Supplementary Materials for

Transition of the Coordination Modes in Sodiated Uridine Radicals Revealed by Infrared Multiphoton Dissociation Spectroscopy and Theoretical Calculations

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1 Experimental and Calculational Methods

1.1 Experimental Methods

All experiments were performed on an experimental setup combining a dual-beam laser system and an FT ICR mass spectrometer.[32] Mass spectrometry measurements were performed using the 7.0 T FT ICR mass spectrometer (Varian IonSpec, Lake Forest, CA, USA). The dual-beam laser system utilized one UV OPO laser (NT-342C, EKSPLA, Vilnius, Lithuania) and one IR OPO laser (Firefly-IR, M Squared, Glasgow, UK). Tunable triggers were generated by one pulse generator (DG535, Stanford, CA, USA) and connected to the multi-channel mechanical shutter controller (SSH-C4RA, Sigma-Koki, Tokyo, Japan) to control the irradiation time of the two lasers.

The Na^+-containing 5-iodouridine solution was prepared by weighing 0.037 g of 5-iodouridine solid (Shanghai Haohong Bio-pharmaceutical Technology Co.) and dissolving it in 1 ml of water to form a 10 mM solution, followed by taking 100 μL of this solution and mixing it well with 390 μL of water, 490 μL of methanol, and 20 μL of 1 mM NaCl, to ultimately obtain a 1 mM solution of [I-Urd+Na]. The precursor ion of $[I\text{-}Urd+Na]^+$ was generated by spraying the solution of [I-Urd+Na] at a flow rate of 2 μL/min, followed by subsequent injection of the generated ions into the ICR analysis cell by a quadrupole ion guide. The target ions were then mass-selected using the stored waveform inverse Fourier transform (SWIFT) method.[35] The selected $[I\text{-}Urd+Na]^+$ complex ions were irradiated by the UV laser to produce radical cations. The target ions were mass-selected using the stored waveform Fourier inverse transform (SWIFT) method and characterized by CID/IRMPD/UVPD-MS^3. N_2 was used as the cone gas and desolvent gas, and the probe and cone voltages were set to 3.8 kV and 22 V. For the CID experiments, sustained off-resonance radiation (SORI) with a frequency shift of 1000 Hz was used with a typical amplitude of 2.2 V ($V_{p\text{-}p}$).[38] For the IRMPD spectroscopy experiments, the UV wavelength was set at 282 nm, and the average UV laser pulse energy was 0.7 mJ. The UV laser has a frequency of 10 Hz and a 5 ns pulse duration. The typical UV irradiation time was 15 s. For the IRMPD experiments, the scanning wavelength range of IR laser was set between 2750 cm^{-1} and 3750 cm^{-1} with a step size of 5 cm^{-1}, and the irradiation time was 15 s. The spectral intensity at each wave number is given by the equation I_{IR} =

-ln ($I_p/(I_P/(\sum I_{fi} + I_p))$), where I_p and I_{fi} are the intensities of the parent ion and the *i*th fragment ion in the corresponding experiment.

1.2 Calculational Methods

Conformational searches for $[I\text{-}Urd+Na]^+$ and $[Urd+Na\text{-}H]^{\bullet+}$ were performed using the program Molclus.[39] Besides, some structures and conformations were also constructed manually to avoid the loss of some important isomers. The initial configurations were first optimized at the semi-empirical quantum mechanics level of the GFN-xTB method.45 Then some isomers were picked out for further optimization with DFT calculation at the level of B3LYP/6-31+G(d)/def2-QZVDP for $[I\text{-}Urd+Na]^+$ and B3LYP/6-31+G(d) for $[Urd+Na\text{-}H]^{\bullet+}$ using the Gaussian 09 program.[40] Finally, the selected isomers shown in the article and the supporting information were optimized at the level of B3LYP/6-311+G(d,p)/def2-QZVDP for $[I\text{-}Urd+Na]^+$ and B3LYP/6-311+G(d,p) for $[Urd+Na\text{-}H]^{\bullet+}$. Based on these optimized structures, the vibrational frequencies were calculated. For all structures, their electronic energies were calculated at 0 K with zero-point energy (ZPE) corrected, while their free energies were calculated at 298 K. A single scaling factor of 0.962 was applied to the calculated harmonic frequencies in the range 2750-3750 cm^{-1}.[20,32,41] The calculated IR spectra shown in the paper are drawn after the fitting process, in which the Lorentzian line shape and a half-width of 4 cm^{-1} are applied for all vibrational modes.

2 Supplementary Figures

Figures. S1–S20

Fig. S1 Mass spectra of the fragment ion at m/z 238.08 that is generated with the method shown in Figure 1 in the article, after its (a) isolation and (b) CID.

Fig. S2 Selected isomers of the precursor ions. Their relative energies and Gibbs free energies are shown in the parentheses in the unit of kcal/mol. The calculation was performed on the level of B3LYP/6-311+G(d,p)/def2-QZVDP.

Fig. S3 A comparison among the experimental IRMPD spectrum and the calculated IR spectra of the isomers of $[I\text{-}Urd+Na]^+$. Their relative energies and Gibbs free energies are shown in the parentheses in the unit of kcal/mol. Their corresponding structures are shown in **Fig. S2**. The calculation was performed on the level of B3LYP/6-311+G(d,p)/def2-QZVDP.

Fig. S4 Structures of the top two isomers of the precursor ion that bind one or two water molecules. Their relative energies and Gibbs free energies are shown in the parentheses in the unit of kcal/mol. The calculation was performed on the level of B3LYP/6-311+G(d,p)/def2-QZVDP.

Fig. S5 Some selected isomers of $[Urd+Na-H]^{\bullet+}$ with the tridentate coordination mode. Some of them have H transfers from the positions of O2', O3' or O5'. Their relative energies and Gibbs free energies are shown in the parentheses in kcal/mol. The calculation was performed on the level of B3LYP/6-311+G(d,p).

Fig. S6 Some selected isomers of $[Urd+Na-H]^{\bullet+}$ with the tridentate coordination mode, which have H transfers from the positions of C6, C1' ,C2'or C3'. Their relative energies and Gibbs free energies are shown in the parentheses in kcal/mol. The calculation was performed on the level of B3LYP/6-311+G(d,p).

Fig. S7 Some selected isomers of $[Urd+Na-H]^{\bullet+}$ with the tridentate coordination mode that have H transfers from the positions of C4' or C5', along with some selected isomers with the bidentate that have no H transfer or H transfers from the position of O2'. Some structures are

characterized by their opening sugar rings. Their relative energies and Gibbs free energies are shown in the parentheses in kcal/mol. The calculation was performed on the level of B3LYP/6-311+G(d,p).

Fig. S8 Some selected isomers of $[Urd+Na-H]^{\bullet+}$ with the bidentate that have H transfers from the position of O3', O5', C6 or C1'. Their relative energies and Gibbs free energies are shown in the parentheses in kcal/mol. The calculation was performed on the level of B3LYP/6-311+G(d,p).

Fig. S9 Some selected isomers of $[Urd+Na-H]^{\bullet+}$ with the bidentate that have H transfers from the position of C2', C3', C4' or C5'. Their relative energies and Gibbs free energies are shown in the parentheses in kcal/mol. The calculation was performed on the level of B3LYP/6-311+G(d,p).

Fig. S10 A comparison among the experimental IRMPD spectrum and the calculated IR spectra of some isomers of the radical ion of $[Urd+Na-H]^{\bullet+}$. Their corresponding relative energies and Gibbs free energies are shown in parentheses in kcal/mol. The structures of these isomers can be found in **Fig. S5**. All calculations were performed on the level of B3LYP/6-311+G (d, p).

Fig. S11 A comparison among the experimental IRMPD spectrum and the calculated IR spectra of some isomers of the radical ion of $[Urd+Na-H]^{\bullet+}$. Their corresponding relative energies and Gibbs free energies are shown in parentheses in kcal/mol. The structures of these isomers can be found in **Fig. S5** or **Fig. S6**. All calculations were performed on the level of B3LYP/6-311+G (d, p).

Fig. S12 A comparison among the experimental IRMPD spectrum and the calculated IR spectra of some isomers of the radical ion of $[Urd+Na-H]^{\bullet+}$. Their corresponding relative energies and Gibbs free energies are shown in parentheses in kcal/mol. The structures of these isomers can be found in **Fig. S6** or **Fig. S7**. All calculations were performed on the level of B3LYP/6-311+G (d, p).

Fig. S13 A comparison among the experimental IRMPD spectrum and the calculated IR spectra of some isomers of the radical ion of $[Urd+Na-H]^{\bullet+}$. Their corresponding relative energies and Gibbs

free energies are shown in parentheses in kcal/mol. The structures of these isomers can be found in **Fig. S7**. All calculations were performed on the level of B3LYP/6-311+G (d, p).

Fig. S14 A comparison among the experimental IRMPD spectrum and the calculated IR spectra of some isomers of the radical ion of $[Urd+Na-H]^{\bullet+}$. Their corresponding relative energies and Gibbs free energies are shown in parentheses in kcal/mol. The structures of these isomers can be found in **Fig. S8**. All calculations were performed on the level of B3LYP/6-311+G (d, p).

Fig. S15 A comparison among the experimental IRMPD spectrum and the calculated IR spectra of some isomers of the radical ion of $[Urd+Na-H]^{\bullet+}$. Their corresponding relative energies and Gibbs free energies are shown in parentheses in kcal/mol. The structures of these isomers can be found in **Fig. S8** and **Fig. S9**. All calculations were performed on the level of B3LYP/6-311+G (d, p).

