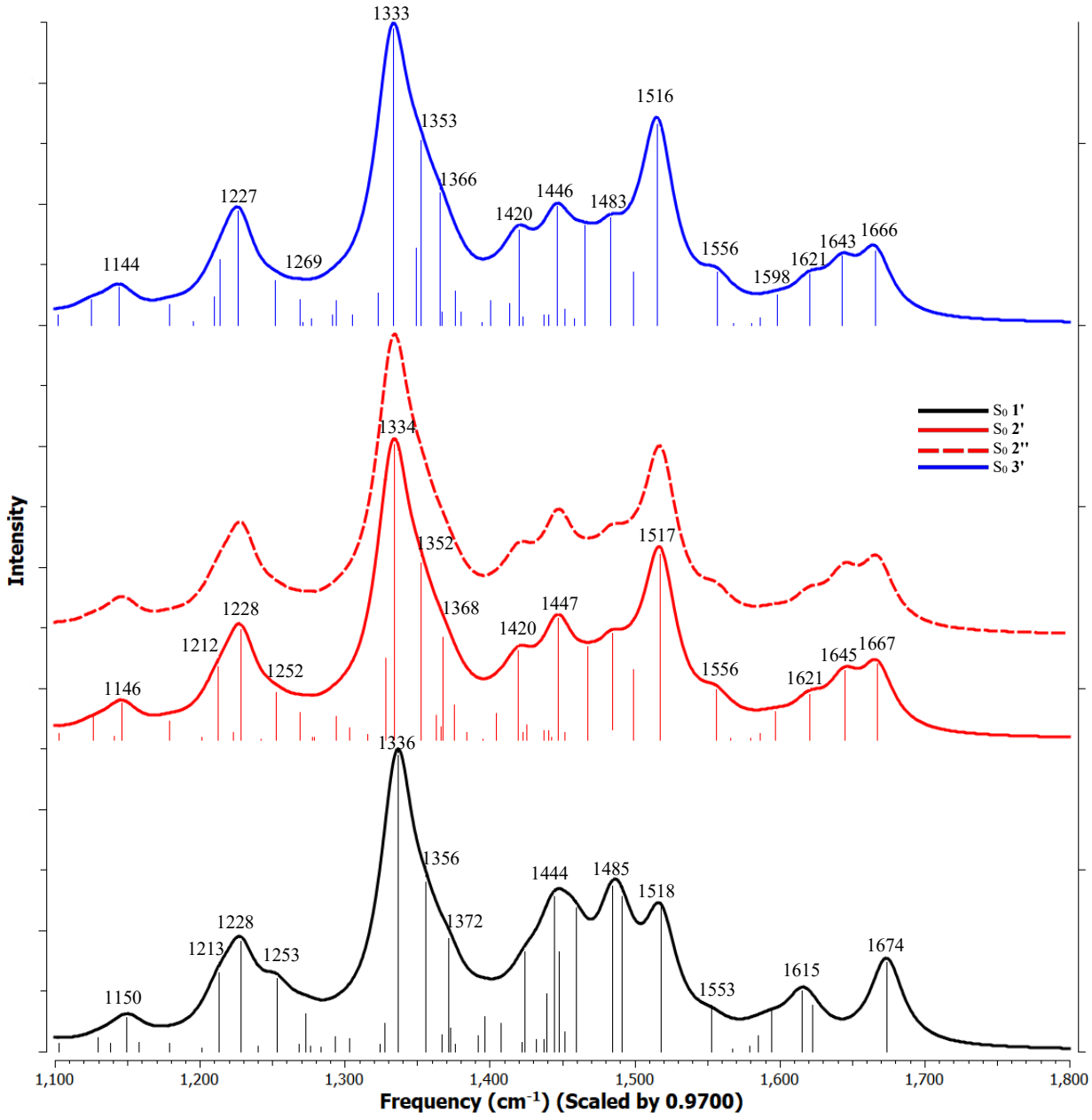


Fig. S13a

Computed ground-state (S_0) Raman spectra (high-frequency region) of **1'** (black), **2'** (red), **2''** (dashed red) and **3'** (blue) lines

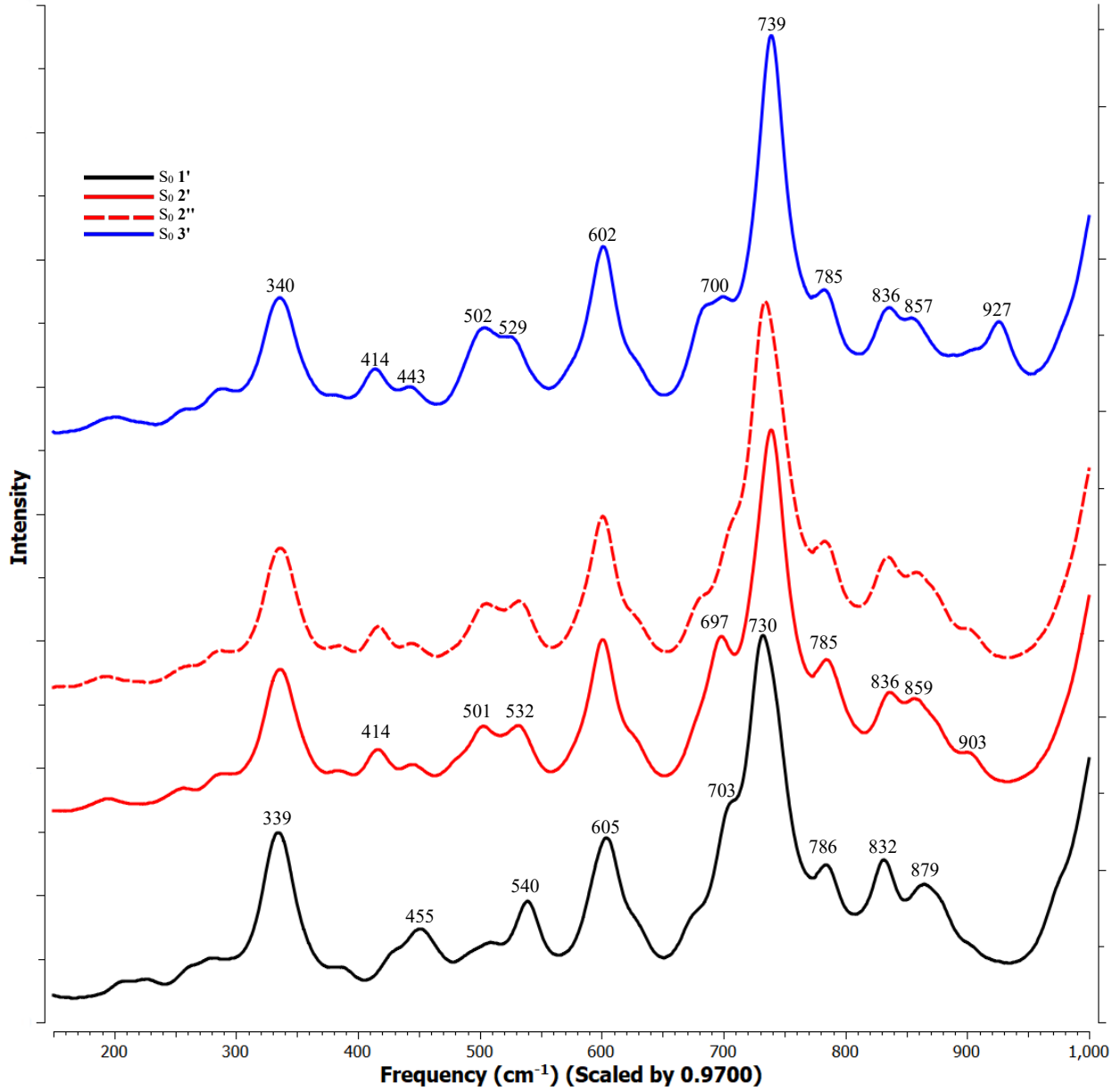


Fig. S13b

Computed ground-state (S_0) Raman spectra (low-frequency region) of models **1'** (black), **2'** (red solid), **2''** (red dashed) and **3'** (blue).

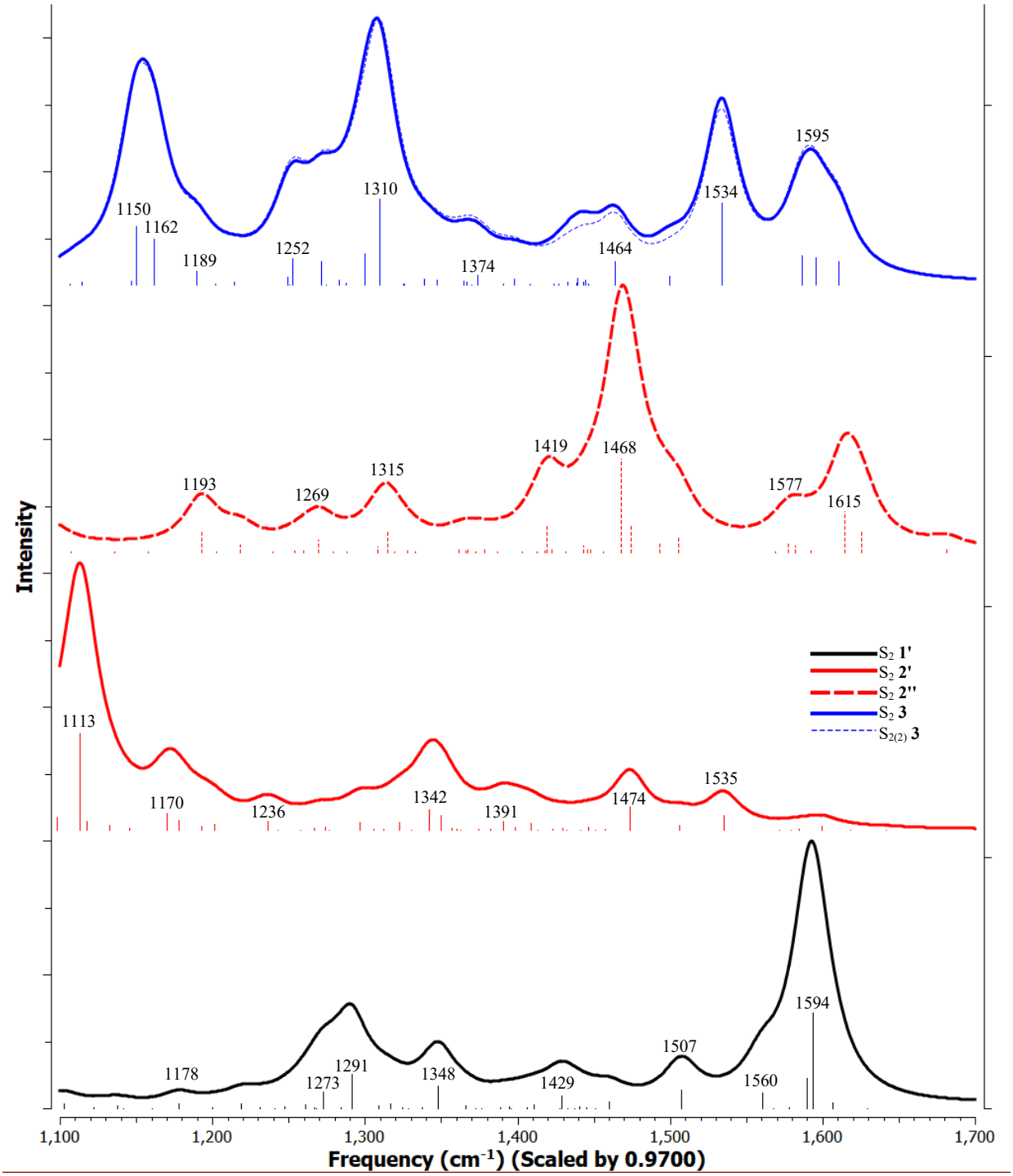


Fig. S14

Computed second excited singlet-State (S_2) Raman spectra of **1'** (black), **2'** (red solid), **2''** (red dashed) and **3** (blue). The Raman spectrum of the second excited-state ($S_{2(2)}$) structure of **3** is also included with a blue dashed line.

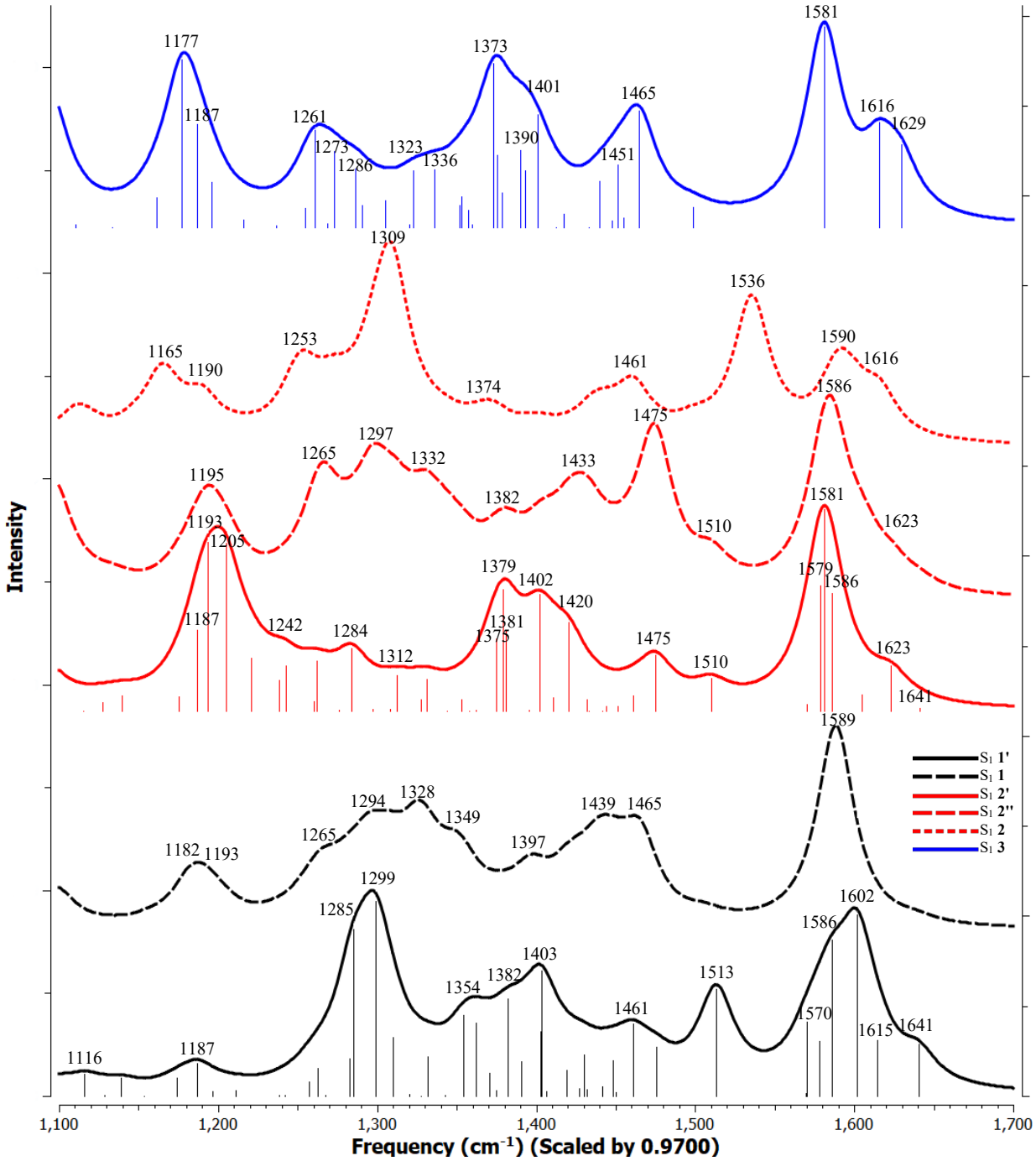


Fig. S15

Calculated excited singlet-state (S_1) Raman spectra (high-frequency region) of **1'** (solid black), **1** (dashed black), **2'** (solid red), **2''** (dashed red), **2** (dotted red) and **3** (solid blue) lines.

