Supporting Information For

Dissecting the Mechanism of the Heat-Induced Phase Separation and Crystallization of Poly(2-isopropyl-2-oxazoline) in Water through Vibrational Spectroscopy and Molecular Orbital Calculations

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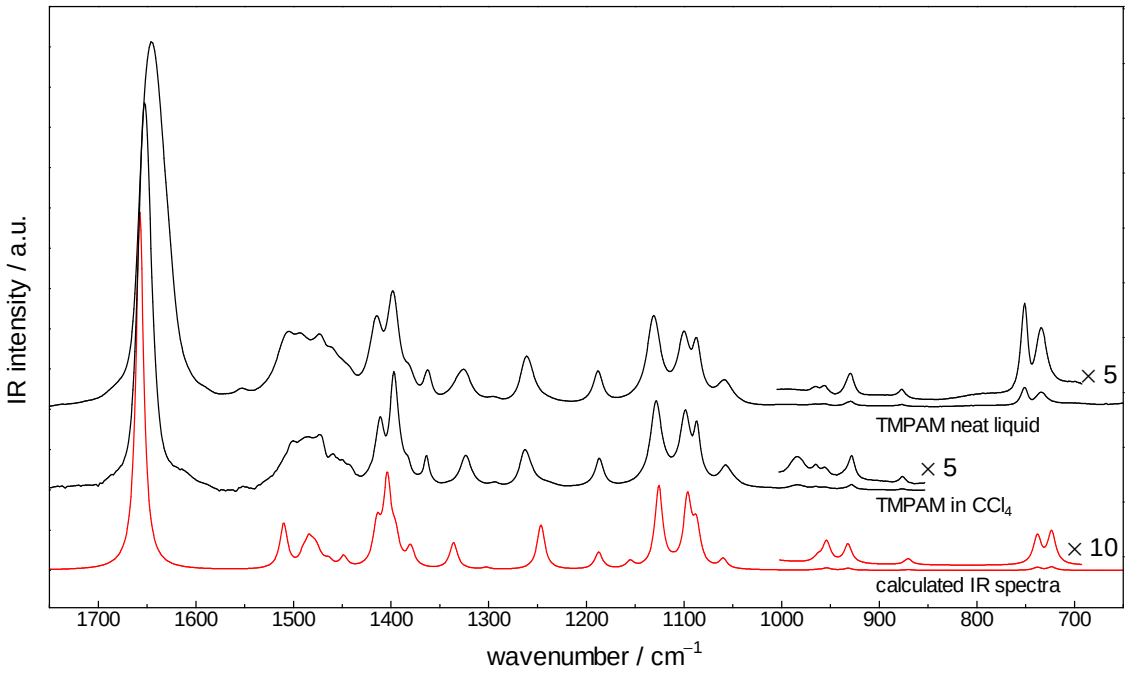

Figure S1. Comparison between the experimental IR spectra of TMPAm, which are observed in the neat liquid and in CCl_4, and the simulated IR spectra for TMPAm calculated at the B3LYP/6-31+G(d) level.

Table S1. Sum of the electronic and zero-point energy E (hatree), relative energy ΔE (kJ mol^{-1}), and ϕ for EMPAm conformers optimized in vacuum

ID	E / hatree	ΔE / kJ mol^{-1}	ϕ / ^{o}	ψ / ^{o}
a1	-731.384475	0.00	180.0	11.30
a2	-731.384305	0.446	177.9	14.12
a3	-731.383417	2.78	180.0	14.22
a4	-731.384086	1.02	178.0	10.26
b1	-731.384442	0.0867	62.60	177.3
b2	-731.383613	2.26	62.97	174.8
b3	-731.382879	4.19	63.52	173.4
c1	-731.381770	7.10	-53.69	158.6
c2	-731.381420	8.02	-54.06	-155.3
c3	-731.381436	7.98	-57.39	-158.4
d1	-731.378061	16.8	176.1	187.0
d2	-731.378263	16.3	173.8	176.7
d3	-731.378321	16.2	170.0	175.6
e1	-731.379424	13.3	75.48	14.33
e2	-731.379687	12.6	75.54	14.95
e3	-731.380007	11.7	78.10	16.88
e4	-731.379772	12.4	78.44	16.59
f1	-731.379778	12.3	-78.44	-4.05
f2	-731.379634	12.7	-76.91	-3.62
f3	-731.379647	12.7	-77.63	-2.52
f4	-731.380011	11.7	-78.09	-2.87

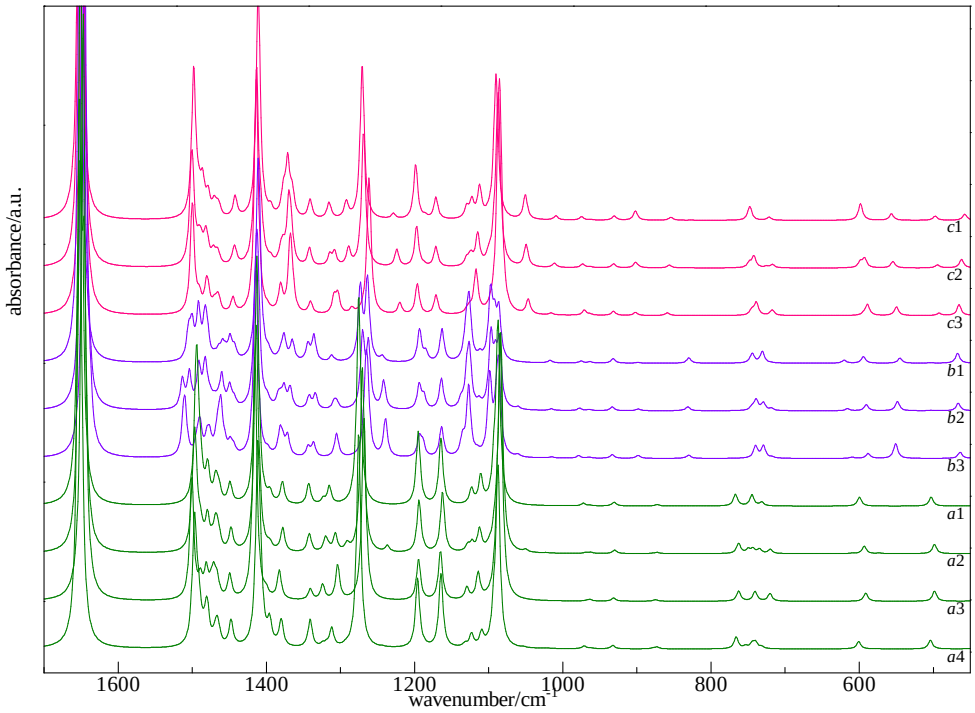

Figure S2. Simulated IR spectra for the nine conformers of EMPAm.

