Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Formation of n→π^+ Interaction Facilitating Dissociative Electron Transfer in Isolated Tyrosine-containing Molecular Peptide Radical Cations

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Supporting Information

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Computational Details: Sampling of Conformers

Conformational spaces were firstly sampled with density functional tight binding molecular dynamics (DFTB-MD) simulations by using CP2K/Quickstep package with electronic energies evaluated using local spin density approximation. An elevated temperature of 500 K controlled by the Nosé–Hoover thermostat was used in order to ensure a better sampling efficiency. The MD trajectories, obtained from integrating the equations of motion of all atoms with a time step of 0.5 fs. **Figure S1a** shows the C-C distances between C-terminal COOH and 1st, 2nd or 3rd amide in two DFTB-MD trajectories for **FY$_O$GG** (Phenoxy(1) and Phenoxy(2)). As shown in the distribution plots, folded geometries could be formed as indicated by the peak of the C-C distance between the C-terminal COOH and the first amide group in the short distance region of 4 – 6 Å. Formation of these folded geometries of **FY$_O$GG** can be attributed to hydrogen bonds formed between the cationic ammonium NH_3^+ moiety and various parts of the peptide chain. Similar folded geometries could also be observed for **FY$_\pi$GG**, **FY$_\beta$GG** and **F$_\alpha$YGG** (**Figure S10b**), albeit less obvious, due to the absence of the NH_3^+ moiety as in **FY$_O$GG**. These DFTB-MD trajectories suggested that **FY$_\pi$GG**, **FY$_\beta$GG** and **F$_\alpha$YGG** preferentially formed unfolded conformers probably due to the higher entropic characters of these more extended geometries.

The DFTB-MD trajectories were served as a guide for constructing possible conformers that occurred at finite temperatures. From each trajectory of different radical tautomers (phenoxy, π-, β- and α-radicals), a geometry was sampled in every 1 ps and optimized using the UM06-2X functional with a small 3-21G basis set (and with the "opt=loose" option). Identical geometries were then discarded. A collection of conformers from these initial geometry optimizations covered a variety of geometries, generally including unfolded peptide chain or folded chain in particular with the C-terminal COOH group hydrogen bonded to different amide linkages or the Tyr side chain. Selected geometries with distinct peptide folding

or orientation of the side chains were further optimized with the 6-31G(d) basis set and subsequently refined with the largest 6-311++G(d,p) basis set used for this study. All optimized geometries were characterized using harmonic vibration analysis to ensure that they were located on the corresponding potential energy surfaces (PES's) with correct curvatures (i.e., all real vibration frequencies for structures on local minima). For comparison with the IRMPD result, the geometries were reoptimized at the UB3LYP/6-311++G(d,p) level (including Grimme's D3 dispersion correction), followed by harmonic vibration analysis at the same level to obtain theoretical IR absorption spectra. Note that in these reoptimizations with the B3LYP functional some conformers originally obtained from the M06-2X functional were converged to identical or very similar geometries. Nonetheless, both unfolded or folded peptide conformers were be able to located for spectral comparisons.

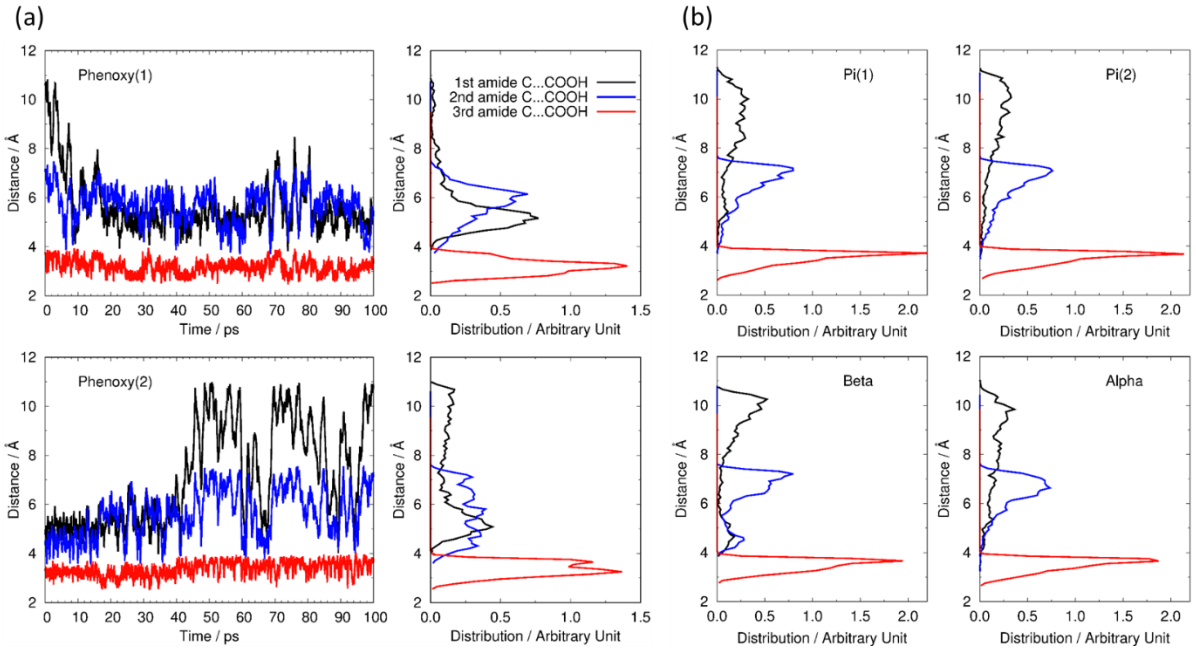


Figure S1. (a) C-C distances between COOH and 1st amide (black), 2nd amide (blue) or 3rd amide (red) in two DFTB-MD trajectories for **FY$_O$GG** (Phenoxy(1) and Phenoxy(2)) at 500 K for 100 ps and their distributions. (b) Distributions of C-C distances between COOH and 1st amide (black), 2nd amide (blue) or 3rd amide (red) in DFTB-MD trajectories for **FY$_\pi$GG** (Pi(1) and Pi(2)), **FY$_\beta$GG** (Beta), and **F$_\alpha$YGG** (Alpha).

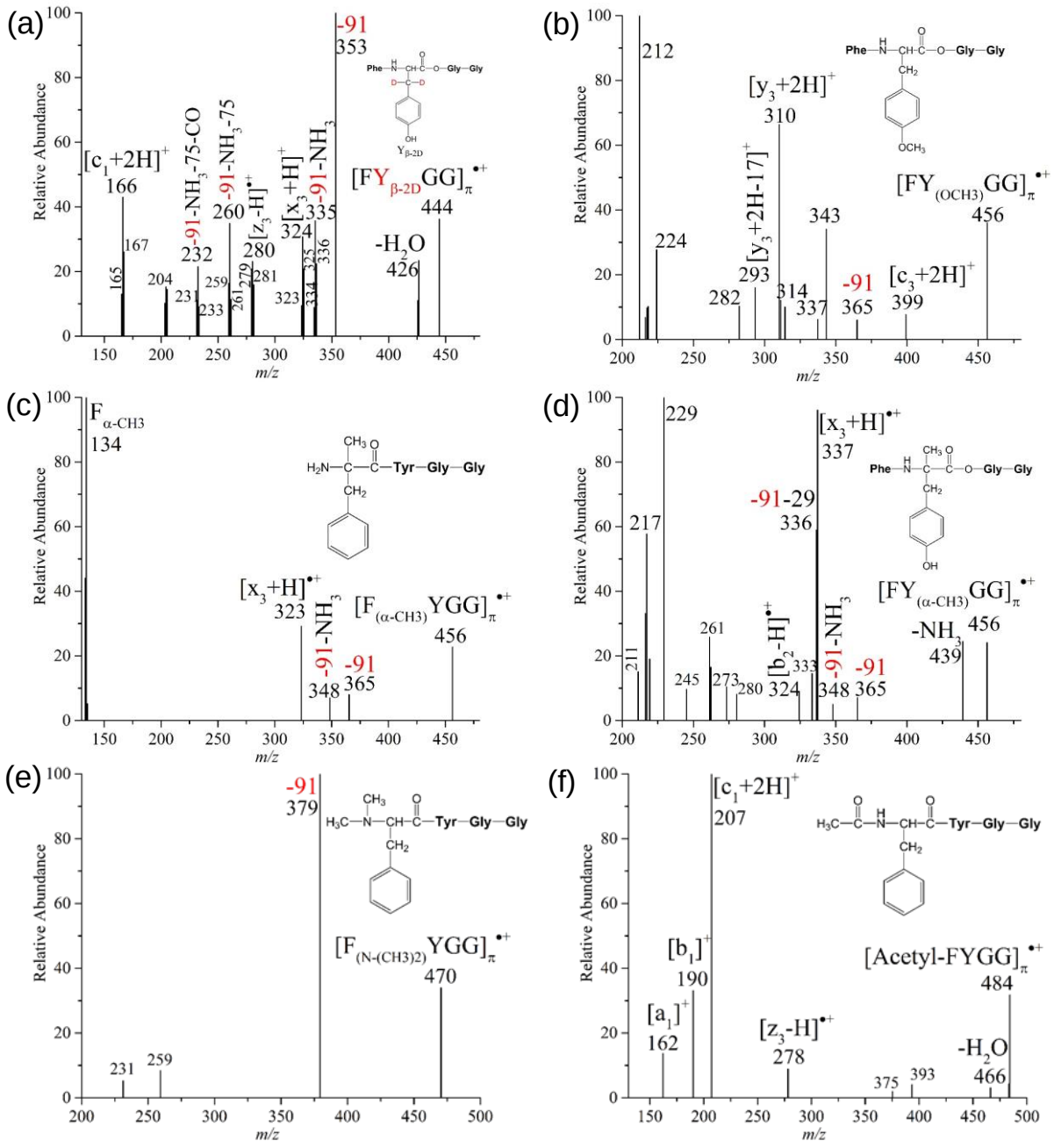


Figure S2. CID spectra of (a) $[FY_{(\beta\text{-}2D)}GG]_{\pi}^{\bullet+}$, (b) $[FY_{(OCH3)}GG]_{\pi}^{\bullet+}$, (c) $[F_{(\alpha\text{-}CH3)}YGG]_{\pi}^{\bullet+}$, (d) $[FY_{(\alpha\text{-}CH3)}GG]_{\pi}^{\bullet+}$; (e) $[F_{N(Me)2}YGG]_{\pi}^{\bullet+}$ and (f) $[Acetyl\text{-}FYGG]_{\pi}^{\bullet+}$.

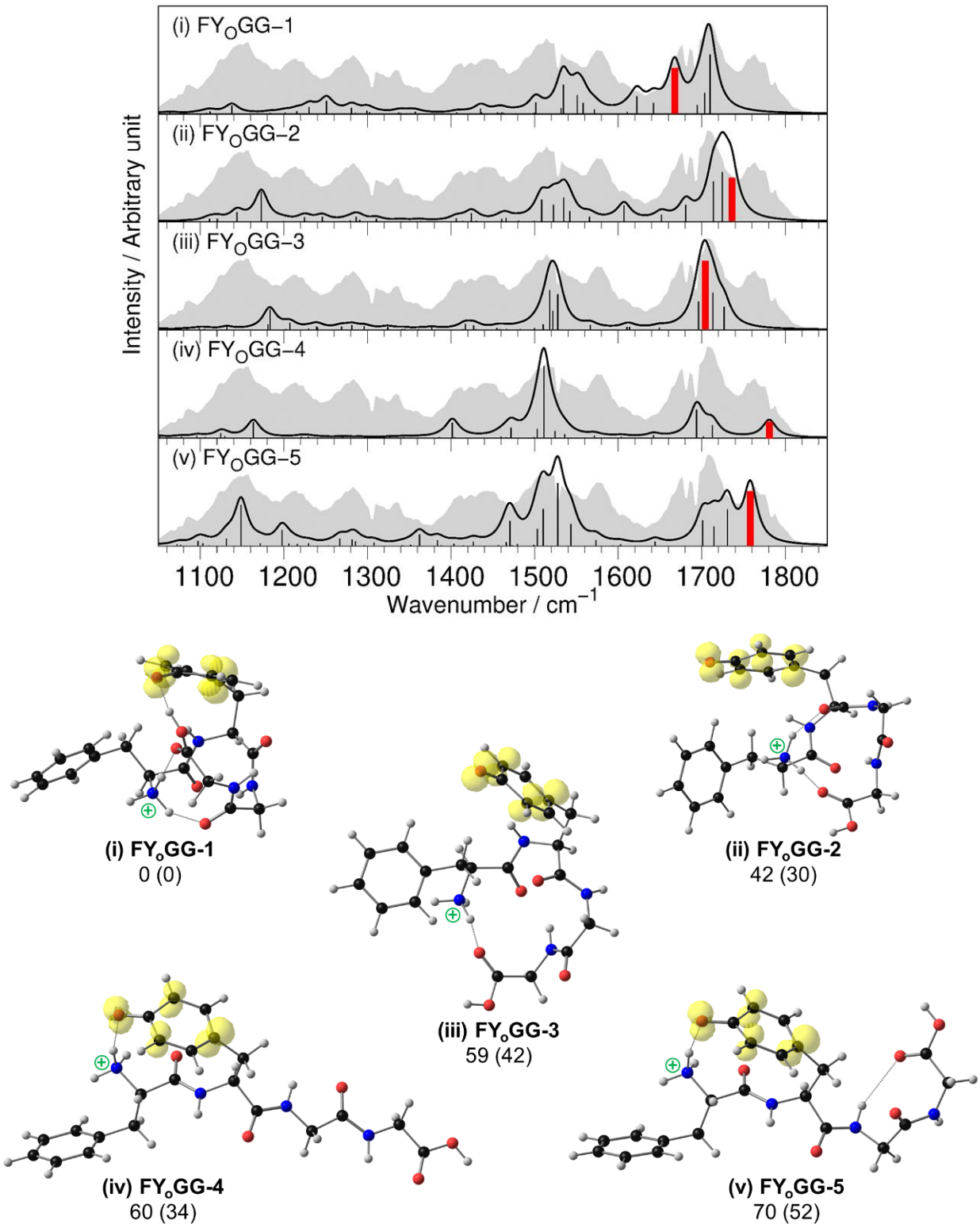


Figure S3. Theoretical IR spectra of $[FY_O^{\bullet}GG]^+$ (black curves and lines) obtained from harmonic vibration analyses including a frequency scaling factor of 0.982 for geometries optimized at the UB3LYP/6-311++G(d,p) level. The theoretical line spectra were arbitrarily broadened using Gaussian profiles of FWHM = 10 cm^{-1} by using GaussView 5.0. Thick red lines highlight the C=O stretches of COOH. Experimental IRMPD spectrum of $[FYGG]^{\bullet+}$ is shown as shaded grey color.

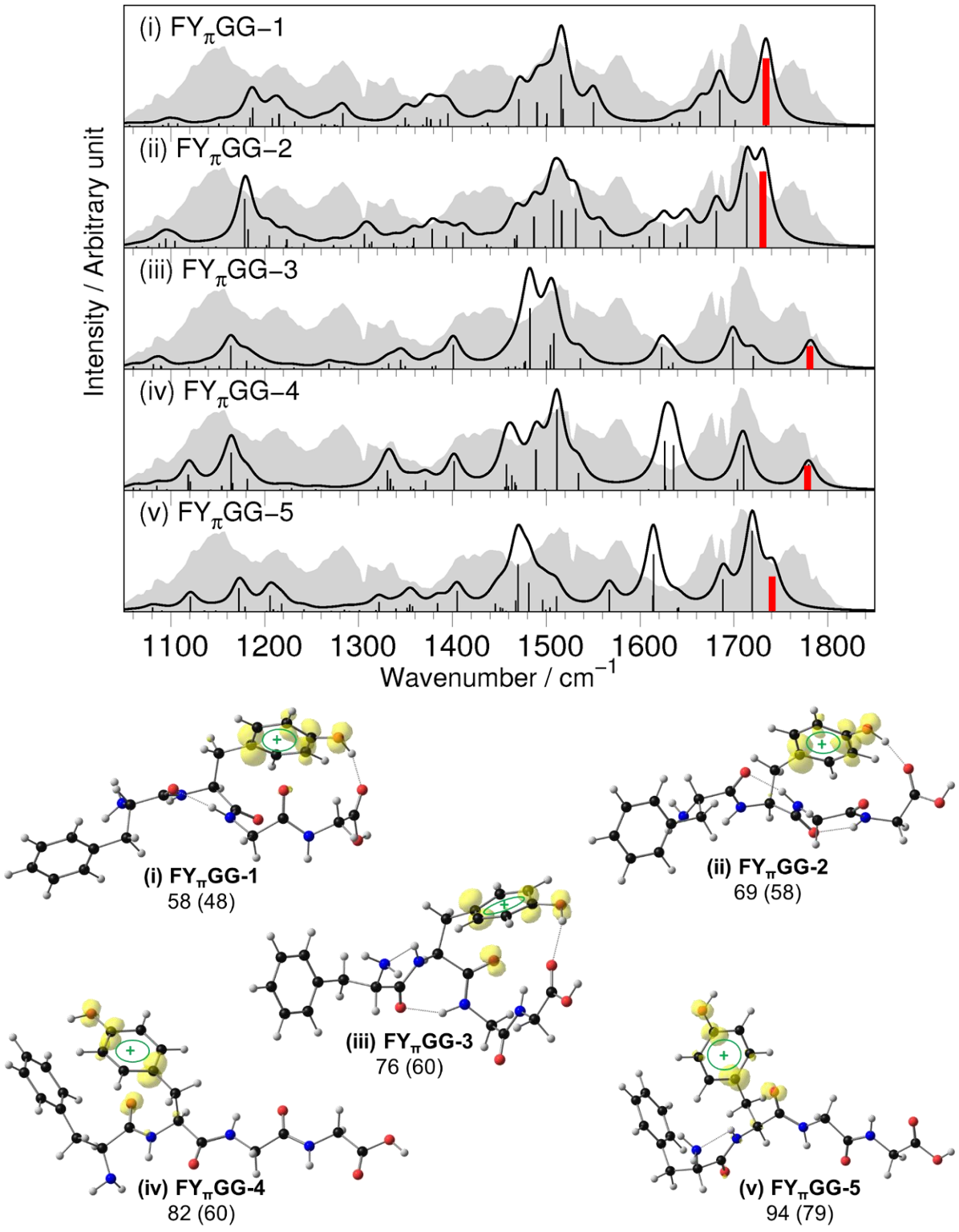


Figure S4. Theoretical IR spectra of $[FY_{\pi}^{\bullet}GG]^{+}$ (black curves and lines) obtained from harmonic vibration analyses including a frequency scaling factor of 0.982 for geometries optimized at the UB3LYP/6-311++G(d,p) level. The theoretical line spectra were arbitrarily broadened using Gaussian profiles of FWHM = 10 cm^{-1} by using GaussView 5.0. Thick red lines highlight the C=O stretches of COOH. Experimental IRMPD spectrum of $[FYGG]^{\bullet+}$ is shown as shaded grey color.