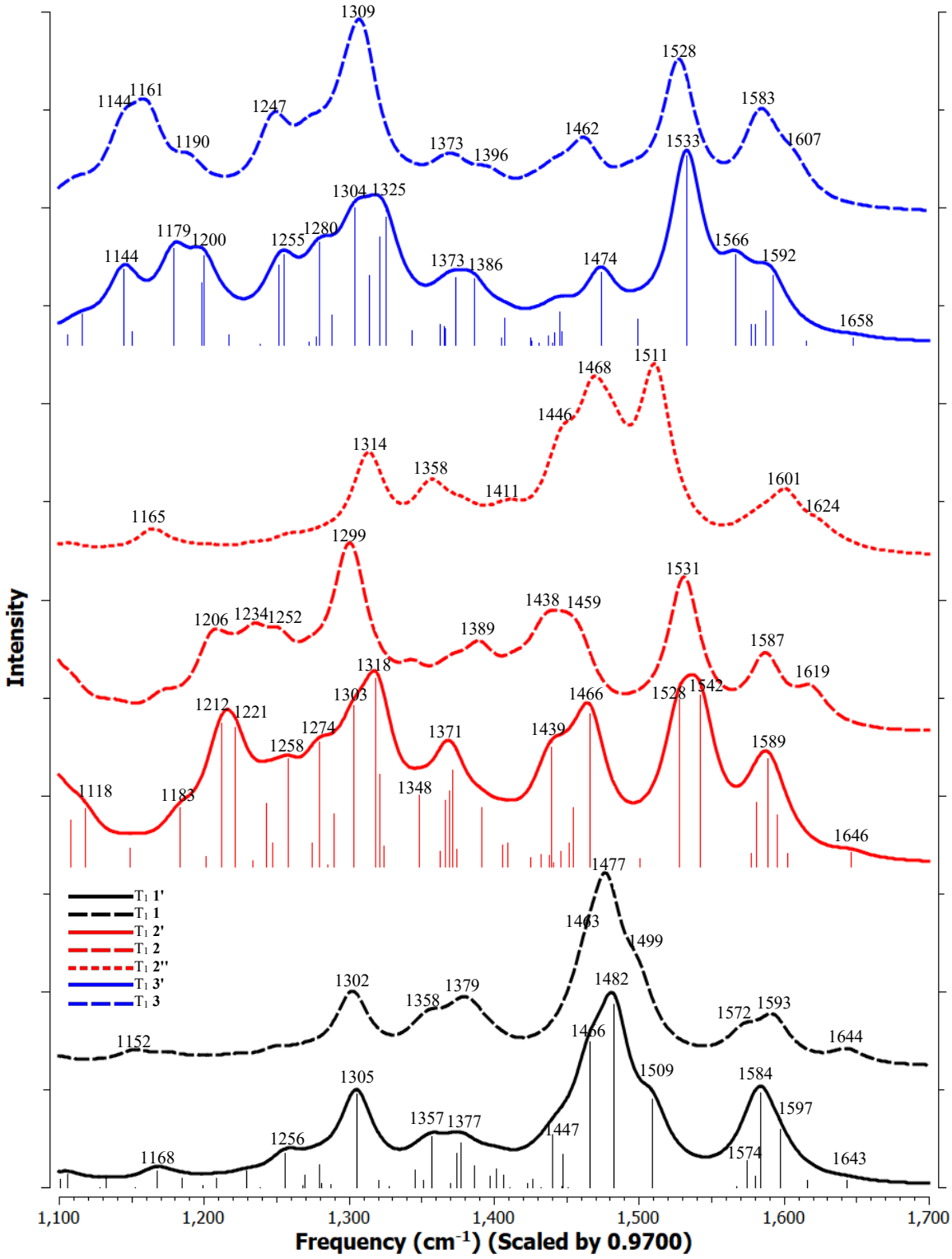


Fig. S16

Calculated excited triplet-state (T_1) Raman spectra (high-frequency region) of **1'** (solid black), **1** (dashed black), **2'** (solid red), **2''** (dashed red), **2** (dotted red) and **3** (solid blue) lines.

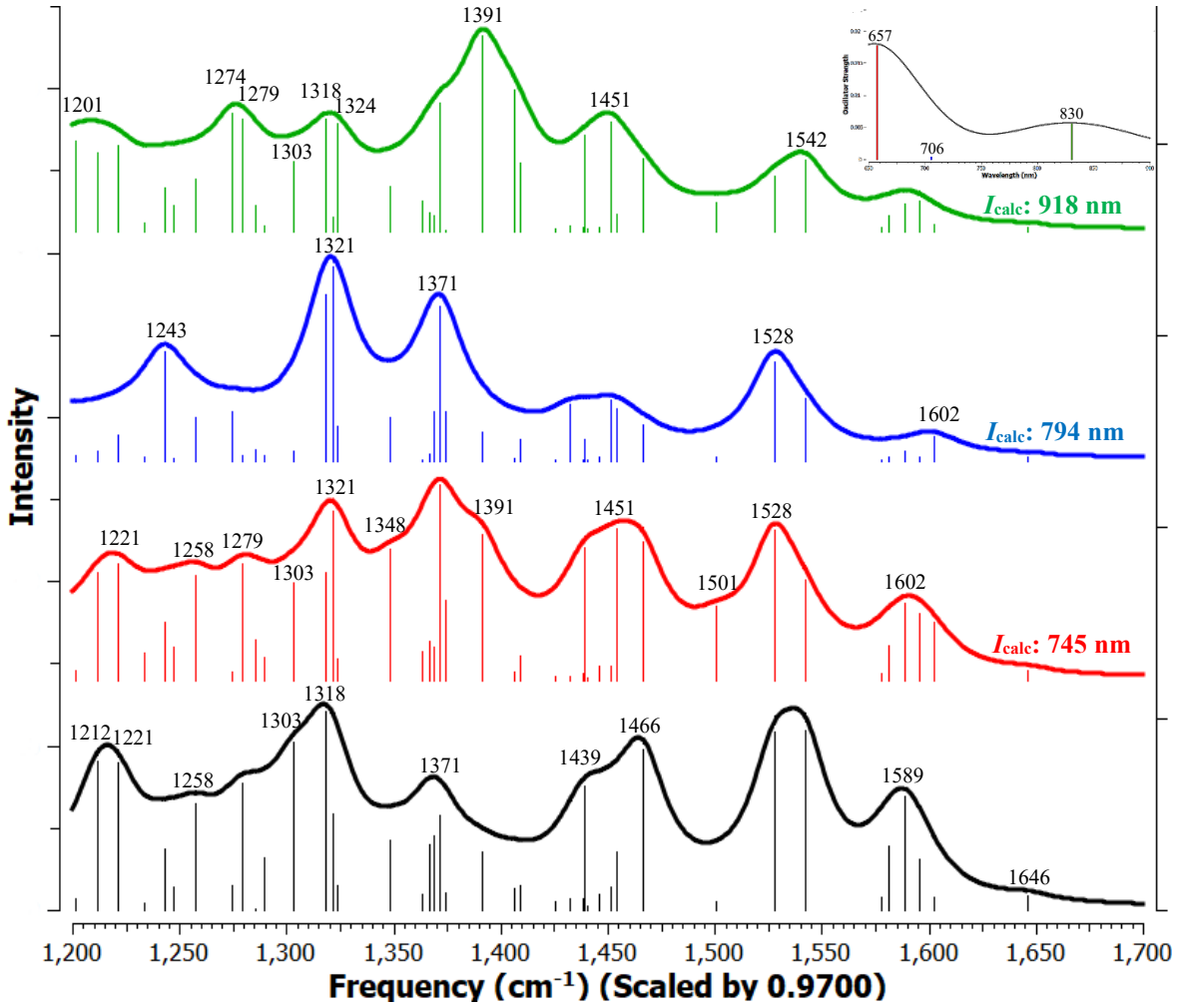


Fig. S17

Calculated pre-resonance Raman spectra for the triplet state of **2'** with the most prominent peaks labelled. The red plot shows the calculated Raman intensities when the 657-nm T–T transition is considered pre-resonant. The blue corresponds to the 706 nm transition and the green to the 830 nm. For comparison, the black plot when the incident light is set to 0 cm^{-1} is included (no pre-resonance, repeated from **Fig. S16**). In the inset Figure (top right corner), the calculated absorption spectrum with the three transitions in matching colours is included.

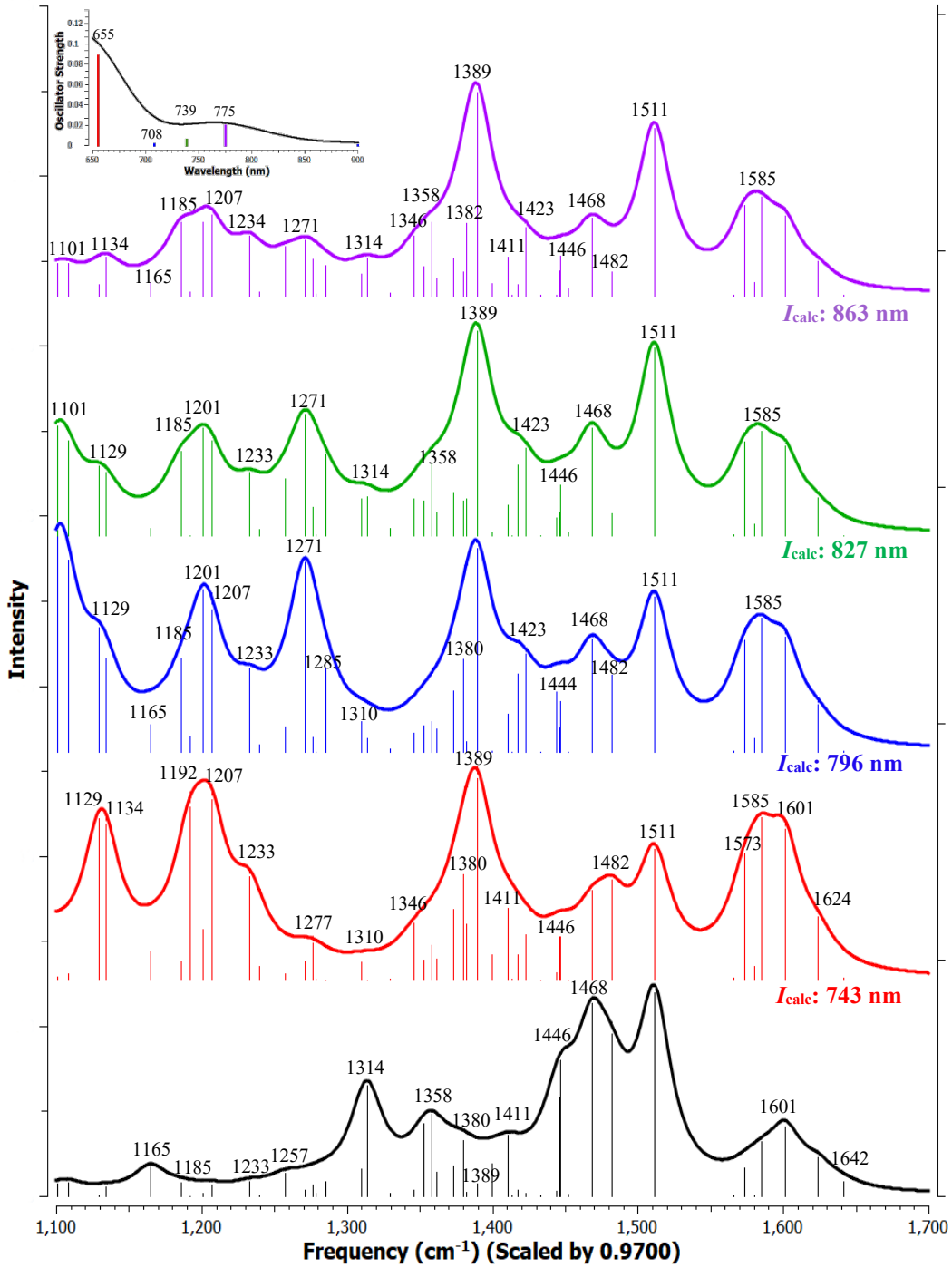


Fig. S18

Calculated pre-resonance Raman spectra for the triplet state of **2''** with the most prominent peaks labelled. The red plot shows the calculated Raman intensities when the 655 nm T–T transition is considered pre-resonant. The blue corresponds to the 708 nm transition, the green to the 739 nm and the violet to the 775 nm. For comparison, the black plot when the incident light is set to 0 cm^{-1} is included (no pre-resonance, repeated from Fig. S16). In the inset Figure (top left corner), the calculated absorption spectrum with the four transitions in matching colours is included.

Table S6

Agreement between the experimental and theoretical Raman spectra. Mean absolute deviations (MAD) are given in cm^{-1}. Two values are included, either over the 3 most prominent peaks (2 for T_1) or over all assigned peaks. MADs for the S_1, S_2 and T_1 spectra are based on the assignments in **Tables 3-4**.

	S_1		S_2		T_1	
	Overall	3 peaks[a]	Overall	3 peaks[a]	Overall	2 peaks[b]
1'	61 $_{48}$[c]	68 $_{47}$[c]	56	70	23	29
2'	32 $_{19}$[c]	30 $_{12}$[c]	34	36	13	13
2''	33 $_{19}$[c]	32 $_{12}$[c]	29	36	9	8
3	31 $_{22}$[c]	38 $_{23}$[c]	42	53	23	18

[a] Excited singlet peaks: 1200, 1384, 1500 cm^{-1}
[b] Triplet peaks: 1396, 1521 cm^{-1}
[c] Correlation of ν_{E2} to 1475 cm^{-1} (**2'**, **2''**) or 1465 cm^{-1} (**1'**, **3**)

Table S7

Calculated triplet–triplet transitions (in nm), with oscillator strengths f, and the corresponding incident light given in nm and cm^{-1}.

T–T transition	f	Incident light	
		nm	cm^{-1}
	2'		
657	0.0251	745	13423
706	0.0003	794	12595
830	0.0082	918	10893
	2''		
655	0.0881	743	13459
708	0.0008	796	12563
739	0.0055	827	12092
775	0.0199	863	11588

Table S8

Equivalent singlet-triplet vibrations for **2'** and **2''**.