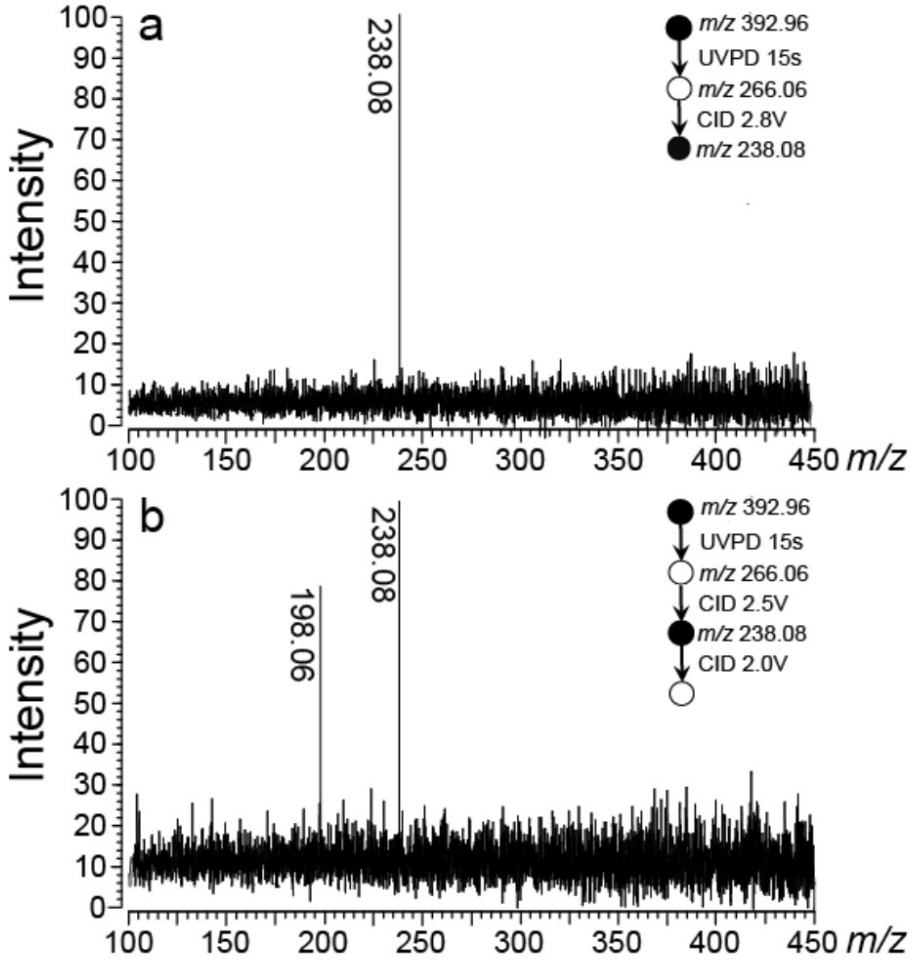
Fig. S16 A comparison among the experimental IRMPD spectrum and the calculated IR spectra of some isomers of the radical ion of $[Urd+Na-H]^{\bullet+}$. Their corresponding relative energies and Gibbs free energies are shown in parentheses in kcal/mol. The structures of these isomers can be found in **Fig. S9**. All calculations were performed on the level of B3LYP/6-311+G(d, p).

Fig. S17 The potential energy change curve (black) from M-B(O2,O2')-1 to M-T(O2,O',O5')-1 for the precursor ion, and that (red) from R-B(O2,O2')-(C5H-C1')-1 to R-T(O2,O',O5')-(C5H-C1')-1 for the radical ion. Both results are achieved through the rotation of the intramolecular C-N bond.

Fig. S18 Some ring-opening structures with tridentate or bidentate coordination modes of the isomers of $[Urd+Na-H]^{\bullet+}$, along with the most stable isomer of R-T(O2,O',O5')-(C5H-C1')-1. The calculation was performed on the level of B3LYP/6-311+G(d,p). Their relative energies and Gibbs free energies are shown in the parentheses in kcal/mol.

Fig. S19 A comparison among the experimental IRMPD spectrum and the calculated IR spectra of the corresponding isomers of the radical ion of $[Urd+Na-H]^{\bullet+}$ shown in **Fig. S18**. Their relative energies and Gibbs free energies are shown in parentheses in kcal/mol. All calculations were performed on the level of B3LYP/6-311+G (d, p).

Fig. S20 Potential energy profile associated with one of the ring-opening isomerization pathways relative to t [Urd+Na-H]$^{\bullet+}$. Relative energies and Gibbs free energies are shown in the parentheses in kcal/mol. All calculations were performed at the level of B3LYP/6-311+G(d, p).



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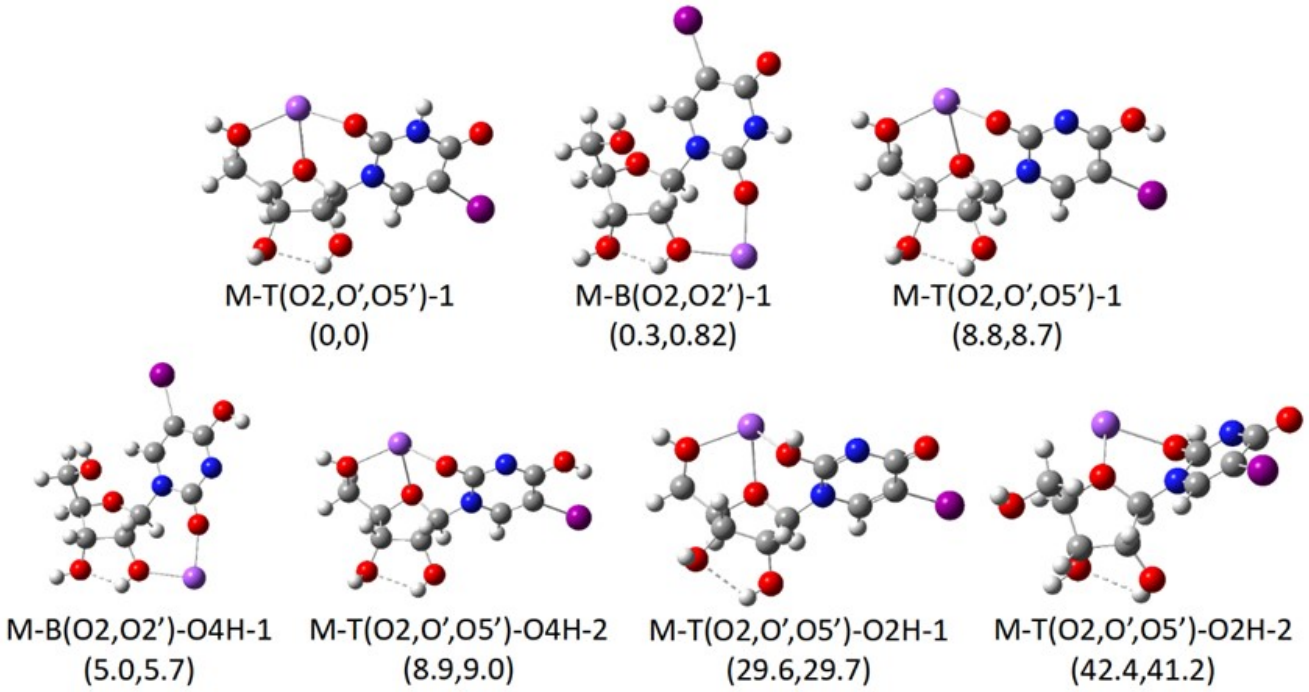
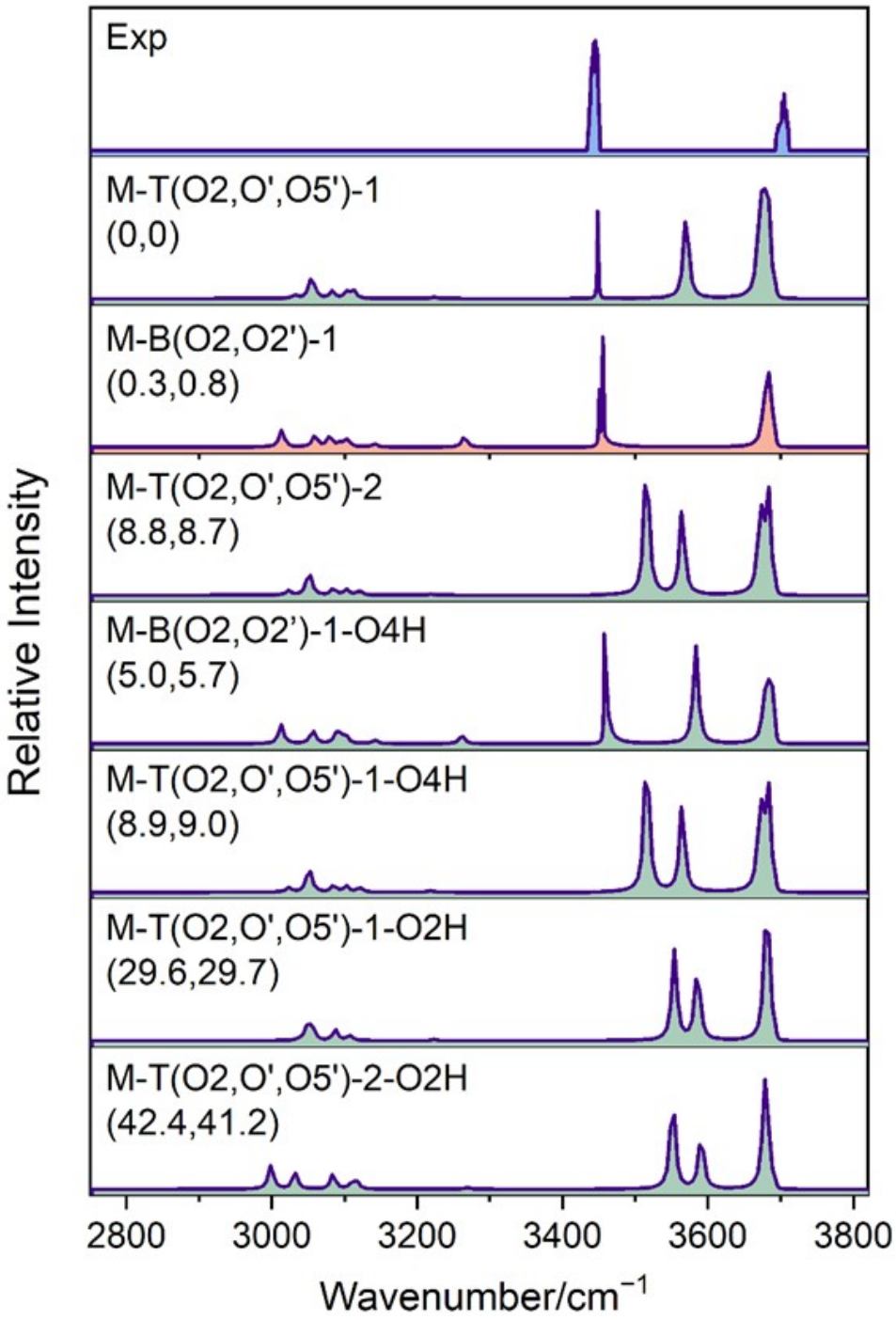


Fig. S2 Selected isomers of the precursor ions. Their relative energies and Gibbs free energies are shown in the parentheses in the unit of kcal/mol. The calculation was performed on the level of B3LYP/6-311+G(d,p)/def2-QZVDP.



