Supplementary Information

to

IR Low-Temperature Matrix, X-ray and *ab Initio* Study on L-Isoserine Conformations.

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Fig. 1SI. The B3LYP/aug-cc-pVDZ optimized 54 stable structures of L-isoserine in the gas phase. The relative free Gibbs energies (ΔG , kcal/mol) referred to the most stable conformer are given in parentheses and square brackets. respectively.







52 (7.04)	53 (7.32)	54 (8.98)

Table 1SI. The total energies (E, hartree), the total energies corrected for zero-point energies (E_0 , hartree), the Gibbs free energies in 298.15 K (G, hartree), relative total energies (ΔE , kcal/mol), and corresponding relative energies referred to the most stable conformer (kcal/mol) for the B3LYP/aug-cc-pVDZ optimized 54 stable structures of L-isoserine in the gas phase (Fig 1SI). The populations X(G) are calculated based on the ΔG values.

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Conformer number	Е	ΔΕ	E_0	ΔE_0	G	ΔG	X(G)
1	-399.036151	0.00	-398.92267	0.00	-398.95377	0.00	60.22
2	-399.033658	1.58	-398.920075	1.63	-398.95193	1.15	8.59
3	-399.032899	2.05	-398.91966	1.89	-398.95158	1.37	5.92
4	-399.032316	2.42	-398.91967	1.88	-398.95152	1.41	5.53
5	-399.031661	2.83	-398.91922	2.16	-398.95151	1.42	5.49
6	-399.031471	2.95	-398.9191	2.24	-398.95148	1.44	5.34
7	-399.031278	3.07	-398.91884	2.40	-398.95116	1.64	3.79
8	-399.029887	3.94	-398.91713	3.47	-398.94964	2.59	0.76
9	-399.0293352	4.29	-398.916496	3.87	-398.949583	2.63	0.71
10	-399.031529	2.91	-398.917957	2.95	-398.94953	2.66	0.68
11	-399.0294159	4.24	-398.917135	3.47	-398.949523	2.66	0.67
12	-399.0291292	4.42	-398.916771	3.70	-398.949133	2.91	0.44
13	-399.028085	5.07	-398.91587	4.26	-398.9485	3.31	0.23
14	-399.0280662	5.09	-398.91591	4.24	-398.948366	3.39	0.20
15	-399.027394	5.51	-398.91536	4.59	-398.94835	3.40	0.19
16	-399.028049	5.10	-398.91571	4.36	-398.9482	3.49	0.17
17	-399.0283496	4.91	-398.91547	4.52	-398.94817	3.51	0.16
18	-399.027837	5.23	-398.91556	4.46	-398.94816	3.52	0.16
19	-399.027516	5.43	-398.91508	4.76	-398.94767	3.82	0.09
20	-399.02724	5.60	-398.91499	4.82	-398.94759	3.87	0.09
21	-399.027734	5.29	-398.91497	4.83	-398.9475	3.94	0.08
22	-399.0273773	5.52	-398.9149	4.87	-398.947424	3.98	0.07
23	-399.0270781	5.71	-398.914787	4.94	-398.94723	4.10	0.06
24	-399.026107	6.31	-398.91419	5.32	-398.94715	4.15	0.05
25	-399.026587	6.01	-398.9143	5.25	-398.94715	4.15	0.05
26	-399.026622	5.99	-398.91449	5.13	-398.94707	4.20	0.05
27	-399.0262109	6.25	-398.914045	5.41	-398.946746	4.41	0.04
28	-399.025536	6.67	-398.91355	5.72	-398.9466	4.50	0.03
29	-399.0266346	5.98	-398.914057	5.40	-398.946271	4.71	0.02
30	-399.0266477	5.98	-398.914066	5.40	-398.946196	4.75	0.02
31	-399.024066	7.60	-398.91194	6.73	-398.94578	5.01	0.01
32	-399.0256654	6.59	-398.913255	5.91	-398.945677	5.08	0.01
33	-399.0255422	6.67	-398.913034	6.04	-398.945392	5.26	0.01
34	-399.024907	7.07	-398.91264	6.29	-398.94521	5.37	0.01
35	-399.023264	8.10	-398.9115	7.01	-398.94521	5.37	0.01
36	-399.0229227	8.31	-398.911244	7.17	-398.945083	5.45	0.01
37	-399.025017	7.00	-398.91262	6.30	-398.94493	5.55	0.01
38	-399.0256978	6.57	-398.912907	6.12	-398.944904	5.56	0.00
39	-399.0239761	7.65	-398.911838	6.79	-398.944852	5.60	0.00
40	-399.0252579	6.85	-398.912667	6.27	-398.944757	5.66	0.00

41	-399.023871	7.72	-398.91175	6.85	-398.94453	5.80	0.00
42	-399.0238842	7.71	-398.911487	7.01	-398.944422	5.87	0.00
43	-399.0242673	7.47	-398.912008	6.69	-398.944243	5.98	0.00
44	-399.0240211	7.62	-398.911905	6.75	-398.944208	6.00	0.00
45	-399.024117	7.56	-398.911868	6.78	-398.944092	6.07	0.00
46	-399.023754	7.79	-398.91155	6.97	-398.94377	6.27	0.00
47	-399.0235252	7.93	-398.911322	7.12	-398.943671	6.34	0.00
48	-399.0231452	8.17	-398.910935	7.36	-398.94359	6.39	0.00
49	-399.0231934	8.14	-398.911068	7.28	-398.94328	6.58	0.00
50	-399.0215859	9.15	-398.909685	8.15	-398.94304	6.73	0.00
51	-399.0219123	8.95	-398.910244	7.79	-398.942908	6.82	0.00
52	-399.0213702	9.29	-398.909546	8.23	-398.942556	7.04	0.00
53	-399.0215822	9.15	-398.90914	8.49	-398.942108	7.32	0.00
54	-399.018297	11.22	-398.906664	10.04	-398.939466	8.98	0.00



Scheme 1SI.

Table 2SI. The selected dihedral angles (deg) for the B3LYP/aug-cc-pVDZ optimized 54 stable structures of L-isoserine in the gas phase (Fig 1SI). Atom numbering as in Scheme 1SI.

	(H12N7C3C2)	(H13N7C3C2)	(N7C3C2C1)	(04C1C2C3)	(H14O5C1C2)	(H8O6C2C1)
1	79.1	-162	63.4	135.4	9.2	-12.1
2	84.6	-155.3	-77.5	-47.5	-2.4	96
3	-81.7	158.4	-168.9	-64.8	2.1	152
4	175.6	-65.8	-56.6	124.9	179.8	-4.9
5	-65.2	53.2	-177.3	111.5	178.3	10.7
6	68	-52	-62	121.7	-178.8	-3.9
7	-179.8	61.7	177.3	177.8	-179.9	5.2
8	78	-160.5	-72.9	88.7	177	80.9
9	83.8	-155.7	-76.5	-75.5	-179.4	85.3
10	171.2	-69.4	-56.9	-153.3	0.8	-54
11	62.6	-57.6	114.8	114.8	178.8	4.8
12	-72.2	168.5	79.1	124.7	-179.1	-5.4
13	68.9	-51.3	-63.5	-37.1	177.3	-39.3
14	172.6	-68.2	-62.6	-55.3	178.5	-20.1
15	-64.8	54.1	176	-48.5	178.1	-37.1
16	-67.3	51.2	176.3	-79.6	-177	42.6
17	-82.5	157.3	-175.5	-75.6	-178.5	158.1
18	-176.9	64.8	170.1	-31.7	177.1	-50.9
19	70.6	-170.5	58.7	82.7	177.2	36.6
20	179.9	60.9	172.1	-75	-178.1	40.2
21	-83	156.7	-172.5	100.4	177.3	157.2
22	-75.5	165.2	69.3	-16.4	179	-50.7
23	70	-50.5	-60.4	-50.4	-0.8	-159
24	-79.7	161	169.4	114.4	179.6	9.4
25	63.3	-56.7	69.4	-33	178.1	-40.7
26	63.8	-55.2	65.9	-75.7	-176.6	42.1
27	63.6	-54.6	68.6	-63.2	2.5	166.4
28	-62.2	178	73	-66	-177.2	33.7
29	-65.4	54.9	175.6	-71.8	3.1	-93.7
30	176.9	-64.4	75.5	-45.9	-2.9	-159.8
31	72.2	-47.4	-63.1	-44.2	178.4	-169.4
32	58.2	-70.5	-66.6	-41.2	-1.5	89.5

33	64.9	-58.9	64.7	-70.7	3.3	-96.5
34	68.1	-172.6	52.1	-110.5	179.5	57
35	-68.9	172.5	172.1	-86	-178.3	65.2
36	-90.2	150.7	159.6	-38.3	176.7	-49.9
37	-68.4	51.3	169.6	-45.9	0.3	91.2
38	-65.3	175.2	71.4	-39.1	-3.2	91.3
39	-77.8	163.7	66.5	-0.4	179.9	-160.1
40	-176.5	63.7	166.1	-39.3	-1.9	84.1
41	69.9	-48.1	-62	102.6	177.4	-171.4
42	78.8	-161.6	59.9	-138.8	177.2	-65.9
43	-178.7	-60.3	-54.1	131.1	10.2	-10.7
44	64.6	-54.9	-61.2	116.2	-2.1	0.6
45	177.9	59.8	175.8	111.3	-3.3	9.8
46	-64	54.4	-176.5	110.6	-3.1	9
47	178.4	-61.5	-60.2	-64.4	178.8	-166.8
48	62.5	-55.8	66.9	-72.7	-177.4	178
49	-178.2	-58.2	-54.5	118.6	178.6	169
50	81.2	-158.5	65.8	48.7	-179.2	-171.7
51	58.1	-77.7	69.5	114.5	1.2	4.1
52	71.4	-168.6	56.7	-120.2	179.6	-167.7
53	74.7	-163.3	-73.5	79.6	-7.9	81.8
54	-77.3	162.5	171.1	113.5	-1.2	7.8

Table 3SI. The B3LYP/aug-cc-pVDZ Cartesian coordinates for L-isoserine conformers in the
gas phase.

<u> </u>	2
C,0,0.232514219,-0.9534289939,0.340543524	C,0,-0.5314738122,-0.0135689623,-1.0605098161
O,0,0.9711641009,-1.5330107326,1.1097655118	O,0,-1.4752623728,0.708880642,-1.2821451429
O,0,-0.3291882708,-1.5487678962,-0.7141576124	O,0,0.4025922687,-0.2908064561,-1.9866874378
H,0,-0.7817246852,-0.8454837812,-1.2602690868	H,0,1.0564166808,-0.8719512738,-1.5472621692
C,0,-0.1249886346,0.524586941,0.5645589404	C,0,-0.3070623402,-0.7141049329,0.2937436038
H,0,-1.1727164017,0.5374709348,0.928703388	H,0,-1.0638393355,-1.5094105218,0.3598372394
C,0,-0.0552539204,1.3611275853,-0.7233128398	C,0,-0.4772536011,0.2564125907,1.4727964025
H,0,0.9405238099,1.250320022,-1.1717143012	H,0,-0.5625515574,-0.3346317902,2.3932221294
H,0,-0.1861209096,2.4196111088,-0.4543443362	H,0,-1.4051441186,0.8291296688,1.3353633742
0,0,0.7284303391,1.0821703008,1.5350134864	0.0.097960971461.3273945298.0.3330975373
H.0.1.1901820997.0.3295759696.1.9453919265	H.0.1.54527480720.6672464688.0.7822661972
N.01.0624066671.0.86655137271.6872114019	N.0.0.7379402837.1.0803001701.1.5717721165
H.01.9915278672.1.21233947931.455864841	H.0.0.6921252722.1.885514099.0.9511614124
H 0 -0 8551372118 1 1844376297 -2 6298522975	H 0 0 8728780506 1 4343777652 2 5133445133
2	11,0,0.0720700200,11.1570777022,2.5755716755
J	4
C,0,-0.606/135509,-1.0633680496,0.426/6/644	C,0,-0.9051592425,-0.2820234991,-0.309671951
0,0,-1.8016892968,-1.1489831423,0.58332/1134	0,0,-1.69/3543632,0.558/898036,-0.6/9283422/
0,0,0.1/85842552,-2.13/4325049,0.2291419169	0,0,-1.2632062679,-1.4106296004,0.3340608943
H,0,1.0950809959,-1.8089283975,0.1450194009	H,0,-2.2261341243,-1.3802355158,0.4568555488
C,0,0.122810177,0.2791594322,0.4077585774	C,0,0.5918160519,-0.1967748419,-0.5763359432
H,0,-0.1399030987,0.8042850274,1.341900481	H,0,0.8546219975,-1.0507048178,-1.2267059071
C,0,-0.3295805368,1.1198348966,-0.8017114074	C,0,1.4189953753,-0.2921235355,0.7091343068
H,0,-1.3902989774,1.3832336184,-0.6807268051	H,0,2.4819892032,-0.2432573976,0.4119489181
H,0,-0.2300072684,0.5134809316,-1.7123203125	H,0,1.2425111635,-1.2718895116,1.171685496
O,0,1.5272422352,0.0545320802,0.3497005848	O,0,0.8773504785,1.0188677014,-1.2455957136
H,0,1.8928597658,0.8385559719,-0.1013623546	H,0,0.0250640071,1.4470925063,-1.4291947908
N,0,0.5833323487,2.2654181029,-0.9216235959	N,0,1.0036118787,0.7555839607,1.641904041
H,0,0.5754545284,2.6514337039,-1.8606435895	H,0,1.4894545438,0.6673508831,2.5297352724
H,0,0.3273284429,3.0160283292,-0.2839776534	H,0,1.2336893583,1.6704538844,1.260463191
5	6
C 0 -1 1353757406 -0 139973085 -0 4109748197	C 0 -1 0166542608 -0 0665183494 0 2268511954
0.0 - 1.7080507872 - 1.2093700966 - 0.3654812383	0.0 -1.4011798378 -1.1079204836.0.7177133467
0,0,1,4400485776,0,8205223057,1,2006182102	0,0, 1.1011/903/0, 1.10/9201050,0.11/115510/
	0 0 -1 72618362 0 6257793839 -0 6901452607
H 0 -2 1650505168 0 4978091978 -1 8562321603	O,0,-1.72618362,0.6257793839,-0.6901452607 H 0 -2 5560274537 0 1435188952 -0 8407392558
H,0,-2.1650505168,0.4978091978,-1.8562321603 C 0 0 0175473066 0 2349463689 0 4995034409	O,0,-1.72618362,0.6257793839,-0.6901452607 H,0,-2.5560274537,0.1435188952,-0.8407392558 C 0 0 3025667492 0 5964094573 0 580931238
H,0,-2.1650505168,0.4978091978,-1.8562321603 C,0,0.0175473066,0.2349463689,0.4995034409 H,0,-0.2043775808,1.2164952445,0.9502160302	O,0,-1.72618362,0.6257793839,-0.6901452607 H,0,-2.5560274537,0.1435188952,-0.8407392558 C,0,0.3025667492,0.5964094573,0.580931238 H 0.0.0588384879 1 5959231424 0 986124688
H,0,-2.1650505168,0.4978091978,-1.8562321603 C,0,0.0175473066,0.2349463689,0.4995034409 H,0,-0.2043775808,1.2164952445,0.9502160302 C,0,1,3442187604,0,3425426022,-0,2988164986	O,0,-1.72618362,0.6257793839,-0.6901452607 H,0,-2.5560274537,0.1435188952,-0.8407392558 C,0,0.3025667492,0.5964094573,0.580931238 H,0,0.0588384879,1.5959231424,0.986124688 C 0,1,2253109341,0,7926265731,-0,6462811443
H,0,-2.1650505168,0.4978091978,-1.8562321603 C,0,0.0175473066,0.2349463689,0.4995034409 H,0,-0.2043775808,1.2164952445,0.9502160302 C,0,1.3442187604,0.3425426022,-0.2988164986 H,0,1.2383915354,1.1166094787, 1.0707737585	O,0,-1.72618362,0.6257793839,-0.6901452607 H,0,-2.5560274537,0.1435188952,-0.8407392558 C,0,0.3025667492,0.5964094573,0.580931238 H,0,0.0588384879,1.5959231424,0.986124688 C,0,1.2253109341,0.7926265731,-0.6462811443 H 0.2,1180388396,1,315374748,0,2777530256
H,0,-2.1650505168,0.4978091978,-1.8562321603 C,0,0.0175473066,0.2349463689,0.4995034409 H,0,-0.2043775808,1.2164952445,0.9502160302 C,0,1.3442187604,0.3425426022,-0.2988164986 H,0,1.2383915354,1.1166094787,-1.0707737585 H 0,1,5151387207,-0.6181911577,-0.8071617473	O,0,-1.72618362,0.6257793839,-0.6901452607 H,0,-2.5560274537,0.1435188952,-0.8407392558 C,0,0.3025667492,0.5964094573,0.580931238 H,0,0.0588384879,1.5959231424,0.986124688 C,0,1.2253109341,0.7926265731,-0.6462811443 H,0,2.1189388396,1.3152374748,-0.2777539256 H 0.0 72851642321,4566438788,-1,3656233862
H,0,-2.1650505168,0.4978091978,-1.8562321603 C,0,0.0175473066,0.2349463689,0.4995034409 H,0,-0.2043775808,1.2164952445,0.9502160302 C,0,1.3442187604,0.3425426022,-0.2988164986 H,0,1.2383915354,1.1166094787,-1.0707737585 H,0,1.5151387207,-0.6181911577,-0.8071617473	O,0,-1.72618362,0.6257793839,-0.6901452607 H,0,-2.5560274537,0.1435188952,-0.8407392558 C,0,0.3025667492,0.5964094573,0.580931238 H,0,0.0588384879,1.5959231424,0.986124688 C,0,1.2253109341,0.7926265731,-0.6462811443 H,0,2.1189388396,1.3152374748,-0.2777539256 H,0,0.7285164232,1.4566438788,-1.3656233862 O,0.0686666688,0.171486100715640380551
H,0,-2.1650505168,0.4978091978,-1.8562321603 C,0,0.0175473066,0.2349463689,0.4995034409 H,0,-0.2043775808,1.2164952445,0.9502160302 C,0,1.3442187604,0.3425426022,-0.2988164986 H,0,1.2383915354,1.1166094787,-1.0707737585 H,0,1.5151387207,-0.6181911577,-0.8071617473 O,0,0.1388813338,-0.7227392948,1.5353641061 H,0,0.4373882065,1.468850405,1.3032546487	O,0,-1.72618362,0.6257793839,-0.6901452607 H,0,-2.5560274537,0.1435188952,-0.8407392558 C,0,0.3025667492,0.5964094573,0.580931238 H,0,0.0588384879,1.5959231424,0.986124688 C,0,1.2253109341,0.7926265731,-0.6462811443 H,0,2.1189388396,1.3152374748,-0.2777539256 H,0,0.7285164232,1.4566438788,-1.3656233862 O,0,09686696688,-0.1714861997,1.5649389551 H 0,0 3704433484,0.00214472101811008057
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0,0,-1.44094837/0,0.8293223037,-1.2990182102 H,0,-2.1650505168,0.4978091978,-1.8562321603 C,0,0.0175473066,0.2349463689,0.4995034409 H,0,-0.2043775808,1.2164952445,0.9502160302 C,0,1.3442187604,0.3425426022,-0.2988164986 H,0,1.2383915354,1.1166094787,-1.0707737585 H,0,1.5151387207,-0.6181911577,-0.8071617473 O,0,0.1388813338,-0.7227392948,1.5353641061 H,0,-0.4373882265,-1.468850405,1.3033546487 N,0,2.5099967428,0.6401239944,0.5197527023 H,0,2.4381663349,1.5649347269,0.9390289079 H,0,2.579850715,-0.0291098801,1.2835886569 7 C,0,-1.1679379268,0.1910708626,0.0490011126 O,0,-1.730086433,1.2449968443,-0.1665257217 O,0,-1.7164388861,-0.8076433151,0.771334156 H,0,-2.5966536232,-0.5110951923,1.0563222097 C,0,0.2218017691,-0.138503228,-0.4672423162	0,0,-1.72618362,0.6257793839,-0.6901452607 H,0,-2.5560274537,0.1435188952,-0.8407392558 C,0,0.3025667492,0.5964094573,0.580931238 H,0,0.0588384879,1.5959231424,0.986124688 C,0,1.2253109341,0.7926265731,-0.6462811443 H,0,2.1189388396,1.3152374748,-0.2777539256 H,0,0.7285164232,1.4566438788,-1.3656233862 O,0,0.9686696688,-0.1714861997,1.5649389551 H,0,0.3794433484,-0.9021447219,1.8110098057 N,0,1.6533336583,-0.4210777788,-1.3265172617 H,0,2.0554228101,-1.0778729108,-0.6616252081 H,0,0.8810041926,-0.8898683413,-1.7941338264 8 C,0,-0.769157215,-0.1899843581,0.7320149415 O,0,-1.5363517489,-0.9435852384,0.1790319617 O,0,-1.1627463472,0.6888028976,1.6929995755 H,0,-2.1210431494,0.5760844151,1.8072046582 C,0,0.722159326,-0.0410640288,0.4201524172
0,0,-1.44094837/0,0.8293223037,-1.2990182102 H,0,-2.1650505168,0.4978091978,-1.8562321603 C,0,0.0175473066,0.2349463689,0.4995034409 H,0,-0.2043775808,1.2164952445,0.9502160302 C,0,1.3442187604,0.3425426022,-0.2988164986 H,0,1.2383915354,1.1166094787,-1.0707737585 H,0,1.5151387207,-0.6181911577,-0.8071617473 O,0,0.1388813338,-0.7227392948,1.5353641061 H,0,-0.4373882265,-1.468850405,1.3033546487 N,0,2.5099967428,0.6401239944,0.5197527023 H,0,2.579850715,-0.0291098801,1.2835886569 7 C,0,-1.1679379268,0.1910708626,0.0490011126 O,0,-1.730086433,1.2449968443,-0.1665257217 O,0,-1.7164388861,-0.8076433151,0.771334156 H,0,-2.5966536232,-0.5110951923,1.0563222097 C,0,0.2218017691,-0.138503228,-0.4672423162 H,0,0.1579502383,-1.0651261239,-1.0614738695	0,0,-1.72618362,0.6257793839,-0.6901452607 H,0,-2.5560274537,0.1435188952,-0.8407392558 C,0,0.3025667492,0.5964094573,0.580931238 H,0,0.0588384879,1.5959231424,0.986124688 C,0,1.2253109341,0.7926265731,-0.6462811443 H,0,2.1189388396,1.3152374748,-0.2777539256 H,0,0.7285164232,1.4566438788,-1.3656233862 O,0,0.9686696688,-0.1714861997,1.5649389551 H,0,0.3794433484,-0.9021447219,1.8110098057 N,0,1.6533336583,-0.4210777788,-1.3265172617 H,0,2.0554228101,-1.0778729108,-0.6616252081 H,0,0.8810041926,-0.8898683413,-1.7941338264 8 C,0,-0.769157215,-0.1899843581,0.7320149415 O,0,-1.5363517489,-0.9435852384,0.1790319617 O,0,-1.1627463472,0.6888028976,1.6929995755 H,0,-2.1210431494,0.5760844151,1.8072046582 C,0,0.722159326,-0.0410640288,0.4201524172 H,0,1.2271071828,0.2989778576,1.3332135829
0,0,-1.4409483770,0.8293223037,-1.2990182102 H,0,-2.1650505168,0.4978091978,-1.8562321603 C,0,0.0175473066,0.2349463689,0.4995034409 H,0,-0.2043775808,1.2164952445,0.9502160302 C,0,1.3442187604,0.3425426022,-0.2988164986 H,0,1.2383915354,1.1166094787,-1.0707737585 H,0,1.5151387207,-0.6181911577,-0.8071617473 O,0,0.1388813338,-0.7227392948,1.5353641061 H,0,-0.4373882265,-1.468850405,1.3033546487 N,0,2.5099967428,0.6401239944,0.5197527023 H,0,2.579850715,-0.0291098801,1.2835886569 7 C,0,-1.1679379268,0.1910708626,0.0490011126 O,0,-1.730086433,1.2449968443,-0.1665257217 O,0,-1.7164388861,-0.8076433151,0.771334156 H,0,-2.5966536232,-0.5110951923,1.0563222097 C,0,0.2218017691,-0.138503228,-0.4672423162 H,0,0.1579502383,-1.0651261239,-1.0614738695 C,0,1.2142877248,-0.3750274519,0.6801741098	0,0,-1.72618362,0.6257793839,-0.6901452607 H,0,-2.5560274537,0.1435188952,-0.8407392558 C,0,0.3025667492,0.5964094573,0.580931238 H,0,0.0588384879,1.5959231424,0.986124688 C,0,1.2253109341,0.7926265731,-0.6462811443 H,0,2.1189388396,1.3152374748,-0.2777539256 H,0,0.7285164232,1.4566438788,-1.3656233862 O,0,0.9686696688,-0.1714861997,1.5649389551 H,0,0.3794433484,-0.9021447219,1.8110098057 N,0,1.6533336583,-0.4210777788,-1.3265172617 H,0,2.0554228101,-1.0778729108,-0.6616252081 H,0,0.8810041926,-0.8898683413,-1.7941338264 8 C,0,-0.769157215,-0.1899843581,0.7320149415 O,0,-1.5363517489,-0.9435852384,0.1790319617 O,0,-1.1627463472,0.6888028976,1.6929995755 H,0,-2.1210431494,0.5760844151,1.8072046582 C,0,0.722159326,-0.0410640288,0.4201524172 H,0,1.2271071828,0.2989778576,1.3332135829 C,0,0.9042894847,1.0217095356,-0.689185805
0,0,-1.4409483770,0.8293223037,-1.2990182102 H,0,-2.1650505168,0.4978091978,-1.8562321603 C,0,0.0175473066,0.2349463689,0.4995034409 H,0,-0.2043775808,1.2164952445,0.9502160302 C,0,1.3442187604,0.3425426022,-0.2988164986 H,0,1.2383915354,1.1166094787,-1.0707737585 H,0,1.5151387207,-0.6181911577,-0.8071617473 O,0,0.1388813338,-0.7227392948,1.5353641061 H,0,-0.4373882265,-1.468850405,1.3033546487 N,0,2.5099967428,0.6401239944,0.5197527023 H,0,2.4381663349,1.5649347269,0.9390289079 H,0,2.579850715,-0.0291098801,1.2835886569 7 C,0,-1.1679379268,0.1910708626,0.0490011126 O,0,-1.730086433,1.2449968443,-0.1665257217 O,0,-1.7164388861,-0.8076433151,0.771334156 H,0,-2.5966536232,-0.5110951923,1.0563222097 C,0,0.2218017691,-0.138503228,-0.4672423162 H,0,0.1579502383,-1.0651261239,-1.0614738695 C,0,1.2142877248,-0.3750274519,0.6801741098 H,0,0.8498308119,-1.2034351684,1.3021043353	0,0,-1.72618362,0.6257793839,-0.6901452607 H,0,-2.5560274537,0.1435188952,-0.8407392558 C,0,0.3025667492,0.5964094573,0.580931238 H,0,0.0588384879,1.5959231424,0.986124688 C,0,1.2253109341,0.7926265731,-0.6462811443 H,0,2.1189388396,1.3152374748,-0.2777539256 H,0,0.7285164232,1.4566438788,-1.3656233862 O,0,0.9686696688,-0.1714861997,1.5649389551 H,0,0.3794433484,-0.9021447219,1.8110098057 N,0,1.6533336583,-0.4210777788,-1.3265172617 H,0,2.0554228101,-1.0778729108,-0.6616252081 H,0,0.8810041926,-0.8898683413,-1.7941338264 8 C,0,-0.769157215,-0.1899843581,0.7320149415 O,0,-1.5363517489,-0.9435852384,0.1790319617 O,0,-1.1627463472,0.6888028976,1.6929995755 H,0,-2.1210431494,0.5760844151,1.8072046582 C,0,0.722159326,-0.0410640288,0.4201524172 H,0,1.2271071828,0.2989778576,1.3332135829 C,0,0.9042894847,1.0217095356,-0.689185805 H,0,1.9795370009,1.2269396693,-0.7671906001
0,0,-1.4409483770,0.8293223037,-1.2990182102 H,0,-2.1650505168,0.4978091978,-1.8562321603 C,0,0.0175473066,0.2349463689,0.4995034409 H,0,-0.2043775808,1.2164952445,0.9502160302 C,0,1.3442187604,0.3425426022,-0.2988164986 H,0,1.2383915354,1.1166094787,-1.0707737585 H,0,1.5151387207,-0.6181911577,-0.8071617473 O,0,0.1388813338,-0.7227392948,1.5353641061 H,0,-0.4373882265,-1.468850405,1.3033546487 N,0,2.5099967428,0.6401239944,0.5197527023 H,0,2.579850715,-0.0291098801,1.2835886569 7 C,0,-1.1679379268,0.1910708626,0.0490011126 O,0,-1.730086433,1.2449968443,-0.1665257217 O,0,-1.7164388861,-0.8076433151,0.771334156 H,0,-2.5966536232,-0.5110951923,1.0563222097 C,0,0.2218017691,-0.138503228,-0.4672423162 H,0,0.1579502383,-1.0651261239,-1.0614738695 C,0,1.2142877248,-0.3750274519,0.6801741098 H,0,0.8498308119,-1.2034351684,1.3021043353 H,0,1.2412615448,0.5388216181,1.3041744447	0,0,-1.72618362,0.6257793839,-0.6901452607 H,0,-2.5560274537,0.1435188952,-0.8407392558 C,0,0.3025667492,0.5964094573,0.580931238 H,0,0.0588384879,1.5959231424,0.986124688 C,0,1.2253109341,0.7926265731,-0.6462811443 H,0,2.1189388396,1.3152374748,-0.2777539256 H,0,0.7285164232,1.4566438788,-1.3656233862 O,0,0.9686696688,-0.1714861997,1.5649389551 H,0,0.3794433484,-0.9021447219,1.8110098057 N,0,1.6533336583,-0.4210777788,-1.3265172617 H,0,2.0554228101,-1.0778729108,-0.6616252081 H,0,0.8810041926,-0.8898683413,-1.7941338264 8 C,0,-0.769157215,-0.1899843581,0.7320149415 O,0,-1.5363517489,-0.9435852384,0.1790319617 O,0,-1.1627463472,0.6888028976,1.6929995755 H,0,-2.1210431494,0.5760844151,1.8072046582 C,0,0.722159326,-0.0410640288,0.4201524172 H,0,1.2271071828,0.2989778576,1.3332135829 C,0,0.9042894847,1.0217095356,-0.689185805 H,0,1.9795370009,1.2269396693,-0.7671906001 H,0,0.3979195694,1.95732626,-0.3961050892