	S_1 **2'**	S_1 **2''**	T_1 **2'**	T_1 **2''**	S_1 **2'/2''** Modes	T_1 **2'** Modes	T_1 **2''** Modes
$\nu_{E/T1}$	1641 vw	1641 w	1646 vw	1642 vw	*sc*H_2O, *r*N_3-H, *s*C_4=$O_{4'}$	Same as S_1	Same as S_1
$\nu_{E1/T2''}$	1623 m	1623 m	—	1624 m	*sc*H_2O, *r*N_3-H, *s*C_2=$O_{2'}$	—	Same as S_1
$\nu_{T2'}$	1604 vw	1606 s	1602 vw	1601 m	*sc*H_2O, *s*C_4=$O_{4'}$, *r*N_3-H	Same as S_1	S_1 + *s*C_2=$O_{2'}$
v	1586 m	1586 vs	1589 m	1573 m	*sc*H_2O, *r*N_3-H, *r*$C_{6,9}$-H, *s*C_6-C_{5a}, *s*C_8-C_9	Same as S_1	Same as S_1
$\nu_{E2/T3'}$	1581 vs	1582 s	1542 s 1528 m	1585 m	*sc*H_2O, *s*C_2=$O_{2'}$, *s*C_4=$O_{4'}$	*r*N_3-H, *s*C_2=$O_{2'}$, *s*C_4=$O_{4'}$, *s*C_8-C_7, *s*C_{9a}-C_{5a}, *s*C_{10a}-C_{4a} ‡	S_1 - *s*C_4=$O_{4'}$
$\nu_{T3''}$	1510 w	1510 m	—	1511 vs	*r*$C_{6,9}$-H, *s*N_1-C_{10a}, *s*N_{10}-C_{9a}, *s*C_4-C_{4a}, *r*N_3-H	—	Same as S_1
ν_{E2}	1475 m	1475 vs	1466 m	—	*r*$C_{6,9}$-H, *r*N_3-H, *ar*CH_3, *sc*$C_{11}H_2$, *s*N_1-C_{10a}, *s*C_4-C_{4a}, *s*C_7-C_8, *s*C_6-C_{5a}	*s*N_1-C_{10a}, *s*C_4-C_{4a}, *s*N_1-C_2, *sc*$C_{11}H_2$, *ar*CH_3	—
$\nu_{T4''}$	1451 vw	1451 w	1446 vw	1468 s	*sc*$C_{11}H_2$, *ar*CH_3	Same as S_1	Same as S_1
$\nu_{T4'}$	1442 vw	1445 vw	1451 s	1444 vw	*sc*$C_{15}H_2$	Same as S_1	Same as S_1
ν_{E3}	1402 s	1403 m	—	—	*s*N_5=C_{4a}	—	—
ν_{T5}	1395 vw	1397 vw	1391 vs	1389 vs	*r*$C_{12,13,14}$-H, *r*$O_{12',14''}$-H, *sc*$C_{11,15}H_2$	*sc*$C_{11}H_2$, *r*$C_{12,13,14}$-H, *r*$O_{13',14'}$-H	*t*$C_{11}H_2$, *r*$C_{12,14}$-H, *r*C_6-H
ν_{E4}	1379 m	1379 w	1374 vw	1373 vw	*t*$C_{11}H_2$, *r*C_{13}-H, *r*$O_{13''}$-H, *sr*CH_3	*sr*CH_3	*sr*CH_3
$\nu_{T6'}$	1362 vw	1362 vw	1371 s	1362 vw	*t*$C_{15}H_2$	Same as S_1	Same as S_1
$\nu_{T6''}$	1358 vw	1358 vw	1363 w	1358 m	*sc*$C_{11,15}H_2$, *r*$C_{12,14}$-H, *r*$O_{12',13''}$-H, *r*C_9-H, *sr*CH_3	*r*N_3-H + S_1 - *sr*CH_3	Same as S_1
v	1328 vw	1328 m	1324 s	1329 w	*r*$C_{12,13,14}$-H	Same as S_1	Same as S_1
v	1308 vw	1309 m	1318 s	1310 w	*r*C_{14}-H, *r*$O_{14''}$-H, *t*$C_{15}H_2$	Same as S_1	Same as S_1
v	1312 w	1314 m	1303 m	1314 w	*r*C_{11}H, *s*N_{10}-C_{10a}, *s*N_5-C_{5a}, *r*$C_{6,9}$-H	Same as S_1	Same as S_1
v	1297 vw	1297 s	—	—	*t*$C_{11}H_2$, *s*C_9-C_{9a}, *s*N_5-C_{4a}, *s*N_{10}-C_{10a}	—	—
ν_{E5}	1284 w	1283 w	1279 m	1277 vw	*r*$C_{6,9}$-H	Same as S_1	Same as S_1
ν_{T7}	1262 w	1265 s	1274 s	1271 m	*r*$C_{12,13,14}$-H	Same as S_1	Same as S_1
v	1243 w	1243 vw	1221 m	1233 m	*t*$C_{15}H_2$, *r*$C_{12,14}$-H, *r*$O_{12',14''}$-H	*r*C_{12}-H, *r*$O_{12''}$-H, *r*C_9-H, rO_{16}H	*r*C_{12}-H, *r*$O_{12''}$-H
$\nu_{E6/T8''}$	1205 s	1195 s	1212 m	1207 s	*r*$C_{12,13}$-H, *r*$O_{12',13''}$-H, *t*$C_{11}H_2$	S_1 + *r*$C_{6,9}$-H	S_1 + *r*C_6-H
$\nu_{T8'}$	1194 s	-	1201 m	1201 w	*r*$C_{12,13,14}$-H, *r*$O_{12',13''}$-H	*r*C_{13}-H, *r*$O_{13''}$-H	Same as S_1
ν_{T9}	1187 m	1187 m	1183 w	1185 s	*r*$C_{6,9}$-H, *t*$C_{11}H_2$, *r*C_{12}-H, *r*$O_{12''}$-H *s*N_3-C_2, *s*C_{4a}-C_{10a}	S_1 - *s*N_3-C_2 - *s*C_{4a}-C_{10a}	Same as T_1 **2'**

Intensities (based on pre-resonance conditions for Triplets) vs: very strong, s: strong, m: medium, w: weak, vw: very weak br: broad
Assignments: *s*: stretch, *a*-: antisymmetric, *s*-: symmetric, *w*: wag, *t*: twist, *sc*: scissor, *r*: rock
‡: Similar modes for both 1542 and 1528 cm^{-1}

5. Cartesian coordinates of all optimised ground–state and excited–state species

1 S_0

N	2.29098300	-8.27933700	18.16522000
C	2.58148000	-7.00646400	17.79603400
O	2.02997400	-6.45225000	16.83794100
N	3.51798200	-6.28378000	18.51671600
C	4.21765100	-6.72430500	19.61775500
O	5.00849700	-6.01601000	20.20611500
C	3.90973800	-8.13062700	19.98204100
N	4.52933100	-8.66269900	20.99535500
C	4.25755300	-9.94309000	21.32379700
C	4.91009500	-10.51814000	22.43275900
C	4.67740200	-11.81472900	22.81382800
C	5.38221000	-12.40730900	23.99775800
C	3.74326900	-12.58798300	22.06369600
C	3.45106800	-14.00163700	22.46208800
C	3.09410100	-12.04267500	20.97126800
C	3.33699800	-10.72523900	20.57550900
N	2.72466700	-10.14062200	19.48085700
C	2.94780600	-8.83225100	19.17812100
C	1.87286300	-10.93130000	18.57152200
C	0.38972500	-10.91668600	18.95215500
O	0.16025000	-12.04541500	19.79743000
C	-0.53001800	-11.02003500	17.72643000
O	-0.27020500	-12.21460600	17.00432800
C	-0.36276000	-9.85298300	16.75216400
O	-0.36348500	-8.62091000	17.47814700
C	-1.47925900	-9.82100000	15.72677200
O	-1.17551100	-9.04481200	14.55097400
P	-0.62864300	-7.54613700	14.53193000
O	-1.26581000	-6.80306900	15.77904900
O	0.91659700	-7.67826000	14.81336700
O	-0.96063200	-6.91025100	13.25000900
H	3.69630900	-5.33816800	18.20324000
H	5.60557500	-9.89155000	22.97474200
H	5.96457200	-13.28571000	23.71103000
H	6.05635700	-11.68268500	24.45018000
H	4.66925800	-12.73373000	24.75815800
H	3.07670400	-14.04780800	23.48733100
H	2.71281300	-14.45348200	21.80322800
H	4.35919100	-14.60840800	22.43282700
H	2.36243000	-12.63893200	20.45283400
H	2.24479600	-11.94947800	18.55909800
H	2.02620100	-10.51384300	17.58435200
H	0.15723000	-9.99555200	19.48674200
H	-0.64730300	-11.90090900	20.30522400
H	-1.56047400	-11.01771000	18.10606600
H	-0.34314500	-12.94955000	17.62786500
H	0.58386000	-9.96775800	16.21889000
H	0.56618000	-8.45413200	17.76869700
H	-2.38951100	-9.42948500	16.18613600
H	-1.66865700	-10.82750500	15.36414300
H	1.29498200	-7.21299600	15.61621600
H	-1.02500100	-7.29342300	16.60658800

1 S_1

N	-0.45832868	1.25260389	-0.12446228
C	-1.10710916	2.46005711	-0.04353521
O	-2.34429412	2.52832774	-0.07879878
N	-0.35929594	3.59194335	0.08621371
C	1.03535180	3.65377271	0.14621108
O	1.59353408	4.73630853	0.27334962
C	1.69571821	2.36403372	0.02896036
N	3.03407275	2.31262921	0.07359480
C	3.58923919	1.07100564	-0.02426615
C	4.97076237	0.94605297	0.02762138
C	5.64304622	-0.29881255	-0.06507732
C	7.12627565	-0.33968033	0.00466261
C	4.88531299	-1.47637027	-0.21822292
C	5.54680481	-2.81830934	-0.30479009
C	3.50564725	-1.36860800	-0.28239316
C	2.83490037	-0.12065139	-0.19662094
N	1.46462867	-0.02663584	-0.28431019
C	0.86460270	1.22305155	-0.12384296
C	0.62153976	-1.18229423	-0.61062405
C	0.15512975	-1.96491811	0.62372776
O	1.12513340	-2.97991301	0.87766178
C	-1.21529770	-2.62863552	0.40776813
O	-1.17179313	-3.52816020	-0.68822413
C	-2.32554709	-1.61663552	0.12229335
O	-2.24496739	-0.53765865	1.05766742
C	-3.69795973	-2.25336193	0.22724387
O	-4.74160944	-1.50818341	-0.42904691
P	-5.05676420	0.04300865	-0.23034699
O	-4.72218321	0.39616240	1.27909976
O	-3.99532933	0.78866693	-1.12555112
O	-6.45415895	0.31812103	-0.58917230
H	-0.85590483	4.47110196	0.14588688
H	5.54972814	1.85291866	0.13949159
H	7.54176192	-0.80428520	-0.89521362
H	7.55447149	0.65285779	0.11828933
H	7.45493790	-0.96516402	0.84098875
H	6.13139258	-3.02844391	0.59398172
H	4.80868001	-3.60879081	-0.42392660
H	6.23630652	-2.86449227	-1.15092835
H	2.92298376	-2.27099532	-0.36406234
H	1.17175207	-1.83785802	-1.27772321
H	-0.22383850	-0.79850361	-1.16593578
H	0.08517868	-1.29184712	1.47802462
H	1.10136754	-3.21952950	1.81184020
H	-1.45247620	-3.16499637	1.33606627
H	-0.46149823	-4.16061622	-0.51624775
H	-2.20680687	-1.23577311	-0.89472751
H	-1.61232240	0.12276979	0.69194633
H	-3.96216905	-2.38722855	1.27847728
H	-3.68630242	-3.22285240	-0.26306135
H	-3.36183682	1.42478850	-0.68143669
H	-3.77663965	0.17047594	1.46564541

1 S_2

N	-0.48972548	1.23934437	-0.07636884
C	-1.11268866	2.43901288	-0.01723252
O	-2.35288360	2.54927574	-0.02138518
N	-0.34828769	3.58102910	0.06165810
C	1.03147824	3.63254253	0.09600576
O	1.62689508	4.69903939	0.17678160
C	1.68598819	2.32213444	0.00930873
N	3.03478063	2.29115600	0.02290398
C	3.58669634	1.05593981	-0.04677166
C	5.01902598	0.94562410	0.02480272
C	5.68740387	-0.25368294	-0.02696933
C	7.18386368	-0.31193900	0.04924207
C	4.91889795	-1.43295822	-0.14847679
C	5.56120690	-2.76877018	-0.19944546
C	3.50136440	-1.34829124	-0.21807888
C	2.83120743	-0.13097186	-0.18889798
N	1.44290447	-0.04310509	-0.27588261
C	0.84806983	1.18719081	-0.10455120
C	0.61814357	-1.19731968	-0.64241174
C	0.13777457	-2.02464577	0.55582137
O	1.09380296	-3.06961458	0.75846620

C	-1.24243011	-2.65598496	0.32592519
O	-1.22090390	-3.51291787	-0.80647671
C	-2.34044516	-1.61746220	0.08861421
O	-2.23335611	-0.57344810	1.05983652
C	-3.71929334	-2.24188183	0.18349679
O	-4.76255620	-1.46590639	-0.43775719
P	-5.05509224	0.08202618	-0.18126492
O	-4.68762921	0.37764626	1.33256018
O	-4.00109537	0.84259186	-1.06991996
O	-6.45658454	0.38438521	-0.50290374
H	-0.84212106	4.46301881	0.10097848
H	5.56212269	1.87702686	0.11813419
H	7.60482953	-0.78414445	-0.84093069
H	7.60578385	0.68699237	0.13832140
H	7.51099952	-0.90023072	0.90933006
H	6.16405498	-2.94282632	0.69935188
H	4.83186652	-3.56892672	-0.29469791
H	6.26522748	-2.82886604	-1.03718575
H	2.94326310	-2.27006102	-0.25682349
H	1.18743138	-1.82786127	-1.31940972
H	-0.22291276	-0.80538646	-1.20186303
H	0.08803570	-1.38860203	1.43938523
H	1.03631758	-3.38181977	1.66953723
H	-1.48463025	-3.22692340	1.23228299
H	-0.50427348	-4.14760442	-0.67307023
H	-2.22399100	-1.20264716	-0.91531193
H	-1.59874378	0.09770844	0.70358250
H	-3.97582863	-2.40843651	1.23209258
H	-3.72238823	-3.19475168	-0.33864294
H	-3.36014724	1.47330125	-0.61746744
H	-3.73931070	0.13204455	1.48930463