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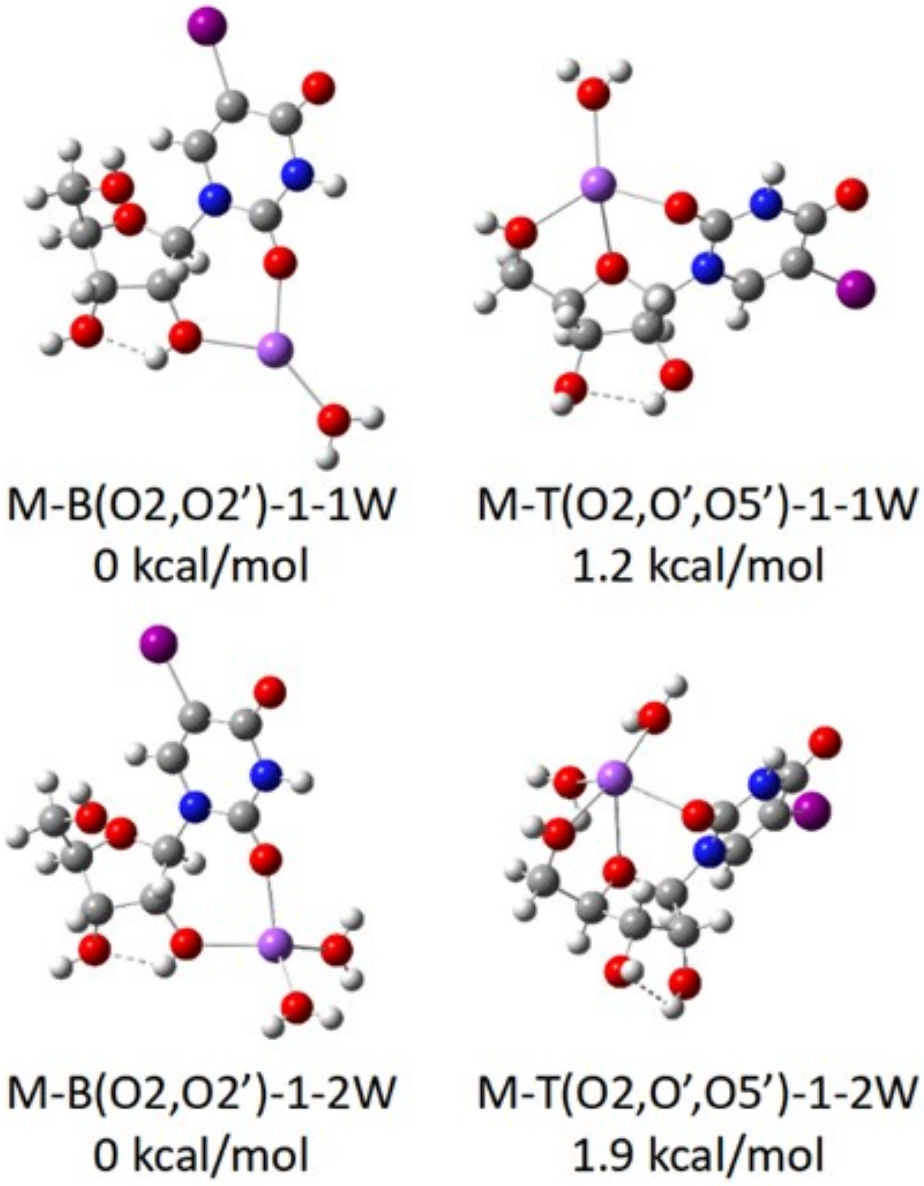

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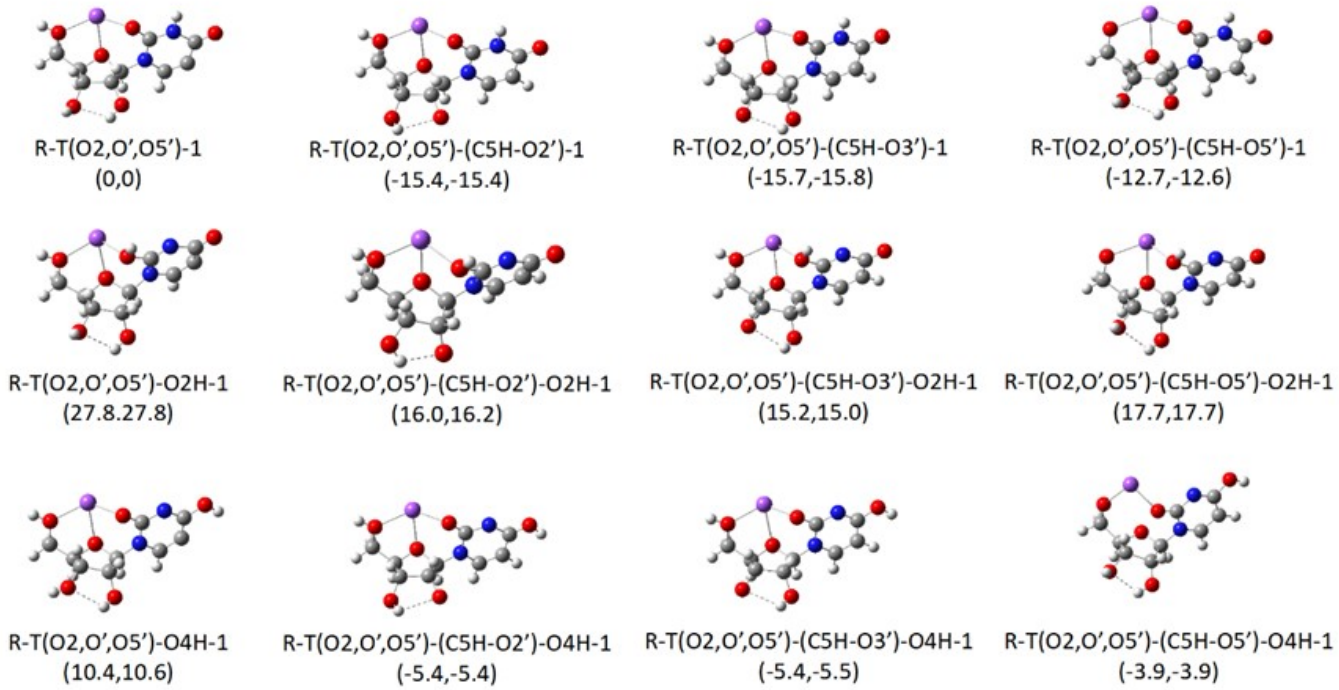

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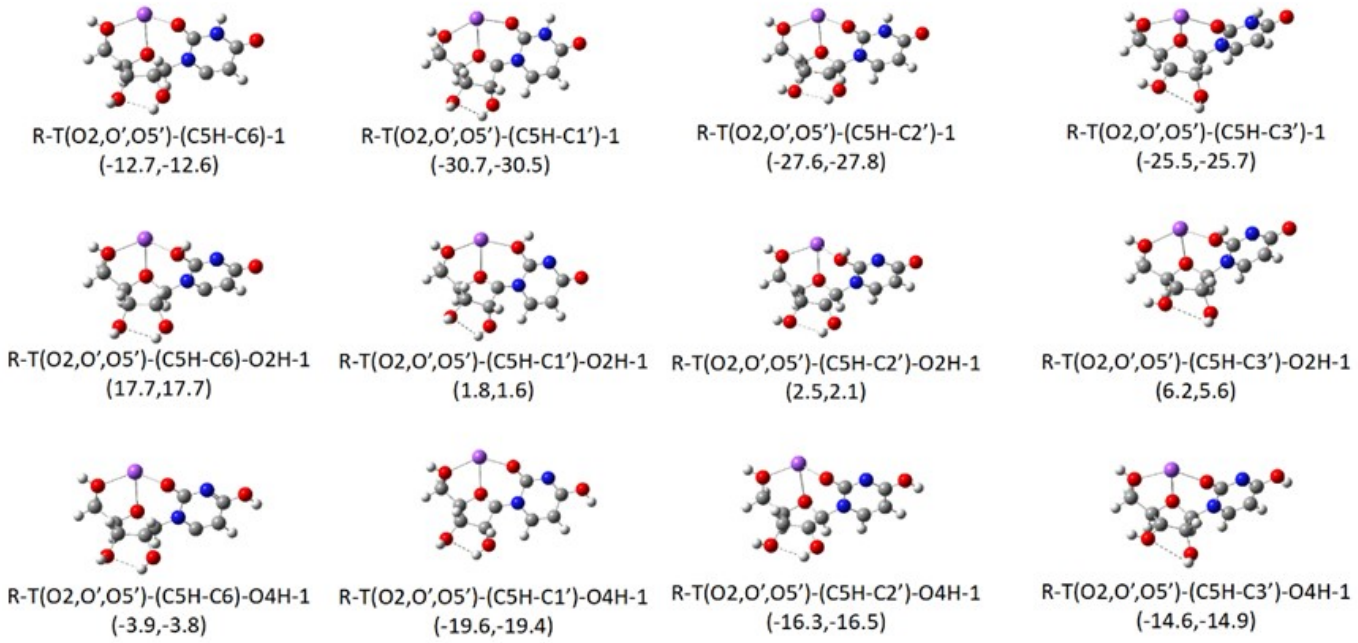

