

Supporting information

Structural characterization of nucleotide 5'-triphosphates by infrared ion spectroscopy and theoretical studies

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Table T1 | Predicted relative free energies of the lowest-energy conformers of doubly deprotonated ATP, GTP and CTP at four levels of theory.

Structure	ΔG° (kJ mol ⁻¹) B3LYP/ 6-31++G(d,p)	ΔG° (kJ mol ⁻¹) B3LYP/ 6-311+G(d,p)	ΔG° (kJ mol ⁻¹) M06-2X/ 6-311+G(d,p)	ΔG° (kJ mol ⁻¹) MP2/ 6-311++G(2d,2p)
[ATP-2H]²⁻				
$\alpha\beta$	0.0	0.0	0.0	0.0
$\alpha\gamma$	12.7	14.7	18.1	8.2
$\beta\gamma$	16.6	19.7	21.1	12.6
$\alpha\beta 2$	5.3	5.2	4.7	6.6
[CTP-2H]²⁻				
$\alpha\beta$	0.0	0.0	0.0	0.0
$\alpha\gamma$	21.4	23.0	33.1	24.7
$\beta\gamma$	26.9	29.9	37.5	29.9
[GTP-2H]²⁻				
$\alpha\beta$	0.0	6.6	0.0	7.9
$\alpha\gamma$	8.0	8.0	17.0	15.4
$\beta\gamma$	40.2	42.8	58.0	45.5
$\alpha\beta 2$	8.5	0.0	11.5	0.0

Table T2 | Predicted relative free energies relative of the lowest-energy conformers of singly deprotonated ATP, GTP and CTP at four levels of theory.

Structure	ΔG° (kJ mol ⁻¹) B3LYP/ 6-31++G(d,p)	ΔG° (kJ mol ⁻¹) B3LYP/ 6-311+G(d,p)	ΔG° (kJ mol ⁻¹) M06-2X/ 6-311+G(d,p)	ΔG° (kJ mol ⁻¹) MP2/ 6-311++G(2d,2p)
[ATP-H]¹⁻				
β	0.0	0.0	12.9	13.9
γ	5.5	6.0	19.7	20.3
α	13.4	9.2	0.0	9.3
$\alpha 2$	29.6	26.1	33.3	42.7
$\beta 2$	11.0	10.9	5.1	0.0
[CTP-H]¹⁻				
β	4.3	1.0	12.7	13.8
γ	12.5	9.3	21.9	24.6
α	27.7	20.8	23.7	34.9
$\beta 2$	0.0	0.0	0.0	0.0
$\gamma 2$	5.5	3.8	7.5	7.9
$\alpha 2$	18.6	13.6	4.6	15.6
[GTP-H]¹⁻				
β	3.6	2.5	0.0	4.1
γ	6.4	6.7	17.0	10.0
α	3.2	3.9	2.5	0.0
$\beta 2$	0.0	0.0	9.3	2.2
$\alpha 2$	32.3	28.9	32.8	34.7

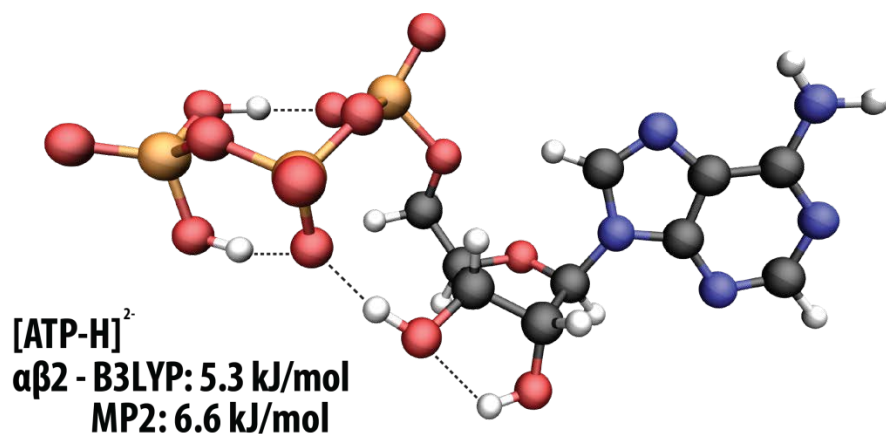


Figure S1 | B3LYP optimized structure and predicted free energy relative to the ground state conformer of the $\alpha\beta$ -deprotonated ATP-conformer proposed by Burke *et al.*

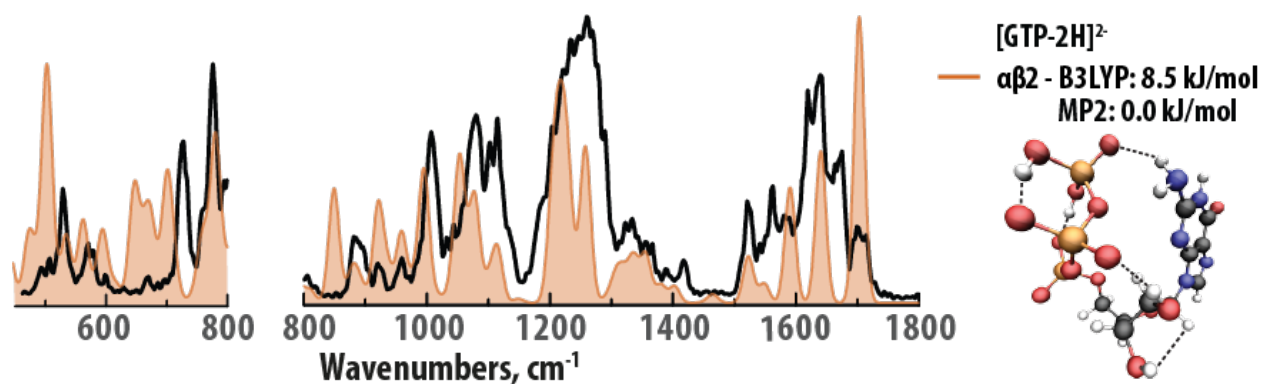


Figure S2 | IRMPD spectrum of [GTP-2H]²⁻ in comparison with the predicted linear infrared spectrum of the $\alpha\beta$ 2-deprotonated structure. The spectra are divided in two wavelength regions and subsequently normalized. The calculated structure, deprotonation sites and relative energies are presented next to the panel.

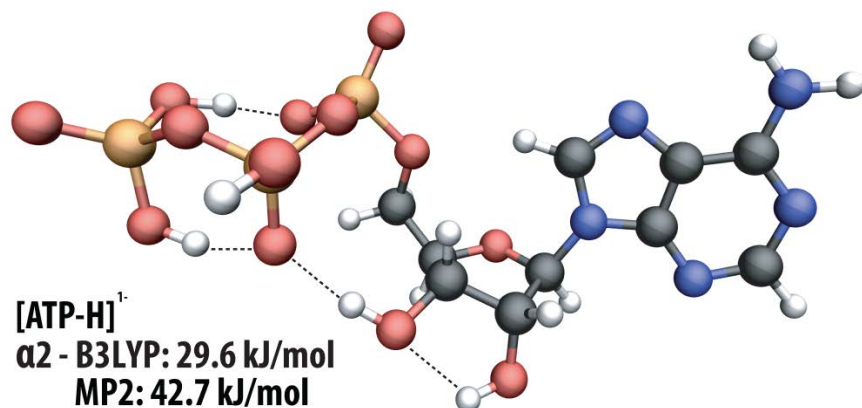


Figure S3 | B3LYP optimized structure and predicted free energy relative to the ground state conformer of the α -deprotonated ATP-conformer proposed by Burke *et al.*

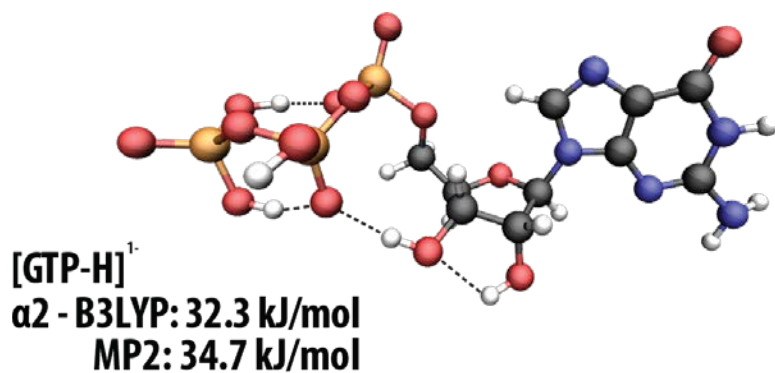


Figure S4 | B3LYP optimized structure and predicted free energy relative to the ground state conformer of the α 2-structure of [GTP-H]¹⁻.

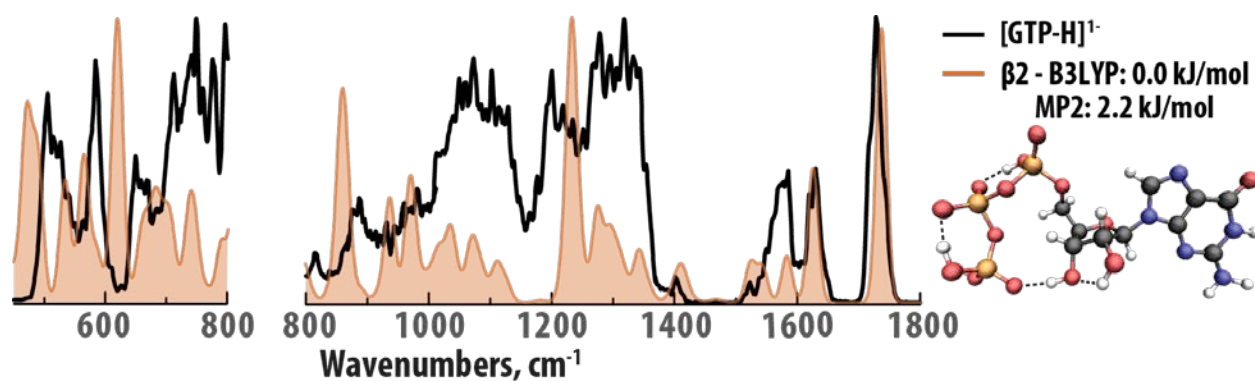


Figure S5 | IRMPD spectrum of [GTP-H]¹⁻ in comparison with the predicted linear infrared spectrum of the β₂-structure. The spectra are divided in two wavelength regions and subsequently normalized. The calculated structure, deprotonation sites and relative energies are presented next to the panel. The C=O stretching vibration is slightly blue-shifted compared to the experimental spectrum due to the absence of a hydrogen-bond with the phosphate-tail. On the other hand, the location of the observed vibration just above 1600 cm⁻¹ is better predicted by the spectrum of the β₂- and γ-structure (see Fig. S11), than by the folded conformers (labelled β and α). However, the intensity of the band below 1600 cm⁻¹ is better predicted by the folded conformers. Moreover, both the observed bands in the 1150-1400 cm⁻¹ (symmetric P=O stretching) and the 950-1150 cm⁻¹ (asymmetric P=O stretching) spectral region are better explained by the predicted spectrum of the β-structure. Additionally, the experimental band around 900 cm⁻¹ is blue-shifted compared to the β₂-spectrum while it is well predicted by the β-spectrum and, finally, the 450-800 cm⁻¹ is much better predicted by the β-spectrum.