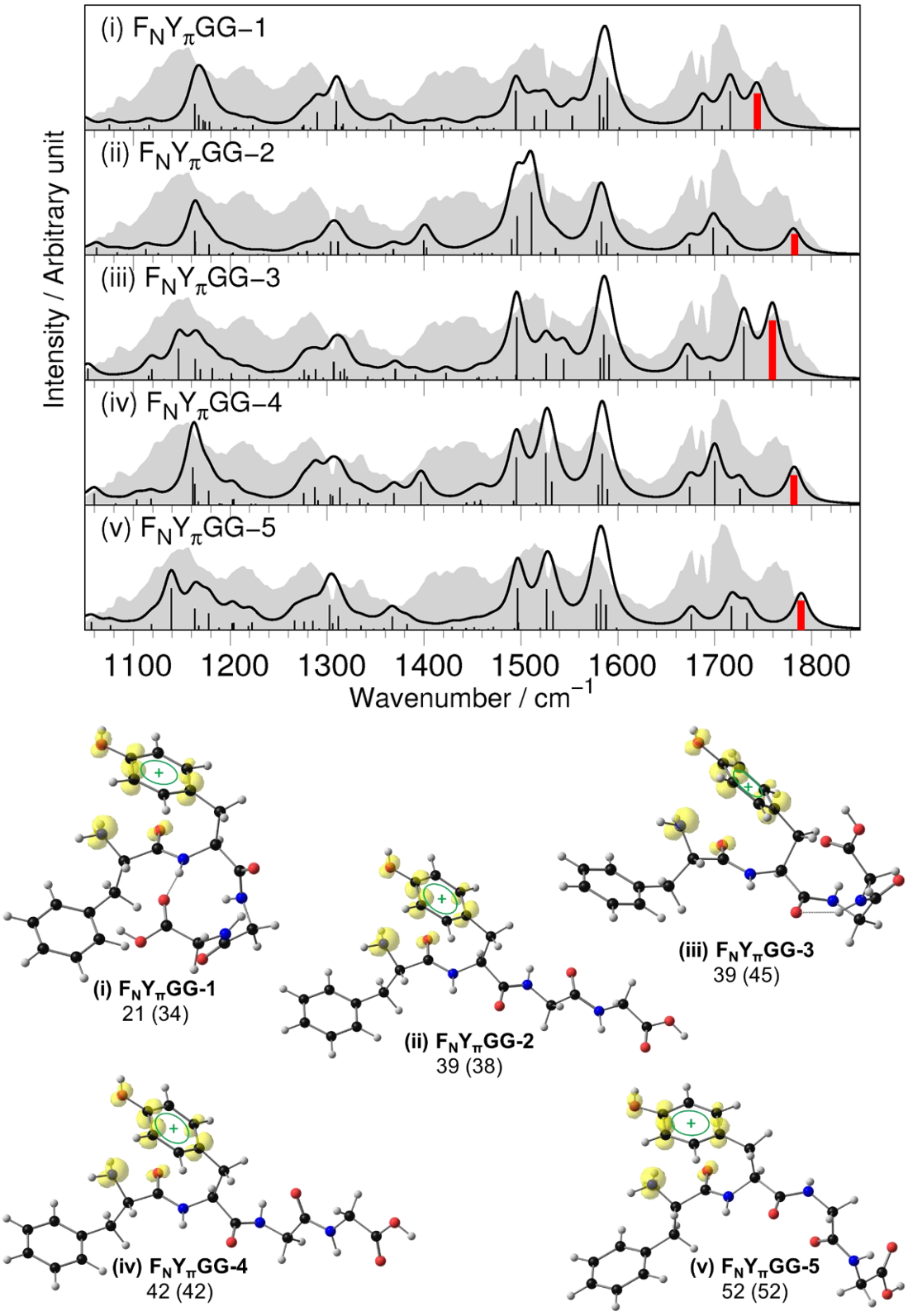


Figure S5. Theoretical IR spectra of $[F_NY_\pi^{\bullet}GG]^+$ (black curves and lines) obtained from harmonic vibration analyses including a frequency scaling factor of 0.982 for geometries optimized at the UB3LYP/6-311++G(d,p) level. The theoretical line spectra were arbitrarily broadened using Gaussian profiles of FWHM = 10 cm^{-1} by using GaussView 5.0. Thick red lines highlight the C=O stretches of COOH. Experimental IRMPD spectrum of $[FYGG]^{\bullet+}$ is shown as shaded grey color.

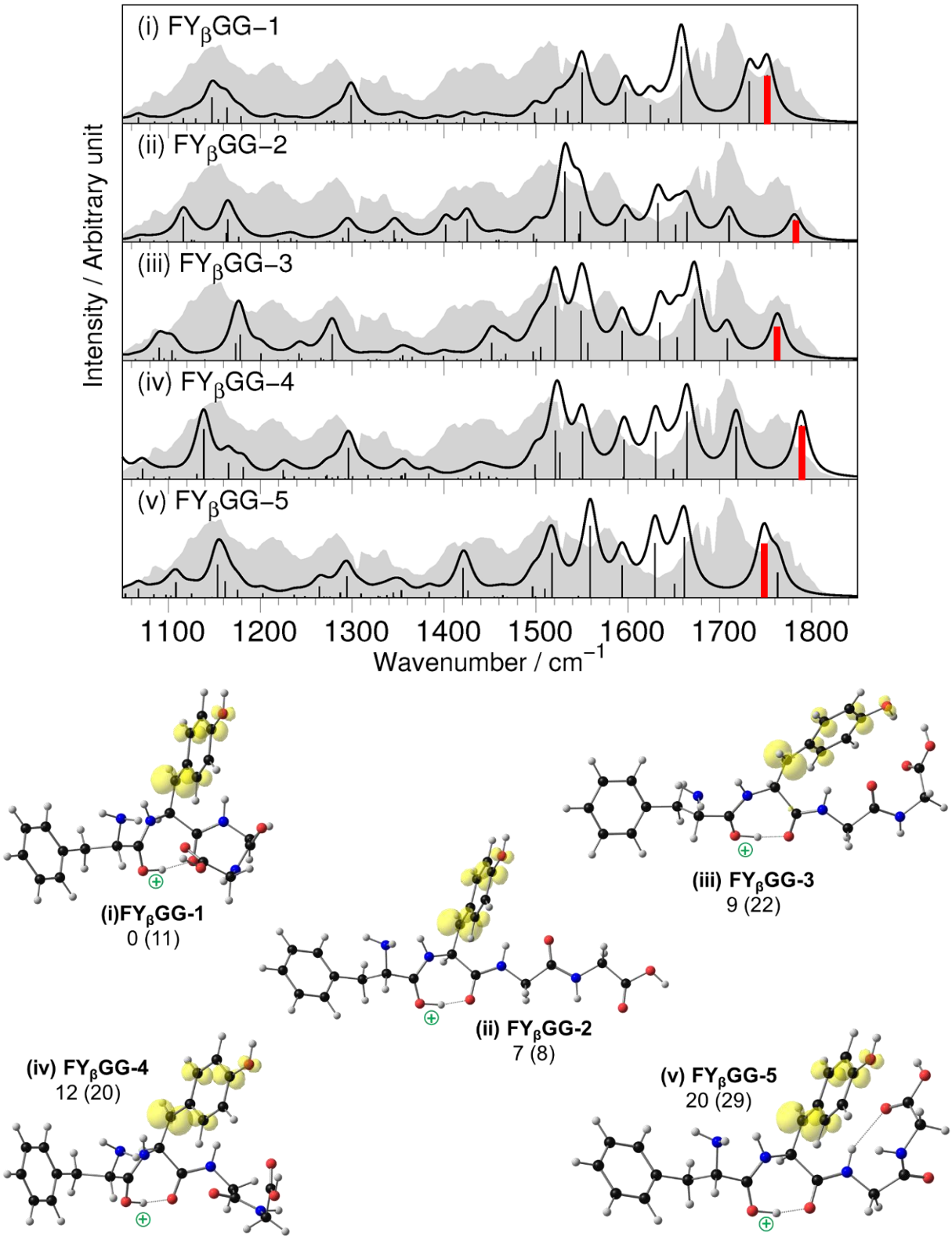


Figure S6. Theoretical IR spectra of $[FY_{\beta}^{\bullet}GG]^{+}$ (black curves and lines) obtained from harmonic vibration analyses including a frequency scaling factor of 0.982 for geometries optimized at the UB3LYP/6-311++G(d,p) level. The theoretical line spectra were arbitrarily broadened using Gaussian profiles of FWHM = 10 cm^{-1} by using GaussView 5.0. Thick red lines highlight the C=O stretches of COOH. Experimental IRMPD spectrum of $[FYGG]^{\bullet+}$ is shown as shaded grey color.

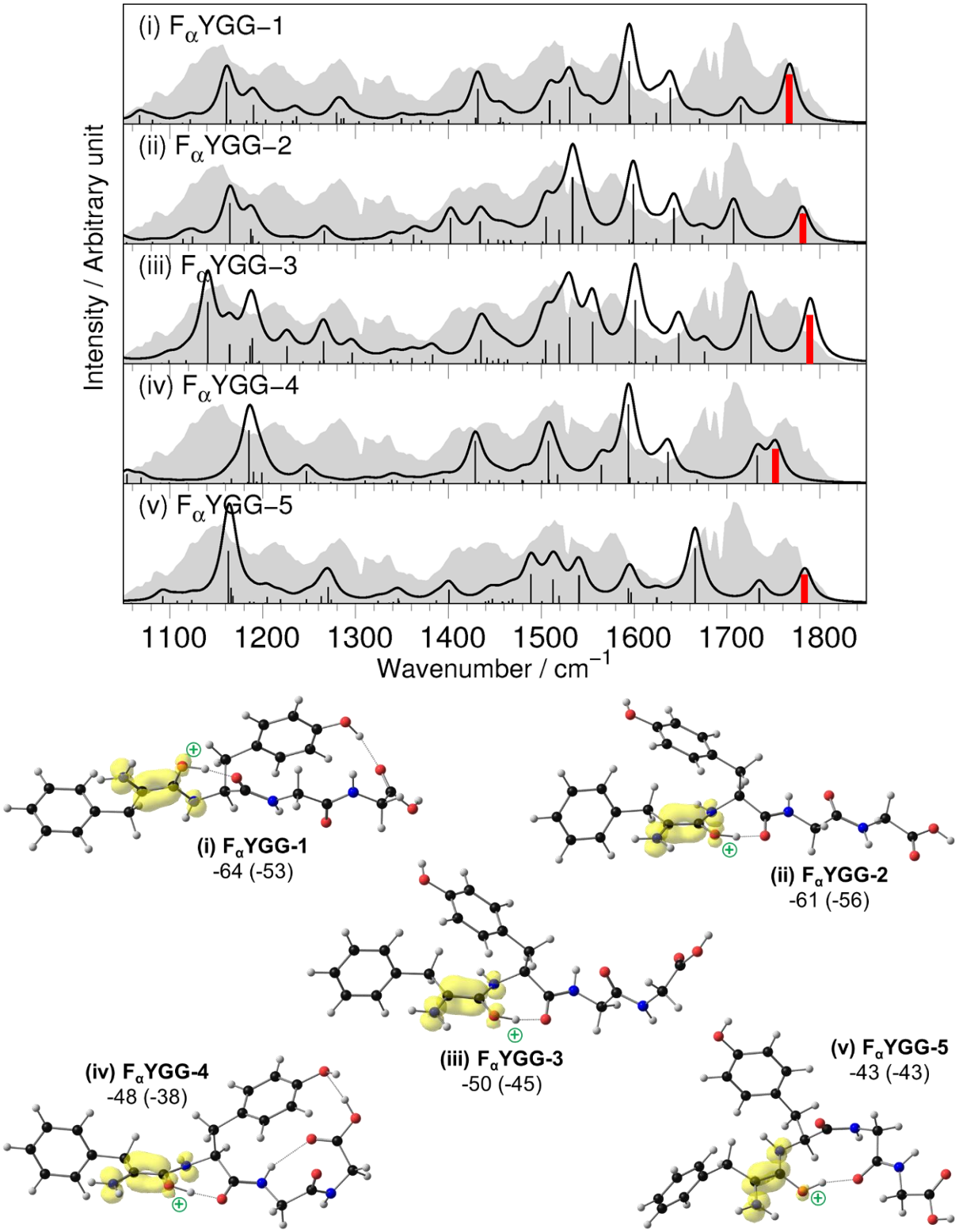


Figure S7. Theoretical IR spectra of $[F_{\alpha}^{\bullet}YGG]^{+}$ (black curves and lines) obtained from harmonic vibration analyses including a frequency scaling factor of 0.982 for geometries optimized at the UB3LYP/6-311++G(d,p) level. The theoretical line spectra were arbitrarily broadened using Gaussian profiles of FWHM = 10 cm^{-1} by using GaussView 5.0. Thick red lines highlight the C=O stretches of COOH. Experimental IRMPD spectrum of $[FYGG]^{\bullet+}$ is shown as shaded grey color.

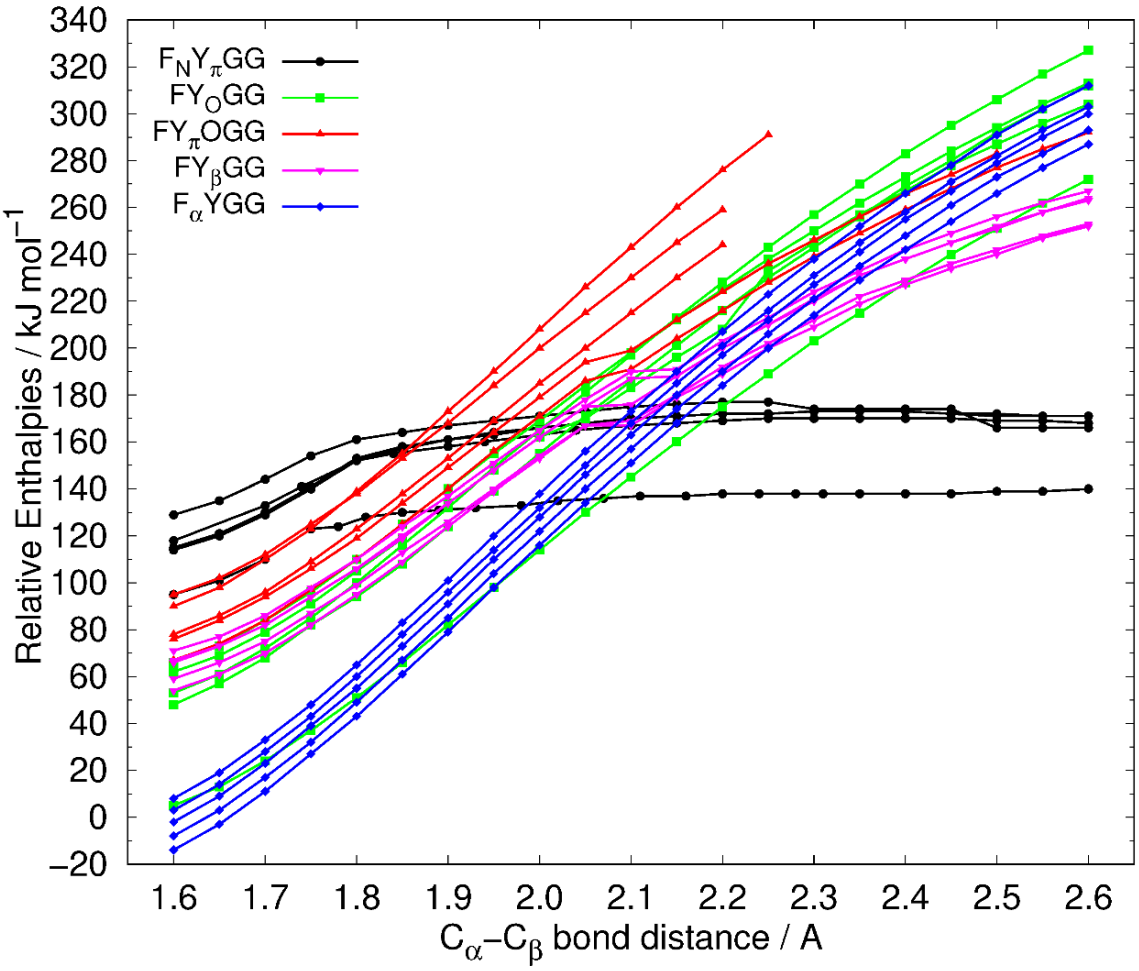


Figure S8. Potential energy surface scans along the C_α–C_β bond of the N-terminal Phe residue of different geometries of $[FYGG]^{\bullet+}$ at the UM06-2X/6-311++G(d,p) level of theory (without zero-point energy correction). The energy of all structures are generally increasing with the C_α–C_β distance monotonically. Only for the π-radical structures featuring the n→π^+ interaction $F_NY_\pi GG$'s, plateaus are observed beyond 2.2 Å.

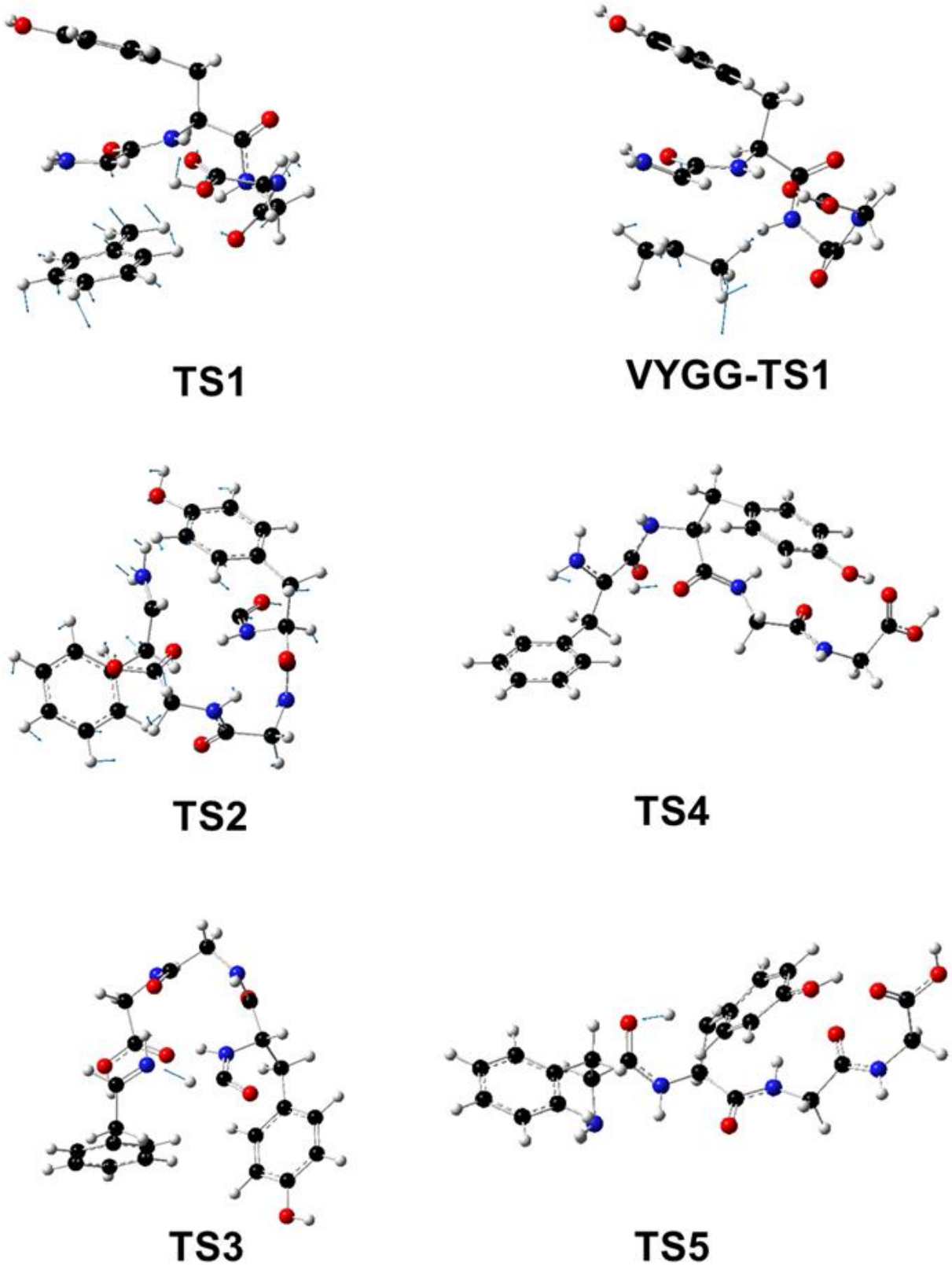


Figure S9. Optimized geometries of **TS1** – **TS5** of **FYGG** and **VYGG-TS1** with displacement vectors of respective imaginary normal mode evaluated at the UM06-2X/6-311++G(d,p) level of theory. Animated gif files of these TS are also available in SI.