H,0,0.010603305,1.617153527,-1.2633541182	H,0,1.0661133775,-1.3857960538,-0.8991976053
N,0,2.5071888841,-0.749382657,0.108733223	N,0,0.4578537101,0.4567907056,-1.9657887212
H,0,2.8627541326,0.0091713833,-0.4695541159	H,0,-0.5553858908,0.4527178446,-2.0516778752
H,0,3.1901966918,-0.9168539192,0.8425488439	H,0,0.8376855474,0.9673881753,-2.7559938022
9	10
C.00.64424951621.03491470340.2345698918	C.0.0.3179085457.0.71378762170.7674559376
0,0,-1.1121887361,-1.5102522299,-1.247533029	O,0,1.08780149,1.5844334365,-1.1141110809
0,0,0.1685520465,-1.7287519433,0.5944783627	0,0,-0.8116754335,0.4485066141,-1.4326626383
H.0.0.2491635432.6219992193.0.22050507	H.01.3087851360.26506106890.938358309
C.00.8734898785.0.4168017764.0.1973871679	C.0.0.59050479830.1031566723.0.5169229909
H.01.9317617532.0.61852512670.0150158984	H.0.1.68450946930.1781198213.0.6091355068
C.00.0074686004.1.36012383410.6687722439	C.00.00833999631.5064089596.0.5453990485
H,0,-0.3713192366,2.3806536178,-0.4959700812	H.0.0.2757486641,-1.9819019906,1.4976840056
H.O0.1497816239,1.1173582341,-1.73375252	H,0,0.4300056866,-2.0938986065,-0.272616034
0,0,-0.6519300092,0.6500871601,1.5666457893	0,0,0.0400862873,0.5993570612,1.6409257353
H,0,0.3024082837,0.814892388,1.6566768013	H.0,0.3938969012,1.4984909036,1.6436252383
N,0,1.3849049775,1.2925667122,-0.2074358285	N.0,-1.4688612034,-1.4447338066,0.3417320155
H,0,1.884911836,0.5068869664,-0.6157275568	H,0,-1.8637084718,-2.3719203589,0.2139466352
H,0,1.8979986073,2.1352722401,-0.4449161216	H,0,-1.9175916016,-1.0253743726,1.1533328437
11	12
C 0 -0 5130918358 -0 5510949145 -0 6969854627	C 0 0 2112846688 -1 0117927666 0 078778712
0.0 - 0.3522193733 - 0.945061304 - 1.8335580955	0.0.8266468985 - 1.7512170497.0.8182819398
0.0 -1 7181973995 -0 1649245214 -0 2178868276	0.0.0603178326 - 1.257222355 - 1.2425409809
H 0 -2 3597734108 -0 2656338389 -0 9413051039	H 0 0 5141982516 -2 0952294666 -1 4324691529
C 0 0 6114258431 -0 4228215391 0 3140425111	C 0 -0 4682710282 0 2672994321 0 5430829255
H 0 0 3215284376 -0 9873647804 1 217376771	H 0 -1 5518227691 0 1414899369 0 3693066877
C 0 0 8698193142 1 0584936568 0 7250885332	C 0 -0 0179019883 1 5188993349 -0 2371015149
H 0 0 9420210815 1 6702503363 -0 1860118818	H 0 1 0868998659 1 5369969671 -0 2769250749
H 0 1 8653946246 1 0614056648 1 1872268086	H 0 -0 334931125 2 371797175 0 3760177866
0.017919945399 - 0.9788905421 - 0.2297402979	0.0 = 0.2066639921.0.4541885815.1.9200873349
H 0 1 5988078005 -1 2333108284 -1 146344068	H 0 0 2691453916 -0 3305852434 2 2354689344
N 0 -0 0771339494 1 6756990213 1 6406412077	N 0 -0 6810128671 1 6151447808 -1 5380147189
1,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	
H.01.0251354724.1.654691507.1.2753268739	H.00.5207263243.2.5289458329-1.951936543
H,0,-1.0251354724,1.654691507,1.2753268739 H.0,-0.0881902401,1.2015621028,2.5403790919	H,0,-0.5207263243,2.5289458329,-1.951936543 H,0,-0.3241628348.0.9202847206,-2.1885363954
H,0,-1.0251354724,1.654691507,1.2753268739 H,0,-0.0881902401,1.2015621028,2.5403790919 13	H,0,-0.5207263243,2.5289458329,-1.951936543 H,0,-0.3241628348,0.9202847206,-2.1885363954 14
H,0,-1.0251354724,1.654691507,1.2753268739 H,0,-0.0881902401,1.2015621028,2.5403790919 13 C 0 -0 0494377932 0 7038775983 -0 7414966114	H,0,-0.5207263243,2.5289458329,-1.951936543 H,0,-0.3241628348,0.9202847206,-2.1885363954 14
H,0,-1.0251354724,1.654691507,1.2753268739 H,0,-0.0881902401,1.2015621028,2.5403790919 13 C,0,-0.0494377932,0.7038775983,-0.7414966114 O,0,0,4084661534,1,7920363262,-0,4788009923	H,0,-0.5207263243,2.5289458329,-1.951936543 H,0,-0.3241628348,0.9202847206,-2.1885363954 14 C,0,-0.0890685567,0.2952033119,1.007396668 O,0,-0,1586076543,-0,4713953908,1,9380331791
H,0,-1.0251354724,1.654691507,1.2753268739 H,0,-0.0881902401,1.2015621028,2.5403790919 13 C,0,-0.0494377932,0.7038775983,-0.7414966114 O,0,0.4084661534,1.7920363262,-0.4788009923 O 0 -0 0582866434 0 1980163985 -2 0039420581	H,0,-0.5207263243,2.5289458329,-1.951936543 H,0,-0.3241628348,0.9202847206,-2.1885363954 14 C,0,-0.0890685567,0.2952033119,1.007396668 O,0,-0.1586076543,-0.4713953908,1.9380331791 O 0 0 5705572414 1 4819843805 1 0755022823
H,0,-1.0251354724,1.654691507,1.2753268739 H,0,-0.0881902401,1.2015621028,2.5403790919 13 C,0,-0.0494377932,0.7038775983,-0.7414966114 O,0,0.4084661534,1.7920363262,-0.4788009923 O,0,-0.0582866434,0.1980163985,-2.0039420581 H 0 0 3481386132 0 863354247 -2 5832655681	H,0,-0.5207263243,2.5289458329,-1.951936543 H,0,-0.3241628348,0.9202847206,-2.1885363954 14 C,0,-0.0890685567,0.2952033119,1.007396668 O,0,-0.1586076543,-0.4713953908,1.9380331791 O,0,0.5705572414,1.4819843805,1.0755022823 H 0 0 9568833812 1 5437291659 1 9642891352
H,0,-1.0251354724,1.654691507,1.2753268739 H,0,-0.0881902401,1.2015621028,2.5403790919 13 C,0,-0.0494377932,0.7038775983,-0.7414966114 O,0,0.4084661534,1.7920363262,-0.4788009923 O,0,-0.0582866434,0.1980163985,-2.0039420581 H,0,0.3481386132,0.863354247,-2.5832655681 C,0,-0.7260294047,-0.2276630979,0.2604539311	H,0,-0.5207263243,2.5289458329,-1.951936543 H,0,-0.3241628348,0.9202847206,-2.1885363954 14 C,0,-0.0890685567,0.2952033119,1.007396668 O,0,-0.1586076543,-0.4713953908,1.9380331791 O,0,0.5705572414,1.4819843805,1.0755022823 H,0,0.9568833812,1.5437291659,1.9642891352 C,0,-0,7805833281,0.0804644448,-0.3358544748
H,0,-1.0251354724,1.654691507,1.2753268739 H,0,-0.0881902401,1.2015621028,2.5403790919 13 C,0,-0.0494377932,0.7038775983,-0.7414966114 O,0,0.4084661534,1.7920363262,-0.4788009923 O,0,-0.0582866434,0.1980163985,-2.0039420581 H,0,0.3481386132,0.863354247,-2.5832655681 C,0,-0.7260294047,-0.2276630979,0.2604539311 H,0,-1,7564626086,0.1659167462,0.3685523784	H,0,-0.5207263243,2.5289458329,-1.951936543 H,0,-0.3241628348,0.9202847206,-2.1885363954 14 C,0,-0.0890685567,0.2952033119,1.007396668 O,0,-0.1586076543,-0.4713953908,1.9380331791 O,0,0.5705572414,1.4819843805,1.0755022823 H,0,0.9568833812,1.5437291659,1.9642891352 C,0,-0.7805833281,0.0804644448,-0.3358544748 H,0,-1.8619447775,0.0560956552,-0.1094653974
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H,0,-1.0251354724,1.654691507,1.2753268739 H,0,-0.0881902401,1.2015621028,2.5403790919 13 C,0,-0.0494377932,0.7038775983,-0.7414966114 O,0,0.4084661534,1.7920363262,-0.4788009923 O,0,-0.0582866434,0.1980163985,-2.0039420581 H,0,0.3481386132,0.863354247,-2.5832655681 C,0,-0.7260294047,-0.2276630979,0.2604539311 H,0,-1.7564626086,0.1659167462,0.3685523784 C,0,-0.0468168714,-0.1760296035,1.6400267336 H,0,-0.6477085107,-0.8071444222,2.3096683603 H,0,-0.0983559315,0.8529093395,2.0157470797 O,0,-0,7565501884,-1.5842311783,-0.1619922374	H,0,-0.5207263243,2.5289458329,-1.951936543 H,0,-0.3241628348,0.9202847206,-2.1885363954 14 C,0,-0.0890685567,0.2952033119,1.007396668 O,0,-0.1586076543,-0.4713953908,1.9380331791 O,0,0.5705572414,1.4819843805,1.0755022823 H,0,0.9568833812,1.5437291659,1.9642891352 C,0,-0.7805833281,0.0804644448,-0.3358544748 H,0,-1.8619447775,0.0560956552,-0.1094653974 C,0,-0.3790531986,-1.2702058417,-0.9318884677 H,0,-1.0051810873,-1.431332472,-1.8277674119 H,0,-0.6190314715,-2.0529022325,-0.2016566894 O,0,-0.5125503759,1.0931662106,-1.298821075
$\begin{array}{c} \text{H,0,-1.0251354724,1.654691507,1.2753268739} \\ \text{H,0,-0.0881902401,1.2015621028,2.5403790919} \\ \hline \textbf{13} \\ \hline \textbf{C,0,-0.0494377932,0.7038775983,-0.7414966114} \\ \text{O,0,0.4084661534,1.7920363262,-0.4788009923} \\ \text{O,0,-0.0582866434,0.1980163985,-2.0039420581} \\ \text{H,0,0.3481386132,0.863354247,-2.5832655681} \\ \text{C,0,-0.7260294047,-0.2276630979,0.2604539311} \\ \text{H,0,-1.7564626086,0.1659167462,0.3685523784} \\ \text{C,0,-0.0468168714,-0.1760296035,1.6400267336} \\ \text{H,0,-0.6477085107,-0.8071444222,2.3096683603} \\ \text{H,0,-0.0983559315,0.8529093395,2.0157470797} \\ \text{O,0,-0.7565501884,-1.5842311783,-0.1619922374} \\ \text{H,0,-0.9380185118,-1.6214961688,-1.1091892065} \\ \end{array}$	H,0,-0.5207263243,2.5289458329,-1.951936543 H,0,-0.3241628348,0.9202847206,-2.1885363954 14 C,0,-0.0890685567,0.2952033119,1.007396668 O,0,-0.1586076543,-0.4713953908,1.9380331791 O,0,0.5705572414,1.4819843805,1.0755022823 H,0,0.9568833812,1.5437291659,1.9642891352 C,0,-0.7805833281,0.0804644448,-0.3358544748 H,0,-1.8619447775,0.0560956552,-0.1094653974 C,0,-0.3790531986,-1.2702058417,-0.9318884677 H,0,-1.0051810873,-1.431332472,-1.8277674119 H,0,-0.6190314715,-2.0529022325,-0.2016566894 O,0,-0.5125503759,1.0931662106,-1.298821075 H,0,-0.2029019798,1.8874413232,-0.8462692181
$\begin{array}{c} \text{H,0,-1.0251354724,1.654691507,1.2753268739} \\ \text{H,0,-0.0881902401,1.2015621028,2.5403790919} \\ \hline \textbf{13} \\ \hline \textbf{C,0,-0.0494377932,0.7038775983,-0.7414966114} \\ \text{O,0,0.4084661534,1.7920363262,-0.4788009923} \\ \text{O,0,-0.0582866434,0.1980163985,-2.0039420581} \\ \text{H,0,0.3481386132,0.863354247,-2.5832655681} \\ \text{C,0,-0.7260294047,-0.2276630979,0.2604539311} \\ \text{H,0,-1.7564626086,0.1659167462,0.3685523784} \\ \text{C,0,-0.0468168714,-0.1760296035,1.6400267336} \\ \text{H,0,-0.0983559315,0.8529093395,2.0157470797} \\ \text{O,0,-0.7565501884,-1.5842311783,-0.1619922374} \\ \text{H,0,-0.9380185118,-1.6214961688,-1.1091892065} \\ \text{N,0,1.3360324336,-0.6305699064,1.6892655143} \\ \end{array}$	H,0,-0.5207263243,2.5289458329,-1.951936543 H,0,-0.3241628348,0.9202847206,-2.1885363954 14 C,0,-0.0890685567,0.2952033119,1.007396668 O,0,-0.1586076543,-0.4713953908,1.9380331791 O,0,0.5705572414,1.4819843805,1.0755022823 H,0,0.9568833812,1.5437291659,1.9642891352 C,0,-0.7805833281,0.0804644448,-0.3358544748 H,0,-1.8619447775,0.0560956552,-0.1094653974 C,0,-0.3790531986,-1.2702058417,-0.9318884677 H,0,-1.0051810873,-1.431332472,-1.8277674119 H,0,-0.6190314715,-2.0529022325,-0.2016566894 O,0,-0.5125503759,1.0931662106,-1.298821075 H,0,-0.2029019798,1.8874413232,-0.8462692181 N,0,1.0605291547,-1.2828484353,-1.1903518598
$\begin{array}{c} \text{H,0,-1.0251354724,1.654691507,1.2753268739} \\ \text{H,0,-0.0881902401,1.2015621028,2.5403790919} \\ \hline \textbf{13} \\ \hline \textbf{C,0,-0.0494377932,0.7038775983,-0.7414966114} \\ \text{O,0,0.4084661534,1.7920363262,-0.4788009923} \\ \text{O,0,-0.0582866434,0.1980163985,-2.0039420581} \\ \text{H,0,0.3481386132,0.863354247,-2.5832655681} \\ \text{C,0,-0.7260294047,-0.2276630979,0.2604539311} \\ \text{H,0,-1.7564626086,0.1659167462,0.3685523784} \\ \text{C,0,-0.0468168714,-0.1760296035,1.6400267336} \\ \text{H,0,-0.0983559315,0.8529093395,2.0157470797} \\ \text{O,0,-0.7565501884,-1.5842311783,-0.1619922374} \\ \text{H,0,-0.9380185118,-1.6214961688,-1.1091892065} \\ \text{N,0,1.3360324336,-0.6305699064,1.6892655143} \\ \text{H,0,1.4293625161,-1.5468319462,1.2579546832} \\ \end{array}$	H,0,-0.5207263243,2.5289458329,-1.951936543 H,0,-0.3241628348,0.9202847206,-2.1885363954 14 C,0,-0.0890685567,0.2952033119,1.007396668 O,0,-0.1586076543,-0.4713953908,1.9380331791 O,0,0.5705572414,1.4819843805,1.0755022823 H,0,0.9568833812,1.5437291659,1.9642891352 C,0,-0.7805833281,0.0804644448,-0.3358544748 H,0,-1.8619447775,0.0560956552,-0.1094653974 C,0,-0.3790531986,-1.2702058417,-0.9318884677 H,0,-1.0051810873,-1.431332472,-1.8277674119 H,0,-0.6190314715,-2.0529022325,-0.2016566894 O,0,-0.5125503759,1.0931662106,-1.298821075 H,0,-0.605291547,-1.2828484353,-1.1903518598 H,0,1.3731134512,-2.2071804306,-1.4721693809
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H,0,-1.0251354724,1.654691507,1.2753268739 H,0,-0.0881902401,1.2015621028,2.5403790919 13 C,0,-0.0494377932,0.7038775983,-0.7414966114 O,0,0.4084661534,1.7920363262,-0.4788009923 O,0,-0.0582866434,0.1980163985,-2.0039420581 H,0,0.3481386132,0.863354247,-2.5832655681 C,0,-0.7260294047,-0.2276630979,0.2604539311 H,0,-1.7564626086,0.1659167462,0.3685523784 C,0,-0.0468168714,-0.1760296035,1.6400267336 H,0,-0.6477085107,-0.8071444222,2.3096683603 H,0,-0.0983559315,0.8529093395,2.0157470797 O,0,-0.7565501884,-1.5842311783,-0.1619922374 H,0,-0.9380185118,-1.6214961688,-1.1091892065 N,0,1.3360324336,-0.6305699064,1.6892655143 H,0,1.9549168074,0.0116056474,1.2005179732 15 C,0,-1.072181772,0.2343402719,-0.5355779331 O,0,-1.7810458275,-0.6659275212,-0.9231690112 O,0,-1.5386433865,1.4903872484,-0.3044404613 H,0,-2.4883316248,1.4835909635,-0.5090831051 C,0,0.4275805481,0.1079421167,-0.2964172922 H,0,0.8722096504,-0.0210952726,-1.3023183817	H,0,-0.5207263243,2.5289458329,-1.951936543 H,0,-0.3241628348,0.9202847206,-2.1885363954 14 C,0,-0.0890685567,0.2952033119,1.007396668 O,0,-0.1586076543,-0.4713953908,1.9380331791 O,0,0.5705572414,1.4819843805,1.0755022823 H,0,0.9568833812,1.5437291659,1.9642891352 C,0,-0.7805833281,0.0804644448,-0.3358544748 H,0,-1.8619447775,0.0560956552,-0.1094653974 C,0,-0.3790531986,-1.2702058417,-0.9318884677 H,0,-1.0051810873,-1.431332472,-1.8277674119 H,0,-0.6190314715,-2.0529022325,-0.2016566894 O,0,-0.5125503759,1.0931662106,-1.298821075 H,0,-0.2029019798,1.8874413232,-0.8462692181 N,0,1.0605291547,-1.2828484353,-1.1903518598 H,0,1.3731134512,-2.2071804306,-1.4721693809 H,0,1.2865892013,-0.6382197492,-1.9437272896 16 C,0,0.3707438744,0.6167551116,0.9738104865 O,0,0.3041992974,0.3170078068,2.1436129982 O,0,1.3112745568,1.4682809245,0.4818842602 H,0,1.8596663707,1.7556656445,1.2302767093 C,0,-0.510440898,0.0386422117,-0.121344804 H,0,-1.5148699312,-0.076810697,0.306220592
H,0,-1.0251354724,1.654691507,1.2753268739 H,0,-0.0881902401,1.2015621028,2.5403790919 13 C,0,-0.0494377932,0.7038775983,-0.7414966114 O,0,0.4084661534,1.7920363262,-0.4788009923 O,0,-0.0582866434,0.1980163985,-2.0039420581 H,0,0.3481386132,0.863354247,-2.5832655681 C,0,-0.7260294047,-0.2276630979,0.2604539311 H,0,-1.7564626086,0.1659167462,0.3685523784 C,0,-0.0468168714,-0.1760296035,1.6400267336 H,0,-0.6477085107,-0.8071444222,2.3096683603 H,0,-0.0983559315,0.8529093395,2.0157470797 O,0,-0.7565501884,-1.5842311783,-0.1619922374 H,0,-0.9380185118,-1.6214961688,-1.1091892065 N,0,1.3360324336,-0.6305699064,1.6892655143 H,0,1.4293625161,-1.5468319462,1.2579546832 H,0,1.9549168074,0.0116056474,1.2005179732 15 C,0,-1.072181772,0.2343402719,-0.5355779331 O,0,-1.7810458275,-0.6659275212,-0.9231690112 O,0,-1.5386433865,1.4903872484,-0.3044404613 H,0,-2.4883316248,1.4835909635,-0.5090831051 C,0,0.4275805481,0.1079421167,-0.2964172922 H,0,0.8722096504,-0.0210952726,-1.3023183817 C,0,0.7469423742,-1.1463784827,0.543429504	H,0,-0.5207263243,2.5289458329,-1.951936543 H,0,-0.3241628348,0.9202847206,-2.1885363954 14 C,0,-0.0890685567,0.2952033119,1.007396668 O,0,-0.1586076543,-0.4713953908,1.9380331791 O,0,0.5705572414,1.4819843805,1.0755022823 H,0,0.9568833812,1.5437291659,1.9642891352 C,0,-0.7805833281,0.0804644448,-0.3358544748 H,0,-1.8619447775,0.0560956552,-0.1094653974 C,0,-0.3790531986,-1.2702058417,-0.9318884677 H,0,-1.0051810873,-1.431332472,-1.8277674119 H,0,-0.6190314715,-2.0529022325,-0.2016566894 O,0,-0.5125503759,1.0931662106,-1.298821075 H,0,-0.2029019798,1.8874413232,-0.8462692181 N,0,1.0605291547,-1.2828484353,-1.1903518598 H,0,1.3731134512,-2.2071804306,-1.4721693809 H,0,1.2865892013,-0.6382197492,-1.9437272896 16 C,0,0.3707438744,0.6167551116,0.9738104865 O,0,0.3041992974,0.3170078068,2.1436129982 O,0,1.3112745568,1.4682809245,0.4818842602 H,0,1.8596663707,1.7556656445,1.2302767093 C,0,-0.510440898,0.0386422117,-0.121344804 H,0,-1.5148699312,-0.076810697,0.306220592 C,0,0.0273149586,-1.3600583824,-0.5274084023
H,0,-1.0251354724,1.654691507,1.2753268739 H,0,-0.0881902401,1.2015621028,2.5403790919 13 C,0,-0.0494377932,0.7038775983,-0.7414966114 O,0,0.4084661534,1.7920363262,-0.4788009923 O,0,-0.0582866434,0.1980163985,-2.0039420581 H,0,0.3481386132,0.863354247,-2.5832655681 C,0,-0.7260294047,-0.2276630979,0.2604539311 H,0,-1.7564626086,0.1659167462,0.3685523784 C,0,-0.0468168714,-0.1760296035,1.6400267336 H,0,-0.6477085107,-0.8071444222,2.3096683603 H,0,-0.0983559315,0.8529093395,2.0157470797 O,0,-0.7565501884,-1.5842311783,-0.1619922374 H,0,-0.9380185118,-1.6214961688,-1.1091892065 N,0,1.3360324336,-0.6305699064,1.6892655143 H,0,1.4293625161,-1.5468319462,1.2579546832 H,0,1.9549168074,0.0116056474,1.2005179732 15 C,0,-1.072181772,0.2343402719,-0.5355779331 O,0,-1.7810458275,-0.6659275212,-0.9231690112 O,0,-1.5386433865,1.4903872484,-0.3044404613 H,0,-2.4883316248,1.4835909635,-0.5090831051 C,0,0.4275805481,0.1079421167,-0.2964172922 H,0,0.8722096504,-0.0210952726,-1.3023183817 C,0,0.7469423742,-1.1463784827,0.543429504 H,0,0.2870856447,-2.0153382892,0.0579259851	H,0,-0.5207263243,2.5289458329,-1.951936543 H,0,-0.3241628348,0.9202847206,-2.1885363954 14 C,0,-0.0890685567,0.2952033119,1.007396668 O,0,-0.1586076543,-0.4713953908,1.9380331791 O,0,0.5705572414,1.4819843805,1.0755022823 H,0,0.9568833812,1.5437291659,1.9642891352 C,0,-0.7805833281,0.0804644448,-0.3358544748 H,0,-1.8619447775,0.0560956552,-0.1094653974 C,0,-0.3790531986,-1.2702058417,-0.9318884677 H,0,-1.0051810873,-1.431332472,-1.8277674119 H,0,-0.6190314715,-2.0529022325,-0.2016566894 O,0,-0.5125503759,1.0931662106,-1.298821075 H,0,-0.2029019798,1.8874413232,-0.8462692181 N,0,1.0605291547,-1.2828484353,-1.1903518598 H,0,1.3731134512,-2.2071804306,-1.4721693809 H,0,1.2865892013,-0.6382197492,-1.9437272896 16 C,0,0.3707438744,0.6167551116,0.9738104865 O,0,0.3041992974,0.3170078068,2.1436129982 O,0,1.3112745568,1.4682809245,0.4818842602 H,0,1.8596663707,1.7556656445,1.2302767093 C,0,-0.510440898,0.0386422117,-0.121344804 H,0,-1.5148699312,-0.076810697,0.306220592 C,0,0.0273149586,-1.3600583824,-0.5274084023 H,0,0.1132166598,-1.9830196105,0.3731827697
	H,0,3.1901966918,-0.9168539192,0.8425488439 9 C,0,-0.6442495162,-1.0349147034,-0.2345698918 O,0,-1.1121887361,-1.5102522299,-1.247533029 O,0,0.1685520465,-1.7287519433,0.5944783627 H,0,0.249163543,-2.6219992193,0.22050507 C,0,-0.8734898785,0.4168017764,0.1973871679 H,0,-1.9317617532,0.6185251267,-0.0150158984 C,0,-0.0074686004,1.3601238341,-0.6687722439 H,0,-0.3713192366,2.3806536178,-0.4959700812 H,0,-0.3713192366,2.3806536178,-0.4959700812 H,0,-0.497816239,1.1173582341,-1.73375252 O,0,-0.6519300092,0.6500871601,1.5666457893 H,0,0.3024082837,0.814892388,1.6566768013 N,0,1.3849049775,1.2925667122,-0.2074358285 H,0,1.884911836,0.5068869664,-0.6157275568 H,0,1.8979986073,2.1352722401,-0.4449161216 11 C,0,-0.5130918358,-0.5510949145,-0.6969854627 O,0,-0.3522193733,-0.945061304,-1.8335580955 O,0,-1.7181973995,-0.1649245214,-0.2178868276 H,0,-2.3597734108,-0.2656338389,-0.9413051039 C,0,0.6114258431,-0.4228215391,0.3140425111 H,0,0.3215284376,-0.9873647804,1.217376771 C,0,0.8698193142,1.0584936568,0.7250885332 H,0,1.8653946246,1.0614056648,1.1872268086 O,0,1.79199