1 T_1

N	2.29672816	-8.24436262	18.22318929
C	2.54057918	-6.94744152	17.84527429
O	1.94746014	-6.43220444	16.88792422
N	3.45471925	-6.22553644	18.55756634
C	4.18773930	-6.68130146	19.65038441
O	4.97537036	-5.93880344	20.21616247
C	3.92900128	-8.07446656	20.00535444
N	4.58775733	-8.60517662	21.04462252
C	4.28309331	-9.89943569	21.35081755
C	4.91643735	-10.50828275	22.41846159
C	4.65665934	-11.83760584	22.80080962
C	5.37474341	-12.42399191	23.96343770
C	3.70498826	-12.60435388	22.07328261
C	3.39234624	-14.01586000	22.46712563
C	3.07127122	-12.02263288	20.99877550
C	3.33537924	-10.69253078	20.60390249
N	2.73075720	-10.13052173	19.51348138
C	2.98390521	-8.76741162	19.22152239
C	1.90391114	-10.90963681	18.58259934
C	0.41424103	-10.92272077	18.94619935
O	0.19275801	-12.05278286	19.79071343
C	-0.48834803	-11.04635779	17.70890928
O	-0.19877601	-12.23708286	16.99286023
C	-0.33064002	-9.87894272	16.73437223
O	-0.36948503	-8.64415264	17.45610723
C	-1.43482511	-9.87132670	15.69523311
O	-1.13235908	-9.09111464	14.52232105
P	-0.62698304	-7.57850756	14.50451503
O	-1.30369209	-6.84672248	15.73777113
O	0.91776107	-7.66466053	14.81037704
O	-0.95421107	-6.95761448	13.21457293
H	3.61916326	-5.27108138	18.26482633
H	5.64039340	-9.92517170	22.97071065
H	5.92965344	-13.31734995	23.66227668
H	6.06625641	-11.71377085	24.40931478
H	4.66411833	-12.75313593	24.72734877
H	3.01923122	-14.06712500	23.49248768
H	2.63977419	-14.44373304	21.80805056
H	4.28422931	-14.64504905	22.42153262
H	2.32338317	-12.58839892	20.46874348
H	2.28468916	-11.92498385	18.55000233
H	2.05816915	-10.47878873	17.60207125
H	0.15876901	-10.00506572	19.47576242
H	-0.60406304	-11.90709486	20.31467246
H	-1.52298311	-11.06142680	18.07647030
H	-0.27474902	-12.97318291	17.61460529
H	0.62500205	-9.97445371	16.21346819
H	0.54416204	-8.45737160	17.76822629
H	-2.35850417	-9.49828367	16.14288415
H	-1.59849511	-10.88220077	15.33243908
H	1.26309009	-7.20489954	15.62764913
H	-1.06328207	-7.32135155	16.57260719

2 S_0

N	2.44918918	-8.12203859	18.39703534
C	2.71706219	-6.80553550	18.14324331
O	2.16564015	-6.18392046	17.24719822
N	3.65538726	-6.14716545	18.94618639
C	4.35053632	-6.67507547	20.00357746
O	5.14306237	-6.02167143	20.65534148
C	4.03323129	-8.10492759	20.25503344
N	4.63143533	-8.71521665	21.23332253
C	4.34217231	-10.01630470	21.46673457
C	4.97558736	-10.67461279	22.53876263
C	4.71905934	-11.99027787	22.83208167
C	5.40597439	-12.67204290	23.97858371
C	3.77683627	-12.69394089	22.02842161
C	3.45375725	-14.12498101	22.33261259
C	3.14695723	-12.06501389	20.97012950
C	3.41802125	-10.72928876	20.65977948
N	2.82984121	-10.06111474	19.60123141
C	3.07709722	-8.73727064	19.38149839
C	1.94133714	-10.74689676	18.65187234
C	0.46810803	-10.52886478	18.97870735
O	0.13889001	-11.43878183	20.03163746
C	-0.43955103	-10.79387177	17.77359131
O	-0.30576002	-12.14410985	17.34366723
C	-0.15231101	-9.89687273	16.56316619
O	-0.00218100	-8.53513059	16.96203222
C	-1.29562609	-9.98893174	15.56608110
O	-0.95829407	-9.44564869	14.29372203
P	-1.26599409	-7.87685458	13.92261902
O	-2.53414718	-7.46200353	14.60096605
O	0.00111800	-7.10991450	14.58913603
O	-1.11914908	-7.76273353	12.44323089
H	3.82509828	-5.17524037	18.72236537
H	5.67596539	-10.09720775	23.12742867
H	5.97539441	-13.53994397	23.63848667
H	6.08995546	-11.99052388	24.48080377
H	4.68346834	-13.03502696	24.71307876
H	3.06525322	-14.22933503	23.34834069
H	2.71528620	-14.51988403	21.63811756
H	4.35023731	-14.74674507	22.27463159
H	2.41188417	-12.61650093	20.40885749
H	2.17656716	-11.80389587	18.65067836
H	2.18186216	-10.35428275	17.67052927
H	0.31662002	-9.50235569	19.31222639
H	-0.65007805	-11.12036582	20.48637249
H	-1.46861810	-10.60457676	18.10836931
H	-0.43285603	-12.70243593	18.12262429
H	0.75992805	-10.24924471	16.07027817
H	0.86388306	-8.41035563	17.40953826
H	-2.17116316	-9.47711468	15.97223216
H	-1.53791311	-11.03994681	15.41196611
H	0.10002301	-7.39782052	15.52077914

2 S_1

N	-0.30272190	1.35655302	-0.02140586
C	-0.86851543	2.58814070	0.05996843
O	-2.09264182	2.76365972	0.08945562
N	-0.02280259	3.68291324	0.12228984
C	1.36256561	3.66013942	0.12191510
O	1.99320700	4.71761050	0.19607606
C	1.93463376	2.33148057	0.01725416
N	3.27995575	2.21082532	-0.01851224
C	3.78093318	0.95239456	-0.09333183
C	5.17695437	0.76296308	-0.09712489
C	5.76437503	-0.48714188	-0.15761576
C	7.26183843	-0.62640324	-0.15913089
C	4.93542484	-1.62549760	-0.20790904
C	5.52430282	-3.00784252	-0.25092898
C	3.55229653	-1.46196144	-0.20886958
C	2.96106049	-0.20264182	-0.16834426
N	1.56703721	-0.01972754	-0.20387512
C	1.03668789	1.24444643	-0.06051176
C	0.67013756	-1.12881558	-0.51215192
C	0.07195043	-1.80684177	0.72135438
O	0.97949191	-2.83347674	1.13824865
C	-1.29348425	-2.44995189	0.44852214
O	-1.18093872	-3.47726438	-0.52791306
C	-2.33555173	-1.45297093	-0.05917892
O	-2.30788997	-0.26967562	0.73421553
C	-3.72787111	-2.04769270	-0.01000614
O	-4.65317840	-1.24126448	-0.77431268
P	-5.49826052	-0.03196748	-0.20258102
O	-6.88580370	-0.41769917	0.25429412
O	-4.66825393	0.59134521	0.95519094
O	-5.79867281	0.90880577	-1.35507220
H	-0.46173600	4.59003662	0.18824129
H	5.79208249	1.65291903	-0.04873605
H	7.61399800	-1.14148042	-1.05654765
H	7.74416121	0.34939236	-0.11805540
H	7.60941649	-1.21256232	0.69548281
H	6.15489667	-3.20310436	0.62058862
H	4.74176558	-3.76521775	-0.27661519
H	6.15699777	-3.14701324	-1.13171539
H	2.93453623	-2.34539607	-0.20742799
H	1.20969142	-1.86028818	-1.10571479
H	-0.11755766	-0.72774468	-1.13982489
H	-0.04321102	-1.06835712	1.51493640
H	0.79273707	-3.06240869	2.05670481
H	-1.64495236	-2.87071115	1.40074910
H	-0.44355532	-4.04086257	-0.25598937
H	-2.11664164	-1.20922621	-1.10236405
H	-1.56167076	0.33663123	0.42200862
H	-4.06962303	-2.14196426	1.02141790
H	-3.72947023	-3.02765869	-0.47791721
H	-3.66722313	0.37343348	0.90509215

2 S_2

N	-0.10984402	1.54193309	-0.11576515
C	-0.59281610	2.83121605	0.03822208
O	-1.79856639	3.04758214	0.06981910
N	0.32409047	3.84618745	0.15349354
C	1.71218744	3.71222937	0.15475453
O	2.42461157	4.70474895	0.27595621
C	2.18124648	2.34749462	0.00312308
N	3.50057445	2.10293429	-0.00192488
C	3.87340935	0.79697535	-0.10498464
C	5.22372540	0.47688708	-0.08718689
C	5.70250833	-0.84672762	-0.17148834
C	7.16735420	-1.10594665	-0.14201066
C	4.77763389	-1.91004437	-0.27556903
C	5.24129268	-3.33362157	-0.34734034
C	3.42661624	-1.61092833	-0.30558402
C	2.94619675	-0.28366375	-0.23536719
N	1.60479818	0.01442944	-0.29636755
C	1.19234538	1.33327089	-0.13432893
C	0.58114789	-1.00867552	-0.51790941
C	-0.01929280	-1.51927973	0.79176713
O	0.90670072	-2.45547122	1.34393371
C	-1.36995402	-2.21369663	0.57559889
O	-1.21278107	-3.34750262	-0.26787947
C	-2.44255400	-1.31893659	-0.05681847
O	-2.47391068	-0.03549903	0.56810983
C	-3.81039315	-1.96525069	0.09753883
O	-4.79684896	-1.36615163	-0.73490790
P	-5.73975559	-0.13474721	-0.19834820
O	-5.99794646	-0.32764036	1.26305446
O	-4.78247974	1.15764761	-0.43038195
O	-6.86769303	-0.02146857	-1.16639669
H	-0.04052644	4.78271679	0.26264917
H	5.92795361	1.29386205	-0.00348481
H	7.48417966	-1.64403530	-1.04062825
H	7.73825485	-0.18385772	-0.06609044
H	7.42855043	-1.75175698	0.70222670
H	5.82812856	-3.60423023	0.53376526
H	4.39536797	-4.01492168	-0.41491016
H	5.88167733	-3.49792524	-1.21744577
H	2.72400960	-2.42549488	-0.35378215
H	1.01471766	-1.82925210	-1.07717376
H	-0.18332164	-0.56133676	-1.14072351
H	-0.16003392	-0.68397280	1.47695344
H	0.81394739	-2.46812593	2.30380090
H	-1.71852555	-2.52681913	1.56896992
H	-0.51956190	-3.89737053	0.12146626
H	-2.23234693	-1.21416090	-1.12605758
H	-1.71113793	0.50078956	0.27087945
H	-4.11864551	-1.91026203	1.14403633
H	-3.73346234	-3.01125688	-0.19733738
H	-3.91283612	0.99245526	-0.01290071

2 S_2 (b)

N	-0.10977000	1.54201512	-0.11601678
C	-0.59271121	2.83133876	0.03786866
O	-1.79845564	3.04776347	0.06913576
N	0.32422635	3.84624866	0.15342173
C	1.71231894	3.71221821	0.15489780
O	2.42477093	4.70468983	0.27631170
C	2.18134028	2.34748135	0.00319861
N	3.50064587	2.10287704	-0.00166423
C	3.87343619	0.79690697	-0.10481128
C	5.22373278	0.47677765	-0.08702533
C	5.70247643	-0.84684760	-0.17141015
C	7.16730843	-1.10611875	-0.14195218
C	4.77757186	-1.91013713	-0.27559111
C	5.24119812	-3.33372010	-0.34743511
C	3.42657041	-1.61098250	-0.30560552
C	2.94619069	-0.28369987	-0.23533784
N	1.60481934	0.01444800	-0.29645699
C	1.19240778	1.33330094	-0.13443629
C	0.58113098	-1.00862136	-0.51802160
C	-0.01928948	-1.51917701	0.79168051
O	0.90674366	-2.45534883	1.34381654
C	-1.36995807	-2.21356901	0.57558748
O	-1.21280412	-3.34746806	-0.26777913
C	-2.44258126	-1.31888794	-0.05688814
O	-2.47391909	-0.03533901	0.56783206
C	-3.81040356	-1.96516755	0.09770510
O	-4.79698003	-1.36624927	-0.73473568
P	-5.73983200	-0.13480965	-0.19820803
O	-5.99790063	-0.32754345	1.26324895
O	-4.78257985	1.15758249	-0.43047947
O	-6.86791597	-0.02163735	-1.16609864
H	-0.04035775	4.78279395	0.26255158
H	5.92798960	1.29372210	-0.00326839

H	7.48415262	-1.64365814	-1.04090280
H	7.73823485	-0.18409336	-0.06547139
H	7.42844793	-1.75247704	0.70187331
H	5.82788514	-3.60443329	0.53373863
H	4.39526273	-4.01498709	-0.41520314
H	5.88171654	-3.49795575	-1.21745401
H	2.72393587	-2.42552298	-0.35381428
H	1.01467360	-1.82920645	-1.07729497
H	-0.18333363	-0.56126139	-1.14082307
H	-0.15996339	-0.68383893	1.47684431
H	0.81378440	-2.46823588	2.30366269
H	-1.71852835	-2.52661062	1.56898758
H	-0.51947308	-3.89721076	0.12154789
H	-2.23246222	-1.21427426	-1.12616066
H	-1.71111805	0.50089106	0.27059412
H	-4.11853621	-1.90997807	1.14423042
H	-3.73350347	-3.01123419	-0.19696749
H	-3.91288811	0.99242529	-0.01309453

2 T_1

N	2.30585516	-8.26928560	18.10923431
C	2.59156818	-7.02039750	17.73495930
O	2.05398015	-6.45516047	16.73612222
N	3.49328625	-6.28488943	18.45306934
C	4.18369930	-6.72298851	19.57986641
O	4.96369036	-5.95878745	20.14799248
C	3.89875828	-8.09471156	19.94916143
N	4.55676233	-8.62412561	21.00901450
C	4.26649631	-9.91112569	21.32327356
C	4.91134535	-10.51197376	22.42269062
C	4.67167233	-11.81673885	22.81090765
C	5.39122839	-12.40599788	23.99199570
C	3.73583727	-12.57943889	22.08253660
C	3.42599824	-13.99677501	22.47339363
C	3.08605022	-12.00623087	20.99139851
C	3.33723724	-10.69762877	20.59101046
N	2.71078719	-10.11572975	19.47433539
C	2.96603122	-8.79883761	19.16433140
C	1.88454614	-10.92141079	18.57340536
C	0.39729303	-10.96366178	18.94567134
O	0.18143801	-12.12039187	19.76519841
C	-0.52816704	-11.06478179	17.72646627
O	-0.27048102	-12.26005487	16.99839320
C	-0.37340203	-9.88800970	16.76264521
O	-0.38335003	-8.66273761	17.47261127
C	-1.50030911	-9.85158569	15.75498516
O	-1.24553909	-8.96361166	14.64515605
P	-0.58166704	-7.52851053	14.68810604
O	-1.30904609	-6.54457947	15.60950015
O	0.91483707	-7.72144855	14.99017808
O	-0.85673206	-6.89109949	13.33376693
H	3.67947326	-5.34200236	18.14103029
H	5.62140039	-9.90150573	22.96701567
H	5.97016841	-13.28819197	23.70676668
H	6.07385244	-11.68137584	24.43391274
H	4.69011934	-12.72798990	24.76632876
H	3.04869022	-14.05670899	23.49789571
H	2.67687919	-14.42993003	21.81187857
H	4.31841931	-14.62737004	22.43232159
H	2.34489917	-12.59275289	20.47380649
H	2.28311116	-11.93198487	18.55098332
H	2.01026115	-10.50319778	17.58240925
H	0.14196801	-10.06099171	19.50100338
H	-0.64921005	-12.01227688	20.24384743
H	-1.55798511	-11.07246581	18.11060429
H	-0.27229102	-12.98354092	17.63994225
H	0.56671704	-10.00642570	16.21762117
H	0.54971104	-8.47248363	17.73085426
H	-2.42146617	-9.53000568	16.24443617
H	-1.64819112	-10.83301877	15.31215609
H	1.39185110	-7.17688849	15.80271515