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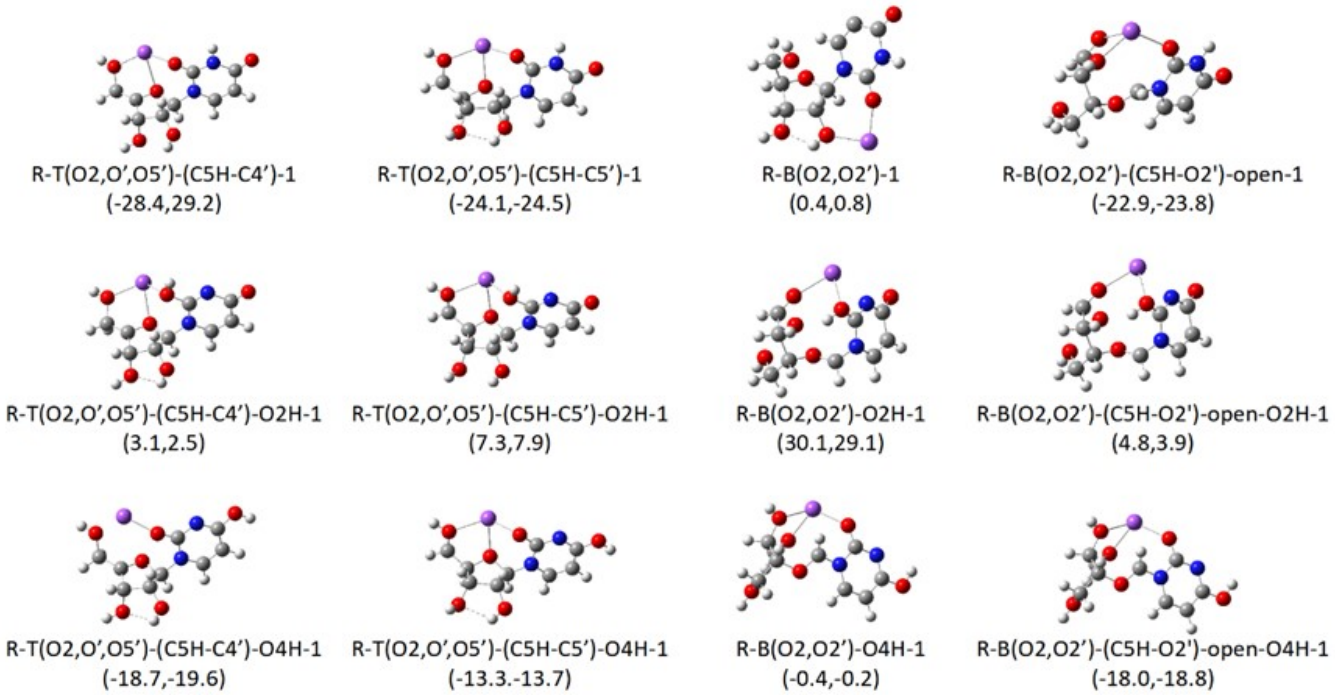

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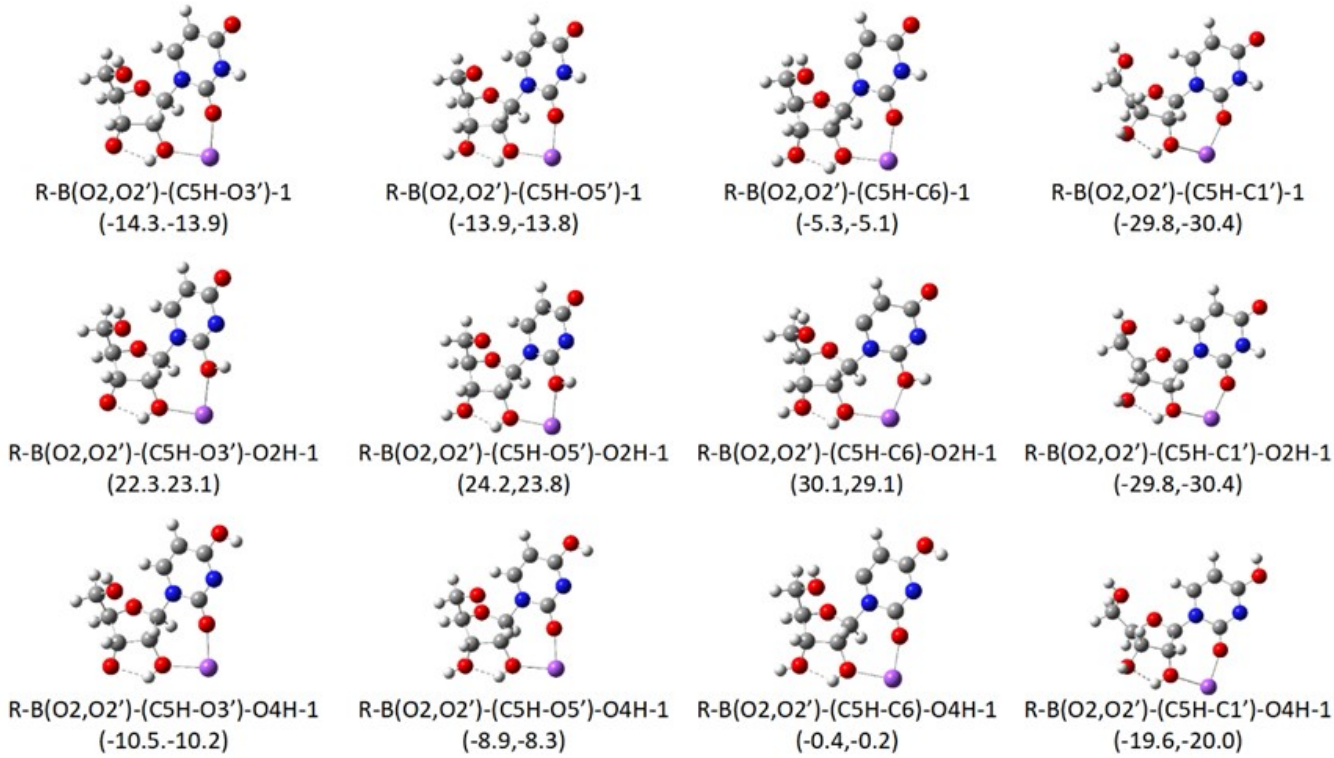

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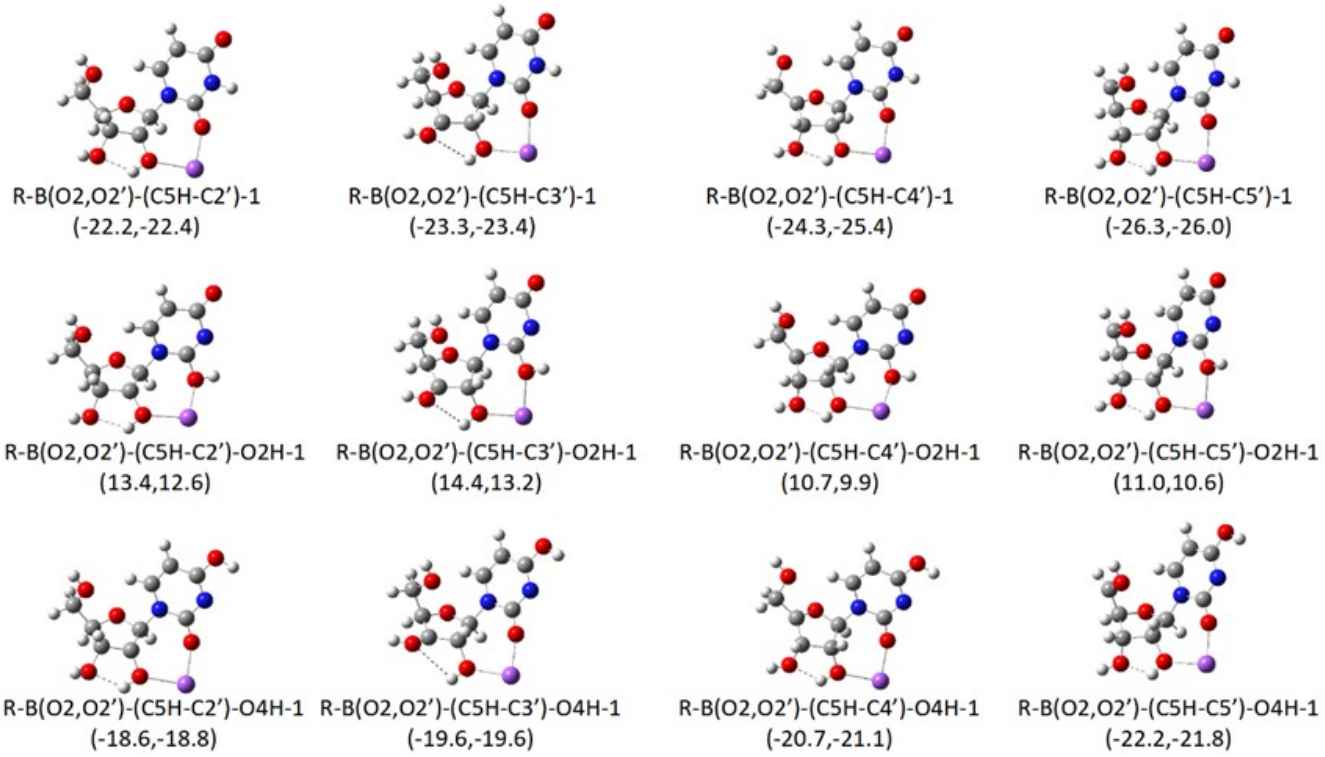

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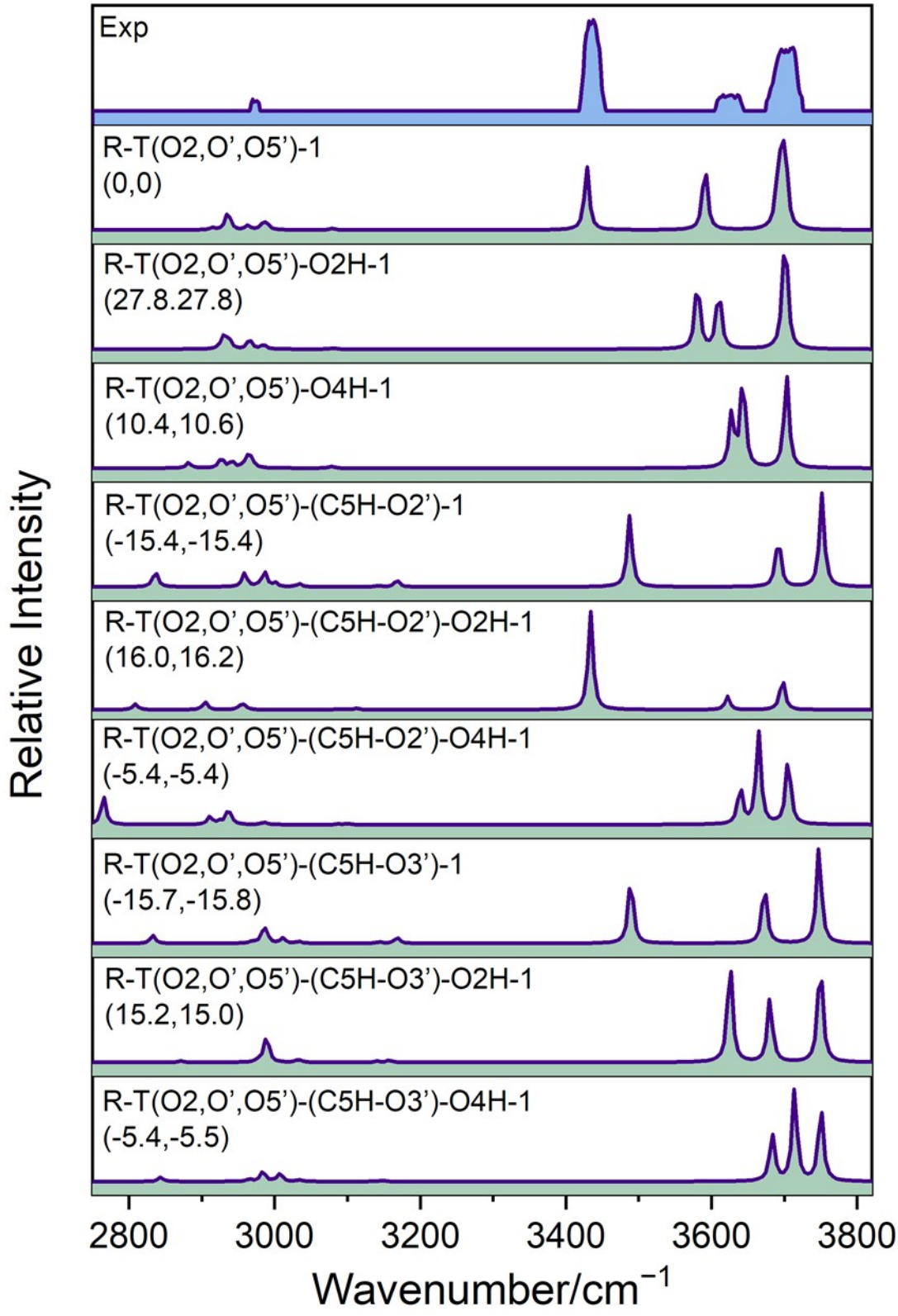