1		
	0,0,1.0079613977,1.2265490533,0.3581220719	0,0,-0.6521119447,0.8908572208,-1.2503577123
	H,0,0.5877814072,2.0367474396,0.0450834297	H,0,0.2111365734,1.2713501008,-1.461641441
	N,0,2.1667135162,-1.3988239511,0.7461648651	N,0,-0.7876218753,-2.0533582107,-1.5137238185
	H,0,2.6335714457,-1.6083487338,-0.1335997648	H,0,-1.6924212612,-2.3107022243,-1.125125264
	H,0,2.6212515487,-0.5780096806,1.1394925396	H,0,-0.9673203992,-1.4464419489,-2.310958012
	17	18
	C,0,0.9526742321,-0.1775652104,0.8850325998	C,0,0.4443688796,0.8883654008,-0.6959735848
	0,0,2.1136252634,0.1691775079,0.8151412544	0,0,-0.3276391414,1.5386488523,-1.3616775977
	0,0,0.2563774231,-0.1964918932,2.0392042631	0,0,1.7338740364,1.2664325339,-0.4891964204
	H,0,0.8694097006,0.0957913325,2.734223714	H,0,1.8655409056,2.1044014396,-0.9621135021
	C,0,0.1421676181,-0.5756237909,-0.3372720893	C,0,0.1418646363,-0.4629404139,-0.0523303429
	H,0,0.8289638641,-1.1744732735,-0.9626727558	H,0,0.350495994,-1.2239844786,-0.8280437727
	C,0,-0.2522766422,0.6956027236,-1.1239155803	C,0,-1.3237057722,-0.5848706577,0.3479866911
	H,0,0.6588147011,1.2313688915,-1.431661637	H,0,-1.9404651062,-0.3248401046,-0.5201322752
	H,0,-0.8346353104,1.3489709521,-0.4603355795	H,0,-1.5241546453,0.1592741869,1.1405860859
	O,0,-1.0037005046,-1.3200665329,0.0072852589	O,0,0.9288469572,-0.7135026101,1.1073217504
	H,0,-1.6059772271,-1.2147994768,-0.7494311448	H,0,1.8592554399,-0.5629259668,0.9002866273
	N,0,-1.1229342503,0.2852612181,-2.2324819692	N,0,-1.6026593577,-1.9685792919,0.7358442341
	H,0,-1.7043232369,1.0520575233,-2.5554994653	H,0,-1.0747108934,-2.2129355435,1.5707004937
	H,0,-0.5829356708,-0.0444600114,-3.0291168489	H,0,-2.5874119329,-2.0855433064,0.9579915733
	19	20
	C.0.0.7610981156.0.55508522020.2214487803	C.0.0.0847464177.1.0224060633.0.6378949163
	0.0.0.9461808167.1.5855777369.0.3929921474	O.0.0.9364563153.1.3308407161.1.4381868627
	0.0.1.0989055148.0.38751641771.5132691914	0.00.6714428428.1.93903245770.0240182418
	H.0.1.4438707623.1.2372897451.8356806886	H.00.3909802653.2.8171499405.0.2819017048
	C.0.0.13479459830.6804874307.0.4139008078	C.00.22801086560.4058168942.0.2112760662
	H,0,0.4486294758,-1.5715327227,-0.1464277597	H,0,-0.2099663339,-1.0278192453,1.1149838933
	C,0,-1.4029634262,-0.5700660654,0.4178905975	C,0,0.8697518776,-0.9102706799,-0.7405687399
	H,0,-1.674104665,0.3231687397,0.9982708682	H,0,1.8445193934,-0.7746293292,-0.2528699596
	H,0,-1.7770879071,-1.450753331,0.9681601206	H,0,0.8562441311,-0.2807847524,-1.6526227144
	O,0,0.6230926085,-0.827285258,1.7383417024	0,0,-1.5238966057,-0.5608800516,-0.355121903
	H,0,0.7174951559,0.0638556936,2.1082716463	H,0,-1.707743772,0.1986902026,-0.9237702898
	N,0,-1.9349419954,-0.4161738297,-0.9373126892	N,0,0.6591681218,-2.3344077221,-0.9902910234
	H,0,-1.8407830083,-1.2766040412,-1.4724723072	H,0,-0.2468747383,-2.4831189023,-1.4291999782
	H,0,-2.9249359859,-0.1898408143,-0.9124665138	H,0,1.3685291667,-2.7018918632,-1.6182806132
	21	22
	C,0,1.0047749082,0.1064006778,0.7415381426	C,0,-0.6015018356,-0.4927316591,-0.5019120133
	O,0,1.43657773,-0.7749604591,1.4409106836	O,0,-1.6849094163,-0.0841639267,-0.1494688174
	O,0,1.1870576359,1.4297598776,1.0186329322	O,0,-0.4495441002,-1.3440099249,-1.5509692606
	H,0,1.6881429675,1.4748447546,1.8491710753	H,0,-1.3334649414,-1.5206424577,-1.9125869906
	C,0,0.1656288496,-0.0543890353,-0.5174629673	C,0,0.7436634795,-0.1741571164,0.1504301653
	H,0,0.5026524314,0.7165446414,-1.2355374236	H,0,1.0058668064,-1.0562426075,0.7628470282
	C,0,-1.3253311035,0.1940092056,-0.1920345837	C,0,0.6674439169,1.0403993873,1.0755495982
	H,0,-1.4610318364,1.2284420995,0.1606190513	H,0,0.3004930607,1.9042505214,0.494476286
	H,0,-1.6189526121,-0.4914503148,0.6141511031	H,0,1.6979189871,1.2598281917,1.3829371448
	0,0,0.348825256,-1.3456548685,-1.0426157645	O,0,1.7446487685,0.0854194289,-0.8293193387
	H,0,-0.4441756908,-1.5119942538,-1.5803082613	H,0,1.7443571101,-0.632305889,-1.4749903416
	N,0,-2.1106074689,-0.1461377033,-1.3850840668	N,0,-0.1239304683,0.7294458553,2.2677747214
	H,0,-3.0713324963,-0.3731120687,-1.148752742	H,0,0.0133421711,1.4397829614,2.9807326339
	H,0,-2.1329785305,0.6224475069,-2.0509772188	H,0,-1.1143835586,0.7156271951,2.0362491645
	23	24
	C,0,-0.5291161511,0.366476785,0.8375497261	C,0,-0.9995030822,-0.1636246192,0.603735206
	0,0,-0.114/8/01/5,0.1611855573,1.9530358118	0,0,-1.9728396534,-0.8013840058,0.2599815447
	0,0,-1.159443/322,1.5081/85228,0.5053971285	0,0,-1.046466/6/8,0.808899562/,1.5403174379
	н, U, -1.391941/U22, 1.452682/4/9, -0.4399236173	H,U,-1.90/2232998,U.8/51062686,1.8433414762
	$U_{0} = 1.0275741189 = 1.510250569 = 0.0278500627$	U.0.1.0810182280 0.5162210427 0.8781000062
	$\Pi, U, -1.02/3/41100, -1.310300000, -0.02/839002/$	$\pi_{0,1}$, $0,10010105503$, -0.5102510427 , 0.764990005
	(0,1,1,0,1,2,1,2,0,3,0,0,1,1,1,2,1,0,2,0,1,0,0,0,0,0,0,0,0,0	U 0 0 6022007268 1 7725055262 0 12/7011596
	1,0,1.10/9912034,-1.91/3413/33,-1.201903383	n,0,0.000309/000,1.//23033202,-0.184/911380

H,0,1.343925415,-1.6567391825,0.5328956035	H,0,0.2880088392,0.8942530506,-1.7026516665
O,0,-0.8312830742,-0.0410609021,-1.505812574	O,0,0.4039253916,-1.5397786297,-0.76752359
H,0,-1.0622762624,-0.7178536112,-2.1521719365	H,0,-0.5179555831,-1.8271347431,-0.8638046884
N.0.2.08074793710.14025321860.6989109358	N.0.2.279714039.0.7479437911.0928273026
H.0.1.8095801709.0.42780331991.4977554692	H.0.2.532648936.1.3701296621.8545530127
H.0.2.2207363314.0.4811057736.0.0940989575	H.0.2.8634694124.0.99490691410.2970849271
25	26
0.0.1.0027066596.0.0771140766.0.500202020	C,0,-0.0846054752,0.5605378785,0.3997136885
0,0,-1.693/866586,0.0//1140/66,-0.5092823238	0,0,-1./448508932,0.6140195494,-0.184248/233
0,0,-0.336011/331,-1.303948556,-1.6591/64328	0,0,-0.5886/22353,0.6382822/,1./533643168
H,0,-1.14030/53/3,-1.3//0213543,-2.199045/61/	H,0,-1.4894/30/9,0.746666068/,2.0999492204
C,0,0.5/5356015,-0.2902/5448/,0.309324/88/	C,0,0.6577733707,0.3045529017,-0.262635838
H,0,0.4115251948,-1.0373647967,1.1115798418	H,0,0.6/508/10/3,0.8892303311,-1.1918485502
C,0,0.6254025857,1.1122668975,0.9537241595	$C_{0,0,1/59826504,-1.2089695093,-0.623842/5/6}$
H,0,0.6030524022,1.8653794384,0.1540802093	H,0,0.6583061471,-1.8005081554,0.2975728166
H,0,1.6059951909,1.1908330483,1.4414003513	H,0,1.8093415902,-1.3530316351,-0.9660447169
0,0,1.8245849058,-0.5127451712,-0.3294494622	0,0,1./6562084/,0./38352//4,0.51064/4869
H,0,1.7475194848,-1.2631610353,-0.9319592722	H,0,1.6183415806,0.5001707934,1.4353407256
N,0,-0.41/1229504,1.422090841/,1.921159/516	N,0,-0.1369481069,-1./20/502593,-1.633692949/
H,0,-1.33//36198,1.30/8/4/388,1.5046966383	H,0,-1.10/202/999,-1.534681241/,-1.389/99441/
H,0,-0.366268/926,0.8118695385,2.733401137	H,0,0.0287993362,-1.2789217858,-2.5349752572
27	28
C,0,0.7301046734,0.561126246,-0.4700468254	C,0,-0.7604946831,0.4970085779,0.3184799793
O,0,0.3008233185,1.0833192784,-1.4735825474	O,0,-1.6299333452,0.6129883899,-0.5170914288
O,0,1.7770680928,1.0684505478,0.2039554315	0,0,-1.0222412708,0.5226716607,1.6515071063
H,0,1.9531551428,0.484102051,0.9646489277	H,0,-1.9801049129,0.6481360667,1.7530152186
C,0,0.0911400173,-0.6897997903,0.1336208579	C,0,0.7079415641,0.2372308506,0.0099622969
H,0,0.077058352,-1.4620111757,-0.652583125	H,0,1.0135969708,0.977454205,-0.7420889727
C,0,-1.3625796385,-0.3953040266,0.5924727452	C,0,0.8622878753,-1.163420792,-0.6255218632
H,0,-1.345067581,0.4652112793,1.2775631465	H,0,0.3936439203,-1.9129223669,0.0428746896
H,0,-1.7021571957,-1.2637733761,1.1804145382	H,0,1.9410633527,-1.3656700487,-0.6396886597
O,0,0.9206250799,-1.1068561659,1.2269294823	O,0,1.5604911428,0.3959191879,1.1320114065
H,0,0.4533130332,-1.7555154107,1.7667895411	H,0,1.0920936162,0.1217371485,1.9306078459
N,0,-2.3333446901,-0.1445096486,-0.4588543032	N,0,0.3633758863,-1.1729210721,-1.9995305789
H,0,-2.0114664016,0.6068998133,-1.0663264534	H,0,0.4962889537,-2.0861546367,-2.4246223182
H,0,-2.454922223,-0.9650895819,-1.0482514759	H,0,-0.6310090903,-0.9578071108,-2.0316647017
29	30
C,0,-0.5817304932,0.5402710892,1.007932087	C,0,1.0592481736,-0.2415289301,-0.1497144458
0,0,-0.9539222473,0.0113140971,2.0272630206	0,0,1.7577455677,0.7460825689,-0.1519646667
O,0,-0.4394041121,1.8774945217,0.8983944997	0,0,1.5795145871,-1.4805373549,-0.1753115951
H,0,-0.146600876,2.060980434,-0.0140358148	H,0,0.8364944289,-2.1112953936,-0.1311245403
C,0,-0.1888819704,-0.2578823478,-0.2402862047	C,0,-0.4719083521,-0.1663945923,-0.1341021591
H,0,-0.9756963698,-1.0041712706,-0.4203504556	H,0,-0.7812465744,0.1741655417,-1.1358999771
C,0,1.157145029,-0.9749815117,-0.0053485867	C,0,-0.9838492188,0.8479223861,0.9003188682
H,0,1.0757250442,-1.5531708053,0.9233635874	H,0,-0.5043473584,0.6332287866,1.8729643581
H,0,1.9285576124,-0.2063285667,0.152494086	H,0,-2.0633033576,0.6734332566,1.0214699844
0,0,-0.0359236926,0.609083221,-1.3807354523	0,0,-0.9567435718,-1.4928725451,0.1261313009
H,0,-0.8634296652,0.6445319059,-1.87466666391	H,0,-1.8737240946,-1.5670968952,-0.1614286182
N,0,1.5938407815,-1.8488579645,-1.0829771273	N,0,-0.7899248204,2.2107810444,0.4069307385
H,0,0.9686247972,-2.6427856479,-1.1996335971	H,0,-1.1729348804,2.8855944194,1.0633749093
H,U,1.02/9401823,-1.34//4/1143,-1.90/163363	н,0,0.2057294312,2.4025176874,0.309605883
31	32
C,0,0.2586378963,0.9330678947,-0.3081169111	C,0,0.1606712428,0.3986371112,1.0772868961
0,0,1.2143503804,1.0412559353,-1.0478475503	0,0,0.2758267813,1.5920594763,1.2223727955
0,0,-0.7808722579,1.7896836536,-0.320462315	0,0,-0.4724810999,-0.3762466314,1.980244528
H,0,-0.582102914,2.4526536299,-1.0028522402	H,0,-0.4396992443,-1.2909140481,1.6405672911
C,0,0.1497635755,-0.1720777814,0.7358696432	C,0,0.7424653022,-0.362417096,-0.1283634376
H,0,0.8737202067,0.1054739986,1.5251786283	H,0,1.8220207268,-0.4624531045,0.0606141255
(0.0, 5751846265 - 1, 5315458436, 0, 1404781877)	$C_0.0.5439819423.0.40880862481.4458326429$

