Conformational profile of a proline-arginine hybrid

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Figure SI1. Rational design of arginine surrogates with a proline skeleton. Combination of the latter frame with the guanidilated side chain of arginine generates the proline-like analogues studied previously [($^{\gamma}$Pro)Arg (ref. 8)] and in the present work [*trans*-($^{\beta}$Pro)Arg and *cis*-($^{\beta}$Pro)Arg]. The arginine surrogates are named according to the γ/β position of the proline skeleton bearing the guanidilated side chain and to the *trans*/*cis* relative orientation between this side chain and the carboxylic acid.

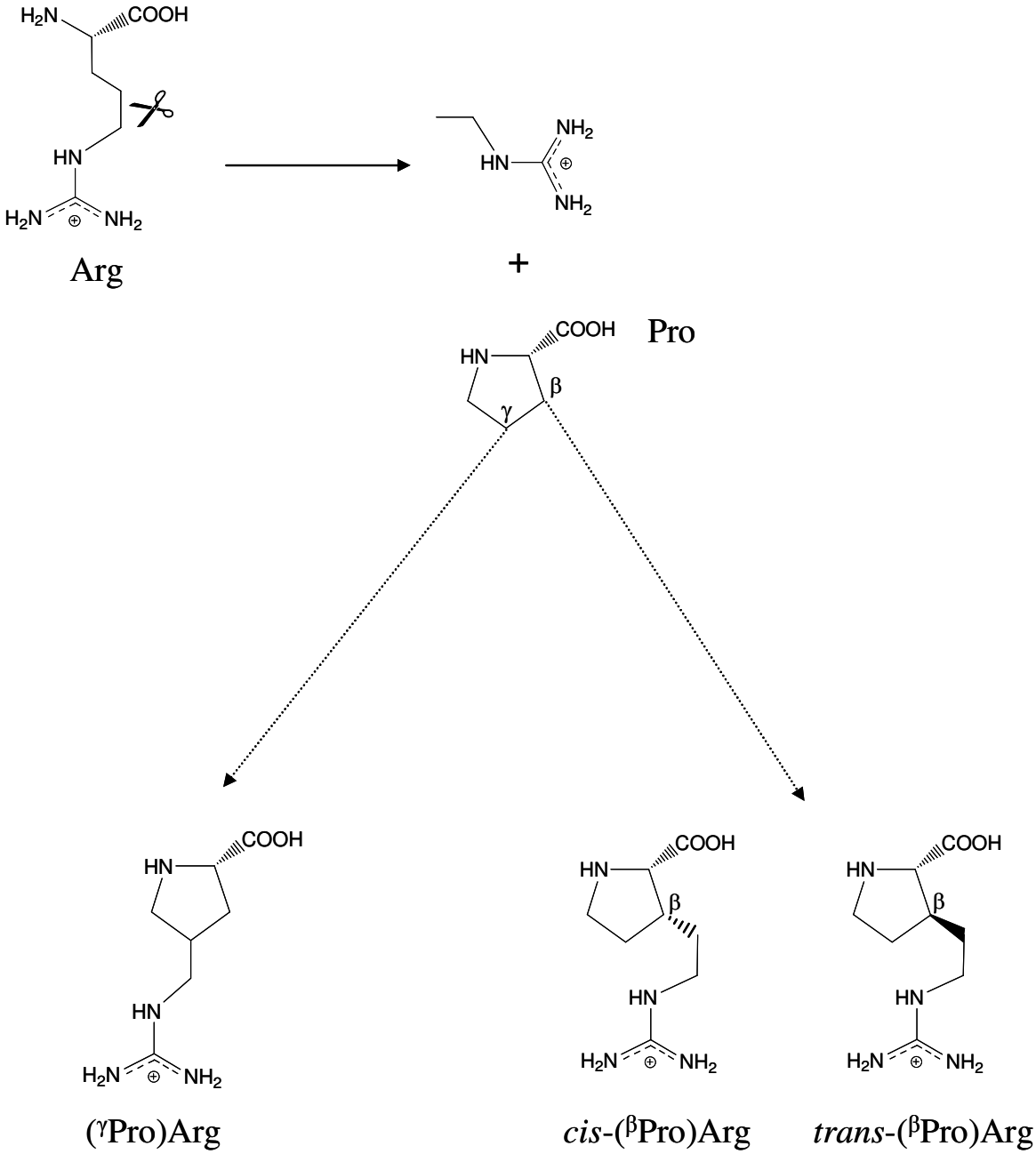

Table SI1. Dihedral angles (in degrees; see Figure 2 for definition) and relative energy (ΔE^{gp}; in kcal/mol) of the minimum energy conformations characterized for Ac-*t*-($^{\beta}$Pro)Arg-NHMe in the gas phase at the B3LYP/6-31+G(d,p) level.

Conformation	ω_0	φ	ψ	ω	χ^0	χ^1	χ^2	χ^3	χ^4	ξ^1	ξ^2	ξ^3	ΔE^{gp}
γ_L[u]s$^-$g$^+$t	–169.6	–77.8	54.8	178.2	–1.7	–22.3	37.5	–38.2	25.2	–127.0	61.1	162.8	0.0
γ_L[u]g$^-$g$^-$s$^+$	–170.3	–79.9	59.5	179.1	–5.7	–18.4	34.9	–38.0	27.5	–84.2	–77.5	117.9	1.1
γ_L[u]g$^-$g$^-$s$^-$	–170.3	–80.5	56.1	179.3	–8.7	–15.1	32.5	–37.3	29.1	–59.8	–49.6	–115.6	1.5
α_L[u]s$^-$g$^+$t	–169.7	–89.7	–3.5	176.5	–13.5	–9.2	27.4	–35.4	30.7	–92.4	61.2	156.5	2.1
α_L[u]g$^+$g$^-$t	–170.2	–73.1	–20.2	179.0	9.7	–30.7	40.2	–34.5	15.5	39.5	–77.7	–173.8	3.0
α_L[u]g$^-$tg$^-$	–169.9	–76.5	–16.0	177.2	3.0	–24.6	36.8	–35.1	20.0	–88.4	155.2	–86.1	3.5
γ_L[u]s$^-$tg$^-$	–169.4	–73.5	44.0	177.3	3.2	–26.6	39.6	–37.4	21.5	–126.2	157.4	–87.1	3.7
α_L[u]g$^+$tg$^+$	–169.9	–72.3	–17.7	178.0	11.5	–32.6	41.3	–34.4	14.3	52.8	–159.1	88.0	5.0
γ_L[u]tg$^+$g$^+$	–169.8	–76.6	53.3	177.1	0.1	–23.6	37.7	–37.2	23.5	–167.7	51.1	64.1	5.4
δ_L[^{a}]g$^-$g$^+$t	–177.6	–122.4	17.2	174.7	–36.8	40.9	–31.2	10.0	16.6	–59.1	81.9	177.8	7.0
γ_L[u]g$^-$g$^+$s$^-$	–171.9	–81.5	75.6	–163.6	–7.1	–17.0	33.7	–37.2	27.9	–74.5	68.7	–147.1	10.4
γ_L[^{a}]g$^+$g$^-$t	179.0	–113.3	88.4	–175.7	–35.3	15.4	8.4	–28.9	40.3	70.9	–64.7	–166.6	10.4
γ_L[^{a}]g$^+$g$^-$g$^-$	173.3	–92.3	75.2	–176.5	–34.2	16.8	4.8	–24.7	37.2	65.2	–61.4	–85.4	10.6
γ_L[u]g$^-$tt	–171.1	–79.0	49.1	177.9	–6.5	–17.6	34.3	–37.8	28.0	–69.4	–175.2	–175.4	10.6
γ_L[u]ttt	–171.9	–78.5	57.2	178.0	–2.5	–21.3	36.3	–37.3	25.2	–164.1	173.7	172.8	14.5
ε_L[^{a}]g$^+$ts$^+$	173.3	–108.1	179.8	–178.0	–39.7	24.2	–2.1	–20.5	38.0	59.5	–151.5	96.3	15.1
γ_L[u]tts$^+$	–172.1	–78.5	57.4	178.1	–2.0	–21.9	36.8	–37.4	25.0	–162.7	166.5	91.1	15.3
γ_L[^{a}]g$^+$g$^+$s$^-$	–179.5	–99.4	74.5	–176.4	–23.2	–1.9	24.7	–38.0	38.6	37.9	67.3	–143.0	15.8
γ_L[u]g$^+$tg$^-$	–172.8	–79.6	57.7	178.7	–4.1	–20.5	36.6	–38.5	27.1	65.0	–171.1	–80.5	18.3
γ_L[d]s$^-$g$^-$s$^-$	–173.5	–83.5	67.1	–179.1	–13.5	30.7	–37.7	28.9	–9.3	–140.8	–57.7	–96.9	19.0
ε_L[^{a}]tg$^-$t	166.3	–80.7	179.7	–176.0	–31.9	41.6	–34.7	15.5	10.0	–175.0	–80.0	–169.4	25.3

[a] Different envelope or twisted (half-chair) conformations with one or two atoms of the five-membered ring other than the γ carbon deviating out of the ring plane.

Table SI2. Dihedral angles (in degrees; see Figure 2 for definition) and relative energy (ΔE^{gp}; in kcal/mol) of the minimum energy conformations characterized for Ac-*c*-($^{\beta}$Pro)Arg-NHMe in the gas phase at the B3LYP/6-31+G(d,p) level.

Conformation	ω_0	φ	ψ	ω	χ^0	χ^1	χ^2	χ^3	χ^4	ξ^1	ξ^2	ξ^3	ΔE^{gp}
α_L[d]g^+g^-t	–169.7	–86.3	–11.6	175.3	–12.4	31.7	–39.6	32.0	–12.2	75.3	–71.4	178.9	0.0
α_L[d]g^+ts^+	–169.2	–90.1	–4.3	174.5	–14.8	33.5	–40.1	31.0	–10.0	69.2	–172.0	95.2	1.3
γ_L[d]s^-g^+t	–171.1	–84.1	75.5	–176.7	–18.1	35.0	–39.5	28.3	–6.3	–116.3	70.4	164.2	2.0
γ_L[d]s^-ts^-	–170.3	–83.1	66.4	–178.5	–16.0	34.1	–40.0	30.0	–8.8	–104.8	168.1	–93.4	3.1
γ_L[u]s^+g^-t	–168.7	–66.8	31.8	174.5	8.9	–32.1	43.4	–38.2	18.1	127.7	–65.4	178.3	3.9
γ_L[d]$g^-g^-s^+$	–175.9	–83.6	80.9	–175.2	–19.1	36.1	–40.2	28.2	–5.9	–76.4	–70.6	122.9	5.1
γ_L[u]s^+ts^+	–169.1	–73.5	47.9	174.7	4.1	–28.8	42.7	–40.4	22.6	112.6	–170.4	92.2	5.4
ε_L[u]g^-g^+t	–172.3	–56.3	133.9	–177.1	15.6	–31.5	36.5	–27.8	7.4	–75.9	72.2	169.3	5.4
ε_L[u]g^-ct	–162.4	–79.9	169.9	175.2	16.6	–39.5	45.7	–36.8	12.7	–71.3	–7.3	–165.5	5.5
α_L[u]$g^+g^+s^-$	–168.5	–78.5	–8.5	173.3	0.6	–23.2	37.0	–37.0	22.7	84.3	55.7	–110.0	5.7
γ_L[u]$s^+g^+s^-$	–168.5	–64.1	20.3	174.8	11.9	–33.8	43.6	–36.7	15.3	97.7	54.4	–107.7	6.0
γ_L[u]g^-tg^-	–171.6	–80.2	83.7	–177.3	–5.7	–16.8	32.5	–36.0	26.0	–71.0	176.4	–90.0	6.5
γ_L[^{a}]$g^-g^-s^-$	–173.4	–84.8	82.6	–173.7	–22.4	37.8	–40.5	26.8	–2.6	–52.0	–53.1	–108.5	7.3
γ_L[u]tg^-g^-	–169.0	–68.3	32.5	–174.8	7.7	–29.9	41.0	–36.6	18.0	158.1	–51.3	–68.2	8.9
γ_L[^{a}]ttt	–174.5	–84.6	78.3	–174.8	–20.0	35.4	–38.5	26.3	–3.9	172.4	178.1	–172.5	13.7
γ_L[^{a}]g^+g^+t	–173.4	–85.4	67.9	–175.6	–20.0	35.5	–38.9	26.6	–4.0	45.5	61.0	–158.6	13.8
γ_L[^{a}]$g^+g^+g^+$	–174.3	–85.2	72.4	–175.6	–20.1	35.4	–38.6	26.3	–3.7	49.3	59.2	89.5	14.7
γ_L[^{a}]tg^-t	–175.7	–84.3	80.0	–174.7	–21.5	36.0	–38.0	25.0	–2.0	175.4	–66.9	–166.9	15.4
γ_L[^{a}]tg^-g^-	–175.6	–83.5	78.9	–174.4	–21.1	35.9	–38.2	25.4	–2.6	172.0	–67.7	–87.5	15.7
α_L[d]ttc	–168.5	–88.8	0.7	172.8	–13.4	31.8	–38.7	30.7	–10.9	169.1	174.6	26.7	17.3
γ_L[u]ttc	–172.0	–84.2	78.4	–175.7	–16.2	–7.3	26.8	–36.3	33.2	173.2	172.8	26.5	18.1
γ_L[u]g^-g^+t	–166.3	–60.7	3.5	172.2	12.7	–29.0	33.4	–25.1	7.5	–69.9	71.5	175.0	18.8
α_L[d]$g^-g^-s^-$	–168.5	–72.6	–27.2	162.5	–2.4	25.3	–38.3	36.0	–21.5	–50.8	–45.5	–99.6	21.6

[a] Envelope conformation with the β carbon deviating out of the ring plane.