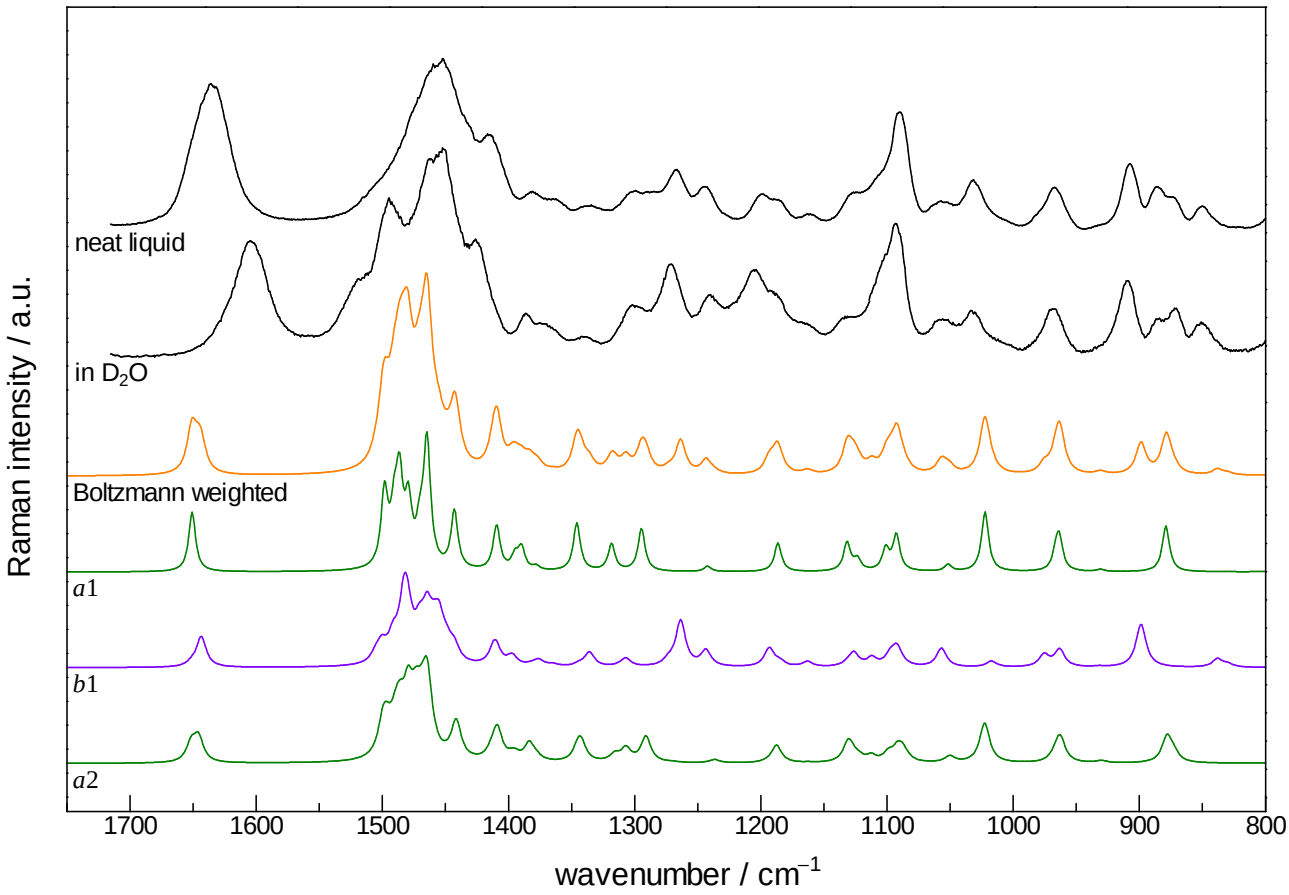

Figure S3. Comparison between the simulated and observed Raman spectra of EMPAm.

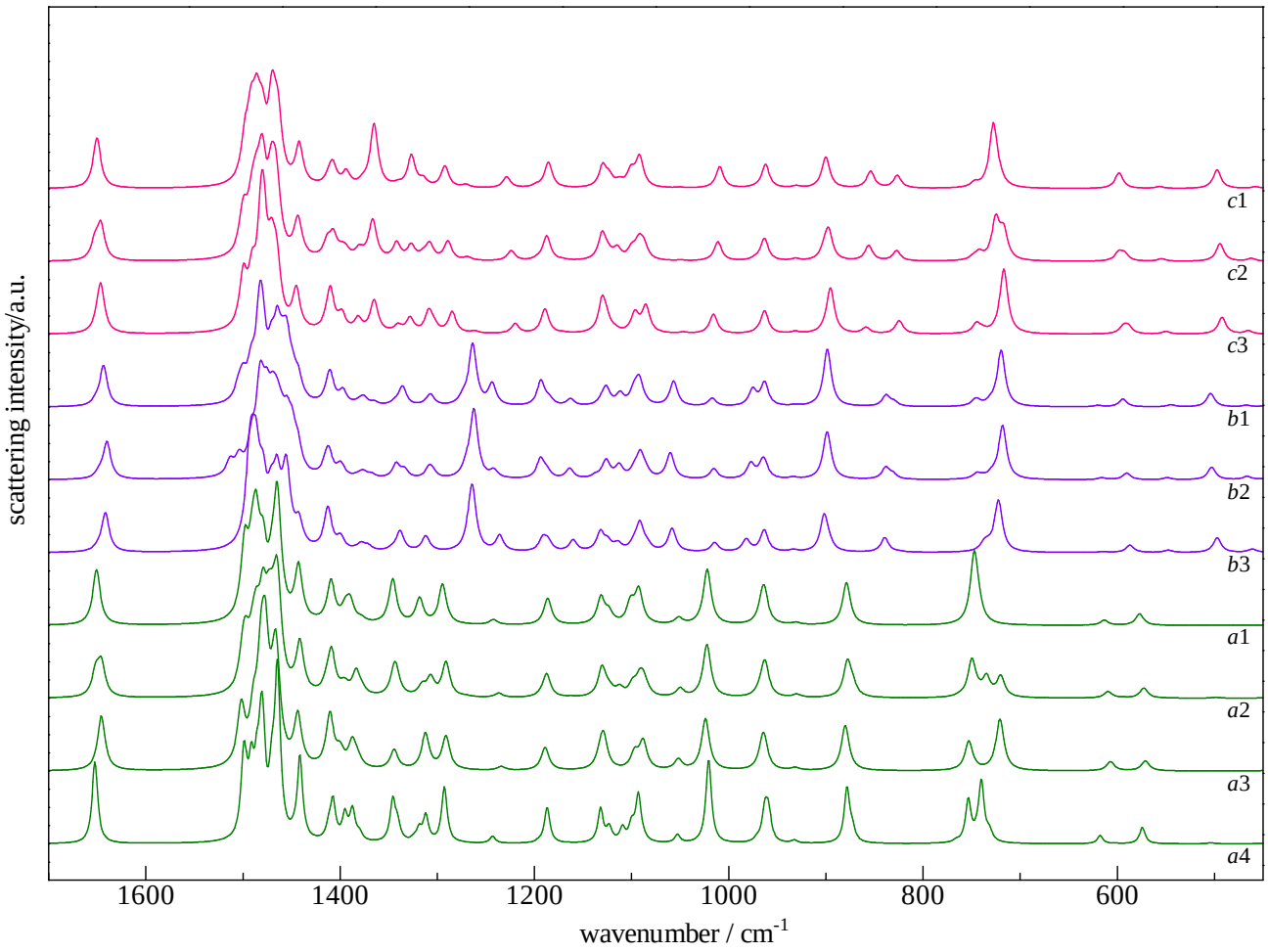

Figure S4. Simulated Raman spectra for the nine conformers of EMPAm.

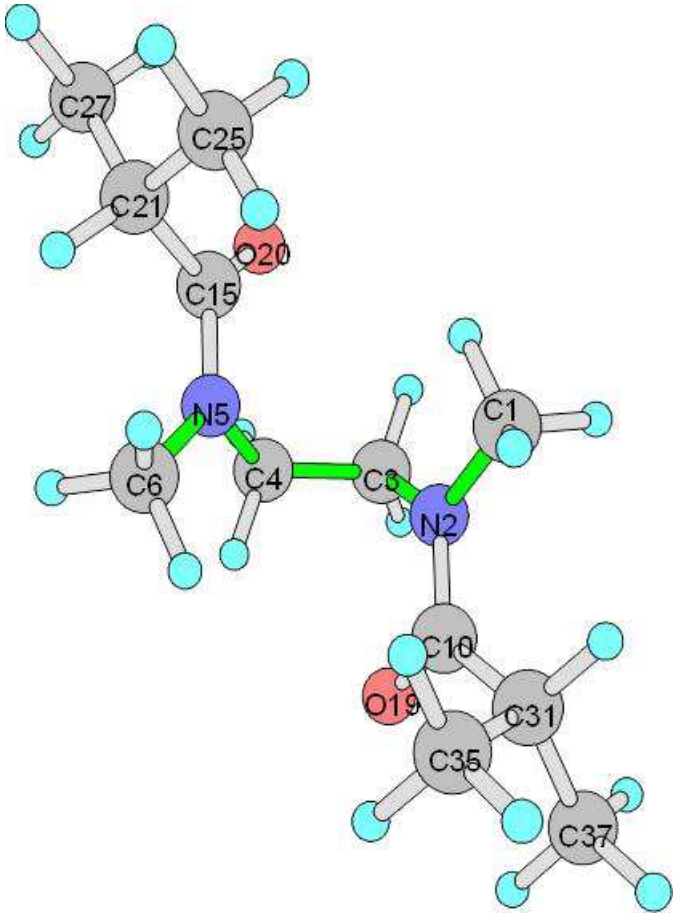

Figure S5. Definition of the atom number for the dimer model.

Example for the definition of redundant coordinates with scan and constraint information.

ϕ scan with a fixed ψ:

Freeze the coordinate in the optimization (the numbers are defined in Figure S5).

Dihedral angle: 2 3 4 5
Dihedral angle: 10 2 3 4
Valence angle: 10 2 1
Valence angle: 2 10 19
Valence angle: 31 10 19
Valence angle: 6 5 15
Valence angle: 20 15 21
Valence angle: 5 15 21

Perform a relaxed potential energy surface scan for the dihedral angle (3 4 5 15) with the increment the coordinate by 12 degree and a total of 30 times.

***a*1:**

Number of imaginary frequencies: 0

Optimized geometries in Cartesian coordinate. See Figure S5 for the definition of the atom numbers.