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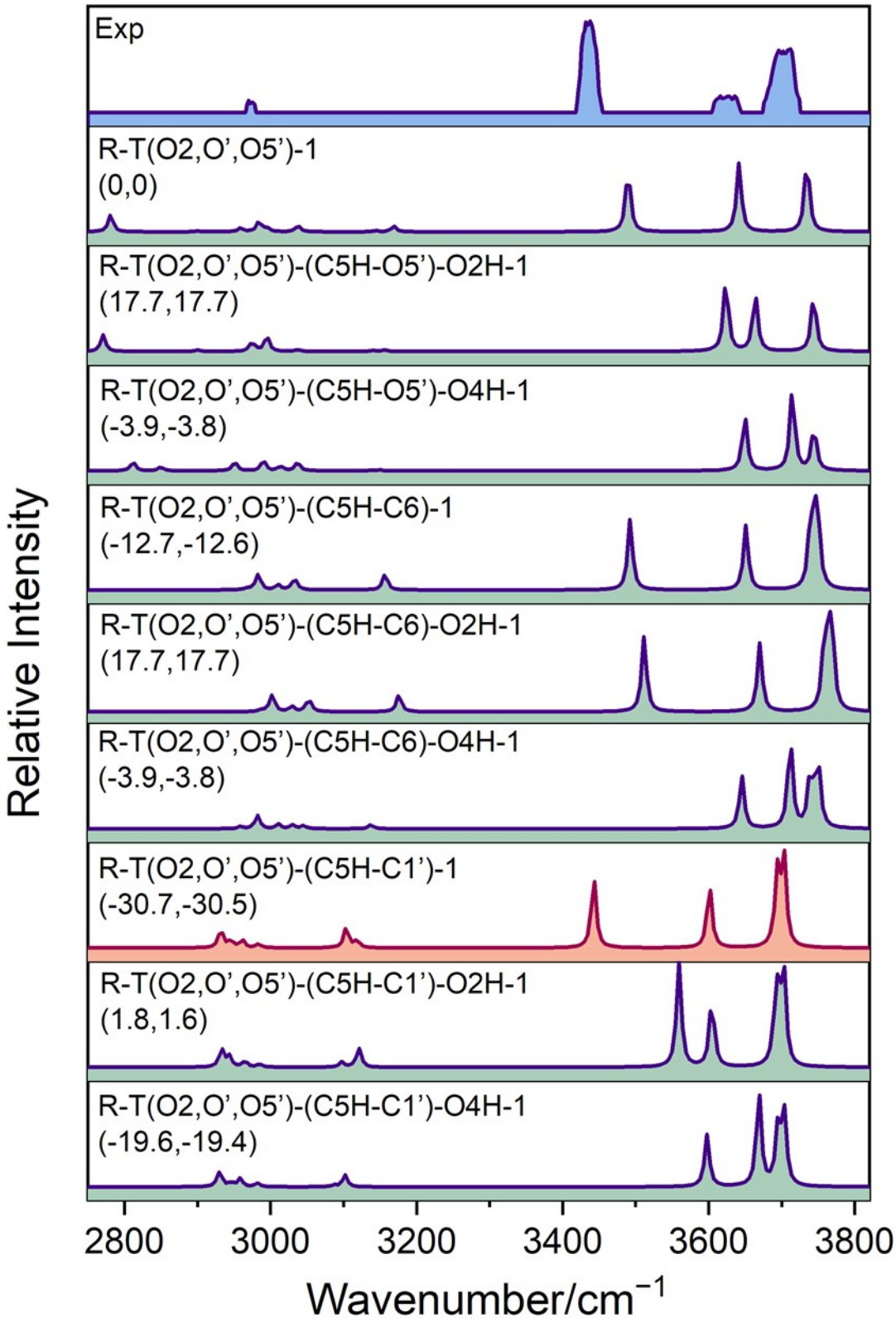

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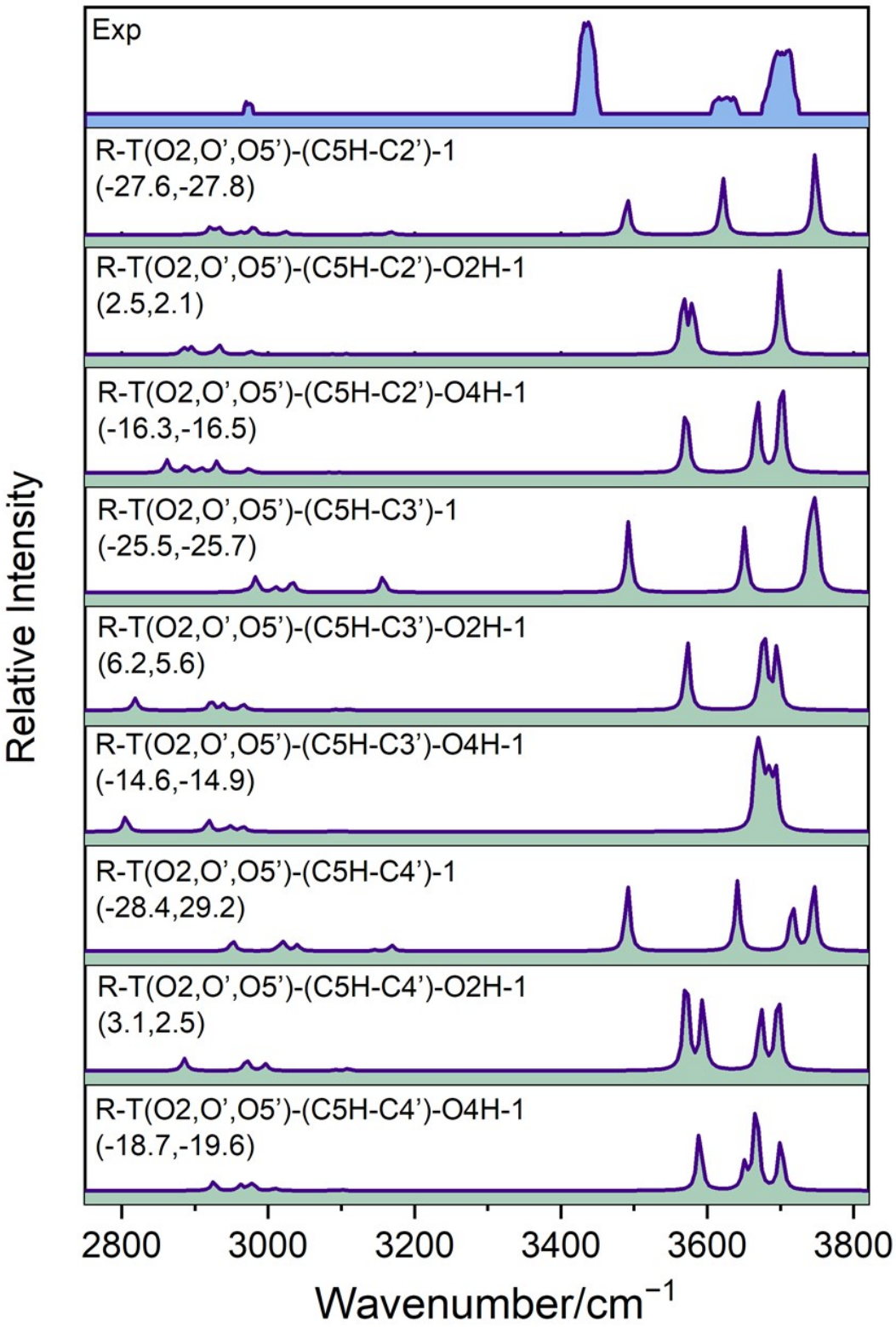