3 S_0

N	2.65427419	-7.92413757	18.59890636
C	2.96966121	-6.60423245	18.44570732
O	2.47392718	-5.90227941	17.57652628
N	3.89691828	-6.02952241	19.32546936
C	4.54411133	-6.64970645	20.36160646
O	5.33210839	-6.06615841	21.08261851
C	4.18161530	-8.08410960	20.49954646
N	4.73260734	-8.77941665	21.44826554
C	4.39968032	-10.08477373	21.57950557
C	4.98471736	-10.83654277	22.61699064
C	4.68247633	-12.16107888	22.80933863
C	5.31720739	-12.94294091	23.92164175
C	3.74357527	-12.77684693	21.93321558
C	3.37175224	-14.21560203	22.12561358
C	3.16074723	-12.05539085	20.90781449
C	3.47619825	-10.70883277	20.70135249
N	2.93306521	-9.94887471	19.68188940
C	3.23224423	-8.62246363	19.55674242
C	2.02541815	-10.53074076	18.68257637
C	0.56189104	-10.27967675	19.02452139
O	0.21558002	-11.20518680	20.06087646
C	-0.35850703	-10.49028876	17.82064527
O	-0.24873002	-11.83232185	17.35241924
C	-0.07637101	-9.55090569	16.63945820
O	0.09024501	-8.20943861	17.08450622
C	-1.23061309	-9.59475771	15.65654411
O	-0.87093506	-8.98631066	14.43975506
P	-2.07697715	-8.82770661	13.26274695
O	-3.16663723	-7.98520658	13.91751601
O	-1.31935309	-8.12726659	12.14491590
O	-2.51503518	-10.25325175	12.94033894
H	4.10015530	-5.04989736	19.17574036
H	5.68537040	-10.32402773	23.26266065
H	5.87284843	-13.80031500	23.53507269
H	6.00427441	-12.31920090	24.49045776
H	4.56419833	-13.33681097	24.60803777
H	2.95120121	-14.37956104	23.12054365
H	2.64238519	-14.53769005	21.38541452
H	4.25132331	-14.85890207	22.04733758
H	2.42700617	-12.54415590	20.28982346
H	2.22204416	-11.59261186	18.60434032
H	2.27930017	-10.07446673	17.73277830
H	0.44272403	-9.25725767	19.38217737
H	-0.57434804	-10.88499477	20.51247347
H	-1.38187810	-10.29912274	18.17288131
H	-0.37153203	-12.40798891	18.11926729
H	0.82669606	-9.89841173	16.12412317
H	0.97225107	-8.09946558	17.48497825
H	-2.08635015	-9.07824267	16.10995413
H	-1.51569511	-10.63972376	15.49812712

3 S_1

N	0.34858596	1.88358806	-0.08265397
C	0.13539565	3.24676430	0.03295236
O	-1.00171767	3.70017092	0.09364574
N	1.23706828	4.06548939	0.07694261
C	2.57065593	3.66066201	0.03521446
O	3.46818600	4.49753263	0.09005161
C	2.75652973	2.22664396	-0.07664008
N	4.00155127	1.72708149	-0.11779305
C	4.10764817	0.37166142	-0.18858460
C	5.36976972	-0.20643995	-0.20915588
C	5.57751233	-1.59813140	-0.26705993
C	6.96470212	-2.13877867	-0.28134756
C	4.45943431	-2.46144934	-0.30525070
C	4.63260713	-3.94996971	-0.34712357

C	3.19170573	-1.90493786	-0.29745769
C	2.98173485	-0.50918633	-0.24812436
N	1.72227691	0.04460116	-0.26444150
C	1.58293808	1.42283551	-0.13841347
C	0.51087777	-0.76582450	-0.41140714
C	-0.10061080	-1.15153585	0.93455986
O	0.66630632	-2.24151724	1.45122519
C	-1.56587219	-1.58267901	0.79401951
O	-1.66540387	-2.70261386	-0.07917132
C	-2.49292567	-0.47989018	0.26685798
O	-2.26140828	0.73976670	0.96466240
C	-3.94643904	-0.87922158	0.44977056
O	-4.78767233	0.02861915	-0.21668520
P	-6.41339568	-0.39733243	-0.41562484
O	-6.92438045	-0.70348498	0.98835114
O	-6.98188260	0.86961369	-1.03787882
O	-6.40012974	-1.60824890	-1.34363593
H	1.06751864	5.05863270	0.15909405
H	6.22191343	0.45920847	-0.17809627
H	7.13674405	-2.74279464	-1.17744592
H	7.70637203	-1.34421038	-0.24808331
H	7.12837426	-2.80783110	0.56905406
H	5.18292763	-4.30959116	0.52584153
H	3.66766357	-4.45283166	-0.37100745
H	5.19983008	-4.25910754	-1.22848317
H	2.34316403	-2.56749972	-0.29703090
H	0.74873940	-1.65359344	-0.98587441
H	-0.19295092	-0.18042063	-0.98884389
H	-0.04916951	-0.30151909	1.61375407
H	0.59874356	-2.24824546	2.41312949
H	-1.90239234	-1.86077646	1.80238936
H	-1.06469444	-3.38026944	0.25856360
H	-2.31257847	-0.34514560	-0.80528416
H	-1.50847357	1.20268112	0.56038116
H	-4.16770698	-0.90001338	1.52529727
H	-4.07862734	-1.89384861	0.06126181

3 S_2

N	-0.12306415	1.71811863	0.35109018
C	-0.45287015	3.02920574	0.42960653
O	-1.60773016	3.42742154	0.63412862
N	0.56229563	3.96422626	0.27924361
C	1.90266085	3.70136571	0.05143568
O	2.70112104	4.63704718	-0.06138592
C	2.22147686	2.29111083	-0.04096262
N	3.50181986	1.93057583	-0.28459165
C	3.76272641	0.60113743	-0.34804040
C	5.08369880	0.16539195	-0.57489634
C	5.43345134	-1.17067900	-0.63965873
C	6.86117314	-1.57439916	-0.88641113
C	4.43077003	-2.14458335	-0.46143965
C	4.76233375	-3.61042872	-0.49920618
C	3.11766879	-1.73730620	-0.23914062
C	2.76056279	-0.39222787	-0.19454672
N	1.43551132	0.03367439	-0.00704689
C	1.15213135	1.37867799	0.11258219
C	0.32273211	-0.90887940	-0.04558195
C	-0.15956065	-1.34935912	1.33392065
O	0.69575216	-2.41687538	1.77030393
C	-1.60744457	-1.84700887	1.32288425
O	-1.72905990	-2.98707592	0.47352074
C	-2.60376412	-0.78485830	0.84920848
O	-2.41967649	0.42363643	1.56797711
C	-4.02961901	-1.26359324	1.05208615
O	-5.00250758	-0.37569587	0.49195439
P	-5.29341850	-0.33593579	-1.10224298
O	-5.32255833	-1.77091037	-1.62444667
O	-6.52207456	0.49357103	-1.25789071
O	-4.04412992	0.20420309	-1.82387402
H	0.29590524	4.93598705	0.34452648
H	5.83748785	0.93303793	-0.69955197
H	6.95393776	-2.18259817	-1.78992557
H	7.49955136	-0.69924170	-1.00122556
H	7.25504247	-2.17530795	-0.06259241
H	5.49790682	-3.87633547	0.26481093
H	3.87218375	-4.21638183	-0.33413596
H	5.19304124	-3.90023856	-1.46155813
H	2.37212777	-2.49652234	-0.06658477
H	0.61596566	-1.77546117	-0.62931342
H	-0.48470484	-0.41763477	-0.57571030
H	-0.08420006	-0.50872533	2.02330313
H	0.59195506	-2.52546642	2.72326405
H	-1.86095455	-2.12396874	2.35655179
H	-1.00002647	-3.57962914	0.70279012
H	-2.45681174	-0.61714319	-0.21865497
H	-1.68605963	0.92290506	1.14862895
H	-4.24446534	-1.30952648	2.12127201
H	-4.14439966	-2.25884977	0.62354615

3 S_2 (b)

N	0.25324141	1.83143044	0.03029449
C	0.01835766	3.16327764	0.11340403
O	-1.11797730	3.64959901	0.18581098
N	1.11350563	4.01703452	0.12353819
C	2.44804664	3.65321881	0.05391904
O	3.32516218	4.52305750	0.07220434
C	2.66533004	2.22517791	-0.04394726
N	3.93490589	1.76872146	-0.13473412
C	4.10115271	0.42573595	-0.20801045
C	5.40433103	-0.10612161	-0.28287997
C	5.65921354	-1.46325353	-0.34551633
C	7.07278885	-1.97066229	-0.42611246
C	4.57229135	-2.35982656	-0.32337385
C	4.79655358	-3.84563459	-0.36499493
C	3.27533597	-1.85670385	-0.25291633
C	3.01579040	-0.48952826	-0.21035299
N	1.71385928	0.03656287	-0.17290274
C	1.51945105	1.39711971	-0.05431240
C	0.54352379	-0.81828734	-0.33441162
C	-0.11139504	-1.20108748	0.98877901
O	0.64613351	-2.28395634	1.54817481
C	-1.56557907	-1.64795703	0.82551572
O	-1.63503133	-2.81489316	0.00865026
C	-2.47052168	-0.57821142	0.20271915
O	-2.28724691	0.67590269	0.83382028
C	-3.92239011	-0.97880758	0.34418078
O	-4.72458032	-0.12804932	-0.47746124
P	-6.33225847	-0.32404219	-0.47765004
O	-6.82419313	-0.23704766	0.97238154
O	-6.86121659	0.69468614	-1.42810082
O	-6.63390570	-1.79281636	-0.79671997
H	0.91520206	5.00490224	0.18943032
H	6.22260152	0.60336569	-0.28854941
H	7.23324465	-2.56426274	-1.32984590
H	7.78328223	-1.14495895	-0.43363659
H	7.31453586	-2.61798328	0.42087551
H	5.40647632	-4.18387418	0.47711027
H	3.85039873	-4.38462887	-0.33265187
H	5.32474193	-4.14686334	-1.27376282
H	2.46115293	-2.56095466	-0.19820073
H	0.82945533	-1.71133058	-0.87993861
H	-0.16322019	-0.27442068	-0.95100280
H	-0.08281896	-0.34359618	1.66073156
H	0.43761348	-2.35253722	2.48757451
H	-1.94390762	-1.87555995	1.83264142
H	-0.96780374	-3.42781413	0.34687777
H	-2.24459518	-0.51196052	-0.86763259
H	-1.45655277	1.09069184	0.51186979
H	-4.22426345	-0.87839295	1.39048415
H	-4.05109085	-2.01798480	0.03878976

3 T_1

N	2.42216217	-8.08967458	18.40765334
C	2.69530119	-6.79117246	18.12999631
O	2.14511616	-6.16286042	17.21587622
N	3.63370326	-6.14211646	18.91989538
C	4.34624331	-6.68682046	19.97743442
O	5.15497537	-5.98616142	20.59678246
C	4.04700129	-8.07755457	20.23432647
N	4.71128034	-8.71218563	21.23252754
C	4.38843931	-10.00952573	21.45664056
C	5.03406136	-10.71171277	22.49475260
C	4.75105334	-12.03044586	22.79964162
C	5.47361737	-12.72693192	23.91957674
C	3.76696427	-12.70323790	22.04786157
C	3.40434324	-14.12960401	22.35293860
C	3.11804922	-12.03016889	21.01396353
C	3.41600925	-10.70907577	20.69200547
N	2.79802020	-10.02647374	19.63203841
C	3.08084322	-8.69494763	19.40691742
C	1.90987314	-10.71340677	18.70017733
C	0.43103403	-10.52744976	19.02561235
O	0.09897001	-11.45176583	20.07184445
C	-0.48053703	-10.79126779	17.82488430
O	-0.34646602	-12.14236786	17.38853723
C	-0.20012001	-9.87573273	16.62728220
O	-0.10124301	-8.52405661	17.03314321
C	-1.31922210	-9.99133674	15.60942014
O	-0.94835907	-9.42596668	14.35212405
P	-1.36192110	-7.92971557	13.89382400
O	-2.56845818	-7.48093554	14.64802208
O	-0.11641301	-7.02688050	13.99161998
O	-1.47338411	-8.01477155	12.36454790
H	3.81674128	-5.17338437	18.70105233
H	5.77881839	-10.16768072	23.06310267
H	6.00829642	-13.61084398	23.56199871
H	6.19693547	-12.06174088	24.38973178
H	4.77937335	-13.07154796	24.69055476
H	3.04432422	-14.24233204	23.37941266
H	2.62420519	-14.48674605	21.68161053
H	4.26710131	-14.79386809	22.25072558
H	2.34189317	-12.55278392	20.47851346
H	2.15804316	-11.76965086	18.68753534
H	2.12081815	-10.31866372	17.71256828
H	0.26846002	-9.50575370	19.36823742
H	-0.72363205	-11.16531181	20.48654050
H	-1.51131211	-10.60964474	18.16228332
H	-0.40883803	-12.69488193	18.17976130
H	0.72683805	-10.20628171	16.14496016
H	0.78174906	-8.36196962	17.43295525
H	-2.21342216	-9.49609769	15.99159316
H	-1.53849011	-11.04330582	15.43075011