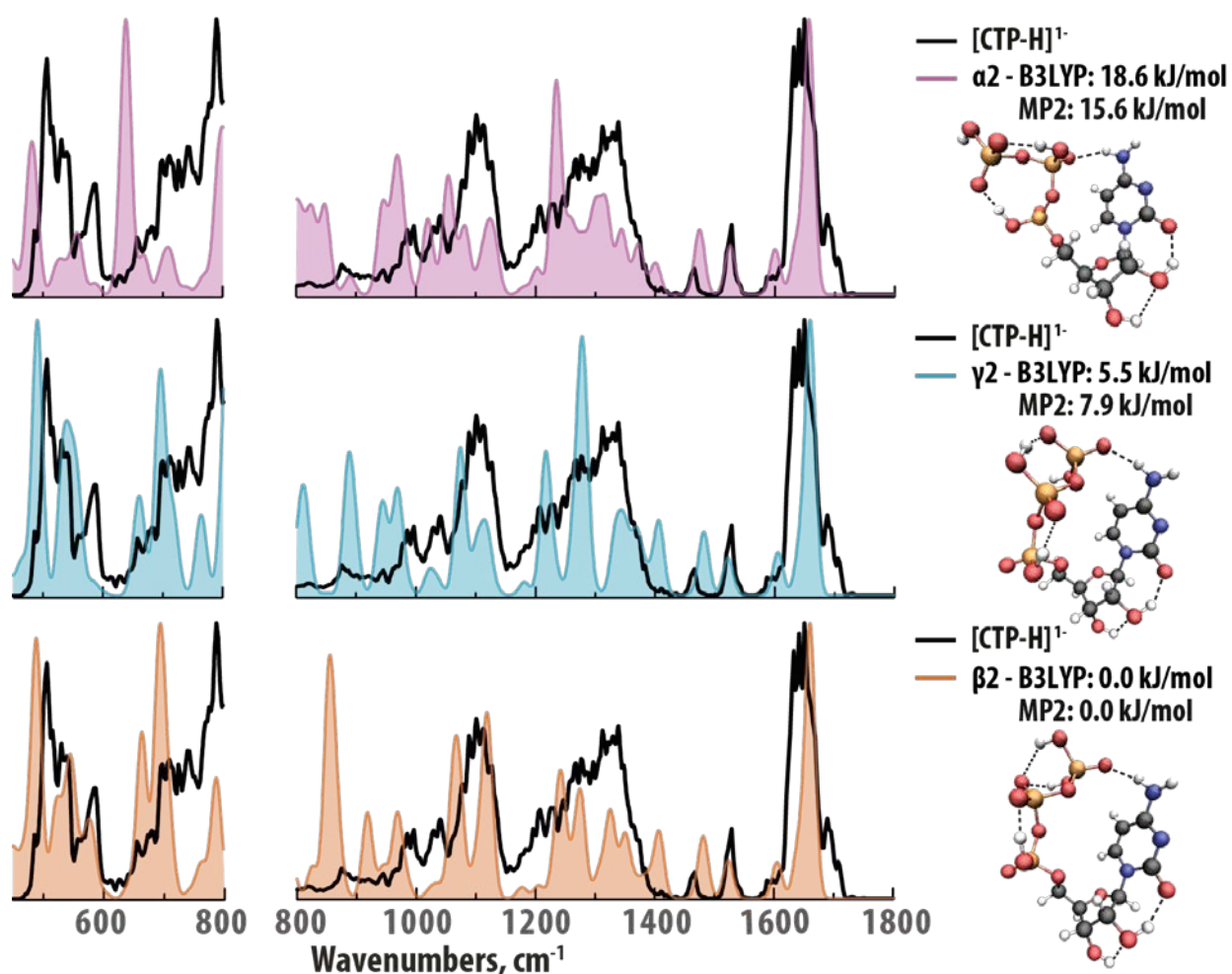


Figure S6 | IRMPD spectrum of $[\text{CTP-H}]^{1-}$ in comparison with the predicted linear infrared spectra of the $\alpha 2$, $\beta 2$ and $\gamma 2$ -deprotonated structures. The spectra are divided in two wavelength regions and subsequently normalized. The calculated structures, deprotonation sites and relative energies are presented next to each panel. In all three predicted spectra, the C=O stretch vibration is redshifted due to its hydrogen-bond interaction with the ribose 2'-OH group. This causes the experimental band around 1700 cm^{-1} to be unexplained by this calculation while the calculated bands around 1650 cm^{-1} are shifted relative to the experiment. This hydrogen-bond also causes a vibration of the ribose 2'-OH to be predicted just above 1400 cm^{-1} which is not observed. Moreover, all predicted spectra shown in Fig. 6 do much better predict the intensity of the band just below 1500 cm^{-1} . Therefore, we assign the β -conformer, which does not have a hydrogen-bond interaction between the cytosine-base and the phosphate tail.

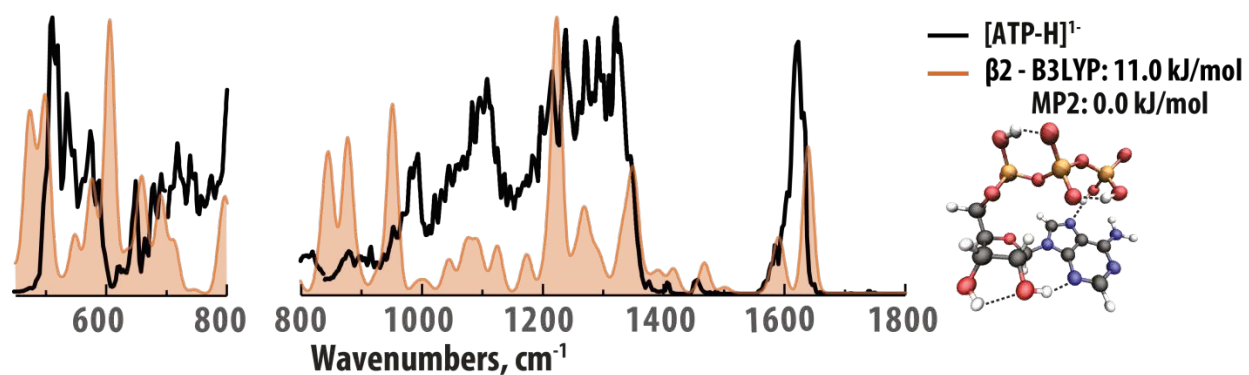


Figure S7 | IRMPD spectrum of $[\text{ATP-H}]^{1-}$ in comparison with the predicted linear infrared spectrum of the folded $\beta 2$ -deprotonated structure. The spectra are divided in two wavelength regions and subsequently normalized. The calculated structure, deprotonation sites and relative energies are presented next to the panel. The band just above 1600 cm^{-1} , which corresponds to the NH_2 -group of the nucleobase, is shifted compared to the experiment. Moreover, the band just below 1000 cm^{-1} and the $450\text{--}800\text{ cm}^{-1}$ region are explained better by the β -conformer. Therefore, we conclude that the β -conformer shows a slightly better spectral match than the $\beta 2$ -conformer.

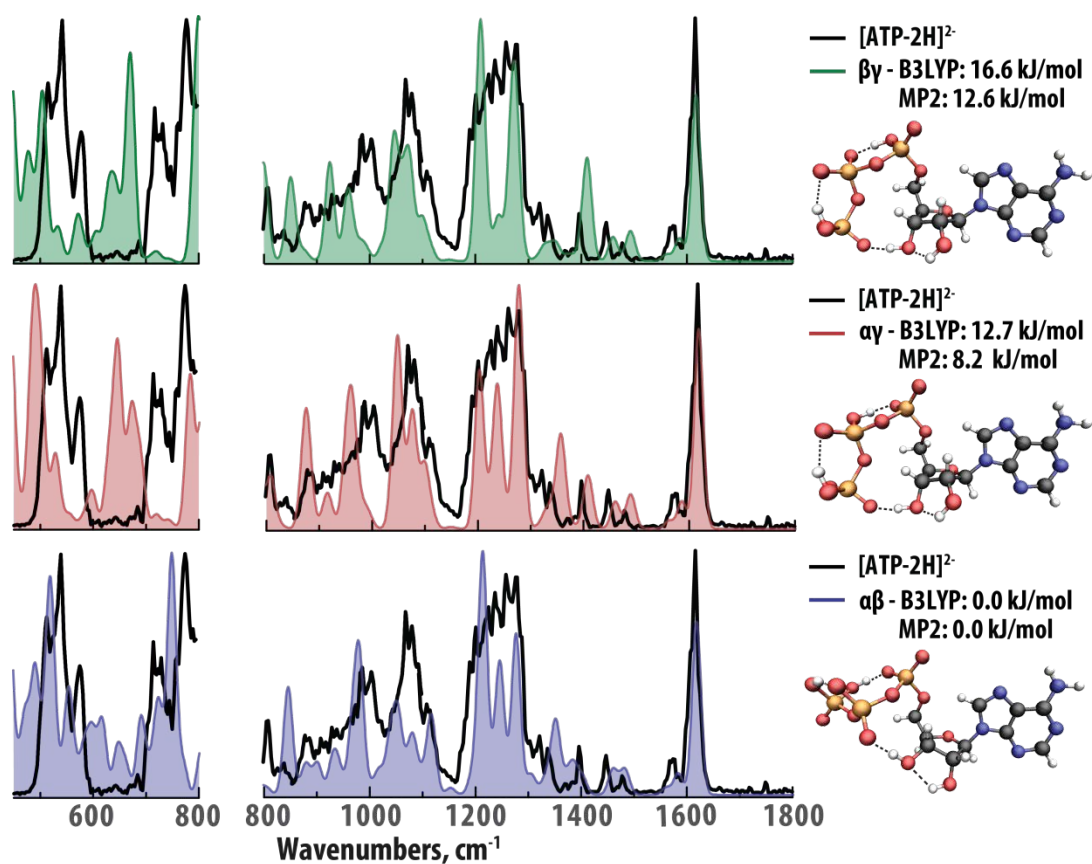


Figure S8 | IRMPD spectrum of $[\text{ATP-2H}]^{2-}$ (black traces) in comparison with the predicted linear infrared spectra of three low-energy conformers (coloured traces). The spectra are divided in two wavelength regions and subsequently normalized. Calculated structures, deprotonation sites and relative energies are presented next to each panel.

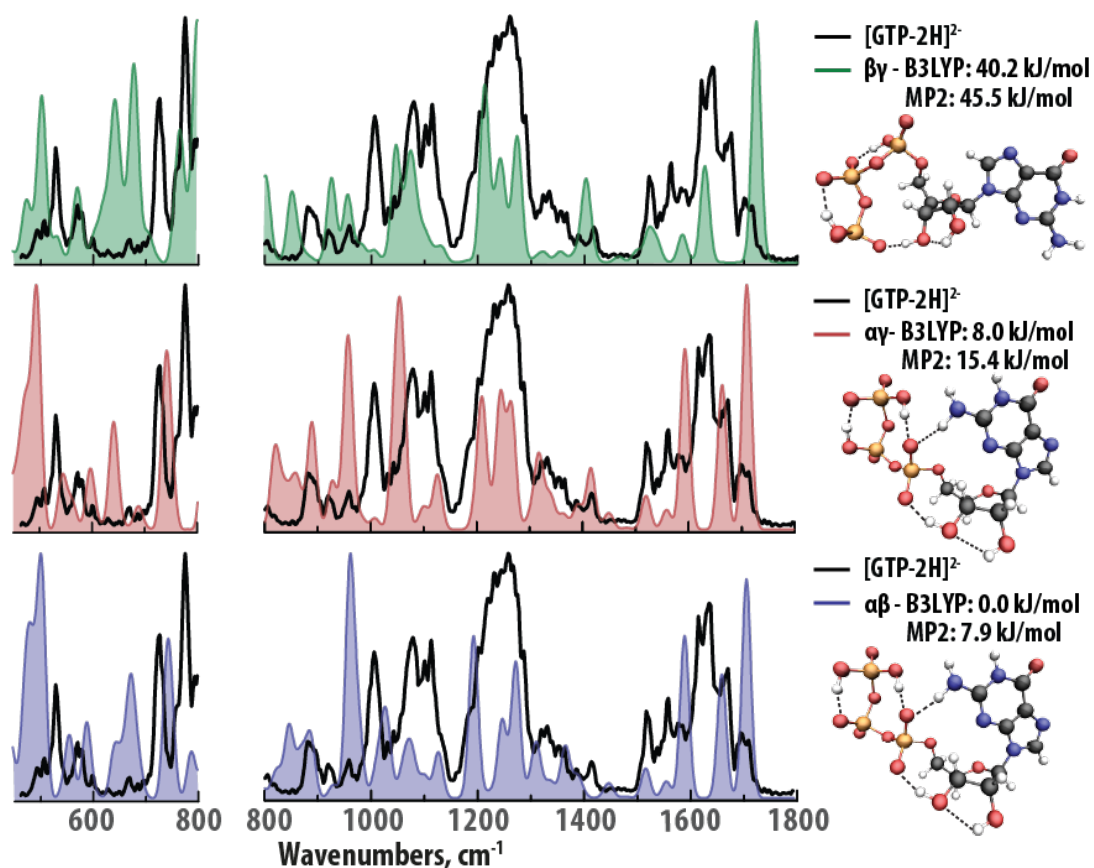


Figure S9 | IRMPD spectrum of $[GTP-2H]^{2-}$ (black traces) compared with the predicted linear infrared spectra of three low-energy conformers (coloured traces). The spectra are divided in two wavelength regions and subsequently normalized. Calculated structures, deprotonation sites and relative energies are presented next to each panel.

