

Supplementary Material for
Infrared Multiple Photon Dissociation Action Spectroscopy of Protonated Glycine,
Histidine, Lysine, and Arginine Complexed with 18-Crown-6 Ether

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Table S1. Relative energies at 0 K (Gibbs energies at 298 K) in kJ/mol of the (Gly)H⁺(18C6) complexes.^a

| (Gly)H ⁺ (18C6) | B3LYP | B3P86 | M06 | MP2(full) |
|---|------------------|---------------------|------------------|------------------|
| H ⁺ G[N]-tt(-00/+00/-00/+00/-00/+00) | 0.0 (0.0) | 0.01 (0.0) | 0.0 (0.0) | 0.0 (0.0) |
| H ⁺ G[N]-tt(+0+/-00/-00/+00/-0/-00) | 0.8 (3.2) | 0.0 (2.4) | 6.4 (8.9) | 1.5 (4.0) |
| H ⁺ G[N]-tt(+00/-00/+00/-00/+00/-00) | 2.7 (3.2) | 2.3 (2.8) | 6.5 (7.0) | 3.4 (3.9) |
| H ⁺ G[N]-tt(+0+/-00/-00/+0+/-00/-00) | 6.9 (6.7) | 6.7 (6.5) | 12.6 (12.4) | 8.6 (8.4) |
| H ⁺ G[N]-tt(+0+/-00/-00/+0+/-00/-00) | 7.4 (8.0) | 7.1 (7.8) | 13.3 (13.9) | 9.0 (9.6) |
| H ⁺ G[N]-tt(++0/+00/--0/-00/+0+/-0+) | 13.3 (15.4) | 11.7 (13.9) | 18.7 (20.9) | 13.7 (15.8) |
| H ⁺ G[N]-tt(+00/-00/+00/--0/-00/+0+) | 8.5 (5.4) | 8.4 (5.3) | 16.2 (13.1) | 13.7 (10.6) |
| H ⁺ G[N]-tt(+00/-00/+00/--0/-00/+0+) | 8.9 (7.0) | 8.9 (7.0) | 16.7 (14.8) | 14.3 (12.4) |
| H ⁺ G[N]-tt(--0/-00/+00/-00/+0+/-00) | 11.7 (10.5) | 11.9 (10.7) | 20.3 (19.1) | 16.1 (14.9) |
| H ⁺ G[N]-tt(+00/-00/+00/--0/+00/+0+) | 11.0 (10.6) | 11.1 (10.7) | 20.4 (19.9) | 16.5 (16.0) |
| H ⁺ G[N]-tt(--0/-00/+00/-00/+0+/-00) | 12.1 (11.9) | 12.3 (12.1) | 20.7 (20.5) | 16.5 (16.2) |
| H ⁺ G[N]-tt(+00/--0/-00/-00/+00/-00) | 12.9 (11.6) | 13.0 (11.7) | 20.4 (19.1) | 16.6 (15.3) |
| H ⁺ G[N]-tt(+00/--0/--0/-00/+00/-00) | 13.0 (11.7) | 13.1 (11.8) | 20.4 (19.1) | 16.6 (15.4) |
| H ⁺ G[N]-tt(+0+/-00/+00/-00/+00/-00) | 17.3 (18.2) | 16.1 (17.0) | 22.0 (22.9) | 16.8 (17.7) |
| H ⁺ G[N]-tc(-00/+00/-00/+00/-00/+00) | 16.6 (14.2) | 17.4 (15.0) | 18.2 (15.8) | 16.9 (14.5) |
| H ⁺ G[N]-tt(+00/-00/+0+/-00/+00/-00) | 16.1 (18.0) | 16.0 (17.9) | 22.6 (24.5) | 17.5 (19.4) |