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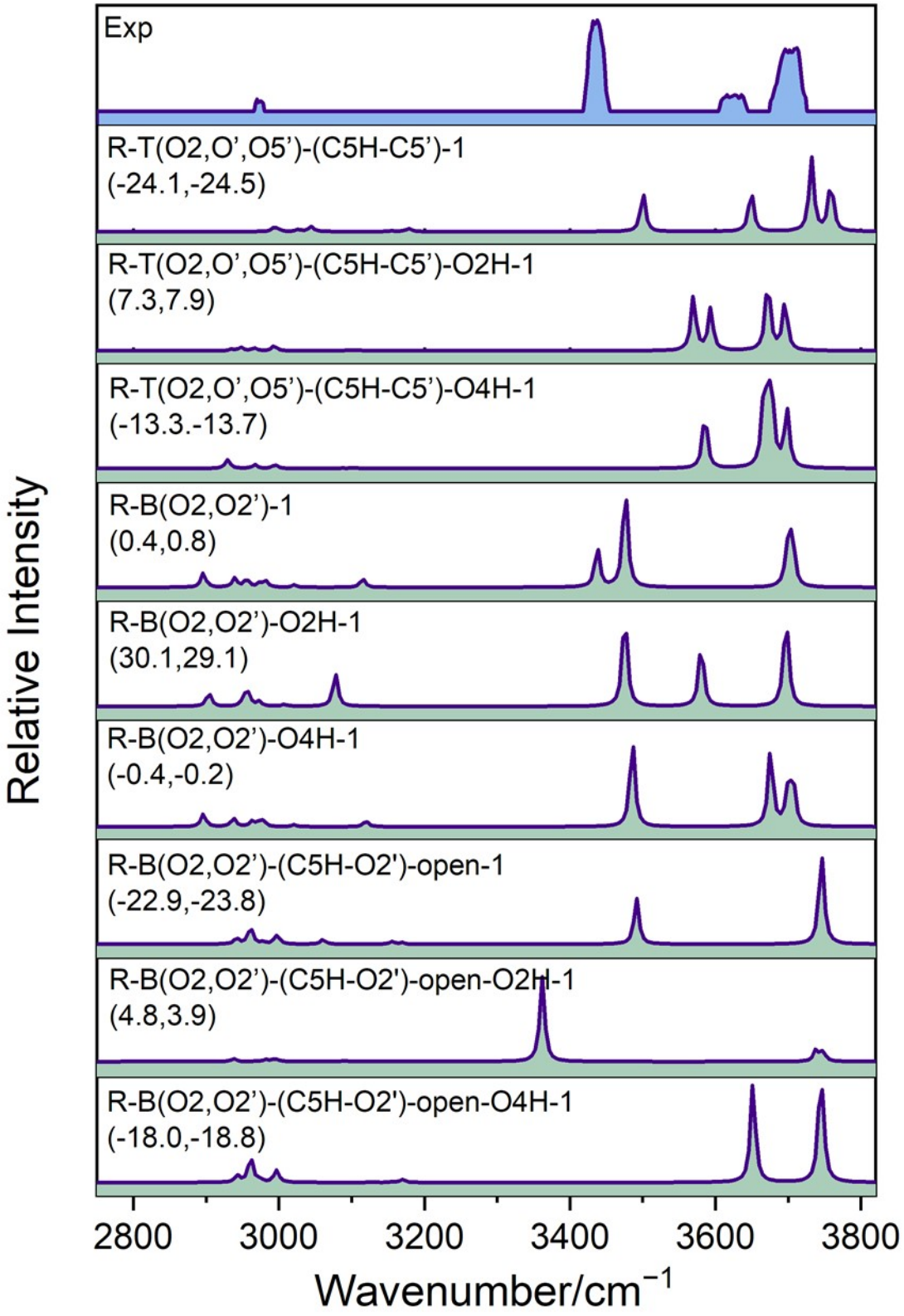

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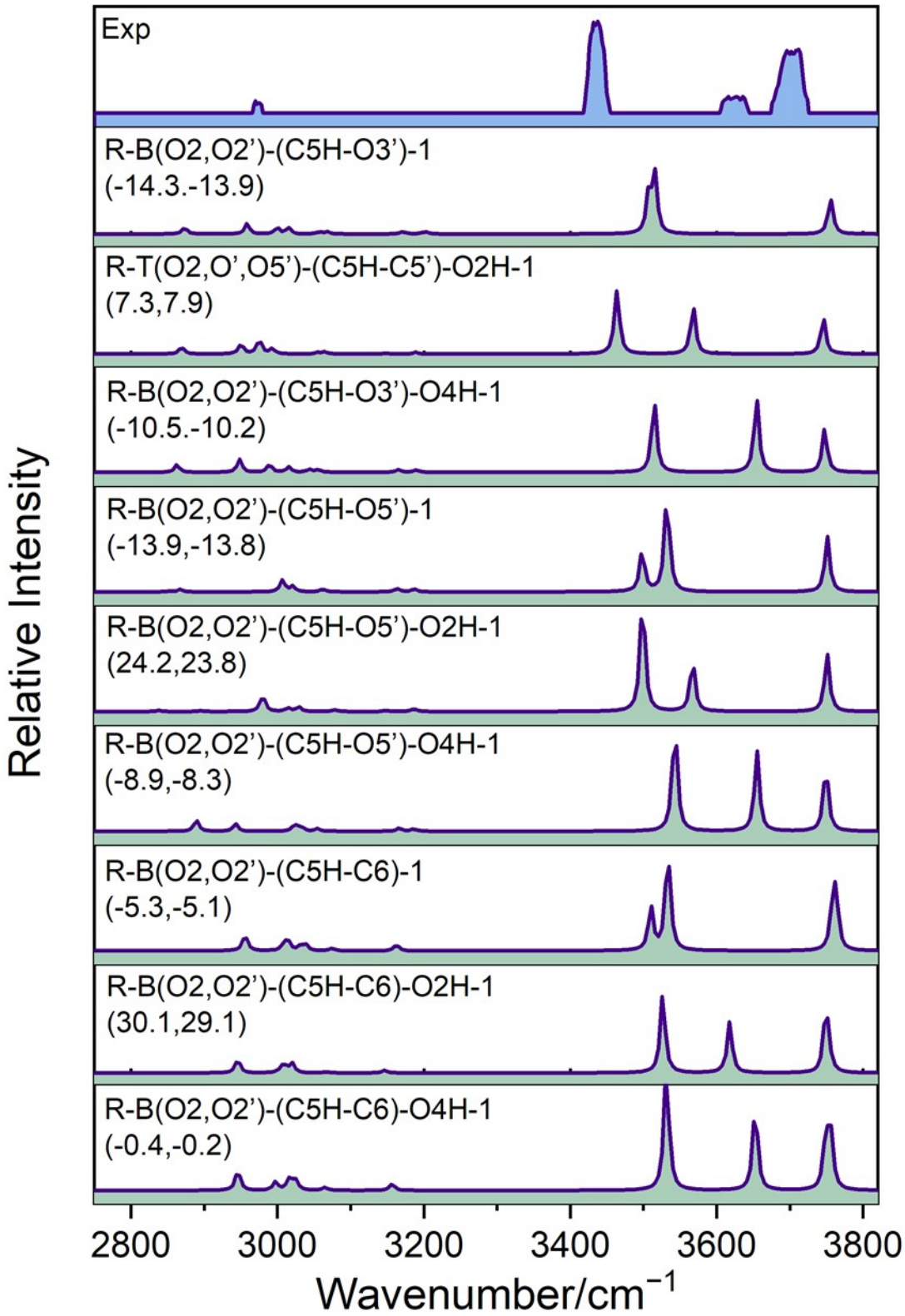

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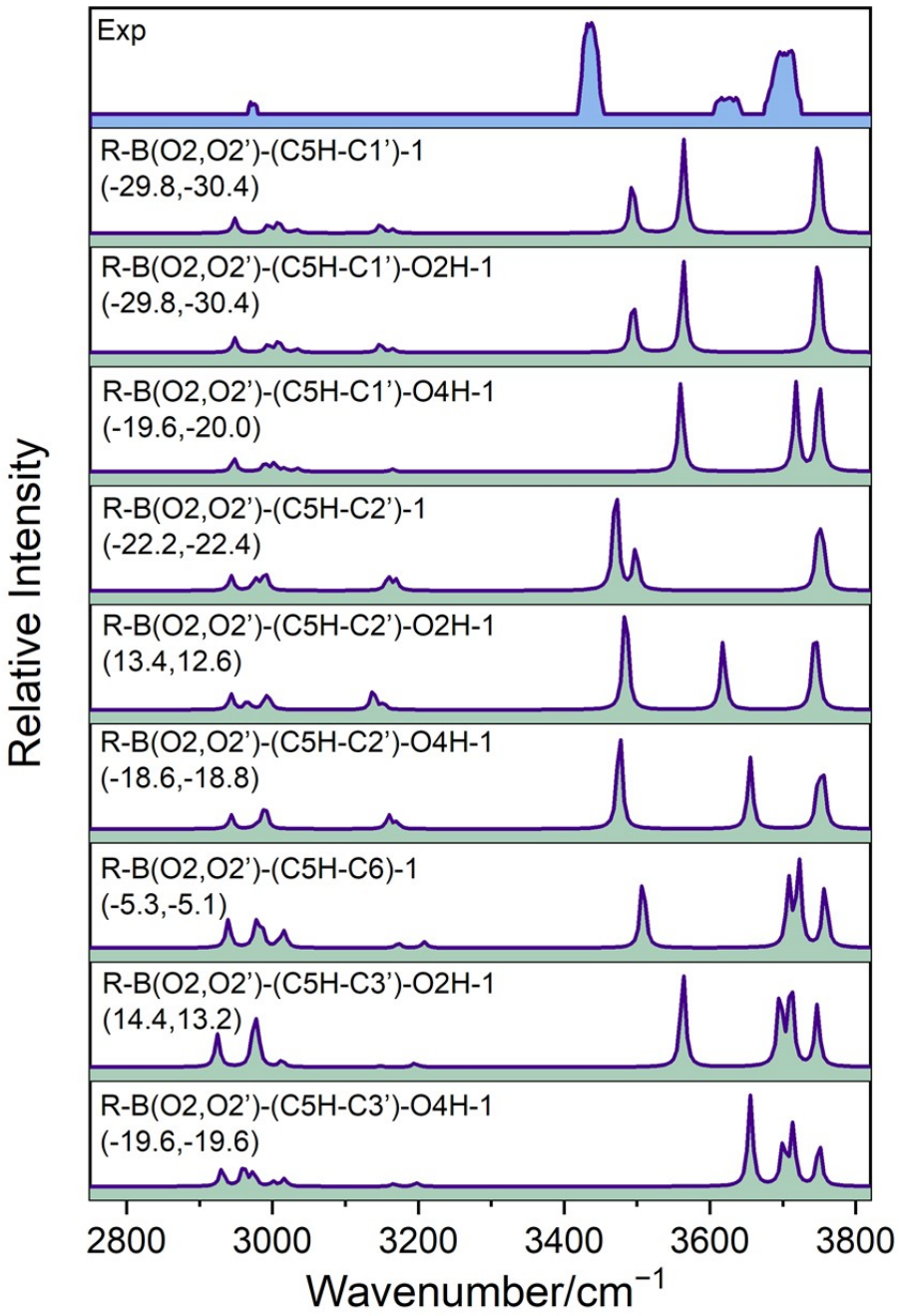