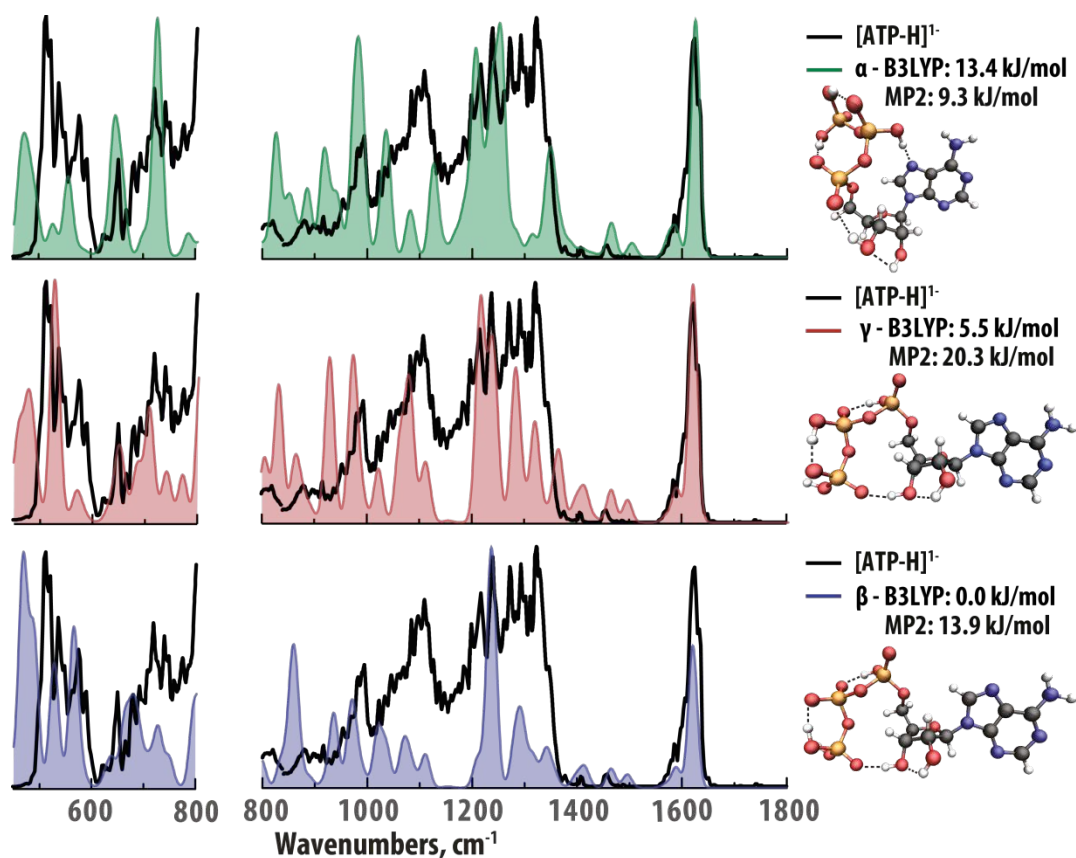


Figure S10 | IRMPD spectrum of $[\text{ATP-H}]^{1-}$ (black traces) in comparison with the predicted linear infrared spectra of three low-energy conformers (coloured traces). The spectra are divided in two wavelength regions and subsequently normalized. Calculated structures, deprotonation sites and relative energies are presented next to each panel.

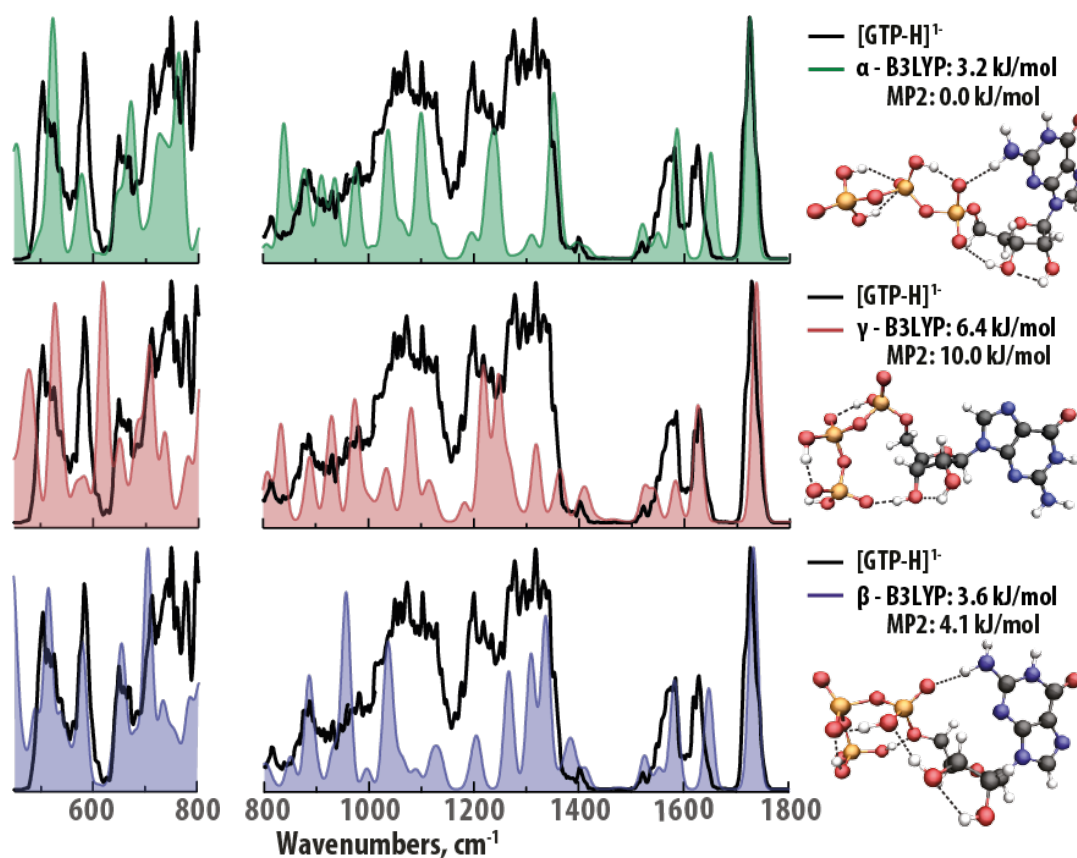


Figure S11 | IRMPD spectrum of $[GTP-H]^{1-}$ (black traces) in comparison with the predicted linear infrared spectra of three low-energy conformers (coloured traces). The spectra are divided in two wavelength regions and subsequently normalized. Calculated structures, deprotonation sites and relative energies are presented next to each panel.

Optimized coordinates of [ATP-2H]²⁻ αβ

P	3.098334000	0.179339000	1.480879000
P	1.415215000	-1.885813000	-0.127504000
O	2.488082000	1.437716000	2.056073000
O	2.605642000	-2.164531000	-1.025764000
O	0.293922000	-0.986414000	-0.972754000
O	4.093435000	-0.641840000	2.273907000
O	0.642680000	-2.970708000	0.544786000
C	0.685316000	0.210142000	-1.647386000
C	-0.207230000	1.372722000	-1.238144000
C	-2.520604000	1.506521000	-0.751174000
O	-1.560466000	1.134804000	-1.712394000
O	-1.811293000	3.540512000	0.335679000
H	-0.913137000	3.817762000	0.605755000
H	0.169634000	2.287897000	-1.714973000
H	0.598224000	0.045097000	-2.728571000
H	1.724353000	0.478942000	-1.429399000
N	-3.330332000	0.323098000	-0.399634000
C	-2.899304000	-0.980821000	-0.200484000
C	-4.694127000	0.310995000	-0.214908000
C	-5.009254000	-1.021393000	0.091868000
C	-6.361851000	-1.299316000	0.344271000
N	-3.879529000	-1.812847000	0.096241000
N	-6.798117000	-2.571152000	0.622684000
N	-7.264147000	-0.303045000	0.282914000
N	-5.572731000	1.325222000	-0.296180000
C	-6.819905000	0.929622000	-0.035543000
H	-1.853226000	-1.249469000	-0.309826000
H	-7.702073000	-2.643132000	1.065884000
C	-1.775678000	2.124021000	0.447439000
H	-3.227970000	2.232456000	-1.162819000
H	-2.226055000	1.808241000	1.397647000
O	1.834586000	-0.724136000	0.990224000
C	-0.321109000	1.622374000	0.282069000
H	-6.090352000	-3.236399000	0.901672000
H	-7.585221000	1.701861000	-0.079648000
H	-0.174095000	0.685054000	0.825577000
O	0.570733000	2.615012000	0.733555000
H	1.321513000	2.193310000	1.262601000
P	5.231362000	0.089675000	-0.657030000
O	3.833878000	0.606483000	0.045241000
O	5.994382000	-0.676401000	0.526611000
O	6.021009000	1.190705000	-1.270325000
H	5.374205000	-0.802001000	1.317897000
H	3.893473000	-1.483786000	-1.435745000
O	4.740101000	-0.981449000	-1.721272000

Optimized coordinates of [ATP-2H]²⁻ αβ2

P	2.858592000	-0.014428000	1.482094000
P	1.621669000	-1.807015000	-0.662390000
O	2.610278000	1.240709000	0.613506000
O	2.770613000	-1.474808000	-1.603857000
O	0.358239000	-0.797523000	-1.076450000
O	2.639150000	0.030505000	2.954553000
O	1.047503000	-3.175812000	-0.512674000
C	0.602022000	0.402945000	-1.809617000
C	-0.365378000	1.489930000	-1.379129000
C	-2.665589000	1.529479000	-0.843283000
O	-1.715891000	1.172607000	-1.820457000
O	-1.957031000	3.636114000	0.091044000
H	-1.070830000	3.949865000	0.348899000
H	-0.063598000	2.432681000	-1.856236000
H	0.477111000	0.203941000	-2.882209000
H	1.620704000	0.761321000	-1.640641000
N	-3.386005000	0.313702000	-0.416918000
C	-2.878305000	-0.969702000	-0.270870000
C	-4.723977000	0.237572000	-0.104220000
C	-4.946407000	-1.108835000	0.221050000
C	-6.255499000	-1.450169000	0.596837000
N	-3.786100000	-1.846961000	0.111473000
N	-6.605002000	-2.740452000	0.905576000
N	-7.203961000	-0.495932000	0.626756000
N	-5.651148000	1.210945000	-0.096023000
C	-6.849003000	0.756778000	0.277494000
H	-1.835426000	-1.187580000	-0.478925000
H	-7.462136000	-2.857889000	1.425300000
C	-1.913375000	2.229051000	0.305062000
H	-3.426347000	2.198384000	-1.256641000
H	-2.350186000	1.980270000	1.280421000
O	2.003469000	-1.261690000	0.863408000
C	-0.474002000	1.715048000	0.142475000
H	-5.846253000	-3.375993000	1.109392000
H	-7.649792000	1.492681000	0.310770000
H	-0.354647000	0.757011000	0.660869000
O	0.426179000	2.678603000	0.636129000
H	1.316970000	2.225400000	0.733178000
P	5.497164000	-0.041942000	-0.005819000
O	4.431533000	-0.453555000	1.168732000
O	5.245227000	-1.084077000	-1.175726000
O	6.906887000	-0.034838000	0.465741000
H	4.253162000	-1.268270000	-1.362905000
H	4.029599000	1.533357000	-0.193755000
O	4.976705000	1.401751000	-0.496028000