C	−1.893797	1.996345	0.756331
N	−1.735037	0.563891	0.502694
C	−0.392246	0.000094	0.661967
C	0.392246	−0.000094	−0.661967
N	1.735037	−0.563891	−0.502694
C	1.893797	−1.996345	−0.756331
H	−2.603116	2.451632	0.061951
H	−0.927765	2.485204	0.605871
H	−2.223499	2.199132	1.785104
C	−2.751418	−0.287853	0.149876
H	0.149039	0.594293	1.403984
H	−0.493071	−1.022333	1.034106
H	0.493071	1.022333	−1.034106
H	−0.149039	−0.594293	−1.403984
C	2.751418	0.287853	−0.149876
H	2.223499	−2.199132	−1.785104
H	0.927765	−2.485204	−0.605871
H	2.603116	−2.451632	−0.061951
O	−2.524467	−1.476283	−0.099775
O	2.524467	1.476283	0.099775
C	4.177309	−0.271431	−0.049288
H	5.117351	1.691603	0.020996
H	4.999694	1.021208	−1.611628
H	6.205067	0.372661	−0.480832
C	5.185441	0.768292	−0.561408
H	4.269591	−1.168973	−0.67118
C	4.473674	−0.656461	1.415534
H	5.494551	−1.045754	1.50759
H	4.382389	0.222847	2.063157
H	3.785295	−1.424049	1.789831
C	−4.177309	0.271431	0.049288
H	−4.382389	−0.222847	−2.063157
H	−3.785295	1.424049	−1.789831
H	−5.494551	1.045754	−1.50759
C	−4.473674	0.656461	−1.415534
H	−4.269591	1.168973	0.67118
C	−5.185441	−0.768292	0.561408
H	−6.205067	−0.372661	0.480832
H	−5.117351	−1.691603	−0.020996
H	−4.999694	−1.021208	1.611628

***a*2:**

Number of imaginary frequencies: 0

Optimized geometries in Cartesian coordinate. See Figure S5 for the definition of the atom numbers.

C	1.893519	2.100351	0.056423
N	1.75106	0.687456	−0.297167
C	0.418444	0.235816	−0.705109
C	−0.398032	−0.293821	0.486954
N	−1.749323	−0.698727	0.087415
C	−1.939739	−2.126391	−0.149718
H	2.593376	2.239744	0.882927
H	0.920353	2.476452	0.382895
H	2.226311	2.707087	−0.797655
C	2.771207	−0.230202	−0.296116
H	−0.108941	1.079769	−1.158776
H	0.537339	−0.550955	−1.453808
H	−0.480449	0.480881	1.2538
H	0.110116	−1.162785	0.915299
C	−2.719202	0.274297	0.055747
H	−1.914203	−2.6905	0.793346
H	−1.136186	−2.502728	−0.79231
H	−2.888738	−2.324872	−0.645482
O	2.55553	−1.41843	−0.555722
O	−2.429995	1.448875	0.306951
C	−4.170873	−0.121077	−0.255764
H	−4.845684	0.102327	1.806352
H	−4.335103	−1.550797	1.417144
H	−5.885927	−0.938468	0.815325
C	−4.844781	−0.664271	1.022585
H	−4.183076	−0.912485	−1.014784
C	−4.940892	1.080252	−0.81961
H	−5.971414	0.786087	−1.052755
H	−4.963497	1.90229	−0.098483
H	−4.475634	1.457919	−1.736603
C	4.186872	0.24645	0.057681
H	4.351225	−1.046434	1.804502
H	3.732081	0.569172	2.191232
H	5.454055	0.345503	1.83084
C	4.442465	0.018531	1.562462
H	4.281741	1.317606	−0.153766
C	5.220767	−0.500996	−0.797684
H	6.232764	−0.166243	−0.539802
H	5.151998	−1.579921	−0.631574
H	5.062527	−0.31694	−1.866534

***a*3:**

Number of imaginary frequencies: 0

Optimized geometries in Cartesian coordinate. See Figure S5 for the definition of the atom numbers.

C	1.899118	2.082844	0.48444
N	1.75026	0.719029	−0.014203
C	0.420601	0.372327	−0.525806
C	−0.420601	−0.372327	0.525806
N	−1.75026	−0.719029	0.014203
C	−1.899118	−2.082844	−0.48444
H	2.823396	2.203014	1.047457
H	1.062673	2.323624	1.149596
H	1.896431	2.808108	−0.341545
C	2.739727	−0.228825	−0.118554
H	−0.091185	1.297043	−0.806641
H	0.541076	−0.252199	−1.414683
H	−0.541076	0.252199	1.414683
H	0.091185	−1.297043	0.806641
C	−2.739727	0.228825	0.118554
H	−1.896431	−2.808108	0.341545
H	−1.062673	−2.323624	−1.149596
H	−2.823396	−2.203014	−1.047457
O	2.486165	−1.344419	−0.584579
O	−2.486165	1.344419	0.584579
C	−4.170582	−0.128651	−0.313237
H	−4.919583	−0.293227	1.728893
H	−4.356113	−1.839288	1.067734
H	−5.90055	−1.156234	0.528694
C	−4.873833	−0.905421	0.820479
H	−4.137724	−0.770578	−1.2018
C	−4.949277	1.140878	−0.681458
H	−5.964263	0.875796	−1.001438
H	−5.014871	1.81986	0.173445
H	−4.462419	1.684429	−1.498461
C	4.170582	0.128651	0.313237
H	5.014871	−1.81986	−0.173445
H	4.462419	−1.684429	1.498461
H	5.964263	−0.875796	1.001438
C	4.949277	−1.140878	0.681458
H	4.137724	0.770578	1.2018
C	4.873833	0.905421	−0.820479
H	5.90055	1.156234	−0.528694
H	4.919583	0.293227	−1.728893
H	4.356113	1.839288	−1.067734

***a*4:**

Number of imaginary frequencies: 0

Optimized geometries in Cartesian coordinate. See Figure S5 for the definition of the atom numbers.

C	1.937524	−2.078139	−0.19366
N	1.745362	−0.676523	0.185118
C	0.391929	−0.236396	0.533015
C	−0.422284	0.178161	−0.706112
N	−1.757283	0.661066	−0.345105
C	−1.904713	2.095649	−0.095032
H	2.119965	−2.200259	−1.269013
H	1.027298	−2.628447	0.053561
H	2.766047	−2.534799	0.357537
C	2.732034	0.277542	0.119909
H	−0.122229	−1.05374	1.046845
H	0.480707	0.609681	1.217931
H	−0.539089	−0.674905	−1.378623
H	0.103974	0.977688	−1.236917
C	−2.776423	−0.255258	−0.273825
H	−2.275011	2.632702	−0.979555
H	−0.925415	2.50471	0.166296
H	−2.57615	2.291606	0.743963
O	2.490098	1.463345	0.365365
O	−2.55998	−1.459831	−0.440812
C	−4.192395	0.245939	0.041777
H	−5.15716	−1.61675	−0.54307
H	−5.060142	−0.428676	−1.850084
H	−6.236225	−0.198909	−0.540098
C	−5.223528	−0.549439	−0.772951
H	−4.283435	1.30263	−0.233894
C	−4.455821	0.109293	1.55615
H	−5.468352	0.452838	1.798899
H	−4.366668	−0.939282	1.861813
H	−3.747992	0.696487	2.154035
C	4.160221	−0.176799	−0.210941
H	4.934108	1.843533	−0.456091
H	4.384859	1.107664	−1.967285
H	5.915627	0.579926	−1.239125
C	4.892235	0.90535	−1.01693
H	4.128688	−1.090779	−0.814532
C	4.903207	−0.491565	1.105378
H	5.92867	−0.817352	0.894485
H	4.950762	0.402815	1.736941
H	4.407751	−1.284312	1.678816

***b*1:**

Number of imaginary frequencies: 0

Optimized geometries in Cartesian coordinate. See Figure S5 for the definition of the atom numbers.

C	1.853112	−1.641037	−1.080493
N	0.396878	−1.480454	−1.112496
C	−0.158708	−0.754818	−2.252289
C	0.158708	0.754818	−2.252289
N	−0.396878	1.480454	−1.112496
C	−1.853112	1.641037	−1.080493
H	2.13648	−2.6062	−0.656082
H	2.339587	−0.831007	−0.524863
H	2.221256	−1.618527	−2.110787
C	−0.440403	−1.826755	−0.079515
H	0.250161	−1.186879	−3.17615
H	−1.237186	−0.921402	−2.248656
H	−0.250161	1.186879	−3.17615
H	1.237186	0.921402	−2.248656
C	0.440403	1.826755	−0.079515
H	−2.13648	2.6062	−0.656082
H	−2.339587	0.831007	−0.524863
H	−2.221256	1.618527	−2.110787
O	−1.653344	−1.59287	−0.124131
O	1.653344	1.59287	−0.124131
C	−0.158708	2.573326	1.121868
H	1.67097	2.522317	2.303995
H	0.583504	1.163992	2.620278
H	0.185097	2.772588	3.25425
C	0.619521	2.237063	2.401534
H	−1.199424	2.2638	1.26693
C	−0.129092	4.09151	0.842081
H	−0.546662	4.642778	1.692927
H	0.903014	4.427978	0.690422
H	−0.7055	4.360991	−0.050858
C	0.158708	−2.573326	1.121868
H	−1.67097	−2.522317	2.303995
H	−0.583504	−1.163992	2.620278
H	−0.185097	−2.772588	3.25425
C	−0.619521	−2.237063	2.401534
H	1.199424	−2.2638	1.26693
C	0.129092	−4.09151	0.842081
H	0.546662	−4.642778	1.692927
H	−0.903014	−4.427978	0.690422
H	0.7055	−4.360991	−0.050858

***b*2:**

Number of imaginary frequencies: 0

Optimized geometries in Cartesian coordinate. See Figure S5 for the definition of the atom numbers.