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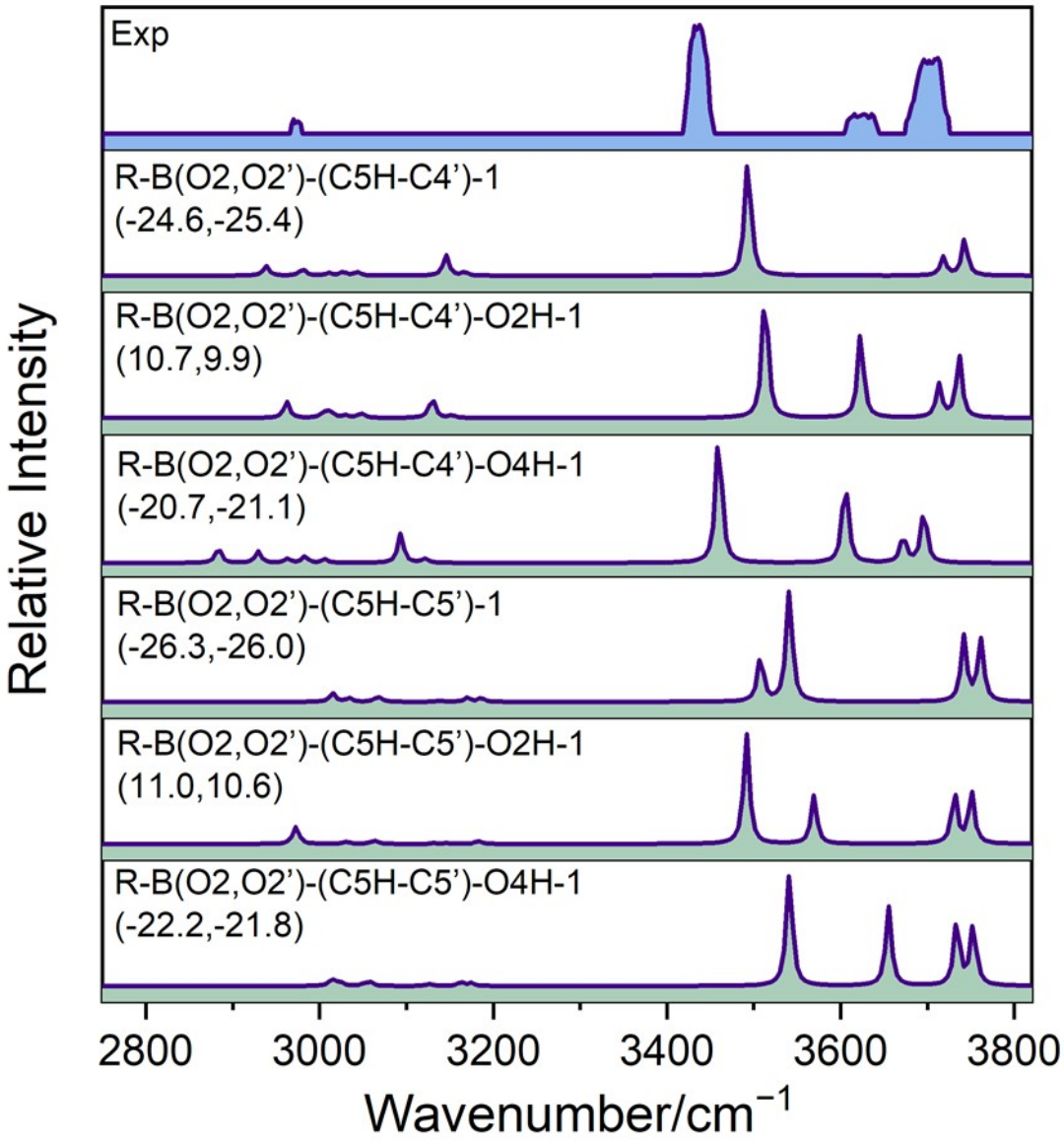

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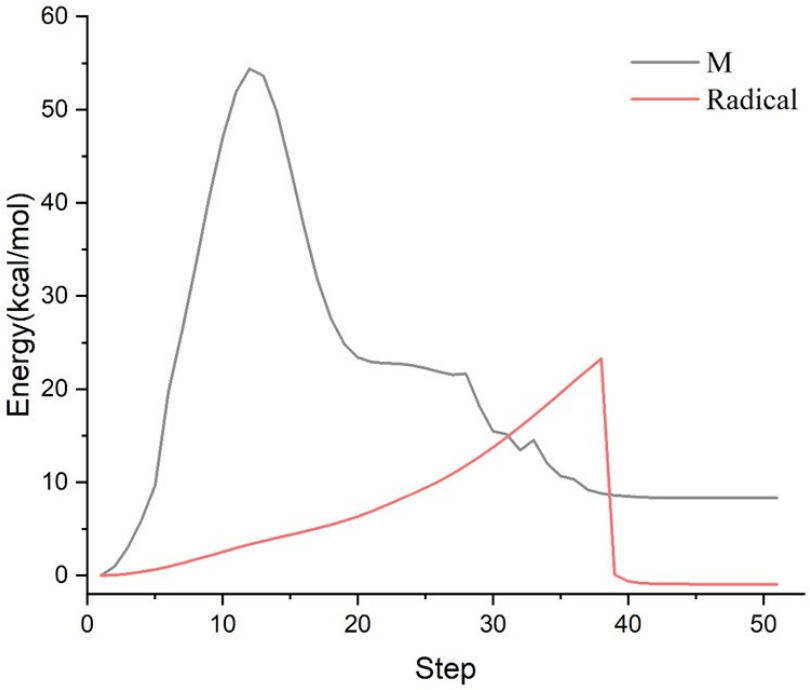

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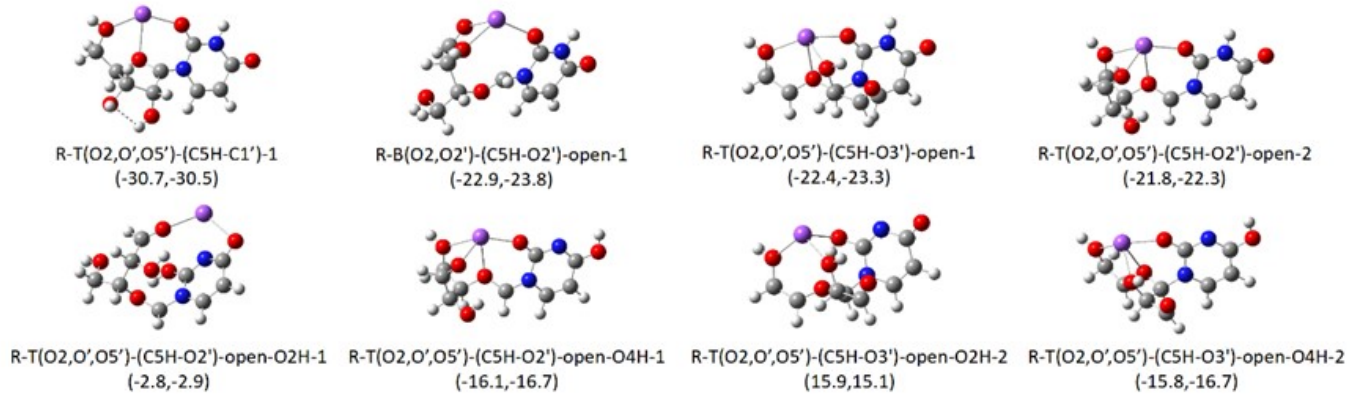

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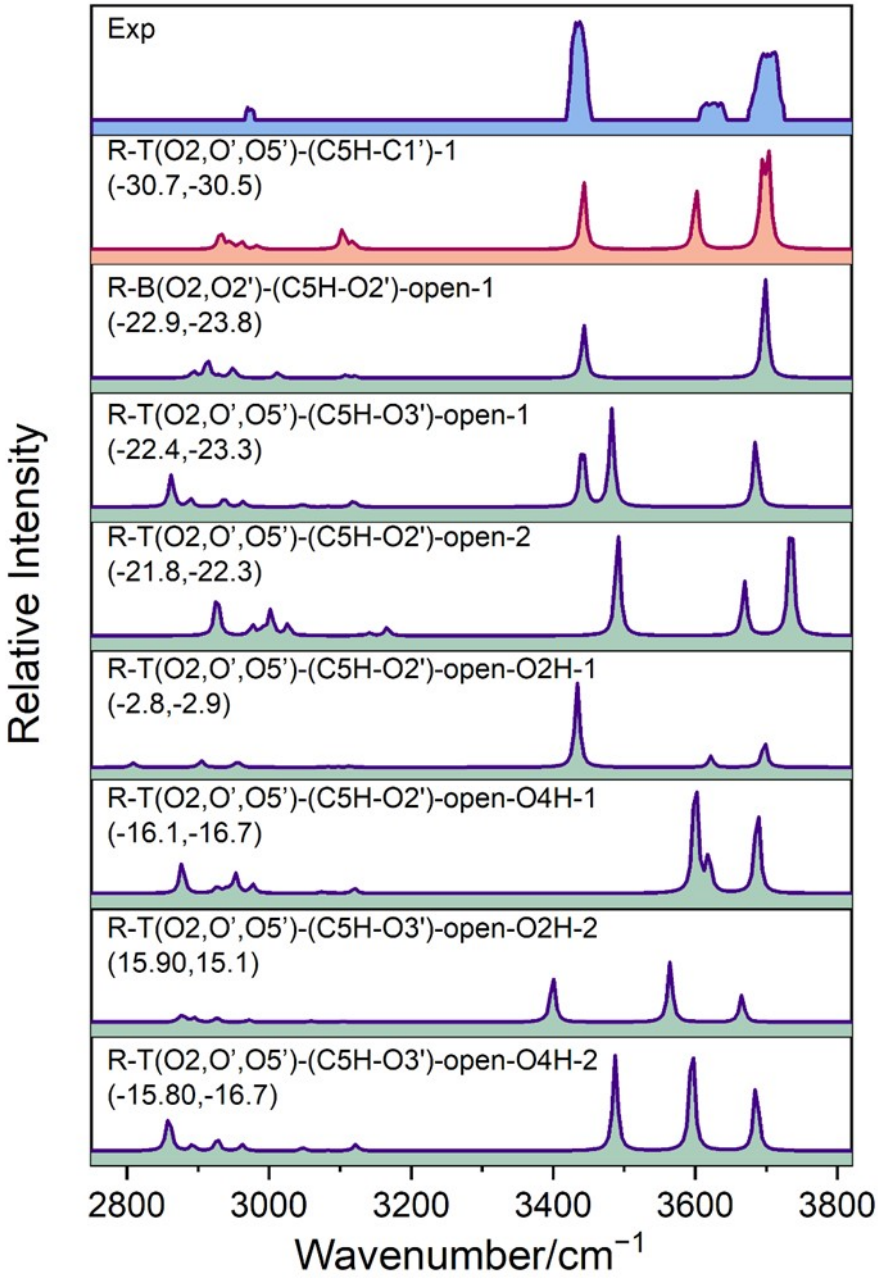