Optimized coordinates of [ATP-2H]²⁻ αγ

P	-3.806801000	1.111181000	0.465515000
P	-1.222178000	2.565561000	-0.050584000
O	-4.328237000	2.155477000	-0.613069000
O	-2.035256000	3.122809000	-1.214236000
O	-0.193015000	1.405695000	-0.616114000
O	-4.680542000	0.949110000	1.668342000
O	-0.442402000	3.403456000	0.902944000
C	-0.576233000	0.541416000	-1.697630000
C	-0.022867000	-0.852938000	-1.458760000
C	2.053832000	-1.241463000	-0.385580000
O	1.427819000	-0.844157000	-1.588317000
O	1.171569000	-2.299480000	1.660010000
H	0.553400000	-3.000035000	1.366510000
H	-0.417133000	-1.521101000	-2.232585000
H	-0.174881000	0.950809000	-2.632431000
H	-1.663863000	0.469249000	-1.783054000
N	3.162990000	-0.319748000	-0.114004000
C	3.078523000	1.049973000	0.073051000
C	4.502849000	-0.631213000	-0.064355000
C	5.154096000	0.590523000	0.169236000
C	6.551301000	0.540432000	0.287888000
N	4.249004000	1.630834000	0.250786000
N	7.302998000	1.674876000	0.484842000
N	7.182651000	-0.641489000	0.174750000
N	5.106296000	-1.824134000	-0.195939000
C	6.429887000	-1.735401000	-0.063384000
H	2.119689000	1.555891000	0.052448000
H	8.233538000	1.526912000	0.847375000
C	0.968509000	-1.264851000	0.721327000
H	2.513570000	-2.230653000	-0.480993000
H	0.957449000	-0.306177000	1.246839000
O	-2.310803000	1.616506000	0.834705000
C	-0.346786000	-1.442212000	-0.072107000
H	6.803296000	2.487201000	0.818919000
H	6.983005000	-2.667955000	-0.154824000
H	-1.166239000	-0.894836000	0.397575000
O	-0.641498000	-2.826078000	-0.119997000
H	-1.643645000	-2.904460000	-0.205032000
O	-3.532473000	-0.276170000	-0.293643000
O	-3.221751000	-2.815262000	-0.449925000
O	-5.616785000	-1.783270000	-0.778078000
O	-4.438548000	-1.816650000	1.553034000
H	-4.749989000	-0.932424000	1.851031000
H	-3.522610000	2.642182000	-1.010275000
P	-4.296117000	-1.815305000	-0.075459000

Optimized coordinates of [ATP-2H]²⁻ βγ

N	-5.102806000	-1.829898000	0.226500000
C	-4.519854000	-0.627676000	0.089966000
C	-5.193040000	0.585687000	-0.124816000
C	-6.591472000	0.515437000	-0.218340000
N	-7.202670000	-0.676267000	-0.099579000
C	-6.429735000	-1.760163000	0.119070000
N	-3.183866000	-0.296838000	0.116978000
C	-3.123555000	1.073990000	-0.063743000
N	-4.304606000	1.639836000	-0.216701000
H	-6.967293000	-2.701140000	0.216028000
H	-0.997600000	-0.237717000	-1.283640000
N	-7.363802000	1.638901000	-0.395902000
H	-8.299446000	1.478078000	-0.739361000
H	-6.884074000	2.460593000	-0.736044000
C	-0.995147000	-1.204896000	-0.773092000
C	0.335670000	-1.397815000	-0.009666000
C	0.043656000	-0.813845000	1.387769000
O	-1.403603000	-0.784861000	1.544198000
C	-2.053667000	-1.199684000	0.359425000
H	1.152591000	-0.856396000	-0.493189000
H	-2.492155000	-2.197144000	0.467990000
H	0.447275000	-1.492235000	2.147625000
O	-1.218999000	-2.223662000	-1.722670000
H	-0.600019000	-2.931582000	-1.447122000
O	0.611454000	-2.782561000	0.025288000
H	1.618915000	-2.874232000	0.126866000
O	0.201514000	1.466627000	0.580068000
H	-2.172528000	1.593322000	-0.057660000
P	1.257313000	2.493042000	-0.130334000
O	0.500385000	3.323865000	-1.099926000
O	2.013503000	3.235398000	1.051097000
O	2.369191000	1.528713000	-0.798364000
H	3.006735000	2.893867000	1.079598000
C	0.614473000	0.571446000	1.633875000
H	1.703364000	0.488029000	1.684902000
H	0.238151000	0.973172000	2.581303000
P	3.939184000	1.120986000	-0.271250000
O	4.246458000	2.158847000	0.803890000
O	3.614037000	-0.306889000	0.417505000
O	4.796023000	0.957927000	-1.493535000
H	4.727743000	-0.862216000	-1.791486000
P	4.274093000	-1.857528000	0.075028000
O	4.397069000	-1.760406000	-1.551436000
O	5.601677000	-1.969022000	0.758802000
O	3.151262000	-2.827338000	0.400181000

Optimized coordinates of [CTP-2H]²⁻ αβ

P	2.580564000	0.140198000	1.478363000
P	0.911839000	-1.801936000	-0.281549000
O	1.976513000	1.382503000	2.089352000
O	2.139784000	-2.117166000	-1.112923000
O	-0.114576000	-0.820635000	-1.149649000
O	3.536557000	-0.736629000	2.259883000
O	0.033873000	-2.872165000	0.284104000
C	0.276002000	0.450940000	-1.667500000
C	-0.689531000	1.534107000	-1.203961000
C	-3.008862000	1.559902000	-0.720094000
O	-2.026549000	1.241685000	-1.687079000
O	-2.313983000	3.631717000	0.310910000
H	-1.439125000	3.926004000	0.627275000
H	-0.363208000	2.491388000	-1.634495000
H	0.264502000	0.392420000	-2.762977000
H	1.287678000	0.728589000	-1.352061000
C	-2.282316000	2.217594000	0.466809000
H	-3.763510000	2.229454000	-1.131943000
H	-2.740152000	1.931404000	1.422218000
O	1.313724000	-0.722885000	0.915110000
C	-0.827721000	1.715484000	0.323327000
H	-0.698788000	0.755422000	0.832152000
O	0.062956000	2.678188000	0.838284000
H	0.809524000	2.220912000	1.334830000
P	4.772098000	0.099017000	-0.602524000
O	3.360890000	0.607937000	0.079240000
O	5.488165000	-0.725472000	0.570772000
O	5.594016000	1.211505000	-1.148376000
H	4.841575000	-0.875967000	1.336406000
H	3.442039000	-1.427076000	-1.477609000
O	4.297632000	-0.921210000	-1.723392000
N	-3.740394000	0.319755000	-0.330953000
C	-3.072941000	-0.857714000	-0.207458000
C	-5.142964000	0.408239000	-0.077625000
H	-2.013859000	-0.859141000	-0.449681000
C	-3.721775000	-1.997208000	0.174661000
N	-5.796133000	-0.751927000	0.260420000
O	-5.711107000	1.498300000	-0.177808000
H	-3.164683000	-2.918576000	0.293183000
C	-5.121161000	-1.881972000	0.394445000
N	-5.846239000	-2.988243000	0.795456000
H	-6.847725000	-2.895457000	0.698033000
H	-5.457978000	-3.897272000	0.592826000

Optimized coordinates of [CTP-2H]²⁻ αγ

P	-3.283923000	1.300300000	0.449735000
P	-0.613594000	2.500474000	-0.205507000
O	-3.755986000	2.294606000	-0.699637000
O	-1.391102000	3.041234000	-1.399226000
O	0.271905000	1.193055000	-0.680368000
O	-4.162689000	1.270721000	1.658639000
O	0.282110000	3.326333000	0.655371000
C	-0.150418000	0.331044000	-1.748989000
C	0.402611000	-1.063035000	-1.505972000
C	2.464641000	-1.554523000	-0.428829000
O	1.850199000	-1.040681000	-1.599412000
O	1.504320000	-2.806964000	1.471164000
H	0.808201000	-3.409896000	1.136445000
H	0.023428000	-1.728097000	-2.291379000
H	0.227947000	0.731870000	-2.696802000
H	-1.241044000	0.267611000	-1.798860000
C	1.366048000	-1.658647000	0.662724000
H	2.922553000	-2.528339000	-0.607551000
H	1.403058000	-0.774602000	1.307545000
O	-1.765904000	1.760588000	0.785270000
C	0.033312000	-1.666634000	-0.134183000
H	-0.720138000	-1.052291000	0.363291000
O	-0.422795000	-3.002774000	-0.233671000
H	-1.428860000	-2.967854000	-0.212710000
O	-3.078399000	-0.148160000	-0.209454000
O	-3.010197000	-2.710536000	-0.265499000
O	-5.298688000	-1.468846000	-0.633545000
O	-4.119875000	-1.522137000	1.695059000
H	-4.374209000	-0.607873000	1.950669000
H	-2.930962000	2.688146000	-1.146344000
P	-3.983188000	-1.600686000	0.067367000
N	3.579681000	-0.650636000	-0.068622000
C	3.303129000	0.660478000	0.159260000
C	4.923725000	-1.140672000	-0.051149000
H	2.265669000	0.966626000	0.052182000
C	4.291547000	1.546569000	0.478404000
N	5.913393000	-0.237949000	0.271728000
O	5.157571000	-2.316961000	-0.321697000
H	4.055293000	2.584756000	0.676324000
C	5.613578000	1.021139000	0.528343000
N	6.664718000	1.846438000	0.888397000
H	7.578691000	1.475473000	0.666960000
H	6.543612000	2.838058000	0.744181000

Optimized coordinates of [CTP-2H]²⁻ βγ

H	1.465822000	-0.618595000	1.302838000
C	1.401927000	-1.539776000	0.714152000
C	0.044239000	-1.589995000	-0.033235000
C	0.360514000	-1.008577000	-1.428644000
O	1.804065000	-0.983254000	-1.574950000
C	2.454524000	-1.500673000	-0.425441000
H	-0.705980000	-0.980663000	0.477842000
H	2.868775000	-2.493929000	-0.604460000
H	-0.048287000	-1.686526000	-2.187408000
O	1.568843000	-2.638250000	1.582143000
H	0.879316000	-3.269618000	1.288149000
O	-0.377718000	-2.936059000	-0.088938000
H	-1.391515000	-2.920306000	-0.122619000
O	0.281285000	1.280333000	-0.660626000
P	-0.661514000	2.434094000	0.008497000
O	0.199190000	3.246884000	0.906707000
O	-1.381793000	3.174021000	-1.195503000
O	-1.831597000	1.616805000	0.762071000
H	-2.405137000	2.923624000	-1.176772000
C	-0.200963000	0.379416000	-1.680593000
H	-1.292502000	0.315122000	-1.672816000
H	0.135458000	0.759675000	-2.651544000
P	-3.437428000	1.302639000	0.276719000
O	-3.691894000	2.328658000	-0.824276000
O	-3.229445000	-0.162191000	-0.375998000
O	-4.275722000	1.240024000	1.520552000
H	-4.307702000	-0.578316000	1.886670000
P	-3.975360000	-1.656030000	0.040934000
O	-4.032746000	-1.499551000	1.666939000
O	-5.332161000	-1.696933000	-0.591622000
O	-2.932268000	-2.707340000	-0.289741000
N	3.614024000	-0.629222000	-0.134329000
C	3.394524000	0.698596000	0.050563000
C	4.937698000	-1.172490000	-0.119928000
H	2.367985000	1.038812000	-0.053011000
C	4.422079000	1.553756000	0.328380000
N	5.961844000	-0.308704000	0.204787000
O	5.123089000	-2.359161000	-0.377994000
H	4.237985000	2.611369000	0.470351000
C	5.718135000	0.969877000	0.415357000
N	6.811641000	1.771995000	0.696757000
H	7.637833000	1.257406000	0.971109000
H	6.634828000	2.620229000	1.215152000