| H ⁺ G[N]-tt(+0+/-00/--0/-00/+00/-00) | 14.7 (14.1) | 14.6 (14.0) | 20.5 (19.9) | 17.6 (17.0) |
| H ⁺ G[N]-tt(+00/-00/+0+/-00/+00/-00) | 17.4 (19.3) | 16.1 (18.0) | 22.9 (24.8) | 17.9 (19.8) |
| H ⁺ G[N]-tc(+0+/-00/-00/+00/--0/-00) | 17.2 (17.7) | 17.2 (17.7) | 23.8 (24.3) | 18.6 (19.1) |
| H ⁺ G[N]-tt(-00/+00/--0/-0/-00/-00) | 16.8 (16.0) | 16.0 (15.3) | 23.8 (23.0) | 18.8 (18.0) |
| H ⁺ G[N]-tt(--0/-00/+00/-00/+00/-00) | 19.1 (17.2) | 18.4 (16.5) | 23.9 (22.0) | 19.4 (17.5) |
| H ⁺ G[N]-tt(+00/-00/+00/-0/-00/-00) | 21.2 (21.9) | 20.2 (20.9) | 22.1 (22.8) | 20.8 (21.5) |
| H ⁺ G[N]-tt(-00/+0+/-00/-00/-00/-00) | 18.6 (17.4) | 18.4 (17.2) | 25.7 (24.5) | 21.2 (20.0) |
| H ⁺ G[N]-tt(--0/-00/+00/-00/+0+/-00) | 17.0 (14.7) | 17.5 (15.1) | 25.4 (23.1) | 21.7 (19.3) |
| H ⁺ G[N]-tt(-00/+00/--0/--0/-00/-00) | 19.5 (16.0) | 18.9 (15.4) | 26.5 (23.1) | 22.4 (18.9) |
| H ⁺ G[N]-tt(-00/+0+/-0+/-00/--0/--0) | 15.8 (11.4) | 16.4 (12.1) | 27.1 (22.7) | 22.5 (18.2) |
| H ⁺ G[N]-tt(+00/+00/--0/-00/+0+/-0+) | 22.1 (21.3) | 21.3 (20.5) | 28.2 (27.4) | 22.6 (21.8) |
| H ⁺ G[N]-tt(-0/-00/+0+/-00/+00/--0) | 22.7 (23.8) | 21.8 (22.9) | 29.5 (30.6) | 24.1 (25.2) |
| H ⁺ G[N]-tt(-0/-00/+0+/-00/--0/--0) | 21.7 (21.0) | 21.3 (20.6) | 29.6 (28.9) | 24.9 (24.2) |
| H ⁺ G[N]-tt(-00/+00/--+/-00/-00/-00) | 21.6 (20.3) | 21.0 (19.7) | 29.8 (28.6) | 25.1 (23.9) |
| H ⁺ G[N]-tt(+0+/-00/--0/-00/-00/-00) | 26.4 (24.9) | 25.6 (24.0) | 30.4 (28.9) | 27.1 (25.5) |
| H ⁺ G[N]-tt(--0/-00/--0/-00/+00/-00) | 23.9 (21.2) | 23.9 (21.2) | 31.2 (28.5) | 27.6 (24.9) |
| H ⁺ G[N]-tt(-00/+0+/-0+/-00/+00/--0) | 25.6 (23.1) | 25.1 (22.6) | 32.3 (29.8) | 28.3 (25.7) |

^a Gibbs energies in parentheses. **Ground conformations in bold.** All values calculated at the level of theory indicated using the 6-311+G(2d,2p) basis set with conformations, zero-point energies, and thermal energies calculated at B3LYP/6-311+G(d,p) level of theory.