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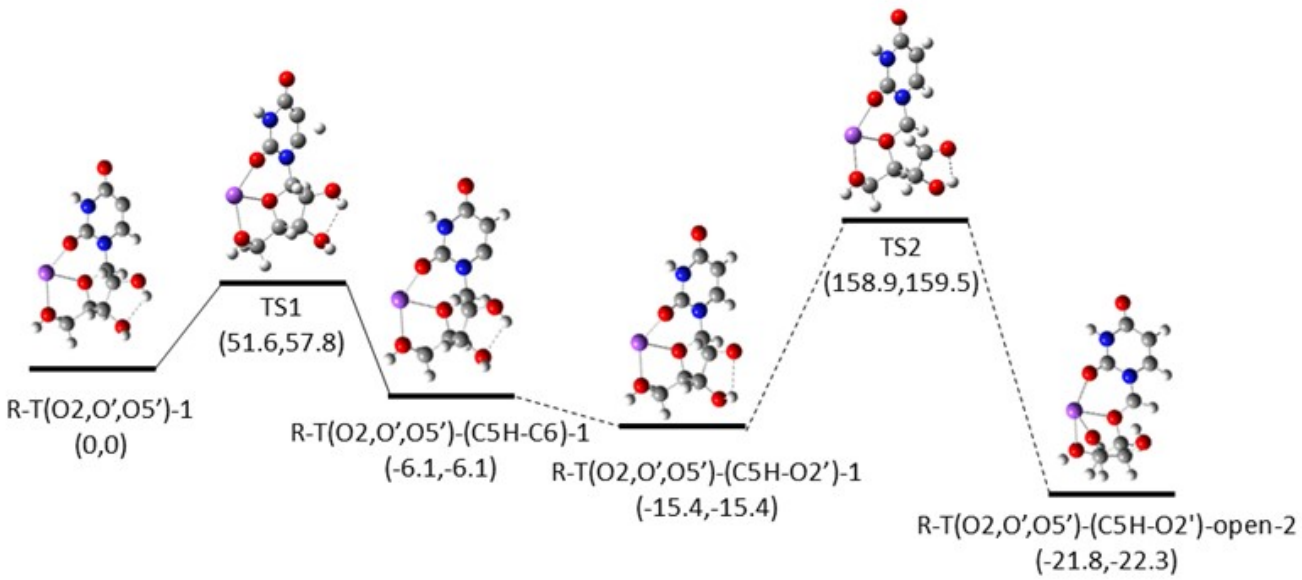

Fig. S20 Potential energy profile associated with one of the ring-opening isomerization pathways relative to t $[Urd+Na-H]^{\bullet+}$. Relative energies and Gibbs free energies are shown in the parentheses in kcal/mol. All calculations were performed at the level of B3LYP/6-311+G(d, p).

3 Supplementary Data

Data S1 The XYZ coordinates of M-T(O2,O',O5')-1

Element	X	Y	Z
C	-0.28455600	1.49124000	0.59456700
N	-0.21971400	0.22495700	0.03924000
C	1.01573000	-0.36551000	-0.24584800
C	2.22068300	1.55449500	0.63680600
C	-1.41854400	-0.57925100	-0.11204300
O	-2.38485300	0.03627100	-0.97673900
C	-2.19936500	-0.91501200	1.17725700
H	-1.09184200	-1.51949400	-0.56512100
C	-3.53672000	-0.83264000	-0.86823800
C	-3.63709500	-1.19648300	0.62780900
H	-2.20579000	-0.04743800	1.83627200
C	-4.74485000	-0.17659900	-1.49167400
H	-3.33822000	-1.76096400	-1.41773700
H	-4.37633300	-0.57743300	1.13835900
O	-3.97334600	-2.57084400	0.71621200
O	-4.98739400	1.09059900	-0.84005500
H	-4.58021500	-0.01511200	-2.56041400
H	-5.60077800	-0.84309700	-1.36116500
H	-4.51844800	-2.73302500	1.49350900
H	-5.90714700	1.34683600	-0.96331000
O	-1.63101000	-1.98371600	1.87674500
H	-2.05579100	-2.80116700	1.57691100
O	3.18523900	2.20649200	0.94010300
O	-1.35640200	2.06759700	0.81298100
H	0.95475200	-1.34767100	-0.69186300
Na	-3.10341100	2.27497600	-0.47963900
C	2.19490800	0.22754400	0.01450800
N	0.91486800	2.06945200	0.86548300
H	0.87708200	2.99549600	1.27767300
I	4.01198400	-0.67548000	-0.43496200

Data S2 The XYZ coordinates of M-B(O2,O2')-1

Element	X	Y	Z
C	2.15420300	-2.34576300	-0.24761800
O	1.60359600	-1.40282900	-1.19716500
C	3.33613000	-1.61101800	0.39158300
C	1.86762900	-0.08553900	-0.82706600
C	2.92237800	-0.12057800	0.31638600
H	3.51426600	-1.92331300	1.42145600
H	2.46925200	0.18818900	1.25485000
O	4.05582200	0.70338900	0.05040900
H	4.74770300	0.09671700	-0.27332000
O	4.52457500	-1.72676400	-0.39116300
H	5.03506400	-2.49930900	-0.12903100
C	1.11882800	-2.82093200	0.75720400
H	1.54295500	-3.65591900	1.32855800
H	0.23559900	-3.18458400	0.22157000
O	0.79897700	-1.72247000	1.60919800
H	0.09316300	-1.97100300	2.21468800
H	2.25564400	0.46008900	-1.68922400
Na	3.81457300	2.91915700	-0.01806400
C	0.64523100	1.90819900	-0.06560200
N	0.58858300	0.58763000	-0.42275600
C	-0.61961800	-0.08858700	-0.46750200
C	-1.82328200	1.87026100	0.33539100
O	-2.77745900	2.50973800	0.70121000
O	1.71017400	2.54618700	-0.05949300
H	-0.54770900	-1.10102000	-0.82685300
C	-1.78862500	0.47807500	-0.10674900
N	-0.53791000	2.47649000	0.29080100
H	-0.50526600	3.45279900	0.56102200
I	-3.58222200	-0.57712500	-0.15747400
H	2.49935900	-3.19732900	-0.83534800

Data S3 The XYZ coordinates of R-T(O2,O',O5')-1

Element	X	Y	Z
C	-1.77239000	0.97617200	-0.20928900
N	-1.16554600	-0.27143300	-0.02188700
C	-1.94160400	-1.41676900	0.22035300
C	-3.99841400	-0.12711800	0.08482900

C	0.22344900	-0.36761800	-0.17897800
O	1.00437500	0.40250600	0.67275500
C	0.96724000	-1.56323600	-0.66130500
C	2.34621700	-0.16658900	0.69924200
C	2.41624700	-1.02561800	-0.56986000
H	0.67880100	-1.84846700	-1.67778000
C	3.36359500	0.94314800	0.83043600
H	2.42016200	-0.82445700	1.56923800
H	2.64386900	-0.40733800	-1.44266800
O	3.37312300	-2.04557500	-0.37837500
O	3.11263900	1.94016300	-0.18639300
H	3.29793300	1.40647900	1.81864900
H	4.35946500	0.50978300	0.71241400
H	-3.85919700	-2.27190200	0.45422500
H	3.93704200	2.38088800	-0.41597300
O	0.79673100	-2.66039700	0.23776100
H	1.59223700	-3.21147600	0.19232300
O	-5.19142800	0.04618300	0.10460600
O	-1.11473300	1.99296400	-0.43788300
H	-1.36570300	-2.31775300	0.37568400
Na	0.93989100	2.67006600	-0.18663600
C	-3.28178600	-1.37946900	0.26408000
N	-3.12536300	0.98151200	-0.12585000
H	-3.57560100	1.88021000	-0.26070000
H	3.78757800	-2.28141900	-1.21506100

Data S4 The XYZ coordinates of R-B(O2,O2')-1

Element	X	Y	Z
C	2.45608900	-0.74103400	-0.66643600
O	1.06791900	-0.69512100	-1.09168300
C	2.47386100	-0.04195900	0.70684200
C	0.37373100	0.19908900	-0.35090100
C	1.22853700	0.88187300	0.66631900
H	2.35261300	-0.78096300	1.49912300
H	0.73409900	0.97630400	1.63485700
O	1.63161200	2.20054200	0.21985600
H	2.57880400	2.27900200	0.43072800
O	3.66964600	0.70701900	0.86087800
H	4.06515500	0.54106500	1.72274300
C	2.88902500	-2.19026900	-0.64531800

H	3.95559300	-2.22853000	-0.39178600
H	2.75027000	-2.62261400	-1.64147700
O	2.09018400	-2.85747500	0.32746500
H	2.35035100	-3.78237100	0.38123800
Na	-0.02888000	3.45192600	-0.58892200
C	-1.91964300	0.84359200	-0.03561000
N	-0.97403700	-0.17024700	-0.13445400
C	-1.34952100	-1.51830800	-0.08301800
C	-3.68387700	-0.90960100	0.21456500
O	-4.86281400	-1.11177300	0.36926800
O	-1.60426500	2.03644700	-0.11143800
H	-0.52314200	-2.20900500	-0.17643000
C	-2.62617600	-1.89858400	0.07768100
N	-3.19724600	0.43104800	0.15467500
H	-3.89706700	1.16031700	0.23497500
H	3.05958300	-0.17377300	-1.37899300
H	-2.90001100	-2.94212700	0.12209800

4 Supplementary References

38 J. W. Gauthier, T. R. Trautman, D. B. Jacobson. Sustained off-resonance irradiation for collision-activated dissociation involving Fourier-transform mass-spectrometry-collision-activated dissociation technique that emulates infrared multiphoton dissociation. *Analytica Chimica Acta*, 1991, **246(1)**: 211-225.

39 T. Lu, Molclus program, Version 3.8, http://www.keinsci.com/research/molclus.html accessed 4 1, 2022.

40 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman and G. Scalmani, Gaussian09 (2009). Gaussian Inc, Wallingford, CT.

41 A. P. Scott, L. Radom, Harmonic Vibrational Frequencies: An Evaluation of Hartree−Fock, Møller−Plesset, Quadratic Configuration Interaction, Density Functional Theory, and Semiempirical Scale Factors, J. Phys. Chem. 1996 100, 16502-16513.