H,0,0.5515265441,-2.266437622,0.9613221862	H,0,1.1127753026,-0.1057055297,-2.2319900426
H,0,1.6157589477,-1.4569932806,-0.1981208587	H,0,0.9834260172,1.4050206911,-1.3124915484
O,0,-1.1734688059,-0.2069610537,1.2609420505	O,0,0.2305931647,-1.701738525,-0.1727280419
H,0,-1.1789655681,-0.7902356437,2.0294838352	H,0,-0.5841209607,-1.6918496332,-0.6962459137
N,0,-0.2456423214,-2.0309418536,-0.9545625966	N,0,-0.8293272466,0.5652465536,-1.9040332285
H,0,-1.2348417512,-1.9628858505,-0.7257135735	H,0,-1.27083549,-0.2849283948,-2.2380142419
H,0,-0.0877985987,-1.4940562431,-1.8038484457	H,0,-1.4315464183,1.0372304457,-1.2363865387
33	34
C.0.0.1702362592,-0.9793342865,-0.2487655366	C.0.0.0086319590.9442512694.0.2838213433
0.00.39042851851.43313383121.2198728391	0.00.69349030151.8982948251.0.053263251
0.0.1.28682435381.5366176223.0.2590581482	0.0.1.35515265881.0400985412.0.4651623223
H.0.1.54128513911.0044401673.1.0373182486	H.0.1.59240788051.9758246009.0.3623186368
C.00.2929301919.0.2987094659.0.456299759	C.00.463673245.0.500175811.0.4395413322
H.01.3755417654.0.218423243.0.6274759652	H.01.5592364464.0.4603610124.0.4765619244
C.00.0029685618.1.54198049080.4273421143	C.00.0026251756.1.3788119880.7347016651
H.0.1.0782969104.1.57514320210.6277595834	H.0.1.0937312892.1.45542501820.701997626
H.00.2407922018.2.4228787378.0.1837508247	H.00.4129944192.2.38904885940.560007672
0.0.0.4173721418.0.4734602929.1.6973831448	0.00.0531627335.1.0465599683.1.6890330923
H,0,-0.1131647998,0.1304682856,2.4260166307	H,0,0.9094857004,0.9801163788,1.7502460478
N,0,-0.7222482645,1.6252221741,-1.6870136557	N,0,-0.3752190965,0.7705920529,-2.0129046495
H,0,-0.5922898458,0.7810920783,-2.2407086209	H,0,-1.3840385244,0.7731382321,-2.1466413581
H,0,-1.7231505948,1.7231479166,-1.5333403313	H,0,0.0300303939,1.2814898756,-2.7916949194
35	36
C.00.94148548770.0841452869.0.7720753597	C.01.20218461790.00529953770.0984281317
0.01.2451639693.0.6131802791.1.7129298575	0.01.682021245.0.53291255351.0705761197
0,0,-1.8477678905,-0.8128206562,0.0709826477	0,0,-1.9237649122,-0.8194626046,0.7153146909
H,0,-2.714748743,-0.6602282224,0.4812026457	H,0,-2.8252016006,-0.8525168842,0.3552535657
C,0,0.4680721608,-0.2086550181,0.1946761327	C,0,0.2277244065,0.1970133267,0.4074109821
H 0 1 1551684614 0 0500800650 1 0381767645	H 0 0 2034771132 1 1691326371 0 9388765919
11,0,1.1551004014,-0.0599009059,1.0501707045	11,0,0.205 1771152,1.1071520571,0.7500705717
C,0,0.6789030775,0.9264209772,-0.8297593928	C,0,1.2278454278,0.3151236617,-0.7501024905
C,0,0.6789030775,0.9264209772,-0.8297593928 H,0,0.3182904811,1.8635955229,-0.3670746262	C,0,1.2278454278,0.3151236617,-0.7501024905 H,0,0.7279427101,0.8263095023,-1.5858200346
C,0,0.6789030775,0.9264209772,-0.8297593928 H,0,0.3182904811,1.8635955229,-0.3670746262 H,0,0.0431676244,0.7297157492,-1.7067201004	C,0,1.2278454278,0.3151236617,-0.7501024905 H,0,0.7279427101,0.8263095023,-1.5858200346 H,0,1.4694055517,-0.7060821197,-1.0733131595
C,0,0.6789030775,0.9264209772,-0.8297593928 H,0,0.3182904811,1.8635955229,-0.3670746262 H,0,0.0431676244,0.7297157492,-1.7067201004 O,0,0.7473852821,-1.5009468852,-0.3034800142	C,0,1.2278454278,0.3151236617,-0.7501024905 H,0,0.7279427101,0.8263095023,-1.5858200346 H,0,1.4694055517,-0.7060821197,-1.0733131595 O,0,0.666299935,-0.8330773839,1.2749798943
C,0,0.6789030775,0.9264209772,-0.8297593928 H,0,0.3182904811,1.8635955229,-0.3670746262 H,0,0.0431676244,0.7297157492,-1.7067201004 O,0,0.7473852821,-1.5009468852,-0.3034800142 H,0,0.1744176863,-1.6802194302,-1.0603263138	C,0,1.2278454278,0.3151236617,-0.7501024905 H,0,0.7279427101,0.8263095023,-1.5858200346 H,0,1.4694055517,-0.7060821197,-1.0733131595 O,0,0.666299935,-0.8330773839,1.2749798943 H,0,0.0034088662,-0.9770015207,1.9613380807
C,0,0.6789030775,0.9264209772,-0.8297593928 H,0,0.3182904811,1.8635955229,-0.3670746262 H,0,0.0431676244,0.7297157492,-1.7067201004 O,0,0.7473852821,-1.5009468852,-0.3034800142 H,0,0.1744176863,-1.6802194302,-1.0603263138 N,0,2.0694514103,0.9699853695,-1.2769649931	C,0,1.2278454278,0.3151236617,-0.7501024905 H,0,0.7279427101,0.8263095023,-1.5858200346 H,0,1.4694055517,-0.7060821197,-1.0733131595 O,0,0.666299935,-0.8330773839,1.2749798943 H,0,0.0034088662,-0.9770015207,1.9613380807 N,0,2.4607987032,0.9732786649,-0.3051986347
C,0,0.6789030775,0.9264209772,-0.8297593928 H,0,0.3182904811,1.8635955229,-0.3670746262 H,0,0.0431676244,0.7297157492,-1.7067201004 O,0,0.7473852821,-1.5009468852,-0.3034800142 H,0,0.1744176863,-1.6802194302,-1.0603263138 N,0,2.0694514103,0.9699853695,-1.2769649931 H,0,2.1817084905,1.6326244784,-2.0393188047	C,0,1.2278454278,0.3151236617,-0.7501024905 H,0,0.7279427101,0.8263095023,-1.5858200346 H,0,1.4694055517,-0.7060821197,-1.0733131595 O,0,0.666299935,-0.8330773839,1.2749798943 H,0,0.0034088662,-0.9770015207,1.9613380807 N,0,2.4607987032,0.9732786649,-0.3051986347 H,0,3.2603441051,0.65356119,-0.8423786316
 H,0,1.1531034014,00.0595805053,1.0581707045 C,0,0.6789030775,0.9264209772,-0.8297593928 H,0,0.3182904811,1.8635955229,-0.3670746262 H,0,0.0431676244,0.7297157492,-1.7067201004 O,0,0.7473852821,-1.5009468852,-0.3034800142 H,0,0.1744176863,-1.6802194302,-1.0603263138 N,0,2.0694514103,0.9699853695,-1.2769649931 H,0,2.1817084905,1.6326244784,-2.0393188047 H,0,2.685101356,1.2742240687,-0.5256491225 	C,0,1.2278454278,0.3151236617,-0.7501024905 H,0,0.7279427101,0.8263095023,-1.5858200346 H,0,1.4694055517,-0.7060821197,-1.0733131595 O,0,0.666299935,-0.8330773839,1.2749798943 H,0,0.0034088662,-0.9770015207,1.9613380807 N,0,2.4607987032,0.9732786649,-0.3051986347 H,0,3.2603441051,0.65356119,-0.8423786316 H,0,2.4044255768,1.9811084745,-0.4273565433
C,0,0.6789030775,0.9264209772,-0.8297593928 H,0,0.3182904811,1.8635955229,-0.3670746262 H,0,0.0431676244,0.7297157492,-1.7067201004 O,0,0.7473852821,-1.5009468852,-0.3034800142 H,0,0.1744176863,-1.6802194302,-1.0603263138 N,0,2.0694514103,0.9699853695,-1.2769649931 H,0,2.1817084905,1.6326244784,-2.0393188047 H,0,2.685101356,1.2742240687,-0.5256491225 37	C,0,1.2278454278,0.3151236617,-0.7501024905 H,0,0.7279427101,0.8263095023,-1.5858200346 H,0,1.4694055517,-0.7060821197,-1.0733131595 O,0,0.666299935,-0.8330773839,1.2749798943 H,0,0.0034088662,-0.9770015207,1.9613380807 N,0,2.4607987032,0.9732786649,-0.3051986347 H,0,3.2603441051,0.65356119,-0.8423786316 H,0,2.4044255768,1.9811084745,-0.4273565433 38
C,0,0.6789030775,0.9264209772,-0.8297593928 H,0,0.3182904811,1.8635955229,-0.3670746262 H,0,0.0431676244,0.7297157492,-1.7067201004 O,0,0.7473852821,-1.5009468852,-0.3034800142 H,0,0.1744176863,-1.6802194302,-1.0603263138 N,0,2.0694514103,0.9699853695,-1.2769649931 H,0,2.1817084905,1.6326244784,-2.0393188047 H,0,2.685101356,1.2742240687,-0.5256491225 37 C,0,-0.6512280746,0.6368049759,-0.5557405988	C,0,1.2278454278,0.3151236617,-0.7501024905 H,0,0.7279427101,0.8263095023,-1.5858200346 H,0,1.4694055517,-0.7060821197,-1.0733131595 O,0,0.666299935,-0.8330773839,1.2749798943 H,0,0.0034088662,-0.9770015207,1.9613380807 N,0,2.4607987032,0.9732786649,-0.3051986347 H,0,3.2603441051,0.65356119,-0.8423786316 H,0,2.4044255768,1.9811084745,-0.4273565433 38 C,0,-0.6512280746,0.6368049759,-0.5557405988
H,0,1.1531084014,00.0393809039,100381707043 C,0,0.6789030775,0.9264209772,-0.8297593928 H,0,0.3182904811,1.8635955229,-0.3670746262 H,0,0.0431676244,0.7297157492,-1.7067201004 O,0,0.7473852821,-1.5009468852,-0.3034800142 H,0,0.1744176863,-1.6802194302,-1.0603263138 N,0,2.0694514103,0.9699853695,-1.2769649931 H,0,2.1817084905,1.6326244784,-2.0393188047 H,0,2.685101356,1.2742240687,-0.5256491225 37 C,0,-0.6512280746,0.6368049759,-0.5557405988 O,0,0.0001108866,1.5698189501,-0.9659740947	C,0,1.2278454278,0.3151236617,-0.7501024905 H,0,0.7279427101,0.8263095023,-1.5858200346 H,0,1.4694055517,-0.7060821197,-1.0733131595 O,0,0.666299935,-0.8330773839,1.2749798943 H,0,0.0034088662,-0.9770015207,1.9613380807 N,0,2.4607987032,0.9732786649,-0.3051986347 H,0,3.2603441051,0.65356119,-0.8423786316 H,0,2.4044255768,1.9811084745,-0.4273565433 38 C,0,-0.6512280746,0.6368049759,-0.5557405988 O,0,0.0001108866,1.5698189501,-0.9659740947
H,0,1.1531084014,00.0393809039,100381707043 C,0,0.6789030775,0.9264209772,-0.8297593928 H,0,0.3182904811,1.8635955229,-0.3670746262 H,0,0.0431676244,0.7297157492,-1.7067201004 O,0,0.7473852821,-1.5009468852,-0.3034800142 H,0,0.1744176863,-1.6802194302,-1.0603263138 N,0,2.0694514103,0.9699853695,-1.2769649931 H,0,2.1817084905,1.6326244784,-2.0393188047 H,0,2.685101356,1.2742240687,-0.5256491225 37 C,0,-0.6512280746,0.6368049759,-0.5557405988 O,0,0.0001108866,1.5698189501,-0.9659740947 O,0,-1.8477766092,0.3187140419,-1.0843786799	C,0,1.2278454278,0.3151236617,-0.7501024905 H,0,0.7279427101,0.8263095023,-1.5858200346 H,0,1.4694055517,-0.7060821197,-1.0733131595 O,0,0.666299935,-0.8330773839,1.2749798943 H,0,0.0034088662,-0.9770015207,1.9613380807 N,0,2.4607987032,0.9732786649,-0.3051986347 H,0,3.2603441051,0.65356119,-0.8423786316 H,0,2.4044255768,1.9811084745,-0.4273565433 38 C,0,-0.6512280746,0.6368049759,-0.5557405988 O,0,0.0001108866,1.5698189501,-0.9659740947 O,0,-1.8477766092,0.3187140419,-1.0843786799
H,0,1.1531034014,00.0393809039,100381707043 C,0,0.6789030775,0.9264209772,-0.8297593928 H,0,0.3182904811,1.8635955229,-0.3670746262 H,0,0.0431676244,0.7297157492,-1.7067201004 O,0,0.7473852821,-1.5009468852,-0.3034800142 H,0,0.1744176863,-1.6802194302,-1.0603263138 N,0,2.0694514103,0.9699853695,-1.2769649931 H,0,2.1817084905,1.6326244784,-2.0393188047 H,0,2.685101356,1.2742240687,-0.5256491225 37 C,0,-0.6512280746,0.6368049759,-0.5557405988 O,0,0.0001108866,1.5698189501,-0.9659740947 O,0,-1.8477766092,0.3187140419,-1.0843786799 H,0,-2.1612043759,-0.4797136217,-0.6178280151	C,0,1.2278454278,0.3151236617,-0.7501024905 H,0,0.7279427101,0.8263095023,-1.5858200346 H,0,1.4694055517,-0.7060821197,-1.0733131595 O,0,0.666299935,-0.8330773839,1.2749798943 H,0,0.0034088662,-0.9770015207,1.9613380807 N,0,2.4607987032,0.9732786649,-0.3051986347 H,0,3.2603441051,0.65356119,-0.8423786316 H,0,2.4044255768,1.9811084745,-0.4273565433 38 C,0,-0.6512280746,0.6368049759,-0.5557405988 O,0,0.0001108866,1.5698189501,-0.9659740947 O,0,-1.8477766092,0.3187140419,-1.0843786799 H,0,-2.1612043759,-0.4797136217,-0.6178280151
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H,0,1.1531034014,00.0393809039,110381707043 C,0,0.6789030775,0.9264209772,-0.8297593928 H,0,0.3182904811,1.8635955229,-0.3670746262 H,0,0.0431676244,0.7297157492,-1.7067201004 O,0,0.7473852821,-1.5009468852,-0.3034800142 H,0,0.1744176863,-1.6802194302,-1.0603263138 N,0,2.0694514103,0.9699853695,-1.2769649931 H,0,2.1817084905,1.6326244784,-2.0393188047 H,0,2.685101356,1.2742240687,-0.5256491225 37 C,0,-0.6512280746,0.6368049759,-0.5557405988 O,0,0.0001108866,1.5698189501,-0.9659740947 O,0,-1.8477766092,0.3187140419,-1.0843786799 H,0,-2.1612043759,-0.4797136217,-0.6178280151 C,0,-0.2076741866,-0.2595302793,0.6130909667 H,0,-0.4423328991,0.2846937341,1.5392245999 C,0,1.2970112354,-0.5530240494,0.5921624179 H,0,1.5582248079,-0.9839174034,-0.3965089564	C,0,1.2278454278,0.3151236617,-0.7501024905 H,0,0.7279427101,0.8263095023,-1.5858200346 H,0,1.4694055517,-0.7060821197,-1.0733131595 O,0,0.666299935,-0.8330773839,1.2749798943 H,0,0.0034088662,-0.9770015207,1.9613380807 N,0,2.4607987032,0.9732786649,-0.3051986347 H,0,3.2603441051,0.65356119,-0.8423786316 H,0,2.4044255768,1.9811084745,-0.4273565433 38 C,0,-0.6512280746,0.6368049759,-0.5557405988 O,0,0.0001108866,1.5698189501,-0.9659740947 O,0,-1.8477766092,0.3187140419,-1.0843786799 H,0,-2.1612043759,-0.4797136217,-0.6178280151 C,0,-0.2076741866,-0.2595302793,0.6130909667 H,0,-0.4423328991,0.2846937341,1.5392245999 C,0,1.2970112354,-0.5530240494,0.5921624179 H,0,1.5582248079,-0.9839174034,-0.3965089564 H,0,1.40260275
H,0,1.1531034014,00.0393809039,10.0381707043 C,0,0.6789030775,0.9264209772,-0.8297593928 H,0,0.3182904811,1.8635955229,-0.3670746262 H,0,0.0431676244,0.7297157492,-1.7067201004 O,0,0.7473852821,-1.5009468852,-0.3034800142 H,0,0.1744176863,-1.6802194302,-1.0603263138 N,0,2.0694514103,0.9699853695,-1.2769649931 H,0,2.1817084905,1.6326244784,-2.0393188047 H,0,2.685101356,1.2742240687,-0.5256491225 37 C,0,-0.6512280746,0.6368049759,-0.5557405988 O,0,0.0001108866,1.5698189501,-0.9659740947 O,0,-1.8477766092,0.3187140419,-1.0843786799 H,0,-2.1612043759,-0.4797136217,-0.6178280151 C,0,-0.2076741866,-0.2595302793,0.6130909667 H,0,-0.4423328991,0.2846937341,1.5392245999 C,0,1.2970112354,-0.5530240494,0.5921624179 H,0,1.4836626075,-1.3233513446,1.3538381537 O,0,0.0117228407 O,1.4011722880	C,0,1.2278454278,0.3151236617,-0.7501024905 H,0,0.7279427101,0.8263095023,-1.5858200346 H,0,1.4694055517,-0.7060821197,-1.0733131595 O,0,0.666299935,-0.8330773839,1.2749798943 H,0,0.0034088662,-0.9770015207,1.9613380807 N,0,2.4607987032,0.9732786649,-0.3051986347 H,0,3.2603441051,0.65356119,-0.8423786316 H,0,2.4044255768,1.9811084745,-0.4273565433 38 C,0,-0.6512280746,0.6368049759,-0.5557405988 O,0,0.0001108866,1.5698189501,-0.9659740947 O,0,-1.8477766092,0.3187140419,-1.0843786799 H,0,-2.1612043759,-0.4797136217,-0.6178280151 C,0,-0.2076741866,-0.2595302793,0.6130909667 H,0,-0.4423328991,0.2846937341,1.5392245999 C,0,1.2970112354,-0.5530240494,0.5921624179 H,0,1.458826075,-1.3233513446,1.3538381537 O,0,0.001042135
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11,0,11531034014,00.0393809039,10.0381707043 C,0,0.6789030775,0.9264209772,-0.8297593928 H,0,0.3182904811,1.8635955229,-0.3670746262 H,0,0.0431676244,0.7297157492,-1.7067201004 O,0,0.7473852821,-1.5009468852,-0.3034800142 H,0,0.1744176863,-1.6802194302,-1.0603263138 N,0,2.0694514103,0.9699853695,-1.2769649931 H,0,2.1817084905,1.6326244784,-2.0393188047 H,0,2.685101356,1.2742240687,-0.5256491225 37 C,0,-0.6512280746,0.6368049759,-0.5557405988 O,0,0.0001108866,1.5698189501,-0.9659740947 O,0,-1.8477766092,0.3187140419,-1.0843786799 H,0,-2.1612043759,-0.4797136217,-0.6178280151 C,0,-0.2076741866,-0.2595302793,0.6130909667 H,0,-0.4423328991,0.2846937341,1.5392245999 C,0,1.2970112354,-0.5530240494,0.5921624179 H,0,1.4836626075,-1.3233513446,1.3538381537 O,0,-1.0011723882,-1.4577901007,0.6441912125 H,0,-0.5610195226,-2.1411869139,0.1204482806 N,0,2.0596992324,0.6404581126,0.9476683306 H,0,3.0510933556,0.4267239409,1.010374139 H,0,1.9343559709,1.3585499175,0.2366822441	C,0,1.2278454278,0.3151236617,-0.7501024905 H,0,0.7279427101,0.8263095023,-1.5858200346 H,0,1.4694055517,-0.7060821197,-1.0733131595 O,0,0.666299935,-0.8330773839,1.2749798943 H,0,0.0034088662,-0.9770015207,1.9613380807 N,0,2.4607987032,0.9732786649,-0.3051986347 H,0,3.2603441051,0.65356119,-0.8423786316 H,0,2.4044255768,1.9811084745,-0.4273565433 38 C,0,-0.6512280746,0.6368049759,-0.5557405988 O,0,0.0001108866,1.5698189501,-0.9659740947 O,0,-1.8477766092,0.3187140419,-1.0843786799 H,0,-2.1612043759,-0.4797136217,-0.6178280151 C,0,-0.2076741866,-0.2595302793,0.6130909667 H,0,-0.4423328991,0.2846937341,1.5392245999 C,0,1.2970112354,-0.5530240494,0.5921624179 H,0,1.4836626075,-1.3233513446,1.3538381537 O,0,-1.0011723882,-1.4577901007,0.6441912125 H,0,-0.5610195226,-2.1411869139,0.1204482806 N,0,2.0596992324,0.6404581126,0.9476683306 H,0,3.0510933556,0.4267239409,1.010374139 H,0,1.9343559709,1.3585499175,0.2366822441 40
11,0,11531034014,00.0393809039,10.0381707043 C,0,0.6789030775,0.9264209772,-0.8297593928 H,0,0.3182904811,1.8635955229,-0.3670746262 H,0,0.0431676244,0.7297157492,-1.7067201004 O,0,0.7473852821,-1.5009468852,-0.3034800142 H,0,0.1744176863,-1.6802194302,-1.0603263138 N,0,2.0694514103,0.9699853695,-1.2769649931 H,0,2.1817084905,1.6326244784,-2.0393188047 H,0,2.685101356,1.2742240687,-0.5256491225 37 C,0,-0.6512280746,0.6368049759,-0.5557405988 O,0,0.0001108866,1.5698189501,-0.9659740947 O,0,-1.8477766092,0.3187140419,-1.0843786799 H,0,-2.1612043759,-0.4797136217,-0.6178280151 C,0,-0.2076741866,-0.2595302793,0.6130909667 H,0,-0.4423328991,0.2846937341,1.5392245999 C,0,1.2970112354,-0.5530240494,0.5921624179 H,0,1.4836626075,-1.3233513446,1.3538381537 O,0,-1.0011723882,-1.4577901007,0.6441912125 H,0,-0.5610195226,-2.1411869139,0.1204482806 N,0,2.0596992324,0.6404581126,0.9476683306 H,0,3.0510933556,0.4267239409,1.010374139 H,0,1.9343559709,1.3585499175,0.2366822441	C,0,1.2278454278,0.3151236617,-0.7501024905 H,0,0.7279427101,0.8263095023,-1.5858200346 H,0,1.4694055517,-0.7060821197,-1.0733131595 O,0,0.666299935,-0.8330773839,1.2749798943 H,0,0.0034088662,-0.9770015207,1.9613380807 N,0,2.4607987032,0.9732786649,-0.3051986347 H,0,3.2603441051,0.65356119,-0.8423786316 H,0,2.4044255768,1.9811084745,-0.4273565433 38 C,0,-0.6512280746,0.6368049759,-0.5557405988 O,0,0.0001108866,1.5698189501,-0.9659740947 O,0,-1.8477766092,0.3187140419,-1.0843786799 H,0,-2.1612043759,-0.4797136217,-0.6178280151 C,0,-0.2076741866,-0.2595302793,0.6130909667 H,0,-0.4423328991,0.2846937341,1.5392245999 C,0,1.2970112354,-0.5530240494,0.5921624179 H,0,1.4836626075,-1.3233513446,1.3538381537 O,0,-1.0011723882,-1.4577901007,0.6441912125 H,0,-0.5610195226,-2.1411869139,0.1204482806 N,0,2.0596992324,0.6404581126,0.9476683306 H,0,3.0510933556,0.4267239409,1.010374139 H,0,1.9343559709,1.3585499175,0.2366822441 40 C,0,-0.3029013508,0.7719650995,-0.9864710759 O,0-0.6278928182,0.2669515036 -2.0331712232
11,0,11531034014,00.0393809039,10.0381707043 C,0,0.6789030775,0.9264209772,-0.8297593928 H,0,0.3182904811,1.8635955229,-0.3670746262 H,0,0.0431676244,0.7297157492,-1.7067201004 O,0,0.7473852821,-1.5009468852,-0.3034800142 H,0,0.1744176863,-1.6802194302,-1.0603263138 N,0,2.0694514103,0.9699853695,-1.2769649931 H,0,2.1817084905,1.6326244784,-2.0393188047 H,0,2.685101356,1.2742240687,-0.5256491225 37 C,0,-0.6512280746,0.6368049759,-0.5557405988 O,0,0.0001108866,1.5698189501,-0.9659740947 O,0,-1.8477766092,0.3187140419,-1.0843786799 H,0,-2.1612043759,-0.4797136217,-0.6178280151 C,0,-0.2076741866,-0.2595302793,0.6130909667 H,0,-0.4423328991,0.2846937341,1.5392245999 C,0,1.2970112354,-0.5530240494,0.5921624179 H,0,1.4836626075,-1.3233513446,1.3538381537 O,0,-1.0011723882,-1.4577901007,0.6441912125 H,0,-0.5610195226,-2.1411869139,0.1204482806 N,0,2.0596992324,0.6404581126,0.9476683306 H,0,3.0510933556,0.4267239409,1.010374139 H,0,1.9343559709,1.3585499175,0.2366822441 39 C,0,0.3744945407,0.8476566909,-0.3730570425 O,0,-0.47969663,1.4116195041,-1.0233852843 O,0,1.6721278536,1.2173716452 -0 3911641742 </th <th>C,0,1.2278454278,0.3151236617,-0.7501024905 H,0,0.7279427101,0.8263095023,-1.5858200346 H,0,1.4694055517,-0.7060821197,-1.0733131595 O,0,0.666299935,-0.8330773839,1.2749798943 H,0,0.0034088662,-0.9770015207,1.9613380807 N,0,2.4607987032,0.9732786649,-0.3051986347 H,0,3.2603441051,0.65356119,-0.8423786316 H,0,2.4044255768,1.9811084745,-0.4273565433 38 C,0,-0.6512280746,0.6368049759,-0.5557405988 O,0,0.0001108866,1.5698189501,-0.9659740947 O,0,-1.8477766092,0.3187140419,-1.0843786799 H,0,-2.1612043759,-0.4797136217,-0.6178280151 C,0,-0.2076741866,-0.2595302793,0.6130909667 H,0,-0.4423328991,0.2846937341,1.5392245999 C,0,1.2970112354,-0.5530240494,0.5921624179 H,0,1.4582248079,-0.9839174034,-0.3965089564 H,0,1.4836626075,-1.3233513446,1.3538381537 O,0,-1.0011723882,-1.4577901007,0.6441912125 H,0,-0.5610195226,-2.1411869139,0,1204482806 N,0,2.0596992324,0.6404581126,0.9476683306 H,0,3.0510933556,0.4267239409,1.010374139 H,0,1.9343559709,1.3585499175,0.2366822441 40 C,0,-0.3029013508,0.7719650995,-0.9864710759 O,0,-0.6278928182,0.2669515036,-2.0331712232 O,0,-0.5366078449,2.0726054896,-0.714944992</th>	C,0,1.2278454278,0.3151236617,-0.7501024905 H,0,0.7279427101,0.8263095023,-1.5858200346 H,0,1.4694055517,-0.7060821197,-1.0733131595 O,0,0.666299935,-0.8330773839,1.2749798943 H,0,0.0034088662,-0.9770015207,1.9613380807 N,0,2.4607987032,0.9732786649,-0.3051986347 H,0,3.2603441051,0.65356119,-0.8423786316 H,0,2.4044255768,1.9811084745,-0.4273565433 38 C,0,-0.6512280746,0.6368049759,-0.5557405988 O,0,0.0001108866,1.5698189501,-0.9659740947 O,0,-1.8477766092,0.3187140419,-1.0843786799 H,0,-2.1612043759,-0.4797136217,-0.6178280151 C,0,-0.2076741866,-0.2595302793,0.6130909667 H,0,-0.4423328991,0.2846937341,1.5392245999 C,0,1.2970112354,-0.5530240494,0.5921624179 H,0,1.4582248079,-0.9839174034,-0.3965089564 H,0,1.4836626075,-1.3233513446,1.3538381537 O,0,-1.0011723882,-1.4577901007,0.6441912125 H,0,-0.5610195226,-2.1411869139,0,1204482806 N,0,2.0596992324,0.6404581126,0.9476683306 H,0,3.0510933556,0.4267239409,1.010374139 H,0,1.9343559709,1.3585499175,0.2366822441 40 C,0,-0.3029013508,0.7719650995,-0.9864710759 O,0,-0.6278928182,0.2669515036,-2.0331712232 O,0,-0.5366078449,2.0726054896,-0.714944992
11,0,11531034014,00.0393809039,10.0381707043 C,0,0.6789030775,0.9264209772,-0.8297593928 H,0,0.3182904811,1.8635955229,-0.3670746262 H,0,0.0431676244,0.7297157492,-1.7067201004 O,0,0.7473852821,-1.5009468852,-0.3034800142 H,0,0.1744176863,-1.6802194302,-1.0603263138 N,0,2.0694514103,0.9699853695,-1.2769649931 H,0,2.1817084905,1.6326244784,-2.0393188047 H,0,2.685101356,1.2742240687,-0.5256491225 37 C,0,-0.6512280746,0.6368049759,-0.5557405988 O,0,0001108866,1.5698189501,-0.9659740947 O,0,-1.8477766092,0.3187140419,-1.0843786799 H,0,-2.1612043759,-0.4797136217,-0.6178280151 C,0,-0.2076741866,-0.2595302793,0.6130909667 H,0,-0.4423328991,0.2846937341,1.5392245999 C,0,1.2970112354,-0.5530240494,0.5921624179 H,0,1.4836626075,-1.3233513446,1.3538381537 O,0,-1.0011723882,-1.4577901007,0.6441912125 H,0,-0.5610195226,-2.1411869139,0.1204482806 N,0,2.0596992324,0.6404581126,0.9476683306 H,0,3.0510933556,0.4267239409,1.010374139 H,0,1.9343559709,1.3585499175,0.2366822441 39 C,0,0.3744945407,0.8476566909,-0.3730570425 O,0,-0.47969663,1.4116195041,-1.0233852843 O,0,1.6721278536,1.2173716452,-0.3911641742	C,0,1.2278454278,0.3151236617,-0.7501024905 H,0,0.7279427101,0.8263095023,-1.5858200346 H,0,1.4694055517,-0.7060821197,-1.0733131595 O,0,0.666299935,-0.8330773839,1.2749798943 H,0,0.0034088662,-0.9770015207,1.9613380807 N,0,2.4607987032,0.9732786649,-0.3051986347 H,0,3.2603441051,0.65356119,-0.8423786316 H,0,2.4044255768,1.9811084745,-0.4273565433 38 C,0,-0.6512280746,0.6368049759,-0.5557405988 O,0,0.0001108866,1.5698189501,-0.9659740947 O,0,-1.8477766092,0.3187140419,-1.0843786799 H,0,-2.1612043759,-0.4797136217,-0.6178280151 C,0,-0.2076741866,-0.2595302793,0.6130909667 H,0,-0.4423328991,0.2846937341,1.5392245999 C,0,1.2970112354,-0.5530240494,0.5921624179 H,0,1.4836626075,-1.3233513446,1.3538381537 O,0,-1.0011723882,-1.4577901007,0.6441912125 H,0,-0.5610195226,-2.1411869139,0.1204482806 N,0,2.0596992324,0.6404581126,0.9476683306 H,0,3.0510933556,0.4267239409,1.010374139 H,0,1.9343559709,1.3585499175,0.2366822441 40 C,0,-0.3029013508,0.7719650995,-0.9864710759 O,0,-0.6278928182,0.2669515036,-2.0331712232 O,0,-0.5366078449,2.0726054896,-0.714944992 H,0,-0.1889694858,2.2472051559.0.1796663776
11,0,11131034014,00.0393809039,10.0381707043 C,0,0.6789030775,0.9264209772,-0.8297593928 H,0,0.3182904811,1.8635955229,-0.3670746262 H,0,0.0431676244,0.7297157492,-1.7067201004 O,0,0.7473852821,-1.5009468852,-0.3034800142 H,0,0.1744176863,-1.6802194302,-1.0603263138 N,0,2.0694514103,0.9699853695,-1.2769649931 H,0,2.1817084905,1.6326244784,-2.0393188047 H,0,2.685101356,1.2742240687,-0.5256491225 37 C,0,-0.6512280746,0.6368049759,-0.5557405988 O,0,0001108866,1.5698189501,-0.9659740947 O,0,-1.8477766092,0.3187140419,-1.0843786799 H,0,-2.1612043759,-0.4797136217,-0.6178280151 C,0,-0.2076741866,-0.2595302793,0.6130909667 H,0,-0.4423328991,0.2846937341,1.5392245999 C,0,1.2970112354,-0.5530240494,0.5921624179 H,0,1.4836626075,-1.3233513446,1.3538381537 O,0,-1.0011723882,-1.4577901007,0.6441912125 H,0,-0.5610195226,-2.1411869139,0.1204482806 N,0,2.0596992324,0.6404581126,0.9476683306 H,0,3.0510933556,0.4267239409,1.010374139 H,0,1.9343559709,1.3585499175,0.2366822441 39 C,0,0.3744945407,0.8476566909,-0.3730570425 O,0,-0.47969663,1.4116195041,-1.0233852843 O,0,1.6721278536,1.2173716452,-0.3911641742	C,0,1.2278454278,0.3151236617,-0.7501024905 H,0,0.7279427101,0.8263095023,-1.5858200346 H,0,1.4694055517,-0.7060821197,-1.0733131595 O,0,0.666299935,-0.8330773839,1.2749798943 H,0,0.0034088662,-0.9770015207,1.9613380807 N,0,2.4607987032,0.9732786649,-0.3051986347 H,0,3.2603441051,0.65356119,-0.8423786316 H,0,2.4044255768,1.9811084745,-0.4273565433 38 C,0,-0.6512280746,0.6368049759,-0.5557405988 O,0,0.0001108866,1.5698189501,-0.9659740947 O,0,-1.8477766092,0.3187140419,-1.0843786799 H,0,-2.1612043759,-0.4797136217,-0.6178280151 C,0,-0.2076741866,-0.2595302793,0.6130909667 H,0,-0.4423328991,0.2846937341,1.5392245999 C,0,1.2970112354,-0.5530240494,0.5921624179 H,0,1.5582248079,-0.9839174034,-0.3965089564 H,0,1.4836626075,-1.3233513446,1.3538381537 O,0,-1.0011723882,-1.4577901007,0.6441912125 H,0,-0.5610195226,-2.1411869139,0.1204482806 N,0,2.0596992324,0.6404581126,0.9476683306 H,0,3.0510933556,0.4267239409,1.010374139 H,0,1.9343559709,1.3585499175,0.2366822441 40 C,0,-0.3029013508,0.7719650995,-0.9864710759 O,0,-0.6278928182,0.2669515036,-2.0331712232 O,0,-0.5366078449,2.0726054896,-0.714944992 H,0,-0.1889694858,2.2472051559,0.1796663776 C,0,0.4455287874,0.0133026098.0.1230564903