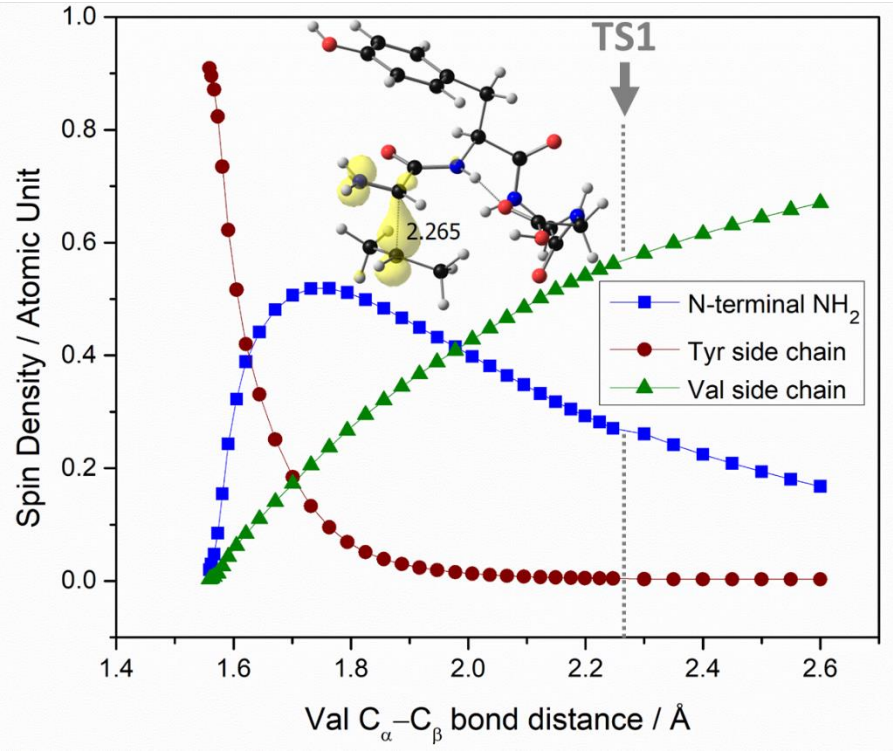


Figure S10. Spin densities on the N-terminal NH_2, Tyr side chain and Val side chain of $V_NY_\pi GG$-1 at different C_α–C_β bond lengths of the Val residue. Geometrical optimizations were calculated at the M06-2X/6-311++G(d,p) level of theory.. The spin densities were evaluated from the difference in natural populations between alpha and beta electrons.

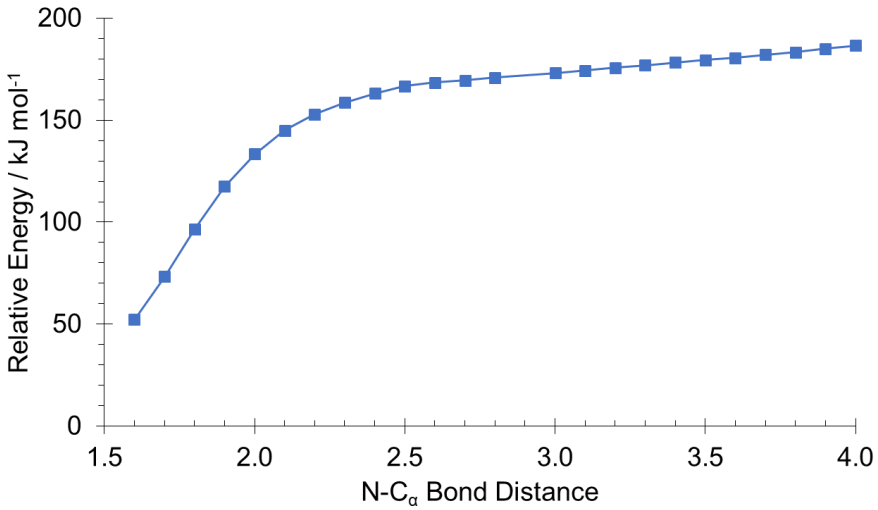
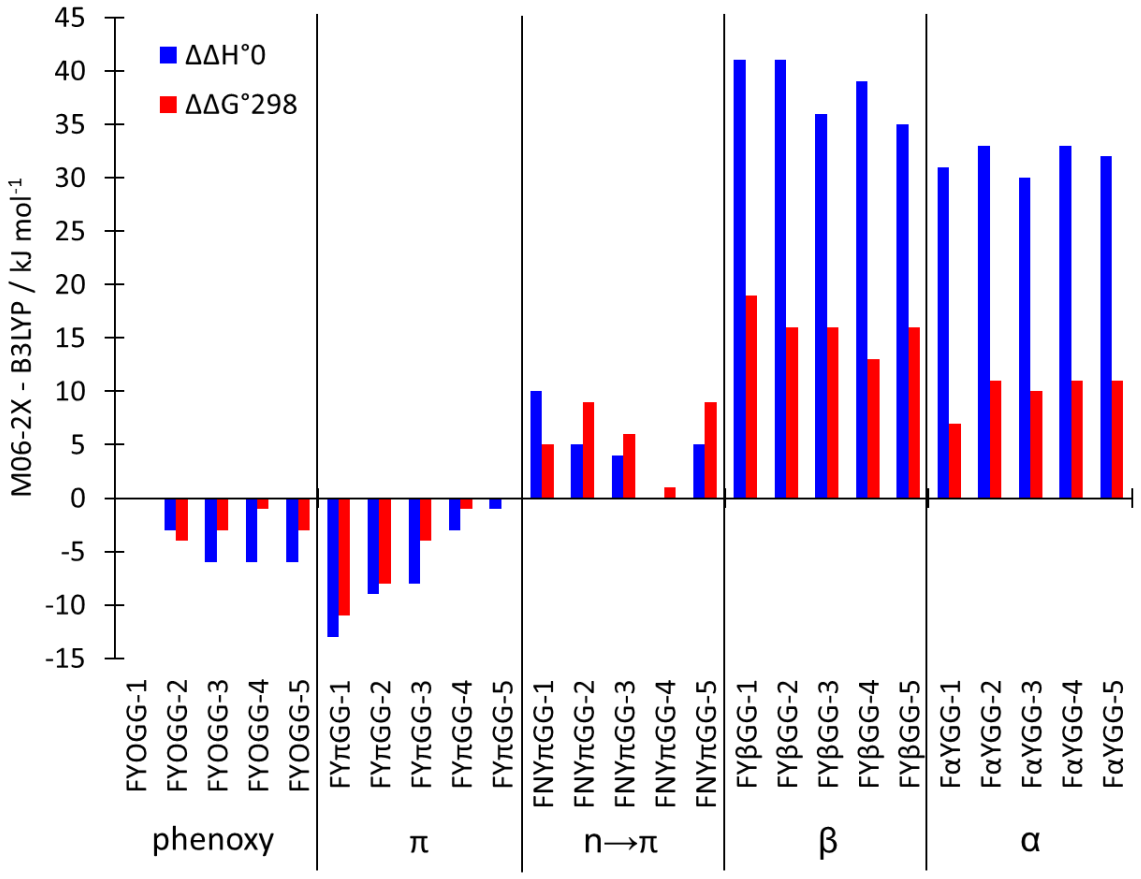


Figure S11 Potential energy surface scan along the N–C_α bond of the Tyr residue of the β-radical **FYβGG-1** at the UM06-2X/6-311++G(d,p) level of theory (without zero-point energy correction). The energy increases rapidly with N–C_α distance to higher than 170 kJ mol^{-1} (without zero-point correction) and reaches a flat plateau beyond 2.5 Å, then further increases gradually even up to 4 Å.

Table S1. Comparison of relative energies (kJ mol^{-1}) calculated with B3LYP and UM06-2X.

	B3LYP/6-311++G(d,p)				UM06-2X/6-311++G(d,p)			
	ΔE	$\Delta H°_0$	$\Delta H°_{298}$	$\Delta G°_{298}$	ΔE	$\Delta H°_0$	$\Delta H°_{298}$	$\Delta G°_{298}$
FY_OGG-1	0	0	0	0	0	0	0	0
FY_OGG-2	47	42	45	30	43	39	41	26
FY_OGG-3	65	59	63	42	58	53	56	39
FY_OGG-4	70	60	65	34	62	54	58	33
FY_OGG-5	77	70	74	52	69	64	67	49
$FY_\pi GG$-1	78	71	74	59	64	58	61	48
$FY_\pi GG$-2	84	78	80	66	73	69	71	58
$FY_\pi GG$-3	97	84	90	64	86	76	81	60
$FY_\pi GG$-4	98	85	91	61	92	82	87	60
$FY_\pi GG$-5	105	95	99	79	101	94	97	79
$F_NY_\pi GG$-1	89	80	84	69	97	90	93	74
$F_NY_\pi GG$-2	114	99	105	73	116	104	109	82
$F_NY_\pi GG$-3	110	99	104	79	112	103	108	85
$F_NY_\pi GG$-4	115	102	108	76	112	102	107	77
$F_NY_\pi GG$-5	124	111	117	86	126	116	121	95
$FY_\beta GG$-1	-1	0	-2	11	51	41	44	30
$FY_\beta GG$-2	14	7	7	8	64	48	52	24
$FY_\beta GG$-3	12	9	7	22	57	45	47	38
$FY_\beta GG$-4	13	12	10	20	63	51	55	33
$FY_\beta GG$-5	23	20	18	29	68	55	57	45
$F_\alpha YGG$-1	-64	-64	-66	-53	-22	-33	-30	-46
$F_\alpha YGG$-2	-59	-61	-61	-56	-17	-28	-24	-45
$F_\alpha YGG$-3	-50	-50	-51	-45	-11	-20	-16	-35
$F_\alpha YGG$-4	-48	-48	-49	-38	-6	-15	-12	-27
$F_\alpha YGG$-5	-41	-43	-42	-43	-1	-11	-6	-32



Cartesian coordinates, harmonic vibration analyses (frequency in cm^{-1}, IR intensity in km mol^{-1}) and energies (E, E_{zpc}, H_{298}, G_{298} in au) of the optimized geometries discussed in main text.

FY_OGG-1

N	-1.330703	-1.829664	0.355168
C	-1.393777	-1.582999	-1.124767
C	0.038532	-1.737505	-1.661753
O	0.428149	-2.832323	-2.021829
H	-0.806956	-1.062201	0.824271
H	-1.962200	-2.408751	-1.553793
C	-2.096477	-0.246377	-1.379123
C	-3.439573	-0.204440	-0.686418
H	-1.486746	0.583126	-1.011270
C	-5.877800	-0.206195	0.676852
C	-4.495449	-1.004924	-1.129750
C	-3.615890	0.594810	0.444568
C	-4.832838	0.595351	1.122428
C	-5.709132	-1.004522	-0.451771
H	-4.376894	-1.615266	-2.020336
H	-2.804225	1.234945	0.779976
H	-4.965556	1.228754	1.991094
H	-6.526437	-1.618844	-0.809369
H	-6.825766	-0.202578	1.200586
N	0.794405	-0.619339	-1.655927
C	2.222999	-0.620903	-1.980173
C	2.966075	-1.025029	-0.693883
O	3.604034	-0.232505	-0.026137
H	0.456793	0.173872	-1.122644
H	2.378867	-1.385904	-2.743706
C	2.674196	0.760719	-2.521124
C	1.987874	1.887012	-1.799046
H	2.430950	0.801697	-3.584327
H	3.757230	0.824918	-2.406962
C	0.302082	3.331417	-0.075450
C	2.505774	2.410562	-0.587810
C	0.715837	2.324127	-2.251566
C	-0.108419	3.050611	-1.437406
C	1.703327	3.131212	0.248474
H	3.521026	2.165125	-0.305532
H	0.375365	2.011794	-3.233719
H	-1.111081	3.339807	-1.730407
H	2.058873	3.502676	1.202930
O	-0.536892	3.633052	0.798063
H	-0.827438	-2.690093	0.606399
H	-2.280243	-1.851397	0.741492
H	-2.201029	-0.129260	-2.460993
N	2.759219	-2.311063	-0.316297
H	2.170594	-2.899115	-0.896010
C	2.971258	-2.688757	1.071998
C	1.857560	-2.040384	1.893715
H	2.888456	-3.769373	1.165584
H	3.961950	-2.367982	1.393434
O	0.729913	-2.520257	1.930036
N	2.182581	-0.881374	2.500172
H	3.073783	-0.466791	2.258342
C	1.209591	-0.073719	3.198823
C	0.438884	0.850468	2.262694
H	0.486291	-0.736025	3.681903
H	1.700677	0.520002	3.967138
O	0.032214	0.494422	1.164498
O	0.256408	2.036894	2.769588
H	-0.183196	2.669468	2.133261

20.9, 0.2; 29.8, 0.4; 34.9, 0.2; 49.1, 0.1; 61.7, 0.7; 73.7, 1.5; 85.8, 1.8; 92.8, 3.7; 97.4, 4.5; 102.3, 2.9; 110.7, 12.9; 118.6, 8.2; 130.9, 9.4; 138.4, 2.5; 145.9, 11.1; 148.7, 4.3; 161.9, 7.5; 187.9, 9.9; 204.4, 12.6; 229.1, 40.6; 240.2, 7.5; 262.4, 2.7; 271.4, 21.9; 281.7, 17.8; 303.1, 2.6; 311.4, 12.3; 325.1, 14.1; 328.0, 7.6; 334.5, 13.0; 348.4, 27.6; 365.4, 3.3; 371.7, 9.1; 380.4, 5.3; 387.4, 14.5; 406.8, 11.9; 412.8, 0.1; 467.6, 15.0; 475.2, 6.9; 483.8, 9.0; 498.5, 27.0; 517.5, 16.5; 543.6, 12.6; 558.9, 48.9; 571.6, 60.0; 580.9, 21.4; 587.4, 54.0; 606.3, 44.0; 616.9, 41.5; 630.8, 2.6; 634.5, 72.9; 650.7, 24.8; 662.0, 38.3; 703.8, 47.9; 724.4, 25.6; 747.8, 2.6; 758.2, 18.3; 765.9, 28.7; 778.1, 8.3; 785.8, 21.5; 794.2, 0.7; 801.1, 11.3; 813.8, 5.7; 833.3, 5.3; 844.7, 3.2; 857.3, 2.5; 875.6, 16.5; 881.1, 7.9; 886.6, 61.0; 903.7, 11.1; 925.2, 22.8; 942.8, 18.9; 955.7, 5.4; 964.4, 12.0; 972.9, 169.3; 980.1, 12.0; 991.3, 0.9; 1000.3, 3.0; 1009.9, 6.9; 1012.5, 17.5; 1014.7, 0.6; 1017.9, 3.2; 1033.9, 5.2; 1036.7, 0.1; 1061.3, 2.0; 1061.7, 1.2; 1072.5, 4.6; 1090.9, 3.9; 1101.7, 1.9; 1115.2, 17.0; 1126.2, 3.3; 1133.8, 18.0; 1148.2, 3.3; 1164.6, 60.4; 1175.2, 0.9; 1185.4, 1.6; 1208.0, 16.4; 1209.0, 0.9; 1233.4, 11.3; 1236.7, 4.0; 1248.8, 16.5; 1265.6, 46.1; 1269.7, 3.9; 1288.0, 81.2; 1293.1, 6.8; 1294.7, 4.7; 1307.0, 3.2; 1313.9, 93.2; 1333.2, 15.9; 1334.1, 9.5; 1339.6, 6.6; 1351.0, 7.8; 1359.9, 1.1; 1372.2, 8.0; 1372.9, 42.3; 1383.3, 5.1; 1395.9, 3.0; 1397.3, 10.2; 1412.4, 1.8; 1447.9, 12.8; 1452.1, 5.8; 1462.8, 26.6; 1475.7, 1.5; 1483.8, 14.0; 1485.1, 6.3; 1486.1, 73.8; 1499.1, 15.7; 1534.8, 5.9; 1539.0, 14.6; 1549.8, 87.4; 1570.2, 166.6; 1579.8, 84.6; 1587.5, 194.7; 1597.5, 230.7; 1622.7, 54.9; 1632.0, 140.1; 1656.1, 16.0; 1664.2, 79.1; 1674.7, 2.8; 1748.6, 290.2; 1775.9, 261.5; 1789.1, 264.3; 1796.5, 547.4; 3078.3, 4.5; 3095.4, 3.6; 3097.9, 15.0; 3115.4, 0.9; 3120.5, 3.3; 3124.7, 4.7; 3134.0, 835.9; 3141.0, 92.9; 3152.7, 0.5; 3173.5, 6.9; 3179.1, 0.3; 3185.8, 69.2; 3186.4, 49.1; 3187.3, 403.4; 3195.9, 1.1; 3214.0, 0.5; 3214.7, 0.0; 3222.4, 1.5; 3223.6, 0.7; 3233.9, 1.1; 3239.5, 1.6; 3410.7, 79.6; 3477.7, 208.8; 3573.0, 102.7; 3595.7, 111.1; 3621.2, 77.2;

-1524.023214270 -1523.544303 -1523.514612 -1523.604177

$FY_\pi GG$-1

N	-4.233769	-1.271485	1.424565
C	-3.831439	-0.932279	0.063886
C	-2.315489	-0.991405	-0.094443
O	-1.792238	-0.987239	-1.203648
H	-4.368523	-2.271389	1.529293
H	-4.240247	-1.607739	-0.696280
C	-4.264240	0.506553	-0.287038
C	-5.764446	0.659920	-0.261792
H	-3.804549	1.192274	0.432137
C	-8.555333	0.859453	-0.186315
C	-6.543063	0.117092	-1.286627
C	-6.401336	1.306087	0.797326
C	-7.790247	1.405908	0.836545
C	-7.928052	0.216500	-1.250933
H	-6.058427	-0.377307	-2.123216
H	-5.806342	1.745667	1.592219
H	-8.271078	1.914911	1.663263
H	-8.520004	-0.202235	-2.055966
H	-9.635220	0.939002	-0.160099
N	-1.619728	-0.989566	1.065083
C	-0.172889	-1.027061	1.180147
C	0.543076	0.266096	0.741348
O	1.321011	0.817218	1.502988
H	-2.198174	-0.971140	1.900037
H	0.046694	-1.086170	2.245806
C	0.400584	-2.284951	0.466670
C	1.877552	-2.243183	0.237224
H	-0.108876	-2.419961	-0.487161
C	4.534405	-1.745721	-0.382936
C	2.413369	-2.679473	-1.005938
C	2.759610	-1.740452	1.236767
C	4.060986	-1.483092	0.941473
C	3.721324	-2.465566	-1.313616
H	1.747903	-3.129838	-1.732847
H	2.373057	-1.495678	2.217845
H	4.736521	-1.044033	1.664636
H	4.147256	-2.719663	-2.275881
O	5.694985	-1.337661	-0.793679
H	-5.122197	-0.833079	1.648788

H	-3.870274	0.740970	-1.278208
N	0.324037	0.711263	-0.512492
H	-0.307249	0.198118	-1.122702
C	1.087266	1.840980	-0.975854
C	2.581917	1.517905	-0.993651
H	0.778702	2.085172	-1.993528
H	0.907304	2.711434	-0.339101
O	2.999497	0.384675	-1.130879
N	3.419178	2.584599	-0.901711
H	3.059673	3.481477	-0.611402
C	4.848687	2.363142	-0.893822
C	5.340430	1.901354	0.468830
H	5.102538	1.601259	-1.628673
H	5.360978	3.293844	-1.142449
O	5.952256	0.877080	0.684199
O	5.030921	2.764274	1.420790
H	5.345306	2.437360	2.276798
H	6.049757	-0.626861	-0.206611
H	0.159969	-3.153704	1.093502