1' S_0

N	2.35885017	-8.29507659	18.06862032
C	2.67492020	-7.04340353	17.66326727
O	2.09089015	-6.51029248	16.70139819
N	3.64877726	-6.31755248	18.31815634
C	4.32046631	-6.73575147	19.43079141
O	5.12625537	-6.02752043	20.01980844
C	3.99987729	-8.11832958	19.85066244
N	4.61914833	-8.62717262	20.87892252
C	4.33397031	-9.88890570	21.25717752
C	4.99130536	-10.43566576	22.37830763
C	4.74116434	-11.71399882	22.80392965
C	5.44979339	-12.27860888	23.99850474
C	3.78473727	-12.49723788	22.09004758
C	3.47551725	-13.89106498	22.53938463
C	3.13133023	-11.97928485	20.98745953
C	3.39026024	-10.68039378	20.54430549
N	2.77502520	-10.12331175	19.43898741
C	3.01974422	-8.83172063	19.08751635
C	1.88677314	-10.92355078	18.57239733
C	0.41348203	-10.86273080	18.98675036
O	0.17982201	-11.96124985	19.86907140
C	-0.53751904	-10.97927780	17.78598427
O	-0.32006402	-12.19812790	17.09146421
C	-0.37085503	-9.84442872	16.77391722
O	-0.32232902	-8.59104764	17.46113225
C	-1.51692711	-9.81501970	15.78148614
O	-1.23188609	-9.08242566	14.57326404
P	-0.63756005	-7.60547857	14.48429405
O	-1.20408909	-6.79752651	15.72464012
O	0.91297507	-7.78201056	14.71971909
O	-0.98801307	-7.00166653	13.19233696
H	3.86913628	-5.37006040	17.93996029
H	5.70438040	-9.80630870	22.89331065
H	6.01178942	-13.17711094	23.73469671
H	6.14274745	-11.55176683	24.41741976
H	4.74010934	-12.56513592	24.77771676
H	3.11669122	-13.89636501	23.57114268
H	2.72012919	-14.35205705	21.90705359
H	4.37354431	-14.51299102	22.51710764
H	2.38443617	-12.58071093	20.49760946
H	2.23694416	-11.94930786	18.58405934
H	2.02712215	-10.53989177	17.56983425
H	0.21473702	-9.92163373	19.49989439
H	-0.61123505	-11.78434484	20.39245247
H	-1.55781211	-10.94457478	18.19050032
H	-0.39877703	-12.91507793	17.73488728
H	0.55681704	-9.99827971	16.21767816
H	0.61755105	-8.43796862	17.72188926
H	-2.40255217	-9.38672168	16.25590619
H	-1.74192613	-10.82678977	15.45580713
H	1.32299309	-7.30934754	15.49717709
H	-0.96026107	-7.27037152	16.56144118
O	6.57222347	-7.13341949	22.50992761
H	6.68633346	-6.25974246	22.12005458
H	5.92381444	-7.55909856	21.91919260
O	5.07539336	-3.21881023	19.92767641
H	5.13690837	-4.18795330	20.04303446
H	4.44798332	-2.91730721	20.59457950
O	1.52414911	-3.75276527	16.55361719
H	1.62519112	-4.72379534	16.53176719
H	1.32091709	-3.49137625	15.64828911
O	4.18577930	-3.76328227	17.35865924
H	4.39934432	-3.32881324	18.20880329
H	3.28115924	-3.49768725	17.09921523

1' S_1

N	-0.44818946	0.43064433	-0.33916242
C	-1.11098784	1.62811346	-0.36722745
O	-2.35889622	1.65313982	-0.39068666
N	-0.40305445	2.78655706	-0.36041328
C	0.97711122	2.86685023	-0.26763190
O	1.53579432	3.96759269	-0.20891477
C	1.67257108	1.59597091	-0.26302394
N	3.01085348	1.57507937	-0.19006471
C	3.59886041	0.34348576	-0.17322246
C	4.98339603	0.25845094	-0.08141167
C	5.68635763	-0.97459594	-0.05185105
C	7.16737685	-0.97119671	0.05716039
C	4.95861973	-2.17501064	-0.12268366
C	5.64789693	-3.50474847	-0.08538805
C	3.57726683	-2.10428423	-0.22771822
C	2.87521552	-0.86854353	-0.25759991
N	1.50394150	-0.81666283	-0.36963666
C	0.87357281	0.42482306	-0.32625334
C	0.68680447	-2.01658572	-0.58215108

C	0.23855040	-2.68026913	0.72615007
O	1.23395841	-3.63824415	1.07953047
C	-1.11666229	-3.39438703	0.58220594
O	-1.05548348	-4.39574776	-0.41988360
C	-2.25058256	-2.44055451	0.20177690
O	-2.19329991	-1.27055977	1.02236695
C	-3.60819325	-3.09308203	0.37918337
O	-4.67089324	-2.44165599	-0.34341907
P	-5.01661859	-0.88526983	-0.31644643
O	-4.68564824	-0.35709320	1.14145977
O	-3.96996262	-0.22320373	-1.29438677
O	-6.41853579	-0.67750528	-0.70037143
H	-0.93747666	3.67701755	-0.41305552
H	5.54352391	1.18261212	-0.03472079
H	7.61728213	-1.51186405	-0.78130663
H	7.57013159	0.03788262	0.08398446
H	7.48600050	-1.50313052	0.95963997
H	6.23304515	-3.61906802	0.82981725
H	4.92727858	-4.31828251	-0.13371369
H	6.34117241	-3.61121898	-0.92296228
H	3.01723456	-3.02407016	-0.25365716
H	1.25047068	-2.72317021	-1.18229993
H	-0.16582590	-1.70584706	-1.17117745
H	0.15095621	-1.92645129	1.50820198
H	1.22647217	-3.77206009	2.03496799
H	-1.33868860	-3.84080487	1.56036888
H	-0.34021271	-5.00134698	-0.18422056
H	-2.14338067	-2.16276559	-0.84943284
H	-1.57721102	-0.63616657	0.58960532
H	-3.86554730	-3.12402627	1.44012142
H	-3.57722510	-4.10712740	-0.00958127
H	-3.35150693	0.46394749	-0.91882743
H	-3.73729601	-0.54703552	1.35201025
O	4.54772192	3.97203958	0.13110189
H	3.87038225	4.65521748	0.07041521
H	4.02153910	3.15115964	0.01962351
O	0.35736792	6.21875657	0.88954624
H	0.83850058	5.44311422	0.52869397
H	0.42659187	6.14551896	1.84810319
O	-3.82681488	3.67369640	0.90571007
H	-3.41472588	2.90777086	0.46061815
H	-4.72919847	3.71587147	0.56931325
O	-1.86927137	5.17702923	-0.38964001
H	-1.26542956	5.69137937	0.18349242
H	-2.62377427	4.88009236	0.15642591

1' S_2

N	-0.47698463	0.42494413	-0.27458490
C	-1.10365793	1.62223193	-0.31486174
O	-2.35423737	1.69797118	-0.32514242
N	-0.36958028	2.77886156	-0.33030223
C	0.99754916	2.83203269	-0.25197707
O	1.60623972	3.90507331	-0.21095376
C	1.67536108	1.53540231	-0.24067489
N	3.02243314	1.52105143	-0.19905484
C	3.59938720	0.29331127	-0.16724835
C	5.02902688	0.21474463	-0.06900450
C	5.71068931	-0.97438747	-0.01599738
C	7.20576887	-1.00682460	0.08728016
C	4.95714058	-2.17440536	-0.05550163
C	5.61964976	-3.49862313	0.00527551
C	3.54252469	-2.11812556	-0.15609201
C	2.85739542	-0.91209466	-0.22714556
N	1.46998758	-0.84889649	-0.34300568
C	0.85929523	0.38059849	-0.28452610
C	0.65858734	-2.04223909	-0.60428835
C	0.18097978	-2.75570123	0.66595592
O	1.14828875	-3.76360655	0.97181590
C	-1.19110346	-3.42307982	0.49305765
O	-1.15540575	-4.38248226	-0.55299687
C	-2.30258135	-2.42683610	0.15602766
O	-2.21452869	-1.29426495	1.02506304
C	-3.67274729	-3.05840372	0.30992309
O	-4.72757036	-2.35890710	-0.37933604
P	-5.04011186	-0.79781704	-0.28611763
O	-4.67704102	-0.33598006	1.18616102
O	-3.99320150	-0.12149066	-1.25259076
O	-6.44320699	-0.54593943	-0.64001191
H	-0.89070126	3.67834330	-0.39302162
H	5.56173216	1.15606689	-0.03928641
H	7.64665766	-1.55297828	-0.74923212
H	7.61425105	0.00156115	0.09130383
H	7.52555327	-1.50941076	1.00275638
H	6.26204924	-3.57355877	0.88943074
H	4.90157816	-4.31429165	0.01638478
H	6.29090973	-3.63172482	-0.85203955
H	2.99814896	-3.04839391	-0.13915571
H	1.23846412	-2.72676755	-1.21637592
H	-0.18252266	-1.71273001	-1.20237598
H	0.11864943	-2.03831146	1.48431984
H	1.08743714	-3.99046704	1.90768428
H	-1.42848778	-3.90787950	1.44955552
H	-0.43545449	-4.99667873	-0.35656035
H	-2.18871003	-2.10744929	-0.88252260
H	-1.58664001	-0.65268115	0.61246022
H	-3.92690363	-3.12912995	1.36978966
H	-3.66279131	-4.05592934	-0.12054738
H	-3.36069500	0.54774147	-0.86157488
H	-3.72925418	-0.55957027	1.37409968
O	4.66775271	3.88181584	-0.00547835
H	4.06582164	4.63352804	-0.03544068
H	4.06402166	3.11399172	-0.07844459
O	0.48635488	6.25489736	0.79137589
H	0.95276314	5.45769697	0.46440000
H	0.57605419	6.23383695	1.75088052
O	-3.74679875	3.76615486	0.96260272
H	-3.35546134	2.98310520	0.52720656
H	-4.65280048	3.81926663	0.63769907
O	-1.78019782	5.18990105	-0.39851175
H	-1.16119951	5.71913403	0.14367367
H	-2.53295677	4.92846746	0.16814320

1' T_1

N	2.39897917	-8.27593360	18.10943132
C	2.68508919	-7.00520752	17.68496528
O	2.05731015	-6.50676949	16.72967620
N	3.65210626	-6.29072647	18.31890634
C	4.36113231	-6.72999651	19.42041239
O	5.18297137	-5.99618345	19.97251645
C	4.07059829	-8.09220156	19.84186143
N	4.72579134	-8.60543163	20.89218349
C	4.38858731	-9.87775070	21.26082154
C	5.02318036	-10.46084375	22.33861462
C	4.72537534	-11.76860187	22.78088763
C	5.45152438	-12.33229888	23.94799472
C	3.73397027	-12.52757190	22.10540457
C	3.37719624	-13.90827001	22.56498062
C	3.10079422	-11.96776386	21.01863950
C	3.40262025	-10.66339576	20.56367846
N	2.79411020	-10.12542174	19.46460038
C	3.08719622	-8.78726265	19.10983535
C	1.90726914	-10.90496978	18.58986536
C	0.43169903	-10.84150677	19.00317237
O	0.19586901	-11.92797587	19.89849943
C	-0.51754204	-10.97449981	17.80179629
O	-0.29820902	-12.20046787	17.12176924
C	-0.34912903	-9.85128469	16.77778619
O	-0.30751602	-8.58913964	17.45032428
C	-1.49268211	-9.83329071	15.78230716
O	-1.20479609	-9.11119967	14.56899803

P	-0.62484104	-7.62987057	14.46594404
O	-1.20771309	-6.81165051	15.69232914
O	0.92678407	-7.78536856	14.71305304
O	-0.97140007	-7.04550849	13.16445995
H	3.86745428	-5.34047040	17.94969430
H	5.77898143	-9.88602671	22.85565064
H	5.98323941	-13.24519393	23.66241872
H	6.16503846	-11.62399286	24.36059073
H	4.74828334	-12.62692393	24.73239977
H	3.01531422	-13.89869101	23.59555468
H	2.60158119	-14.33770301	21.93452556
H	4.24600730	-14.56961103	22.53810264
H	2.32447317	-12.52780490	20.52468047
H	2.24672116	-11.93515586	18.58368336
H	2.04654815	-10.51596576	17.58983424
H	0.23180502	-9.89430770	19.50401440
H	-0.56524604	-11.72384385	20.45504948
H	-1.53823311	-10.93541779	18.20455828
H	-0.38970303	-12.91158594	17.76986727
H	0.58013204	-10.00888272	16.22522116
H	0.62394005	-8.43022258	17.72057526
H	-2.38059617	-9.40295070	16.25044619
H	-1.71405312	-10.84856176	15.46533713
H	1.31968109	-7.31688254	15.49911711
H	-0.96391907	-7.26613651	16.53720819
O	6.57300650	-7.07020250	22.45800061
H	6.60935748	-6.23223344	21.98326760
H	5.94296542	-7.59109553	21.91486255
O	5.03160236	-3.21811723	19.94465744
H	5.11655737	-4.19134530	20.02607644
H	4.39520232	-2.95505321	20.61909649
O	1.49093211	-3.74798627	16.56456121
H	1.59589711	-4.71856034	16.54388419
H	1.28652609	-3.48869225	15.65888715
O	4.15779630	-3.71752927	17.36417724
H	4.36099431	-3.29650724	18.22374731
H	3.24698723	-3.46868325	17.11060323

2' S_0

N	2.47260718	-8.18075858	18.16576531
C	2.76804520	-6.89560750	17.82422029
O	2.16968416	-6.32299745	16.91360922
N	3.76217427	-6.20919846	18.51799235
C	4.43914232	-6.67931450	19.60014940
O	5.25870738	-6.00540542	20.21539643
C	4.10529329	-8.07460658	19.96602641
N	4.71393434	-8.62917365	20.97399853
C	4.41008032	-9.90262070	21.30792752
C	5.05885336	-10.49690274	22.40875961
C	4.78537834	-11.78343285	22.79596865
C	5.48770137	-12.39882091	23.96967173
C	3.81078227	-12.52315592	22.06331757
C	3.47171625	-13.92342999	22.47174361
C	3.16603923	-11.95706988	20.97951150
C	3.45208725	-10.65124379	20.57203147
N	2.85067020	-10.04689374	19.48490841
C	3.11773623	-8.74775063	19.16856439
C	1.92167114	-10.77570776	18.60679332
C	0.46247203	-10.51242377	18.96442935
O	0.15061201	-11.35910181	20.07330546
C	-0.48517003	-10.82353480	17.80125727
O	-0.38063103	-12.19417087	17.43328027
C	-0.22535202	-9.98889374	16.54086819
O	-0.04881600	-8.61200560	16.87098621
C	-1.39743810	-10.11168371	15.58111715
O	-1.08656508	-9.63450469	14.27590003
P	-1.37947910	-8.08061158	13.83645299
O	-2.62375619	-7.61287355	14.52437902
O	-0.08466001	-7.30258253	14.43341504
O	-1.26665109	-8.04037257	12.35026588
H	3.98947929	-5.25140238	18.18386433
H	5.78470840	-9.89811873	22.94224663
H	6.03634245	-13.29608496	23.67485470
H	6.19255446	-11.69682384	24.41087278
H	4.77625834	-12.70098890	24.74137779
H	3.10744122	-13.95109601	23.50128869
H	2.70975719	-14.35088006	21.82367658
H	4.35644031	-14.56335007	22.43506363
H	2.40821517	-12.53133790	20.47432746
H	2.14190515	-11.83425086	18.66485332
H	2.13824616	-10.44820875	17.59664025
H	0.33818602	-9.46700067	19.24664836
H	-0.61374604	-10.99943178	20.53922147
H	-1.50058011	-10.60422978	18.15834132
H	-0.50117904	-12.71423092	18.23920431
H	0.66796805	-10.37444276	16.03831216
H	0.83670206	-8.47787758	17.27381223
H	-2.25414916	-9.56763071	15.98550413
H	-1.65849012	-11.16496779	15.48387410
H	0.03365800	-7.54497657	15.37528910
O	6.69959448	-7.22603752	22.63165261
H	6.80845852	-6.34437446	22.25845760
H	6.03696841	-7.63360756	22.04275056
O	5.16900937	-3.20738323	20.28462049
H	5.23884838	-4.18250630	20.33400447
H	4.52087432	-2.95953021	20.95369352
O	1.71610912	-3.58931426	16.79524322
H	1.80978413	-4.56492633	16.76751920
H	1.55286011	-3.31581624	15.88560912
O	4.35145031	-3.60146726	17.65755125
H	4.53312433	-3.21451223	18.53669533
H	3.44700925	-3.34167524	17.38974825