C,0,-1.3359746136,-0.7928852284,0.5250658453	C,0,-0.0560709304,-1.4164722466,0.285755149
H,0,-1.947152714,0.0492839387,0.8909251601	H,0,-0.1165969175,-1.8646044099,-0.7128665222
H,0,-1.4335413834,-1.6146015473,1.2494547817	H,0,-1.0916006789,-1.3807937537,0.6852469957
O,0,0.5856689252,0.0000446218,1.8322761601	O,0,0.4233892214,0.7560876746,1.3570472454
H,0,0.7450075392,-0.8038231651,2.3400649179	H,0,-0.406626172,0.5661927477,1.8171128814
N,0,-1.7200786632,-1.2961198939,-0.7962525025	N,0,0.8807680998,-2.1892715541,1.0996755143
H.0,-2.5883394269,-1.8205513017,-0.7434692322	H,0,0.9445609483,-1.8225691277,2.0462552176
H,0,-1.8738855052,-0.5162471827,-1.4311041951	H,0,0.5885890706,-3.1598485285,1.1689225363
41	42
C.00.9933932716.0.1509097740.2477505601	C,0,-0.003406329,1.0016518949,-0.1675582389
0.01.46388723510.72598275290.9287066933	0.00.7026051387.1.91018703690.5616980893
0.01.2957748433.1.46840829570.4223685364	O.0.1.0653983068.1.1933756725.0.6371443387
H.01.9203911157.1.51748080451.1642368959	H.0.1.118353218.2.1469099776.0.8131788225
C.0.0.03505653970.0069341783.0.8597624412	C.00.18380261760.45836933970.5948565118
H.00.2632350184.0.663112392.1.6840067404	H.01.20437826210.52247917141.0035484303
C.0.1.4418190065.0.4230108186.0.3620490859	C.00.01706823591.4516978337.0.5516879289
H.0.2.1236085335.0.3359801978.1.2233589851	H.0.0.98472896681.3272153974.0.9794488669
H.0.1.4137130684.1.4851298973.0.0842027099	H.00.07509330642.466804.0.1232409959
0.0.01491014121.3677490989.1.2677015246	0.0.0.78136190850.78871451441.5966154272
H.0.0.56193175631.4529061406.2.0579629775	H.0.0.59560955160.27507189692.3924117001
N.0.1.99378532330.34949214380.7412900278	N.01.01365313851.1672064979.1.5883229828
H.0.1.90386547411.34612015830.5534693009	H.01.92842154051.533973893.1.3373022526
H,0,1.489991681,-0.1715977672,-1.6072224502	H,0,-0.7542733228,-1.5905920374,2.473612189
43	44
C.0.0.3265138678.0.80561157850.5745340928	C.0.0.092982791.0.8574972952.0.6175106173
0.00.1386435364.1.91303353180.4400746191	0.0.1.0922921502.0.8710268103.1.2972329556
O,0,0.7563473095,0.383082942,-1.7817518795	O,0,-1.0768622669,1.3270066087,1.111990102
H,0,1.0091592319,-0.5502367671,-1.7473907779	H,0,-1.7791534858,1.2716484687,0.4476692961
C,0,0.5346398589,-0.1254236843,0.6289464403	C,0,0.0818917691,0.3075247952,-0.8072938545
H,0,1.628318989,-0.1898902807,0.7919474305	H,0,-0.306920996,1.1021260394,-1.4735287773
C,0,-0.0104145246,-1.5429532011,0.4304100964	C,0,-0.8317300323,-0.9381847928,-0.9544110574
H,0,0.1891983917,-2.0922048702,1.3681296261	H,0,-0.7919528124,-1.2257163027,-2.0141030722
H,0,0.5588375805,-2.0600408721,-0.3597692004	H 0 -1 8777646966 -0 6643672134 -0 7427582056
	11,0, 1.0777010900, 0.0019072191, 0.7127902090
0,0,-0.0847334549,0.4509959559,1.761403679	O,0,1.3991739507,-0.0208109276,-1.1914408629
O,0,-0.0847334549,0.4509959559,1.761403679 H,0,-0.3251263361,1.3591972103,1.5077486524	O,0,1.3991739507,-0.0208109276,-1.1914408629 H,0,1.9717300943,0.1841895916,-0.4329747266
O,0,-0.0847334549,0.4509959559,1.761403679 H,0,-0.3251263361,1.3591972103,1.5077486524 N,0,-1.4171913345,-1.4874773128,0.0418233908	O,0,1.3991739507,-0.0208109276,-1.1914408629 H,0,1.9717300943,0.1841895916,-0.4329747266 N,0,-0.4748796852,-2.0952561021,-0.1508274553
O,0,-0.0847334549,0.4509959559,1.761403679 H,0,-0.3251263361,1.3591972103,1.5077486524 N,0,-1.4171913345,-1.4874773128,0.0418233908 H,0,-1.8044367341,-2.4197370225,-0.0741113816	O,0,1.3991739507,-0.0208109276,-1.1914408629 H,0,1.9717300943,0.1841895916,-0.4329747266 N,0,-0.4748796852,-2.0952561021,-0.1508274553 H,0,0.490247894,-2.3630656285,-0.3291634445
O,0,-0.0847334549,0.4509959559,1.761403679 H,0,-0.3251263361,1.3591972103,1.5077486524 N,0,-1.4171913345,-1.4874773128,0.0418233908 H,0,-1.8044367341,-2.4197370225,-0.0741113816 H,0,-1.9544692685,-1.0264571678,0.7732226958	N,0, 1.3991739507,-0.0208109276,-1.1914408629 H,0,1.9717300943,0.1841895916,-0.4329747266 N,0,-0.4748796852,-2.0952561021,-0.1508274553 H,0,0.490247894,-2.3630656285,-0.3291634445 H,0,-0.5600546942,-1.9111186021,0.84634848853
O,0,-0.0847334549,0.4509959559,1.761403679 H,0,-0.3251263361,1.3591972103,1.5077486524 N,0,-1.4171913345,-1.4874773128,0.0418233908 H,0,-1.8044367341,-2.4197370225,-0.0741113816 H,0,-1.9544692685,-1.0264571678,0.7732226958 45	0,0,1.3991739507,-0.0208109276,-1.1914408629 H,0,1.9717300943,0.1841895916,-0.4329747266 N,0,-0.4748796852,-2.0952561021,-0.1508274553 H,0,0.490247894,-2.3630656285,-0.3291634445 H,0,-0.5600546942,-1.9111186021,0.8463484853 46
O,0,-0.0847334549,0.4509959559,1.761403679 H,0,-0.3251263361,1.3591972103,1.5077486524 N,0,-1.4171913345,-1.4874773128,0.0418233908 H,0,-1.8044367341,-2.4197370225,-0.0741113816 H,0,-1.9544692685,-1.0264571678,0.7732226958 45 C,0,-0.2434816486,0.2817084927,1.1652862692	0,0,1.3991739507,-0.0208109276,-1.1914408629 H,0,1.9717300943,0.1841895916,-0.4329747266 N,0,-0.4748796852,-2.0952561021,-0.1508274553 H,0,0.490247894,-2.3630656285,-0.3291634445 H,0,-0.5600546942,-1.9111186021,0.8463484853 46 C,0,-1.0224673522,-0.5608352629,0.343131366
O,0,-0.0847334549,0.4509959559,1.761403679 H,0,-0.3251263361,1.3591972103,1.5077486524 N,0,-1.4171913345,-1.4874773128,0.0418233908 H,0,-1.8044367341,-2.4197370225,-0.0741113816 H,0,-1.9544692685,-1.0264571678,0.7732226958 45 C,0,-0.2434816486,0.2817084927,1.1652862692 O,0,-1.1800385586,-0.1972013327,1.7597913725	0,0,1.3991739507,-0.0208109276,-1.1914408629 H,0,1.9717300943,0.1841895916,-0.4329747266 N,0,-0.4748796852,-2.0952561021,-0.1508274553 H,0,0.490247894,-2.3630656285,-0.3291634445 H,0,-0.5600546942,-1.9111186021,0.8463484853 46 C,0,-1.0224673522,-0.5608352629,0.343131366 O,0,-1.3214767328,-0.7096396609,1.5047151632
O,0,-0.0847334549,0.4509959559,1.761403679 H,0,-0.3251263361,1.3591972103,1.5077486524 N,0,-1.4171913345,-1.4874773128,0.0418233908 H,0,-1.8044367341,-2.4197370225,-0.0741113816 H,0,-1.9544692685,-1.0264571678,0.7732226958 45 C,0,-0.2434816486,0.2817084927,1.1652862692 O,0,-1.1800385586,-0.1972013327,1.7597913725 O,0,0.2979057492,1.4550843903,1.5665956919 H,0,0.2979057492,1.4550843903,1.5665956919	0,0,1.3991739507,-0.0208109276,-1.1914408629 H,0,1.9717300943,0.1841895916,-0.4329747266 N,0,-0.4748796852,-2.0952561021,-0.1508274553 H,0,0.490247894,-2.3630656285,-0.3291634445 H,0,-0.5600546942,-1.9111186021,0.8463484853 46 C,0,-1.0224673522,-0.5608352629,0.343131366 O,0,-1.3214767328,-0.7096396609,1.5047151632 O,0,-1.5474097071,-1.367833693,-0.6089666899
O,0,-0.0847334549,0.4509959559,1.761403679 H,0,-0.3251263361,1.3591972103,1.5077486524 N,0,-1.4171913345,-1.4874773128,0.0418233908 H,0,-1.8044367341,-2.4197370225,-0.0741113816 H,0,-1.9544692685,-1.0264571678,0.7732226958 45 C,0,-0.2434816486,0.2817084927,1.1652862692 O,0,-1.1800385586,-0.1972013327,1.7597913725 O,0,0.2979057492,1.4550843903,1.5665956919 H,0,1.0632195752,1.6849464996,1.0195633279 C,0.0201500,02000127	0,0,1.3991739507,-0.0208109276,-1.1914408629 H,0,1.9717300943,0.1841895916,-0.4329747266 N,0,-0.4748796852,-2.0952561021,-0.1508274553 H,0,0.490247894,-2.3630656285,-0.3291634445 H,0,-0.5600546942,-1.9111186021,0.84634848853 46 C,0,-1.0224673522,-0.5608352629,0.343131366 O,0,-1.3214767328,-0.7096396609,1.5047151632 O,0,-1.5474097071,-1.367833693,-0.6089666899 H,0,-1.2372529303,-1.1106088685,-1.4891510318
O,0,-0.0847334549,0.4509959559,1.761403679 H,0,-0.3251263361,1.3591972103,1.5077486524 N,0,-1.4171913345,-1.4874773128,0.0418233908 H,0,-1.8044367341,-2.4197370225,-0.0741113816 H,0,-1.9544692685,-1.0264571678,0.7732226958 45 C,0,-0.2434816486,0.2817084927,1.1652862692 O,0,-1.1800385586,-0.1972013327,1.7597913725 O,0,0.2979057492,1.4550843903,1.5665956919 H,0,1.0632195752,1.6849464996,1.0195633279 C,0,0.3694071509,-0.3899320514,-0.062399437	0,0,1.3991739507,-0.0208109276,-1.1914408629 H,0,1.9717300943,0.1841895916,-0.4329747266 N,0,-0.4748796852,-2.0952561021,-0.1508274553 H,0,0.490247894,-2.3630656285,-0.3291634445 H,0,-0.5600546942,-1.9111186021,0.84634848853 46 C,0,-1.0224673522,-0.5608352629,0.343131366 O,0,-1.3214767328,-0.7096396609,1.5047151632 O,0,-1.5474097071,-1.367833693,-0.6089666899 H,0,-1.2372529303,-1.1106088685,-1.4891510318 C,0,-0.0280724881,0.5058189327,-0.1086968133 H,0,0,491240018,10971474762,003200674
O,0,-0.0847334549,0.4509959559,1.761403679 H,0,-0.3251263361,1.3591972103,1.5077486524 N,0,-1.4171913345,-1.4874773128,0.0418233908 H,0,-1.8044367341,-2.4197370225,-0.0741113816 H,0,-1.9544692685,-1.0264571678,0.7732226958 45 C,0,-0.2434816486,0.2817084927,1.1652862692 O,0,-1.1800385586,-0.1972013327,1.7597913725 O,0,0.2979057492,1.4550843903,1.5665956919 H,0,1.0632195752,1.6849464996,1.0195633279 C,0,0.3694071509,-0.3899320514,-0.062399437 H,0,1.4623436787,-0.4688631843,0.0747808717 C 0,0 0090641020,0 4170328166,1 3420460165	0,0,1.3991739507,-0.0208109276,-1.1914408629 H,0,1.9717300943,0.1841895916,-0.4329747266 N,0,-0.4748796852,-2.0952561021,-0.1508274553 H,0,0.490247894,-2.3630656285,-0.3291634445 H,0,-0.5600546942,-1.9111186021,0.84634848853 46 C,0,-1.0224673522,-0.5608352629,0.343131366 O,0,-1.3214767328,-0.7096396609,1.5047151632 O,0,-1.5474097071,-1.367833693,-0.6089666899 H,0,-1.2372529303,-1.1106088685,-1.4891510318 C,0,-0.0280724881,0.5058189327,-0.1086968133 H,0,-0.481360018,1.0871747863,-0.933209674 C,0,1.205656482,0.132337867,0.6100773000
O,0,-0.0847334549,0.4509959559,1.761403679 H,0,-0.3251263361,1.3591972103,1.5077486524 N,0,-1.4171913345,-1.4874773128,0.0418233908 H,0,-1.8044367341,-2.4197370225,-0.0741113816 H,0,-1.9544692685,-1.0264571678,0.7732226958 45 C,0,-0.2434816486,0.2817084927,1.1652862692 O,0,-1.1800385586,-0.1972013327,1.7597913725 O,0,0.2979057492,1.4550843903,1.5665956919 H,0,1.0632195752,1.6849464996,1.0195633279 C,0,0.3694071509,-0.3899320514,-0.062399437 H,0,1.4623436787,-0.4688631843,0.0747808717 C,0,0.0990641029,0.4179328166,-1.3429469165 H,0,0.493740200,1.4402326166,-1.3429469165	0,0,1.3991739507,-0.0208109276,-1.1914408629 H,0,1.9717300943,0.1841895916,-0.4329747266 N,0,-0.4748796852,-2.0952561021,-0.1508274553 H,0,0.490247894,-2.3630656285,-0.3291634445 H,0,-0.5600546942,-1.9111186021,0.84634848853 46 C,0,-1.0224673522,-0.5608352629,0.343131366 O,0,-1.3214767328,-0.7096396609,1.5047151632 O,0,-1.5474097071,-1.367833693,-0.6089666899 H,0,-1.2372529303,-1.1106088685,-1.4891510318 C,0,-0.0280724881,0.5058189327,-0.1086968133 H,0,-0.481360018,1.0871747863,-0.933209674 C,0,1.295656482,-0.132337867,-0.6100773009 H 0,1.0964464081,0.7858093410,14730175865
O,0,-0.0847334549,0.4509959559,1.761403679 H,0,-0.3251263361,1.3591972103,1.5077486524 N,0,-1.4171913345,-1.4874773128,0.0418233908 H,0,-1.8044367341,-2.4197370225,-0.0741113816 H,0,-1.9544692685,-1.0264571678,0.7732226958 45 C,0,-0.2434816486,0.2817084927,1.1652862692 O,0,-1.1800385586,-0.1972013327,1.7597913725 O,0,0.2979057492,1.4550843903,1.5665956919 H,0,1.0632195752,1.6849464996,1.0195633279 C,0,0.3694071509,-0.3899320514,-0.062399437 H,0,1.4623436787,-0.4688631843,0.0747808717 C,0,0.0990641029,0.4179328166,-1.3429469165 H,0,0.493749209,1.4403226166,-1.2348179459 H 0, 0.9970016637,0.4941400178,1.468960254	0,0,1.3991739507,-0.0208109276,-1.1914408629 H,0,1.9717300943,0.1841895916,-0.4329747266 N,0,-0.4748796852,-2.0952561021,-0.1508274553 H,0,0.490247894,-2.3630656285,-0.3291634445 H,0,-0.5600546942,-1.9111186021,0.84634848853 46 C,0,-1.0224673522,-0.5608352629,0.343131366 O,0,-1.3214767328,-0.7096396609,1.5047151632 O,0,-1.5474097071,-1.367833693,-0.6089666899 H,0,-1.2372529303,-1.1106088685,-1.4891510318 C,0,-0.0280724881,0.5058189327,-0.1086968133 H,0,-0.481360018,1.0871747863,-0.933209674 C,0,1.295656482,-0.132337867,-0.6100773009 H,0,1.0964464981,-0.7858083419,-1.4739175865 H 0,1.6910507835, 0.7677480096,0.195262812
Ö,0,-0.0847334549,0.4509959559,1.761403679 H,0,-0.3251263361,1.3591972103,1.5077486524 N,0,-1.4171913345,-1.4874773128,0.0418233908 H,0,-1.8044367341,-2.4197370225,-0.0741113816 H,0,-1.9544692685,-1.0264571678,0.7732226958 45 C,0,-0.2434816486,0.2817084927,1.1652862692 O,0,-1.1800385586,-0.1972013327,1.7597913725 O,0,0.2979057492,1.4550843903,1.5665956919 H,0,1.0632195752,1.6849464996,1.0195633279 C,0,0.3694071509,-0.3899320514,-0.062399437 H,0,1.4623436787,-0.4688631843,0.0747808717 C,0,0.0990641029,0.4179328166,-1.3429469165 H,0,0.493749209,1.4403226166,-1.2348179459 H,0,-0.9970016637,0.4941400178,-1.4689960254 O,0,01556348457,1.6961654814,0.1937212181	N,0, 1.3991739507,-0.0208109276,-1.1914408629 H,0,1.9717300943,0.1841895916,-0.4329747266 N,0,-0.4748796852,-2.0952561021,-0.1508274553 H,0,0.490247894,-2.3630656285,-0.3291634445 H,0,-0.5600546942,-1.9111186021,0.84634848853 46 C,0,-1.0224673522,-0.5608352629,0.343131366 O,0,-1.3214767328,-0.7096396609,1.5047151632 O,0,-1.5474097071,-1.367833693,-0.6089666899 H,0,-0.280724881,0.5058189327,-0.1086968133 H,0,-0.481360018,1.0871747863,-0.933209674 C,0,1.295656482,-0.132337867,-0.6100773009 H,0,1.0964464981,-0.7858083419,-1.4739175865 H,0,1.6919507835,-0.7677480096,0.195262812 O,0.0235041488 1.3856563888.0.063880824
O,0,-0.0847334549,0.4509959559,1.761403679 H,0,-0.3251263361,1.3591972103,1.5077486524 N,0,-1.4171913345,-1.4874773128,0.0418233908 H,0,-1.8044367341,-2.4197370225,-0.0741113816 H,0,-1.9544692685,-1.0264571678,0.7732226958 45 C,0,-0.2434816486,0.2817084927,1.1652862692 O,0,-1.1800385586,-0.1972013327,1.7597913725 O,0,0.2979057492,1.4550843903,1.5665956919 H,0,1.0632195752,1.6849464996,1.0195633279 C,0,0.3694071509,-0.3899320514,-0.062399437 H,0,1.4623436787,-0.4688631843,0.0747808717 C,0,0.0990641029,0.4179328166,-1.3429469165 H,0,0.493749209,1.4403226166,-1.2348179459 H,0,-0.9970016637,0.4941400178,-1.4689960254 O,0,-0.1556348457,-1.6961654814,-0.1937212181 H 0 -0 8867244965 -1 7658952848 0 4438486843	0,0,1.3991739507,-0.0208109276,-1.1914408629 H,0,1.9717300943,0.1841895916,-0.4329747266 N,0,-0.4748796852,-2.0952561021,-0.1508274553 H,0,0.490247894,-2.3630656285,-0.3291634445 H,0,-0.5600546942,-1.9111186021,0.84634848853 46 C,0,-1.0224673522,-0.5608352629,0.343131366 O,0,-1.3214767328,-0.7096396609,1.5047151632 O,0,-1.5474097071,-1.367833693,-0.6089666899 H,0,-1.2372529303,-1.1106088685,-1.4891510318 C,0,-0.0280724881,0.5058189327,-0.1086968133 H,0,-0.481360018,1.0871747863,-0.933209674 C,0,1.295656482,-0.132337867,-0.6100773009 H,0,1.0964464981,-0.7858083419,-1.4739175865 H,0,1.6919507835,-0.7677480096,0.195262812 O,0,0.235041488,1.3856563888,0.9638808924 H 0,-0.1788375601 0.9923068857 1.7514297163
O,0,-0.0847334549,0.4509959559,1.761403679 H,0,-0.3251263361,1.3591972103,1.5077486524 N,0,-1.4171913345,-1.4874773128,0.0418233908 H,0,-1.8044367341,-2.4197370225,-0.0741113816 H,0,-1.9544692685,-1.0264571678,0.7732226958 45 C,0,-0.2434816486,0.2817084927,1.1652862692 O,0,-1.1800385586,-0.1972013327,1.7597913725 O,0,0.2979057492,1.4550843903,1.5665956919 H,0,1.0632195752,1.6849464996,1.0195633279 C,0,0.3694071509,-0.3899320514,-0.062399437 H,0,1.4623436787,-0.4688631843,0.0747808717 C,0,0.0990641029,0.4179328166,-1.3429469165 H,0,0.493749209,1.4403226166,-1.2348179459 H,0,-0.9970016637,0.4941400178,-1.4689960254 O,0,-0.1556348457,-1.6961654814,-0.1937212181 H,0,-0.8867244965,-1.7658952848,0.4438486843 N 0 0 7941486278 -0 2258189597 -2 4560871006	0,0,1.3991739507,-0.0208109276,-1.1914408629 H,0,1.9717300943,0.1841895916,-0.4329747266 N,0,-0.4748796852,-2.0952561021,-0.1508274553 H,0,0.490247894,-2.3630656285,-0.3291634445 H,0,-0.5600546942,-1.9111186021,0.84634848853 46 C,0,-1.0224673522,-0.5608352629,0.343131366 O,0,-1.3214767328,-0.7096396609,1.5047151632 O,0,-1.5474097071,-1.367833693,-0.6089666899 H,0,-1.2372529303,-1.1106088685,-1.4891510318 C,0,-0.0280724881,0.5058189327,-0.1086968133 H,0,-0.481360018,1.0871747863,-0.933209674 C,0,1.295656482,-0.132337867,-0.6100773009 H,0,1.0964464981,-0.7858083419,-1.4739175865 H,0,1.6919507835,-0.7677480096,0.195262812 O,0,0.235041488,1.3856563888,0.9638808924 H,0,-0.1788375601,0.9923068857,1.7514297163 N 0 2 3221517682 0 8282777413 -0 9835683875
$\begin{array}{c} 0,0,-0.0847334549,0.4509959559,1.761403679\\ H,0,-0.3251263361,1.3591972103,1.5077486524\\ N,0,-1.4171913345,-1.4874773128,0.0418233908\\ H,0,-1.8044367341,-2.4197370225,-0.0741113816\\ H,0,-1.9544692685,-1.0264571678,0.7732226958\\ \\ \hline \\ \hline \\ \hline \\ \hline \\ C,0,-0.2434816486,0.2817084927,1.1652862692\\ O,0,-1.1800385586,-0.1972013327,1.7597913725\\ O,0,0.2979057492,1.4550843903,1.5665956919\\ H,0,1.0632195752,1.6849464996,1.0195633279\\ C,0,0.3694071509,-0.3899320514,-0.062399437\\ H,0,1.4623436787,-0.4688631843,0.0747808717\\ C,0,0.0990641029,0.4179328166,-1.3429469165\\ H,0,0.493749209,1.4403226166,-1.2348179459\\ H,0,-0.9970016637,0.4941400178,-1.4689960254\\ O,0,-0.1556348457,-1.6961654814,-0.1937212181\\ H,0,-0.8867244965,-1.7658952848,0.4438486843\\ N,0,0.7941486278,-0.2258189597,-2.4560871006\\ H,0,0.4521281029,-1.1786343961,-2.5662739905\\ \end{array}$	N,0, 1.3991739507,-0.0208109276,-1.1914408629 H,0,1.9717300943,0.1841895916,-0.4329747266 N,0,-0.4748796852,-2.0952561021,-0.1508274553 H,0,0.490247894,-2.3630656285,-0.3291634445 H,0,-0.5600546942,-1.9111186021,0.8463484853 46 C,0,-1.0224673522,-0.5608352629,0.343131366 O,0,-1.3214767328,-0.7096396609,1.5047151632 O,0,-1.5474097071,-1.367833693,-0.6089666899 H,0,-0.280724881,0.5058189327,-0.1086968133 H,0,-0.481360018,1.0871747863,-0.933209674 C,0,1.295656482,-0.132337867,-0.6100773009 H,0,1.0964464981,-0.7858083419,-1.4739175865 H,0,1.6919507835,-0.7677480096,0.195262812 O,0,0.235041488,1.3856563888,0.9638808924 H,0,-0.1788375601,0.9923068857,1.7514297163 N,0,2.3221517682,0.8282777413,-0.9835683875 H,0,2.030055402,1.394095783,-1.7778170996
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Ö,0,-0.0847334549,0.4509959559,1.761403679 H,0,-0.3251263361,1.3591972103,1.5077486524 N,0,-1.4171913345,-1.4874773128,0.0418233908 H,0,-1.8044367341,-2.4197370225,-0.0741113816 H,0,-1.9544692685,-1.0264571678,0.7732226958 45 C,0,-0.2434816486,0.2817084927,1.1652862692 O,0,-1.1800385586,-0.1972013327,1.7597913725 O,0,0.2979057492,1.4550843903,1.5665956919 H,0,1.0632195752,1.6849464996,1.0195633279 C,0,0.3694071509,-0.3899320514,-0.062399437 H,0,1.4623436787,-0.4688631843,0.0747808717 C,0,0.0990641029,0.4179328166,-1.3429469165 H,0,0.493749209,1.4403226166,-1.2348179459 H,0,-0.9970016637,0.4941400178,-1.4689960254 O,0,-0.1556348457,-1.6961654814,-0.1937212181 H,0,-0.8867244965,-1.7658952848,0.4438486843 N,0,0.7941486278,-0.2258189597,-2.4560871006 H,0,0.4521281029,-1.1786343961,-2.5662739905 H,0,0.6099149565,0.2631258767,-3.3281236435 47 C,0,0.733193977,-0.7537962467,-0.0272564352 O,0,0.7265910528,-1.787237009,0.6062535363	0,0,1.3991739507,-0.0208109276,-1.1914408629 H,0,1.9717300943,0.1841895916,-0.4329747266 N,0,-0.4748796852,-2.0952561021,-0.1508274553 H,0,0.490247894,-2.3630656285,-0.3291634445 H,0,-0.5600546942,-1.9111186021,0.8463484853 46 C,0,-1.0224673522,-0.5608352629,0.343131366 O,0,-1.3214767328,-0.7096396609,1.5047151632 O,0,-1.5474097071,-1.367833693,-0.6089666899 H,0,-1.2372529303,-1.1106088685,-1.4891510318 C,0,-0.0280724881,0.5058189327,-0.1086968133 H,0,-0.481360018,1.0871747863,-0.933209674 C,0,1.295656482,-0.132337867,-0.6100773009 H,0,1.0964464981,-0.7858083419,-1.4739175865 H,0,1.6919507835,-0.7677480096,0.195262812 O,0,0.235041488,1.3856563888,0.9638808924 H,0,-0.1788375601,0.9923068857,1.7514297163 N,0,2.3221517682,0.8282777413,-0.9835683875 H,0,2.030055402,1.394095783,-1.7778170996 H,0,2.4953243667,1.467481166,-0.2105153064 48 C,0,-0.023356838,0.9925756724,0.1016147835 O,0,-0.815356004,1.3624883896,0.9462454865
Ö,0,-0.0847334549,0.4509959559,1.761403679 H,0,-0.3251263361,1.3591972103,1.5077486524 N,0,-1.4171913345,-1.4874773128,0.0418233908 H,0,-1.8044367341,-2.4197370225,-0.0741113816 H,0,-1.9544692685,-1.0264571678,0.7732226958 45 C,0,-0.2434816486,0.2817084927,1.1652862692 O,0,-1.1800385586,-0.1972013327,1.7597913725 O,0,0.2979057492,1.4550843903,1.5665956919 H,0,1.0632195752,1.6849464996,1.0195633279 C,0,0.3694071509,-0.3899320514,-0.062399437 H,0,1.4623436787,-0.4688631843,0.0747808717 C,0,0.0990641029,0.4179328166,-1.3429469165 H,0,0.493749209,1.4403226166,-1.2348179459 H,0,-0.9970016637,0.4941400178,-1.4689960254 O,0,-0.1556348457,-1.6961654814,-0.1937212181 H,0,-0.8867244965,-1.7658952848,0.4438486843 N,0,0.7941486278,-0.2258189597,-2.4560871006 H,0,0.4521281029,-1.1786343961,-2.5662739905 H,0,0.6099149565,0.2631258767,-3.3281236435 47 C,0,0.733193977,-0.7537962467,-0.0272564352 O,0,0,7265910528,-1.787237009,0.6062535363 O,0,1.1832350105,-0.660274811,-1.2914345508	N,0, 1.3991739507,-0.0208109276,-1.1914408629 H,0,1.9717300943,0.1841895916,-0.4329747266 N,0,-0.4748796852,-2.0952561021,-0.1508274553 H,0,0.490247894,-2.3630656285,-0.3291634445 H,0,-0.5600546942,-1.9111186021,0.8463484853 46 C,0,-1.0224673522,-0.5608352629,0.343131366 O,0,-1.3214767328,-0.7096396609,1.5047151632 O,0,-1.5474097071,-1.367833693,-0.6089666899 H,0,-0.280724881,0.5058189327,-0.1086968133 H,0,-0.481360018,1.0871747863,-0.933209674 C,0,1.295656482,-0.132337867,-0.6100773009 H,0,1.0964464981,-0.7858083419,-1.4739175865 H,0,1.6919507835,-0.7677480096,0.195262812 O,0,0.235041488,1.3856563888,0.9638808924 H,0,-0.1788375601,0.9923068857,1.7514297163 N,0,2.3221517682,0.8282777413,-0.9835683875 H,0,2.030055402,1.394095783,-1.7778170996 H,0,2.4953243667,1.467481166,-0.2105153064 48 C,0,-0.023356838,0.9925756724,0.1016147835 O,0,-0.815356004,1.3624883896,0.9462454865 O,0,1.0857246587,1.6866022941,-0.217980863
Ö,0,-0.0847334549,0.4509959559,1.761403679 H,0,-0.3251263361,1.3591972103,1.5077486524 N,0,-1.4171913345,-1.4874773128,0.0418233908 H,0,-1.8044367341,-2.4197370225,-0.0741113816 H,0,-1.9544692685,-1.0264571678,0.7732226958 45 C,0,-0.2434816486,0.2817084927,1.1652862692 O,0,-1.1800385586,-0.1972013327,1.7597913725 O,0,0.2979057492,1.4550843903,1.5665956919 H,0,1.0632195752,1.6849464996,1.0195633279 C,0,0.3694071509,-0.3899320514,-0.062399437 H,0,1.4623436787,-0.4688631843,0.0747808717 C,0,0.0990641029,0.4179328166,-1.3429469165 H,0,0.493749209,1.4403226166,-1.2348179459 H,0,-0.9970016637,0.4941400178,-1.4689960254 O,0,-0.1556348457,-1.6961654814,-0.1937212181 H,0,-0.8867244965,-1.7658952848,0.4438486843 N,0,0.7941486278,-0.2258189597,-2.4560871006 H,0,0.4521281029,-1.1786343961,-2.5662739905 H,0,0.6099149565,0.2631258767,-3.3281236435 47 C,0,0.733193977,-0.7537962467,-0.0272564352 O,0,0,7265910528,-1.787237009,0.6062535363 O,0,1.1832350105,-0.660274811,-1.2914345508 H,0,1.4485005369,-1.5575186943,-1.5535490325	0,0,1.3991739507,-0.0208109276,-1.1914408629 H,0,1.9717300943,0.1841895916,-0.4329747266 N,0,-0.4748796852,-2.0952561021,-0.1508274553 H,0,0.490247894,-2.3630656285,-0.3291634445 H,0,-0.5600546942,-1.9111186021,0.8463484853 46 C,0,-1.0224673522,-0.5608352629,0.343131366 O,0,-1.3214767328,-0.7096396609,1.5047151632 O,0,-1.5474097071,-1.367833693,-0.6089666899 H,0,-1.2372529303,-1.1106088685,-1.4891510318 C,0,-0.0280724881,0.5058189327,-0.1086968133 H,0,-0.481360018,1.0871747863,-0.933209674 C,0,1.295656482,-0.132337867,-0.6100773009 H,0,1.0964464981,-0.7858083419,-1.4739175865 H,0,1.6919507835,-0.7677480096,0.195262812 O,0,0.235041488,1.3856563888,0.9638808924 H,0,-0.1788375601,0.9923068857,1.7514297163 N,0,2.3221517682,0.8282777413,-0.9835683875 H,0,2.030055402,1.394095783,-1.7778170996 H,0,2.4953243667,1.467481166,-0.2105153064 48 C,0,-0.023356838,0.9925756724,0.1016147835 O,0,-0.815356004,1.3624883896,0.9462454865 O,0,1.0857246587,1.6866022941,-0.217980863 H,0,1.0812286055,2.4841944441,0.3373210803