C	−1.645958	−0.986811	1.981282
N	−1.553104	−1.125465	0.528448
C	−0.794863	−2.281718	0.054056
C	0.722355	−2.21932	0.321526
N	1.41402	−1.12269	−0.351149
C	1.507108	−1.204793	−1.811096
H	−2.427756	−0.283469	2.263176
H	−0.693882	−0.644945	2.404428
H	−1.899303	−1.961202	2.416992
C	−1.99621	−0.207349	−0.396065
H	−1.182909	−3.176838	0.561159
H	−0.992972	−2.383147	−1.014042
H	1.158061	−3.168311	−0.021471
H	0.924041	−2.123464	1.38924
C	1.809474	−0.03698	0.392292
H	0.653342	−0.719441	−2.298081
H	1.507867	−2.262102	−2.094968
H	2.439936	−0.770805	−2.174466
O	−1.739914	−0.338289	−1.598242
O	1.615554	0.015898	1.612229
C	2.56638	1.094279	−0.320451
H	2.68157	2.380973	1.433862
H	1.275639	2.70027	0.410733
H	2.884796	3.229279	−0.119027
C	2.337084	2.431414	0.396968
H	2.197936	1.193045	−1.347641
C	4.070821	0.747731	−0.36561
H	4.629139	1.546671	−0.867757
H	4.465281	0.644277	0.651941
H	4.267694	−0.189538	−0.899109
C	−2.824344	0.994519	0.085187
H	−1.280989	2.476947	−0.322266
H	−1.205973	1.835459	1.328872
H	−2.475333	2.992262	0.882673
C	−1.887106	2.138207	0.526262
H	−3.436165	0.698379	0.945149
C	−3.776179	1.458854	−1.025981
H	−4.378244	2.303502	−0.669485
H	−3.21778	1.773745	−1.912134
H	−4.456898	0.656469	−1.330991

***b*3:**

Number of imaginary frequencies: 0

Optimized geometries in Cartesian coordinate. See Figure S5 for the definition of the atom numbers.

C	1.939973	1.535376	1.14353
N	0.478884	1.486285	1.159328
C	−0.114567	0.76205	2.281337
C	0.114567	−0.76205	2.281337
N	−0.478884	−1.486285	1.159328
C	−1.939973	−1.535376	1.14353
H	2.303143	2.292873	0.451289
H	2.359271	0.564187	0.855334
H	2.300689	1.796309	2.146405
C	−0.351053	1.961923	0.170503
H	0.324917	1.154977	3.20988
H	−1.180557	0.993337	2.289401
H	−0.324917	−1.154977	3.20988
H	1.180557	−0.993337	2.289401
C	0.351053	−1.961923	0.170503
H	−2.359271	−0.564187	0.855334
H	−2.300689	−1.796309	2.146405
H	−2.303143	−2.292873	0.451289
O	−1.566619	1.737438	0.194773
O	1.566619	−1.737438	0.194773
C	−0.255147	−2.793965	−0.971654
H	0.027285	−1.281804	−2.513297
H	−1.549989	−1.167029	−1.713882
H	−1.240835	−2.463866	−2.885586
C	−0.792335	−1.867374	−2.082111
H	−1.090412	−3.389396	−0.584582
C	0.792335	−3.768686	−1.527953
H	0.34749	−4.372507	−2.328199
H	1.653422	−3.228589	−1.931756
H	1.161363	−4.446421	−0.750401
C	0.255147	2.793965	−0.971654
H	−0.027285	1.281804	−2.513297
H	1.549989	1.167029	−1.713882
H	1.240835	2.463866	−2.885586
C	0.792335	1.867374	−2.082111
H	1.090412	3.389396	−0.584582
C	−0.792335	3.768686	−1.527953
H	−0.34749	4.372507	−2.328199
H	−1.653422	3.228589	−1.931756
H	−1.161363	4.446421	−0.750401

***c*1:**

Number of imaginary frequencies: 0

Optimized geometries in Cartesian coordinate. See Figure S5 for the definition of the atom numbers.

C	1.983006	−0.594664	0.462731
N	1.003913	−1.129623	−0.484182
C	0.697095	−0.323244	−1.674503
C	−0.697095	0.323244	−1.674503
N	−1.003913	1.129623	−0.484182
C	−1.983006	0.594664	0.462731
H	1.734762	−0.869257	1.490435
H	1.967253	0.495129	0.400302
H	3.0047	−0.936745	0.242288
C	0.474081	−2.392097	−0.412932
H	1.456235	0.456711	−1.753963
H	0.761766	−0.965049	−2.560084
H	−1.456235	−0.456711	−1.753963
H	−0.761766	0.965049	−2.560084
C	−0.474081	2.392097	−0.412932
H	−1.967253	−0.495129	0.400302
H	−3.0047	0.936745	0.242288
H	−1.734762	0.869257	1.490435
O	−0.350163	−2.777971	−1.248716
O	0.350163	2.777971	−1.248716
C	−0.898726	3.3121	0.741725
H	1.118933	3.487268	1.546181
H	0.183784	2.175124	2.290352
H	−0.159752	3.860278	2.719973
C	0.121074	3.196173	1.893952
H	−1.882733	3.010025	1.116974
C	−1.003913	4.761523	0.243584
H	−1.299512	5.420549	1.068791
H	−0.044985	5.103285	−0.156298
H	−1.750353	4.856525	−0.553292
C	0.898726	−3.3121	0.741725
H	−1.118933	−3.487268	1.546181
H	−0.183784	−2.175124	2.290352
H	0.159752	−3.860278	2.719973
C	−0.121074	−3.196173	1.893952
H	1.882733	−3.010025	1.116974
C	1.003913	−4.761523	0.243584
H	1.299512	−5.420549	1.068791
H	0.044985	−5.103285	−0.156298
H	1.750353	−4.856525	−0.553292

***c*2:**

Number of imaginary frequencies: 0

Optimized geometries in Cartesian coordinate. See Figure S5 for the definition of the atom numbers.

C	−1.027411	−0.308066	1.893983
N	−1.352335	−0.741221	0.534041
C	−0.49025	−1.755665	−0.088604
C	0.429815	−1.218772	−1.195917
N	1.27579	−0.08211	−0.799077
C	1.009145	1.174704	−1.49359
H	−1.199162	0.763384	2.023847
H	0.032564	−0.496113	2.073521
H	−1.60568	−0.853428	2.65367
C	−2.485909	−0.365245	−0.13977
H	0.113795	−2.212649	0.696431
H	−1.12537	−2.527689	−0.536051
H	−0.182056	−0.894598	−2.040033
H	1.071712	−2.044272	−1.525293
C	2.363976	−0.34598	−0.005002
H	−0.054819	1.418399	−1.414604
H	1.263687	1.098843	−2.560624
H	1.579331	1.996553	−1.063268
O	−2.70376	−0.771244	−1.286084
O	2.545619	−1.484291	0.440212
C	3.365054	0.777951	0.307659
H	4.626209	−0.441685	1.599992
H	3.363691	0.436698	2.468212
H	4.782476	1.313664	1.858374
C	4.076917	0.503194	1.639082
H	2.83283	1.732077	0.403264
C	4.381113	0.899669	−0.848401
H	5.107913	1.691872	−0.633212
H	4.930689	−0.041034	−0.969938
H	3.899286	1.13565	−1.804188
C	−3.466599	0.598906	0.544777
H	−3.205791	2.165216	−0.948339
H	−2.11379	2.337362	0.440344
H	−3.829451	2.749522	0.60784
C	−3.12846	2.048914	0.13885
H	−3.373867	0.513045	1.633263
C	−4.909555	0.241809	0.15865
H	−5.609021	0.935804	0.640117
H	−5.044473	0.298276	−0.925263
H	−5.16676	−0.775813	0.473874

***c*3:**

Number of imaginary frequencies: 0

Optimized geometries in Cartesian coordinate. See Figure S5 for the definition of the atom numbers.