15.5, 0.1; 20.4, 0.4; 24.4, 1.0; 30.8, 0.4; 45.6, 0.7; 47.7, 2.0; 64.6, 2.8; 67.1, 1.3; 73.2, 0.7; 85.2, 0.8; 100.1, 4.4; 102.7, 3.9; 119.7, 3.8; 120.6, 3.4; 132.1, 1.4; 160.7, 9.9; 169.9, 11.5; 177.0, 1.4; 187.7, 14.9; 188.9, 5.6; 208.0, 2.6; 255.3, 4.7; 260.8, 1.1; 270.1, 2.3; 282.8, 7.6; 289.5, 3.3; 291.9, 38.0; 299.3, 10.3; 346.1, 1.4; 353.9, 6.6; 371.2, 42.3; 375.0, 2.1; 399.1, 23.1; 410.3, 0.4; 413.8, 0.3; 427.1, 7.0; 446.0, 107.2; 451.2, 3.4; 462.4, 8.5; 490.8, 5.7; 503.4, 28.6; 529.5, 23.3; 533.7, 14.9; 556.1, 5.3; 579.1, 59.9; 590.6, 11.7; 599.1, 25.9; 607.9, 3.5; 632.3, 0.0; 640.1, 75.7; 646.5, 47.0; 664.0, 100.5; 692.8, 18.7; 705.1, 22.9; 715.7, 8.2; 721.5, 50.8; 733.1, 16.7; 759.5, 4.0; 761.6, 75.8; 762.8, 66.0; 776.9, 40.9; 793.3, 11.2; 821.6, 42.5; 826.2, 27.0; 847.4, 74.6; 859.7, 14.6; 861.6, 39.9; 875.2, 1.3; 879.2, 22.5; 888.6, 9.7; 907.0, 3.3; 911.2, 41.3; 919.0, 5.3; 944.8, 26.1; 955.3, 14.7; 972.9, 31.3; 992.6, 32.5; 996.1, 0.6; 1006.7, 3.5; 1008.8, 1.1; 1010.1, 17.1; 1018.8, 1.1; 1029.0, 0.0; 1034.2, 14.2; 1054.1, 9.5; 1061.9, 4.4; 1062.8, 10.6; 1105.1, 12.3; 1107.9, 12.9; 1131.3, 10.0; 1146.9, 6.6; 1152.7, 5.4; 1160.8, 19.4; 1174.3, 9.0; 1184.8, 4.0; 1194.1, 0.9; 1201.5, 2.5; 1206.0, 0.1; 1229.6, 152.1; 1238.6, 1.4; 1243.2, 11.2; 1246.7, 90.5; 1258.7, 56.8; 1260.9, 17.9; 1293.9, 23.1; 1298.0, 1.4; 1299.4, 7.2; 1306.8, 6.0; 1308.9, 1.6; 1330.1, 7.8; 1337.2, 17.6; 1337.7, 9.8; 1355.4, 1.5; 1372.0, 37.0; 1379.6, 13.3; 1381.2, 5.1; 1385.2, 7.9; 1410.1, 13.1; 1414.6, 29.3; 1425.1, 101.3; 1434.0, 14.5; 1439.7, 91.8; 1464.1, 16.6; 1465.0, 13.8; 1470.3, 16.0; 1489.0, 2.8; 1497.7, 7.6; 1522.4, 123.2; 1540.1, 16.1; 1547.6, 26.6; 1551.6, 208.6; 1560.2, 602.9; 1572.2, 238.6; 1590.9, 247.1; 1658.7, 2.3; 1669.6, 40.4; 1678.1, 5.8; 1709.3, 17.9; 1749.2, 161.2; 1770.6, 324.2; 1791.3, 53.9; 1827.9, 633.0; 3039.2, 13.0; 3056.5, 4.5; 3069.5, 14.9; 3081.7, 12.4; 3111.4, 3.1; 3127.3, 3.2; 3131.7, 4.6; 3144.0, 0.9; 3149.7, 0.9; 3176.9, 0.7; 3186.1, 5.0; 3186.6, 4.5; 3210.2, 0.3; 3218.7, 6.5; 3219.0, 0.1; 3229.3, 0.3; 3230.5, 5.1; 3241.1, 9.0; 3242.4, 1.3; 3415.4,1112.1; 3511.3, 393.7; 3536.9, 64.7; 3553.5, 169.9; 3611.6, 34.9; 3663.6, 75.8; 3808.9, 137.2;

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F_NY_πGG-1

C	-2.931080	0.757936	1.325333
O	-3.954231	1.228304	0.867978
N	-2.882947	-0.389890	2.040978
H	-1.970986	-0.778238	2.237347
C	-4.003733	-1.323357	1.989333
C	-3.898674	-2.025397	0.638602
H	-3.898948	-2.056750	2.785021
H	-4.933679	-0.769152	2.109288
O	-3.201204	-3.004148	0.474806
N	-4.539198	-1.395628	-0.388185
H	-4.893330	-0.462876	-0.216885
C	-4.185332	-1.771487	-1.727330
C	-2.756822	-1.389110	-2.077333
H	-4.279900	-2.850192	-1.859882
H	-4.849720	-1.288360	-2.446044
O	-2.045441	-0.645652	-1.439868
O	-2.380039	-1.958506	-3.216226
H	-1.472523	-1.697488	-3.423721
N	2.924545	0.727777	0.039321
C	1.796550	-0.120112	0.396496
C	0.756614	0.783595	1.043444
O	1.087433	1.738468	1.721949
H	3.244855	1.223025	0.868458
H	1.383441	-0.548655	-0.523890
C	2.133702	-1.280531	1.367961
C	3.158682	-2.207506	0.768037
H	2.502351	-0.847331	2.302461
C	5.063959	-3.862819	-0.441903
C	2.768386	-3.193530	-0.140534
C	4.514270	-2.064401	1.065799
C	5.463055	-2.886947	0.464446
C	3.713221	-4.017346	-0.741156
H	1.713981	-3.330485	-0.362990
H	4.827799	-1.317192	1.788421
H	6.511364	-2.772283	0.712675
H	3.395940	-4.787732	-1.433685
H	5.800041	-4.508910	-0.904335
N	-0.553177	0.463677	0.823092
C	-1.574692	1.447227	1.119101
H	-0.775301	-0.191705	0.078275
H	-1.282241	1.950113	2.044033
C	-1.742219	2.511516	-0.016187
C	-0.412305	3.017482	-0.440251
H	-2.384749	3.305958	0.366363
H	-2.250563	2.023041	-0.849382
C	2.239782	3.677500	-0.966873
C	0.290565	2.340040	-1.457232
C	0.226519	4.093550	0.254769
C	1.522756	4.427678	-0.002803
C	1.604925	2.628779	-1.706500
H	-0.210908	1.545144	-1.998001
H	-0.331131	4.624028	1.018154
H	2.016492	5.229212	0.535080
H	2.194174	2.108061	-2.449252
O	3.497223	3.908590	-1.260756
H	3.872951	4.631296	-0.738973
H	3.693040	0.162626	-0.312611
H	1.214280	-1.829700	1.593240

11.8, 1.3; 15.2, 1.2; 18.9, 2.7; 33.0, 0.5; 35.9, 2.1; 38.9, 0.7; 51.5, 5.8; 62.6, 1.3; 69.0, 1.6; 78.8, 1.6; 80.2, 1.4; 87.7, 2.6; 99.1, 2.5; 106.0, 2.4; 123.7, 11.8; 129.9, 10.8; 136.2, 10.7; 166.6, 2.2; 178.4, 5.9; 184.5, 7.0; 246.2, 12.9; 254.2, 1.7; 260.9, 3.1; 285.1, 5.9; 303.8, 2.9; 310.6, 17.2; 324.4, 2.4; 331.0, 7.1; 346.3, 3.5; 351.5, 2.8; 372.8, 4.9; 383.8, 2.8; 397.0, 5.9; 405.3, 13.7; 415.0, 1.4; 432.1, 16.6; 437.5, 28.1; 472.8, 6.6; 482.4, 14.6; 486.7, 36.6; 502.1, 8.5; 510.5, 32.7; 519.6, 18.7; 559.2, 37.5; 569.3, 71.3; 572.8, 97.4; 581.6, 97.1; 582.7, 33.0; 613.2, 1.9; 626.4, 154.0; 632.0, 0.6; 657.7, 46.2; 674.4, 15.6; 704.0, 14.3; 720.1, 18.0; 722.4, 34.4; 726.1, 25.4; 742.7, 10.1; 755.3, 14.5; 775.3, 30.3; 785.7, 39.0; 799.8, 30.8; 808.3, 9.9; 811.9, 8.0; 847.4, 5.9; 853.3, 14.3; 863.0, 6.1; 874.9, 0.8; 883.0, 19.1; 885.1, 7.7; 891.2, 18.0; 901.6, 4.5; 906.9, 5.3; 931.3, 1.6; 952.4, 5.1; 973.8, 21.1; 994.6, 13.7; 1002.1, 23.5; 1002.9, 40.1; 1008.9, 0.1; 1012.7, 13.8; 1018.5, 2.5; 1029.2, 12.7; 1030.7, 0.7; 1040.3, 14.7; 1062.0, 2.3; 1064.7, 7.9; 1091.7, 14.1; 1109.6, 4.3; 1115.0, 46.2; 1134.6, 11.0; 1140.4, 45.2; 1165.0, 12.2; 1169.5, 1.6; 1181.0, 13.1; 1186.7, 49.0; 1191.4, 74.3; 1199.1, 39.8; 1204.9, 180.1; 1206.3, 35.5; 1216.3, 12.7; 1237.3, 0.2; 1239.1, 5.2; 1245.6, 20.5; 1264.4, 5.5; 1287.8, 72.7; 1295.0, 142.4; 1300.6, 13.0; 1312.3, 7.2; 1316.6, 40.1; 1332.7, 4.2; 1334.0, 9.0; 1336.2, 11.9; 1347.7, 24.3; 1350.5, 11.6; 1362.0, 8.4; 1365.6, 11.5; 1381.1, 4.9; 1405.2, 172.0; 1409.1, 21.8; 1442.7, 42.3; 1446.5, 18.2; 1457.9, 61.7; 1484.1, 17.0; 1485.1, 4.2; 1488.7, 4.7; 1496.3, 7.8; 1503.4, 43.0; 1523.3, 222.9; 1539.8, 17.4; 1541.2, 87.7; 1546.9, 679.4; 1560.6, 26.6; 1574.5, 253.5; 1626.2, 48.1; 1658.1, 2.3; 1677.2, 12.3; 1683.4, 148.0; 1783.1, 227.8; 1791.0, 162.2; 1810.8, 445.5; 1828.2, 414.3; 3058.4, 8.1; 3064.9, 10.0; 3095.8, 1.4; 3106.6, 4.9; 3109.2, 10.0; 3116.2, 6.5; 3126.3, 4.7; 3155.3, 1.1; 3156.2, 0.2; 3181.9, 6.3; 3186.2, 6.3; 3193.5, 0.0; 3208.8, 0.6; 3210.2, 1.8; 3210.9, 0.2; 3219.7, 5.4; 3222.1, 3.2; 230.9, 3.7; 3250.3, 3.7; 3508.5, 63.3;

3565.0, 230.3; 3596.2, 41.3; 3613.2, 84.6; 3640.7, 61.1; 3820.2, 346.2; 3834.7, 79.9;

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FY$_\beta$GG-1

N	-1.896875	0.888476	0.390411
C	-2.257586	-0.265001	-0.413220
C	-1.079092	-0.640662	-1.275857
O	-1.092619	-1.795037	-1.831587
H	-1.369683	0.604693	1.210095
H	-2.490262	-1.162548	0.171686
C	-3.457587	0.047913	-1.334833
C	-4.691939	0.349855	-0.521468
H	-3.199216	0.905781	-1.962641
C	-6.930240	0.903002	1.060291
C	-5.391252	-0.685406	0.102314
C	-5.128265	1.662932	-0.347817
C	-6.243085	1.939333	0.440154
C	-6.504158	-0.411717	0.887451
H	-5.072155	-1.713452	-0.041956
H	-4.604022	2.473635	-0.844720
H	-6.577351	2.962659	0.560814
H	-7.046088	-1.223565	1.357369
H	-7.800976	1.115611	1.668283
N	-0.130494	0.242808	-1.427053
C	1.068867	0.202093	-2.299467
C	1.872266	-1.067231	-1.948514
O	1.326189	-2.175797	-2.065781
H	-0.293035	1.090157	-0.873938
H	0.726409	0.047871	-3.327455
C	1.798652	1.503317	-2.201900
C	2.215985	2.087360	-0.986806
H	1.961398	2.040779	-3.126541
C	3.127800	3.334500	1.375076
C	2.097255	1.450988	0.286386
C	2.814868	3.378667	-1.008892
C	3.255993	3.989717	0.141023
C	2.550234	2.058410	1.433330
H	1.673412	0.455698	0.376714
H	2.920457	3.889327	-1.959471
H	3.706658	4.975622	0.096444
H	2.489254	1.557903	2.391569
O	3.541796	3.870963	2.534687
H	-2.724930	1.391407	0.693223
H	-3.626776	-0.812403	-1.986372
N	3.123830	-0.940025	-1.531277
H	3.491084	-0.007028	-1.389504
C	3.805256	-2.068050	-0.902136
C	3.186201	-2.237805	0.488525
H	3.695157	-2.951414	-1.529920
H	4.858161	-1.821155	-0.789274
O	3.460260	-1.481146	1.394612
N	2.275328	-3.240198	0.605737
H	1.921590	-3.663941	-0.240033
C	1.510550	-3.338772	1.817733
C	0.489290	-2.223857	1.968321
H	0.981034	-4.292088	1.854980
H	2.173946	-3.295387	2.683404
O	0.203986	-1.403627	1.129432
O	-0.080650	-2.283125	3.168223
H	-0.732310	-1.574527	3.258238
H	3.936477	4.738217	2.397413
H	-0.132500	-2.064646	-2.107994

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F$_\alpha$YGG-1

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O	0.050079	-0.310598	1.857330
H	-0.185884	-0.738803	-1.366480
C	-0.374630	1.342451	-0.766797
C	1.055209	1.775272	-0.570945
H	-0.732288	1.526827	-1.782646
H	-1.024716	1.884692	-0.076497
C	3.767176	2.057870	0.077922
C	2.046819	1.419503	-1.485554
C	1.445248	2.342165	0.643784
C	2.784843	2.499738	0.965297
C	3.393493	1.548204	-1.170776
H	1.769959	1.001638	-2.450077
H	0.689338	2.636234	1.365066
H	3.091444	2.935189	1.908799
H	4.157450	1.240821	-1.875039
O	5.053252	2.142331	0.475626
H	5.610420	1.623942	-0.126765
N	1.557132	-1.083423	0.378757
H	1.809316	-1.273011	-0.586582
C	2.675616	-1.117553	1.300349
C	3.918928	-1.429343	0.471351
H	2.757737	-0.157708	1.817247
H	2.547283	-1.907223	2.046408
O	3.828336	-1.922569	-0.635881
N	5.110116	-1.194967	1.068672
H	5.161019	-0.622560	1.897636
C	6.317034	-1.663516	0.433384
C	6.685226	-0.887414	-0.819091
H	7.152076	-1.581158	1.131315
H	6.212938	-2.713754	0.156683
O	6.318535	0.226907	-1.091601
O	7.515529	-1.590560	-1.577737
H	7.768610	-1.058074	-2.345961
N	-4.875885	0.324230	1.556251
C	-4.145191	-0.117774	0.527545
C	-2.741101	-0.057310	0.662341
O	-2.252050	0.503371	1.732230
H	-5.885482	0.330775	1.498689
C	-4.816966	-0.677196	-0.703835
C	-6.318202	-0.508848	-0.688531
H	-4.398712	-0.180597	-1.586336
C	-9.085279	-0.155907	-0.575786
C	-7.135717	-1.513438	-0.170537
C	-6.896663	0.675228	-1.147843
C	-8.275022	0.850495	-1.093171
C	-8.515123	-1.337854	-0.115005

H	-6.694034	-2.439295	0.184267
H	-6.267462	1.460436	-1.555116
H	-8.716233	1.769264	-1.459653
H	-9.142719	-2.126485	0.281565
H	-10.159228	-0.021156	-0.537742
N	-1.918342	-0.587035	-0.276871
H	-2.359566	-1.081291	-1.037732
H	-4.415544	0.690893	2.378464
H	-4.571698	-1.743271	-0.786504
H	-1.246796	0.214849	1.888547

11.5, 0.2; 19.3, 0.1; 25.8, 0.1; 36.4, 2.6; 41.1, 0.6; 45.0, 3.2; 52.9, 1.2; 62.6, 2.1; 71.4, 1.6; 73.7, 3.8; 83.7, 1.0; 103.7, 2.4; 107.7, 7.8; 110.6, 2.9; 140.4, 5.6; 142.0, 3.3; 153.0, 7.8; 171.5, 31.8; 175.2, 3.1; 203.6, 2.4; 235.6, 0.9; 258.5, 5.0; 267.8, 5.6; 275.9, 12.6; 312.6, 20.6; 321.5, 20.2; 332.0, 6.1; 337.2, 20.5; 344.2, 0.6; 360.5, 5.9; 386.2, 125.4; 387.8, 6.0; 405.0, 16.9; 411.1, 0.4; 422.7, 2.5; 430.7, 73.2; 439.7, 10.9; 450.9, 11.1; 459.5, 25.3; 462.8, 148.9; 491.0, 13.6; 503.5, 38.0; 510.6, 2.5; 535.5, 56.0; 557.0, 58.4; 576.3, 25.6; 580.6, 21.2; 597.9, 11.6; 605.1, 6.5; 626.0, 136.1; 631.7, 0.1; 644.0, 120.6; 653.5, 1.2; 659.7, 51.7; 665.3, 100.5; 686.3, 26.3; 698.4, 48.7; 717.9, 24.4; 727.6, 15.4; 736.8, 14.6; 741.6, 7.8; 773.2, 34.7; 790.5, 6.2; 817.6, 21.3; 850.7, 4.5; 852.4, 12.3; 861.3, 35.8; 873.7, 4.5; 877.2, 0.0; 884.2, 9.2; 890.1, 7.4; 900.4, 43.2; 935.9, 1.1; 945.9, 32.8; 956.6, 5.9; 972.6, 2.3; 980.5, 4.8; 993.9, 2.7; 1004.2, 5.5; 1008.3, 4.8; 1012.1, 0.0; 1019.6, 4.5; 1030.8, 0.4; 1035.6, 0.0; 1039.8, 12.4; 1060.3, 38.3; 1061.5, 3.0; 1096.2, 9.0; 1114.2, 5.3; 1124.8, 34.8; 1134.2, 3.2; 1144.2, 97.2; 1165.5, 25.0; 1183.7, 0.1; 1188.2, 53.1; 1196.2, 8.9; 1207.9, 1.8; 1208.2, 3.3; 1216.4, 382.9; 1223.2, 136.5; 1236.3, 7.7; 1240.9, 52.0; 1245.8, 15.0; 1255.7, 41.9; 1266.3, 27.6; 1286.4, 3.6; 1312.6, 1.4; 1319.1, 43.0; 1325.4, 2.5; 1330.2, 232.9; 1334.8, 1.0; 1339.3, 21.9; 1347.2, 3.8; 1354.8, 3.9; 1360.0, 0.2; 1382.1, 14.9; 1392.2, 40.2; 1414.7, 18.0; 1425.9, 6.9; 1449.4, 45.4; 1466.3, 539.7; 1468.4, 48.6; 1482.8, 150.7; 1487.7, 124.6; 1490.3, 11.9; 1495.5, 12.3; 1497.6, 7.6; 1515.2, 15.0; 1541.0, 27.8; 1563.6, 11.6; 1570.9, 484.8; 1581.4, 130.6; 1624.3, 134.4; 1630.6, 971.3; 1658.3, 19.3; 1659.5, 2.0; 1677.0, 2.7; 1687.1, 84.9; 1700.8, 651.1; 1736.4, 23.8; 1800.0, 204.9; 1860.7, 510.5; 2206.9,2895.1; 3038.2, 8.8; 3075.8, 11.6; 3080.6, 2.0; 3081.8, 15.4; 3103.8, 4.1; 3119.5, 3.7; 3122.8, 0.2; 3139.0, 3.3; 3154.7, 1.0; 3176.3, 5.3; 3191.2, 3.3; 3192.2, 3.5; 3193.4, 3.0; 3215.0, 0.2; 3222.6, 0.5; 3223.8, 2.4; 3224.9, 0.3; 3233.9, 1.5; 3570.5, 154.1; 3575.5, 192.4; 3659.5, 53.9; 3665.8, 68.3; 3702.4, 190.1; 3728.9, 716.1; 3816.8, 139.0;