Table S2. Relative energies at 0 K (Gibbs energies at 298 K) in kJ/mol of the (His)H⁺(18C6) complexes.^a

| (His)H ⁺ (18C6) | B3LYP | B3P86 | M06 | MP2(full) |
|--|------------------|------------------|------------------|--------------------|
| H ⁺ H[N _α]-cggc(-00/+00/--0/-00/+00/--0) | 0.0 (0.0) | 0.0 (0.0) | 0.4 (2.4) | 0.0 (0.6) |
| H ⁺ H[N _α]-cggc(--0/-00/+0+/-00/-00/+00) | 2.5 (4.3) | 2.2 (3.9) | 2.9 (6.6) | 2.8 (5.1) |
| H ⁺ H[N _α]-cggc(-00/+00/-00/+00/-00/+00) | 4.1 (2.0) | 4.0 (1.9) | 0.0 (0.0) | 1.5 (0.0) |
| H ⁺ H[N _α]-cggc(+00/-00/+00/--0/-00/+0+) | 5.5 (2.9) | 6.2 (3.7) | 7.5 (7.0) | 8.4 (6.4) |
| H ⁺ H[N _α]-cggc(+0+/-00/-00/+0+/-00/-00) | 5.5 (3.4) | 5.4 (3.2) | 4.3 (4.2) | 6.6 (5.0) |
| H ⁺ H[N _α]-cggc(+00/-00/+0+/-00/-00/+0+) | 5.6 (4.6) | 5.9 (4.9) | 6.1 (7.2) | 7.2 (6.8) |
| H ⁺ H[N _α]-cggc(+00/-00/+00/--0/-00/+0+) | 5.7 (1.9) | 5.8 (2.0) | 5.5 (3.7) | 9.0 (5.8) |
| H ⁺ H[N _α]-cggc(+00/-00/+00/-00/+00/-00) | 7.0 (7.1) | 6.7 (6.7) | 7.5 (9.6) | 8.8 (9.4) |
| H ⁺ H[N _α]-cggc(-0/-00/-00/-00/-00/--0) | 7.8 (9.1) | 6.5 (7.8) | 3.7 (7.0) | 3.4 (5.3) |
| H ⁺ H[N _α]-cggc(-00/+00/-00/+00/+00/--0) | 8.1 (6.5) | 8.5 (6.9) | 6.7 (7.1) | 7.6 (6.5) |
| H ⁺ H[N _α]-cggc(-00/+00/--0/-00/+00/--0) | 8.6 (6.9) | 8.1 (6.4) | 9.4 (9.7) | 10.6 (9.5) |
| H ⁺ H[N _α]-cggc(+00/+00/+00/+00/-00/+00) | 8.8 (8.5) | 8.4 (8.1) | 5.5 (7.2) | 6.7 (7.0) |
| H ⁺ H[N _α]-cggc(++0/+00/-00/+00/-00/+0+) | 9.7 (9.6) | 8.5 (8.4) | 4.9 (6.9) | 6.9 (7.4) |
| H ⁺ H[N _α]-cggc(+00/--0/-00/+00/-00/+0+) | 9.9 (7.2) | 10.8 (8.1) | 11.1 (10.4) | 13.9 (11.7) |
| H ⁺ H[N _α]-cggc(++0/+00/-+0/-00/+0+/-+0+) | 10.3 (11.0) | 9.1 (9.8) | 10.8 (13.5) | 9.7 (11.0) |
| H ⁺ H[N _α]-cggc(--0/--0/-00/+00/-00/+00) | 10.9 (8.0) | 11.4 (8.5) | 12.7 (11.8) | 13.1 (10.8) |
| H ⁺ H[N _α]-cggc(--0/-00/-00/--0/-0/--0) | 11.4 (11.0) | 10.7 (10.3) | 12.9 (14.5) | 11.8 (12.0) |
| H ⁺ H[N _α]-cggc(-00/+00/--0/--0/-00/--0) | 11.4 (9.9) | 11.6 (10.1) | 12.4 (12.9) | 12.2 (11.3) |
| H ⁺ H[N _α]-cggc(++0/+0+/-+00/-0/-00/+0+) | 11.8 (9.9) | 11.5 (9.6) | 13.0 (13.2) | 14.9 (13.6) |
| H ⁺ H[N _α]-cggc(++0/+0+/-+00/-0/-00/+0+) | 11.9 (10.6) | 11.7 (10.4) | 12.7 (13.5) | 14.9 (14.2) |