C	−0.141504	2.095754	−0.593182
N	−0.886087	1.233216	0.320132
C	−0.141504	0.754167	1.495591
C	0.141504	−0.754167	1.495591
N	0.886087	−1.233216	0.320132
C	0.141504	−2.095754	−0.593182
H	−0.702384	2.286605	−1.506917
H	0.800573	1.610906	−0.867047
H	0.095224	3.06129	−0.123216
C	−2.242539	1.017291	0.298421
H	0.804546	1.297542	1.536084
H	−0.717728	0.985654	2.398183
H	−0.804546	−1.297542	1.536084
H	0.717728	−0.985654	2.398183
C	2.242539	−1.017291	0.298421
H	−0.800573	−1.610906	−0.867047
H	−0.095224	−3.06129	−0.123216
H	0.702384	−2.286605	−1.506917
O	−2.779156	0.351748	1.190029
O	2.779156	−0.351748	1.190029
C	3.089938	−1.629793	−0.828533
H	4.96771	−0.753121	−0.154307
H	4.107708	0.238342	−1.335806
H	4.949389	−1.231711	−1.869949
C	4.355135	−0.792699	−1.059481
H	2.516988	−1.634769	−1.763646
C	3.446967	−3.088133	−0.469278
H	4.063557	−3.533859	−1.258816
H	4.018169	−3.119155	0.465893
H	2.557121	−3.715585	−0.342837
C	−3.089938	1.629793	−0.828533
H	−4.96771	0.753121	−0.154307
H	−4.107708	−0.238342	−1.335806
H	−4.949389	1.231711	−1.869949
C	−4.355135	0.792699	−1.059481
H	−2.516988	1.634769	−1.763646
C	−3.446967	3.088133	−0.469278
H	−4.063557	3.533859	−1.258816
H	−4.018169	3.119155	0.465893
H	−2.557121	3.715585	−0.342837

***d*1:**

Number of imaginary frequencies: 0

Optimized geometries in Cartesian coordinate. See Figure S5 for the definition of the atom numbers.

C	−2.365011	2.030045	−0.450979
N	−1.890859	0.770787	0.120072
C	−0.503089	0.724705	0.584135
C	0.503079	0.724681	−0.584167
N	1.890849	0.770782	−0.120106
C	2.364975	2.030037	0.450974
H	−3.370795	2.276899	−0.100854
H	−2.366509	2.026133	−1.549383
H	−1.699521	2.83204	−0.118061
C	−2.664154	−0.367932	0.219159
H	−0.327825	1.587208	1.242447
H	−0.381569	−0.187716	1.169366
H	0.327808	1.587156	−1.242516
H	0.381562	−0.187764	−1.169362
C	2.664193	−0.367894	−0.219287
H	3.37073	2.276949	0.100809
H	2.366527	2.026079	1.549377
H	1.699432	2.832015	0.118123
O	−2.233448	−1.394899	0.742591
O	2.233492	−1.394891	−0.742661
C	4.104585	−0.314643	0.311568
H	4.365141	−2.476009	0.274238
H	3.804443	−1.857954	1.833308
H	5.496445	−1.617295	1.350497
C	4.46363	−1.64893	0.983011
H	4.201344	0.478551	1.061001
C	5.063126	−0.005819	−0.857848
H	6.100274	0.020862	−0.502997
H	4.982591	−0.783036	−1.625942
H	4.843372	0.959453	−1.330844
C	−4.104592	−0.314668	−0.311563
H	−4.365224	−2.476022	−0.274084
H	−3.804632	−1.85808	−1.833237
H	−5.496586	−1.61733	−1.350299
C	−4.463741	−1.648981	−0.982897
H	−4.201397	0.478487	−1.061031
C	−5.063014	−0.005744	0.857923
H	−6.100195	0.020939	0.503171
H	−4.982424	−0.782913	1.62606
H	−4.843189	0.959553	1.330835

***d*2:**

Number of imaginary frequencies: 0

Optimized geometries in Cartesian coordinate. See Figure S5 for the definition of the atom numbers.

C	−2.349791	1.991057	−0.529565
N	−1.863745	0.745401	0.060832
C	−0.460251	0.702315	0.475568
C	0.50601	0.68069	−0.725496
N	1.905954	0.785505	−0.306898
C	2.421121	2.125936	−0.03566
H	−3.333592	2.264745	−0.139001
H	−2.406306	1.949811	−1.625753
H	−1.658622	2.794549	−0.258189
C	−2.648225	−0.376097	0.239528
H	−0.255799	1.573979	1.113497
H	−0.318831	−0.20101	1.069659
H	0.290592	1.509953	−1.412992
H	0.385717	−0.258485	−1.267842
C	2.68366	−0.353596	−0.309513
H	2.969895	2.542779	−0.892549
H	3.072458	2.14161	0.841595
H	1.577859	2.788286	0.177058
O	−2.2118	−1.387376	0.787568
O	2.206267	−1.452782	−0.588854
C	4.162116	−0.223335	0.086368
H	3.9488	−1.494213	1.843481
H	3.724881	0.226919	2.200724
H	5.354222	−0.409006	1.904364
C	4.303398	−0.486263	1.600886
H	4.520112	0.790609	−0.125207
C	5.013342	−1.208311	−0.728215
H	6.066786	−1.124569	−0.435109
H	4.680304	−2.236533	−0.56125
H	4.94062	−1.004982	−1.802822
C	−4.108094	−0.322658	−0.235919
H	−4.392152	−2.477385	−0.107875
H	−3.886946	−1.925032	−1.709998
H	−5.555373	−1.644541	−1.170386
C	−4.509178	−1.675875	−0.842743
H	−4.225585	0.443937	−1.009756
C	−5.015273	0.041434	0.958203
H	−6.065361	0.069597	0.643884
H	−4.913496	−0.708122	1.750848
H	−4.764391	1.020245	1.385718

***d*3:**

Number of imaginary frequencies: 0

Optimized geometries in Cartesian coordinate. See Figure S5 for the definition of the atom numbers.

C	−2.376538	2.104275	−0.008367
N	−1.876565	0.756347	0.24957
C	−0.462964	0.636676	0.6163
C	0.462907	0.636542	−0.616284
N	1.876506	0.756271	−0.249564
C	2.376471	2.104168	0.00862
H	−2.815595	2.565294	0.888736
H	−3.118261	2.115149	−0.809676
H	−1.542303	2.731804	−0.33467
C	−2.675418	−0.366718	0.312723
H	−0.210549	1.469715	1.286824
H	−0.332271	−0.298473	1.162426
H	0.210478	1.469424	−1.287
H	0.332232	−0.298733	−1.162196
C	2.675457	−0.366716	−0.312832
H	2.816665	2.56488	−0.888076
H	3.11727	2.115106	0.810803
H	1.541974	2.731934	0.333768
O	−2.203416	−1.471668	0.576775
O	2.203615	−1.471673	−0.577143
C	4.173355	−0.212407	−0.007889
H	4.092494	−1.49474	1.751632
H	3.869727	0.22125	2.133998
H	5.484113	−0.39096	1.727004
C	4.4167	−0.480599	1.492597
H	4.500429	0.808264	−0.237025
C	4.988206	−1.178562	−0.88035
H	6.056958	−1.072376	−0.658308
H	4.689162	−2.213831	−0.693841
H	4.838826	−0.975936	−1.947062
C	−4.173382	−0.212509	0.008039
H	−4.092644	−1.494114	−1.75202
H	−3.870184	0.222056	−2.133735
H	−5.48441	−0.390544	−1.726698
C	−4.416943	−0.480123	−1.492514
H	−4.500561	0.80802	0.237667
C	−4.987966	−1.179127	0.880236
H	−6.056767	−1.072975	0.658414
H	−4.688831	−2.214285	0.693257
H	−4.838431	−0.976923	1.947005

***e*1:**

Number of imaginary frequencies: 0

Optimized geometries in Cartesian coordinate. See Figure S5 for the definition of the atom numbers.

C	2.579315	1.999689	0.576578
N	1.717251	1.075062	−0.161031
C	0.533169	1.642416	−0.82166
C	−0.644055	1.953758	0.120022
N	−1.391254	0.775159	0.560482
C	−0.907873	0.03309	1.723377
H	3.610742	1.983692	0.2072
H	2.590774	1.79406	1.654292
H	2.196004	3.013263	0.437463
C	1.992584	−0.265009	−0.304891
H	0.838441	2.572433	−1.319857
H	0.204779	0.938834	−1.587199
H	−1.341858	2.599663	−0.418272
H	−0.296777	2.492925	1.010171
C	−2.397732	0.32635	−0.265398
H	−1.73542	−0.285338	2.363944
H	−0.272879	0.69747	2.315586
H	−0.316389	−0.845525	1.437914
O	1.231906	−1.019745	−0.914489
O	−2.712645	0.953244	−1.279752
C	−3.156154	−0.946729	0.132372
H	−5.060128	0.087613	0.36912
H	−4.13435	−0.018387	1.877929
H	−4.962333	−1.454115	1.245499
C	−4.399643	−0.55735	0.959873
H	−2.513462	−1.585121	0.74774
C	−3.549046	−1.739417	−1.122691
H	−4.095105	−2.646563	−0.836262
H	−4.184729	−1.136599	−1.777717
H	−2.663974	−2.038258	−1.694917
C	3.305765	−0.802667	0.284325
H	2.728749	−2.892844	0.091523
H	2.358713	−2.20066	1.677245
H	4.037682	−2.59747	1.263208
C	3.093387	−2.209018	0.863333
H	3.654184	−0.150116	1.092051
C	4.378651	−0.814516	−0.825597
H	5.326489	−1.202246	−0.433849
H	4.059196	−1.457727	−1.653033
H	4.565399	0.18789	−1.22987

***e*2:**

Number of imaginary frequencies: 0

Optimized geometries in Cartesian coordinate. See Figure S5 for the definition of the atom numbers.