Cartesian coordinates and relative energies of all the structures calculated for Ac-*t*-($^{\beta}$Pro)Arg-NHMe

γ_L[u]s$^-$g$^+$t	0.0000000		
C	0.00000	0.00000	0.00000
H	1.09000	0.00000	0.00000
H	-0.36500	1.03100	0.00000
H	-0.34500	-0.48200	0.92200
C	-0.46200	-0.77200	-1.21800
O	0.33900	-1.43800	-1.89000
N	-1.78200	-0.70500	-1.57000
C	-2.85800	-0.15100	-0.72100
H	-2.51300	-0.00900	0.30200
H	-3.18800	0.82100	-1.10900
C	-3.96000	-1.20400	-0.84100
H	-4.94700	-0.81500	-0.57500
H	-3.73800	-2.05300	-0.18300
C	-3.86600	-1.62600	-2.31800
H	-4.30600	-0.81400	-2.90900
C	-4.57800	-2.95900	-2.67400
H	-3.88000	-3.65200	-3.15900
H	-4.91700	-3.45700	-1.76000
C	-5.79700	-2.79300	-3.59200
H	-6.25200	-3.77400	-3.77600
H	-6.55000	-2.14900	-3.11600
N	-5.36200	-2.20200	-4.86100
H	-4.42000	-1.74600	-4.85700
C	-6.02300	-2.18900	-6.00400
N	-7.29100	-2.63500	-6.10300
H	-7.72300	-2.78400	-7.00300
H	-7.79700	-2.94500	-5.28900
N	-5.40200	-1.73100	-7.11200
H	-5.93000	-1.45200	-7.92500
H	-4.45400	-1.38300	-7.03000
C	-2.34000	-1.61200	-2.60500
H	-1.89900	-2.60600	-2.44900
C	-2.01600	-1.21700	-4.07200
O	-2.92600	-1.10300	-4.93100
N	-0.73300	-1.06000	-4.38000
H	-0.05900	-1.23000	-3.62600
C	-0.28000	-0.72900	-5.72700
H	-0.77400	0.17800	-6.08600
H	0.79700	-0.56300	-5.69500
H	-0.49600	-1.54400	-6.42500

γ_L[u]g⁻g⁻s⁺	1.1000000		
C	0.00000	0.00000	0.00000
H	1.09000	0.00000	0.00000
H	-0.36400	1.03100	0.00000
H	-0.34600	-0.48200	0.92100
C	-0.46200	-0.76900	-1.22000
O	0.33800	-1.42600	-1.90100
N	-1.78500	-0.71100	-1.56200
C	-2.86600	-0.16600	-0.72100
H	-2.52000	0.00600	0.29700
H	-3.22200	0.78900	-1.12800
C	-3.94100	-1.24800	-0.81600
H	-4.93900	-0.88100	-0.55800
H	-3.69700	-2.07400	-0.13700
C	-3.85000	-1.71200	-2.28300
H	-4.37700	-0.97600	-2.90100
C	-4.46600	-3.10500	-2.51300
H	-3.75100	-3.87800	-2.20500
H	-5.33300	-3.22500	-1.84900
C	-4.91900	-3.42800	-3.94600
H	-4.17700	-3.12400	-4.68600
H	-5.06400	-4.50800	-4.05200
N	-6.20600	-2.79000	-4.29200
H	-7.01700	-3.13500	-3.79500
C	-6.44600	-1.88300	-5.25100
N	-5.46800	-1.17400	-5.80200
H	-5.65200	-0.63900	-6.63800
H	-4.52000	-1.10200	-5.38100
N	-7.72500	-1.68800	-5.64200
H	-7.98000	-0.88500	-6.19600
H	-8.43800	-2.38200	-5.47500
C	-2.33400	-1.60800	-2.61100
H	-1.83700	-2.58200	-2.50200
C	-2.04800	-1.12900	-4.05700
O	-2.97000	-0.92000	-4.87600
N	-0.76500	-0.99800	-4.39000
H	-0.07800	-1.21000	-3.66000
C	-0.33700	-0.57500	-5.71900
H	0.75200	-0.51200	-5.72500
H	-0.66000	-1.29300	-6.47900
H	-0.75700	0.40300	-5.96800

γ_L[u]g¯g¯s¯	1.5000000		
C	0.00000	0.00000	0.00000
H	1.08900	0.00000	0.00000
H	-0.36300	1.03200	0.00000
H	-0.35000	-0.48100	0.92000
C	-0.46300	-0.76100	-1.22400
O	0.34400	-1.36600	-1.94700
N	-1.79600	-0.75900	-1.52600
C	-2.87700	-0.21400	-0.68800
H	-2.52700	-0.01700	0.32500
H	-3.24800	0.72900	-1.11100
C	-3.93800	-1.31100	-0.75400
H	-4.94000	-0.94800	-0.50700
H	-3.68500	-2.11300	-0.04900
C	-3.84100	-1.81700	-2.20800
H	-4.40900	-1.12600	-2.83900
C	-4.43000	-3.23000	-2.36700
H	-3.90600	-3.92400	-1.69600
H	-5.47400	-3.19800	-2.03200
C	-4.38400	-3.84800	-3.77600
H	-3.35400	-4.09600	-4.05800
H	-4.93900	-4.78900	-3.77400
N	-4.90200	-2.94000	-4.80400
H	-4.30700	-2.08900	-4.91600
C	-5.96500	-3.07500	-5.57600
N	-6.70600	-4.19900	-5.61700
H	-7.60500	-4.21000	-6.07400
H	-6.42500	-5.03400	-5.13000
N	-6.34800	-2.03500	-6.35200
H	-6.93100	-2.18800	-7.16100
H	-5.80100	-1.18400	-6.34300
C	-2.33900	-1.65200	-2.57700
H	-1.79200	-2.60300	-2.51400
C	-2.13100	-1.11000	-4.02100
O	-3.09100	-0.97300	-4.81700
N	-0.87700	-0.83700	-4.37200
H	-0.15200	-1.02500	-3.67200
C	-0.52200	-0.33700	-5.69700
H	-1.06700	0.58500	-5.91800
H	0.54900	-0.13600	-5.71200
H	-0.76200	-1.07400	-6.46900

α_L[u]s$^-$g$^+$t	2.1000000		
C	0.00000	0.00000	0.00000
H	1.09000	0.00000	0.00000
H	-0.36500	1.03200	0.00000
H	-0.34700	-0.47800	0.92300
C	-0.46400	-0.77700	-1.21500
O	0.30700	-1.43100	-1.91100
N	-1.80900	-0.71000	-1.55100
C	-2.90500	-0.21000	-0.70400
H	-2.54900	0.04200	0.29400
H	-3.34800	0.69300	-1.14500
C	-3.89400	-1.37500	-0.71100
H	-4.91700	-1.07300	-0.46900
H	-3.57900	-2.12000	0.03000
C	-3.79100	-1.98200	-2.13300
H	-4.49700	-1.45800	-2.79100
C	-4.14600	-3.49200	-2.10000
H	-3.26100	-4.06800	-1.80300
H	-4.88800	-3.64100	-1.30800
C	-4.76900	-4.12200	-3.35500
H	-4.97800	-5.17300	-3.12600
H	-5.72600	-3.63400	-3.58600
N	-3.88100	-4.03300	-4.51300
H	-3.34400	-3.13900	-4.62100
C	-3.88400	-4.80600	-5.58900
N	-4.60900	-5.93900	-5.66700
H	-4.62200	-6.49600	-6.50700
H	-5.19300	-6.23900	-4.90400
N	-3.12700	-4.43900	-6.64200
H	-2.97000	-5.05400	-7.42400
H	-2.58700	-3.58400	-6.58900
C	-2.32000	-1.62900	-2.57600
H	-1.68100	-2.51800	-2.58500
C	-2.22900	-1.06300	-4.00000
O	-2.57500	-1.77300	-4.97400
N	-1.78300	0.18300	-4.15400
H	-1.44900	0.64800	-3.32000
C	-1.57900	0.81000	-5.45700
H	-1.57000	1.89300	-5.32800
H	-0.63100	0.49100	-5.90100
H	-2.39400	0.53100	-6.12600

$\alpha_L[u]g^+g^-t$	3.0000000		
C	0.00000	0.00000	0.00000
H	1.09000	0.00000	0.00000
H	-0.37000	1.02900	0.00000
H	-0.34000	-0.48000	0.92500
C	-0.47000	-0.78900	-1.20400
O	0.26600	-1.55700	-1.81900
N	-1.77800	-0.60500	-1.62500
C	-2.87600	-0.06100	-0.79000
H	-2.59900	-0.05500	0.26500
H	-3.11000	0.96900	-1.08600
C	-4.04800	-1.00200	-1.09400
H	-5.02000	-0.53400	-0.91300
H	-3.98200	-1.90000	-0.46700
C	-3.83400	-1.35500	-2.57700
H	-4.09000	-0.46100	-3.16100
C	-4.71300	-2.50000	-3.13300
H	-5.71600	-2.37800	-2.71000
H	-4.82900	-2.38400	-4.21600
C	-4.27100	-3.95000	-2.86700
H	-3.95600	-4.08300	-1.82200
H	-5.12800	-4.61100	-3.04700
N	-3.17900	-4.31200	-3.77800
H	-2.70700	-3.52500	-4.28800
C	-2.63400	-5.51100	-3.90900
N	-3.06600	-6.57100	-3.19900
H	-2.73800	-7.50300	-3.40200
H	-3.85500	-6.48900	-2.57600
N	-1.62500	-5.67600	-4.78800
H	-1.06700	-6.51600	-4.79000
H	-1.23600	-4.86200	-5.24700
C	-2.28900	-1.52900	-2.64700
H	-1.99000	-2.54700	-2.37100
C	-1.74700	-1.32100	-4.06200
O	-1.88700	-2.24300	-4.90000
N	-1.21400	-0.13800	-4.36800
H	-1.06100	0.50300	-3.60000
C	-0.64400	0.17800	-5.67600
H	-0.73000	1.25100	-5.85200
H	0.41000	-0.11400	-5.72400
H	-1.19700	-0.36200	-6.44500

α_L[u]g⁻tg⁻	3.5000000		
C	0.00000	0.00000	0.00000
H	1.09000	0.00000	0.00000
H	-0.36800	1.03000	0.00000
H	-0.34200	-0.47900	0.92500
C	-0.46700	-0.78700	-1.20700
O	0.28200	-1.52100	-1.84600
N	-1.78700	-0.63900	-1.60400
C	-2.88000	-0.08500	-0.77600
H	-2.57900	-0.00400	0.26800
H	-3.16100	0.91600	-1.12700
C	-4.01800	-1.08600	-0.99000
H	-5.00400	-0.65600	-0.79300
H	-3.88600	-1.94900	-0.32500
C	-3.85100	-1.52500	-2.45800
H	-4.25400	-0.72700	-3.09800
C	-4.56600	-2.85200	-2.78600
H	-3.92100	-3.68800	-2.49100
H	-5.47200	-2.93300	-2.17400
C	-4.95800	-3.00400	-4.27300
H	-5.92200	-2.52800	-4.47000
H	-4.23100	-2.52300	-4.92600
N	-5.08800	-4.40700	-4.69700
H	-5.96600	-4.87200	-4.50900
C	-4.07400	-5.17400	-5.12900
N	-2.84200	-4.69200	-5.25200
H	-2.12400	-5.27100	-5.66300
H	-2.57100	-3.70900	-5.03600
N	-4.32500	-6.47000	-5.42600
H	-3.59500	-7.06700	-5.78500
H	-5.26900	-6.81800	-5.49500
C	-2.29800	-1.56600	-2.62500
H	-1.91600	-2.57200	-2.41500
C	-1.84400	-1.26200	-4.05500
O	-2.01700	-2.11700	-4.95000
N	-1.32900	-0.05500	-4.30500
H	-1.13700	0.52900	-3.50200
C	-0.80300	0.34000	-5.60900
H	-0.84300	1.42700	-5.69300
H	0.23200	0.00500	-5.73200
H	-1.41400	-0.10800	-6.39400