| H ⁺ H[N _α]-cggc(++0/+0+/-+00/-0/-00/+0+) | 11.9 (10.7) | 11.7 (10.4) | 12.7 (13.5) | 14.8 (14.2) |
| H ⁺ H[N _α]-cggc(++0/+00/--0/-00/+00/--+) | 12.6 (12.2) | 11.9 (11.5) | 12.2 (13.8) | 11.8 (12.0) |
| H ⁺ H[N _α]-cggc(+00/-+0/-00/--0/-00/-0+) | 12.8 (8.5) | 13.5 (9.2) | 14.8 (12.5) | 15.4 (11.6) |
| H ⁺ H[N _α]-cggc(--0/-00/+0+/-+00/-0/--0) | 13.1 (14.2) | 11.9 (13.0) | 13.5 (16.7) | 13.1 (14.8) |
| H ⁺ H[N _α]-cggc(++0/0+0/+00/-00/+0+/-+00) | 13.1 (12.7) | 12.6 (12.2) | 14.6 (16.2) | 15.1 (15.2) |
| H ⁺ H[N _α]-cggc(+0+/-+00/-00/+00/-00/+00) | 13.2 (7.1) | 13.7 (7.7) | 13.9 (9.8) | 15.1 (9.6) |
| H ⁺ H[N _α]-cggc(+0+/-+00/-00/+0+/-+00/+00) | 13.2 (11.7) | 12.2 (10.7) | 13.8 (14.3) | 13.9 (12.9) |
| H ⁺ H[N _α]-cggc(+0+/-+00/-0+/-+00/-00/+0+) | 13.5 (11.5) | 13.8 (11.9) | 16.3 (16.4) | 16.5 (15.1) |
| H ⁺ H[N _α]-cggc(-0/--0/-00/+00/-00/+00) | 13.6 (12.7) | 12.7 (11.8) | 9.5 (10.7) | 12.1 (11.8) |
| H ⁺ H[N _α]-cggc(++0/+00/--0/--0/-00/+0+) | 14.4 (12.1) | 14.0 (11.7) | 16.3 (16.0) | 16.7 (14.9) |
| H ⁺ H[N _α]-cggc(+0+/-+00/+00/-0/-00/+00) | 14.9 (13.1) | 14.8 (13.1) | 14.9 (15.1) | 14.9 (13.7) |
| H ⁺ H[N _α]-cggc(-0/-00/+0+/-+00/-0/--0) | 15.4 (15.6) | 14.6 (14.8) | 15.5 (17.7) | 15.4 (16.2) |
| H ⁺ H[N _α]-cggc(-0/-00/+0+/-+00/+00/--0) | 15.5 (15.4) | 14.6 (14.5) | 14.3 (16.2) | 13.5 (14.0) |
| H ⁺ H[N _π]-tgg.g.(+00/-00/+0+/-+00/-00/+0+) | 18.6 (11.0) | 26.0 (18.5) | 27.5 (22.0) | 36.2 (29.1) |
| H ⁺ H[N _π]-tgtg(+00/-00/+0+/-+00/-00/+0+) | 19.9 (9.4) | 28.1 (17.6) | 36.7 (28.2) | 48.3 (38.3) |
| H ⁺ H[N _π]-tgg.g.(-00/-00/-00/-00/+00/--0) | 23.2 (15.3) | 29.8 (21.8) | 25.2 (19.2) | 34.7 (27.2) |
| H ⁺ H[N _π]-tgtg(+00/-00/+00/--0/-00/+0+) | 23.5 (14.2) | 31.2 (21.9) | 38.6 (31.3) | 50.1 (41.4) |
| H ⁺ H[N _π]-tgg.g(+00/-00/+0+/-+00/-00/+0+) | 26.7 (27.0) | 32.3 (32.6) | 30.0 (32.3) | 33.1 (33.9) |
| H ⁺ H[N _π]-tgg.g.(-00/+00/--0/-00/+00/--0) | 25.5 (21.4) | 32.8 (28.7) | 29.0 (26.9) | 35.3 (31.8) |

^a Gibbs energies in parentheses. **Ground conformations in bold.** All values calculated at the level of theory indicated using the 6-311+G(2d,2p) basis set with conformations, zero-point energies, and thermal energies calculated at B3LYP/6-311+G(d,p) level of theory.