C	2.571456	2.037206	0.49239
N	1.663452	1.10517	−0.177676
C	0.463235	1.672466	−0.808976
C	−0.677923	2.015638	0.165269
N	−1.419967	0.851287	0.650859
C	−0.932152	0.142583	1.834252
H	3.579794	2.009978	0.063958
H	2.644726	1.848796	1.570676
H	2.184432	3.050169	0.360099
C	1.910872	−0.243167	−0.28947
H	0.761598	2.588192	−1.336708
H	0.100141	0.957644	−1.547903
H	−1.386648	2.658449	−0.362437
H	−0.296795	2.568985	1.032278
C	−2.447706	0.391849	−0.141407
H	−1.707092	0.061396	2.605256
H	−0.103307	0.713107	2.258674
H	−0.561137	−0.859468	1.591526
O	1.10929	−1.004796	−0.835052
O	−2.770307	0.989329	−1.171732
C	−3.166677	−0.900063	0.261461
H	−4.930027	−0.467697	−0.937116
H	−5.077263	0.055931	0.748261
H	−5.195878	−1.670152	0.349362
C	−4.685137	−0.733423	0.095447
H	−2.959853	−1.14089	1.309197
C	−2.62851	−2.052546	−0.61388
H	−3.108105	−2.99673	−0.328336
H	−2.850498	−1.857137	−1.668828
H	−1.543406	−2.17032	−0.517044
C	3.246967	−0.781262	0.24492
H	2.648446	−2.870464	0.123835
H	2.358715	−2.143041	1.710502
H	4.013617	−2.560626	1.224914
C	3.05363	−2.173468	0.862969
H	3.641776	−0.114865	1.019341
C	4.261314	−0.825975	−0.918368
H	5.224804	−1.214605	−0.567941
H	3.894015	−1.483135	−1.714388
H	4.435472	0.165988	−1.352834

***e*3:**

Number of imaginary frequencies: 0

Optimized geometries in Cartesian coordinate. See Figure S5 for the definition of the atom numbers.

C	2.659393	2.126383	0.070817
N	1.677277	1.127337	−0.343425
C	0.423555	1.655593	−0.902059
C	−0.657713	2.002592	0.137797
N	−1.385104	0.845642	0.660483
C	−0.835821	0.126423	1.81052
H	3.286475	2.46334	−0.767935
H	3.304276	1.752557	0.867374
H	2.128776	2.997751	0.466325
C	1.927862	−0.222886	−0.411868
H	0.673749	2.565623	−1.463967
H	0.02305	0.923716	−1.604623
H	−1.388162	2.656713	−0.344419
H	−0.22046	2.545408	0.984494
C	−2.435644	0.380799	−0.097678
H	−1.591209	−0.021823	2.589673
H	−0.034059	0.730441	2.2409
H	−0.412408	−0.842981	1.524887
O	1.048811	−1.018743	−0.751411
O	−2.793252	0.976689	−1.117915
C	−3.139224	−0.912074	0.328064
H	−4.94265	−0.484079	−0.811416
H	−5.03332	0.043237	0.876781
H	−5.163452	−1.683892	0.485936
C	−4.662581	−0.747196	0.212856
H	−2.896823	−1.153755	1.367731
C	−2.629134	−2.063789	−0.564995
H	−3.099354	−3.008157	−0.264653
H	−2.885621	−1.867942	−1.612103
H	−1.541599	−2.180867	−0.502054
C	3.326007	−0.731965	−0.024818
H	2.611853	−1.907249	1.666743
H	3.107629	−0.266225	2.121112
H	4.33479	−1.491671	1.753258
C	3.344511	−1.116369	1.469511
H	4.068335	0.056922	−0.190792
C	3.706551	−1.931348	−0.90589
H	4.703206	−2.295942	−0.629618
H	2.986035	−2.745183	−0.785235
H	3.724692	−1.657332	−1.966732

***e*4:**

Number of imaginary frequencies: 0

Optimized geometries in Cartesian coordinate. See Figure S5 for the definition of the atom numbers.

C	2.679509	2.10226	0.161999
N	1.734531	1.096339	−0.316727
C	0.496019	1.617089	−0.914755
C	−0.627364	1.93691	0.089092
N	−1.365671	0.767046	0.564697
C	−0.840332	0.025756	1.710289
H	3.332513	2.473104	−0.642013
H	3.299439	1.719684	0.973866
H	2.116646	2.952775	0.558345
C	2.01593	−0.246497	−0.414188
H	0.754984	2.538129	−1.454579
H	0.131439	0.890044	−1.641485
H	−1.344337	2.594408	−0.408526
H	−0.226066	2.466721	0.961657
C	−2.387933	0.309606	−0.235648
H	−1.647769	−0.320128	2.361414
H	−0.212835	0.701005	2.298299
H	−0.230732	−0.831253	1.399874
O	1.169142	−1.048575	−0.814771
O	−2.723771	0.927623	−1.249387
C	−3.138464	−0.959223	0.189649
H	−5.027451	0.085463	0.491996
H	−4.050776	−0.026506	1.967807
H	−4.90847	−1.457272	1.363762
C	−4.350646	−0.56355	1.059476
H	−2.476667	−1.599396	0.782427
C	−3.578587	−1.752029	−1.04943
H	−4.115371	−2.657902	−0.742245
H	−4.236693	−1.148969	−1.681748
H	−2.715633	−2.053308	−1.653282
C	3.405392	−0.739743	0.02172
H	2.640708	−1.961713	1.657259
H	3.09108	−0.323738	2.166686
H	4.351605	−1.522222	1.824101
C	3.368064	−1.155593	1.507411
H	4.139904	0.064917	−0.096552
C	3.844591	−1.913824	−0.866063
H	4.835107	−2.266747	−0.55465
H	3.134673	−2.742514	−0.792794
H	3.902631	−1.617618	−1.919451

***f*1:**

Number of imaginary frequencies: 0

Optimized geometries in Cartesian coordinate. See Figure S5 for the definition of the atom numbers.

C	0.840457	0.025314	1.709872
N	1.366018	0.766755	0.564499
C	0.627658	1.936643	0.089023
C	−0.495991	1.616853	−0.914543
N	−1.734455	1.09637	−0.316203
C	−2.678911	2.102033	0.164262
H	1.647867	−0.32229	2.360075
H	0.229365	−0.830557	1.399228
H	0.214454	0.701028	2.298968
C	2.388458	0.309569	−0.235787
H	0.226595	2.466501	0.961675
H	1.344562	2.594068	−0.408786
H	−0.13172	0.889549	−1.641165
H	−0.754834	2.537797	−1.454585
C	−2.016509	−0.246282	−0.414049
H	−3.294034	1.72077	0.980477
H	−3.336675	2.46945	−0.637415
H	−2.115486	2.954607	0.555228
O	2.724446	0.927881	−1.24929
O	−1.170455	−1.048697	−0.815508
C	−3.40592	−0.738892	0.022639
H	−3.138727	−2.739679	−0.797872
H	−3.907516	−1.610878	−1.920104
H	−4.838255	−2.262838	−0.555487
C	−3.84792	−1.91006	−0.867635
H	−4.139635	0.066962	−0.092234
C	−3.366684	−1.158755	1.507132
H	−4.350101	−1.525212	1.824406
H	−2.639879	−1.96597	1.653682
H	−3.08785	−0.328884	2.168139
C	3.138947	−0.959389	0.18923
H	4.237932	−1.148135	−1.681841
H	2.716993	−2.052691	−1.654376
H	4.116449	−2.657503	−0.743056
C	3.579664	−1.751564	−1.050043
H	2.476949	−1.599928	0.781391
C	4.350742	−0.564048	1.059744
H	4.908534	−1.45787	1.363792
H	5.027713	0.085317	0.492863
H	4.050475	−0.027486	1.968227

***f*2:**

Number of imaginary frequencies: 0

Optimized geometries in Cartesian coordinate. See Figure S5 for the definition of the atom numbers.