-1524.031729810 -1523.556865 -1523.525961 -1523.621660

FY_OGG-2

N	-0.079137	1.348404	-0.137118
C	-0.557496	1.138620	1.274664
C	0.361454	0.017503	1.781684
O	1.533714	0.260926	1.990635
H	-0.055292	0.445683	-0.639796
H	-0.314319	2.048496	1.824210
C	-2.066349	0.885457	1.269472
C	-2.811479	2.019376	0.600667
H	-2.296018	-0.038404	0.726651
C	-4.108567	4.130220	-0.688287
C	-2.840940	3.289691	1.182074
C	-3.439815	1.815140	-0.628853
C	-4.087962	2.868521	-1.270388
C	-3.487168	4.339418	0.540744
H	-2.376448	3.455928	2.149660
H	-3.453040	0.825145	-1.077444
H	-4.583387	2.695492	-2.217851
H	-3.515269	5.318240	1.003726
H	-4.616569	4.948173	-1.184093
N	-0.149662	-1.237133	1.791745
C	0.730771	-2.337578	1.429315
C	1.538576	-1.885672	0.196113
O	1.049919	-1.145357	-0.647645
H	-1.114846	-1.342373	1.512696
H	1.418469	-2.551627	2.250487
C	-0.103761	-3.612179	1.122106
C	-1.295410	-3.311170	0.250744
H	-0.433621	-4.033478	2.073658
H	0.556279	-4.341783	0.646320
C	-3.450986	-2.301570	-1.293709
C	-1.149298	-3.138177	-1.143698
C	-2.554663	-3.081532	0.851039
C	-3.609585	-2.597932	0.118400
C	-2.182448	-2.657411	-1.902670
H	-0.196333	-3.364303	-1.608861
H	-2.676779	-3.281392	1.911838
H	-4.578604	-2.400910	0.562141
H	-2.085598	-2.499893	-2.970378
O	-4.352053	-1.745263	-1.943252
H	0.901730	1.710572	-0.176228
H	-0.702080	2.003931	-0.621156
H	-2.392727	0.755157	2.305380
N	2.803235	-2.328122	0.102839
H	3.198785	-2.881239	0.848761
C	3.651455	-1.871326	-0.986316
C	4.080264	-0.404272	-0.901648
H	4.558216	-2.475839	-1.006682
H	3.136124	-1.994933	-1.938100
O	4.582474	0.131476	-1.863606
N	3.943632	0.226307	0.296641
H	3.323655	-0.126619	1.011530
C	4.408062	1.583478	0.398260
C	3.562972	2.565347	-0.391135
H	4.377954	1.898610	1.443665
H	5.435237	1.662098	0.041913
O	2.373867	2.458432	-0.603166
O	4.267095	3.608612	-0.787648
H	3.692108	4.224763	-1.264808

15.6, 0.6; 19.0, 2.9; 28.1, 0.3; 30.0, 0.5; 35.4, 2.2; 41.1, 0.5; 50.7, 4.4; 57.6, 1.7; 64.8, 2.1; 69.8, 7.1; 88.4, 1.1; 95.9, 0.8; 103.4, 1.5; 117.9, 1.0; 140.2, 7.4; 152.8, 1.6; 161.5, 15.0; 173.1, 4.7; 194.4, 7.8; 200.3, 27.6; 234.3, 0.8; 247.1, 22.2; 269.1, 25.3; 286.4, 8.2; 294.7, 3.4; 308.8, 8.8; 325.9, 1.9; 341.0, 12.1; 346.2, 19.0; 347.9, 2.6; 368.0, 18.0; 384.2, 2.0; 393.6, 24.9; 396.4, 32.7; 412.9, 0.3; 433.8, 13.0; 455.4, 40.0; 457.6, 2.9; 472.3, 60.8; 475.9, 22.9; 496.6, 2.7; 522.3, 17.0; 524.5, 9.3; 534.0, 123.6; 553.4, 24.3; 577.0, 6.2; 597.2, 29.3; 609.5, 9.1; 613.7, 55.0; 622.4, 8.7; 630.1, 0.1; 651.8, 54.2; 685.0, 26.0; 689.8, 16.0; 711.7, 2.9; 725.2, 32.5; 729.7, 27.7; 744.0, 8.0; 769.1, 10.7; 777.5, 14.5; 786.1, 22.4; 815.3, 2.3; 819.0, 1.3; 824.7, 9.6; 846.6, 4.3; 865.1, 2.8; 873.2, 20.4; 881.1, 1.9; 881.8, 11.0; 888.6, 42.6; 906.4, 28.5; 954.2, 7.1; 957.4, 1.6; 962.3, 3.6; 979.5, 4.0; 991.7, 2.3; 997.2, 0.9; 1010.1, 0.7; 1015.2, 0.4; 1017.6, 3.1; 1021.1, 18.3; 1038.4, 0.0; 1052.7, 2.4; 1058.1, 9.8; 1060.5, 3.4; 1066.2, 7.4; 1098.5, 7.5; 1101.7, 1.0; 1120.1, 5.5; 1130.0, 13.6; 1145.5, 4.6; 1160.8, 29.1; 1165.0, 67.5; 1167.0, 2.6; 1184.5, 2.0; 1210.5, 1.8; 1212.2, 10.2; 1227.5, 255.1; 1230.5, 11.2; 1236.8, 2.3; 1253.6, 22.6; 1257.4, 16.8; 1267.0, 3.0; 1278.6, 18.0; 1284.5, 4.6; 1299.4, 3.6; 1301.3, 8.0; 1319.5, 24.2; 1324.1, 24.4; 1331.4, 9.8; 1345.9, 14.2; 1349.4, 32.4; 1359.6, 2.0; 1368.7, 14.0; 1373.7, 14.3; 1388.6, 7.5; 1399.9, 7.7; 1406.0, 4.7; 1443.0, 7.8; 1448.5, 4.3; 1452.1, 25.9; 1461.0, 29.2; 1472.1, 105.8; 1482.6, 8.7; 1489.5, 13.1; 1500.6, 28.9; 1502.1, 21.0; 1538.4, 10.8; 1539.1, 15.4; 1552.5, 39.5; 1558.0, 67.3; 1563.9, 441.8; 1578.1, 314.8; 1620.5, 40.0; 1626.9, 173.4; 1657.5, 4.0; 1670.4, 66.4; 1674.6, 4.6; 1760.5, 220.3; 1801.3, 425.6; 1813.2, 441.6; 1823.6, 470.8; 3054.1, 10.1; 3076.2,1213.4; 3084.0, 2.6; 3103.1, 8.7; 3104.8, 13.8; 3109.1, 0.4; 3119.2, 3.5; 3136.4, 1.6; 3138.0, 1.5; 3159.3, 1.1; 3173.5, 0.3; 3175.8, 0.1; 3185.2, 2.9; 3185.4, 1.4; 3206.4, 2.5; 3215.5, 0.3; 3223.6, 0.7; 3224.8, 0.9; 3228.6, 0.3; 3234.5, 1.0; 3327.8, 182.9; 3455.9, 218.5; 3629.6, 169.3; 3645.2, 182.1; 3654.9, 91.5; 3814.8, 128.6;

-1524.006711370 -1523.529616 -1523.498914 -1523.594253

FY_OGG-3

N	1.239738	1.993025	1.745832
C	-0.097155	1.330561	1.657840
C	0.163659	-0.150451	1.926938
O	1.300015	-0.535924	2.150823
H	1.674897	1.829477	2.655413

H	-0.736910	1.766916	2.429193
C	-0.677847	1.586661	0.253535
C	-0.701676	3.066581	-0.048023
H	-0.079359	1.035646	-0.477002
C	-0.669477	5.821730	-0.513377
C	-1.671680	3.891854	0.525626
C	0.284996	3.633916	-0.856926
C	0.299429	5.007570	-1.088966
C	-1.657573	5.262076	0.292541
H	-2.457000	3.458421	1.138301
H	1.030869	2.993287	-1.318219
H	1.059414	5.438333	-1.729543
H	-2.423296	5.891684	0.728952
H	-0.663341	6.888397	-0.700700
N	-0.904535	-0.970139	1.851334
C	-0.651250	-2.359844	1.495996
C	0.237260	-2.345936	0.237016
O	0.181358	-1.433488	-0.563762
H	-1.755017	-0.576244	1.465953
H	-0.112238	-2.842079	2.314470
C	-1.982402	-3.109528	1.256555
C	-2.898627	-2.375168	0.313570
H	-2.471070	-3.244059	2.223750
H	-1.743211	-4.101538	0.865199
C	-4.497802	-0.809791	-1.433160
C	-2.720104	-2.464865	-1.083352
C	-3.908398	-1.535315	0.834701
C	-4.689392	-0.771126	0.004619
C	-3.486163	-1.718624	-1.938745
H	-1.958132	-3.128901	-1.477920
H	-4.071728	-1.512143	1.908594
H	-5.474586	-0.126718	0.382062
H	-3.361673	-1.768330	-3.013729
O	-5.170504	-0.094676	-2.193239
H	1.143941	2.997503	1.564773
H	1.879433	1.586123	1.017529
H	-1.689242	1.172294	0.215131
N	1.096407	-3.379740	0.092333
H	1.173023	-4.085983	0.808329
C	2.017279	-3.373921	-1.029241
C	3.058156	-2.254912	-0.993106
H	2.554994	-4.321993	-1.054299
H	1.474312	-3.261047	-1.967432
O	3.668343	-1.956350	-1.994244
N	3.325425	-1.677275	0.215129
H	2.654545	-1.713381	0.969844
C	4.357126	-0.672349	0.252936
C	3.957425	0.608352	-0.462937
H	4.566217	-0.415829	1.293538
H	5.266228	-1.053305	-0.210415
O	2.914509	1.208685	-0.273379
O	4.885981	1.045043	-1.285577
H	4.587381	1.861219	-1.713373

16.0, 1.8; 18.3, 0.3; 23.9, 0.7; 31.9, 0.9; 35.9, 1.9; 51.4, 6.8; 56.6, 2.3; 57.2, 3.0; 61.3, 0.7; 66.7, 2.3; 78.4, 1.3; 86.3, 1.0; 95.2, 2.5; 106.7, 2.2; 111.6, 10.8; 147.8, 1.1; 160.5, 8.6; 166.4, 8.6; 194.3, 9.3; 201.2, 46.0; 224.5, 4.7; 259.3, 9.4; 267.6, 14.2; 282.3, 2.4; 290.8, 7.2; 314.6, 3.1; 317.9, 15.0; 330.9, 5.1; 353.5, 13.1; 355.6, 4.5; 363.9, 7.6; 383.0, 1.6; 391.3, 41.4; 408.6, 48.7; 413.1, 1.1; 430.1, 22.8; 439.5, 2.9; 447.8, 20.8; 458.1, 7.3; 475.9, 3.6; 496.1, 2.0; 506.5, 6.5; 511.0, 103.3; 552.3, 12.5; 554.8, 73.8; 586.9, 5.5; 602.8, 38.1; 611.3, 12.4; 614.2, 81.4; 623.7, 7.0; 631.1, 0.2; 657.5, 54.2; 686.7, 8.7; 691.8, 12.3; 706.3, 13.0; 723.5, 42.9; 737.7, 1.3; 755.2, 28.2; 759.3, 36.2; 765.4, 2.4; 783.4, 36.6; 817.1, 0.4; 818.8, 0.1; 823.8, 6.4; 855.8, 3.3; 867.9, 4.6; 872.5, 20.7; 879.1, 7.3; 880.9, 3.4; 888.5, 28.3; 914.9, 24.0; 949.1, 4.6; 956.6, 7.9; 963.2, 5.1; 971.1, 14.3; 991.9, 1.5; 997.1, 0.5; 1005.6, 0.2; 1014.6, 0.3; 1018.1, 2.2; 1025.3, 22.9; 1036.3, 0.0; 1053.0, 10.7; 1059.7, 6.9; 1061.8, 1.7; 1081.2, 1.7; 1094.0, 0.4; 1101.7, 20.0; 1119.0, 2.3; 1125.2, 8.3; 1140.8, 20.0; 1153.0, 15.1; 1157.6, 15.4; 1166.0, 1.8; 1185.1, 0.8; 1208.1, 0.8; 1216.8, 11.6; 1229.4, 182.2; 1232.0, 51.0; 1236.9, 1.2; 1242.1, 35.8; 1260.0, 9.1; 1266.7, 8.6; 1272.2, 17.5; 1284.6, 5.5; 1291.9, 10.0; 1297.2, 9.4; 1317.9, 42.5; 1323.0, 14.9; 1334.0, 11.3; 1339.4, 30.8; 1358.0, 1.2; 1359.9, 31.7; 1369.4, 18.3; 1373.2, 8.2; 1389.4, 2.8; 1391.3, 7.6; 1412.7, 16.7; 1442.1, 6.8; 1448.5, 3.8; 1461.3, 37.2; 1463.4, 7.4; 1472.7, 104.2; 1476.8, 3.7; 1489.7, 15.2; 1495.6, 11.9; 1496.5, 10.2; 1538.5, 55.4; 1541.5, 15.2; 1543.6, 76.3; 1549.2, 178.6; 1561.3, 273.5; 1569.9, 454.7; 1623.2, 71.4; 1632.3, 38.5; 1657.7, 4.7; 1670.8, 24.5; 1674.5, 0.8; 1777.7, 247.0; 1789.3, 710.9; 1800.0, 361.2; 1817.1, 253.0; 2987.9, 996.2; 3077.4, 2.2; 3082.8, 3.8; 3104.0, 5.2; 3104.4, 1.2; 3106.2, 9.1; 3114.2, 3.1; 3131.8, 4.8; 3134.3, 2.3; 3166.5, 0.7; 3168.3, 0.3; 3181.2, 2.8; 3183.0, 4.6; 3190.1, 0.2; 3198.2, 3.7; 3214.7, 0.0; 3223.5, 1.8; 3224.8, 0.1; 3231.1, 0.2; 3233.6, 1.2; 3447.4, 94.0; 3534.2, 113.5; 3591.3, 135.8; 3638.8, 163.0; 3662.1, 81.1; 3812.2, 111.6;

-1524.001018170 -1523.524146 -1523.493274 -1523.589228

FY_OGG-4

N	-4.222712	0.377797	-0.844316
C	-3.141796	-0.337851	-0.089464
C	-1.829297	0.330146	-0.528165
O	-1.828443	0.986085	-1.556491
H	-3.837077	0.616666	-1.771404
H	-3.330477	-0.189940	0.974829
C	-3.161549	-1.833807	-0.451782
C	-4.527188	-2.435791	-0.222709
H	-2.860405	-1.947307	-1.497793
C	-7.107159	-3.421899	0.207470
C	-4.985051	-2.675577	1.075238
C	-5.373604	-2.698195	-1.301777
C	-6.660037	-3.189781	-1.087329
C	-6.266337	-3.168262	1.288931
H	-4.329456	-2.495458	1.922188
H	-5.017640	-2.546616	-2.316998
H	-7.304064	-3.400164	-1.932388
H	-6.607783	-3.362690	2.298297
H	-8.104256	-3.809423	0.375891
N	-0.759961	0.129538	0.254628
C	0.510943	0.794595	0.019966
C	1.597403	-0.150161	0.544380
O	1.321159	-0.972547	1.401959
H	-0.777726	-0.501660	1.049896
H	0.604683	0.975115	-1.052164
C	0.629842	2.155899	0.794553
C	-0.667759	2.894779	0.702414
H	1.456643	2.722084	0.360875
H	0.870016	1.939024	1.838947
C	-3.352133	3.374133	0.071703
C	-1.677521	2.595182	1.655198
C	-0.988275	3.692577	-0.418945
C	-2.293167	3.970781	-0.721273
C	-2.987695	2.839318	1.372726
H	-1.394041	2.099718	2.578427
H	-0.195569	4.001733	-1.091677
H	-2.577666	4.498363	-1.623415
H	-3.790456	2.572213	2.051864
O	-4.499996	3.200441	-0.384807
H	-4.498511	1.287687	-0.426957
H	-5.051706	-0.220797	-0.938252
H	-2.404190	-2.333121	0.157601
N	2.825961	0.048071	0.054542
H	3.024656	0.713053	-0.686652
C	3.965462	-0.711487	0.517199
C	5.183889	-0.211615	-0.255673
H	4.112358	-0.571921	1.591864
H	3.816501	-1.780498	0.339874
O	5.080228	0.669954	-1.090259
N	6.347354	-0.809178	0.050431
H	6.408998	-1.544561	0.744189
C	7.573689	-0.434161	-0.614485
C	8.691716	-1.291916	-0.071948
H	7.501084	-0.577562	-1.696070
H	7.813809	0.619336	-0.446628
O	8.545974	-2.134237	0.770143
O	9.854934	-0.992788	-0.647590
H	10.540683	-1.563574	-0.272339