γ_L[u]s$^-$tg$^-$	3.7000000		
C	0.00000	0.00000	0.00000
H	1.09000	0.00000	0.00000
H	-0.36500	1.03100	0.00000
H	-0.34600	-0.48200	0.92200
C	-0.46200	-0.77300	-1.21700
O	0.33800	-1.44600	-1.88500
N	-1.78100	-0.70100	-1.57100
C	-2.84500	-0.11500	-0.72300
H	-2.51700	-0.03300	0.31300
H	-3.10700	0.88900	-1.08100
C	-4.01000	-1.09100	-0.90500
H	-4.97500	-0.63900	-0.65800
H	-3.86900	-1.96900	-0.26400
C	-3.88800	-1.47300	-2.38600
H	-4.20900	-0.60400	-2.97400
C	-4.68800	-2.70700	-2.86400
H	-4.01600	-3.41000	-3.36700
H	-5.11100	-3.24700	-2.00900
C	-5.81100	-2.32300	-3.84700
H	-6.70100	-1.97000	-3.32000
H	-5.48000	-1.51100	-4.49800
N	-6.24100	-3.43200	-4.71300
H	-6.93700	-4.07100	-4.35500
C	-5.66900	-3.74500	-5.88400
N	-4.57200	-3.12300	-6.30900
H	-4.26700	-3.25400	-7.26200
H	-3.98900	-2.50000	-5.72100
N	-6.23100	-4.71200	-6.64200
H	-5.75900	-5.07300	-7.45700
H	-7.17900	-5.01700	-6.48400
C	-2.35900	-1.60000	-2.60000
H	-2.01700	-2.62400	-2.38200
C	-1.99700	-1.33600	-4.08300
O	-2.88900	-1.42500	-4.95900
N	-0.72700	-1.06800	-4.37600
H	-0.05600	-1.15900	-3.60600
C	-0.26200	-0.86000	-5.74300
H	0.73200	-0.41200	-5.70600
H	-0.20500	-1.80600	-6.29300
H	-0.94300	-0.18900	-6.27100

$\alpha_L[u]g^+tg^+$	5.0000000		
C	0.00000	0.00000	0.00000
H	1.09000	0.00000	0.00000
H	-0.37000	1.02900	0.00000
H	-0.33900	-0.48000	0.92600
C	-0.46900	-0.79100	-1.20400
O	0.26600	-1.56500	-1.81100
N	-1.77300	-0.59700	-1.63500
C	-2.86800	-0.04100	-0.80300
H	-2.60100	-0.05200	0.25500
H	-3.07900	0.99700	-1.08900
C	-4.06100	-0.95400	-1.12300
H	-5.02200	-0.46300	-0.94500
H	-4.01900	-1.85700	-0.50100
C	-3.83000	-1.29100	-2.60600
H	-4.03600	-0.37500	-3.17700
C	-4.69000	-2.39200	-3.25000
H	-5.74700	-2.14300	-3.09900
H	-4.51800	-2.35800	-4.33100
C	-4.42900	-3.83000	-2.76300
H	-3.36600	-4.01700	-2.60000
H	-4.93500	-4.03500	-1.81600
N	-4.89500	-4.84900	-3.71700
H	-5.85900	-5.14800	-3.65800
C	-4.16700	-5.34100	-4.73200
N	-3.00200	-4.80400	-5.08100
H	-2.40900	-5.30600	-5.72700
H	-2.69300	-3.83400	-4.85000
N	-4.63800	-6.42200	-5.39300
H	-4.23100	-6.71200	-6.26900
H	-5.33800	-7.02300	-4.98400
C	-2.29300	-1.52200	-2.65100
H	-2.02500	-2.54400	-2.35900
C	-1.75400	-1.37500	-4.07000
O	-1.97200	-2.29600	-4.88600
N	-1.14300	-0.23500	-4.40400
H	-0.92700	0.40100	-3.64700
C	-0.54900	0.00600	-5.71600
H	-0.53400	1.08000	-5.90700
H	0.47200	-0.38500	-5.76200
H	-1.15200	-0.49000	-6.47700

γ_L[u]tg$^+$g$^+$	5.4000000		
C	0.00000	0.00000	0.00000
H	1.08961	0.00000	0.00000
H	-0.36516	1.03107	0.00000
H	-0.34510	-0.48225	0.92181
C	-0.46244	-0.77257	-1.21739
O	0.33438	-1.44513	-1.88639
N	-1.78281	-0.70034	-1.56983
C	-2.85451	-0.13352	-0.72622
H	-2.52149	-0.02011	0.30499
H	-3.15270	0.85474	-1.09989
C	-3.99216	-1.14871	-0.87891
H	-4.96553	-0.71669	-0.62774
H	-3.81896	-2.00857	-0.21985
C	-3.87071	-1.55924	-2.35520
H	-4.27247	-0.74000	-2.96233
C	-4.55593	-2.86435	-2.77339
H	-4.16171	-3.19580	-3.73792
H	-4.30499	-3.66052	-2.06000
C	-6.08644	-2.82011	-2.84066
H	-6.45986	-3.77262	-3.23347
H	-6.50095	-2.69774	-1.83715
N	-6.69784	-1.71233	-3.62461
H	-7.50141	-1.28138	-3.18726
C	-6.59447	-1.48199	-4.94850
N	-5.47195	-1.72919	-5.61707
H	-5.49570	-1.67240	-6.62642
H	-4.52549	-1.61549	-5.19046
N	-7.66600	-0.97372	-5.59300
H	-7.56704	-0.52525	-6.49219
H	-8.59876	-1.06127	-5.21752
C	-2.34556	-1.60008	-2.60587
H	-1.94113	-2.60810	-2.43081
C	-2.01689	-1.25160	-4.08101
O	-2.92903	-1.17929	-4.93642
N	-0.73415	-1.09567	-4.39746
H	-0.05619	-1.24651	-3.64460
C	-0.28981	-0.82792	-5.76159
H	0.78973	-0.67663	-5.74693
H	-0.52765	-1.66730	-6.42234
H	-0.77546	0.06922	-6.15402

$\delta_L[^a]g^-g^+t$	7.0000000		
C	0.00000	0.00000	0.00000
H	1.09075	0.00000	0.00000
H	-0.37137	1.02678	0.00000
H	-0.33069	-0.48319	0.92746
C	-0.47181	-0.80051	-1.19189
O	0.24459	-1.70720	-1.66886
N	-1.69111	-0.50283	-1.72357
C	-2.81581	0.09060	-0.94632
H	-2.62387	-0.01807	0.12214
H	-2.91806	1.15716	-1.16592
C	-4.06944	-0.71167	-1.41141
H	-4.71118	-0.08751	-2.03831
H	-4.66992	-1.03970	-0.55838
C	-3.52186	-1.89712	-2.24562
H	-4.20765	-2.16184	-3.05454
C	-3.27136	-3.14275	-1.36736
H	-2.70986	-2.88048	-0.45965
H	-4.24606	-3.49593	-1.01433
C	-2.57764	-4.33847	-2.04445
H	-2.80732	-5.25056	-1.48082
H	-2.95072	-4.46229	-3.06910
N	-1.11717	-4.14623	-2.07747
H	-0.74898	-3.20524	-1.91452
C	-0.21320	-4.99913	-2.55209
N	-0.52256	-6.28627	-2.78449
H	0.11009	-6.89563	-3.28053
H	-1.40658	-6.67190	-2.49105
N	1.02522	-4.54764	-2.81218
H	1.80181	-5.17933	-2.93427
H	1.21324	-3.55229	-2.73450
C	-2.24238	-1.27137	-2.85158
H	-1.50044	-1.98914	-3.19394
C	-2.58412	-0.42919	-4.10324
O	-3.29884	-0.92568	-4.97027
N	-2.03313	0.80377	-4.18423
H	-1.40118	1.09101	-3.45063
C	-2.18689	1.65061	-5.36467
H	-2.12599	2.69905	-5.06670
H	-1.41277	1.44153	-6.11087
H	-3.16170	1.45465	-5.81254

$\gamma_L[u]g^-g^+s^-$	10.4000000		
C	0.00000	0.00000	0.00000
H	1.08970	0.00000	0.00000
H	-0.36493	1.03113	0.00000
H	-0.34555	-0.48216	0.92168
C	-0.46411	-0.77217	-1.21755
O	0.32704	-1.45127	-1.88663
N	-1.78538	-0.69828	-1.56566
C	-2.87480	-0.13812	-0.76071
H	-2.55590	0.01447	0.27012
H	-3.20116	0.82709	-1.16818
C	-3.95765	-1.20082	-0.89289
H	-4.96052	-0.82976	-0.66223
H	-3.72759	-2.02554	-0.20656
C	-3.81077	-1.66753	-2.33404
H	-4.30447	-0.91933	-2.96490
C	-4.43031	-3.03640	-2.65136
H	-3.81690	-3.84295	-2.22779
H	-5.41961	-3.09008	-2.17647
C	-4.59413	-3.23771	-4.16057
H	-5.19501	-4.13505	-4.34455
H	-5.11404	-2.38560	-4.60826
N	-3.28206	-3.37208	-4.82641
H	-2.55586	-3.88559	-4.34388
C	-3.02845	-2.94302	-6.06203
N	-4.01552	-2.43718	-6.81426
H	-3.82369	-1.97730	-7.69175
H	-4.97821	-2.47423	-6.50980
N	-1.78137	-3.00492	-6.56406
H	-1.59918	-2.84020	-7.54277
H	-0.99203	-3.24111	-5.98164
C	-2.30789	-1.56685	-2.62631
H	-1.78828	-2.53040	-2.53303
C	-2.06917	-1.02146	-4.06432
O	-3.00184	-0.57537	-4.74360
N	-0.79711	-1.13608	-4.50581
H	-0.11666	-1.37559	-3.78126
C	-0.31163	-0.37935	-5.65768
H	-0.05696	0.64941	-5.37790
H	0.57800	-0.86909	-6.05856
H	-1.08587	-0.34745	-6.42499

$\gamma_L[^a]g^+g^-t$	10.4000000		
C	0.00000	0.00000	0.00000
H	1.09045	0.00000	0.00000
H	-0.36407	1.02966	0.00000
H	-0.34071	-0.48129	0.92458
C	-0.47133	-0.77928	-1.20650
O	0.28617	-1.60462	-1.77579
N	-1.72969	-0.58015	-1.65577
C	-2.87739	-0.04550	-0.89548
H	-2.59132	0.19773	0.12720
H	-3.24975	0.85776	-1.38679
C	-3.90256	-1.19571	-0.99232
H	-4.92753	-0.81997	-0.95998
H	-3.77473	-1.87019	-0.13865
C	-3.59507	-1.91907	-2.33958
H	-4.36937	-1.64730	-3.06091
C	-3.58104	-3.46657	-2.29232
H	-4.61097	-3.80077	-2.12019
H	-3.30665	-3.84453	-3.28496
C	-2.74182	-4.20931	-1.23682
H	-3.04644	-3.92700	-0.22131
H	-2.96055	-5.27553	-1.36029
N	-1.29051	-4.00507	-1.38294
H	-0.94769	-3.13084	-1.78223
C	-0.32987	-4.71189	-0.78143
N	-0.59376	-5.89106	-0.19097
H	0.12718	-6.40261	0.29459
H	-1.49013	-6.33994	-0.29237
N	0.91646	-4.21834	-0.76631
H	1.70476	-4.78267	-0.48895
H	1.07404	-3.26531	-1.10072
C	-2.27142	-1.27895	-2.83863
H	-1.53926	-1.99980	-3.20259
C	-2.51425	-0.22658	-3.95305
O	-3.59310	0.34929	-4.05993
N	-1.44916	0.00496	-4.75810
H	-0.57562	-0.46205	-4.55712
C	-1.46942	1.02848	-5.80110
H	-0.75043	0.76069	-6.57725
H	-2.47031	1.07392	-6.23195
H	-1.21796	2.01618	-5.39965