C	0.965229	0.031058	1.764423
N	1.406836	0.77713	0.587245
C	0.633594	1.944425	0.163
C	−0.543123	1.619322	−0.77487
N	−1.723798	1.052156	−0.104835
C	−2.653274	2.041376	0.428088
H	1.81452	−0.270294	2.384586
H	0.382009	−0.857943	1.495362
H	0.333234	0.685976	2.369937
C	2.39064	0.33612	−0.268339
H	0.28065	2.465708	1.061047
H	1.314434	2.611128	−0.371799
H	−0.20898	0.918992	−1.541214
H	−0.860171	2.546405	−1.271893
C	−1.965311	−0.300274	−0.212902
H	−3.399602	1.586508	1.077214
H	−3.172057	2.578417	−0.379793
H	−2.102709	2.779584	1.022524
O	2.666212	0.963455	−1.294297
O	−1.137661	−1.04898	−0.736564
C	−3.297975	−0.865036	0.307954
H	−4.126851	−1.174482	−1.685146
H	−4.552426	0.40183	−0.993997
H	−5.349692	−1.066854	−0.404257
C	−4.396116	−0.656786	−0.75715
H	−3.596191	−0.334298	1.220074
C	−3.147083	−2.35055	0.661055
H	−4.098263	−2.740908	1.042628
H	−2.853667	−2.932958	−0.216876
H	−2.381645	−2.503418	1.429866
C	3.174201	−0.928001	0.108533
H	4.155728	−1.104684	−1.827576
H	2.647789	−2.023331	−1.706288
H	4.107564	−2.616215	−0.885586
C	3.544003	−1.715091	−1.156888
H	2.554018	−1.573857	0.73904
C	4.433749	−0.525825	0.905036
H	5.013504	−1.416608	1.174936
H	5.072206	0.127333	0.299161
H	4.185726	0.008743	1.830428

***f*3:**

Number of imaginary frequencies: 0

Optimized geometries in Cartesian coordinate. See Figure S5 for the definition of the atom numbers.

C	−0.967314	−0.086428	1.852278
N	−1.433829	−0.835404	0.684832
C	−0.663003	−1.99381	0.231849
C	0.474361	−1.651933	−0.747863
N	1.678403	−1.085656	−0.119694
C	2.641479	−2.075566	0.348715
H	−1.755415	0.016163	2.606915
H	−0.594709	0.907378	1.580732
H	−0.143269	−0.639729	2.307847
C	−2.452309	−0.407834	−0.135684
H	−0.271866	−2.513677	1.114579
H	−1.354891	−2.667233	−0.279626
H	0.105896	−0.945807	−1.492898
H	0.776912	−2.571539	−1.266924
C	1.897523	0.271879	−0.202592
H	3.419576	−1.624727	0.962392
H	3.118685	−2.597101	−0.494049
H	2.128752	−2.826302	0.961338
O	−2.746181	−1.031272	−1.159726
O	1.036577	1.022117	−0.667589
C	3.247321	0.84091	0.266824
H	3.982435	1.190033	−1.756311
H	4.452248	−0.393073	−1.111347
H	5.262891	1.073309	−0.534069
C	4.297881	0.659983	−0.850101
H	3.590698	0.298078	1.155782
C	3.100533	2.319146	0.650631
H	4.064592	2.711099	0.996525
H	2.764973	2.913282	−0.204063
H	2.368366	2.453374	1.454456
C	−3.199934	0.879855	0.226571
H	−2.86751	1.796765	−1.720279
H	−1.588266	2.163706	−0.552137
H	−3.1725	2.962511	−0.412719
C	−2.66869	2.021838	−0.666553
H	−3.013789	1.148135	1.27141
C	−4.71249	0.682171	0.041232
H	−5.243538	1.615447	0.264453
H	−4.936544	0.387461	−0.988237
H	−5.101067	−0.098146	0.706945

***f*4:**

Number of imaginary frequencies: 0

Optimized geometries in Cartesian coordinate. See Figure S5 for the definition of the atom numbers.

C	0.835833	0.125974	1.810201
N	1.385056	0.845408	0.660253
C	0.657736	2.002512	0.137834
C	−0.423736	1.655731	−0.901869
N	−1.677358	1.127406	−0.343083
C	−2.659494	2.126324	0.071467
H	1.590669	−0.020529	2.590247
H	0.414338	−0.844299	1.524725
H	0.032545	0.728844	2.239318
C	2.435735	0.380784	−0.097825
H	0.220713	2.54533	0.984655
H	1.38819	2.656573	−0.344458
H	−0.023373	0.923934	−1.6046
H	−0.673991	2.56585	−1.463605
C	−1.928026	−0.222799	−0.411843
H	−3.303563	1.752677	0.868782
H	−3.287417	2.462662	−0.766901
H	−2.128818	2.998052	0.466079
O	2.793348	0.976734	−1.118023
O	−1.049078	−1.018621	−0.751714
C	−3.326153	−0.731874	−0.024729
H	−2.986542	−2.74474	−0.786227
H	−3.725455	−1.656259	−1.966986
H	−4.703642	−2.295457	−0.629916
C	−3.707037	−1.930796	−0.906282
H	−4.068416	0.057183	−0.190158
C	−3.344373	−1.116977	1.469424
H	−4.334647	−1.492256	1.753221
H	−2.611789	−1.908059	1.66611
H	−3.107217	−0.26717	2.121367
C	3.139481	−0.91195	0.328071
H	2.886104	−1.868017	−1.612011
H	1.542172	−2.181242	−0.501967
H	3.100156	−3.008084	−0.264498
C	2.629676	−2.063858	−0.564881
H	2.897069	−1.153501	1.367775
C	4.662817	−0.746842	0.212948
H	5.163816	−1.683384	0.486318
H	4.942946	−0.483921	−0.811356
H	5.033353	0.043829	0.876703

***a*1w:**

Number of imaginary frequencies: 0

Optimized geometries in Cartesian coordinate. See Figure S5 for the definition of the atom numbers.

C	−2.00666225	1.8312876	0.72307532
N	−1.80257117	0.40846447	0.45912851
C	−0.42919617	−0.08944653	0.63515051
C	0.421245	0.064692	−0.643136
N	1.79462	−0.433219	−0.467114
C	1.98910182	−1.86548949	−0.68281011
H	−2.66133405	2.29106292	−0.01987549
H	−1.03860895	2.33455856	0.66224676
H	−2.42097863	2.0048155	1.7244785
C	−2.83633436	−0.42087522	0.11740766
H	0.0374877	0.47495531	1.44949535
H	−0.48361216	−1.14010382	0.92946338
H	0.47566099	1.11534928	−0.93744887
H	−0.04543887	−0.49970985	−1.45748084
C	2.83631555	0.40278524	−0.16843176
H	2.38962581	−2.07649974	−1.68262685
H	1.01974899	−2.36163545	−0.59168789
H	2.65136696	−2.30168654	0.06759074
O	−2.68069893	−1.63502486	−0.13440924
O	2.68922347	1.62585314	0.04195441
C	4.22281088	−0.2516743	−0.07790098
H	5.35561338	1.61377943	−0.0701867
H	5.10553432	0.9351231	−1.68896168
H	6.28007973	0.18613388	−0.58864034
C	5.30329489	0.68193982	−0.64047465
H	4.2363566	−1.17013305	−0.6750261
C	4.5182161	−0.62284735	1.39133249
H	5.50399285	−1.09673854	1.46671195
H	4.52152735	0.27492837	2.02001011
H	3.77690446	−1.32061174	1.79950831
C	−4.22467459	0.23038166	0.03221199
H	−4.49394217	−0.2224523	−2.08679939
H	−3.75986036	1.36743201	−1.80005154
H	−5.48998127	1.12436828	−1.49787847
C	−4.50299293	0.65236739	−1.42660521
H	−4.25027529	1.12692187	0.6613929
C	−5.30779739	−0.72734935	0.54715517
H	−6.28620155	−0.2342475	0.50030619
H	−5.34833471	−1.638503	−0.05653878
H	−5.12228533	−1.01685807	1.58845534

***b*1w:**

Number of imaginary frequencies: 0

Optimized geometries in Cartesian coordinate. See Figure S5 for the definition of the atom numbers.