Optimized coordinates of [GTP-2H]²⁻ αβ

P	-4.273857000	1.010975000	0.589151000
P	-1.348284000	1.217565000	-0.243046000
O	-4.953027000	1.726863000	1.705440000
O	-1.373442000	-0.111916000	-0.989226000
O	-0.171926000	1.030280000	0.906351000
O	-4.704483000	1.110355000	-0.864915000
O	-1.089810000	2.501736000	-1.001186000
C	0.472205000	2.172353000	1.460853000
C	1.823233000	2.490661000	0.814977000
C	3.918322000	1.503295000	0.409550000
O	2.877100000	1.663302000	1.365659000
O	4.035383000	3.366149000	-1.128532000
H	3.337873000	3.922324000	-1.518474000
H	2.059064000	3.545164000	1.029932000
H	0.628096000	1.972221000	2.527070000
H	-0.163662000	3.058874000	1.361433000
N	4.321089000	0.101186000	0.365967000
C	5.495485000	-0.423707000	0.889582000
C	3.552021000	-0.989774000	0.014766000
C	4.322996000	-2.112481000	0.337078000
C	3.749522000	-3.411694000	0.121258000
N	5.542720000	-1.731553000	0.877857000
N	2.422210000	-3.288092000	-0.384498000
N	2.317991000	-0.932143000	-0.514598000
C	1.750782000	-2.113075000	-0.678277000
H	6.274872000	0.230140000	1.258923000
C	3.416018000	2.092517000	-0.930001000
H	4.811941000	2.059302000	0.720241000
H	3.646632000	1.429253000	-1.771289000
O	-2.651880000	1.369051000	0.711408000
C	1.910607000	2.253049000	-0.700911000
H	1.425858000	1.305121000	-0.936173000
O	1.391573000	3.312532000	-1.475810000
H	0.404773000	3.159605000	-1.465834000
P	-4.323220000	-1.929387000	-0.036662000
O	-4.243490000	-0.633727000	0.952389000
O	-5.084284000	-1.384436000	-1.335909000
O	-4.951519000	-3.121943000	0.589381000
H	-5.002374000	-0.369399000	-1.360059000
H	-2.291412000	-1.365667000	-0.666176000
O	-2.798845000	-2.211189000	-0.450594000
O	4.218052000	-4.535997000	0.310008000
H	1.959731000	-4.175940000	-0.538023000
N	0.500734000	-2.195731000	-1.187939000
H	-0.058202000	-1.324301000	-1.165543000
H	-0.048325000	-3.025020000	-1.004150000

Optimized coordinates of [GTP-2H]²⁻ αγ

P	4.178731000	-0.915550000	0.742439000
P	1.348634000	-1.380060000	-0.350075000
O	4.837491000	-1.585235000	1.893090000
O	1.426472000	-0.112529000	-1.179153000
O	0.210353000	-1.080131000	0.809980000
O	1.043159000	-2.710501000	-1.003775000
C	-0.467579000	-2.162240000	1.443002000
C	-1.841263000	-2.466475000	0.836737000
C	-3.913055000	-1.421016000	0.445254000
O	-2.857804000	-1.593776000	1.384705000
O	-4.131778000	-3.319180000	-1.035600000
H	-3.464241000	-3.913927000	-1.420866000
H	-2.099974000	-3.506564000	1.091360000
H	-0.598396000	-1.889934000	2.496109000
H	0.135083000	-3.075132000	1.388818000
N	-4.265077000	-0.007013000	0.376399000
C	-5.392043000	0.576521000	0.942461000
C	-3.453678000	1.045057000	0.000445000
C	-4.153440000	2.204492000	0.351223000
C	-3.514988000	3.472910000	0.130725000
N	-5.372542000	1.884778000	0.932392000
N	-2.209771000	3.281705000	-0.409509000
N	-2.241779000	0.924973000	-0.567399000
C	-1.614134000	2.075605000	-0.734699000
H	-6.190290000	-0.037371000	1.339180000
C	-3.460319000	-2.065312000	-0.886447000
H	-4.818531000	-1.936825000	0.788773000
H	-3.683046000	-1.417262000	-1.741478000
O	2.682858000	-1.565634000	0.578968000
C	-1.956703000	-2.277590000	-0.684598000
H	-1.441574000	-1.358693000	-0.966077000
O	-1.500004000	-3.385090000	-1.432975000
H	-0.507366000	-3.288984000	-1.436612000
P	4.172675000	1.972087000	-0.131877000
O	3.932860000	0.664291000	0.952214000
O	5.014485000	1.360607000	-1.257798000
O	4.634481000	3.164410000	0.635593000
H	2.248143000	1.313589000	-0.892784000
O	2.642671000	2.190267000	-0.634206000
O	-3.917651000	4.618327000	0.341478000
H	-1.699807000	4.142640000	-0.566778000
N	-0.377910000	2.094876000	-1.282399000
H	0.107825000	1.185824000	-1.302301000
H	0.251241000	2.858339000	-1.062166000
O	4.873506000	-1.055443000	-0.672236000
H	5.004312000	-0.092837000	-1.075755000

Optimized coordinates of [GTP-2H]²⁻ βγ

N	4.912229000	-1.420861000	-0.184646000
C	4.394568000	-0.165044000	-0.061570000
C	5.085201000	1.037553000	0.138664000
C	6.517257000	1.012356000	0.213716000
C	6.212670000	-1.450409000	-0.116396000
N	3.068476000	0.167247000	-0.091076000
C	3.014962000	1.542715000	0.074285000
N	4.199869000	2.094033000	0.215364000
H	0.828157000	0.207444000	1.300380000
C	0.912412000	-0.782418000	0.842805000
C	-0.392138000	-1.142253000	0.099226000
C	-0.182057000	-0.540752000	-1.308366000
O	1.249864000	-0.309545000	-1.461765000
C	1.942695000	-0.742509000	-0.309747000
H	-1.266934000	-0.703694000	0.586523000
H	2.383167000	-1.736502000	-0.444447000
H	-0.486994000	-1.279595000	-2.058125000
O	1.243179000	-1.726198000	1.838446000
H	0.714447000	-2.512381000	1.590036000
O	-0.483871000	-2.552058000	0.081036000
H	-1.464477000	-2.781145000	-0.073328000
O	-0.670512000	1.700017000	-0.522167000
H	2.068070000	2.066728000	0.066724000
P	-1.882715000	2.550529000	0.167309000
O	-1.291643000	3.472274000	1.168553000
O	-2.706942000	3.191055000	-1.030379000
O	-2.860113000	1.421689000	0.789071000
H	-3.640688000	2.721796000	-1.084561000
C	-0.931917000	0.750950000	-1.575645000
H	-1.996559000	0.514632000	-1.651026000
H	-0.593545000	1.194016000	-2.519049000
P	-4.349651000	0.812287000	0.228128000
O	-4.781467000	1.812261000	-0.838871000
O	-3.821941000	-0.547651000	-0.474943000
O	-5.194858000	0.511738000	1.432893000
H	-4.850220000	-1.267892000	1.727939000
P	-4.226750000	-2.181328000	-0.132704000
O	-4.383872000	-2.105543000	1.491786000
O	-5.508649000	-2.510660000	-0.833351000
O	-2.957632000	-2.958872000	-0.440743000
O	7.345375000	1.909117000	0.361478000
N	6.891089000	-2.657383000	-0.289702000
H	7.656652000	-2.814307000	0.355633000
H	6.237435000	-3.432106000	-0.294046000
N	6.991306000	-0.335991000	0.072286000
H	8.000191000	-0.410751000	0.030589000

Optimized coordinates of [GTP-2H]²⁻ αβ2

P	2.337956000	-0.032770000	-1.289226000
P	2.119605000	-1.686086000	1.333235000
O	0.490579000	-1.824343000	1.653460000
O	3.831972000	0.163188000	-1.461156000
C	-0.133209000	-3.103415000	1.751615000
C	-1.075335000	-3.427865000	0.589930000
C	-2.487417000	-1.865489000	-0.493198000
O	-2.312656000	-2.659096000	0.680687000
O	-1.061454000	-1.432312000	-2.463595000
H	-0.223222000	-0.922630000	-2.608132000
H	-1.347980000	-4.489424000	0.665046000
H	-0.718915000	-3.109881000	2.679865000
H	0.635379000	-3.883843000	1.804935000
C	-1.075065000	-1.723390000	-1.083937000
H	-3.141775000	-2.391594000	-1.201990000
H	-0.519200000	-0.981882000	-0.513032000
O	2.015160000	-1.259040000	-0.270178000
C	-0.507347000	-3.124135000	-0.789844000
H	0.584337000	-3.124227000	-0.808581000
O	-1.022191000	-4.059010000	-1.751074000
H	-1.010619000	-3.563107000	-2.588759000
O	1.783726000	1.310641000	-0.449530000
O	2.570370000	1.994021000	1.886142000
O	1.938801000	3.809604000	0.194171000
P	2.586139000	2.473012000	0.383197000
H	2.591210000	0.963352000	2.001023000
N	-3.178859000	-0.638113000	-0.096000000
C	-4.395484000	-0.636937000	0.569796000
C	-2.796792000	0.685217000	-0.168276000
H	-4.905815000	-1.566274000	0.781643000
C	-3.812109000	1.406049000	0.474753000
N	-4.808840000	0.555158000	0.923815000
C	-3.675851000	2.832308000	0.586661000
O	-4.429354000	3.669857000	1.091602000
N	-1.681278000	1.160886000	-0.754645000
C	-1.536542000	2.462362000	-0.656525000
N	-2.458509000	3.260501000	-0.010327000
H	-2.309237000	4.261915000	0.005499000
N	-0.476835000	3.083184000	-1.265356000
H	0.159921000	2.373889000	-1.622694000
H	0.077243000	3.717098000	-0.681100000
O	2.758305000	-3.038674000	1.427186000
O	2.624106000	-0.503273000	2.132893000
O	1.418280000	-0.205991000	-2.471036000
O	4.078860000	2.396687000	-0.186007000
H	4.198298000	1.526644000	-0.698597000

Optimized coordinates of [ATP-H]¹⁻ β

P	4.181517000	1.061783000	-0.206411000
P	1.551583000	2.507811000	-0.140583000
O	4.561017000	2.013009000	0.895556000
O	2.254901000	3.156371000	1.131572000
O	0.396456000	1.539643000	0.436586000
O	5.059025000	0.771525000	-1.397446000
O	1.002682000	3.404589000	-1.175055000
C	0.634541000	0.623567000	1.528583000
C	-0.122740000	-0.667757000	1.275933000
C	-2.243960000	-0.971221000	0.305202000
O	-1.539867000	-0.418877000	1.409927000
O	-1.530487000	-1.965840000	-1.843869000
H	-1.054770000	-2.773452000	-1.576999000
H	0.179208000	-1.396177000	2.039552000
H	0.282467000	1.096331000	2.450234000
H	1.699530000	0.394804000	1.625913000
N	-3.415837000	-0.151030000	0.060848000
C	-3.445519000	1.205104000	-0.218011000
C	-4.733974000	-0.556019000	0.124749000
C	-5.482496000	0.598100000	-0.139255000
C	-6.880743000	0.443835000	-0.147760000
N	-4.659796000	1.690972000	-0.349409000
N	-7.726208000	1.494972000	-0.361269000
N	-7.405835000	-0.770969000	0.092083000
N	-5.227469000	-1.776785000	0.377283000
C	-6.561842000	-1.790363000	0.341128000
H	-2.531924000	1.779262000	-0.293728000
H	-8.689778000	1.275635000	-0.563750000
C	-1.225179000	-1.011338000	-0.857321000
H	-2.617112000	-1.979137000	0.520010000
H	-1.180295000	-0.026673000	-1.331694000
O	2.668779000	1.449797000	-0.727722000
C	0.102249000	-1.291702000	-0.122089000
H	-7.337522000	2.344964000	-0.741491000
H	-7.035626000	-2.749826000	0.534762000
H	0.947193000	-0.829808000	-0.639006000
O	0.270749000	-2.700266000	-0.062420000
H	1.235161000	-2.883750000	-0.049857000
O	3.845016000	-0.423516000	0.502797000
O	3.003271000	-2.829789000	0.008369000
O	5.259711000	-2.470299000	1.085261000
O	4.965219000	-1.757449000	-1.362395000
H	5.092818000	-0.760330000	-1.577044000
H	3.219400000	2.863467000	1.211093000
P	4.185354000	-1.932460000	0.002564000
H	6.086686000	-1.966860000	1.065470000