$\gamma_L[^a]g^+g^-g^-$	10.6000000		
C	0.00000	0.00000	0.00000
H	1.08954	0.00000	0.00000
H	-0.36333	1.03211	0.00000
H	-0.35252	-0.47463	0.92252
C	-0.47422	-0.74968	-1.22446
O	0.33519	-1.34120	-1.97752
N	-1.80100	-0.78561	-1.49014
C	-2.91930	-0.27332	-0.67701
H	-2.62191	-0.14375	0.36369
H	-3.24834	0.69487	-1.07126
C	-4.02671	-1.30632	-0.90809
H	-5.04084	-0.90472	-0.85206
H	-3.92236	-2.03680	-0.09783
C	-3.71557	-1.97433	-2.29028
H	-4.45557	-1.60203	-3.00347
C	-3.76875	-3.51801	-2.35975
H	-4.79203	-3.84215	-2.13246
H	-3.57783	-3.82588	-3.39529
C	-2.85559	-4.33015	-1.42025
H	-3.06772	-4.10761	-0.37095
H	-3.06825	-5.39251	-1.55520
N	-1.41262	-4.09856	-1.61935
H	-1.03151	-3.28616	-1.15048
C	-0.57868	-4.68332	-2.48869
N	-0.88202	-5.86617	-3.05363
H	-0.31825	-6.23830	-3.80296
H	-1.59577	-6.46583	-2.67036
N	0.56848	-4.07003	-2.79752
H	1.31886	-4.57163	-3.24927
H	0.71237	-3.08385	-2.54215
C	-2.35097	-1.36495	-2.72959
H	-1.65345	-2.10494	-3.12083
C	-2.50045	-0.24314	-3.79822
O	-3.59322	0.23592	-4.08434
N	-1.33021	0.14339	-4.36068
H	-0.46941	-0.25544	-4.00585
C	-1.26107	1.23635	-5.32843
H	-0.32209	1.16033	-5.87898
H	-2.09778	1.15711	-6.02431
H	-1.31271	2.21368	-4.83649

γ_L[u]g¯tt	10.6000000		
C	0.00000	0.00000	0.00000
H	1.08958	0.00000	0.00000
H	−0.36328	1.03199	0.00000
H	−0.34805	−0.48108	0.92105
C	−0.46210	−0.76610	−1.22276
O	0.34202	−1.39516	−1.92603
N	−1.78986	−0.73724	−1.54172
C	−2.86610	−0.18056	−0.70437
H	−2.52217	−0.01346	0.31583
H	−3.21075	0.77906	−1.11184
C	−3.95661	−1.24755	−0.80416
H	−4.94927	−0.86159	−0.55515
H	−3.72915	−2.07400	−0.11889
C	−3.85850	−1.70906	−2.26912
H	−4.37644	−0.97936	−2.90125
C	−4.49848	−3.08636	−2.51249
H	−3.92827	−3.86253	−1.98417
H	−5.50940	−3.07351	−2.08195
C	−4.59856	−3.43327	−3.99862
H	−5.11959	−2.62978	−4.52845
H	−3.60388	−3.52835	−4.43988
N	−5.31949	−4.70796	−4.20178
H	−5.79852	−5.11990	−3.41154
C	−5.46754	−5.28296	−5.39422
N	−5.00478	−4.67393	−6.49485
H	−4.98668	−5.14526	−7.38678
H	−4.61634	−3.74161	−6.45353
N	−6.07363	−6.47973	−5.50714
H	−6.32057	−6.86190	−6.40761
H	−6.32575	−7.01953	−4.69301
C	−2.34276	−1.61469	−2.60145
H	−1.84747	−2.59274	−2.50801
C	−2.10554	−1.14118	−4.06426
O	−3.04031	−1.15137	−4.88133
N	−0.85060	−0.79046	−4.38185
H	−0.13015	−0.95136	−3.67666
C	−0.48285	−0.37179	−5.72874
H	0.50726	0.08481	−5.69282
H	−0.45871	−1.22086	−6.42161
H	−1.20468	0.35650	−6.10470

γ_L[u]ttt	14.5000000		
C	0.00000	0.00000	0.00000
H	1.08967	0.00000	0.00000
H	-0.36425	1.03157	0.00000
H	-0.34563	-0.48150	0.92207
C	-0.46262	-0.77061	-1.22042
O	0.33365	-1.43498	-1.89687
N	-1.78493	-0.70444	-1.56234
C	-2.86051	-0.14887	-0.72129
H	-2.53388	-0.03900	0.31271
H	-3.16659	0.83887	-1.09045
C	-3.98981	-1.17228	-0.88657
H	-4.96667	-0.74733	-0.63409
H	-3.81073	-2.03285	-0.22900
C	-3.86034	-1.57341	-2.36488
H	-4.28243	-0.77906	-2.99095
C	-4.51454	-2.89339	-2.79169
H	-4.12217	-3.15646	-3.78163
H	-4.25119	-3.69691	-2.09098
C	-6.03663	-2.77763	-2.90152
H	-6.49173	-2.60609	-1.91970
H	-6.28594	-1.94046	-3.56620
N	-6.59494	-4.02756	-3.45898
H	-5.93696	-4.66286	-3.89355
C	-7.89007	-4.31935	-3.56175
N	-8.81931	-3.40657	-3.24339
H	-9.79413	-3.65538	-3.16333
H	-8.57288	-2.43855	-3.10228
N	-8.28145	-5.54086	-3.96700
H	-9.23240	-5.71969	-4.25410
H	-7.62168	-6.29934	-4.05769
C	-2.33748	-1.56921	-2.63084
H	-1.89921	-2.57037	-2.50884
C	-2.05672	-1.12443	-4.09758
O	-2.99666	-0.97384	-4.88894
N	-0.76601	-0.98116	-4.43693
H	-0.06887	-1.18181	-3.72044
C	-0.36398	-0.61169	-5.78857
H	0.71501	-0.45206	-5.79695
H	-0.61700	-1.39976	-6.50551
H	-0.86832	0.30651	-6.10143

$\varepsilon_L[^a]g^+ts^+$	15.1000000		
C	0.00000	0.00000	0.00000
H	1.09004	0.00000	0.00000
H	-0.37005	1.02790	0.00000
H	-0.33959	-0.48698	0.92215
C	-0.46829	-0.77135	-1.21188
O	0.30732	-1.55050	-1.81081
N	-1.75100	-0.61679	-1.61185
C	-2.88366	-0.09519	-0.83035
H	-2.61686	0.00568	0.22151
H	-3.17293	0.88493	-1.21968
C	-3.98605	-1.15890	-1.07568
H	-4.96888	-0.69238	-1.17456
H	-4.04577	-1.84783	-0.22718
C	-3.57595	-1.91586	-2.38223
H	-4.35841	-1.79546	-3.13671
C	-3.34831	-3.43761	-2.21924
H	-4.29378	-3.92219	-1.94787
H	-3.06285	-3.84524	-3.19717
C	-2.25633	-3.82765	-1.19409
H	-1.48003	-3.06887	-1.12969
H	-2.67205	-3.92534	-0.18821
N	-1.59697	-5.10742	-1.50097
H	-2.09141	-5.95079	-1.24365
C	-0.43653	-5.26565	-2.15626
N	0.32943	-4.23588	-2.50916
H	1.18258	-4.41525	-3.01953
H	0.19414	-3.24948	-2.21426
N	-0.04840	-6.51875	-2.48324
H	0.88864	-6.70186	-2.80877
H	-0.61710	-7.32200	-2.26340
C	-2.27535	-1.19703	-2.84601
H	-1.54303	-1.88923	-3.26761
C	-2.51367	-0.06706	-3.88755
O	-2.29536	1.10830	-3.62341
N	-3.00756	-0.48179	-5.08428
H	-3.04731	-1.47003	-5.28790
C	-3.24334	0.45727	-6.18099
H	-3.86879	-0.02840	-6.93171
H	-3.75846	1.33907	-5.79685
H	-2.30419	0.77999	-6.64243

$\gamma_L[u]tts^+$	15.3000000		
C	0.00000	0.00000	0.00000
H	1.08968	0.00000	0.00000
H	-0.36448	1.03140	0.00000
H	-0.34500	-0.48168	0.92227
C	-0.46266	-0.77172	-1.21965
O	0.33115	-1.44620	-1.88872
N	-1.78239	-0.69468	-1.56976
C	-2.85846	-0.13619	-0.73128
H	-2.53492	-0.03074	0.30415
H	-3.15978	0.85343	-1.09882
C	-3.99384	-1.15300	-0.90461
H	-4.96958	-0.72447	-0.65432
H	-3.81867	-2.01820	-0.25103
C	-3.85823	-1.54392	-2.38515
H	-4.26419	-0.73470	-3.00311
C	-4.53271	-2.84469	-2.84065
H	-4.12827	-3.11224	-3.82252
H	-4.28584	-3.66531	-2.15112
C	-6.05268	-2.68723	-2.98898
H	-6.56716	-2.57396	-2.02956
H	-6.27159	-1.78926	-3.57267
N	-6.68690	-3.80530	-3.71955
H	-6.66365	-3.74986	-4.73037
C	-7.19033	-4.91822	-3.19031
N	-7.01206	-5.21010	-1.89284
H	-7.56231	-5.92350	-1.43792
H	-6.31947	-4.72967	-1.33910
N	-7.90737	-5.76292	-3.95373
H	-8.08988	-6.71075	-3.65837
H	-8.24293	-5.48904	-4.86565
C	-2.33449	-1.55643	-2.64075
H	-1.90616	-2.56147	-2.51493
C	-2.04138	-1.11749	-4.10690
O	-2.97546	-0.95797	-4.90354
N	-0.74763	-0.98913	-4.44051
H	-0.05546	-1.19585	-3.72115
C	-0.33571	-0.62448	-5.79068
H	0.74475	-0.47499	-5.79410
H	-0.59283	-1.41053	-6.50836
H	-0.82995	0.29818	-6.10630

$\gamma_L[^a]g^+g^+s^-$	15.8000000		
C	0.00000	0.00000	0.00000
H	1.09017	0.00000	0.00000
H	-0.36586	1.02959	0.00000
H	-0.34232	-0.48017	0.92460
C	-0.47018	-0.77564	-1.21075
O	0.30447	-1.55353	-1.81639
N	-1.74398	-0.60936	-1.63324
C	-2.88830	-0.11459	-0.84518
H	-2.59191	0.12520	0.17550
H	-3.29828	0.78697	-1.31378
C	-3.86471	-1.29554	-0.95015
H	-4.89825	-1.00301	-0.74549
H	-3.58001	-2.06199	-0.21924
C	-3.68052	-1.80012	-2.40543
H	-4.36878	-1.23578	-3.04264
C	-3.98043	-3.29718	-2.65076
H	-4.88484	-3.57303	-2.09208
H	-4.24555	-3.43001	-3.70667
C	-2.88673	-4.34402	-2.39199
H	-3.25277	-5.31694	-2.74145
H	-1.97894	-4.13312	-2.95657
N	-2.50076	-4.50972	-0.96885
H	-3.25567	-4.77658	-0.34789
C	-1.26459	-4.74430	-0.49830
N	-0.17566	-4.24408	-1.08953
H	0.73063	-4.58437	-0.79856
H	-0.15740	-3.32679	-1.56279
N	-1.12778	-5.50080	0.60982
H	-0.27228	-5.48949	1.14619
H	-1.84662	-6.14855	0.89809
C	-2.25526	-1.35122	-2.80317
H	-1.57339	-2.18009	-2.98884
C	-2.22656	-0.44589	-4.06537
O	-3.25006	0.03643	-4.54094
N	-0.98723	-0.25317	-4.57683
H	-0.19474	-0.63866	-4.07804
C	-0.74678	0.62972	-5.71571
H	0.21838	0.37901	-6.15875
H	-1.53493	0.48619	-6.45657
H	-0.74320	1.68303	-5.41491