C	1.836351	−1.640748	−1.055177
N	0.37723	−1.486781	−1.087523
C	−0.173272	−0.751201	−2.227714
C	0.173272	0.751201	−2.227714
N	−0.37723	1.486781	−1.087523
C	−1.836351	1.640748	−1.055177
H	2.124317	−2.628186	−0.690091
H	2.312619	−0.867199	−0.442441
H	2.210431	−1.546903	−2.078379
C	−0.454894	−1.915973	−0.092599
H	0.227531	−1.187568	−3.15257
H	−1.25406	−0.897627	−2.225802
H	−0.227531	1.187568	−3.15257
H	1.25406	0.897627	−2.225802
C	0.454894	1.915973	−0.092599
H	−2.124317	2.628186	−0.690091
H	−2.312619	0.867199	−0.442441
H	−2.210431	1.546903	−2.078379
O	−1.686956	−1.755043	−0.157515
O	1.686956	1.755043	−0.157515
C	−0.162631	2.646957	1.107662
H	1.655111	2.66266	2.316888
H	0.621516	1.253149	2.602358
H	0.147184	2.83778	3.24365
C	0.615575	2.329057	2.392845
H	−1.195874	2.313079	1.252222
C	−0.173272	4.166328	0.831518
H	−0.612884	4.699922	1.682275
H	0.849383	4.535468	0.688697
H	−0.753177	4.421882	−0.06323
C	0.162631	−2.646957	1.107662
H	−1.655111	−2.66266	2.316888
H	−0.621516	−1.253149	2.602358
H	−0.147184	−2.83778	3.24365
C	−0.615575	−2.329057	2.392845
H	1.195874	−2.313079	1.252222
C	0.173272	−4.166328	0.831518
H	0.612884	−4.699922	1.682275
H	−0.849383	−4.535468	0.688697
H	0.753177	−4.421882	−0.06323

***c*1w:**

Number of imaginary frequencies: 0

Optimized geometries in Cartesian coordinate. See Figure S5 for the definition of the atom numbers.

C	−1.040777	0.714364	1.638994
N	−1.384354	−0.365835	0.706525
C	−0.458978	−1.506699	0.619058
C	0.456559	−1.502898	−0.613368
N	1.378466	−0.359119	−0.695725
C	1.023544	0.729422	−1.613907
H	−1.316484	1.691913	1.238353
H	0.040033	0.710743	1.786144
H	−1.522962	0.578686	2.616385
C	−2.577595	−0.44841	0.050339
H	0.145886	−1.516897	1.529681
H	−1.048895	−2.42861	0.592656
H	−0.148597	−1.512399	−1.523884
H	1.050081	−2.422359	−0.58999
C	2.57955	−0.448001	−0.054247
H	−0.058764	0.72556	−1.749673
H	1.495501	0.60369	−2.597651
H	1.30185	1.703501	−1.206951
O	−2.819241	−1.403664	−0.709743
O	2.830258	−1.410181	0.694153
C	3.606234	0.676081	−0.244928
H	3.586913	1.266297	1.858721
H	2.44277	2.188735	0.861869
H	4.178568	2.524084	0.75415
C	3.436845	1.726015	0.874547
H	3.440169	1.170346	−1.2085
C	5.032132	0.104507	−0.251451
H	5.752772	0.915228	−0.410526
H	5.264429	−0.385454	0.699285
H	5.164983	−0.631112	−1.053408
C	−3.607185	0.67291	0.241195
H	−3.551844	1.291013	−1.853797
H	−2.430304	2.204949	−0.824114
H	−4.169123	2.531833	−0.744169
C	−3.421941	1.738367	−0.861085
H	−3.455352	1.153749	1.213958
C	−5.032596	0.10038	0.217954
H	−5.756238	0.908785	0.375297
H	−5.249457	−0.378217	−0.742166
H	−5.177602	−0.644851	1.008833

***d*3w:**

Number of imaginary frequencies: 0

Optimized geometries in Cartesian coordinate. See Figure S5 for the definition of the atom numbers.

C	2.41218	2.117298	−0.106051
N	1.870013	0.768981	−0.30935
C	0.442125	0.676804	−0.634498
C	−0.441012	0.675882	0.628911
N	−1.869458	0.768921	0.30688
C	−2.411942	2.117572	0.107744
H	2.902953	2.498126	−1.011139
H	3.118684	2.146855	0.725669
H	1.58743	2.789233	0.142992
C	2.627478	−0.366553	−0.289704
H	0.187756	1.527011	−1.279317
H	0.273122	−0.242243	−1.197639
H	−0.185822	1.525112	1.274683
H	−0.271783	−0.244239	1.190239
C	−2.626934	−0.366277	0.286783
H	−2.90244	2.49581	1.014042
H	−3.118705	2.149446	−0.72368
H	−1.587358	2.79031	−0.139647
O	2.115289	−1.486574	−0.461448
O	−2.114195	−1.486459	0.455689
C	−4.132325	−0.236458	0.024213
H	−4.082558	−1.427543	−1.80544
H	−3.888863	0.311966	−2.098555
H	−5.482757	−0.342495	−1.680619
C	−4.408346	−0.431691	−1.482298
H	−4.475029	0.763534	0.310897
C	−4.914783	−1.256493	0.865317
H	−5.98948	−1.135153	0.685415
H	−4.632398	−2.281267	0.604526
H	−4.731561	−1.116153	1.937127
C	4.131955	−0.236583	−0.021806
H	4.076255	−1.4259	1.80893
H	3.881283	0.313872	2.099634
H	5.476671	−0.340758	1.687773
C	4.402955	−0.430325	1.485862
H	4.475424	0.763264	−0.308166
C	4.917448	−1.257263	−0.859222
H	5.991494	−1.135455	−0.675736
H	4.634398	−2.281829	−0.598354
H	4.737855	−1.118049	−1.931777

***e*3w:**

Number of imaginary frequencies: 0

Optimized geometries in Cartesian coordinate. See Figure S5 for the definition of the atom numbers.

C	2.506752	2.064173	0.468802
N	1.654708	1.116885	−0.257699
C	0.487279	1.697929	−0.93529
C	−0.692399	2.032738	−0.008369
N	−1.390006	0.862059	0.536126
C	−0.920101	0.304735	1.810925
H	3.316054	2.451596	−0.164848
H	2.936915	1.615168	1.365874
H	1.893072	2.909291	0.790023
C	2.005523	−0.182746	−0.505189
H	0.808746	2.625704	−1.42979
H	0.160068	0.996529	−1.702865
H	−1.412585	2.618481	−0.585368
H	−0.363882	2.650046	0.835263
C	−2.416707	0.326326	−0.18281
H	−1.698522	0.343046	2.581101
H	−0.078424	0.905234	2.157482
H	−0.574136	−0.727887	1.70013
O	1.276872	−0.934918	−1.17315
O	−2.753282	0.807047	−1.28093
C	−3.144087	−0.903253	0.371365
H	−4.927384	−0.658063	−0.862997
H	−5.043696	0.129375	0.722503
H	−5.172022	−1.636233	0.601303
C	−4.663544	−0.753875	0.195128
H	−2.938779	−1.014502	1.440176
C	−2.619228	−2.164113	−0.347315
H	−3.110198	−3.057048	0.057182
H	−2.834002	−2.110557	−1.421041
H	−1.536467	−2.28241	−0.223764
C	3.314637	−0.711698	0.0984
H	2.315862	−2.196887	1.350884
H	2.599622	−0.654861	2.183514
H	3.949841	−1.765746	1.894889
C	3.023288	−1.367069	1.465454
H	4.013571	0.116414	0.255447
C	3.98266	−1.709947	−0.85937
H	4.9311	−2.053764	−0.430001
H	3.342683	−2.581317	−1.030296
H	4.196513	−1.25044	−1.831533

***f*4w:**

Number of imaginary frequencies: 0

Optimized geometries in Cartesian coordinate. See Figure S5 for the definition of the atom numbers.

C	0.92298	0.306942	1.818045
N	1.385825	0.862732	0.540217
C	0.687967	2.034897	−0.00073
C	−0.484155	1.700499	−0.937132
N	−1.655171	1.117374	−0.26794
C	−2.51697	2.060706	0.452215
H	1.694527	0.376036	2.5935
H	0.608609	−0.736435	1.716174
H	0.060721	0.885205	2.151329
C	2.410173	0.32693	−0.182204
H	0.352012	2.646217	0.844343
H	1.409909	2.626187	−0.570065
H	−0.150228	1.000544	−1.703042
H	−0.802826	2.628799	−1.432376
C	−1.999071	−0.184386	−0.513299
H	−2.932151	1.617786	1.359603
H	−3.338184	2.425551	−0.179385
H	−1.914415	2.920417	0.755066
O	2.741248	0.805704	−1.283172
O	−1.265968	−0.935611	−1.177059
C	−3.30837	−0.714991	0.088558
H	−3.296786	−2.606487	−1.002035
H	−4.173748	−1.308895	−1.832102
H	−4.897232	−2.098456	−0.416985
C	−3.954234	−1.7447	−0.85037
H	−4.018467	0.108959	0.217638
C	−3.025231	−1.332825	1.475016
H	−3.955036	−1.715274	1.912104
H	−2.321188	−2.168661	1.385934
H	−2.60052	−0.603499	2.174849
C	3.142189	−0.898887	0.37423
H	2.805734	−2.12375	−1.401195
H	1.52523	−2.28313	−0.185059
H	3.102374	−3.055828	0.08225
C	2.606301	−2.166539	−0.324031
H	2.950099	−0.996806	1.446976
C	4.65938	−0.753314	0.177402
H	5.171367	−1.634531	0.581687
H	4.909711	−0.663472	−0.884493
H	5.047927	0.132052	0.694982