2' S_1

N	-0.19916042	0.68904272	-0.41104959
C	-0.61360044	2.00545545	-0.38748540
O	-1.81987923	2.26503109	-0.36999941
N	0.33201162	2.99240029	-0.38419010
C	1.69755152	2.78422105	-0.30668157
O	2.47358866	3.74845044	-0.24727175
C	2.11587607	1.39979517	-0.30583733
N	3.41993967	1.09578496	-0.22953361
C	3.74122040	-0.23055408	-0.21587827
C	5.07526131	-0.60095143	-0.11805812
C	5.50074104	-1.94870489	-0.08810821
C	6.95017250	-2.26187580	0.02313560
C	4.53663258	-2.97378277	-0.15951458
C	4.93778329	-4.41725583	-0.12017252
C	3.20097655	-2.62010347	-0.26395601
C	2.77473671	-1.27057811	-0.30117336
N	1.44791816	-0.92521538	-0.42076253
C	1.08948550	0.41724521	-0.38369240
C	0.38171065	-1.91985618	-0.55046823
C	-0.22099340	-2.28606932	0.80643857
O	0.66476974	-3.22054314	1.42096271
C	-1.61243176	-2.92032582	0.66983531
O	-1.53846846	-4.11935696	-0.08901550
C	-2.64703923	-2.01364562	-0.00777167
O	-2.58538324	-0.68662736	0.51381591
C	-4.04778995	-2.55910207	0.22480339
O	-5.01287280	-1.96020997	-0.63192924
P	-5.87309444	-0.64108353	-0.16940504
O	-6.11336335	-0.71671570	1.30565046
O	-4.84955242	0.57453211	-0.50799556
O	-7.01147716	-0.53063046	-1.12553178
H	-0.00110262	3.97241151	-0.42397567
H	5.81478250	0.18673135	-0.06438486
H	7.27837860	-2.88013792	-0.81789356
H	7.55718934	-1.36069330	0.05466192
H	7.14791958	-2.85185400	0.92376313

H	5.47978991	-4.65119013	0.79910535
H	4.06564861	-5.06549204	-0.17624520
H	5.60135108	-4.66454678	-0.95227890
H	2.46613193	-3.40645354	-0.29049022
H	0.77403161	-2.80411765	-1.03869586
H	-0.36906388	-1.49509808	-1.20475432
H	-0.30562989	-1.39034664	1.42088376
H	0.61810381	-3.12520231	2.37945918
H	-1.95201001	-3.13801936	1.69124678
H	-0.88805193	-4.69102415	0.34025809
H	-2.45909241	-2.00541638	-1.08617476
H	-1.81298292	-0.21809951	0.13715603
H	-4.32594238	-2.40565801	1.26994513
H	-4.04394246	-3.62708360	0.00920885
H	-3.97912818	0.38899430	-0.10168257
O	5.37828075	3.12796590	0.22914762
H	4.82791027	3.91628290	0.15518834
H	4.72313458	2.41406846	0.06859416
O	1.77947351	6.12768770	0.96332156
H	2.08596795	5.28731648	0.55659382
H	1.80633951	5.98036507	1.91543558
O	-2.84303604	4.56487766	0.80284584
H	-2.57551224	3.72217425	0.37924925
H	-3.70100619	4.78766871	0.42442109
O	-0.59509932	5.67008363	-0.40421756
H	0.08933109	6.00895345	0.20659506
H	-1.40869655	5.50780312	0.11387936

2' S_2

N	-0.19890883	0.68453682	-0.36253262
C	-0.60886170	1.99618449	-0.34833789
O	-1.81542663	2.26713379	-0.33601742
N	0.33938312	2.98349500	-0.34701272
C	1.70392727	2.77541234	-0.27589604
O	2.47984843	3.74186300	-0.22037008
C	2.12065706	1.39165161	-0.27841860
N	3.42838878	1.08841121	-0.21970359
C	3.75366541	-0.23504376	-0.20138492
C	5.09341972	-0.60351413	-0.11887143
C	5.51760042	-1.94440163	-0.08407707
C	6.97069595	-2.26099177	0.00903853
C	4.55125922	-2.96996692	-0.13050332
C	4.95386769	-4.41347754	-0.08036556
C	3.21266286	-2.62015778	-0.21840798
C	2.78705836	-1.27558319	-0.26578875
N	1.45471289	-0.92760425	-0.37688256
C	1.09470151	0.41092086	-0.34250478
C	0.39253842	-1.92410345	-0.52207485
C	-0.23965437	-2.29279679	0.81975992
O	0.62670758	-3.23869741	1.44738214
C	-1.63198122	-2.91578887	0.65707332
O	-1.55376078	-4.11702594	-0.09870844
C	-2.64559636	-2.00379907	-0.04399081
O	-2.58968675	-0.67694843	0.48022457
C	-4.05259493	-2.53981791	0.15542436
O	-4.99518514	-1.90128887	-0.70594121
P	-5.88553582	-0.63204644	-0.20881084
O	-6.29759927	-0.83986898	1.21976172
O	-4.85744493	0.60244916	-0.32062377
O	-6.95614607	-0.43077871	-1.23269944
H	0.00716270	3.96201784	-0.39024885
H	5.83095050	0.18719235	-0.08152318
H	7.28806572	-2.88524647	-0.83140166
H	7.57788869	-1.35898882	0.02260698
H	7.18380098	-2.83983646	0.91303619
H	5.51051971	-4.63758224	0.83274149
H	4.08129334	-5.06293038	-0.11528111
H	5.60460986	-4.67138245	-0.91953036
H	2.47896373	-3.40840936	-0.21977739
H	0.79590953	-2.80807651	-1.00207719
H	-0.34591434	-1.50220804	-1.19258868
H	-0.32735655	-1.39921471	1.43721677
H	0.52663286	-3.17764102	2.40472454
H	-1.99644953	-3.12942335	1.67079156
H	-0.89609508	-4.68088454	0.33028780
H	-2.43253968	-1.99445866	-1.11734130
H	-1.79841715	-0.21131256	0.13194308
H	-4.35030515	-2.41309175	1.19861258
H	-4.06213490	-3.60085416	-0.08879888
H	-3.96097063	0.33390637	-0.01304051
O	5.40532080	3.13306690	-0.04658671
H	4.83268654	3.90835728	-0.08092064
H	4.74726599	2.40476913	-0.10509411
O	1.79019300	6.11203512	0.99180146
H	2.09226032	5.27033865	0.58249047
H	1.81848661	5.96309103	1.94357045
O	-2.82082590	4.54894708	0.85362714
H	-2.54844950	3.70994795	0.42261045
H	-3.68130691	4.76862721	0.47923592
O	-0.59099228	5.67385127	-0.37099579
H	0.09945064	6.00372645	0.23799894
H	-1.39821142	5.50212939	0.15396145

2' T_1

N	2.41158618	-8.28356560	18.02670530
C	2.73550620	-7.05972553	17.60498125
O	2.16908516	-6.52142849	16.60192620
N	3.68973926	-6.33239944	18.25497734
C	4.36328531	-6.75817551	19.38300638
O	5.18499537	-6.00300746	19.93356345
C	4.04984129	-8.09763457	19.81438940
N	4.70425734	-8.61502562	20.88316848
C	4.38415332	-9.88118569	21.25188252
C	5.03316036	-10.45950774	22.35976160
C	4.75903434	-11.74046885	22.79815363
C	5.48252242	-12.31101590	23.98535374
C	3.78399927	-12.49759190	22.11469560
C	3.43692725	-13.88832299	22.56362264
C	3.13180323	-11.94431988	21.01620750
C	3.41721425	-10.65972079	20.56393648
N	2.78800120	-10.09627074	19.44025442
C	3.07799822	-8.80358063	19.07758136
C	1.90429014	-10.89805576	18.58996331
C	0.42779103	-10.85565178	19.00063439
O	0.18779501	-11.96006386	19.88188342
C	-0.53349604	-10.97541380	17.81096127
O	-0.34234302	-12.21133087	17.13290323
C	-0.36025503	-9.85190870	16.78754322
O	-0.30493202	-8.59334660	17.43455125
C	-1.51564311	-9.81895672	15.81296515
O	-1.27361409	-8.97115466	14.66743203
P	-0.54647404	-7.57194656	14.62699405
O	-1.16767508	-6.51471746	15.54253113
O	0.95833307	-7.83462258	14.87452608
O	-0.83705806	-6.97084550	13.26198796
H	3.91983628	-5.39985938	17.87786828
H	5.77461440	-9.85743870	22.86980163
H	6.02446141	-13.22248196	23.72083369
H	6.19843145	-11.59512984	24.38662276
H	4.78665434	-12.57989690	24.78410679
H	3.08038822	-13.89714401	23.59705469
H	2.66050519	-14.32043204	21.93398458
H	4.30817531	-14.54792106	22.52812760
H	2.36201117	-12.52412490	20.53430547
H	2.25713316	-11.92524886	18.59794733
H	2.02459314	-10.52365376	17.58099026
H	0.22613302	-9.91658273	19.51652442
H	-0.62511605	-11.79534686	20.37481346
H	-1.55163911	-10.92359576	18.22147232
H	-0.36012803	-12.90582595	17.80545926

H	0.55842604	-10.03384872	16.22378318
H	0.63787004	-8.43049262	17.67203425
H	-2.41318017	-9.45638866	16.31666415
H	-1.70136712	-10.80923378	15.40613813
H	1.44663010	-7.29792551	15.63149011
O	6.42073945	-6.99667051	22.43570859
H	6.39305448	-6.21664843	21.86823860
H	5.83438444	-7.60877153	21.92964358
O	4.94489136	-3.28905424	19.93111945
H	5.04214536	-4.26929931	19.97995145
H	4.26464131	-3.06198022	20.57482346
O	1.45791110	-3.84754928	16.66730721
H	1.62536412	-4.81123035	16.59311820
H	1.16127309	-3.56665226	15.79445913
O	4.17705730	-3.67179027	17.29074723
H	4.35796731	-3.31709824	18.18476832
H	3.23698623	-3.49505825	17.08988223

2'' S_0

N	2.50830218	-8.17354357	18.16496932
C	2.81228520	-6.88884049	17.82849429
O	2.22344516	-6.31275146	16.91372119
N	3.80271927	-6.20844444	18.53213832
C	4.46926632	-6.68464046	19.61849142
O	5.28605938	-6.01561643	20.24233346
C	4.12716230	-8.07971859	19.97766942
N	4.72473334	-8.63931464	20.98958952
C	4.41223932	-9.91189771	21.31820652
C	5.04902737	-10.51142976	22.42321562
C	4.76647234	-11.79747283	22.80535663
C	5.45574938	-12.41829289	23.98387072
C	3.79496027	-12.53139288	22.06272658
C	3.44703425	-13.93130298	22.46460463
C	3.16155723	-11.95999888	20.97497549
C	3.45677425	-10.65466577	20.57290546
N	2.86688321	-10.04487874	19.48238042
C	3.14306923	-8.74660961	19.17128738
C	1.93955614	-10.76626877	18.59628132
C	0.47969403	-10.49290777	18.94482534
O	0.15161401	-11.34569982	20.04359946
C	-0.46347803	-10.78577679	17.77293327
O	-0.37394503	-12.15422989	17.39537023
C	-0.18291101	-9.94867272	16.51867318
O	0.01790500	-8.57654364	16.85284522
C	-1.35491510	-10.04322273	15.55754214
O	-1.03365608	-9.53989468	14.25923502
P	-1.27974009	-7.98416458	13.85939499
O	-2.54793518	-7.49064255	14.50008206
O	0.00876700	-7.23462850	14.46514006
O	-1.21588709	-7.88994055	12.36653289
H	4.03450429	-5.24937538	18.20413732
H	5.77302343	-9.91701073	22.96402963
H	6.00247743	-13.31774096	23.69224669
H	6.16016347	-11.72047383	24.43231573
H	4.73619634	-12.71825590	24.74888576
H	3.07454822	-13.96030798	23.49115071
H	2.68864520	-14.35400104	21.80930159
H	4.32957231	-14.57451004	22.43316262
H	2.40567617	-12.53006089	20.46213749
H	2.15134716	-11.82647783	18.65478033
H	2.16668416	-10.43979975	17.58805927
H	0.36239803	-9.44874368	19.23480140
H	-0.60786404	-10.97920980	20.51217448
H	-1.47830611	-10.55550578	18.12437428
H	-0.50818004	-12.67937391	18.19585930
H	0.70360605	-10.34950872	16.01636416
H	0.89934706	-8.46028662	17.27436925
H	-2.20894916	-9.49953168	15.96704812
H	-1.62493112	-11.09021378	15.43175512
H	0.14801801	-7.51469456	15.39726811
O	6.69244646	-7.24491650	22.67726663
H	6.81024147	-6.36209745	22.30958258
H	6.03785346	-7.64807855	22.07658859
O	5.19550537	-3.21688923	20.32597246
H	5.26625138	-4.19203530	20.37158447
H	4.54368633	-2.97257521	20.99277252
O	1.77138813	-3.57845926	16.79581521
H	1.86686013	-4.55383433	16.76743818
H	1.63096912	-3.30247424	15.88310913
O	4.39758932	-3.59725526	17.69191227
H	4.57191033	-3.21484223	18.57459632
H	3.49617025	-3.33479724	17.41699426
Na	-3.42779025	-6.89744851	12.36230487