$\gamma_L[u]g^+tg^-$	18.3000000		
C	0.00000	0.00000	0.00000
H	1.08970	0.00000	0.00000
H	-0.36400	1.03158	0.00000
H	-0.34566	-0.48098	0.92238
C	-0.46304	-0.76925	-1.22067
O	0.33176	-1.43467	-1.89909
N	-1.78480	-0.70313	-1.56300
C	-2.86695	-0.15744	-0.72408
H	-2.53676	-0.02652	0.30617
H	-3.19587	0.81742	-1.10668
C	-3.97536	-1.20508	-0.87680
H	-4.96350	-0.80762	-0.62435
H	-3.76415	-2.05051	-0.20902
C	-3.85264	-1.58947	-2.36196
H	-4.28914	-0.78348	-2.96082
C	-4.57043	-2.86495	-2.83657
H	-5.65262	-2.70961	-2.72624
H	-4.38930	-2.96488	-3.91257
C	-4.15166	-4.16487	-2.13140
H	-3.06837	-4.29814	-2.16039
H	-4.43640	-4.18110	-1.07451
N	-4.71544	-5.37703	-2.76621
H	-4.16668	-5.79429	-3.50737
C	-5.94770	-5.85650	-2.59824
N	-6.84734	-5.20671	-1.84554
H	-7.70197	-5.65501	-1.55002
H	-6.70573	-4.24610	-1.57352
N	-6.29477	-7.02875	-3.15991
H	-7.26146	-7.30976	-3.23291
H	-5.60297	-7.64383	-3.56255
C	-2.33022	-1.55342	-2.64631
H	-1.85047	-2.53810	-2.55635
C	-2.06332	-1.06165	-4.10051
O	-3.00592	-0.89501	-4.88155
N	-0.77327	-0.89633	-4.43993
H	-0.06941	-1.10728	-3.73439
C	-0.38314	-0.46752	-5.77815
H	-0.65304	-1.21886	-6.52733
H	-0.88174	0.46887	-6.04280
H	0.69721	-0.31793	-5.79201

$\gamma_L[d]s^-g^-s^-$	19.0000000		
C	0.00000	0.00000	0.00000
H	1.08958	0.00000	0.00000
H	-0.36445	1.03134	0.00000
H	-0.34692	-0.48197	0.92112
C	-0.46357	-0.76776	-1.21911
O	0.33425	-1.41918	-1.90881
N	-1.78880	-0.71273	-1.56020
C	-2.92606	-0.42154	-0.54034
H	-2.65836	-0.33685	0.51235
H	-3.27479	0.56027	-0.88525
C	-4.15797	-0.96445	-1.23781
H	-5.21503	-0.68966	-1.29402
H	-3.97486	-1.41450	-0.25427
C	-3.65910	-2.10983	-2.13669
H	-4.38485	-1.84745	-2.91399
C	-3.79641	-3.60899	-1.82156
H	-2.99985	-4.17015	-2.32714
H	-3.63933	-3.74223	-0.74425
C	-5.13242	-4.26954	-2.21010
H	-5.29294	-4.21623	-3.29251
H	-5.09907	-5.33141	-1.95501
N	-6.28499	-3.62020	-1.57478
H	-6.59981	-2.77097	-2.09140
C	-6.93312	-3.96237	-0.47567
N	-6.70301	-5.11438	0.18342
H	-7.08595	-5.27092	1.10312
H	-6.10820	-5.83125	-0.19894
N	-7.85871	-3.11588	0.02942
H	-8.57787	-3.45527	0.65083
H	-8.04558	-2.24465	-0.44789
C	-2.28269	-1.57542	-2.66591
H	-1.72938	-2.52329	-2.64321
C	-2.03219	-0.91777	-4.05253
O	-2.97403	-0.57349	-4.80532
N	-0.75423	-0.80006	-4.41001
H	-0.05911	-1.06355	-3.70552
C	-0.34058	-0.18959	-5.67004
H	0.74545	-0.25183	-5.74112
H	-0.78879	-0.71711	-6.51613
H	-0.64666	0.85977	-5.71639

ε_L[ª]tg¯t	25.3000000		
C	0.00000	0.00000	0.00000
H	1.08954	0.00000	0.00000
H	-0.36963	1.02982	0.00000
H	-0.35321	-0.48393	0.91777
C	-0.47993	-0.73768	-1.22412
O	0.31172	-1.33893	-1.97969
N	-1.81582	-0.78966	-1.46587
C	-2.93262	-0.33667	-0.54138
H	-2.77752	-0.38229	0.53766
H	-3.00854	0.71360	-0.84346
C	-4.29465	-0.79798	-1.34184
H	-5.18191	-0.28996	-1.72629
H	-4.59692	-1.31475	-0.42535
C	-3.72469	-1.78871	-2.38741
H	-4.39763	-1.86851	-3.24588
C	-3.52215	-3.22114	-1.83645
H	-2.91414	-3.79942	-2.54133
H	-2.93653	-3.14659	-0.91178
C	-4.83169	-3.99535	-1.51938
H	-5.58623	-3.83277	-2.28678
H	-4.65036	-5.07400	-1.48704
N	-5.42027	-3.61057	-0.22517
H	-5.01034	-2.80606	0.23160
C	-6.42320	-4.20875	0.43710
N	-7.20081	-5.14598	-0.09784
H	-7.81972	-5.66476	0.50963
H	-7.25328	-5.43129	-1.09431
N	-6.65225	-3.82011	1.71288
H	-7.49061	-4.10130	2.19831
H	-5.95303	-3.32780	2.24772
C	-2.35397	-1.21751	-2.76043
H	-1.71394	-2.01431	-3.14953
C	-2.32551	-0.07754	-3.81972
O	-1.90579	1.03891	-3.54115
N	-2.80487	-0.41330	-5.04484
H	-3.05084	-1.37442	-5.23298
C	-2.76638	0.52085	-6.17002
H	-3.46985	0.18388	-6.93319
H	-3.05731	1.51304	-5.82236
H	-1.76268	0.58645	-6.60299

Cartesian coordinates and relative energies of all the structures calculated for Ac-*c*-($^{\beta}$Pro)Arg-NHMe

α_L[d]g$^+$g$^-$t	0.0000000		
C	0.00000	0.00000	0.00000
H	1.08900	0.00000	0.00000
H	-0.36300	1.03300	0.00000
H	-0.35600	-0.47300	0.92200
C	-0.47500	-0.76300	-1.21800
O	0.29200	-1.33600	-1.98700
N	-1.84000	-0.77800	-1.45800
C	-2.88200	-0.33400	-0.50700
H	-2.75600	-0.82800	0.46500
H	-2.83700	0.74700	-0.34300
C	-4.18400	-0.77900	-1.18100
H	-4.53500	-0.02000	-1.89000
H	-4.98400	-0.95500	-0.45700
C	-3.77600	-2.06100	-1.93300
C	-2.36200	-1.68800	-2.48500
H	-1.71000	-2.56400	-2.54800
C	-2.33200	-1.08400	-3.90200
O	-2.54100	-1.81600	-4.89600
N	-2.08200	0.22100	-4.02200
H	-1.81500	0.70600	-3.17600
C	-1.92800	0.89200	-5.31100
H	-2.66000	0.49400	-6.01500
H	-2.09800	1.96100	-5.17400
H	-0.92400	0.73400	-5.71700
C	-4.86700	-2.58600	-2.88300
H	-5.81700	-2.54500	-2.33700
H	-4.98800	-1.92900	-3.75200
C	-4.71300	-4.04100	-3.35700
H	-4.54200	-4.69200	-2.48800
H	-5.64600	-4.35700	-3.84100
N	-3.60000	-4.16500	-4.30100
H	-3.13600	-3.26300	-4.58700
C	-3.19000	-5.28100	-4.87800
N	-3.72900	-6.47800	-4.57200
N	-2.20600	-5.22200	-5.79900
H	-4.49200	-6.55100	-3.91800
H	-1.77000	-4.33500	-6.00900
H	-3.47200	-7.31400	-5.07500
H	-1.76600	-6.05500	-6.15800
H	-3.59300	-2.83900	-1.17800

α_L[d]g$^+$ts$^+$	1.3000000		
C	0.00000	0.00000	0.00000
H	1.09000	0.00000	0.00000
H	-0.36500	1.03200	0.00000
H	-0.35300	-0.47400	0.92300
C	-0.47400	-0.77100	-1.21400
O	0.29000	-1.38700	-1.95100
N	-1.83400	-0.73900	-1.48600
C	-2.87500	-0.23200	-0.56400
H	-2.75900	-0.67800	0.43200
H	-2.81500	0.85500	-0.45500
C	-4.18500	-0.69100	-1.21800
H	-4.53000	0.04700	-1.95300
H	-4.98300	-0.83000	-0.48400
C	-3.78600	-2.00000	-1.92200
C	-2.37800	-1.65300	-2.49900
H	-1.73100	-2.53300	-2.56600
C	-2.38600	-1.06500	-3.92100
O	-2.74000	-1.76500	-4.89200
N	-1.99500	0.20600	-4.06800
H	-1.62700	0.66200	-3.24400
C	-1.84600	0.84600	-5.37200
H	-1.72800	1.92000	-5.22200
H	-0.97100	0.45700	-5.90200
H	-2.73400	0.66200	-5.97800
C	-4.84200	-2.56300	-2.88200
H	-4.96400	-1.90500	-3.74600
H	-5.80600	-2.58900	-2.36000
C	-4.49000	-3.98400	-3.35300
H	-4.55900	-4.69200	-2.52200
H	-3.46600	-4.03000	-3.72800
N	-5.37200	-4.49100	-4.41600
H	-6.27400	-4.85700	-4.14200
C	-5.11800	-4.42600	-5.73200
N	-5.92700	-5.09700	-6.58000
N	-4.09300	-3.72400	-6.20200
H	-6.52100	-5.84600	-6.25700
H	-3.58000	-3.02400	-5.63700
H	-5.87300	-4.94700	-7.57600
H	-3.81800	-3.82800	-7.16800
H	-3.60400	-2.75000	-1.13900

γ_L[d]s$^-$g$^+$t	2.0000000		
C	0.00000	0.00000	0.00000
H	1.08900	0.00000	0.00000
H	-0.36300	1.03300	0.00000
H	-0.35700	-0.47700	0.92000
C	-0.47400	-0.75300	-1.22200
O	0.31600	-1.30500	-1.99900
N	-1.82400	-0.80000	-1.44900
C	-2.86900	-0.27700	-0.54300
H	-2.74700	-0.70100	0.46000
H	-2.81200	0.81300	-0.46100
C	-4.18400	-0.74900	-1.18400
H	-4.55700	0.00600	-1.88300
H	-4.95400	-0.92300	-0.42700
C	-3.76500	-2.04000	-1.92000
C	-2.37500	-1.67500	-2.50300
H	-1.74000	-2.56300	-2.57800
C	-2.30800	-0.95400	-3.87300
O	-3.29800	-0.43600	-4.44300
N	-1.08800	-0.90800	-4.40800
H	-0.31900	-1.22600	-3.81200
C	-0.79600	-0.21500	-5.65900
H	-0.92400	0.86700	-5.55200
H	0.23600	-0.42900	-5.93700
H	-1.46300	-0.56900	-6.44900
H	-3.51500	-2.76100	-1.13100
C	-4.79600	-2.76300	-2.83600
H	-4.32300	-3.07200	-3.77500
H	-5.09700	-3.69100	-2.34000
C	-6.10600	-2.03200	-3.17200
H	-6.78300	-2.74400	-3.66100
H	-6.59300	-1.68000	-2.25300
N	-5.84700	-0.90700	-4.07200
H	-4.83200	-0.67200	-4.20600
C	-6.74100	-0.25100	-4.78600
N	-6.32000	0.62300	-5.72700
N	-8.06600	-0.43300	-4.61700
H	-8.73200	-0.07200	-5.28400
H	-5.32700	0.75200	-5.86600
H	-6.93600	1.33500	-6.08800
H	-8.41800	-1.04000	-3.89500

γ_L[d]s$^-$ts$^-$	3.1000000		
C	0.00000	0.00000	0.00000
H	1.08900	0.00000	0.00000
H	-0.36100	1.03400	0.00000
H	-0.35900	-0.47600	0.91900
C	-0.47300	-0.74800	-1.22600
O	0.32300	-1.26700	-2.02200
N	-1.82300	-0.82400	-1.43700
C	-2.86000	-0.32500	-0.50900
H	-2.73700	-0.78300	0.48000
H	-2.79500	0.76100	-0.39200
C	-4.17500	-0.76900	-1.16200
H	-4.51800	-0.00300	-1.86400
H	-4.96000	-0.92800	-0.41700
C	-3.77300	-2.06100	-1.90400
C	-2.37900	-1.70700	-2.48400
H	-1.74400	-2.59900	-2.55000
C	-2.34800	-1.03600	-3.88000
O	-3.38700	-0.73200	-4.50700
N	-1.12500	-0.81900	-4.36900
H	-0.33900	-1.05500	-3.75700
C	-0.89100	-0.16800	-5.65300
H	-1.43800	0.77700	-5.71200
H	0.17700	0.02500	-5.75100
H	-1.21200	-0.80900	-6.48100
C	-4.80900	-2.71800	-2.85400
H	-4.29100	-3.13600	-3.72300
H	-5.26500	-3.57000	-2.33600
C	-5.94200	-1.79900	-3.34400
H	-6.65500	-1.59200	-2.54100
H	-5.55200	-0.84400	-3.69200
N	-6.71600	-2.39800	-4.44500
H	-7.40900	-3.09400	-4.20600
C	-6.47900	-2.20600	-5.75000
N	-5.41500	-1.52700	-6.17100
N	-7.35000	-2.71700	-6.64900
H	-4.63700	-1.25300	-5.54800
H	-8.27500	-3.01100	-6.37500
H	-5.36000	-1.23900	-7.13700
H	-7.13300	-2.72900	-7.63400
H	-3.55200	-2.80500	-1.12800