7.8, 0.0; 19.8, 0.1; 21.0, 0.0; 32.0, 0.2; 33.2, 0.6; 37.3, 0.1; 51.9, 0.8; 54.3, 1.1; 57.4, 1.5; 68.8, 0.5; 82.0, 0.4; 84.3, 7.7; 92.8, 1.2; 96.5, 1.6; 112.7, 6.3; 124.7, 2.8; 137.1, 2.7; 148.1, 16.5; 175.1, 7.8; 182.4, 12.4; 191.3, 29.9; 203.8, 6.2; 217.8, 35.2; 256.9, 19.9; 274.4, 2.6; 281.7, 25.2; 302.5, 16.7; 327.6, 6.7; 339.9, 0.9; 345.7, 10.9; 347.7, 12.9; 367.9, 5.8; 372.1, 28.9; 406.1, 27.8; 413.2, 2.6; 435.8, 17.3; 440.4, 21.2; 465.2, 5.0; 496.3, 16.6; 501.5, 12.3; 502.8, 81.0; 534.3, 1.4; 535.0, 10.1; 552.2, 41.2; 570.9, 72.8; 582.7, 14.0; 595.4, 4.8; 608.2, 67.5; 612.0, 2.6; 630.6, 0.1; 632.3, 7.1; 638.0, 70.2; 664.1, 131.9; 684.3, 11.4; 709.0, 1.7; 725.1, 26.9; 729.1, 19.8; 746.0, 1.3; 755.9, 3.8; 776.9, 29.9; 785.0, 16.4; 788.5, 0.2; 821.9, 14.2; 836.1, 19.9; 862.8, 4.3; 867.1, 6.4; 876.6, 15.4; 880.5, 3.9; 897.5, 12.6; 903.4, 7.3; 943.2, 9.0; 956.1, 5.3; 973.1, 38.2; 986.6, 1.7; 995.5, 16.7; 1000.6, 2.9; 1004.8, 23.7; 1009.1, 5.6; 1013.3, 4.3; 1014.9, 0.4; 1017.8, 3.9; 1024.7, 2.6; 1032.6, 108.8; 1039.0, 0.0; 1060.7, 1.1; 1067.6, 0.7; 1083.0, 8.8; 1103.0, 27.4; 1117.4, 25.9; 1120.1, 8.6; 1137.4, 12.6; 1150.2, 42.3; 1168.5, 8.4; 1171.9, 32.6; 1186.7, 0.4; 1208.0, 0.1; 1210.1, 98.7; 1215.3, 174.0; 1231.6, 2.1; 1233.4, 2.9; 1238.8, 9.0; 1249.1, 0.5; 1250.7, 12.6; 1252.9, 1.1; 1259.6, 1.7; 1268.0, 9.4; 1284.8, 4.3; 1297.5, 11.2; 1307.3, 1.1; 1323.1, 15.5; 1325.5, 0.6; 1334.4, 0.2; 1354.0, 11.0; 1355.4, 2.2; 1372.8, 14.1; 1382.5, 10.1; 1394.2, 0.5; 1417.3, 18.8; 1446.8, 21.7; 1450.5, 11.0; 1460.4, 359.1; 1484.1, 6.5; 1493.3, 26.5; 1493.8, 9.3; 1497.5, 11.0; 1503.2, 6.5; 1511.2, 182.9; 1532.1, 6.6; 1539.0, 14.1; 1559.5, 908.1; 1573.2, 644.4; 1581.9, 94.2; 1594.0, 16.9; 1623.3, 79.6; 1628.0, 44.7; 1657.1, 5.5; 1669.8, 54.3; 1673.9, 0.5; 1779.7, 481.3; 1786.4, 96.4; 1797.9, 249.0; 1879.0, 306.0; 3072.5, 4.5; 3073.3, 19.4; 3078.0, 4.7; 3082.8, 12.5; 3111.6, 1.1; 3118.1, 0.2; 3120.2, 0.2; 3122.2, 2.9; 3133.8, 0.8; 3140.2, 3.3; 3182.5, 2.9; 3183.2, 4.7; 3191.0, 1.7; 3204.8, 2.0; 3212.1, 6.9; 3214.7, 0.1; 3223.5, 57.9; 3223.7, 444.7; 3230.8, 2.0; 3233.6, 0.4; 3358.5, 66.4; 3438.7, 337.8; 3571.4, 163.6; 3575.0, 139.9; 3609.0, 135.2; 3822.3, 158.5;

-1523.999477620 -1523.523801 -1523.492353 -1523.591597

FY_OGG-5

N	-3.596114	1.152035	-0.597612
H	-4.601397	0.943680	-0.587474
H	-3.276423	1.368738	-1.554849
C	-2.808652	-0.036675	-0.132037
H	-2.767598	0.001795	0.957508
C	-3.489328	-1.329765	-0.615152
C	-1.413741	0.128846	-0.755936
H	-3.415530	-1.380458	-1.705893
H	-2.921602	-2.173299	-0.214646
C	-4.932570	-1.388660	-0.175768
O	-1.289638	0.881264	-1.708221
C	-5.254492	-1.641871	1.159903
C	-5.959600	-1.127746	-1.084913
H	-4.466659	-1.866921	1.872800
C	-6.579390	-1.633815	1.577572
C	-7.288628	-1.116626	-0.665416
H	-5.724491	-0.961778	-2.132556
H	-6.819493	-1.844047	2.612646
C	-7.598166	-1.366744	0.665702
H	-8.078018	-0.924142	-1.381639
H	-8.630692	-1.364750	0.992244
N	-0.423870	-0.588726	-0.208829
H	-0.591786	-1.274931	0.520434
C	0.962651	-0.446427	-0.616198
H	0.981469	-0.172795	-1.672762
C	1.744433	0.629627	0.227849
C	1.640843	-1.790847	-0.348885
H	2.045846	0.175247	1.176009
H	2.656462	0.893423	-0.313433
C	0.858097	1.811194	0.455085
O	1.137697	-2.583557	0.418915
C	0.726275	2.835590	-0.510240
C	-0.034889	1.779096	1.559597
H	1.467206	2.913882	-1.298610
C	-0.382008	3.636863	-0.525515
C	-1.160176	2.547116	1.560507
H	0.157103	1.075620	2.363577
H	-0.558388	4.365367	-1.307412
C	-1.462509	3.377761	0.407567
H	-1.894381	2.504613	2.358126
O	-2.635403	3.734783	0.173328
H	-3.416797	2.018376	-0.052659
N	2.833018	-1.964889	-0.972767
H	3.205157	-1.163818	-1.470980
C	3.835092	-2.833426	-0.368337
C	4.715344	-1.910246	0.471485
H	3.320670	-3.545532	0.275209
H	4.388390	-3.370661	-1.139155
O	4.245931	-1.256828	1.378696
N	6.008203	-1.771351	0.062616
H	6.282230	-2.210110	-0.803065
C	6.700402	-0.572232	0.457550
C	6.021785	0.657606	-0.132971
H	6.699111	-0.469266	1.543554
H	7.738048	-0.600718	0.124457
O	5.074688	0.637549	-0.875787
O	6.622485	1.772636	0.276933
H	6.182197	2.534531	-0.124888

11.5, 0.4; 24.5, 0.2; 28.3, 0.5; 34.1, 2.7; 35.1, 0.5; 40.0, 0.9; 47.9, 2.2; 58.2, 1.5; 61.8, 2.2; 69.7, 2.6; 82.7, 3.8; 84.7, 0.7; 96.9, 2.2; 108.9, 5.3; 130.7, 8.1; 136.0, 2.9; 139.7, 6.2; 156.0, 18.2; 175.3, 13.5; 198.7, 23.6; 224.5, 10.2; 261.6, 23.2; 272.3, 3.4; 280.0, 4.7; 294.3, 5.0; 297.2, 11.9; 316.5, 22.1; 341.4, 23.8; 344.5, 3.6; 352.5, 16.6; 357.8, 2.5; 369.6, 1.5; 386.2, 56.8; 412.8, 0.1; 421.7, 11.4; 439.2, 8.1; 449.7, 36.9; 466.0, 5.5; 491.1, 30.5; 501.3, 58.0; 503.7, 2.3; 505.8, 29.3; 521.0, 77.3; 550.1, 15.8; 565.9, 31.9; 579.3, 53.6; 588.4, 9.4; 612.2, 1.4; 622.8, 102.1; 630.7, 0.1; 638.1, 52.2; 653.0, 89.3; 696.1, 12.4; 713.9, 0.9; 718.7, 13.7; 724.5, 26.4; 737.6, 31.8; 756.4, 5.4; 772.6, 31.3; 782.0, 23.1; 786.7, 8.0; 789.0, 1.3; 810.5, 26.7; 835.3, 17.0; 852.1, 2.0; 864.7, 1.4; 874.5, 8.3; 878.3, 3.7; 878.9, 26.9; 893.4, 17.6; 905.5, 0.1; 932.2, 16.7; 953.3, 11.7; 954.2, 7.9; 976.7, 20.6; 987.2, 1.8; 998.2, 34.8; 1003.6, 1.8; 1007.1, 14.6; 1013.4, 0.0; 1018.1, 2.6; 1037.8, 0.1; 1039.4, 7.8; 1060.4, 7.8; 1061.0, 0.4; 1063.6, 6.2; 1083.7, 16.6; 1086.5, 3.1; 1112.1, 8.4; 1119.5, 34.2; 1136.5, 31.7; 1146.6, 16.7; 1152.7, 25.5; 1168.8, 1.1; 1185.2, 0.3; 1202.8, 304.3; 1207.7, 7.3; 1207.8, 4.1; 1232.8, 55.2; 1234.1, 24.5; 1238.6, 21.8; 1243.3, 14.0; 1254.1, 5.3; 1271.2, 1.6; 1283.2, 0.8; 1284.6, 4.0; 1297.1, 65.2; 1308.8, 15.5; 1321.5, 63.5; 1329.7, 11.0; 1335.2, 1.2; 1335.7, 32.4; 1354.4, 1.5; 1364.6, 9.3; 1374.8, 14.0; 1383.1, 5.2; 1390.7, 64.1; 1418.1, 14.2; 1437.8, 71.1; 1446.5, 14.8; 1453.0, 9.0; 1458.7, 33.7; 1484.5, 6.3; 1489.4, 25.4; 1490.9, 26.6; 1497.1, 10.9; 1515.0, 160.2; 1532.3, 5.9; 1539.1, 13.9; 1552.7, 409.0; 1568.4, 263.8; 1577.8, 430.2; 1585.8, 73.2; 1625.0, 98.1; 1629.4, 43.1; 1657.3, 5.5; 1670.2, 58.4; 1674.9, 0.4; 1783.4, 218.4; 1801.1, 136.0; 1821.3, 334.4; 1854.4, 441.2; 3073.0, 4.1; 3075.7, 2.0; 3108.2, 25.2; 3114.1, 4.9; 3118.1, 4.8; 3120.1, 0.2; 3133.7, 0.9; 3134.2, 0.7; 3164.3, 0.6; 3174.5, 2.6; 3182.8, 3.8; 3185.8, 4.5; 3193.5, 5.6; 3202.2, 11.9; 3208.2, 502.3; 3212.7, 18.0; 3216.7, 0.1; 3224.5, 1.4; 3232.8, 1.0; 3235.6, 0.6; 3357.8, 63.0; 3439.3, 336.5; 3580.4, 104.3; 3589.5, 66.8; 3662.7, 59.4; 3827.0, 101.2;

-1523.996957210 -1523.520073 -1523.489187 -1523.585563

TS1

C	0.684744	-2.992008	-0.707442
O	0.579459	-3.774671	0.214502
N	-0.190497	-2.958750	-1.750382
H	-0.115493	-2.190879	-2.402324
C	-1.502091	-3.568455	-1.586383
C	-2.303143	-2.726279	-0.592708
H	-2.023964	-3.562141	-2.540832
H	-1.378072	-4.595310	-1.243906
O	-2.911915	-1.724265	-0.934286
N	-2.245076	-3.126967	0.700387
H	-1.564370	-3.828757	0.961048
C	-2.957834	-2.388105	1.704782
C	-2.458175	-0.967528	1.887482
H	-4.020410	-2.327994	1.458304
H	-2.871728	-2.895410	2.667614
O	-1.401560	-0.522529	1.505376
O	-3.347777	-0.243527	2.557611

H	-3.001661	0.651300	2.687122
N	0.724920	2.815370	-0.240675
C	0.272271	1.600195	-0.084392
C	1.101614	0.535635	-0.767833
O	1.857822	0.863928	-1.658815
H	1.484236	2.951080	-0.907540
H	-0.415814	1.372562	0.722219
C	-1.450027	1.265240	-1.600635
C	-2.435202	2.110391	-1.036448
H	-0.788438	1.634801	-2.377035
C	-4.331574	3.759858	0.183984
C	-3.467172	1.552727	-0.241896
C	-2.392252	3.513255	-1.221064
C	-3.330234	4.325425	-0.611915
C	-4.403275	2.374807	0.358203
H	-3.528896	0.471708	-0.161737
H	-1.629886	3.940475	-1.865057
H	-3.303250	5.397558	-0.763204
H	-5.205561	1.944467	0.946088
H	-5.069804	4.400648	0.651191
N	0.890790	-0.698775	-0.289198
C	1.699667	-1.845434	-0.695229
H	0.224316	-0.820756	0.471457
H	2.071326	-1.633432	-1.701424
C	2.872327	-2.082006	0.270342
C	3.650663	-0.806023	0.463546
H	3.498721	-2.876441	-0.142409
H	2.469281	-2.446181	1.217812
C	4.873289	1.708093	0.669644
C	3.304503	0.081204	1.485439
C	4.640723	-0.417617	-0.435343
C	5.253882	0.825299	-0.338197
C	3.900696	1.329971	1.593213
H	2.558151	-0.215304	2.216936
H	4.934155	-1.088473	-1.236436
H	6.022367	1.111638	-1.048868
H	3.649083	2.012218	2.396299
O	5.411868	2.948331	0.807359
H	6.141461	3.066352	0.192286
H	0.329001	3.610468	0.241389
H	-1.569287	0.189658	-1.496781

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-1523.970611520 -1523.497981 -1523.466778 -1523.561733

COM-1

C	-0.560972	-2.718485	-1.167548
O	-0.871154	-3.659041	-0.466044
N	-1.412130	-2.150231	-2.064783
H	-1.124447	-1.284047	-2.498252
C	-2.844366	-2.377057	-1.924069
C	-3.325751	-1.608297	-0.693683
H	-3.359287	-1.986909	-2.798981
H	-3.026641	-3.447567	-1.837267
O	-3.657268	-0.436357	-0.750262
N	-3.290746	-2.293722	0.476538
H	-2.837805	-3.198289	0.499663
C	-3.686990	-1.640961	1.691760
C	-2.735056	-0.548683	2.141814
H	-4.671380	-1.181275	1.576926
H	-3.757828	-2.370810	2.500361
O	-1.617146	-0.349039	1.724700
O	-3.288004	0.180844	3.101515
H	-2.662791	0.861236	3.388864
N	1.412949	2.515172	0.481867
C	0.657211	1.487909	0.501918
C	1.035183	0.410660	-0.499937
O	1.866347	0.677950	-1.341303
H	2.145064	2.533846	-0.235889
H	-0.147567	1.381537	1.224337
C	-3.043592	2.518772	0.759519
C	-1.998473	2.991039	-0.062601
H	-3.556433	1.599229	0.505219
C	-0.022250	3.973253	-1.822634
C	-1.382748	4.249798	0.160831
C	-1.560362	2.226141	-1.181897
C	-0.605887	2.727786	-2.054507
C	-0.415716	4.727432	-0.707869
H	-1.714963	4.858631	0.995231
H	-2.049506	1.273339	-1.367013
H	-0.304912	2.148640	-2.919754
H	0.015921	5.708862	-0.544040
H	0.711154	4.368574	-2.514971
N	0.390340	-0.743214	-0.305093
C	0.768164	-1.975165	-0.995737
H	-0.293565	-0.800782	0.450577
H	1.187971	-1.686524	-1.963094
C	1.796850	-2.779169	-0.180711
C	2.960000	-1.904984	0.209525
H	2.117532	-3.628833	-0.788044
H	1.294204	-3.184145	0.699947
C	4.960542	-0.040161	0.825993
C	2.941423	-1.202899	1.417364
C	4.017835	-1.675841	-0.666969
C	5.014224	-0.755296	-0.368360
C	3.925613	-0.274561	1.729913
H	2.146255	-1.394630	2.132459
H	4.062216	-2.213238	-1.608837
H	5.828876	-0.588429	-1.065455
H	3.928722	0.254584	2.675449
O	5.884725	0.894311	1.170041
H	6.609774	0.897915	0.538269
H	1.261904	3.324781	1.073634
H	-3.414657	3.121513	1.579094

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701.9, 89.4; 717.5, 5.1; 722.8, 11.0; 740.9, 1.2; 763.1, 56.7; 777.2, 5.3; 787.1, 56.7; 799.3, 33.9; 814.8, 43.0; 819.0, 5.3; 836.6, 0.1; 842.4, 5.6; 854.2, 62.4; 870.3, 4.2; 872.2, 30.6; 874.4, 71.4; 884.2, 22.7; 903.0, 1.4; 907.2, 16.1; 920.8, 7.2; 939.1, 9.3; 968.9, 1.1; 981.8, 11.5; 989.5, 0.4; 989.7, 1.1; 996.9, 2.4; 1010.6, 2.6; 1021.1, 0.9; 1022.1, 3.5; 1032.4, 1.4; 1036.3, 8.7; 1050.3, 1.1; 1059.5, 9.8; 1063.8, 1.7; 1085.7, 7.0; 1115.8, 2.1; 1122.0, 1.6; 1131.4, 6.4; 1133.8, 9.2; 1164.8, 10.4; 1176.3, 6.1; 1186.8, 4.3; 1191.1, 109.1; 1196.1, 8.2; 1207.8, 113.9; 1214.4, 180.9; 1234.5, 3.9; 1237.1, 0.7; 1259.8, 33.8; 1280.2, 11.1; 1299.3, 79.8; 1310.1, 6.5; 1315.7, 138.1; 1319.3, 21.6; 1325.8, 16.8; 1332.6, 3.6; 1337.7, 4.0; 1339.5, 15.4; 1353.9, 21.6; 1356.4, 20.7; 1356.9, 2.0; 1382.0, 1.6; 1393.6, 5.6; 1418.5, 14.9; 1443.5, 40.9; 1463.8, 45.0; 1480.5, 13.8; 1482.2, 14.2; 1482.9, 5.5; 1487.2, 15.7; 1490.5, 11.2; 1509.1, 21.6; 1535.2, 69.2; 1548.2, 181.9; 1565.7, 117.5; 1577.5, 222.9; 1601.7, 15.2; 1619.2, 0.3; 1620.3, 136.4; 1661.7, 14.6; 1690.5, 50.2; 1744.7, 208.4; 1780.8, 194.8; 1806.6, 397.4; 1827.5, 551.2; 1838.8, 87.8; 3088.6, 4.8; 3097.0, 4.1; 3102.3, 1.8; 3125.3, 3.4; 3140.7, 2.4; 3147.0, 1.4; 3162.0, 5.4; 3180.6, 7.5; 3184.8, 6.8; 3189.8, 0.0; 3190.6, 5.8; 3194.4, 0.8; 3204.9, 1.9; 3207.9, 1.9; 3211.9, 17.4; 3214.3, 0.9; 3222.5, 0.6; 3228.2, 0.1; 3275.5, 4.9; 3436.1, 112.2; 3474.1, 406.7; 3622.4, 98.6; 3631.0, 127.1; 3640.1, 37.0; 3823.1, 80.2; 3892.0, 122.5;

-1523.971109770 -1523.498912 -1523.466908 -1523.563656

[M-91]$^+$

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O	1.736237	-2.347690	-1.202898
N	2.076270	-2.136449	1.026710
H	1.659078	-1.824051	1.892466
C	3.523157	-1.998713	0.904622
C	3.828812	-0.541977	0.553384
H	3.990284	-2.228780	1.858891
H	3.878943	-2.689972	0.141200
O	4.106652	0.289503	1.391018
N	3.680298	-0.219819	-0.764333
H	3.377062	-0.924961	-1.422865
C	3.933654	1.127154	-1.184558
C	2.861603	2.114322	-0.762965
H	4.878878	1.490120	-0.774955
H	4.004528	1.172640	-2.273344
O	1.738524	1.846970	-0.387809
O	3.300195	3.355475	-0.895733
H	2.605689	3.983489	-0.655323
N	-1.945271	2.414959	1.684633
C	-0.954652	1.842941	1.128965
C	-0.967176	0.325092	1.240654
O	-1.807407	-0.172941	1.957107
H	-2.625640	1.797404	2.148338
H	-0.182928	2.402039	0.601904
N	-0.050515	-0.270486	0.475149
C	-0.146956	-1.693686	0.143492
H	0.621340	0.311230	-0.031652
H	-0.580672	-2.198079	1.010846
C	-1.028939	-1.907375	-1.105899
C	-2.329943	-1.160583	-0.975694
H	-1.188470	-2.982101	-1.218615
H	-0.466728	-1.572117	-1.979385
C	-4.605598	0.386087	-0.431547
C	-2.438296	0.151325	-1.446430
C	-3.404081	-1.693997	-0.267035
C	-4.534806	-0.935260	0.006827
C	-3.560900	0.926046	-1.180141
H	-1.632958	0.570458	-2.043626
H	-3.352088	-2.713315	0.101481
H	-5.356690	-1.365752	0.569441
H	-3.663096	1.932526	-1.569331
O	-5.659914	1.199844	-0.162908
H	-6.386664	0.697947	0.218501
H	-2.098913	3.418492	1.668752