H,0,0.7770902241,0.6784145028,1.5194218825	H,0,-1.2280828725,-0.416055148,-0.9024177571
C,0,-1.2665914832,0.4537280283,0.8681235076	C,0,0.1913654088,-1.4976451349,0.348087273
H,0,-1.5666146987,1.3878454672,1.3842558318	H,0,1.21051843,-1.3333574834,0.7267516134
H,0,-1.4195172141,-0.3770037662,1.5693569494	H,0,0.2242863467,-2.4159540494,-0.2591221432
0,0,0.5230762951,1.6408477437,-0.3174212044	0,0,0.6714661089,-0.3369814423,-1.7744077157
H,0,0.3909237324,2.4662804281,0.1643346273	H,0,0.5934991345,-1.1972116028,-2.2047092843
N,0,-2.0028547269,0.1784683027,-0.3623505501	N,0,-0.7080752622,-1.7205766771,1.4680304782
H,0,-2.9975110011,0.0771026806,-0.1850226078	H.00.8146949397,-0.8744633494,2.0237129609
H.0,-1.879316916,0.9336629604,-1.0323724262	H.0,-1.6392397225,-1.9740559686,1.1452534415
49	50
C 0 0 7491040634 -0 7078150719 -0 1761149382	C = 0.0.2552877388 = 0.942933068 = 0.104692114
0.0.1.1112213923 -0.9243120342 -1.3035095534	0.013538984753 - 11466145395 - 0.3531403226
0.0.0.658564682 -1.6750156221.0.7777601815	0.0-0.6529196421 -1.9238904246.0.3225168497
H 0 0 8933363949 -2 5124618834 0 3468972503	H 0 -0 2412368051 -2 7580165489 0 0411422951
C 0 0 3600822366 0 6443968767 0 4154922227	C 0 -0 2738672343 0 4288770278 0 5310189029
H 0 1 0130156518 0 8118895694 1 2894762532	H 0 -1 3539526778 0 3338735916 0 725184164
C 0 -1 1014326986 0 6449329829 0 8875684939	C 0 -0 0216034599 1 463516062 -0 5696003087
H 0 -1 3132494136 1 6551226275 1 2924004911	H 0 1 043411015 1 4270838233 -0 8290190005
H.01.20633672520.0688151416.1.7151989429	H.00.2325339821.2.46664969360.1527260261
0.0.0.5923302525.1.62486058810.5879618669	0.0.0.4289743863.0.7441008009.1.7356585563
H.0.0.5182827488.2.4953170940.1789775947	H.0.0.0392992606.1.5394649914.2.1183500665
N.01.9783699861.0.23538345140.2054981073	N.00.814337891.1.12709664811.7541330509
H.02.9546697348.0.2555303974.0.0732621281	H.01.7774056421.1.44092374951.6676440879
H.01.868878844.0.85573620571.0044939233	H.00.4305135415.1.55136817292.5923001919
51	52
C 0 0 5548168009 -0 6450455019 -0 6397122915	C 0 0 8080277602 -0 3907854142 0 4567794196
0.0.0.62777654540.84567235191.8298225737	0.0.1.4568715210.1293523011.1.4431509752
0.0.0.66334667081.6656710787.0.2415903115	0.0.062670626311.64996444080.000332565
H,0,0.5573325496,-1.3260339947,1.1445659979	H.0,1.1055875192,-2.240059148,0.6041163022
C,0,0.3305289149,0.7498612118,-0.0605049729	C,0,0.1090623339,0.6495124925,-0.416660068
H,0,1.1365683176,0.9500440554,0.6711578196	H,0,0.331050371,1.6191033147,0.0558049991
C,0,-1.0368224495,0.8900005358,0.6709192981	C,0,-1.407470833,0.4234042354,-0.4816115695
H,0,-1.8367007702,0.5895751243,-0.0192544214	H,0,-1.5870641762,-0.5574231063,-0.9387656117
H,0,-1.1620430174,1.9659077532,0.8519487037	H,0,-1.8302180543,1.1901293645,-1.1604189788
O,0,0.3981811625,1.7027675298,-1.0965877847	O,0,0.7035186836,0.5707673616,-1.7137444527
H,0,0.5066055398,1.2063513467,-1.9258339381	H,0,0.4229886312,1.3380000604,-2.2271901817
N,0,-1.2128935894,0.1774080871,1.9247714698	N,0,-1.9791311251,0.4261220946,0.8647885376
H,0,-1.3964135022,-0.8156649224,1.85760501	H,0,-1.9824768108,1.3581142932,1.2723791472
H,0,-0.5505331929,0.3984222656,2.6589074118	H,0,-2.9392020839,0.0956811335,0.8584540666
53	54
C,0,-0.0122789687,-1.0641225036,-0.2496492174	C,0,-0.2766310041,0.232770942,-1.1618580926
O,0,-1.1135741492,-1.1539190414,-0.7297322847	O,0,0.374499219,0.8979176909,-1.9318957824
O,0,0.5939038843,-2.1674870675,0.275311022	O,0,-1.6003902137,0.041466328,-1.3752316011
H,0,1.4941450391,-1.9582257183,0.5611322469	H,0,-1.9813536627,-0.5242716804,-0.6883608822
C,0,0.7514205502,0.2656740389,-0.106288176	C,0,0.3451608521,-0.4194359955,0.0772506985
H,0,1.8249073012,0.0644610155,0.0354811652	H,0,0.0765213498,-1.4937412657,0.0642567008
C,0,0.2087604427,1.016205896,1.1342523073	C,0,-0.2100217088,0.2049784943,1.3768985826
H,0,0.8814539825,1.8618970574,1.327750239	H,0,-1.3116180526,0.3019402663,1.2966117083
H,0,0.2367362052,0.3498830632,2.0158464411	H,0,0.2003758128,1.2204336137,1.4554883325
0,0,0.6298866719,1.053661085,-1.2620943748	0,0,1.7455432982,-0.3078187333,0.0085705722
H,0,-0.2282368881,1.5063815051,-1.1827118652	H,0,1.9386408534,0.2666789848,-0.7517001571
N,0,-1.1144821237,1.5527857439,0.8156758805	N,0,0.2281406365,-0.562884223,2.5383735102
H,0,-1.8274436852,0.8275873778,0.8008075573	H,0,0.1236783015,-0.0284282002,3.3953956311
H.01.3989483023.2.2694675879.1.4749690987	H,0,-0.3065456214,-1.4211062019,2.6474508391

	B3L	.YP/aug-cc-p√	/DZ	B3LYP/aug-cc-pVTZ				
	harmonic	anharm	Int	harmonic	anharm	Int	Rot. Str.	
1	3670.4	3465.6	109.8	3673.1	3471.5	110.9	-5.4	
2	3578.5	3404.7	11.0	3579.9	3406.9	12.3	0.6	
3	3494.5	3334.6	2.2	3502.2	3366.1	2.6	-3.4	
4	3164.8	2792.7	766.3	3188.2	2908.3	739.2	-68.6	
5	3103.0	2944.6	13.7	3086.4	2940.8	13.4	10.7	
6	3042.3	2871.2	38.6	3032.2	2875.7	34.6	-3.2	
7	2946.3	2809.6	41.6	2937.7	2807.9	39.3	30.9	
8	1802.8	1768.2	374.1	1808.1	1778.2	382.4	-37.2	
9	1634.9	1574.4	26.8	1652.9	1600.0	27.1	-5.1	
10	1501.1	1473.6	127.7	1513.8	1471.4	11.0	-4.4	
11	1490.3	1452.9	68.4	1485.4	1429.9	172.3	-31.0	
12	1423.8	1377.5	73.0	1427.6	1371.5	91.1	100.2	
13	1397.5	1361.8	0.8	1408.8	1374.6	1.4	-13.0	
14	1340.5	1304.1	2.6	1354.3	1321.0	4.6	-10.1	
15	1297.1	1266.1	38.0	1311.2	1276.3	27.9	-40.2	
16	1274.1	1248.1	32.7	1285.8	1253.9	28.7	-15.9	
17	1244.9	1208.9	61.5	1246.9	1209.5	73.7	26.3	
18	1164.7	1137.2	3.9	1171.0	1143.0	4.3	-10.2	
19	1138.3	1109.6	148.2	1136.0	1106.7	152.2	14.0	
20	1059.6	1032.8	9.9	1057.6	1032.1	14.7	2.0	
21	1032.6	1005.3	39.1	1030.7	1001.5	35.6	-31.6	
22	995.7	944.0	44.5	986.9	946.1	24.2	-8.2	
23	971.1	931.4	46.6	964.4	908.6	69.7	32.5	
24	901.5	868.3	43.6	896.4	860.6	44.7	-8.9	
25	807.7	793.9	15.2	808.1	793.7	17.4	-10.6	
26	735.1	726.5	5.1	741.5	732.2	5.2	-18.4	
27	614.1	608.7	11.4	618.5	609.7	11.4	47.0	
28	540.3	527.5	19.0	541.2	524.9	19.8	56.1	
29	481.2	440.2	49.1	484.3	443.0	50.7	-61.0	
30	424.2	410.3	8.8	424.3	411.6	8.7	10.8	
31	379.7	374.7	24.8	375.4	368.4	22.1	-28.7	
32	322.1	322.0	8.4	320.0	310.8	20.3	121.4	
33	306.6	301.4	21.7	309.4	302.0	9.4	-101.0	
34	271.2	257.7	12.9	269.5	255.4	12.1	32.8	
36	169.4	165.6	2.8	167.1	159.2	2.8	-14.0	
36	100.8	100.3	17	100.9	913	15	10.0	

Table 4SI. The B3LYP/aug-cc-pVDZ and B3LYP/aug-cc-pVTZ calculated harmonic and anharmonic frequencies (cm⁻¹), intensities (km/mol), and rotational strength $(10^{-44} esu^2 cm^2)$ of the **1** L-isoserine conformer.

Table 5SI.	The B3LYP/aug	-cc-pVDZ and	B3LYP/aug-c	c-pVTZ ca	lculated ha	armonic an	ıd
anharmonic	frequencies (cm ⁻¹), intensities (k	m/mol), and ro	otational str	ength (10 ⁻⁴	⁴ esu ² cm ²) o	of
the 2 L-isos	erine conformer.						

	B3LY	P/aug-cc-p	VDZ	B3LYP/aug-cc-pVTZ			
	harmonic	anharm	Int	harmonic	anharm	Int	Rot. Str.
1	3596.9	3374.9	130.6	3609.1	3391.9	126.1	145.4
2	3591.3	3425.0	10.7	3593.0	3431.9	11.8	-1.6
3	3573.2	3341.5	174.5	3588.1	3370.6	170.8	-117.1
4	3502.5	3349.4	4.4	3510.4	3386.5	5.0	-6.7
5	3110.3	2948.6	13.6	3092.3	2950.7	13.2	9.2
6	3068.4	2913.1	20.4	3056.1	2915.7	21.4	11.1
7	3052.9	2947.5	17.7	3042.5	2910.8	15.0	-10.3
8	1822.7	1789.4	269.8	1829.1	1801.5	278.3	-67.0
9	1642.6	1555.1	35.0	1660.2	1608.3	35.0	-0.9
10	1481.9	1450.9	8.7	1499.0	1483.8	9.1	-6.5
11	1414.0	1366.7	47.0	1416.6	1383.6	52.0	-115.7
12	1398.6	1361.6	169.9	1409.5	1377.7	42.7	59.9
13	1378.4	1339.7	277.7	1374.1	1329.6	376.6	76.9
14	1335.3	1317.2	15.4	1350.9	1322.3	29.5	-20.5
15	1315.9	1283.9	8.2	1330.2	1295.1	14.7	25.5
16	1232.0	1186.5	22.4	1242.5	1200.5	25.1	8.7
17	1204.3	1157.9	28.4	1204.7	1168.7	28.9	-43.8
18	1168.8	1142.2	7.7	1174.2	1148.9	10.7	27.6
19	1113.5	1081.9	37.7	1111.5	1078.7	39.4	45.5
20	1053.5	1024.4	27.8	1051.4	1023.8	29.9	29.9
21	967.9	940.9	34.1	970.1	939.9	37.8	-69.6
22	923.2	891.9	30.2	920.2	888.3	27.0	-37.2
23	872.0	832.4	35.4	875.2	843.0	31.3	44.8
24	834.0	790.0	65.6	829.5	787.5	72.6	68.0
25	801.8	760.6	52.0	795.8	724.7	54.2	-174.2
26	752.9	736.7	2.8	755.3	740.6	3.7	14.9
27	661.7	635.8	96.1	650.4	584.4	97.3	7.7
28	588.3	581.4	14.1	589.6	581.7	13.4	26.4
29	549.9	536.8	9.3	553.8	538.0	10.1	-2.7
30	516.0	507.0	4.1	517.7	509.7	3.8	-9.9
31	355.0	348.7	9.2	356.7	353.1	9.2	1.9
32	292.5	271.8	4.8	294.7	288.9	4.7	35.3
33	271.7	265.8	23.2	274.8	275.6	20.8	21.8
34	246.3	237.0	11.8	248.3	244.4	12.9	-13.6
35	99.8	101.4	4.0	100.7	116.1	4.0	-2.7
36	66.5	60.1	8.2	68.4	84.5	8.0	-12.3

Table 6SI. The B3LYP/aug-cc-pVDZ and B3LYP/aug-cc-pVTZ calculated harmonic and anharmonic frequencies (cm⁻¹), intensities (km/mol), and rotational strength $(10^{-44}$ esu²cm²) of the **3** L-isoserine conformer.

	B3L	YP/aug-cc-pV	'DZ	B3LYP/aug-cc-pVTZ			
	harmonic	anharm	Int	harmonic	anharm	Int	Rot. Str.
1	3634.5	3416.7	70.0	3641.5	3425.5	72.2	124.0
2	3615.4	3395.2	230.3	3622.2	3404.1	223.0	-151.5
3	3589.0	3415.7	9.6	3590.6	3420.8	10.6	-2.5
4	3500.3	3339.9	2.8	3508.4	3326.9	3.5	6.0
5	3098.1	2937.3	18.2	3080.3	2937.5	18.0	-14.2
6	3044.2	2878.6	21.4	3034.4	2939.0	20.3	4.5
7	3016.2	2864.2	20.2	3004.4	2863.5	18.9	1.1
8	1827.6	1796.3	292.7	1833.4	1802.5	301.9	-57.2
9	1642.0	1591.2	26.7	1658.1	1692.5	26.4	4.8
10	1485.1	1465.0	3.9	1503.7	1520.3	4.0	4.6
11	1415.0	1379.3	72.5	1416.8	1375.0	23.1	-83.3
12	1397.8	1359.3	78.9	1404.3	1361.8	51.2	-163.4
13	1370.2	1326.6	298.0	1372.4	1322.9	315.0	130.5
14	1332.1	1294.2	46.0	1347.2	1306.0	95.9	32.7
15	1295.7	1269.7	31.2	1310.2	1277.1	25.1	-61.6
16	1275.7	1252.2	23.2	1288.5	1254.7	37.0	-19.3
17	1204.2	1162.5	48.8	1203.4	1162.7	40.8	4.1
18	1158.8	1124.1	56.6	1164.0	1120.5	72.3	181.7
19	1125.7	1087.1	30.2	1124.3	1084.9	31.2	-2.4
20	1064.4	1036.4	12.4	1059.7	1031.1	14.1	-10.3
21	970.4	946.7	1.8	972.6	948.8	3.1	12.9
22	935.6	905.7	27.0	931.5	901.9	28.9	-10.7
23	892.9	860.2	55.4	894.6	861.8	51.8	11.7
24	823.3	774.5	57.9	822.0	888.2	62.6	-68.3
25	729.0	710.9	15.5	731.2	722.0	8.7	18.2
26	716.4	677.5	85.0	717.5	699.7	93.1	110.8
27	634.4	596.9	16.1	635.2	608.6	13.7	-81.5
28	603.3	538.7	76.6	599.2	513.3	80.0	6.4
29	564.0	550.4	16.5	564.3	550.5	17.2	30.8
30	445.1	438.1	4.3	445.9	438.9	4.7	16.8
31	340.8	336.5	4.7	343.9	341.5	4.9	-7.1
32	319.9	313.3	8.4	324.3	314.1	8.2	-3.8
33	271.8	243.9	10.3	270.3	241.2	10.1	-49.3
34	190.0	188.5	14.2	190.9	192.6	13.6	-16.8
36	118.4	101.1	5.2	121.3	109.4	5.0	25.7
36	68.2	75.1	5.3	71.0	90.6	5.2	-1.3

Table '	7SI.	The	B3LY	P/aug-o	cc-pVDZ	Z and	B3LYF	∕/aug-c	c-pVTZ	calcula	ted 1	harmonic	and
anharm	onic	frequ	iencies	(cm^{-1})	, intensit	ies (k	m/mol),	and re	otational	strength	n (10	⁻⁴⁴ esu ² cm	n^2) of
the 4 L-	-isose	erine	confor	mer.									