Optimized coordinates of [ATP-H]¹⁻ β2

P	0.536991000	-1.970052000	-1.021771000
P	-1.893854000	-2.594002000	0.561514000
O	0.688431000	-0.550116000	-1.516532000
O	-1.945093000	-3.831007000	-0.422573000
O	-2.862833000	-1.472394000	-0.123860000
O	0.016149000	-3.086132000	-1.890077000
O	-2.230684000	-2.840596000	1.983561000
C	-3.926484000	-0.860089000	0.615453000
C	-3.819770000	0.654061000	0.572278000
C	-1.909303000	2.006740000	0.613024000
O	-2.661622000	1.071891000	1.342228000
O	-2.102175000	2.904883000	-1.689044000
H	-1.242888000	3.335540000	-1.492826000
H	-4.717101000	1.067813000	1.050173000
H	-3.906430000	-1.205377000	1.652933000
H	-4.876757000	-1.159992000	0.155834000
N	-0.494621000	1.822466000	0.940971000
C	0.097702000	0.834984000	1.689471000
C	0.528088000	2.582438000	0.416277000
C	1.705782000	2.019762000	0.908181000
C	2.911942000	2.610240000	0.473399000
N	1.413643000	0.922684000	1.702331000
N	4.134935000	2.168838000	0.863565000
N	2.839744000	3.679646000	-0.349077000
N	0.431584000	3.619135000	-0.434731000
C	1.638567000	4.107819000	-0.754500000
H	-0.485375000	0.073832000	2.183187000
H	4.909555000	2.501133000	0.305686000
C	-2.214597000	1.748061000	-0.878531000
H	-2.179064000	3.039310000	0.878378000
H	-1.575060000	0.933902000	-1.240434000
O	-0.422791000	-1.940968000	0.349320000
C	-3.685978000	1.298723000	-0.822358000
H	4.203223000	1.210188000	1.187577000
H	1.644402000	4.954179000	-1.436775000
H	-3.919979000	0.587505000	-1.622924000
O	-4.558198000	2.424413000	-0.890337000
H	-4.092043000	3.090781000	-1.423919000
O	1.956825000	-2.421865000	-0.324338000
O	4.563457000	-2.477522000	-0.317364000
O	3.315014000	-1.005957000	1.350341000
O	3.255636000	-0.378177000	-1.141493000
H	2.298644000	-0.237649000	-1.421673000
H	-1.228353000	-3.726168000	-1.139891000
P	3.377038000	-1.617742000	-0.134994000
H	2.535013000	-0.415489000	1.557203000

Optimized coordinates of [ATP-H]¹⁻ α

P	-2.109806000	1.110206000	1.021206000
P	-1.611664000	-1.830650000	0.710554000
O	-3.145746000	1.266982000	2.081964000
O	-3.096292000	-1.920672000	0.473592000
O	-0.798719000	-1.842610000	-0.733861000
O	-0.910946000	-2.725207000	1.692542000
C	-0.087299000	-3.011739000	-1.154363000
C	1.406991000	-2.934442000	-0.876538000
C	3.074067000	-1.286407000	-1.064612000
O	2.054451000	-1.976093000	-1.757666000
O	4.152464000	-3.064311000	0.150691000
H	3.899206000	-3.730581000	0.808804000
H	1.836330000	-3.926227000	-1.073192000
H	-0.254276000	-3.110472000	-2.231573000
H	-0.476730000	-3.906692000	-0.656950000
N	2.642562000	0.117969000	-0.879169000
C	1.341323000	0.554277000	-0.826181000
C	3.429530000	1.187540000	-0.491374000
C	2.532804000	2.227981000	-0.219614000
C	3.097854000	3.445236000	0.209939000
N	1.230095000	1.809334000	-0.434343000
N	2.348896000	4.545437000	0.489212000
N	4.436655000	3.527956000	0.327443000
N	4.764582000	1.242623000	-0.381784000
C	5.176616000	2.445849000	0.029198000
H	0.513576000	-0.099614000	-1.062201000
H	2.808858000	5.316946000	0.948104000
C	3.241442000	-1.983963000	0.299544000
H	4.001667000	-1.280587000	-1.641452000
H	3.589332000	-1.286333000	1.070350000
O	-1.224827000	-0.233213000	1.083835000
C	1.814473000	-2.479982000	0.534660000
H	1.348511000	4.456156000	0.586024000
H	6.250837000	2.570458000	0.141450000
H	1.198351000	-1.629915000	0.839442000
O	1.744191000	-3.495181000	1.507447000
H	0.818119000	-3.453959000	1.835240000
P	-4.334077000	0.978739000	-0.985441000
O	-2.742319000	1.121841000	-0.466998000
O	-4.497025000	-0.576619000	-1.206443000
O	-4.594754000	1.801612000	-2.183321000
H	-3.977824000	-1.158142000	-0.553807000
H	-4.651788000	1.335111000	1.149429000
O	-5.170402000	1.418256000	0.308473000
O	-1.016846000	2.252868000	1.017608000
H	-0.223126000	2.118881000	0.409190000

Optimized coordinates of [ATP-H]¹⁻ γ

N	-5.250684000	-1.767686000	0.386892000
C	-4.763974000	-0.546255000	0.125109000
C	-5.518924000	0.600395000	-0.153344000
C	-6.916052000	0.436558000	-0.168076000
N	-7.434179000	-0.779284000	0.080745000
C	-6.584672000	-1.790563000	0.344144000
N	-3.448218000	-0.133022000	0.064062000
C	-3.485911000	1.219743000	-0.227774000
N	-4.702502000	1.696840000	-0.369563000
H	-7.053051000	-2.751217000	0.544760000
H	-1.213941000	-0.007029000	-1.330133000
N	-7.767486000	1.479854000	-0.396638000
H	-8.728072000	1.251341000	-0.603293000
H	-7.382430000	2.327874000	-0.784880000
C	-1.253000000	-0.988920000	-0.848498000
C	0.076935000	-1.260551000	-0.113510000
C	-0.154224000	-0.645691000	1.289132000
O	-1.567351000	-0.370596000	1.410242000
C	-2.270586000	-0.942884000	0.314825000
H	0.918794000	-0.787888000	-0.626070000
H	-2.635340000	-1.951093000	0.542282000
H	0.128770000	-1.387883000	2.046725000
O	-1.556151000	-1.952263000	-1.826556000
H	-1.057561000	-2.748449000	-1.565343000
O	0.261039000	-2.664533000	-0.063199000
H	1.231373000	-2.826714000	-0.002612000
O	0.402172000	1.572586000	0.492248000
H	-2.575962000	1.799196000	-0.304343000
P	1.584075000	2.473016000	-0.117291000
O	1.088859000	3.346056000	-1.196908000
O	2.304925000	3.142893000	1.138098000
O	2.668891000	1.341852000	-0.641209000
C	0.621745000	0.628261000	1.568398000
H	1.683265000	0.382582000	1.663586000
H	0.273772000	1.093453000	2.494943000
P	4.197113000	1.013957000	-0.158352000
O	4.686038000	2.109258000	0.735305000
O	4.045460000	-0.394451000	0.594104000
O	5.006108000	0.740901000	-1.471784000
H	5.006084000	-0.283237000	-1.655776000
P	4.218496000	-1.972032000	-0.043372000
O	4.829379000	-1.758992000	-1.420216000
O	5.342011000	-2.567371000	0.971368000
O	2.939468000	-2.698048000	0.201890000
H	6.227466000	-2.300489000	0.686486000
H	3.288260000	2.949648000	1.150908000

Optimized coordinates of [ATP-H]⁻ α2

P	2.852591000	-0.090657000	1.314590000
P	1.645193000	-1.625294000	-0.940690000
O	2.702940000	1.320673000	0.798801000
O	2.863910000	-1.071346000	-1.652344000
O	0.365679000	-0.671191000	-1.292955000
O	1.222608000	-3.042169000	-0.895399000
C	0.520585000	0.598980000	-1.949995000
C	-0.498697000	1.592260000	-1.425502000
C	-2.780596000	1.514569000	-0.837442000
O	-1.825827000	1.198704000	-1.835514000
O	-2.117618000	3.617835000	0.110114000
H	-1.284270000	3.993682000	0.439076000
H	-0.266133000	2.574988000	-1.859983000
H	0.372174000	0.451715000	-3.025130000
H	1.528062000	0.993622000	-1.792835000
N	-3.458017000	0.278626000	-0.429618000
C	-2.932957000	-1.003548000	-0.352731000
C	-4.778995000	0.176289000	-0.045361000
C	-4.968952000	-1.179990000	0.246455000
C	-6.258563000	-1.548258000	0.673077000
N	-3.807303000	-1.901408000	0.048985000
N	-6.584909000	-2.841417000	0.956147000
N	-7.207572000	-0.599954000	0.779670000
N	-5.705235000	1.143874000	0.043142000
C	-6.881202000	0.666300000	0.459601000
H	-1.906089000	-1.205571000	-0.628711000
H	-7.455925000	-3.009776000	1.435480000
C	-2.024875000	2.214174000	0.309851000
H	-3.555420000	2.178792000	-1.230138000
H	-2.433738000	1.935366000	1.288801000
O	1.875764000	-1.165154000	0.733652000
C	-0.578882000	1.737588000	0.106379000
H	-5.838547000	-3.513610000	1.051111000
H	-7.684213000	1.392975000	0.558052000
H	-0.440168000	0.758239000	0.578278000
O	0.311471000	2.696969000	0.641106000
H	1.197885000	2.288595000	0.746575000
P	5.612424000	-0.131994000	0.111820000
O	4.371898000	-0.582624000	1.167424000
O	5.350189000	-1.023736000	-1.155724000
O	6.929883000	-0.304223000	0.751860000
H	4.364992000	-1.102377000	-1.424344000
H	4.293830000	1.612778000	-0.036257000
O	5.237512000	1.394049000	-0.219511000
O	2.555598000	-0.254935000	2.885813000
H	3.142457000	0.298704000	3.421359000

Optimized coordinates of [CTP-H]¹⁻ β

P	3.666061000	-1.226022000	-0.059365000
P	0.910452000	-2.292193000	-0.502173000
O	3.927399000	-1.712286000	-1.458036000
O	1.557175000	-2.676926000	-1.905299000
O	-0.005407000	-0.988206000	-0.764440000
O	4.605676000	-1.436061000	1.100331000
O	0.123184000	-3.321549000	0.205080000
C	0.294424000	0.046506000	-1.725118000
C	-0.715550000	1.167220000	-1.566051000
C	-3.000633000	1.307738000	-0.995851000
O	-2.041285000	0.673792000	-1.830322000
O	-2.320939000	3.601348000	-0.792719000
H	-1.489509000	4.058830000	-0.579715000
H	-0.461507000	1.945103000	-2.300067000
H	0.240930000	-0.381070000	-2.730679000
H	1.298536000	0.449248000	-1.555122000
C	-2.242480000	2.341623000	-0.142746000
H	-3.768778000	1.803034000	-1.590014000
H	-2.653546000	2.402183000	0.871898000
O	2.163839000	-1.734001000	0.392264000
C	-0.785372000	1.831345000	-0.175937000
H	-0.619013000	1.089525000	0.612898000
O	0.109829000	2.916425000	-0.055177000
H	0.876012000	2.675817000	0.514248000
O	3.400773000	0.428784000	-0.155033000
O	2.251489000	2.156028000	1.427932000
O	4.468844000	2.684939000	0.322403000
O	4.428727000	0.876428000	2.136351000
H	4.598386000	-0.110947000	1.911802000
H	2.524844000	-2.390805000	-1.952691000
P	3.544451000	1.553455000	1.012747000
H	5.342151000	2.345949000	0.077199000
N	-3.699355000	0.276547000	-0.188036000
C	-3.099018000	-0.898725000	0.136825000
C	-5.039074000	0.567487000	0.228012000
H	-2.089836000	-1.046153000	-0.226143000
C	-3.755468000	-1.841718000	0.871434000
N	-5.703467000	-0.401960000	0.932874000
O	-5.525859000	1.657551000	-0.067650000
H	-3.264477000	-2.770500000	1.134100000
C	-5.097789000	-1.533951000	1.248164000
N	-5.815681000	-2.430710000	1.999682000
H	-6.805867000	-2.249136000	2.079602000
H	-5.515062000	-3.392107000	2.035033000