2'' S_1

N	0.14940622	0.70653261	-0.38896338
C	-0.23281371	2.03309179	-0.36846723
O	-1.43261879	2.32109345	-0.34910099
N	0.73621278	2.99651584	-0.37033364
C	2.09662475	2.75545083	-0.29585403
O	2.89636591	3.69999606	-0.24294056
C	2.48097778	1.36094187	-0.29067336
N	3.77721705	1.02561941	-0.21625700
C	4.06556879	-0.30836166	-0.19545074
C	5.38999599	-0.71108609	-0.09932641
C	5.78228122	-2.06952824	-0.06237888
C	7.22352001	-2.41710137	0.04658935
C	4.79285922	-3.07108377	-0.12346628
C	5.15857167	-4.52358986	-0.07520907
C	3.46639051	-2.68482297	-0.22620882
C	3.07395292	-1.32470092	-0.27350503
N	1.75658824	-0.94765879	-0.39711744
C	1.43092406	0.40340496	-0.36330574
C	0.66725096	-1.91521023	-0.54119744
C	0.03191313	-2.26510864	0.80518880
O	0.88024356	-3.22590581	1.43182445
C	-1.37436606	-2.85965031	0.64512514
O	-1.32092881	-4.06515481	-0.10456398
C	-2.36662887	-1.92895412	-0.06189971
O	-2.28749734	-0.60201210	0.45877803
C	-3.78586840	-2.43496696	0.13130728
O	-4.70768197	-1.79485668	-0.75174685
P	-5.53624825	-0.46748550	-0.31228578
O	-5.93785886	-0.57549476	1.13268564
O	-4.47826884	0.72369747	-0.53786788
O	-6.65227286	-0.29570636	-1.29535342
H	0.42659442	3.98444368	-0.41278889
H	6.14927633	0.05799763	-0.05354329
H	7.53170692	-3.05655466	-0.78608082
H	7.85330227	-1.53128033	0.06230697
H	7.41033107	-2.99863909	0.95520263
H	5.70146750	-4.76355372	0.84191030
H	4.27043675	-5.15051656	-0.12016139
H	5.80969932	-4.79340877	-0.91015408
H	2.71126874	-3.45219483	-0.24245086
H	1.04467621	-2.80992130	-1.02203328
H	-0.06064521	-1.47266138	-1.20947139
H	-0.03626957	-1.36812133	1.41980042
H	0.81809876	-3.13420362	2.38986958
H	-1.74240448	-3.05927535	1.66023629
H	-0.68487162	-4.64664381	0.33326810
H	-2.14976972	-1.92765219	-1.13465533
H	-1.48582846	-0.15580714	0.11419446
H	-4.09268816	-2.28242287	1.16827381
H	-3.81466688	-3.49899543	-0.09654873
H	-3.60909361	0.47939770	-0.15057752
O	5.79389211	3.01024561	0.20236575
H	5.26631376	3.81412265	0.13030301
H	5.11653125	2.31452303	0.05554364
O	2.26863925	6.11098761	0.94301859

H	2.55274613	5.25880924	0.54502453
H	2.30513970	5.97741745	1.89682509
O	-2.40217246	4.65074670	0.81399979
H	-2.15379209	3.80110370	0.39279620
H	-3.24860033	4.89838631	0.42515697
O	-0.12558561	5.69249440	-0.39928994
H	0.57038681	6.02198222	0.20367305
H	-0.94008241	5.55569017	0.12447117
Na	-8.25204320	-0.45001765	0.49004729

2'' S_2

N	2.50277146	-8.14505827	18.16800679
C	2.79697690	-6.86464111	17.82248617
O	2.17521291	-6.28729661	16.91795154
N	3.80302666	-6.20112777	18.49787843
C	4.49986707	-6.70386949	19.56306587
O	5.35233894	-6.03316580	20.15945054
C	4.16766432	-8.07642515	19.93127878
N	4.82733841	-8.64441501	20.96654417
C	4.45529885	-9.90782696	21.28455175
C	5.08017728	-10.54250871	22.41462278
C	4.75811004	-11.80893078	22.84084950
C	5.44633373	-12.42733912	24.02075490
C	3.75554981	-12.50903049	22.13438686
C	3.33580543	-13.87243244	22.54186218
C	3.12699229	-11.90073050	21.01538273
C	3.47996812	-10.63075119	20.56449223
N	2.88710551	-10.03977181	19.45372669
C	3.17395948	-8.72542945	19.16285171
C	1.98532966	-10.76865367	18.56301798
C	0.51598578	-10.54423738	18.91093011
O	0.20699808	-11.42838244	19.99064025
C	-0.42200958	-10.83244292	17.73253747
O	-0.29636937	-12.18645832	17.31672459
C	-0.16068735	-9.95360646	16.50263821
O	0.00772972	-8.58718015	16.87394749
C	-1.33012724	-10.04999794	15.53813636
O	-1.01927537	-9.50621599	14.25383440
P	-1.30092412	-7.94682165	13.89344474
O	-2.58109412	-7.49934545	14.54398228
O	-0.03040452	-7.18294037	14.51797973
O	-1.23833069	-7.81382433	12.40339432
H	4.03886691	-5.24409502	18.17744615
H	5.84031239	-9.96803738	22.92790482
H	5.96677458	-13.34400032	23.73465887
H	6.17399690	-11.74065205	24.44814803
H	4.72907334	-12.69541285	24.79920628
H	2.95434884	-13.86697561	23.56959711
H	2.56917368	-14.27642355	21.88579728
H	4.19167816	-14.55609859	22.55197963
H	2.32903710	-12.44171416	20.53429711
H	2.22506684	-11.82601601	18.60309665
H	2.19892232	-10.42881308	17.55544746
H	0.37200377	-9.50976370	19.22370768
H	-0.54151648	-11.07655778	20.48740152
H	-1.44238588	-10.63879357	18.08960336
H	-0.43370384	-12.73960778	18.09733242
H	0.73499152	-10.31996412	15.99049962
H	0.88917593	-8.45924091	17.29344307
H	-2.19641804	-9.53639015	15.96060894
H	-1.57616187	-11.09926557	15.38502628
H	0.11778089	-7.48000085	15.44325711
O	6.70052461	-7.22092133	22.61770620
H	6.77623480	-6.35239610	22.20714403
H	6.06655609	-7.68032365	22.02739172
O	5.18614946	-3.27138327	20.33060324
H	5.27482848	-4.24884079	20.33309825
H	4.52850710	-3.06825423	21.00531809
O	1.73279491	-3.56721535	16.86447686
H	1.83280426	-4.54363548	16.82224618
H	1.56476354	-3.28183096	15.95940887
O	4.38714333	-3.55424215	17.68244566
H	4.56160825	-3.20953245	18.58054735
H	3.47168252	-3.31213233	17.43663685
Na	-3.47206565	-6.88480249	12.41271642

2'' T_1

N	2.56124519	-8.16075060	18.19737730
C	2.82932520	-6.85221751	17.85023131
O	2.18964716	-6.31749744	16.94103520
N	3.80572428	-6.17920342	18.53267734
C	4.50449732	-6.67672550	19.61203943
O	5.33098738	-5.97668443	20.20506445
C	4.19583630	-8.05081059	19.97373843
N	4.83112335	-8.61850660	21.01142152
C	4.46768932	-9.89561270	21.32633553
C	5.07599337	-10.52959176	22.39585160
C	4.74429434	-11.83482888	22.78871766
C	5.44194638	-12.45864688	23.94542874
C	3.73866027	-12.54945693	22.07775961
C	3.34298524	-13.93314600	22.49403260
C	3.13143723	-11.94328984	21.00231649
C	3.47380325	-10.63844775	20.58854550
N	2.90387521	-10.05008970	19.49318140
C	3.22067923	-8.70907063	19.19249337
C	1.98420514	-10.75543080	18.59566335
C	0.51792604	-10.49966875	18.94123535
O	0.19130701	-11.35998083	20.03337644
C	-0.41739603	-10.80059576	17.76351725
O	-0.30937602	-12.16568785	17.38101423
C	-0.14503701	-9.95590070	16.51318021
O	0.02885700	-8.58018263	16.85305822
C	-1.31093210	-10.06519073	15.54592114
O	-0.99067807	-9.55195669	14.25165403
P	-1.26658909	-8.00094458	13.85276900
O	-2.54538318	-7.53315252	14.49115902
O	0.00581300	-7.22657951	14.46306404
O	-1.19909609	-7.90262159	12.36057992
H	4.02807029	-5.21472338	18.21902033
H	5.83505141	-9.98598872	22.94117865
H	5.95854445	-13.37149299	23.63429570
H	6.16586646	-11.78099684	24.39079373
H	4.72342334	-12.76309192	24.71151277
H	2.96186821	-13.94262600	23.51784469
H	2.57022319	-14.32916601	21.83847259
H	4.19721930	-14.61331107	22.46657862
H	2.34972117	-12.47283688	20.48456148
H	2.19952016	-11.81664386	18.63416136
H	2.20773816	-10.41817873	17.59106124
H	0.38841803	-9.45827067	19.23499037
H	-0.55202004	-10.98642381	20.52163046
H	-1.43561910	-10.58438574	18.11381830
H	-0.45164303	-12.69657889	18.17624529
H	0.75078105	-10.33762277	16.01310215
H	0.90860706	-8.44829060	17.26186124
H	-2.17537116	-9.53662071	15.95333412
H	-1.56336411	-11.11593878	15.41553711
H	0.14515001	-7.50092452	15.39572810
O	6.64037245	-7.15686151	22.67265961
H	6.68118546	-6.30575643	22.22204762
H	6.02399441	-7.66360456	22.09930157
O	5.12605537	-3.21290423	20.35825047
H	5.22745538	-4.18865930	20.36852847
H	4.46229432	-3.01352822	21.02807949
O	1.72174313	-3.57384826	16.81120019
H	1.82230413	-4.54764233	16.77805422
H	1.58310912	-3.29413924	15.89929412
O	4.35128831	-3.54245126	17.71289727
H	4.51087332	-3.17672823	18.60557833
H	3.44293425	-3.30213424	17.44150125

Na	-3.42530224	-6.93934749	12.35199089

3' S_0

N	2.60826619	-8.02209960	18.20674130
C	2.95310721	-6.74065948	17.90592329
O	2.39667417	-6.11969146	16.99984421
N	3.95627028	-6.10475046	18.63819935
C	4.60251833	-6.62779947	19.71376741
O	5.43396538	-5.99851442	20.36083445
C	4.21988130	-8.02178257	20.03159946
N	4.79923335	-8.62645860	21.02785454
C	4.45100532	-9.89931070	21.31837152
C	5.07532336	-10.55095174	22.40084560
C	4.75847134	-11.83988686	22.74408865
C	5.43692941	-12.51800988	23.89715074
C	3.76241327	-12.52160892	21.98465860
C	3.37638024	-13.92316201	22.34465158
C	3.13995022	-11.89809683	20.91990751
C	3.47051125	-10.58943774	20.55561147
N	2.89415421	-9.93034372	19.48751138
C	3.21771823	-8.63545461	19.20345840
C	1.92209114	-10.58995776	18.60171036
C	0.48397903	-10.26607573	18.98979139
O	0.17457001	-11.07367577	20.13037844
C	-0.50172604	-10.57157377	17.85920229
O	-0.44870003	-11.95683286	17.52810725
C	-0.25091402	-9.76793271	16.57604721
O	-0.03401900	-8.39272460	16.87266323
C	-1.44084410	-9.87523573	15.64160110
O	-1.08568408	-9.44370571	14.35006306
P	-2.32273017	-9.30314168	13.20516596
O	-2.98429621	-10.67704975	13.16119895
O	-3.23536523	-8.20002360	13.73212500
O	-1.53712811	-8.93073467	11.95684784
H	4.21835231	-5.14547037	18.33851030
H	5.81878943	-9.99477571	22.95581363
H	5.95828145	-13.42114299	23.57207768
H	6.16201442	-11.85452888	24.36449373
H	4.71381334	-12.82500693	24.65599377
H	3.00009522	-13.97176901	23.36917969
H	2.60860819	-14.30606403	21.67586155
H	4.24124131	-14.58884403	22.29644861
H	2.36608417	-12.43061092	20.39414345
H	2.09295915	-11.65879182	18.62613634
H	2.13626815	-10.24141173	17.59836426
H	0.40550103	-9.21000664	19.24701037
H	-0.57742104	-10.68548479	20.59323549
H	-1.50098511	-10.31385974	18.23701230
H	-0.55102804	-12.44773588	18.35457231
H	0.62056004	-10.19194974	16.06384216
H	0.87113506	-8.26315958	17.20949926
H	-2.25203416	-9.25871566	16.05035015
H	-1.78706613	-10.91318579	15.61996410
O	6.79139647	-7.33111355	22.75938563
H	6.92609652	-6.44240545	22.41216560
H	6.12978944	-7.70656454	22.14804361
O	5.40201641	-3.20874523	20.54628250
H	5.44884637	-4.18667830	20.55495550
H	4.73826134	-2.97497622	21.20503853
O	2.01619214	-3.37267924	17.00237420
H	2.08642515	-4.34852732	16.93277020
H	1.86373213	-3.05615122	16.10489917
O	4.64082733	-3.47827825	17.88472027
H	4.81295835	-3.13464423	18.78356133
H	3.74549727	-3.18995623	17.61526629

3' T_1

N	2.49419018	-8.16252557	18.15012330
C	2.80752020	-6.90620851	17.77055229
O	2.21887316	-6.33385145	16.82981421
N	3.80551727	-6.23339144	18.44660533
C	4.50102832	-6.72100848	19.53079442
O	5.35798638	-6.00276345	20.08889846
C	4.16694430	-8.06486257	19.91940441
N	4.82334835	-8.64164561	20.95794048
C	4.47565332	-9.91100769	21.28815751
C	5.12487937	-10.54520074	22.36560959
C	4.81772735	-11.83023186	22.76989064
C	5.54253038	-12.45996491	23.92644572
C	3.80721027	-12.53422192	22.08210061
C	3.42120625	-13.92582801	22.49645862
C	3.15561023	-11.92596685	21.01254750
C	3.47467425	-10.63770675	20.59206448
N	2.84844320	-10.01748873	19.49964038
C	3.16314123	-8.71984362	19.16818540
C	1.90308614	-10.74024378	18.65148133
C	0.44478403	-10.49606875	19.02952736
O	0.13704701	-11.35688683	20.13467245
C	-0.52489404	-10.79375678	17.88278227
O	-0.43660603	-12.16446286	17.50096824
C	-0.27922702	-9.93637274	16.63587620
O	-0.13585201	-8.57226862	16.98330223
C	-1.43983311	-10.06522174	15.66697012
O	-1.09994408	-9.57487668	14.37025704
P	-1.43227511	-8.07221957	13.86698202
O	-2.57813818	-7.51572852	14.64334404
O	-0.12705201	-7.25196652	13.88038502
O	-1.60750811	-8.21096661	12.34742388
H	4.05654129	-5.29727837	18.10711828
H	5.89333843	-9.98292870	22.88149666
H	6.05326543	-13.37803796	23.62477670
H	6.28584444	-11.77861184	24.33822373
H	4.85216735	-12.73401792	24.72834680
H	3.07613022	-13.95325701	23.53359967
H	2.62383519	-14.31525304	21.86487959
H	4.26989731	-14.61215503	22.43160562
H	2.36043617	-12.46886990	20.52838747
H	2.12785615	-11.80057486	18.69646733
H	2.08106515	-10.41392774	17.63334325
H	0.32325702	-9.45416770	19.32544740
H	-0.65473705	-11.02479980	20.57452749
H	-1.53540411	-10.57487674	18.25701631
H	-0.48820904	-12.68305191	18.31545230
H	0.61986604	-10.30514372	16.12957618
H	0.77644606	-8.41142060	17.30609326
H	-2.30313017	-9.52335466	16.05699815
H	-1.69783212	-11.11674080	15.54780311
O	6.48998748	-7.05666148	22.58213665
H	6.45709445	-6.28558043	22.00146860
H	5.92563142	-7.68108857	22.06445858
O	5.03639936	-3.31779124	20.28168345
H	5.16006137	-4.29781731	20.25251647
H	4.31426431	-3.16496623	20.90112352
O	1.72718513	-3.67961726	16.86319519
H	1.86581714	-4.65804933	16.81079722
H	1.49844611	-3.39879924	15.97037215
O	4.40821032	-3.50467025	17.57292528
H	4.53670233	-3.22195123	18.50008134
H	3.46870525	-3.34969524	17.34676323