	B3LY	P/aug-cc-p	VDZ	B3LYP/aug-cc-pVTZ			
	harmonic	anharm	Int	harmonic	anharm	Int	Rot. Str.
1	3742.5	3545.5	76.3	3738.3	3550.3	76.5	3.2
2	3707.1	3511.1	91.1	3710.0	3519.7	92.4	-10.7
3	3583.9	3411.0	6.2	3586.7	3422.0	7.5	2.7
4	3500.0	3343.3	1.4	3508.6	3362.0	1.6	-3.3
5	3095.1	2943.8	16.3	3081.8	2972.1	15.7	-2.3
6	3002.8	2858.2	46.9	2992.1	2856.3	44.5	12.1
7	2985.6	2872.0	49.8	2974.8	2819.7	48.4	18.7
8	1793.3	1764.1	291.8	1796.9	1774.0	297.1	40.4
9	1630.6	1573.3	33.9	1647.5	1538.0	33.8	3.2
10	1482.9	1477.2	5.7	1502.2	1434.8	5.8	15.7
11	1444.0	1397.0	2.9	1449.1	1403.6	4.8	-9.6
12	1405.7	1364.9	8.4	1418.3	1379.1	9.0	21.4
13	1345.6	1312.2	30.6	1357.4	1328.8	15.2	-13.1
14	1329.7	1303.6	55.8	1336.0	1316.1	77.3	26.6
15	1304.6	1273.3	3.9	1316.0	1286.6	2.2	32.0
16	1240.3	1213.4	53.5	1253.5	1227.4	42.8	-57.3
17	1206.2	1173.3	12.6	1209.7	1183.2	3.7	-28.0
18	1168.7	1129.0	169.6	1165.0	1136.4	175.2	40.4
19	1119.3	1085.9	123.4	1112.1	1077.7	138.1	-68.2
20	1071.8	1042.6	38.2	1072.4	1049.3	35.0	-60.7
21	1008.2	979.8	40.9	1010.3	985.6	46.4	100.8
22	915.5	881.0	7.7	912.5	883.5	7.0	0.0
23	855.6	839.3	13.2	859.1	841.2	15.9	-19.2
24	838.0	756.1	87.7	835.1	724.3	88.6	-98.9
25	740.5	725.9	37.1	742.5	734.5	40.7	85.7
26	639.1	618.3	98.7	642.8	628.5	95.9	51.6
27	586.3	569.7	38.6	588.2	574.3	41.6	-98.0
28	511.2	498.8	4.5	513.1	498.5	5.2	18.5
29	478.7	465.1	19.4	480.0	477.8	18.3	-25.4
30	428.1	350.0	54.4	431.5	401.7	55.3	58.4
31	340.0	320.8	3.0	342.8	348.6	4.7	7.7
32	288.5	274.3	39.0	290.0	311.9	32.4	-28.1
33	238.5	232.1	29.9	236.8	299.3	31.1	-36.4
34	207.5	209.1	1.8	207.2	241.8	3.0	-1.0
35	109.5	109.5	3.8	110.8	169.0	4.1	-2.4
36	84.5	82.6	0.5	87.0	159.6	0.4	3.8

Table 8SI. The B3LYP/aug-cc-pVDZ and B3LYP/aug-cc-pVTZ calculated harmonic and anharmonic frequencies (cm⁻¹), intensities (km/mol), and rotational strength $(10^{-44}$ esu²cm²) of the **5** L-isoserine conformer.

	B3LY	P/aug-cc-p	VDZ	B3LYP/aug-cc-pVTZ			
	harmonic	anharm	Int	harmonic	anharm	Int	Rot. Str.
1	3735.3	3538.5	76.0	3732.7	3535,3	76.1	4.3
2	3717.0	3513.6	88.5	3718.4	3545,9	91.1	-20.2
3	3567.4	3399.5	5.5	3573.0	3413,5	6.7	4.2
4	3484.6	3355.2	2.1	3495.2	3397,3	2.3	-2.8
5	3100.8	2942.5	21.1	3085.5	2952,7	20.2	4.6
6	3043.4	2938.9	27.6	3034.0	2892,9	26.4	-13.0
7	3025.4	2866.0	14.3	3011.0	2867,1	14.3	13.8
8	1787.4	1756.0	311.7	1790.8	1761,0	317.5	-11.8
9	1647.3	1657.1	24.3	1663.5	1712,4	24.8	8.0
10	1463.2	1444.5	2.2	1483.4	1472,4	2.0	-1.2
11	1433.1	1385.4	10.6	1436.6	1390,7	12.3	54.2
12	1382.9	1347.2	0.5	1395.8	1361,3	0.6	-9.9
13	1363.4	1333.2	14.2	1378.8	1350,5	11.5	-3.6
14	1334.9	1302.9	77.3	1340.0	1308,0	64.3	-38.2
15	1306.5	1277.8	23.5	1321.8	1293,7	41.0	2.3
16	1245.2	1214.4	58.3	1256.6	1227,4	43.5	-65.5
17	1191.0	1159.7	6.1	1198.1	1168,2	3.1	6.7
18	1166.7	1132.7	119.1	1165.0	1128,5	131.2	-7.2
19	1113.8	1082.8	19.5	1109.5	1071,9	6.6	-29.4
20	1103.2	1068.3	201.2	1098.5	1067,0	220.4	3.6
21	986.4	964.7	22.9	985.4	968,0	22.6	-3.5
22	914.2	892.3	34.7	910.7	894,3	37.6	36.3
23	871.5	827.7	146.7	869.9	838,1	145.5	-27.2
24	818.8	799.9	74.1	820.7	839,1	82.5	11.5
25	721.8	705.2	49.6	725.1	709,1	53.0	-8.0
26	650.0	636.8	28.8	655.0	641,8	29.4	48.0
27	582.1	552.4	61.6	579.7	533,0	61.0	-44.1
28	528.0	521.3	6.7	530.2	525,9	7.1	9.6
29	416.8	412.3	27.4	419.8	421,0	28.4	-10.5
30	368.0	301.3	63.7	373.2	371,4	66.5	6.1
31	345.1	333.4	20.4	348.7	359,3	14.9	-7.0
32	290.5	280.6	33.1	292.0	314,4	29.6	-5.7
33	278.6	282.4	4.8	279.8	305,0	9.1	20.0
34	177.6	187.8	4.3	178.9	209,9	4.3	8.2
35	109.9	132.1	1.0	110.9	144,1	1.0	-8.4
36	57.9	68.9	1.2	62.3	103,5	0.9	-7.3

Table 9SI. The B3LYP/aug-cc-pVDZ and B3LYP/aug-cc-pVTZ calculated harmonic and anharmonic frequencies (cm⁻¹), intensities (km/mol), and rotational strength $(10^{-44}$ esu²cm²) of the **6** L-isoserine conformer.

	B3LY	P/aug-cc-p	VDZ	B3LYP/aug-cc-pVTZ			
	harmonic	anharm	Int	harmonic	anharm	Int	Rot. Str.
1	3737.4	3541.4	76.4	3734.7	3540.1	74.8	1.6
2	3723.0	3530.7	85.6	3726.6	3546.0	88.4	-13.1
3	3575.5	3406.3	4.7	3581.2	3421.3	5.7	-3.9
4	3489.4	3339.3	2.1	3500.4	3405.5	2.2	0.0
5	3108.1	2951.3	14.6	3092.8	2959.1	14.1	1.8
6	3057.8	2922.8	32.8	3049.4	2964.0	31.4	8.9
7	2992.4	2840.5	27.6	2982.4	2846.1	26.5	23.8
8	1787.4	1758.2	294.8	1791.6	1769.4	300.6	63.9
9	1643.0	1627.5	16.0	1658.5	1694.0	16.0	1.2
10	1464.0	1423.1	5.1	1483.9	1455.1	4.6	7.7
11	1437.9	1395.7	1.7	1445.5	1397.9	3.4	12.2
12	1377.6	1345.5	4.1	1392.0	1358.6	6.5	9.1
13	1362.4	1332.2	12.2	1378.9	1343.0	7.7	4.2
14	1332.6	1321.3	85.7	1337.8	1330.5	91.8	10.1
15	1300.9	1255.9	2.5	1310.9	1307.5	3.0	24.0
16	1247.2	1217.9	31.9	1258.7	1227.0	25.1	-22.7
17	1207.8	1178.2	1.0	1214.7	1189.0	0.7	-11.2
18	1165.6	1125.4	160.4	1161.9	1123.1	158.0	10.4
19	1116.5	1080.9	127.6	1108.5	1069.6	129.0	-238.3
20	1082.7	1054.7	75.1	1082.5	1055.7	82.3	132.4
21	966.1	936.7	20.0	963.4	937.0	23.8	-27.8
22	871.1	851.1	17.1	874.1	857.2	19.1	-23.7
23	855.2	793.2	95.4	854.5	813.6	76.5	16.2
24	821.7	790.8	68.3	821.7	830.0	90.8	-13.9
25	730.7	712.7	77.8	732.0	721.1	81.2	-9.3
26	646.7	647.7	65.0	650.4	653.3	64.6	48.9
27	589.5	582.4	13.6	591.9	578.4	13.3	-75.2
28	524.5	519.5	18.4	527.0	509.0	19.2	45.7
29	472.9	460.4	16.7	474.9	473.1	16.7	-51.5
30	407.5	322.5	49.8	408.0	400.0	50.2	34.6
31	350.3	271.5	68.4	352.7	319.8	67.5	-1.2
32	289.8	246.5	7.4	293.4	298.7	7.2	1.8
33	245.4	203.7	22.1	245.7	245.7	22.8	-39.2
34	207.4	215.7	6.7	208.3	218.2	6.5	13.9
35	102.5	94.1	0.5	104.1	101.6	0.5	5.5
36	52.2	51.6	0.2	55.6	118.4	0.1	-2.3

Table 10SI. The B3LYP/aug-cc-pVDZ and B3LYP/aug-cc-pVTZ calculated harmonic and anharmonic frequencies (cm⁻¹), intensities (km/mol), and rotational strength $(10^{-44} esu^2 cm^2)$ of the **7** L-isoserine conformer.

	B3LY	P/aug-cc-p	VDZ	B3LYP/aug-cc-pVTZ			
	harmonic	anharm	Int	harmonic	anharm	Int	Rot. Str.
1	3737.3	3535.6	76.1	3734.2	3536.4	75.7	2.7
2	3716.5	3526.4	94.5	3719.7	3530.4	96.0	-19.9
3	3578.8	3411.8	6.6	3580.8	3419.9	7.8	-5.5
4	3494.8	3343.0	2.0	3502.6	3357.6	2.1	5.6
5	3090.1	2939.8	18.2	3076.1	2966.1	17.2	11.4
6	3032.5	2870.4	17.3	3020.0	2872.7	17.4	1.1
7	2962.2	2799.2	61.2	2950.9	2831.7	58.6	-13.0
8	1789.6	1758.5	298.4	1793.8	1764.7	304.6	-2.3
9	1633.9	1555.9	32.4	1650.5	1531.1	32.4	-20.7
10	1483.3	1439.1	2.6	1503.5	1460.2	2.7	-2.8
11	1438.2	1393.0	8.0	1441.4	1395.6	10.8	44.6
12	1409.0	1372.1	5.1	1420.4	1398.7	3.9	3.2
13	1346.1	1308.2	12.9	1360.2	1328.2	5.8	-17.9
14	1332.2	1300.1	77.6	1336.1	1302.2	87.9	-22.9
15	1280.1	1247.8	31.5	1292.7	1258.9	27.7	-0.9
16	1238.2	1203.7	37.7	1249.9	1217.0	28.0	-42.2
17	1199.7	1176.5	0.7	1206.8	1177.6	1.0	-10.5
18	1169.6	1130.3	160.7	1166.0	1121.8	165.5	-74.9
19	1118.2	1078.2	121.4	1112.5	1071.4	109.6	-97.3
20	1079.6	1049.1	70.9	1082.4	1054.4	91.0	118.0
21	1055.5	1028.8	19.7	1052.2	1023.1	21.7	-23.1
22	935.3	907.0	20.2	931.9	905.9	23.2	75.2
23	855.1	836.9	18.5	859.1	843.6	20.2	8.7
24	839.7	725.5	115.9	840.0	694.7	118.5	-101.1
25	723.6	708.3	44.9	727.9	714.0	45.7	1.4
26	648.1	632.1	51.5	652.7	636.0	51.1	83.7
27	579.3	547.9	55.1	578.1	539.4	56.3	-73.4
28	520.4	510.0	14.3	522.9	516.9	14.0	14.6
29	414.1	406.6	14.8	416.3	401.5	15.1	-12.8
30	366.9	350.2	14.6	367.8	359.3	18.5	21.5
31	355.7	255.4	73.3	360.9	311.9	69.1	-1.7
32	295.4	277.0	9.8	297.2	298.3	7.9	31.0
33	271.6	263.9	29.7	267.7	293.0	31.6	16.8
34	183.9	183.7	2.8	185.3	192.1	3.0	2.6
35	118.2	120.5	4.0	119.9	122.2	4.0	2.7
36	53.6	45.3	1.6	58.7	62.7	1.3	-3.5

Table 11SI. The B3LYP/aug-cc-pVDZ and B3LYP/aug-cc-pVTZ calculated harmonic and anharmonic frequencies (cm⁻¹), intensities (km/mol), and rotational strength (10⁻⁴⁴esu²cm²) of the **8** L-isoserine conformer.

	B3LY	P/aug-cc-p	VDZ	B3LYP/aug-cc-pVTZ			
	harmonic	anharm	Int	harmonic	anharm	Int	Rot. Str.
1	3732.8	3536.9	59.9	3729.1	3535.3	60.2	5.7
2	3689.9	3416.0	83.3	3688.0	3523.5	87.0	28.0
3	3598.8	3432.5	8.9	3601.2	3439.2	10.5	-0.8
4	3508.1	3358.9	2.2	3516.5	3374.7	2.8	-2.8
5	3099.4	2945.0	17.7	3085.7	2944.8	17.5	-9.3
6	3092.2	2939.0	15.5	3077.2	2938.8	14.6	31.5
7	3004.2	2863.6	47.8	2993.4	2794.5	46.4	-0.9
8	1809.8	1777.9	267.4	1813.6	1788.6	271.4	59.3
9	1639.3	1642.5	39.6	1654.4	1655.9	41.0	-30.4
10	1483.8	1459.7	7.3	1503.1	1371.7	6.9	-3.4
11	1428.5	1382.7	44.6	1436.5	1399.2	41.4	48.9
12	1394.3	1353.9	20.6	1408.7	1371.8	15.0	-50.0
13	1372.2	1323.9	36.4	1378.7	1327.1	39.8	-66.6
14	1326.2	1293.3	4.7	1338.8	1304.4	5.6	16.1
15	1288.4	1248.0	0.8	1294.7	1249.9	3.1	30.9
16	1243.7	1217.8	28.3	1254.2	1228.7	31.4	46.8
17	1175.0	1150.4	14.5	1178.9	1165.6	14.7	-45.0
18	1142.1	1102.0	125.7	1139.3	1104.5	104.4	-119.3
19	1118.5	1086.5	207.4	1113.3	1082.8	241.8	62.2
20	1065.8	1039.0	47.2	1062.4	1039.0	44.2	88.7
21	974.2	934.3	20.8	977.9	941.0	23.0	-38.5
22	917.2	886.4	12.5	913.2	890.1	10.2	-30.6
23	851.4	816.4	8.1	854.8	827.9	7.7	27.1
24	793.5	757.7	94.7	792.4	753.8	100.0	-41.7
25	753.3	716.2	25.1	755.7	715.0	28.0	-92.4
26	688.5	654.7	25.9	693.2	663.2	22.6	144.6
27	613.4	576.0	99.1	614.1	537.5	101.2	-99.4
28	556.9	523.8	57.2	559.0	532.6	57.1	10.6
29	500.5	386.4	97.4	503.6	413.1	97.0	-49.9
30	420.1	422.2	1.6	421.0	433.2	1.4	-4.7
31	315.7	305.5	5.4	317.0	313.0	5.1	12.9
32	274.2	246.3	11.2	275.2	251.0	10.5	38.4
33	255.6	242.0	4.7	260.1	266.2	3.6	9.1
34	192.6	173.5	2.2	194.2	193.8	2.2	12.3
35	113.9	82.7	8.9	114.5	127.5	8.8	5.1
36	37.0	-4.8	1.3	34.4	28.4	1.4	1.1

Table 12SI. The total energies (E, hartree), the total energies corrected for zero-point energies (E_0 , hartree), the Gibbs free energies in 298.15 K (G, hartree), relative total energies (ΔE , kcal/mol), and corresponding relative energies referred to the most stable conformer (kcal/mol) for the IEF-PCM/B3LYP/aug-cc-pVDZ optimized 54 stable structures of L-isoserine in water (Structures as in Fig 1SI).

Conformer						
number	E	ΔE	E ₀	ΔE_0	G	ΔG
1w	-399.051465	0.00	-398.938787	0.00	-398.969847	0.00
10w	-399.047376	2.57	-398.934647	2.60	-398.966078	2.37
2w	-399.046423	3.16	-398.933314	3.43	-398.965215	2.91
3w	-399.046172	3.32	-398.933311	3.44	-398.965185	2.93
5w	-399.042623	5.55	-398.930734	5.05	-398.963407	4.04
4 w	-399.042898	5.38	-398.930872	4.97	-398.963048	4.27
6 w	-399.042408	5.68	-398.930461	5.22	-398.963000	4.30
29w	-399.043137	5.23	-398.930720	5.06	-398.962948	4.33
23w	-399.042254	5.78	-398.930240	5.36	-398.962920	4.35
8 w	-399.042958	5.34	-398.930445	5.23	-398.962785	4.43
7w	-399.041935	5.98	-398.930044	5.49	-398.962703	4.48
21w	-399.042691	5.51	-398.930142	5.42	-398.962501	4.61
9w	-399.042071	5.90	-398.929449	5.86	-398.962030	4.91
27w	-399.040642	6.79	-398.928792	6.27	-398.961816	5.04
17w	-399.041849	6.03	-398.929224	6.00	-398.961776	5.06
11w	-399.040936	6.61	-398.928994	6.15	-398.961540	5.21
15w	-399.040075	7.15	-398.928073	6.72	-398.961239	5.40
33w	-399.041135	6.48	-398.928757	6.29	-398.961164	5.45
37w	-399.041391	6.32	-398.928887	6.21	-398.961098	5.49
24w	-399.039962	7.22	-398.928155	6.67	-398.961012	5.54
16w	-399.040371	6.96	-398.928280	6.59	-398.961000	5.55
13w	-399.039655	7.41	-398.927825	6.88	-398.960941	5.59
30w	-399.040508	6.88	-398.928390	6.52	-398.960790	5.68
18w	-399.039463	7.53	-398.927574	7.04	-398.960700	5.74
12w	-399.040185	7.08	-398.928178	6.66	-398.960672	5.76
32w	-399.040792	6.70	-398.928298	6.58	-398.960576	5.82
14w	-399.039981	7.21	-398.927952	6.80	-398.960545	5.84
20w	-399.039514	7.50	-398.927525	7.07	-398.960479	5.88
40 w	-399.041024	6.55	-398.928350	6.55	-398.960366	5.95
19 w	-399.039278	7.65	-398.927186	7.28	-398.960042	6.15
41w	-399.039312	7.63	-398.927291	7.21	-398.959960	6.20
26w	-399.038720	8.00	-398.926873	7.48	-398.959916	6.23
38w	-399.039759	7.35	-398.927346	7.18	-398.959743	6.34
49 w	-399.039612	7.44	-398.927469	7.10	-398.959693	6.37
46 w	-399.038804	7.94	-398.926933	7.44	-398.959541	6.47
31w	-399.038349	8.23	-398.926304	7.83	-398.959197	6.68
35w	-399.037801	8.57	-398.926003	8.02	-398.959168	6.70
25w	-399.038429	8.18	-398.926301	7.84	-398.959077	6.76
43w	-399.039019	7.81	-398.927014	7.39	-398.959044	6.78
34w	-399.038216	8.31	-398.926218	7.89	-398.959022	6.79
47w	-399.038694	8.01	-398.926571	7.67	-398.958915	6.86

-399.039002	7.82	-398.926589	7.65	-398.958881	6.88
-399.037403	8.82	-398.925525	8.32	-398.958860	6.89
-399.038008	8.44	-398.925956	8.05	-398.958807	6.93
-399.038509	8.13	-398.926504	7.71	-398.958797	6.93
-399.037692	8.64	-398.925699	8.21	-398.958771	6.95
-399.038133	8.37	-398.926178	7.91	-398.958557	7.08
-399.037874	8.53	-398.925706	8.21	-398.958412	7.18
-399.037506	8.76	-398.925446	8.37	-398.958216	7.30
-399.037111	9.01	-398.925118	8.58	-398.958055	7.40
-399.036598	9.33	-398.924606	8.90	-398.957774	7.58
-399.036758	9.23	-398.924839	8.75	-398.957700	7.62
-399.036232	9.56	-398.924376	9.04	-398.957029	8.04
-399.036921	9.13	-398.924765	8.80	-398.956826	8.17
	-399.039002 -399.037403 -399.038008 -399.038509 -399.037692 -399.037692 -399.037874 -399.037506 -399.037506 -399.036598 -399.036758 -399.036232 -399.036921	-399.0390027.82-399.0374038.82-399.0380088.44-399.0385098.13-399.0376928.64-399.0376928.64-399.0378748.53-399.0375068.76-399.0375068.76-399.0375068.76-399.0365989.33-399.0367589.23-399.0362329.56-399.0369219.13	-399.0390027.82-398.926589-399.0374038.82-398.925525-399.0380088.44-398.925956-399.0380098.13-398.926504-399.0376928.64-398.925699-399.0376928.64-398.925699-399.0378748.53-398.925706-399.0375068.76-398.925446-399.0371119.01-398.925118-399.0365989.33-398.924606-399.0367589.23-398.924839-399.0362329.56-398.924376-399.0369219.13-398.924765	-399.0390027.82-398.9265897.65-399.0374038.82-398.9255258.32-399.0380088.44-398.9259568.05-399.0380098.13-398.9265047.71-399.0376928.64-398.9256998.21-399.0376928.64-398.9261787.91-399.03776928.64-398.9257068.21-399.0376928.64-398.9251187.91-399.0376928.64-398.9251188.21-399.0376928.64-398.9251188.58-399.0375068.76-398.9254468.37-399.0375068.76-398.9254468.58-399.0365989.33-398.9246068.90-399.0367589.23-398.9248398.75-399.0362329.56-398.9243769.04-399.0369219.13-398.9247658.80	-399.0390027.82-398.9265897.65-398.958881-399.0374038.82-398.9255258.32-398.958860-399.0380088.44-398.9259568.05-398.958807-399.0385098.13-398.9265047.71-398.958771-399.0376928.64-398.9256998.21-398.958771-399.0381338.37-398.9261787.91-398.958557-399.0378748.53-398.9257068.21-398.958412-399.0375068.76-398.9254468.37-398.958216-399.0375068.76-398.9251188.58-398.958055-399.0365989.33-398.9246068.90-398.957774-399.0367589.23-398.9243769.04-398.957029-399.0362329.56-398.9247658.80-398.956826

Table 13SI. The selected dihedral angles (deg) for the B3LYP/aug-cc-pVDZ optimized 54 stable structures of L-isoserine in water (Fig 1SI). Atom numbering as in Scheme 1SI.