15.5, 1.0; 21.5, 0.4; 31.4, 3.5; 39.6, 1.0; 46.6, 12.8; 63.0, 4.1; 75.0, 10.1; 81.7, 6.7; 94.1, 4.0; 106.0, 13.3; 124.7, 5.6; 127.9, 7.1; 139.8, 7.4; 151.2, 1.0; 168.6, 13.6; 198.1, 0.6; 223.2, 4.3; 260.2, 3.4; 280.3, 3.4; 304.9, 8.3; 316.4, 8.7; 317.3, 11.7; 334.8, 20.1; 350.5, 12.6; 352.7, 110.9; 383.5, 1.8; 416.2, 42.3; 422.4, 2.2; 434.6, 7.7; 460.3, 22.6; 485.3, 27.2; 502.5, 20.3; 504.7, 21.9; 514.7, 33.8; 534.2, 103.4; 545.8, 157.1; 559.9, 17.6; 589.1, 19.6; 618.7, 66.9; 652.2, 0.4; 655.2, 44.7; 683.5, 17.7; 712.0, 1.9; 716.5, 99.4; 725.6, 56.1; 741.5, 1.4; 773.2, 9.8; 798.3, 22.1; 816.5, 1.9; 825.6, 54.0; 844.8, 10.4; 855.4, 34.8; 869.4, 5.9; 881.9, 26.6; 899.2, 9.2; 903.3, 12.1; 916.0, 3.9; 940.3, 132.8; 969.5, 3.0; 978.1, 7.9; 991.1, 1.1; 1017.1, 7.5; 1032.1, 3.8; 1034.3, 5.7; 1059.1, 4.8; 1081.7, 7.7; 1103.4, 4.1; 1116.7, 14.0; 1130.0, 8.5; 1133.2, 6.3; 1168.1, 11.9; 1190.6, 112.1; 1195.9, 4.9; 1207.6, 127.6; 1212.9, 193.9; 1235.6, 2.5; 1238.1, 0.9; 1258.9, 54.8; 1295.8, 21.9; 1312.3, 17.3; 1315.3, 141.7; 1317.4, 21.1; 1325.8, 18.9; 1338.3, 3.3; 1342.0, 42.3; 1355.0, 42.0; 1357.8, 2.4; 1377.0, 1.0; 1389.7, 5.0; 1417.6, 27.3; 1442.7, 30.1; 1468.4, 73.6; 1479.3, 15.8; 1482.2, 15.2; 1487.4, 14.9; 1531.8, 67.0; 1554.2, 177.1; 1565.0, 112.3; 1569.5, 307.2; 1614.9, 91.2; 1658.1, 14.1; 1688.3, 45.6; 1766.9, 348.5; 1801.1, 108.7; 1806.6, 658.6; 1820.8, 473.0; 1842.5, 48.3; 3092.6, 2.9; 3095.7, 5.6; 3105.2, 2.0; 3125.2, 3.0; 3144.6, 1.5; 3145.4, 1.8; 3177.1, 5.7; 3189.7, 47.8; 3193.5, 4.8; 3194.2, 0.0; 3207.3, 0.9; 3217.7, 0.4; 3393.9, 104.5; 3442.6, 568.3; 3615.0, 232.6; 3624.3, 103.5; 3639.9, 48.2; 3836.8, 102.5; 3889.3, 131.7;

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Benzylic radical

C	2.396011	-0.000001	0.000005
C	0.986368	-0.000007	-0.000017
H	2.951428	-0.928051	0.000055
C	-1.832045	0.000001	0.000017
C	0.251997	1.212399	-0.000016
C	0.251994	-1.212400	-0.000010
C	-1.129910	-1.206972	0.000011
C	-1.129898	1.206979	0.000007
H	0.793451	2.152036	-0.000047
H	0.793430	-2.152046	-0.000034
H	-1.670934	-2.145884	0.000008
H	-1.670930	2.145886	0.000011
H	-2.914966	0.000013	0.000042
H	2.951418	0.928053	-0.000024

202.0, 1.9; 358.9, 0.2; 388.2, 0.0; 477.8, 19.2; 483.3, 0.0; 532.0, 0.6; 627.0, 0.0; 685.1, 59.4; 705.5, 0.0; 784.2, 73.7; 839.9, 0.4; 845.8, 0.0; 919.6, 5.3; 974.1, 1.6; 990.9, 0.0; 998.0, 0.6; 1003.7, 0.0; 1051.2, 2.9; 1123.1, 4.0; 1171.7, 0.0; 1181.4, 0.0; 1276.4, 3.2; 1324.7, 0.7; 1350.2, 0.2; 1487.6, 6.0; 1491.2, 2.0; 1505.4, 7.6; 1614.2, 0.6; 1627.5, 0.6; 3182.2, 4.1; 3197.8, 5.3; 3199.6, 1.3; 3211.1, 2.3; 3217.7, 19.3; 3229.4, 7.3; 3286.3, 3.8;

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TS2

C	1.306135	3.148650	0.170810
O	1.245689	3.576372	-0.964731
N	0.449360	3.532049	1.152622
H	0.465818	3.004266	2.014017
C	-0.810778	4.175029	0.802936
C	-1.733563	3.113760	0.201902
H	-1.274358	4.568658	1.704426
H	-0.611938	4.988108	0.105501
O	-2.476196	2.432587	0.884226
N	-1.608129	2.940239	-1.140600
H	-0.846534	3.405523	-1.617739
C	-2.339086	1.893535	-1.793437
C	-1.840902	0.498959	-1.462536
H	-3.391310	1.925716	-1.499843
H	-2.297104	2.021830	-2.876298
O	-0.857508	0.228897	-0.809059
O	-2.634873	-0.413699	-2.000110
H	-2.401426	-1.298136	-1.674494
N	0.680388	-3.296692	1.014369
C	0.031330	-2.194759	0.871475
C	1.749996	-0.058356	1.793407
O	2.657667	-0.171691	2.549863
H	0.517119	-3.885888	1.825478

H	0.241271	-1.603682	-0.017518
C	-1.070033	-1.780648	1.775635
C	-2.401448	-1.862436	1.039701
H	-1.077262	-2.392169	2.682954
C	-4.890740	-2.012365	-0.213344
C	-3.298370	-0.797199	1.134050
C	-2.748967	-2.995254	0.300982
C	-3.991367	-3.067232	-0.328340
C	-4.541932	-0.880210	0.518382
H	-3.023307	0.105077	1.669839
H	-2.069252	-3.839178	0.228283
H	-4.257790	-3.952214	-0.893375
H	-5.234063	-0.051202	0.604570
H	-5.858590	-2.071576	-0.695589
N	1.390921	0.914107	0.958044
C	2.283108	2.033506	0.588098
H	0.597935	0.737190	0.344166
H	2.807811	2.323461	1.501399
C	3.299347	1.690842	-0.541226
C	3.351777	0.209456	-0.808046
H	4.281147	2.064950	-0.248838
H	2.994939	2.228511	-1.439982
C	3.109057	-2.561268	-0.959912
C	2.400295	-0.377588	-1.644930
C	4.229369	-0.619982	-0.114019
C	4.111822	-2.004723	-0.178677
C	2.273572	-1.758316	-1.729130
H	1.728212	0.256643	-2.214484
H	4.980496	-0.184417	0.535640
H	4.768515	-2.638896	0.407457
H	1.539407	-2.224146	-2.377374
O	2.820391	-3.915120	-0.928814
H	3.617037	-4.430661	-0.762511
H	1.398394	-3.603143	0.345783
H	-0.896031	-0.741717	2.063811

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-1523.968919640 -1523.494838 -1523.463759 -1523.557276

COM-2

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O	-2.051691	-2.815770	0.529223
N	-0.726175	-1.528222	1.830314
H	-0.491781	-0.578172	2.083202
C	0.243523	-2.588751	2.061013
C	1.169793	-2.711678	0.853675
H	0.844713	-2.342524	2.933287
H	-0.296558	-3.519699	2.239133
O	2.263891	-2.159473	0.818347
N	0.664819	-3.413164	-0.179402
H	-0.317199	-3.668509	-0.127199
C	1.319791	-3.400268	-1.459780
C	1.241402	-2.039118	-2.127781
H	2.379924	-3.643700	-1.347542
H	0.876494	-4.147375	-2.116996
O	0.907665	-1.015204	-1.582579
O	1.613041	-2.107090	-3.400253
H	1.576153	-1.222432	-3.791880
N	2.265288	0.603282	0.388162
C	3.398444	0.535397	0.970574
C	-1.197280	0.957926	-0.428929
O	-0.389188	1.180013	0.434631
H	1.713486	1.457747	0.326088
H	3.851832	-0.452821	1.014753
C	4.117383	1.710582	1.518807
C	5.376370	1.885530	0.680163
H	3.488607	2.602834	1.490321
C	7.652524	2.169539	-0.897496
C	6.595805	1.371403	1.115819
C	5.297136	2.533454	-0.551945
C	6.434816	2.680056	-1.336698
C	7.732341	1.515790	0.327663
H	6.663467	0.872006	2.076673
H	4.349930	2.940950	-0.892332
H	6.372176	3.197132	-2.286253
H	8.680726	1.124678	0.674753
H	8.539881	2.286474	-1.507288
N	-2.263261	0.176326	-0.403452
C	-2.709694	-0.514899	0.820020
H	-2.886276	0.187236	-1.200422
H	-2.596794	0.189086	1.650020
C	-4.171212	-0.947747	0.675636
C	-5.072669	0.197753	0.289859
H	-4.479823	-1.388476	1.627319
H	-4.216518	-1.746392	-0.068276
C	-6.681745	2.366366	-0.463234
C	-5.599636	0.288986	-1.000006
C	-5.375481	1.211704	1.197844
C	-6.172167	2.288543	0.832661
C	-6.395500	1.359767	-1.381900
H	-5.405352	-0.504646	-1.715879
H	-4.996991	1.158117	2.214205
H	-6.405873	3.064104	1.554780
H	-6.814271	1.427425	-2.378077
O	-7.463930	3.388822	-0.886494
H	-7.638627	4.001550	-0.166648
H	1.826318	-0.235645	-0.009564
H	4.387238	1.500356	2.556871

11.2, 0.3; 16.2, 0.3; 18.8, 0.3; 24.0, 0.1; 30.0, 0.2; 30.5, 0.4; 36.4, 0.4; 40.0, 1.4; 47.7, 0.9; 57.3, 2.1; 58.5, 2.0; 65.3, 0.5; 89.1, 5.1; 95.0, 4.3; 111.9, 5.6; 121.6, 5.7; 145.4, 9.2; 153.1, 20.1; 166.0, 4.3; 169.0, 1.9; 180.8, 6.8; 195.1, 19.0; 198.8, 14.0; 220.3, 14.1; 251.0, 4.3; 272.9, 16.2; 289.4, 11.2; 305.6, 30.9; 308.9, 9.7; 328.0, 0.9; 328.9, 93.7; 331.9, 17.0; 343.4, 13.6; 361.2, 3.3; 394.7, 55.0; 409.7, 0.0; 412.6, 21.1; 423.0, 0.9; 432.8, 7.0; 442.1, 18.2; 488.2, 71.8; 495.7, 57.8; 503.0, 19.1; 506.1, 16.0; 512.5, 23.9; 516.0, 41.5; 555.9, 15.8; 559.9, 26.4; 575.8, 46.1; 608.2, 8.4; 630.5, 0.0; 654.5, 0.5; 661.3, 109.3; 676.6, 160.6; 700.0, 6.8; 711.6, 23.7; 728.1, 1.7; 736.1, 16.0; 740.0, 16.2; 755.4, 9.6; 775.2, 34.0; 797.6, 12.9; 807.9, 10.1; 818.3, 11.7; 838.2, 17.3; 849.1, 19.5; 851.3, 28.4; 869.3, 8.4; 869.9, 0.3; 880.4, 15.4; 882.5, 9.5; 913.2, 14.0; 934.7, 71.9; 939.4, 35.8; 947.3, 3.0; 958.8, 64.2; 964.4, 0.3; 989.6, 0.3; 1009.2, 14.8; 1012.2, 56.7; 1019.2, 2.5; 1027.3, 8.1; 1032.2, 0.8; 1034.6, 0.0; 1039.0, 2.5; 1061.2, 2.0; 1062.1, 6.8; 1093.9, 10.4; 1096.6, 5.5; 1103.7, 9.6; 1124.1, 4.0; 1137.1, 10.6; 1140.9, 17.9; 1163.7, 6.6; 1186.0, 0.8; 1193.8, 134.2; 1197.5, 28.2;

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-1523.978033190 -1523.504411 -1523.471698 -1523.574718

TS3

C	0.595626	-3.268288	-0.528769
O	1.006890	-3.257853	-1.664255
N	1.329204	-3.722632	0.533201
H	0.965566	-3.515770	1.453768
C	2.780124	-3.669985	0.418687
C	3.180434	-2.194485	0.412278
H	3.226826	-4.153514	1.285938
H	3.089045	-4.192261	-0.485171
O	2.977093	-1.484005	1.388803
N	3.697998	-1.714586	-0.737527
H	3.623074	-2.286006	-1.567390
C	3.950212	-0.303706	-0.876507
C	2.672531	0.520367	-0.887095
H	4.570922	0.052255	-0.051483
H	4.492979	-0.111472	-1.802519
O	1.555287	0.067360	-0.843522
O	2.944390	1.815447	-0.953237
H	2.114833	2.323023	-1.002857
N	1.059584	0.613567	2.307107
C	1.378495	1.836697	2.341941
C	-1.092082	-0.827082	1.517544
O	-2.219487	-1.092072	1.873510
H	-0.412688	0.029965	2.029684
H	2.431501	2.132227	2.408259
C	0.369689	2.938984	2.208559
C	0.440214	3.446002	0.780647
H	-0.626614	2.554087	2.433453
C	0.637759	4.266298	-1.884314
C	1.260693	4.519096	0.433730
C	-0.274608	2.781279	-0.217118
C	-0.183137	3.192136	-1.543462
C	1.359799	4.927506	-0.894042
H	1.818715	5.043258	1.202382
H	-0.904196	1.937041	0.048525
H	-0.748314	2.677640	-2.312109
H	1.995879	5.764700	-1.153655
H	0.709649	4.588989	-2.915642
N	-0.337987	-1.446904	0.627464
C	-0.749981	-2.632255	-0.133568
H	0.516569	-0.963868	0.341882
H	-1.298511	-3.281445	0.556441
C	-1.616342	-2.296864	-1.353557
C	-2.756001	-1.399436	-0.957920
H	-1.972047	-3.235820	-1.783501
H	-0.981193	-1.814490	-2.099058
C	-4.794184	0.315419	-0.094053
C	-2.633083	-0.010154	-1.099879
C	-3.932560	-1.908296	-0.385856
C	-4.946608	-1.065666	0.036509
C	-3.630998	0.844309	-0.674163
H	-1.735116	0.390820	-1.561024
H	-4.054649	-2.981348	-0.279300
H	-5.851521	-1.473502	0.473724
H	-3.552141	1.919353	-0.786564
O	-5.726523	1.199927	0.303483
H	-6.492779	0.751885	0.676130
H	1.829472	-0.064001	2.311585
H	0.605986	3.740454	2.910956

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-1523.939499640 -1523.471934 -1523.440396 -1523.536696

COM-3

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O	0.410313	-3.096326	-1.357629
N	1.125144	-3.061311	0.789863
H	1.017450	-2.621087	1.692687
C	2.416678	-3.665261	0.479321
C	3.309690	-2.518433	0.020427
H	2.831794	-4.108643	1.381272
H	2.278115	-4.428739	-0.285220
O	3.886701	-1.807214	0.824124
N	3.302824	-2.269130	-1.314366
H	2.594269	-2.751117	-1.854953
C	3.676026	-0.943042	-1.738148
C	2.636370	0.074663	-1.288365
H	4.642872	-0.666950	-1.318008
H	3.756086	-0.900798	-2.825332
O	1.548606	-0.214570	-0.853305
O	3.066677	1.320079	-1.452712
H	2.362796	1.938944	-1.193829
N	1.964427	0.088881	2.111230
C	2.337920	1.296473	2.186835
C	-1.636076	-0.536869	2.087656
O	-2.810930	-0.805419	1.891382
H	-1.304540	0.114592	2.908614
H	3.393471	1.581003	2.112161
C	1.352741	2.428831	2.314359
C	1.179686	3.088600	0.962434
H	0.399920	2.030228	2.667558
C	0.920449	4.197511	-1.598617
C	1.918868	4.213848	0.598921
C	0.313325	2.519639	0.025757
C	0.179844	3.070271	-1.245457
C	1.791489	4.765200	-0.673960
H	2.597524	4.664319	1.315388
H	-0.222989	1.614065	0.293505

H	-0.483928	2.615140	-1.973307
H	2.371841	5.639460	-0.942165
H	0.821480	4.626386	-2.588111
N	-0.628202	-0.996752	1.318171
C	-0.928758	-1.869172	0.210771
H	0.316244	-0.598546	1.467691
H	-1.698110	-2.572924	0.548823
C	-1.474875	-1.106800	-1.030717
C	-2.849659	-0.605270	-0.796624
H	-1.473860	-1.833483	-1.851179
H	-0.777190	-0.304445	-1.274061
C	-5.441984	0.285681	-0.297455
C	-3.123495	0.786460	-0.673265
C	-3.937391	-1.531090	-0.706470
C	-5.205862	-1.105167	-0.462828
C	-4.386742	1.231927	-0.427509
H	-2.305636	1.491982	-0.762827
H	-3.732123	-2.589014	-0.826118
H	-6.030182	-1.804874	-0.379705
H	-4.624827	2.281904	-0.312259
O	-6.630088	0.775362	-0.030016
H	-7.306276	0.089923	0.062140
H	2.761989	-0.536692	1.964936
H	1.716492	3.155920	3.043749

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-1523.969436220 -1523.496228 -1523.464422 -1523.561513

$[x_3+H]^{\bullet+}$

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N	1.828870	-1.923943	0.567840
H	1.567904	-1.729143	1.524639
C	3.232749	-2.226345	0.303082
C	3.968788	-0.890667	0.285739
H	3.624605	-2.839298	1.111004
H	3.303517	-2.761511	-0.643245
O	4.413833	-0.392089	1.295960
N	3.975888	-0.253443	-0.921258
H	3.382368	-0.629008	-1.650142
C	4.262378	1.154386	-0.919698
C	3.188072	1.942523	-0.188430
H	5.215311	1.352148	-0.427344
H	4.328925	1.531146	-1.941651
O	2.108317	1.509349	0.141348
O	3.570332	3.194538	0.024720
H	2.870523	3.670413	0.493170
C	-1.189798	0.267025	1.973189
O	-2.274998	-0.276537	1.887226
H	-0.957550	1.020317	2.738286
N	-0.160609	-0.002168	1.133258
C	-0.339530	-0.947808	0.053871
H	0.648452	0.615710	1.098590
H	-0.910780	-1.792528	0.451920
C	-1.095923	-0.350498	-1.163047
C	-2.516760	-0.072528	-0.839123
H	-1.029855	-1.092186	-1.965849
H	-0.571923	0.548357	-1.490590
C	-5.171825	0.400572	-0.148298
C	-2.995832	1.259845	-0.699854
C	-3.431202	-1.159633	-0.664227
C	-4.729573	-0.938570	-0.326694
C	-4.292178	1.502285	-0.360609
H	-2.308060	2.082059	-0.858649
H	-3.068214	-2.172970	-0.794256
H	-5.422672	-1.759213	-0.178103
H	-4.687856	2.502236	-0.233335
O	-6.396616	0.700910	0.205615
H	-6.951301	-0.078867	0.350543