γ_L[u]s$^+$g$^-$t	3.9000000		
C	0.00000	0.00000	0.00000
H	1.09000	0.00000	0.00000
H	-0.36700	1.03000	0.00000
H	-0.34100	-0.48300	0.92300
C	-0.45900	-0.78300	-1.21300
O	0.33300	-1.50900	-1.82900
N	-1.76200	-0.65000	-1.61700
C	-2.80800	-0.05400	-0.75100
H	-2.48900	-0.03500	0.29100
H	-3.01900	0.97700	-1.05900
C	-4.01000	-0.97300	-0.97700
H	-4.95900	-0.50500	-0.70100
H	-3.89800	-1.88600	-0.38300
C	-3.90800	-1.28700	-2.48100
C	-2.38000	-1.55100	-2.63500
H	-2.17700	-2.58800	-2.32400
C	-1.88300	-1.50600	-4.10000
O	-2.67300	-1.82200	-5.02500
N	-0.61000	-1.21400	-4.34300
H	0.01600	-1.22000	-3.53100
C	-0.04800	-1.26800	-5.69000
H	0.96300	-0.86000	-5.65600
H	-0.01000	-2.29800	-6.06200
H	-0.65500	-0.67400	-6.37600
C	-4.49200	-0.11400	-3.32900
H	-4.82200	0.69400	-2.66800
H	-3.74200	0.32600	-3.99200
C	-5.71000	-0.51900	-4.17300
H	-6.48600	-0.95900	-3.53100
H	-6.12900	0.37200	-4.65800
N	-5.28600	-1.49100	-5.18300
H	-4.25800	-1.70300	-5.17100
C	-6.05900	-2.08900	-6.06900
N	-7.37200	-1.80500	-6.17100
N	-5.52900	-3.02500	-6.88600
H	-7.79900	-1.10600	-5.58300
H	-4.53500	-3.20500	-6.85000
H	-7.98200	-2.34300	-6.76700
H	-6.02300	-3.34000	-7.70700
H	-4.44400	-2.20900	-2.72400

$\gamma_L[d]g^-g^-s^+$ 5.1000000

C	0.00000	0.00000	0.00000
H	1.08935	0.00000	0.00000
H	-0.36094	1.03403	0.00000
H	-0.36098	-0.47483	0.91866
C	-0.47701	-0.74138	-1.22699
O	0.31524	-1.23624	-2.04575
N	-1.82588	-0.83697	-1.42274
C	-2.90144	-0.36876	-0.49293
H	-2.77526	-0.83396	0.49205
H	-2.86932	0.71675	-0.36565
C	-4.19650	-0.79910	-1.20941
H	-4.57257	-0.02217	-1.88224
H	-4.98370	-1.03895	-0.48981
C	-3.74570	-2.04490	-2.02602
C	-2.35346	-1.61861	-2.54423
H	-1.67068	-2.46379	-2.68229
C	-2.36888	-0.79132	-3.85388
O	-3.38506	-0.28748	-4.32668
N	-1.14861	-0.73711	-4.48904
H	-0.35532	-0.76609	-3.83639
C	-0.99454	0.10226	-5.68701
H	-1.75946	-0.15430	-6.42137
H	-1.09686	1.16550	-5.44673
H	-0.00520	-0.07461	-6.11231
C	-4.83273	-2.50450	-3.01046
H	-4.34571	-3.15188	-3.75040
H	-5.56685	-3.12687	-2.49219
C	-5.55794	-1.42312	-3.82280
H	-4.83827	-0.75055	-4.29903
H	-6.15198	-1.89457	-4.61196
N	-6.46033	-0.60342	-2.98290
H	-6.97218	-1.11577	-2.27058
C	-6.42305	0.72510	-2.83660
N	-5.98521	1.50462	-3.84193
N	-6.84446	1.28054	-1.69180
H	-5.97573	1.16866	-4.79369
H	-6.73402	0.76469	-0.81181
H	-5.79055	2.48360	-3.69185
H	-7.03445	2.27137	-1.64266
H	-3.54049	-2.87518	-1.33414

$\gamma_L[u]s^+ts^+$	5.4000000		
C	0.00000	0.00000	0.00000
H	1.08979	0.00000	0.00000
H	-0.36704	1.02982	0.00000
H	-0.34010	-0.48379	0.92300
C	-0.45919	-0.78198	-1.21350
O	0.33368	-1.51225	-1.82438
N	-1.75929	-0.64351	-1.62487
C	-2.82378	-0.10122	-0.75021
H	-2.47622	-0.00744	0.27749
H	-3.13552	0.89311	-1.09464
C	-3.94247	-1.13160	-0.90779
H	-4.91803	-0.75785	-0.58548
H	-3.70842	-2.02240	-0.31440
C	-3.88850	-1.45015	-2.41455
C	-2.34961	-1.55426	-2.65463
H	-2.02621	-2.57574	-2.40619
C	-1.89614	-1.34752	-4.12332
O	-2.73217	-1.37884	-5.05362
N	-0.58892	-1.23651	-4.34932
H	0.02821	-1.36137	-3.53883
C	-0.03578	-1.15309	-5.69600
H	-0.39026	-0.25262	-6.20625
H	1.05079	-1.11040	-5.61770
H	-0.32190	-2.02572	-6.29114
C	-4.64816	-0.36921	-3.23945
H	-5.23625	0.26083	-2.56090
H	-3.95659	0.29649	-3.75956
C	-5.60491	-1.00720	-4.26032
H	-5.09065	-1.78016	-4.83180
H	-6.44984	-1.48131	-3.75196
N	-6.17809	-0.04242	-5.21422
H	-6.97732	0.49809	-4.91172
C	-5.66314	0.26251	-6.41312
N	-4.46857	-0.18489	-6.78980
N	-6.38479	1.04217	-7.24890
H	-3.79780	-0.62342	-6.13490
H	-7.37692	1.17057	-7.12003
H	-4.18850	-0.10281	-7.75605
H	-5.97472	1.42241	-8.08819
H	-4.33570	-2.42869	-2.61781

ε_L[u]g$^-$g$^+$t 5.4000000

C	0.00000	0.00000	0.00000
H	1.09002	0.00000	0.00000
H	-0.37109	1.02933	0.00000
H	-0.34187	-0.47878	0.92520
C	-0.47389	-0.78856	-1.20276
O	0.26629	-1.54436	-1.83147
N	-1.78495	-0.63277	-1.59016
C	-2.85588	-0.01277	-0.78967
H	-2.69561	-0.17606	0.27905
H	-2.88497	1.07099	-0.95928
C	-4.13095	-0.71417	-1.28959
H	-5.02037	-0.08338	-1.20159
H	-4.31354	-1.61110	-0.68961
C	-3.82130	-1.12410	-2.74924
C	-2.31119	-1.51125	-2.64096
H	-2.26332	-2.55112	-2.28673
C	-1.48222	-1.43371	-3.93086
O	-1.18539	-0.34315	-4.46305
N	-1.16534	-2.60302	-4.50065
H	-1.26889	-3.43790	-3.94034
C	-0.32934	-2.69222	-5.69641
H	0.72135	-2.50570	-5.45133
H	-0.43271	-3.69128	-6.12154
H	-0.65880	-1.95189	-6.42613
C	-4.28693	-0.09180	-3.81330
H	-3.91234	-0.37806	-4.80219
H	-5.37662	-0.19466	-3.86677
C	-4.03231	1.41271	-3.60633
H	-4.62686	1.95638	-4.35225
H	-4.37948	1.72725	-2.61346
N	-2.61676	1.74360	-3.77670
H	-1.97799	0.93111	-3.98872
C	-2.10713	2.95835	-3.86107
N	-2.84141	4.06161	-3.60679
N	-0.81102	3.10443	-4.20716
H	-3.81943	3.98628	-3.37595
H	-0.25346	2.28437	-4.40525
H	-2.49588	4.98044	-3.83902
H	-0.32858	3.98174	-4.08881
H	-4.36697	-2.03908	-2.99971

ε_L[u]g$^-$ct	5.5000000		
C	0.00000	0.00000	0.00000
H	1.11892	0.00000	0.00000
H	-0.36415	1.05418	0.00000
H	-0.35731	-0.51308	0.92715
C	-0.47944	-0.76372	-1.20457
O	0.26115	-1.54546	-1.82452
N	-1.79463	-0.57213	-1.65523
C	-2.84805	-0.02452	-0.80081
H	-2.52596	-0.02356	0.27874
H	-3.07692	1.03675	-1.06182
C	-4.07171	-0.96061	-0.98571
H	-5.02585	-0.44534	-0.73770
H	-3.97698	-1.88916	-0.37620
C	-3.91731	-1.27152	-2.48287
C	-2.39055	-1.57696	-2.56223
H	-2.15353	-2.61841	-2.21297
C	-1.90767	-1.36240	-4.01500
O	-1.48402	-0.24967	-4.39531
N	-2.21831	-2.36151	-4.92200
H	-2.18169	-3.29808	-4.58268
C	-1.90432	-2.20901	-6.31562
H	-0.86202	-2.55941	-6.54728
H	-2.63459	-2.81879	-6.91129
H	-1.99065	-1.12960	-6.61054
C	-4.66793	-0.66767	-3.63908
H	-4.47270	-1.30853	-4.54373
H	-5.75992	-0.79746	-3.37921
C	-4.53366	0.78071	-4.12410
H	-4.08581	0.76644	-5.16416
H	-5.58092	1.19275	-4.20322
N	-3.72962	1.64058	-3.28822
H	-2.83087	1.21733	-3.07853
C	-3.73598	3.02384	-3.40364
N	-4.79304	3.70168	-3.96598
N	-2.68948	3.74213	-2.86534
H	-5.57518	3.21048	-4.33419
H	-1.87284	3.27640	-2.53647
H	-4.84387	4.69414	-3.92225
H	-2.70982	4.73535	-2.83260
H	-4.36084	-2.33242	-2.54680

$\alpha_L[u]g^+g^+s^-$	5.7000000		
C	0.00000	0.00000	0.00000
H	1.08994	0.00000	0.00000
H	-0.36784	1.03017	0.00000
H	-0.34120	-0.47988	0.92473
C	-0.46479	-0.78736	-1.20842
O	0.29055	-1.51148	-1.84971
N	-1.78789	-0.64506	-1.60857
C	-2.87909	-0.12731	-0.76041
H	-2.54560	0.01221	0.26775
H	-3.23243	0.84222	-1.13398
C	-3.95411	-1.21047	-0.89311
H	-4.95330	-0.85247	-0.62932
H	-3.71039	-2.04535	-0.22723
C	-3.84888	-1.66610	-2.36902
C	-2.29992	-1.59847	-2.61102
H	-1.85564	-2.58039	-2.40866
C	-1.88450	-1.30079	-4.05330
O	-2.15420	-2.13010	-4.94915
N	-1.26328	-0.14591	-4.30723
H	-1.00060	0.40754	-3.50214
C	-0.69159	0.19576	-5.60760
H	-1.26735	-0.29733	-6.39036
H	-0.73469	1.27775	-5.74597
H	0.34956	-0.13665	-5.67186
C	-4.75129	-0.81078	-3.29184
H	-5.67881	-0.60132	-2.74418
H	-4.29962	0.16809	-3.49447
C	-5.14529	-1.41431	-4.65453
H	-5.85487	-0.74233	-5.14758
H	-4.28897	-1.51963	-5.31744
N	-5.80406	-2.72919	-4.54882
H	-6.74476	-2.74025	-4.17699
C	-5.29573	-3.91673	-4.91528
N	-4.00787	-4.07151	-5.19896
N	-6.13142	-4.97928	-4.96974
H	-3.28498	-3.33464	-5.02760
H	-7.13063	-4.85825	-5.03547
H	-3.69854	-4.92629	-5.63919
H	-5.77182	-5.91350	-5.09356
H	-4.16945	-2.70922	-2.45111