Optimized coordinates of [CTP-H]¹⁻ γ

H	1.608668000	-0.480490000	1.282534000
C	1.584790000	-1.415959000	0.713973000
C	0.234856000	-1.526530000	-0.034360000
C	0.525358000	-0.886987000	-1.413132000
O	1.950607000	-0.715089000	-1.522909000
C	2.622578000	-1.343611000	-0.432901000
H	-0.553678000	-0.988920000	0.498048000
H	2.986963000	-2.338878000	-0.695228000
H	0.186013000	-1.579439000	-2.194753000
O	1.803738000	-2.475321000	1.611697000
H	1.237545000	-3.202190000	1.291787000
O	-0.108531000	-2.897202000	-0.142479000
H	-1.086425000	-2.955551000	-0.049746000
O	0.200936000	1.350412000	-0.563573000
P	-0.832652000	2.418078000	0.049063000
O	-0.182330000	3.239240000	1.087209000
O	-1.492989000	3.156718000	-1.198784000
O	-2.044104000	1.466520000	0.640778000
C	-0.147931000	0.452967000	-1.647631000
H	-1.230515000	0.304716000	-1.701014000
H	0.203125000	0.904639000	-2.579674000
P	-3.585555000	1.244426000	0.138609000
O	-3.940843000	2.308444000	-0.852661000
O	-3.554642000	-0.226619000	-0.498926000
O	-4.446775000	1.156462000	1.442283000
H	-4.596262000	0.149524000	1.679033000
P	-3.968315000	-1.721738000	0.224575000
O	-4.625344000	-1.332113000	1.540910000
O	-5.102528000	-2.240192000	-0.820157000
O	-2.783310000	-2.617484000	0.116448000
H	-5.960333000	-1.845147000	-0.609062000
H	-2.487035000	3.016421000	-1.237494000
N	3.810878000	-0.544518000	-0.126100000
C	3.663406000	0.781312000	0.141464000
C	5.112827000	-1.149890000	-0.195420000
H	2.652066000	1.171035000	0.095722000
C	4.737195000	1.568948000	0.425751000
N	6.183951000	-0.353139000	0.131430000
O	5.219333000	-2.325831000	-0.523761000
H	4.616504000	2.625557000	0.629367000
C	6.013213000	0.920896000	0.423242000
N	7.143194000	1.652740000	0.698090000
H	7.982066000	1.113538000	0.860617000
H	7.049497000	2.517678000	1.207691000

Optimized coordinates of [CTP-H]¹⁻ α

P	2.371147000	-0.043261000	1.274425000
P	1.164664000	-1.573559000	-0.985876000
O	2.210736000	1.367711000	0.763212000
O	2.386627000	-1.037727000	-1.703008000
O	-0.105877000	-0.608856000	-1.332717000
O	0.713167000	-2.983401000	-0.944743000
C	0.034283000	0.690047000	-1.934609000
C	-1.020745000	1.632432000	-1.387204000
C	-3.282570000	1.446122000	-0.743511000
O	-2.338350000	1.178520000	-1.767334000
O	-2.672132000	3.613529000	0.089338000
H	-1.867357000	4.035393000	0.430721000
H	-0.843241000	2.624367000	-1.826296000
H	-0.088974000	0.581035000	-3.017416000
H	1.028064000	1.102664000	-1.740089000
C	-2.538326000	2.223957000	0.357017000
H	-4.118290000	2.032856000	-1.125593000
H	-2.924565000	1.981995000	1.353452000
O	1.406427000	-1.126874000	0.686836000
C	-1.082675000	1.781295000	0.144671000
H	-0.916936000	0.807978000	0.621345000
O	-0.202609000	2.759838000	0.663372000
H	0.690048000	2.365638000	0.752619000
P	5.129748000	-0.067274000	0.070093000
O	3.893339000	-0.525865000	1.126313000
O	4.874242000	-0.963604000	-1.196258000
O	6.449078000	-0.229485000	0.708624000
H	3.891554000	-1.049009000	-1.467058000
H	3.799409000	1.669483000	-0.075204000
O	4.742694000	1.454669000	-0.264886000
O	2.069585000	-0.217049000	2.843158000
H	2.615802000	0.374147000	3.381597000
N	-3.852701000	0.163497000	-0.254255000
C	-3.181432000	-1.011607000	-0.383267000
C	-5.144182000	0.219845000	0.362053000
H	-2.211845000	-0.970455000	-0.864829000
C	-3.720892000	-2.177667000	0.074617000
N	-5.693053000	-0.961648000	0.784855000
O	-5.692716000	1.314998000	0.477406000
H	-3.173536000	-3.107799000	-0.014222000
C	-5.019536000	-2.093018000	0.662669000
N	-5.615952000	-3.223817000	1.159012000
H	-6.592823000	-3.144386000	1.401510000
H	-5.275994000	-4.128401000	0.873422000

Optimized coordinates of [CTP-H]¹⁻ β2

P	-2.700354000	-1.440052000	0.615763000
P	-0.012051000	-2.654229000	0.236525000
O	-2.435299000	-1.765938000	2.059997000
O	0.032305000	-2.438977000	1.804388000
O	1.175541000	-1.680302000	-0.283034000
O	-3.940322000	-1.872990000	-0.130770000
O	0.105049000	-4.029662000	-0.303562000
C	2.030440000	-2.098847000	-1.365439000
C	3.313247000	-1.282499000	-1.344032000
C	3.241801000	0.960514000	-0.600699000
O	3.055036000	0.097451000	-1.701762000
O	4.556232000	0.608703000	1.468489000
H	4.278756000	1.540574000	1.619426000
H	3.979472000	-1.690793000	-2.112426000
H	1.513560000	-1.940286000	-2.318625000
H	2.258974000	-3.164722000	-1.266689000
C	3.552842000	0.069689000	0.632272000
H	4.079000000	1.639985000	-0.794330000
H	2.626580000	-0.122810000	1.184474000
O	-1.361596000	-1.870685000	-0.258957000
C	4.057044000	-1.237071000	-0.003969000
H	3.825665000	-2.108410000	0.621226000
O	5.456249000	-1.165081000	-0.253549000
H	5.810252000	-0.548787000	0.411309000
O	-2.643230000	0.222922000	0.416591000
O	-3.550030000	2.476580000	-0.487083000
O	-5.180451000	0.630359000	0.285882000
O	-3.806110000	0.318165000	-1.872296000
H	-3.898197000	-0.652260000	-1.749881000
H	-0.886867000	-2.188135000	2.151105000
P	-3.788549000	1.016301000	-0.421980000
H	-5.246499000	-0.347148000	0.338086000
N	2.032877000	1.797992000	-0.414529000
C	0.911939000	1.628531000	-1.170128000
C	2.087274000	2.788815000	0.599617000
H	0.969456000	0.861939000	-1.929239000
C	-0.194397000	2.384322000	-0.949798000
N	0.981556000	3.532669000	0.836699000
O	3.153646000	2.910854000	1.237539000
H	-1.097761000	2.249773000	-1.527725000
C	-0.129958000	3.323144000	0.129902000
N	-1.232946000	4.046142000	0.441686000
H	-2.138638000	3.682485000	0.146263000
H	-1.187411000	4.569906000	1.304058000

Optimized coordinates of [CTP-H]⁻ γ₂

P	-2.377137000	-1.246565000	1.000823000
P	0.020258000	-2.793423000	0.122618000
O	-1.719956000	-1.277973000	2.344240000
O	0.251517000	-2.814528000	1.688830000
O	1.059509000	-1.673645000	-0.422339000
O	0.127408000	-4.080962000	-0.598279000
C	1.935600000	-1.960870000	-1.533124000
C	3.189399000	-1.103395000	-1.443770000
C	3.054358000	1.096971000	-0.585266000
O	2.894046000	0.284352000	-1.730112000
O	4.346815000	0.662959000	1.483334000
H	4.035965000	1.574651000	1.688526000
H	3.878239000	-1.448741000	-2.223394000
H	1.409522000	-1.741038000	-2.468520000
H	2.205889000	-3.021191000	-1.526496000
C	3.369553000	0.148976000	0.603340000
H	3.883068000	1.797739000	-0.736394000
H	2.439613000	-0.093320000	1.129428000
O	-1.433541000	-2.062418000	-0.076888000
C	3.913822000	-1.110660000	-0.092555000
H	3.695853000	-2.018092000	0.484232000
O	5.313843000	-0.992427000	-0.317890000
H	5.644048000	-0.405858000	0.385109000
O	-2.501206000	0.207320000	0.363064000
O	-3.770882000	2.295102000	-0.417548000
O	-4.875307000	-0.136108000	-0.524823000
O	-3.015519000	0.593808000	-2.139949000
H	-3.189064000	-0.303211000	-2.459717000
H	-0.404640000	-2.220786000	2.173481000
P	-3.710174000	0.829474000	-0.677000000
N	1.826270000	1.897826000	-0.374392000
C	0.740548000	1.783723000	-1.192133000
C	1.823286000	2.805901000	0.715962000
H	0.844816000	1.096103000	-2.018863000
C	-0.391262000	2.489919000	-0.945738000
N	0.685162000	3.484350000	0.988963000
O	2.872575000	2.914195000	1.385702000
H	-1.263922000	2.386126000	-1.574161000
C	-0.399718000	3.304378000	0.232729000
N	-1.546571000	3.930519000	0.589673000
H	-2.424614000	3.530347000	0.250331000
H	-1.545968000	4.348651000	1.509518000
O	-3.793915000	-1.912342000	0.885807000
H	-4.413645000	-1.300853000	0.318753000

Optimized coordinates of [CTP-H]⁻ α2

P	-2.185128000	1.200060000	0.028080000
P	-1.183674000	-1.317293000	-1.348729000
O	-1.902257000	2.364339000	-0.843546000
O	-1.931118000	-2.502548000	-0.627840000
O	0.369866000	-1.753096000	-1.272054000
O	-1.568856000	-0.913228000	-2.716559000
C	1.022172000	-2.026226000	-0.024346000
C	2.502135000	-2.322496000	-0.295439000
C	3.705084000	-0.311828000	-0.329822000
O	3.129494000	-1.321725000	-1.125249000
O	4.876187000	-0.647366000	1.833641000
H	5.040435000	0.318028000	1.792287000
H	2.606424000	-3.266964000	-0.834477000
H	0.560188000	-2.897731000	0.454217000
H	0.898954000	-1.161729000	0.637074000
C	3.657659000	-0.812712000	1.143280000
H	4.739166000	-0.146771000	-0.648199000
H	2.842956000	-0.305857000	1.674939000
O	-1.218226000	-0.092599000	-0.238772000
C	3.323997000	-2.310926000	0.998327000
H	2.746810000	-2.677790000	1.859042000
O	4.499064000	-3.087766000	0.830515000
H	5.211109000	-2.610529000	1.287566000
P	-4.383803000	-0.511632000	0.939816000
O	-3.671602000	0.599737000	-0.127473000
O	-5.942881000	-0.086123000	0.801014000
O	-3.873141000	-0.161485000	2.312787000
H	-6.343089000	-0.559941000	0.057603000
H	-2.873789000	-2.289792000	-0.257741000
O	-4.196265000	-1.880524000	0.317811000
O	-1.975387000	1.463159000	1.578411000
H	-2.608633000	0.875688000	2.104115000
N	2.951121000	0.955215000	-0.503652000
C	1.954280000	1.066303000	-1.429588000
C	3.293119000	2.042203000	0.339110000
H	1.804437000	0.208767000	-2.071089000
C	1.174709000	2.176987000	-1.468151000
N	2.467786000	3.118010000	0.357642000
O	4.311056000	1.928952000	1.052396000
H	0.338733000	2.252992000	-2.149199000
C	1.412641000	3.157563000	-0.454583000
N	0.524489000	4.181578000	-0.313975000
H	0.631271000	4.718609000	0.536452000
H	-0.431929000	3.961350000	-0.583577000