15.2, 0.9; 25.9, 0.0; 34.9, 0.2; 46.5, 0.1; 58.1, 10.0; 69.3, 3.6; 73.8, 5.5; 88.1, 2.8; 101.0, 7.2; 121.2, 8.0; 126.6, 6.5; 142.6, 8.1; 160.9, 9.4; 197.3, 12.9; 240.0, 12.4; 257.5, 14.8; 273.5, 8.9; 293.6, 1.3; 313.6, 0.7; 319.2, 1.7; 332.0, 29.6; 353.8, 0.5; 367.7, 3.9; 392.0, 0.1; 433.5, 8.3; 444.9, 61.9; 473.8, 3.9; 488.1, 41.7; 511.2, 10.4; 518.1, 29.6; 534.6, 121.3; 555.1, 21.0; 572.5, 101.9; 575.4, 107.4; 610.6, 0.0; 629.1, 138.1; 651.5, 13.7; 664.9, 60.4; 705.5, 20.7; 720.2, 4.3; 725.3, 1.1; 747.7, 8.0; 786.2, 7.5; 803.6, 13.9; 804.9, 4.1; 814.0, 5.5; 849.4, 29.1; 865.0, 26.3; 885.1, 24.4; 896.7, 11.6; 906.8, 12.0; 963.7, 12.8; 998.6, 106.1; 1000.9, 0.7; 1009.2, 17.8; 1012.4, 6.3; 1029.1, 6.0; 1050.2, 21.4; 1064.4, 6.9; 1074.8, 64.7; 1115.4, 79.0; 1141.2, 24.7; 1162.5, 15.6; 1181.6, 185.1; 1192.5, 21.9; 1202.4, 49.4; 1211.0, 244.6; 1233.4, 10.1; 1244.0, 10.0; 1247.6, 13.8; 1270.1, 43.7; 1294.9, 90.1; 1297.7, 107.4; 1316.4, 32.9; 1336.7, 19.2; 1338.0, 12.3; 1346.3, 18.2; 1380.2, 6.4; 1384.7, 3.4; 1407.1, 101.2; 1411.6, 15.5; 1416.2, 56.4; 1444.8, 54.5; 1458.9, 70.3; 1478.2, 14.6; 1484.8, 17.9; 1515.8, 25.3; 1538.0, 538.9; 1546.1, 514.3; 1552.6, 16.8; 1562.0, 48.4; 1574.4, 274.9; 1716.8, 93.0; 1764.5, 429.6; 1792.9, 174.4; 1818.6, 519.8; 1836.0, 364.2; 3067.7, 32.5; 3071.5, 16.4; 3084.1, 12.7; 3109.8, 5.3; 3124.1, 3.9; 3145.9, 6.0; 3158.7, 0.9; 3191.9, 0.0; 3208.7, 0.7; 3219.9, 0.4; 3222.4, 4.0; 3239.1, 7.4; 3524.1, 578.9; 3612.7, 97.8; 3640.9, 59.0; 3814.9, 388.8; 3827.2, 102.4;

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N	-3.276099	0.633607	-0.213643
C	-2.373774	-0.217249	-0.465913
H	-2.182165	-0.607755	-1.473625
C	-1.457700	-0.730100	0.611677
C	-0.026204	-0.334428	0.318972
H	-1.791915	-0.315440	1.564915
C	2.601224	0.448536	-0.245415
C	0.942493	-1.283269	-0.000294
C	0.334130	1.014888	0.346700
C	1.638339	1.404450	0.069645
C	2.250410	-0.895660	-0.280671
H	0.674100	-2.334400	-0.023882
H	-0.419739	1.757764	0.588195
H	1.905478	2.454285	0.099526
H	2.993922	-1.645430	-0.524499
H	3.618729	0.751608	-0.461467
H	-3.784780	0.881368	-1.063048
H	-1.534444	-1.820251	0.661170

35.2, 1.3; 68.9, 5.0; 148.7, 10.8; 293.3, 9.6; 323.5, 1.7; 412.7, 0.0; 448.0, 9.5; 514.1, 31.5; 561.3, 7.5; 632.1, 0.2; 715.2, 34.4; 740.0, 48.6; 770.5, 32.9; 863.8, 10.0; 874.8, 0.5; 942.0, 2.3; 952.8, 22.1; 1005.6, 0.1; 1018.2, 6.9; 1020.8, 0.5; 1029.6, 30.3; 1062.5, 5.1; 1109.3, 1.2; 1131.0, 7.6; 1171.2, 13.9; 1180.8, 6.5; 1206.6, 0.1; 1227.3, 0.2; 1281.8, 11.5; 1312.9, 4.3; 1336.5, 0.5; 1359.9, 0.7; 1430.5, 13.5; 1474.4, 8.8; 1494.8, 7.1; 1539.8, 14.6; 1658.4, 1.6; 1678.1, 10.6; 1758.8, 99.7; 3050.5, 30.7; 3072.1, 11.1; 3131.2, 4.6; 3190.5, 2.5; 3192.6, 3.2; 3205.9, 1.9; 3214.6, 14.8; 3226.2, 9.5; 3501.1, 2.3;

-364.935354010 -364.783696 -364.774837 -364.817467

TS4

N	-4.479529	1.566193	-0.043004
C	-3.595348	0.749206	-0.694479
C	-2.529606	1.436452	-1.600147
O	-2.240030	0.909806	-2.632838
H	-5.366110	1.174899	0.273524
H	-2.667106	0.434449	0.039017
C	-4.202143	-0.538884	-1.251179
C	-5.181774	-1.142826	-0.276317
H	-3.382004	-1.221821	-1.476804
H	-4.687740	-0.297665	-2.200968
C	-6.987128	-2.165412	1.594913
C	-4.718294	-1.799745	0.866786
C	-6.556325	-1.000127	-0.470301
C	-7.456802	-1.512104	0.462088
C	-5.615974	-2.309973	1.795805
H	-3.649664	-1.918438	1.022082
H	-6.926114	-0.509397	-1.365614
H	-8.522014	-1.408086	0.295539
H	-5.248517	-2.826573	2.674118
H	-7.685986	-2.568553	2.317425
N	-1.809967	2.449895	-1.001845
C	-0.373924	2.145025	-0.906815
C	-0.238436	0.719579	-0.330254
O	-1.123668	0.237595	0.412026
H	-2.155694	2.705665	-0.084305
H	0.060437	2.166314	-1.907442
C	0.319328	3.196513	0.007639
C	1.531272	2.619070	0.690204
H	0.556347	4.069766	-0.602602
H	-0.399010	3.513375	0.770261
C	3.554110	0.994448	1.750008
C	2.738675	2.456578	0.012775
C	1.387260	2.022643	1.944547
C	2.388429	1.228921	2.481741
C	3.744369	1.645116	0.526239
H	2.886949	2.934998	-0.951542
H	0.463208	2.154656	2.498923
H	2.279519	0.760914	3.452938
H	4.666915	1.495797	-0.022368
O	4.454850	0.136718	2.271652
H	5.100464	-0.107641	1.589043
H	-4.276771	2.525232	0.209248
N	0.865224	0.066253	-0.638943
H	1.550862	0.492578	-1.256527
C	1.323127	-1.137470	0.024010
C	2.697097	-1.466138	-0.556666
H	1.363213	-0.978254	1.105007
H	0.649353	-1.973827	-0.184142
O	3.045869	-1.022334	-1.631535
N	3.458998	-2.327743	0.157703
H	3.245616	-2.516256	1.125153
C	4.675437	-2.833025	-0.430324
C	5.758744	-1.779087	-0.584031
H	5.076912	-3.633444	0.193499
H	4.471539	-3.247393	-1.418827
O	5.838263	-0.752789	0.041209
O	6.653070	-2.157274	-1.486972
H	7.352914	-1.489822	-1.537784

-233.4, 440.6; 17.2, 0.3; 20.1, 0.8; 27.8, 1.9; 32.3, 0.8; 44.6, 2.9; 46.9, 0.4; 52.6, 3.7; 73.5, 1.2; 75.5, 1.2; 78.9, 12.2; 85.3, 3.5; 96.7, 0.6; 111.5, 5.9; 113.8, 2.2; 133.2, 0.5; 144.4, 6.0; 169.8, 2.2; 175.6, 19.4; 194.2, 1.1; 227.5, 0.6; 233.3, 7.0; 247.0, 1.9; 271.7, 11.8; 279.1, 1.6; 297.6, 1.3; 315.5, 5.3; 329.8, 43.4; 335.5, 2.9; 349.7, 5.6; 365.2, 44.1; 372.5, 109.0; 384.2, 51.1; 411.8, 3.5; 414.7, 20.8; 422.6, 3.3; 440.1, 9.9; 448.1, 3.2; 468.7, 7.6; 476.5, 23.6; 506.1, 7.6; 515.0, 20.6; 531.5, 29.9; 537.8, 211.8; 552.4, 46.7; 564.2, 94.9; 568.4, 20.9; 602.0, 11.1; 623.0, 134.0; 630.8, 2.1; 645.4, 151.5; 649.4, 61.3; 653.1, 11.2; 663.0, 42.1; 666.4, 38.2; 699.9, 130.5; 713.6, 23.7; 721.6, 64.6; 735.6, 70.0; 745.3, 10.4; 755.4, 8.6; 770.0, 92.1; 791.6, 37.2; 801.2, 0.2; 845.5, 312.3; 850.3, 12.4; 854.6, 139.4; 869.1, 203.8; 877.9, 46.2; 879.8, 1.0; 882.0, 37.4; 899.0, 23.0; 909.6, 486.7; 936.7, 67.5; 942.1, 134.5; 946.7, 106.8; 963.2, 16.2; 972.8, 2.9; 993.8, 5.3; 999.5, 27.4; 1003.2, 5.8; 1013.7, 0.2; 1018.6, 1.3; 1030.7, 1.4; 1035.6, 0.0; 1059.3, 4.1; 1060.8, 0.9; 1062.9, 23.7; 1093.1, 3.8; 1111.7, 10.5; 1121.5, 19.5; 1134.6, 1.0; 1156.1, 67.5; 1162.6, 16.4; 1173.3, 122.9; 1184.6, 6.0; 1195.8, 8.4; 1205.0, 83.0; 1206.6, 1.2; 1212.1, 92.9; 1217.6, 362.6; 1229.3, 8.7; 1238.5, 13.2; 1242.1, 20.7; 1250.1, 17.1; 1256.4, 48.1; 1263.6, 11.6; 1300.0, 17.1; 1304.3, 14.0; 1314.0, 9.2; 1318.9, 10.5; 1322.8, 21.2; 1330.6, 201.4; 1337.5, 2.1; 1339.6, 14.7; 1348.9, 3.6; 1358.8, 0.6; 1374.8, 13.7; 1387.4, 14.6; 1390.1, 29.4; 1408.6, 30.7; 1450.9, 49.4; 1469.5, 65.0; 1479.2, 14.3; 1482.0, 26.7; 1486.2, 19.7; 1492.6, 51.3; 1495.9, 10.1; 1515.4, 27.4; 1538.7, 8.1; 1563.1, 32.3; 1571.5, 424.1; 1582.9, 571.2; 1631.6, 379.0; 1641.3, 551.2; 1656.9, 1.7; 1657.9, 10.6; 1675.2, 1.9; 1686.2, 91.2; 1770.0, 255.2; 1804.9, 149.5; 1860.4, 484.0; 1887.1, 165.7; 3066.4, 19.1; 3074.3, 8.6; 3085.6, 2.3; 3103.9, 4.2; 3120.5, 0.2; 3120.8, 5.6; 3135.1, 3.7; 3141.1, 0.9; 3154.9, 0.9; 3181.7, 2.9; 3183.4, 3.0; 3189.2, 2.4; 3189.8, 5.9; 3215.0, 0.1; 3223.0, 0.6; 3223.5, 0.2; 3223.8, 2.1; 3233.9, 1.4; 3489.9, 421.3; 3559.2, 179.0; 3590.8, 11.0; 3655.2, 119.7; 3667.4, 64.8; 3720.3, 707.8; 3814.7, 146.3;

-1523.946896200 -1523.476252 -1523.445753 -1523.540028

TS5

N	4.141475	-1.781651	-0.681868
C	3.941146	-1.044480	0.553690
C	2.546256	-1.307522	1.094887
O	2.252663	-0.942738	2.259649
H	4.807647	-1.300743	-1.278281
H	4.634750	-1.318712	1.357228
C	4.056067	0.477162	0.313555
C	5.447421	0.859297	-0.126134
H	3.788918	0.990392	1.239760
H	3.330750	0.759721	-0.456793
C	8.049790	1.479295	-0.940763
C	5.720092	1.153129	-1.461746
C	6.492402	0.883864	0.799873
C	7.785101	1.192655	0.396338
C	7.015981	1.461381	-1.868797
H	4.912389	1.153744	-2.187676
H	6.289428	0.670824	1.845184
H	8.586501	1.215919	1.124891
H	7.214122	1.691989	-2.908563
H	9.057596	1.722339	-1.254331
N	1.666353	-1.865111	0.277457
C	0.284589	-2.136149	0.639538
C	-0.563992	-2.039184	-0.648935
O	-0.050116	-1.826913	-1.725867
H	1.984211	-2.049665	-0.675338
H	0.216598	-3.159059	1.024317
C	-0.234869	-1.184325	1.737871
C	-0.809826	0.063176	1.320660
H	-0.809839	-1.699860	2.505256
H	0.914720	-0.948480	2.266566
C	-2.228453	2.219994	0.244681
C	-1.982564	0.557103	1.960402
C	-0.301605	0.784033	0.197523
C	-0.984395	1.845422	-0.322388
C	-2.696513	1.590001	1.422237
H	-2.355771	0.043728	2.839031
H	0.614959	0.456047	-0.278647
H	-0.634551	2.384243	-1.194008
H	-3.634000	1.909378	1.859110

O	-2.907109	3.166029	-0.373030
H	-3.841306	3.141116	-0.107233
H	4.513585	-2.709192	-0.509421
N	-1.892640	-2.170917	-0.449360
H	-2.263841	-2.211380	0.493557
C	-2.849829	-1.747129	-1.445112
C	-4.069891	-1.188401	-0.715736
H	-2.395188	-0.987744	-2.088279
H	-3.167892	-2.577463	-2.083542
O	-4.188906	-1.272701	0.491536
N	-5.023700	-0.635919	-1.504047
H	-4.864415	-0.539458	-2.494822
C	-6.283853	-0.227019	-0.942622
C	-6.233437	1.105176	-0.217273
H	-7.036555	-0.152804	-1.728731
H	-6.633191	-0.971123	-0.222559
O	-5.271997	1.824893	-0.125165
O	-7.419789	1.381405	0.311030
H	-7.385714	2.236753	0.762326

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-1523.976554280 -1523.505880 -1523.475106 -1523.571107

$[z_3+H]^{\bullet+}$

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C	0.139642	2.509238	-0.340334
O	1.133268	2.474611	-1.035989
H	-1.248468	3.823507	-1.400479
C	-2.270323	2.011629	-1.017356
C	-2.335875	0.652615	-0.575109
H	-3.190498	2.431710	-1.414359
C	-2.576542	-1.941313	0.414945
C	-1.180021	-0.173297	-0.412586
C	-3.627619	0.094287	-0.301024
C	-3.752612	-1.164143	0.201113
C	-1.292628	-1.435885	0.082398
H	-0.199212	0.164467	-0.722957
H	-4.508621	0.703105	-0.468664
H	-4.725227	-1.581325	0.438424
H	-0.419486	-2.058432	0.227312
O	-2.622121	-3.158099	0.900409
N	0.149589	2.283215	0.992760
H	-0.711311	2.272218	1.517730
C	1.401107	1.927802	1.638128
C	1.794047	0.488414	1.288278
H	2.169305	2.642421	1.339198
H	1.264277	1.979386	2.716960
O	1.135168	-0.453884	1.684185
N	2.918238	0.360280	0.545171
H	3.239085	1.169797	0.032719
C	3.393322	-0.941510	0.157991
C	2.532905	-1.603932	-0.902459
H	4.416409	-0.871173	-0.211389
H	3.401980	-1.603504	1.027643
O	1.486849	-1.185211	-1.319034
O	3.092977	-2.743761	-1.308220
H	2.532357	-3.146753	-1.986111
H	-3.521524	-3.454648	1.097361

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N	-1.144642	-1.344277	1.007093
C	-1.366427	-0.023674	0.437437
C	-2.819611	0.113469	0.029402
O	-3.133392	1.406612	-0.208009
H	-1.547253	-1.410070	1.935954
H	-1.150387	0.798411	1.133936
C	-0.482376	0.166236	-0.810422
C	0.985137	0.136520	-0.465297
H	-0.721497	-0.631422	-1.518961
C	3.690501	0.066530	0.264658
C	1.587749	1.239442	0.145215
C	1.758112	-0.999860	-0.705367
C	3.102474	-1.036451	-0.343174
C	2.928900	1.207150	0.506782
H	0.998477	2.132563	0.329899
H	1.302177	-1.860340	-1.184853
H	3.689421	-1.925933	-0.539957
H	3.382854	2.073359	0.973750
H	4.736918	0.041294	0.544171
N	-3.675593	-0.799397	-0.118017
H	-3.240850	-1.698400	0.088449
H	-0.149910	-1.524915	1.095094
H	-0.744072	1.120816	-1.271929
H	-4.053855	1.421286	-0.500407

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C	-1.234092	-1.756586	-1.471580
O	-1.659420	-2.839372	-1.128262
N	-2.008689	-0.799706	-2.057354
H	-1.602913	0.124595	-2.105281
C	-3.459084	-0.861753	-1.926667
C	-3.805286	-0.379323	-0.520118
H	-3.920759	-0.193737	-2.650157
H	-3.784204	-1.885600	-2.107632
O	-4.088941	0.778683	-0.277937
N	-3.661424	-1.311345	0.459403
H	-3.320252	-2.233577	0.220265
C	-3.827632	-0.923538	1.830231
C	-2.735933	0.002340	2.334601
H	-4.778890	-0.406872	1.977289
H	-3.830384	-1.807644	2.470395
O	-1.691197	0.258638	1.777063
O	-3.062124	0.499051	3.519087
H	-2.345414	1.058612	3.848406
N	2.169170	2.607262	0.614267
C	1.033242	1.964373	0.455615
C	1.097818	0.886098	-0.601576
O	1.975538	0.942843	-1.436979
H	2.910731	2.412596	-0.058534
H	0.304214	1.945725	1.260372
C	-0.345359	3.334406	-0.706672
N	0.133278	-0.046342	-0.494377
C	0.214093	-1.320500	-1.205642
H	-0.467305	-0.027761	0.330062
H	0.731459	-1.130128	-2.150046
C	0.977962	-2.375067	-0.380753
C	2.311633	-1.834930	0.062714
H	1.083838	-3.271509	-0.994651
H	0.363545	-2.650561	0.479932
C	4.692026	-0.533947	0.769728
C	2.433194	-1.172453	1.286450
C	3.419400	-1.863182	-0.781756
C	4.602495	-1.222184	-0.438843
C	3.607444	-0.522985	1.644593
H	1.593652	-1.170602	1.976673
H	3.355487	-2.377743	-1.735068
H	5.452543	-1.249345	-1.112746
H	3.714309	-0.027210	2.602265
O	5.805591	0.144266	1.153889
H	6.529816	-0.025946	0.544341
H	2.348176	3.234630	1.385797
C	-1.710551	2.740185	-0.649276
H	-1.983611	2.271488	-1.597702
H	-1.825906	1.982010	0.132751
H	-2.456414	3.505719	-0.418680
C	0.361939	3.474424	-2.002100
H	1.425350	3.686778	-1.888312
H	0.232621	2.598575	-2.640304
H	-0.088947	4.331151	-2.524807
H	-0.102496	4.072125	0.053224

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