$\gamma_L[u]s^+g^+s^-$	6.0000000		
C	0.00000	0.00000	0.00000
H	1.08973	0.00000	0.00000
H	-0.36756	1.02987	0.00000
H	-0.34161	-0.48186	0.92356
C	-0.46008	-0.78421	-1.21202
O	0.32968	-1.50236	-1.83758
N	-1.76674	-0.65519	-1.60842
C	-2.80274	-0.03372	-0.74985
H	-2.50648	-0.05544	0.29877
H	-2.96255	1.01354	-1.03499
C	-4.03933	-0.89073	-1.02381
H	-4.97167	-0.37913	-0.77109
H	-3.98960	-1.81247	-0.43370
C	-3.90901	-1.21077	-2.52533
C	-2.38944	-1.55774	-2.61945
H	-2.24697	-2.59470	-2.27873
C	-1.87072	-1.56854	-4.06965
O	-2.61301	-2.05452	-4.95509
N	-0.65275	-1.10982	-4.35082
H	-0.01710	-1.02996	-3.55476
C	-0.08677	-1.20789	-5.69496
H	-0.77833	-0.78365	-6.42488
H	0.84818	-0.64715	-5.71421
H	0.10943	-2.25015	-5.96753
C	-4.38071	0.00160	-3.37853
H	-5.11096	0.56603	-2.78511
H	-3.55208	0.69681	-3.56028
C	-5.02289	-0.28100	-4.74843
H	-5.40293	0.65876	-5.16134
H	-4.29823	-0.67805	-5.45600
N	-6.16554	-1.21245	-4.69475
H	-7.03550	-0.85646	-4.32120
C	-6.17471	-2.48187	-5.12860
N	-5.04699	-3.12426	-5.41186
N	-7.36457	-3.11215	-5.25389
H	-4.10796	-2.73789	-5.17236
H	-8.22757	-2.59428	-5.32113
H	-5.08440	-3.99995	-5.91313
H	-7.40865	-4.10578	-5.42175
H	-4.49973	-2.09479	-2.77844

γ_L[u]g⁻tg⁻	6.5000000		
C	0.00000	0.00000	0.00000
H	1.08988	0.00000	0.00000
H	-0.36707	1.02999	0.00000
H	-0.33995	-0.48390	0.92307
C	-0.46325	-0.78071	-1.21204
O	0.31185	-1.51894	-1.83005
N	-1.76998	-0.63554	-1.61740
C	-2.86110	-0.13600	-0.76392
H	-2.52388	-0.00647	0.26432
H	-3.21479	0.83914	-1.12204
C	-3.92901	-1.22753	-0.90001
H	-4.93284	-0.87844	-0.63904
H	-3.68650	-2.05186	-0.22179
C	-3.82054	-1.70293	-2.37208
C	-2.29197	-1.53061	-2.68159
H	-1.80878	-2.50326	-2.53838
C	-1.85967	-1.04381	-4.08928
O	-2.57624	-0.34454	-4.83314
N	-0.63757	-1.44360	-4.45645
H	-0.04845	-1.81804	-3.71193
C	-0.02764	-1.04234	-5.71900
H	0.19345	0.03047	-5.73343
H	0.90002	-1.60107	-5.84603
H	-0.70078	-1.27023	-6.54825
C	-4.88742	-1.07497	-3.30143
H	-4.70784	-1.40014	-4.32851
H	-5.85049	-1.50635	-2.99760
C	-5.02842	0.45606	-3.27637
H	-5.37900	0.80848	-2.30309
H	-4.07820	0.94819	-3.48465
N	-6.01318	0.94090	-4.26137
H	-6.98979	0.88898	-4.00431
C	-5.74258	1.28356	-5.52858
N	-4.53102	1.11055	-6.04744
N	-6.72924	1.82052	-6.27973
H	-3.79984	0.54994	-5.58066
H	-7.56354	2.19855	-5.85743
H	-4.30258	1.52793	-6.93755
H	-6.61119	1.95685	-7.27202
H	-4.02365	-2.77714	-2.41672

γ_L[^{a}]g$^-$g$^-$s$^-$	7.3000000		
C	0.00000	0.00000	0.00000
H	1.08937	0.00000	0.00000
H	-0.36177	1.03373	0.00000
H	-0.35752	-0.47616	0.91965
C	-0.47453	-0.74923	-1.22526
O	0.31388	-1.27630	-2.01999
N	-1.82707	-0.81580	-1.43469
C	-2.87745	-0.31701	-0.52488
H	-2.73431	-0.72708	0.48174
H	-2.85568	0.77473	-0.45251
C	-4.17684	-0.84518	-1.15342
H	-4.58139	-0.10939	-1.85551
H	-4.93578	-1.06094	-0.39549
C	-3.71767	-2.11072	-1.91197
C	-2.36928	-1.65166	-2.52684
H	-1.69789	-2.50638	-2.65811
C	-2.34089	-0.83345	-3.82826
O	-3.31831	-0.19968	-4.25890
N	-1.14395	-0.84310	-4.44178
H	-0.36500	-1.21721	-3.89873
C	-0.85846	-0.02617	-5.61502
H	-1.06486	1.03208	-5.42394
H	0.19485	-0.14510	-5.87015
H	-1.46129	-0.35114	-6.46825
C	-4.82822	-2.89126	-2.65728
H	-4.45542	-3.91315	-2.81343
H	-5.61754	-3.01535	-1.90208
C	-5.54050	-2.60152	-3.99900
H	-4.83875	-2.74250	-4.82491
H	-6.32675	-3.35291	-4.11268
N	-6.15665	-1.27373	-4.18724
H	-6.78634	-0.98565	-3.44670
C	-5.74591	-0.27686	-4.97813
N	-5.26403	-0.51693	-6.21012
N	-6.00307	0.99325	-4.62580
H	-5.23896	-1.46898	-6.54488
H	-5.95942	1.26349	-3.65417
H	-4.52156	0.08295	-6.54439
H	-5.88795	1.72955	-5.30756
H	-3.40764	-2.82751	-1.14030

γ_L[u]tg$^-$g$^-$	8.9000000		
C	0.00000	0.00000	0.00000
H	1.08978	0.00000	0.00000
H	-0.36714	1.02988	0.00000
H	-0.34027	-0.48289	0.92352
C	-0.45951	-0.78397	-1.21231
O	0.32942	-1.51490	-1.82537
N	-1.76053	-0.64465	-1.62104
C	-2.80714	-0.04853	-0.76101
H	-2.49436	-0.03364	0.28262
H	-3.01064	0.98597	-1.06452
C	-4.01615	-0.96016	-0.99073
H	-4.95969	-0.46912	-0.73368
H	-3.92758	-1.85904	-0.37109
C	-3.90261	-1.31511	-2.48585
C	-2.36817	-1.54591	-2.64306
H	-2.14871	-2.58069	-2.33720
C	-1.87679	-1.47085	-4.10925
O	-2.67409	-1.73102	-5.04060
N	-0.60403	-1.16524	-4.34654
H	0.03080	-1.19290	-3.54409
C	-0.08804	-0.96535	-5.69695
H	-0.76121	-0.31666	-6.26147
H	0.89285	-0.49477	-5.62192
H	0.00920	-1.91431	-6.23448
C	-4.51690	-0.19864	-3.36285
H	-4.38287	0.77997	-2.88575
H	-4.01677	-0.12498	-4.32591
C	-6.02968	-0.34160	-3.58919
H	-6.57015	-0.18886	-2.65171
H	-6.36601	0.43312	-4.28707
N	-6.51562	-1.65963	-4.07516
H	-7.28671	-2.05469	-3.55446
C	-6.30030	-2.21978	-5.28060
N	-5.17659	-2.00532	-5.95552
N	-7.25696	-3.02269	-5.79321
H	-4.26238	-1.82401	-5.48399
H	-8.21415	-2.97187	-5.47764
H	-5.12047	-2.32497	-6.91292
H	-7.04678	-3.67125	-6.53771
H	-4.41079	-2.25740	-2.70877

γ_L[ª]ttt	13.7000000		
C	0.00000	0.00000	0.00000
H	1.08944	0.00000	0.00000
H	-0.35932	1.03489	0.00000
H	-0.36021	-0.47564	0.91867
C	-0.47407	-0.74126	-1.23176
O	0.31661	-1.21903	-2.05489
N	-1.82520	-0.85863	-1.40886
C	-2.87105	-0.39088	-0.47944
H	-2.72526	-0.83665	0.51228
H	-2.84806	0.69746	-0.36780
C	-4.18004	-0.87982	-1.12429
H	-4.58326	-0.11655	-1.79659
H	-4.93155	-1.10941	-0.36247
C	-3.74038	-2.10896	-1.94796
C	-2.37066	-1.66664	-2.51446
H	-1.70509	-2.51988	-2.68015
C	-2.43259	-0.82664	-3.81973
O	-3.48300	-0.32321	-4.23686
N	-1.24250	-0.69805	-4.44102
H	-0.42001	-1.00663	-3.92496
C	-1.07642	0.14572	-5.61878
H	-1.10261	1.21041	-5.36001
H	-0.11647	-0.08674	-6.08237
H	-1.88039	-0.05202	-6.33033
C	-4.74309	-2.62402	-2.99003
H	-5.01069	-1.79983	-3.65672
H	-4.26018	-3.40164	-3.59819
C	-6.00390	-3.21748	-2.35703
H	-5.75147	-4.08451	-1.73207
H	-6.51604	-2.47125	-1.73952
N	-6.92554	-3.64262	-3.43200
H	-6.57168	-3.58335	-4.37892
C	-8.17379	-4.07218	-3.26427
N	-8.64792	-4.31701	-2.03349
N	-8.97822	-4.25827	-4.32599
H	-8.03951	-4.31142	-1.22915
H	-8.71161	-3.94425	-5.24750
H	-9.62775	-4.49872	-1.87463
H	-9.85081	-4.75869	-4.24428
H	-3.51795	-2.92820	-1.24774

$\gamma_L[^a]g^+g^+t$	13.8000000		
C	0.00000	0.00000	0.00000
H	1.08941	0.00000	0.00000
H	-0.35984	1.03444	0.00000
H	-0.36063	-0.47389	0.91942
C	-0.47485	-0.74255	-1.22975
O	0.31897	-1.23675	-2.04440
N	-1.82337	-0.84086	-1.42145
C	-2.86701	-0.36896	-0.48588
H	-2.70861	-0.80420	0.50819
H	-2.84532	0.72026	-0.38686
C	-4.17327	-0.87445	-1.11522
H	-4.58769	-0.12527	-1.79700
H	-4.92945	-1.10396	-0.35934
C	-3.73508	-2.11351	-1.92321
C	-2.37280	-1.66910	-2.51433
H	-1.69158	-2.51571	-2.66020
C	-2.43870	-0.88326	-3.85228
O	-3.51034	-0.59028	-4.39393
N	-1.23249	-0.58540	-4.37894
H	-0.41000	-0.80657	-3.81825
C	-1.09950	0.22971	-5.58188
H	-1.38747	1.26979	-5.39476
H	-0.05910	0.19977	-5.90868
H	-1.74130	-0.16038	-6.37528
C	-4.83634	-2.64168	-2.85873
H	-5.63558	-3.07965	-2.24434
H	-5.27332	-1.80887	-3.41167
C	-4.40161	-3.65475	-3.91903
H	-5.26325	-3.92466	-4.54148
H	-3.63915	-3.20459	-4.55941
N	-3.83856	-4.88378	-3.31473
H	-4.18616	-5.14466	-2.40034
C	-3.02916	-5.74791	-3.92487
N	-2.74750	-5.61991	-5.22925
N	-2.47383	-6.76066	-3.23357
H	-3.25224	-4.96933	-5.81237
H	-2.50103	-6.78473	-2.22515
H	-1.98845	-6.13258	-5.65332
H	-2.02606	-7.53385	-3.70281
H	-3.48328	-2.90336	-1.19870

$\gamma_L[^a]g^+g^+g^+$	14.7000000		
C	0.00000	0.00000	0.00000
H	1.08940	0.00000	0.00000
H	-0.36081	1.03401	0.00000
H	-0.35989	-0.47481	0.91933
C	-0.47512	-0.74363	-1.22888
O	0.31577	-1.25360	-2.03541
N	-1.82452	-0.82812	-1.42708
C	-2.87209	-0.34429	-0.50372
H	-2.73012	-0.78213	0.49176
H	-2.83869	0.74455	-0.40355
C	-4.17840	-0.83089	-1.14975
H	-4.57697	-0.07196	-1.82981
H	-4.94302	-1.05777	-0.40136
C	-3.74775	-2.06900	-1.96162
C	-2.37119	-1.64022	-2.52984
H	-1.69472	-2.49189	-2.67530
C	-2.41195	-0.83559	-3.85755
O	-3.47186	-0.44530	-4.35798
N	-1.19997	-0.62919	-4.41447
H	-0.38382	-0.88880	-3.86197
C	-1.03521	0.18730	-5.61295
H	-1.19682	1.24980	-5.40046
H	-0.02212	0.04762	-5.99276
H	-1.75471	-0.11987	-6.37475
C	-4.82743	-2.57223	-2.93252
H	-5.67173	-2.94294	-2.33347
H	-5.19104	-1.73693	-3.53500
C	-4.37461	-3.64791	-3.92791
H	-5.19061	-3.92910	-4.60086
H	-3.57518	-3.26449	-4.56492
N	-3.85142	-4.89067	-3.31173
H	-2.86014	-4.92479	-3.11119
C	-4.56686	-5.96235	-2.97689
N	-5.90796	-5.92793	-2.98409
N	-3.94862	-7.10747	-2.63236
H	-6.40862	-5.05546	-3.05945
H	-2.96743	-7.25174	-2.82048
H	-6.45190	-6.77769	-2.95641
H	-4.44501	-7.85126	-2.16424
H	-3.52727	-2.87326	-1.24318