Table S3. Relative energies at 0 K (Gibbs energies at 298 K) in kJ/mol of the (Lys)H⁺(18C6) complexes.^a

| (Lys)H ⁺ (18C6) | B3LYP | B3P86 | M06 | MP2(full) |
|--|--------------------|---------------------------|---------------------------|---------------------------|
| H ⁺ K[N _e]-ctg.gtt(-00/+00/-00/+00/-00/+00) | 0.0 (3.7) | 0.0 (0.0) | 1.1 (0.7) | 0.6 (0.2) |
| H ⁺ K[N _e]-tg.tttt(-00/+00/-00/+00/-00/+00) | 1.3 (0.0) | 6.4 (1.4) | 15.7 (10.3) | 18.1 (12.7) |
| H ⁺ K[N _e]-ctgttg(+00/-00/+00/--0/+00/+0+) | 2.8 (8.1) | 3.3 (4.9) | 11.6 (12.8) | 5.2 (6.4) |
| H ⁺ K[N _e]-ctg.ggt(-00/+00/--0/-00/+00/--0) | 3.2 (11.2) | 3.1 (7.4) | 14.7 (18.5) | 8.8 (12.7) |
| H ⁺ K[N _e]-cgg.gtt(+00/-00/+0+/-00/-00/+0+) | 3.4 (8.9) | 3.3 (5.1) | 10.3 (11.7) | 4.6 (6.1) |
| H ⁺ K[N _e]-ctgttg(+00/-00/+0+/-00/-00/+0+) | 4.3 (8.5) | 5.6 (6.1) | 15.6 (15.7) | 12.3 (12.4) |
| H ⁺ K[N _e]-cggg.tt(-00/+00/--0/-00/+00/--0) | 4.5 (10.1) | 5.5 (7.3) | 17.9 (19.4) | 11.7 (13.1) |
| H ⁺ K[N _e]-ctgg.g.t(+0+/-00/-00/+0+/-00/-00) | 5.5 (11.8) | 6.7 (9.4) | 16.8 (19.0) | 13.4 (15.7) |
| H ⁺ K[N _e]-ttttt(-00/+00/-00/+00/-00/+00) | 5.7 (0.6) | 10.5 (1.7) | 20.2 (10.9) | 23.6 (14.3) |
| H ⁺ K[N _e]-tggggt(-00/+00/-00/+00/-00/+00) | 6.1 (11.2) | 9.3 (10.7) | 7.5 (8.4) | 3.8 (4.7) |
| H ⁺ K[N _e]-ctg.ggt(+00/-00/+00/-00/+00/-00) | 6.2 (13.8) | 6.3 (10.1) | 12.2 (15.6) | 7.5 (10.9) |
| H ⁺ K[N _e]-tg.tttg(+0+/-00/--0/-00/+00/-00) | 6.4 (9.1) | 10.3 (9.3) | 17.2 (15.9) | 15.9 (14.5) |
| H ⁺ K[N _e]-cg.g.gtt(-00/+0+/-00/-00/+00/--0) | 7.1 (11.8) | 8.4 (9.3) | 15.7 (16.2) | 11.5 (12.0) |
| H ⁺ K[N _e]-cgggtg(+00/-00/+0+/-00/--0/-00) | 7.5 (11.6) | 8.1 (8.5) | 0.0 (0.0) | 0.0 (0.0) |
| H ⁺ K[N _e]-ttttgt(-00/+00/-00/+00/-00/+00) | 7.6 (5.1) | 12.6 (6.3) | 19.2 (12.5) | 22.7 (16.0) |
| H ⁺ K[N _e]-tg.g.ttg(+00/-00/+00/--0/-00/+00) | 7.7 (10.3) | 11.3 (10.2) | 15.4 (13.9) | 12.3 (10.8) |