	(H12N7C3C2)	(H13N7C3C2)	(N7C3C2C1)	(05C1C2C3)	(H14O4C1C2)	(H8O6C2C1)
1w	81,3	-160,1	59,0	137,7	10,2	-14,8
10w	163,7	-77,6	-55,5	-146,9	-5,4	-65,0
2 w	-150,3	89,7	-84,2	-55,5	-0,7	100,9
3w	-83,8	156,5	-163,6	-69,6	2,4	147,2
5w	-63,0	54,1	-179,0	109,0	177,6	19,3
4 w	174,9	-68,5	-56,0	122,6	-179,2	-1,7
6w	67,7	-50,9	-61,3	119,6	-179,9	0,9
29w	-62,3	44,3	175,8	-65,7	2,5	-101,1
23w	66,5	-52,1	-63,9	-51,6	-0,6	-134,9
8 w	-151,1	89,0	76,1	103,1	177,4	87,8
7w	-177,1	66,7	177,7	114,5	179,1	12,8
21w	-84,8	156,0	-169,1	108,6	177,9	155,4
9w	-152,0	88,5	-80,1	-76,9	-178,0	91,0
27w	62,0	-55,4	69,3	-68,0	3,1	167,1
17w	-84,4	156,2	-171,6	-75,2	-178,0	155,1
11w	59,5	-58,8	74,1	112,2	177,8	9,0
15w	-62,7	54,6	173,6	-102,6	-178,9	-67,6
33w	62,3	-55,2	65,8	-66,7	3,1	-101,2
37w	-61,2	56,9	170,0	-48,8	-0,1	92,7
24w	-75,7	168,0	172,3	114,9	179,2	11,0
16w	-63,1	54,1	174,9	-77,9	-176,8	56,1
13w	67,2	-51,1	-64,1	-48,0	177,3	-48,5
30w	-67,7	175,3	72,6	-48,0	-1,8	-141,3
18w	-176,8	66,9	170,3	-47,8	177,1	-60,8
12w	-73,5	169,6	76,5	118,1	179,2	2,3
32w	54,1	-70,4	-68,5	-46,6	-1,2	93,2
14w	174,1	-69,2	-60,8	-57,7	177,6	-51,6
20w	-177,7	65,9	171,5	-73,7	-177,8	56,0
40w	-175,1	68,4	168,8	-46,0	-1,7	89,7
19w	73,6	-169,7	58,3	78,2	178,4	49,4
41w	67,6	-50,8	-62,0	110,9	178,1	-172,3
26w	59,5	-58,7	64,5	-80,3	-176,3	57,1
38w	-67,3	175,7	70,6	-46,9	-1,9	95,4 170.0
49w	1/6,4	-66,9	-56,1	119,2	180,0	-170,9
40W	-03,0	53,8 50,2	-1/9,5	103,8	-3,0	22,8
31W	00,1	-30,5	-09,9	-01,8	-179,4	-1/1,0
33W	-73,4	106,2	109,1	-60,4	-177,0	48.1
23W	02,5	-34,9	70,4 54.6	-41,0	177,5	-40,1
43W	74.8	-07,4	-34,0	119,9	-0,3	0,1 66.0
34W 47m	175.0	-100,5	54,9 _60 1	-111,3	179,0	_170.6
7/W 52m	-152.0	-07,3	-00,1	100.7	1/7,0 _/ /	-170,0
36w	-152,0	167 3	-75,0	-61 1	- - ,-	-60 0
20w	-73.0	170 /	71.2	-01,1	170,0	-00,9
<u>4</u> 4w	67.0	-51 Q	-61.8	112.8	_35	75
28w	_74 2	169.0	64 3	-86.6	-177 2	58 8
-0.0	, ,,	±07,0	01,0	00,0	± , , , , ,	20,0

45w	-177,4	66,3	177,0	107,7	-4,3	19,2
42w	75,0	-168,1	54,1	-115,7	179,6	-72,7
48 w	60,0	-57,8	66,9	-76,1	-177,0	-175,1
50w	74,3	-168,8	60,9	68,9	177,8	-173,4
39w	-77,0	166,1	69,2	-11,7	178,0	-165,9
52w	74,2	-168,9	57,7	-112,3	-179,7	169,4
54w	-76,0	167,5	177,5	110,0	-3,3	15,5
51w	56,6	-67,8	68,7	101,4	-6,0	20,7

Table 14SI. The B3LYP/aug-cc-pVDZ Cartesian coordinates for L-isoserine neutral (w) and zwitterionic (z) conformers in water.

1	10
IW	IUW
$C_{0,0,2093347972,-0.9467400877,0.3312098464}$	$C_{0,0,0,0}$ $C_{1,0,0}$ $C_$
0,0,0.9322110949,-1.5053134512,1.0987933107	0,0,1.116620597,1.4827045244,-1.2439079858
0,0,-0.3595609103,-1.5069709797,-0.727122333	0,0,-0.8/18530333,0.4/75304559,-1.3543159285
H,0,-0./845/40362,-0./50/6336/,-1.2/98416006	H,0,-1.34/65/5086,-0.261246/91/,-0.82240/0133
C,0,-0.1116968042,0.5331463885,0.5734383299	C,0,0.592/350/1/,-0.08152428/4,0.52563/551/
H,0,-1.1451939832,0.558811156,0.9677308664	H,0,1.683/405365,-0.1495628616,0.6342415855
C,0,-0.0648865221,1.3690070103,-0.7164471723	C,0,-0.0053348257,-1.4861854483,0.5591598049
H,0,0.9375609299,1.2998977776,-1.1564549715	H,0,0.2419302822,-1.94742387,1.5261833207
H,0,-0.2548437213,2.4206482337,-0.4614695083	H,0,0.461284048,-2.0853891433,-0.2326181016
0,0,0.7807273894,1.0739099282,1.5296690648	0,0,0.0201704837,0.6500265455,1.6210601014
H,0,1.2095801446,0.3129777252,1.9572460241	H,0,0.4790798768,1.496314813,1.7075051513
N,0,-1.0415323792,0.8195080673,-1.6814554603	N,0,-1.4608653941,-1.4319669459,0.3039881115
H,0,-1.9825764354,1.1525437805,-1.479851415	H,0,-1.8199784633,-2.350852936,0.0596264467
H,0,-0.8208011639,1.1168368182,-2.6281939812	H,0,-1.9599508619,-1.1269614127,1.1366431783
2w	3w
C,0,-0.5901446227,-0.0820548979,-1.0859137311	C,0,-0.5957145006,-1.0719595836,0.4291606882
O,0,-1.6186916344,0.4997034594,-1.3688771472	O,0,-1.7854673723,-1.2224365212,0.6237992769
O,0,0.3982318999,-0.2420373679,-1.9772493928	O,0,0.2102985661,-2.1085911002,0.1554391751
H,0,1.102556964,-0.7435763662,-1.5113350694	H,0,1.1148377357,-1.7425047494,0.0572770238
C,0,-0.3208383215,-0.7148650041,0.2873524725	C,0,0.0909128793,0.2868040625,0.4423270306
H,0,-1.0611430224,-1.5190212508,0.4017021723	H,0,-0.2053202478,0.8016628329,1.3699228163
C,0,-0.4743242452,0.2931928107,1.449569357	C,0,-0.3414268939,1.1256703945,-0.7851090896
H,0,-0.6453585939,-0.2782294011,2.3689275698	H,0,-1.3847583695,1.4462126431,-0.655293638
H,0,-1.3527497939,0.9279217195,1.2704248866	H,0,-0.2816306964,0.5011284989,-1.6859011662
O,0,0.9843318494,-1.2848606638,0.313203373	O,0,1.5010462305,0.0914334308,0.4129694918
H,0,1.5146066167,-0.6107318713,0.797520932	H,0,1.8351940378,0.861797307,-0.094727677
N,0,0.787388423,1.0303739045,1.5978435568	N,0,0.6213841248,2.2222011907,-0.9317736205
H,0,0.8067544557,1.8716734108,1.0266866173	H,0,0.6401024095,2.5675069083,-1.8865105152
H,0,0.9336300254,1.3180125181,2.5601444031	H,0,0.3850410969,3.0083246857,-0.3303297959
5w	4w
C 0 -1 1387972429 -0 1287177882 -0 4132776768	C 0 -0 9075519831 -0 2849986434 -0 3108290511
0.01.69518036021.21138885630.3839362686	0.01.6925235419.0.57789781940.659290394
0.0 - 1.4521421798 0.850153913 - 1.2760670449	0.0 -1 2679521804 -1 4128353304 0 3167427515
H.02.1686289313.0.53821235911.8558976201	H.02.2322362481.4031967506.0.4444648422
C.0.0.0140635223.0.2398157226.0.502097186	C.0.0.58864814940.2051426640.5796886255
H.00.1931343576.1.225182799.0.9455142227	H.0.0.85224612791.06617912861.2166449477
C.0.1.3414199336.0.31906738510.2964596927	C.0.1.4133719316 -0.2828601678.0.708851765
H.0.1.234927697.1.07081790361.0892214517	H.0.2.475991479-0.2281410134.0.4163077766
H.0.1.5136717460.65574988860.7757784053	H.0.1.24708370081.2619255738.1.1748466799
0.0.0.109519236 -0.7076808062 1.556157313	0.0.87283853051.0022902769 - 1.275238621
H.00.36768579711.5026417322.1.2675898423	H.0.0.0235762572.1.4506271281.4219844442
N.0.2.5071198343.0.6476635633.0.5178112452	N.0.0.9982858601.0.7672580016.1.6442875766
H.0.2.4065027115.1.5752198936.0.9271548343	H.0.1.4883248035.0.6592158344.2.5289125773
H 0 2 5793431882 -0 0052044678 1 2960645164	H 0 1 2671471134 1 6784902118 1 2782611143
6w	20xv/
	27 W C 0 0 5567280867 0 5480221854 1 0162718252
$0.0 \pm 1.2722305841 \pm 1.125608274.0.7042487012$	0.0.08510521472.0027100055.20725712122
0,0,-1.5752595641,-1.125006574,0.7042467912 0,0,17328444032,06207703245,0660366610	0,0,-0.8519521475,0.027199955,2.0755712122 0,0,0,5214100602,1,881786207,0,8766544402
$U_{0,2} = 558676228 \ 0.1402050775 \ 0.8502200019$	$U_{0} = 0.0276485205620611212825 = 0.0550211586$
C = 0.0.2001065201 = 0.6067202440 = 0.5704220581	C = 0.01652578161 = 0.2476725187 = 0.2212541415
H 0 0 05528181/8 1 607117/552 0 0751200012	$C_{,0,-0,10,33,70101,-0,2470733107,-0,2313341413}$ H 0 _0 9652360088 _0 9751381752 _0 λ 256000 λ 7 λ
$\begin{array}{c} 11,0,0.0000001140,1.00711740000,0007010000000000000000000000$	$\begin{array}{c} 11,0,-0.7052500000,-0.7751501752,-0.4250909474\\ C \cap 1 1630250405 \cap 0.0050272440 \cap 0.072054092 \end{array}$
H 0 2 12016/572/ 1 212026250 0 275020040	H 0 1 0620605071 1 5001254647 0 0220247410
$H \cap O = 7335074008 + 4552023856 + 2660281072$	H 0 1 0515861888 0 24707020646 0 1707820252
$\begin{array}{c} 11,0,0,1535774000,1.4552025050,-1.5009201072\\ 0,0,0,0508186664,-0,151644676,1,5827276221 \end{array}$	$ \begin{array}{c} 11, 0, 1.7515001000, -0.2472220040, 0.1757020255 \\ 0, 0, 0, 0, 0007764772, 0, 6307667353, 1, 2766829016 \end{array} $
0,0,0.7570100004,-0.151044070,1.5027570551	0,0,00007704472,0.037700233,-1.3400626910

H,0,0.3991266389,-0.9209287521,1.7750914921	H,0,-0.7825755264,0.6064909132,-1.9105103604
N,0,1.6527329644,-0.428237626,-1.3205708389	N,0,1.5798501379,-1.8636607676,-1.0883269688
H,0,2.0317156597,-1.0901672631,-0.6460762994	H,0,0.896833153,-2.6043036946,-1.2386490288
H,0,0.8715747953,-0.8895769816,-1.7826830533	H,0,1.6300653767,-1.3334768481,-1.9561142462
1z	2z
C,0,2.8691863995,-0.1382334424,0.0475492037	C,0,-2.3014851921,0.7840427797,-0.2460927684
O,0,3.6005940784,-1.1074785975,-0.2500104281	O,0,-1.8773947192,1.5746608345,0.6544756639
O,0,3.207212122,1.0884568873,0.1297975408	O,0,-3.3685670836,0.8712308525,-0.8947932616
H,0,1.8177144,1.892277381,0.0779010997	C,0,-1.4295670555,-0.4640178407,-0.5846511831
C,0,1.3848047102,-0.4688789879,0.3578092251	H,0,-0.9201997373,-0.2515185294,-1.5406616372
H,0,1.2396879992,-0.3346339189,1.4448266361	O,0,-2.2807240277,-1.603689537,-0.7328406461
O,0,1.0932561868,-1.806623528,-0.0026557555	H,0,-3.1220166385,-1.2378285615,-1.0555297765
H,0,1.9716088694,-2.1716983637,-0.2327753791	N,0,-0.8315385785,-0.5322673339,1.8290076947
N,0,0.7443788225,1.883300047,-0.0036844279	H,0,-0.0847691571,-0.5891697685,2.522790097
H,0,0.4147946919,2.5584797903,-0.6940632059	H,0,-1.2356094329,0.4412495922,1.7803833903
H,0,0.3366874151,2.1378002111,0.8979303574	H,0,-1.5634584178,-1.1920212644,2.0997662763
C,0,0.426169484,0.4681540419,-0.3906562281	C,0,-0.3390569719,-0.7809124097,0.4328033289
H,0,0.5761203207,0.3810636041,-1.4715442764	H,0,0.5202284586,-0.1207629236,0.2886946258
H,0,-0.6184138298,0.2498162758,-0.1502142719	H,0,-0.0153864367,-1.8225720203,0.349400146
3z	4z
C,0,1.8233728163,-1.239746466,0.0430128649	C,0,2.8789563907,-0.1926739796,0.0399143303
O,0,1.799457923,-1.9148704166,-1.0124821448	O,0,3.1829766921,1.0582534522,0.0757400161
O,0,1.7711734132,-1.6404442464,1.2407237862	O,0,3.6646802315,-1.1273873723,-0.1718316812
C,0,1.920338918,0.3052548964,-0.1077113021	C,0,1.3817201133,-0.4902151171,0.3360872319
H,0,2.8420547412,0.5500635572,-0.658815723	H,0,1.248158835,-0.3454327289,1.4221171581
H,0,0.8453695692,2.5867771956,0.233887577	O,0,1.0628871126,-1.8271232978,-0.0242918177
N,0,0.6961500869,2.3391582285,-0.7525221593	H,0,0.2163283986,-2.0617888172,0.378510049
H,0,1.4453940892,2.7731630043,-1.2986739469	N,0,0.7970127646,1.8877694683,-0.0595796698
H,0,-0.1890346021,2.7462364481,-1.0631108866	H,0,1.8919129862,1.8341303572,0.0231246105
O,0,1.9617840774,0.9192951127,1.1767629751	H,0,0.3939446162,2.1718884082,0.8345282947
H,0,1.8613332311,0.1452732197,1.7757824416	H,0,0.4919595754,2.5565474324,-0.7666270435
C,0,0.7067427383,0.8370115862,-0.8677070432	C,0,0.4451885016,0.4765812373,-0.4172271266
H,0,0.7272557735,0.5740000531,-1.9277149067	H,0,0.5863682928,0.3645148983,-1.4972182361
H,0,-0.2260081951,0.4896940672,-0.4118059822	H,0,-0.6040923207,0.285453239,-0.1705406057
5z	
C,0,-1.7759178358,1.0436810471,-0.3477611081	
O,0,-2.3575345911,1.1510539135,0.7912510636	
O,0,-1.4046042645,1.9668068494,-1.0945890386	
C,0,-1.5241693118,-0.4280487461,-0.7686907114	
H,0,-1.1040199381,-0.4670382732,-1.7796265084	
0,0,-2.7555931135,-1.1667498027,-0.7717835831	
H,0,-3.370180628,-0.7011163578,-0.1846943133	
N,0,-1.1099503839,-1.0422688598,1.5862393973	
H,0,-0.3918345841,-1.0720462513,2.3104617913	
H,0,-1.6659296812,-0.1363574558,1.6330744547	
H,0,-1.7509084989,-1.8206125006,1.7487294362	
C,0,-0.5316790576,-1.0884253941,0.1963924011	
H,0,0.418249574,-0.5442305552,0.2122427674	
H,0,-0.3495504256,-2.1333764535,-0.0709982688	

Table 15SI. The total energies (E, hartree), the total energies corrected for zero-point energies (E_0 , hartree), the Gibbs free energies in 298.15 K (G, hartree), relative total energies (ΔE , kcal/mol), and corresponding relative energies referred to the most stable conformer (kcal/mol) for the zwitterion structures of L-isoserine in water. (Structures as in Fig in the Manuscript).

Conformer number	Е	ΔΕ	E ₀	ΔE_0	G	ΔG				
	B3LYP/aug-cc-pVDZ									
1z	-399.051051	0.00	-398.937216	0.00	-398.968350	0.00				
2z	-399.045750	3.33	-398.931723	3.45	-398.964079	2.68				
3z	-399.044176	4.31	-398.929574	4.80	-398.961633	4.21				
4z	-399.043488	4.75	-398.930697	4.09	-398.962227	3.84				
5z	-399.043212	4.92	-398.929278	4.98	-398.961069	4.57				
			B3LYP/aug-	cc-pVTZ						
1z	-399.151468	0.00	-399.037205	0.00	-399.068305	0.00				
2z	-399.146239	3.28	-399.031896	3.33	-399.064210	2.57				
3z	-399.144826	4.17	-399.029912	4.58	-399.061954	3.99				
4z	-399.143696	4.88	-399.030510	4.20	-399.062057	3.92				
5z	-399.143650	4.91	-399.029281	4.97	-399.061055	4.55				
			MP2/aug-co	e-pVDZ						
1z	-398.012847	0.00	-397.898127	0.00	-397.929325	0.00				
2z	-398.008851	2.51	-397.893482	2.91	-397.925347	2.50				
3z	-398.006721	3.84	-397.891289	4.29	-397.923330	3.76				
4z	-398.004984	4.93	-397.890943	4.51	-397.922340	4.38				
5z	-398.007193	3.55	-397.892114	3.77	-397.923934	3.38				



Scheme 2SI

Table 16SI. The selected dihedral angles (deg) and N-H bond length (Å) for the B3LYP/augcc-pVDZ optimized 5 stable zwitterions structures of L-isoserine in water. Atom numbering as in Scheme 2SI.

	(H12N7C3C2)	(H13N7C3C2)	(H14N7C3C2)	(N7C3C2C1)	(O4C1C2C3)	(H8O6C2C1)	H14-N
1z	-80.2	158.3	37.5	-57.8	48.2	7.7	1.076
2z	-170.8	67.4	-50.5	38.3	14.3	29.8	1.055
3z	70.9	-167.7	-47.7	168.8	61.2	-3.2	1.029
4 z	-80.8	157.3	61.6	-56.4	166.4	165.0	1.099
5z	-154.8	83.9	-33.4	59.6	-65.1	-22.6	1.064

Table 17SI. The B3LYP/aug-cc-pVTZ and MP2/aug-cc-pVDZ relative energies (kcal/mol) referred to the most stable **1w** of L-isoserine conformer in water. The populations X(G) were calculated based on ΔG MP2/aug-cc-pVDZ values separately for the structures of each type.

	B3LYP/aug-cc-pVTZ				MP2/aug-cc-pVDZ			
	ΔE^{1w}	ΔE_0^{1w}	ΔG^{1w}	X(G)	ΔE^{1w}	ΔE_0^{1w}	ΔG^{1w}	X(G)
1w	0.00	0.00	0.00	83.4	0.00	0.00	0.00	56.7
10w	2.76	2.72	2.44	1.4	2.07	2.13	1.94	2.2
2w	2.97	3.23	2.70	0.9	2.71	3.04	2.55	0.8
3w	3.10	3.21	2.72	0.8	3.17	3.39	2.96	0.4
5w	5.16	4.70	3.80	0.1	5.35	5.01	4.14	0.1
4 w	5.05	4.66	4.01	0.1	4.47	4.18	3.62	0.1
6w	5.24	4.84	4.02	0.1	5.04	4.66	3.73	0.1
29w	4.83	4.65	3.91	0.1	5.03	5.02	4.39	0.0
1z	0.25	1.13	1.11	12.8	-0.70	0.27	0.22	38.9
2z	3.53	4.47	3.68	0.0	1.81	3.19	2.72	0.6
3z	4.42	5.71	5.09	0.2	3.15	4.57	3.99	0.1
4z	5.13	5.34	5.03	0.0	4.24	4.78	4.61	0.0
5z	5.16	6.11	5.66	0.0	2.85	4.05	3.61	0.1

X-ray Measurements

Experimental

The crystals of L-isoserine suitable for X-ray diffraction were obtained by slow evaporation from ethanol, methanol or from water. To dissolve the compound in the former cases some drops of water were added to pure solvents, otherwise large amount of L-isoserine suspended in the solution. In all cases the crystals had the same structure, as confirmed by the X-ray diffraction on single crystal. For this paper we used a single crystal from methanol. The measurement was performed at 100 (2) K on a KUMA CCD k-axis diffractometer with graphite-monochromated Mo Kα radiation (0.71073 Å). The crystal was positioned at 62.25 mm from the KM4CCD camera; 1200 frames were measured at 1° intervals on a counting time of 10s. Data reduction and analysis were carried out with the Kuma Diffraction programs. The data were corrected for Lorentz and polarization effects and multi-scan absorption correction 1 was applied. The structure was solved by direct methods 2 and refined by using SHELXL.³ The refinement was based on F^2 for all reflections except for those with very negative F^2 . The weighted R factor, wR and all goodness-of-fit S values are based on F^2 . The non-hydrogen atoms were refined anisotropically. The hydrogen atoms, except at carbons, were located from a difference maps and their positions refined isotropically. The other hydrogen atoms were placed in calculated positions and refined within riding model. The atomic scattering factors were taken from the International Tables.⁴

Details of crystal data and structure refinement, atomic coordinates and equivalent isotropic displacement parameters, anisotropic displacement parameters, hydrogen coordinates and isotropic displacement parameters are presented in Tables 18-21SI.

Crystal data for L-isoserine: C₃H₇NO₃; Mr=105.10, T=100(2)K, orthorhombic, space group P2₁2₁2, a=9.9244(12)Å, b=10.3690(15)Å, c=4.0380(6)Å, V=415.53(10)Å³, Z=4, d=1.680 gcm⁻³, μ =0.150 mm⁻¹, F(000)=224, 20 range 2.84° to 28.59°, 7815 reflections collected, 648 unique R_{int} = 0.0168 which were used in all calculations, GOF=1.093. The final R₁ and wR₂ (F²) were 0.0235, 0.0625 (all data), 0.0229 and 0.0622 (I>2 σ (I)), extinction coefficient: 0.081(12). Largest diff. peak and hole: 0.363 and -0.150 eÅ⁻³. Crystallographic data have been deposited at the Cambridge Crystallographic Data Centre with the deposition number CCDC 770483 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

References

- 1 CrysAlis RED, Oxford Diffraction Ltd., Version 1.171.28cycle4 beta (release 11-11-2005 CrysAlis171 .NET) (compiled Nov 11 2005,15:50:43). Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
- 2 Sheldrick G. M. Acta Cryst. 1990, A46, 467-473.
- 3 Sheldrick G. M., SHELXL93. *Program for the Refinement of Crystal Structures.*, University of Göttingen, Germany.
- 4 *International Tables for Crystallography*, Ed. A. J. C. Wilson, Kluwer:Dordrecht, 1992, Vol.C.

Table 18SI. Crystal data and structure refinement for L-isoserine

Empirical formula	C ₃ H ₇ NO ₃
Formula weight (M)	105.10
Temperature (K)	100(2)
Wavelength (Å)	0.71073
Crystal system	Orthorhombic
Space group	P2 ₁ 2 ₁ 2
Unit cell dimensions	
	a = 9.9244(12) Å
	b = 10.3690(15) Å
	c = 4.0380(6) Å
Volume	415.53(10) Å ³
Z	4
Calculated density	1.680 Mg/m ³
Absorption coefficient	0.150 mm ⁻¹
F(000)	224
Crystal size	0.25 x 0.0.2 x 0.2 mm
Theta range for data collection	2.84° to 28.59°
Limiting indices	$\text{-13} \leq h \leq 13, \text{-13} \leq k \leq 13, \text{-5} \leq l \leq 5$
Reflections collected / unique	7815 / 648 R(int) = 0.0168
Completeness to theta = 28.59°	98.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.03390 and 0.96734
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	648 / 0 / 81
Goodness-of-fit on F ²	1.093
Final R indices I>2sigma(I)	$R_1 = 0.0229, wR_2 = 0.0622$
R indices (all data)	$R_1 = 0.0235, wR_2 = 0.0625$
Extinction coefficient	0.081(12)
Largest diff. peak and hole	0.363 and -0.150 e Å ⁻³

Table 19SI. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters $(\text{\AA}^2 \text{ x } 10^3)$ for L-isoserine. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	Х	Y	Z	U(eq)
C1	9525(1)	2488(1)	4350(3)	9(1)
O4	10165(1)	1685(1)	6051(2)	13(1)
05	9910(1)	3598(1)	3515(2)	12(1)
C2	8094(1)	2063(1)	3404(3)	8(1)
O6	7469(1)	2925(1)	1164(2)	10(1)
C3	8100(1)	702(1)	2002(3)	9(1)
N7	6680(1)	300(1)	1282(3)	10(1)

Table 20SI. Anisotropic displacement parameters ($\text{Å}^2 \ge 10^3$) for L-isoserine. The anisotropic displacement factor exponent takes the form: 2 pi² h² a*2U11+2hka*b*U12

	U11	U22	U33	U23	U13	U12
C1	8(1)	10(1)	8(1)	-2(1)	1(1)	0(1)
O4	11(1)	12(1)	16(1)	3(1)	-3(1)	-1(1)
O5	11(1)	9(1)	15(1)	0(1)	0(1)	-2(1)
C2	8(1)	7(1)	9(1)	1(1)	0(1)	0(1)
O6	8(1)	10(1)	11(1)	2(1)	0(1)	2(1)
C3	7(1)	9(1)	13(1)	-1(1)	-1(1)	-1(1)
N7	9(1)	10(1)	11(1)	-1(1)	-1(1)	-2(1)

Table 21SI. Hydrogen coordinates ($x \ 10^4$) and isotropic displacement parameters (Å² x 10^3) for L-isoserine

	Х	У	Z	U(eq)
H8	6640(20)	3110(20)	2070(60)	35(6)
Н9	7541	2052	5475	10
H10	8642	676	-56	11
H11	8511	101	3620	11
H12	6130(20)	338(19)	3100(60)	26(5)
H13	6600(20)	-520(20)	390(60)	28(6)
H14	6240(20)	851(19)	-320(50)	23(5)