γ_L[ª]tg⁻t	15.4000000		
C	0.00000	0.00000	0.00000
H	1.08947	0.00000	0.00000
H	-0.35863	1.03513	0.00000
H	-0.36078	-0.47502	0.91879
C	-0.47445	-0.73911	-1.23290
O	0.31410	-1.20819	-2.06268
N	-1.82591	-0.86663	-1.40317
C	-2.87825	-0.39378	-0.48284
H	-2.72551	-0.82287	0.51522
H	-2.86808	0.69626	-0.38685
C	-4.18626	-0.89631	-1.12770
H	-4.60439	-0.13998	-1.79780
H	-4.93188	-1.13839	-0.36370
C	-3.73743	-2.10873	-1.96314
C	-2.36861	-1.65317	-2.52365
H	-1.70033	-2.49991	-2.70956
C	-2.43813	-0.78003	-3.80595
O	-3.48632	-0.24518	-4.18343
N	-1.25704	-0.65784	-4.44687
H	-0.43018	-0.98617	-3.95189
C	-1.09843	0.21460	-5.60532
H	-1.07076	1.27104	-5.31486
H	-0.16695	-0.04245	-6.11210
H	-1.93630	0.07007	-6.28955
C	-4.73628	-2.62739	-3.00969
H	-4.99006	-1.80645	-3.68422
H	-4.26834	-3.40441	-3.62898
C	-6.04383	-3.17768	-2.43643
H	-6.52159	-2.42987	-1.79137
H	-6.72517	-3.41999	-3.25883
N	-5.81318	-4.41587	-1.65696
H	-4.85736	-4.62193	-1.39603
C	-6.75783	-5.25843	-1.24600
N	-8.05463	-4.93968	-1.37004
N	-6.42406	-6.44481	-0.70540
H	-8.34122	-4.01142	-1.64178
H	-5.48136	-6.80070	-0.76151
H	-8.77982	-5.62764	-1.23076
H	-7.10310	-7.01078	-0.21839
H	-3.49207	-2.91790	-1.25379

$\gamma_L[^a]tg^-g^-$	15.7000000		
C	0.00000	0.00000	0.00000
H	1.08941	0.00000	0.00000
H	-0.35874	1.03511	0.00000
H	-0.36041	-0.47518	0.91886
C	-0.47380	-0.74019	-1.23275
O	0.31605	-1.21299	-2.05914
N	-1.82489	-0.86456	-1.40547
C	-2.87233	-0.38516	-0.48886
H	-2.72696	-0.81532	0.50993
H	-2.85427	0.70489	-0.39315
C	-4.18098	-0.87112	-1.13890
H	-4.58804	-0.10832	-1.80911
H	-4.93059	-1.09601	-0.37254
C	-3.74689	-2.09243	-1.96808
C	-2.37169	-1.65066	-2.52343
H	-1.70928	-2.50405	-2.70025
C	-2.41701	-0.78142	-3.81035
O	-3.45645	-0.24369	-4.20985
N	-1.22425	-0.66142	-4.42857
H	-0.40741	-0.99546	-3.92019
C	-1.04039	0.21161	-5.58287
H	-1.01419	1.26752	-5.29036
H	-0.10004	-0.04818	-6.07154
H	-1.86525	0.07177	-6.28369
C	-4.74907	-2.60051	-3.01882
H	-5.05433	-1.75324	-3.63981
H	-4.24656	-3.31954	-3.68137
C	-6.03279	-3.21205	-2.44862
H	-6.51013	-2.52865	-1.74367
H	-6.76415	-3.39441	-3.24209
N	-5.84486	-4.49033	-1.71940
H	-5.65333	-4.43662	-0.72767
C	-5.84780	-5.70646	-2.26317
N	-5.84978	-5.86857	-3.59436
N	-5.86064	-6.79852	-1.47605
H	-5.65467	-5.09939	-4.21730
H	-6.08286	-6.73568	-0.49356
H	-6.06711	-6.76196	-4.01085
H	-5.64205	-7.71273	-1.84385
H	-3.52645	-2.90755	-1.26196

α_L[d]ttc	17.3000000		
C	0.00000	0.00000	0.00000
H	1.08958	0.00000	0.00000
H	-0.36429	1.03254	0.00000
H	-0.35233	-0.47417	0.92331
C	-0.47259	-0.77446	-1.21453
O	0.29346	-1.40198	-1.93736
N	-1.83213	-0.74039	-1.48824
C	-2.85524	-0.22760	-0.56704
H	-2.72897	-0.67413	0.42770
H	-2.79622	0.85946	-0.45632
C	-4.17418	-0.67137	-1.20962
H	-4.51267	0.06841	-1.94650
H	-4.96075	-0.78529	-0.45771
C	-3.79911	-1.98305	-1.92303
C	-2.38104	-1.66110	-2.48387
H	-1.75645	-2.55945	-2.52077
C	-2.36756	-1.12298	-3.93252
O	-2.82413	-1.82560	-4.84064
N	-1.84883	0.10812	-4.12155
H	-1.69087	0.67225	-3.29861
C	-1.62619	0.69104	-5.43787
H	-2.38194	1.45152	-5.66464
H	-0.63473	1.14906	-5.48465
H	-1.68570	-0.10645	-6.17885
C	-4.82756	-2.51654	-2.93560
H	-5.11148	-1.73191	-3.64056
H	-4.33338	-3.27891	-3.53973
C	-6.08856	-3.04815	-2.24758
H	-5.85954	-3.89640	-1.58938
H	-6.53407	-2.27088	-1.62434
N	-7.18593	-3.46723	-3.17129
H	-8.11337	-3.19690	-2.86870
C	-7.12995	-3.90443	-4.43402
N	-6.10111	-4.63048	-4.88897
N	-8.16637	-3.67271	-5.26069
H	-5.41280	-5.00787	-4.25606
H	-8.81999	-2.92386	-5.08462
H	-5.91483	-4.70748	-5.87904
H	-8.30557	-4.22874	-6.09240
H	-3.65034	-2.74685	-1.14706

γ_L[u]ttc	18.1000000		
C	0.00000	0.00000	0.00000
H	1.08959	0.00000	0.00000
H	-0.36342	1.03192	0.00000
H	-0.34660	-0.48240	0.92095
C	-0.46199	-0.76617	-1.22215
O	0.33661	-1.40174	-1.92124
N	-1.79475	-0.72795	-1.54535
C	-2.88650	-0.23094	-0.70226
H	-2.53279	0.01130	0.29930
H	-3.31949	0.67973	-1.13754
C	-3.88145	-1.39683	-0.72020
H	-4.89562	-1.08066	-0.45657
H	-3.57301	-2.15059	0.01083
C	-3.78008	-1.97046	-2.15853
C	-2.31833	-1.59928	-2.62005
H	-1.70173	-2.50313	-2.62781
C	-2.10101	-0.91466	-4.01456
O	-2.97268	-0.30703	-4.66701
N	-0.83950	-1.02984	-4.45479
H	-0.15111	-1.38613	-3.79032
C	-0.38729	-0.38990	-5.68524
H	-0.44936	0.70096	-5.61282
H	0.64816	-0.68137	-5.86372
H	-1.00260	-0.71384	-6.52805
C	-4.84952	-1.43117	-3.11209
H	-4.79631	-0.33923	-3.09878
H	-4.57176	-1.77367	-4.10570
C	-6.29497	-1.84020	-2.88636
H	-6.44067	-2.91362	-3.05708
H	-6.64007	-1.61000	-1.87441
N	-7.21171	-1.09061	-3.79319
H	-8.17385	-1.07898	-3.48069
C	-7.02944	-0.52533	-4.99907
N	-5.85022	-0.21384	-5.54541
N	-8.14200	-0.22332	-5.70960
H	-4.94355	-0.23709	-5.07276
H	-9.03739	-0.63310	-5.49172
H	-5.82797	0.05023	-6.52001
H	-8.10856	0.43482	-6.47367
H	-3.85595	-3.06314	-2.13325

γ_L[u]g$^-$g$^+$t	18.8000000		
C	0.00000	0.00000	0.00000
H	1.08947	0.00000	0.00000
H	-0.36763	1.03032	0.00000
H	-0.34836	-0.47607	0.92361
C	-0.46310	-0.78221	-1.21175
O	0.33798	-1.43944	-1.88469
N	-1.79967	-0.72103	-1.54060
C	-2.85947	-0.11141	-0.58400
C	-4.20046	-0.98333	-0.95824
C	-3.95962	-1.45659	-2.40878
C	-2.40149	-1.68124	-2.51551
H	-2.19598	-2.71342	-2.19365
C	-1.83384	-1.67922	-3.94562
O	-2.45424	-2.33673	-4.80629
N	-0.78986	-0.88680	-4.25927
H	-0.16736	-0.69063	-3.47940
C	-0.11919	-0.98196	-5.55736
H	0.05131	0.01684	-5.96994
H	0.84867	-1.47976	-5.44261
H	-0.73003	-1.57810	-6.23696
C	-4.89252	-0.72877	-3.41617
H	-4.79028	-1.22134	-4.38913
H	-5.90598	-0.96324	-3.07208
C	-4.89044	0.78403	-3.67599
H	-5.78701	1.02414	-4.26090
H	-4.95022	1.33250	-2.72479
N	-3.69966	1.23050	-4.40951
H	-3.10194	0.47616	-4.77856
C	-3.50336	2.46897	-4.83958
N	-4.27488	3.48495	-4.41226
N	-2.51935	2.72743	-5.72165
H	-5.00042	3.33578	-3.72918
H	-1.95772	1.97500	-6.09225
H	-4.19895	4.40704	-4.81370
H	-2.23640	3.67093	-5.93788
H	-4.35893	-2.47292	-2.47405
H	-4.22126	-1.82873	-0.30267
H	-5.10196	-0.41289	-0.87586
H	-2.53528	-0.25208	0.42595
H	-3.07414	0.91906	-0.77624

α_L[d]g⁻g⁻s⁻	21.6000000		
C	0.00000	0.00000	0.00000
H	1.08954	0.00000	0.00000
H	-0.35730	1.03592	0.00000
H	-0.36055	-0.47311	0.91988
C	-0.47270	-0.75270	-1.22630
O	0.29604	-1.22805	-2.05728
N	-1.83795	-0.87457	-1.40854
C	-2.88998	-0.43871	-0.46724
H	-2.87494	-1.03250	0.45714
H	-2.76156	0.61200	-0.19445
C	-4.17870	-0.69787	-1.25914
H	-4.36950	0.14663	-1.92853
H	-5.04853	-0.81484	-0.60603
C	-3.83705	-1.98681	-2.02858
C	-2.34131	-1.80282	-2.43050
H	-1.80582	-2.75544	-2.38451
C	-2.13033	-1.32501	-3.87516
O	-2.15519	-2.12210	-4.79982
N	-2.06454	0.05062	-4.08424
H	-1.72021	0.54107	-3.26369
C	-1.47983	0.51673	-5.35620
H	-0.42483	0.23668	-5.43413
H	-2.01641	0.06276	-6.18995
H	-1.56844	1.60417	-5.40977
C	-4.79013	-2.55336	-3.09896
H	-4.54121	-3.60913	-3.24767
H	-5.80736	-2.53858	-2.68568
C	-4.84268	-1.93741	-4.50572
H	-4.02269	-2.27410	-5.13557
H	-5.75718	-2.29162	-4.99380
N	-4.89118	-0.46244	-4.54555
H	-4.03120	0.02771	-4.33312
C	-5.98056	0.28861	-4.72149
N	-7.11504	-0.22137	-5.21596
N	-5.93542	1.59996	-4.40790
H	-7.16937	-1.14276	-5.66624
H	-5.21171	1.97365	-3.81200
H	-7.97359	0.30356	-5.13529
H	-6.64720	2.23939	-4.72850
H	-3.80691	-2.77589	-1.26471