Optimized coordinates of [GTP-H]¹⁻ β

N	-3.112047000	-0.796230000	0.101787000
C	-4.131499000	0.024287000	-0.243566000
C	-5.425976000	-0.309792000	-0.648330000
C	-5.786271000	-1.700514000	-0.713667000
C	-3.419577000	-2.076703000	0.040674000
N	-4.078200000	1.400833000	-0.273001000
C	-5.334230000	1.813920000	-0.703061000
N	-6.162156000	0.827574000	-0.929385000
H	-3.051049000	1.598801000	2.109304000
C	-2.361437000	2.129390000	1.441870000
C	-1.050336000	1.345403000	1.223800000
C	-0.674094000	1.674787000	-0.239881000
O	-1.894030000	2.070488000	-0.898098000
C	-2.952145000	2.280815000	0.026419000
H	-1.252569000	0.277888000	1.335072000
H	-3.333428000	3.299930000	-0.087323000
H	0.032713000	2.514275000	-0.245459000
O	-2.098931000	3.434822000	1.936502000
H	-1.283913000	3.370307000	2.462815000
O	-0.093812000	1.789795000	2.172749000
H	0.579382000	1.093760000	2.282353000
O	1.186881000	0.100706000	-0.561890000
H	-5.559657000	2.865458000	-0.821683000
P	1.384820000	-1.143744000	0.482160000
O	0.245836000	-2.094956000	0.455418000
O	1.650974000	-0.456481000	1.900253000
O	2.790046000	-1.726505000	0.012953000
C	-0.118166000	0.507710000	-1.056693000
H	-0.805955000	-0.338355000	-1.023287000
H	0.040064000	0.816495000	-2.092092000
P	4.370678000	-1.372122000	0.553340000
O	4.142592000	-0.277455000	1.614532000
O	4.957154000	-0.625556000	-0.779648000
O	5.081514000	-2.638594000	0.810984000
H	2.668834000	-0.285644000	1.986975000
P	4.850520000	0.928355000	-1.315475000
O	5.947518000	1.297872000	-2.226980000
O	3.417883000	1.002463000	-2.039533000
H	2.658478000	0.723187000	-1.487516000
O	4.735687000	1.783591000	0.034538000
H	4.539958000	1.204261000	0.818943000
O	-6.840609000	-2.244210000	-1.022915000
N	-4.669553000	-2.515478000	-0.336659000
H	-4.876766000	-3.507160000	-0.339418000
N	-2.494602000	-3.008888000	0.396145000
H	-2.609662000	-3.957704000	0.073404000
H	-1.528022000	-2.681148000	0.479021000

Optimized coordinates of [GTP-H]¹⁻ γ

N	5.065100000	-1.377499000	-0.312983000
C	4.621140000	-0.118263000	-0.050043000
C	5.372105000	1.029493000	0.217497000
C	6.805717000	0.936981000	0.215488000
C	6.368719000	-1.470486000	-0.321349000
N	3.307843000	0.273645000	0.020585000
C	3.330725000	1.631853000	0.309153000
N	4.543349000	2.113085000	0.434208000
H	1.054110000	0.341653000	1.430441000
C	1.151127000	-0.647423000	0.971934000
C	-0.162518000	-1.025130000	0.252857000
C	0.022980000	-0.434468000	-1.169195000
O	1.399785000	-0.009433000	-1.280329000
C	2.146764000	-0.564301000	-0.206207000
H	-1.032305000	-0.595932000	0.757111000
H	2.529123000	-1.563655000	-0.444552000
H	-0.163383000	-1.231836000	-1.900857000
O	1.525738000	-1.570008000	1.965417000
H	1.061255000	-2.395614000	1.733462000
O	-0.247025000	-2.439713000	0.242188000
H	-1.198730000	-2.679310000	0.137558000
O	-0.813548000	1.726706000	-0.460481000
H	2.416104000	2.201586000	0.392740000
P	-2.113729000	2.502895000	0.071833000
O	-1.773693000	3.464842000	1.135302000
O	-2.853048000	3.036203000	-1.238564000
O	-3.080838000	1.268709000	0.596183000
C	-0.884677000	0.731849000	-1.509781000
H	-1.906357000	0.359424000	-1.626500000
H	-0.564830000	1.206237000	-2.441848000
P	-4.560415000	0.782680000	0.097771000
O	-5.148265000	1.810933000	-0.814713000
O	-4.255598000	-0.611407000	-0.636437000
O	-5.355004000	0.439141000	1.404196000
H	-5.247695000	-0.575153000	1.601578000
P	-4.244154000	-2.185948000	0.026350000
O	-4.906127000	-2.031124000	1.386936000
O	-5.260039000	-2.933694000	-1.000892000
O	-2.879156000	-2.751113000	-0.180470000
H	-6.178449000	-2.765515000	-0.746669000
H	-3.817148000	2.768676000	-1.256042000
O	7.674193000	1.780898000	0.403892000
N	7.206163000	-0.411812000	-0.075891000
H	8.208676000	-0.526391000	-0.165206000
N	6.969097000	-2.677677000	-0.643690000
H	7.820047000	-2.906223000	-0.146092000
H	6.301716000	-3.438694000	-0.659979000

Optimized coordinates of [GTP-H]¹⁻ α

N	2.931195000	0.870492000	0.514759000
C	4.095360000	0.688143000	-0.148126000
C	5.086078000	1.626013000	-0.453657000
C	4.894712000	2.987198000	-0.033292000
C	2.723273000	2.117475000	0.880101000
N	4.545218000	-0.504503000	-0.675574000
C	5.765375000	-0.213827000	-1.273982000
N	6.123346000	1.037937000	-1.156454000
H	3.954935000	-1.801036000	1.502026000
C	3.486718000	-2.364981000	0.687401000
C	1.960651000	-2.240633000	0.688650000
C	1.623755000	-2.402495000	-0.802430000
O	2.690416000	-1.710769000	-1.477833000
C	3.882222000	-1.798280000	-0.697829000
H	1.706808000	-1.228750000	1.008186000
H	4.590683000	-2.492188000	-1.164790000
H	1.662151000	-3.472611000	-1.061926000
O	3.889512000	-3.731614000	0.735071000
H	3.234606000	-4.184597000	1.291847000
O	1.375229000	-3.218223000	1.523145000
H	0.471986000	-2.888838000	1.722662000
O	-0.088058000	-0.609097000	-0.690212000
H	6.332058000	-0.986954000	-1.775864000
P	-1.034499000	-0.515290000	0.623171000
O	-0.956204000	-1.745903000	1.468565000
O	-0.854062000	0.892747000	1.181407000
O	-2.576679000	-0.506982000	-0.085961000
C	0.265402000	-1.884126000	-1.257237000
H	-0.491117000	-2.633295000	-1.003353000
H	0.274828000	-1.742733000	-2.341466000
P	-3.567828000	0.710412000	-0.379005000
O	-4.071672000	0.777140000	-1.790709000
O	-4.848392000	0.401166000	0.591304000
P	-6.377504000	0.188624000	0.002182000
O	-7.366117000	-0.076324000	1.056720000
O	-6.652147000	1.530075000	-0.847878000
H	-5.931056000	1.673887000	-1.493919000
O	-6.215855000	-0.997412000	-1.076397000
H	-5.511858000	-0.779862000	-1.719399000
O	5.608011000	3.977356000	-0.165191000
N	3.638556000	3.120298000	0.637332000
H	3.452512000	4.062544000	0.959316000
N	1.588200000	2.446733000	1.560069000
H	1.311169000	3.417532000	1.570935000
H	0.806512000	1.787263000	1.480566000
O	-2.888614000	2.003868000	0.196426000
H	-2.016589000	1.741614000	0.683770000

Optimized coordinates of [GTP-H]¹⁻ β2

P	-4.517067000	0.831701000	0.158480000
P	-2.054724000	2.548032000	0.102720000
O	-4.982191000	1.718396000	-0.963707000
O	-2.791095000	3.078453000	-1.205915000
O	-0.787701000	1.697248000	-0.421287000
O	-5.376837000	0.463154000	1.341252000
O	-1.638940000	3.526975000	1.123972000
C	-0.901798000	0.738356000	-1.495132000
C	-0.022943000	-0.462590000	-1.197676000
C	2.104929000	-0.606993000	-0.228723000
O	1.364892000	-0.076455000	-1.319504000
O	1.471486000	-1.601631000	1.9444449000
H	1.037059000	-2.439105000	1.699330000
H	-0.239478000	-1.237184000	-1.945211000
H	-0.579269000	1.224588000	-2.420660000
H	-1.934754000	0.397699000	-1.609924000
N	3.254139000	0.247194000	0.000387000
C	3.258795000	1.609859000	0.270011000
C	4.572257000	-0.130773000	-0.053408000
C	5.307838000	1.029047000	0.204476000
C	6.742354000	0.952835000	0.215936000
N	4.465044000	2.105996000	0.398792000
N	5.032695000	-1.388827000	-0.293908000
C	6.337240000	-1.467058000	-0.289483000
H	2.336783000	2.170076000	0.337889000
C	1.099906000	-0.687140000	0.941848000
H	2.502541000	-1.604264000	-0.449787000
H	0.992282000	0.302950000	1.394574000
O	-3.064051000	1.387198000	0.693691000
C	-0.204599000	-1.075137000	0.213490000
H	-1.082573000	-0.667093000	0.720837000
O	-0.263173000	-2.493887000	0.181407000
H	-1.208209000	-2.759826000	0.132264000
O	-4.007601000	-0.619907000	-0.520851000
O	-2.949232000	-2.935988000	-0.018925000
O	-5.237900000	-2.791758000	-1.075709000
O	-4.983771000	-2.034875000	1.365799000
H	-5.229393000	-1.054662000	1.557544000
H	-3.721626000	2.695144000	-1.289470000
P	-4.207623000	-2.148191000	-0.007481000
H	-6.105551000	-2.362137000	-1.056304000
O	7.599936000	1.808880000	0.399359000
N	7.160456000	-0.395529000	-0.052567000
H	8.164909000	-0.499866000	-0.132025000
N	6.954376000	-2.672246000	-0.588246000
H	7.801769000	-2.883866000	-0.077179000
H	6.295294000	-3.440570000	-0.599131000

Optimized coordinates of [GTP-H]¹⁻ α2

N	2.931195000	0.870492000	0.514759000
C	4.095360000	0.688143000	-0.148126000
C	5.086078000	1.626013000	-0.453657000
C	4.894712000	2.987198000	-0.033292000
C	2.723273000	2.117475000	0.880101000
N	4.545218000	-0.504503000	-0.675574000
C	5.765375000	-0.213827000	-1.273982000
N	6.123346000	1.037937000	-1.156454000
H	3.954935000	-1.801036000	1.502026000
C	3.486718000	-2.364981000	0.687401000
C	1.960651000	-2.240633000	0.688650000
C	1.623755000	-2.402495000	-0.802430000
O	2.690416000	-1.710769000	-1.477833000
C	3.882222000	-1.798280000	-0.697829000
H	1.706808000	-1.228750000	1.008186000
H	4.590683000	-2.492188000	-1.164790000
H	1.662151000	-3.472611000	-1.061926000
O	3.889512000	-3.731614000	0.735071000
H	3.234606000	-4.184597000	1.291847000
O	1.375229000	-3.218223000	1.523145000
H	0.471986000	-2.888838000	1.722662000
O	-0.088058000	-0.609097000	-0.690212000
H	6.332058000	-0.986954000	-1.775864000
P	-1.034499000	-0.515290000	0.623171000
O	-0.956204000	-1.745903000	1.468565000
O	-0.854062000	0.892747000	1.181407000
O	-2.576679000	-0.506982000	-0.085961000
C	0.265402000	-1.884126000	-1.257237000
H	-0.491117000	-2.633295000	-1.003353000
H	0.274828000	-1.742733000	-2.341466000
P	-3.567828000	0.710412000	-0.379005000
O	-4.071672000	0.777140000	-1.790709000
O	-4.848392000	0.401166000	0.591304000
P	-6.377504000	0.188624000	0.002182000
O	-7.366117000	-0.076324000	1.056720000
O	-6.652147000	1.530075000	-0.847878000
H	-5.931056000	1.673887000	-1.493919000
O	-6.215855000	-0.997412000	-1.076397000
H	-5.511858000	-0.779862000	-1.719399000
O	5.608011000	3.977356000	-0.165191000
N	3.638556000	3.120298000	0.637332000
H	3.452512000	4.062544000	0.959316000
N	1.588200000	2.446733000	1.560069000
H	1.311169000	3.417532000	1.570935000
H	0.806512000	1.787263000	1.480566000
O	-2.888614000	2.003868000	0.196426000
H	-2.016589000	1.741614000	0.683770000