| H ⁺ K[N _e]-ctg.tg.g(-00/+0+/-00/-00/+0+/-00) | 7.8 (14.7) | 7.9 (11.1) | 11.1 (13.9) | 7.2 (10.0) |
| H ⁺ K[N _e]-cggg.tt(+0+/-00/-00/+00/--0/-00) | 7.9 (13.6) | 9.2 (11.1) | 17.6 (19.2) | 12.5 (14.0) |
| H ⁺ K[N _e]-ttg.ttg(+00/-00/+00/--0/-00/+0+) | 8.5 (11.7) | 12.9 (12.4) | 17.9 (17.0) | 14.2 (13.3) |
| H ⁺ K[N _e]-cggg.tt(+00/-00/+0+/-00/-00/+0+) | 9.0 (13.4) | 10.4 (11.1) | 19.6 (19.9) | 13.7 (14.0) |
| H ⁺ K[N _e]-cgg.ttg(+00/-00/+00/--0/-00/+0+) | 9.1 (13.9) | 9.6 (10.6) | 9.6 (10.3) | 6.1 (6.8) |
| H ⁺ K[N _e]-ctgttg(-00/-00/+0+/-00/-00/+00) | 9.7 (16.3) | 9.7 (12.6) | 13.0 (15.5) | 9.6 (12.1) |
| H ⁺ K[N _e]-cg.g.g.tg(--0/-00/-00/--0/-0/--0) | 10.0 (18.2) | 9.8 (14.3) | 17.2 (21.2) | 10.2 (14.2) |
| H ⁺ K[N _e]-tg.g.tgg(+0+/-00/-00/+00/--0/-00) | 10.1 (13.0) | 12.8 (12.1) | 15.0 (13.8) | 12.1 (10.8) |
| H ⁺ K[N _e]-cg.gttg(--0/-00/+0+/-00/-00/+00) | 10.2 (16.1) | 10.2 (12.4) | 8.8 (10.6) | 5.9 (7.7) |
| H ⁺ K[N _e]-cg.gg.tt(+00/--0/-00/+00/-00/+0+) | 10.6 (13.8) | 10.2 (12.4) | 19.2 (18.4) | 16.3 (15.5) |
| H ⁺ K[N _e]-cgggtg(-0/-00/-00/-00/+00/--0) | 10.6 (19.1) | 11.3 (11.0) | 15.8 (20.2) | 9.8 (14.2) |
| H ⁺ K[N _e]-tg.g.ttg(--00/+00/--0/-00/+00/--0) | 10.6 (17.6) | 13.6 (16.9) | 10.4 (13.3) | 6.5 (9.3) |
| H ⁺ K[N _e]-tg.g.gtt(+0+/-00/-00/+0+/-00/-00) | 10.7 (13.8) | 14.3 (13.6) | 21.0 (19.9) | 14.8 (13.7) |
| H ⁺ K[N _e]-cgg.gtt(+0+/-00/--0/-00/+00/-00) | 11.3 (16.2) | 12.1 (13.3) | 22.4 (23.2) | 16.1 (16.9) |
| H ⁺ K[N _e]-ctg.ttg(-00/+00/--0/-00/+0+/-00) | 12.0 (16.6) | 12.8 (13.7) | 18.7 (19.2) | 17.5 (18.0) |
| H ⁺ K[N _e]-cg.tgt(-00/+00/-00/+00/-00/+00) | 12.5 (12.1) | 13.8 (9.8) | 23.4 (19.0) | 27.0 (22.5) |
| H ⁺ K[N _e]-cg.tttt(-00/+00/-00/+00/-00/+00) | 13.4 (13.4) | 15.5 (11.8) | 28.6 (24.5) | 32.0 (27.9) |
| H ⁺ K[N _e]-cgggtg(-00/+0+/-00/-00/+0+/-00) | 13.5 (21.1) | 12.9 (16.8) | 19.2 (22.7) | 12.8 (16.3) |
| H ⁺ K[N _e]-ttgg.g.t(+00/-00/+00/-00/+00/-00) | 13.8 (26.7) | 14.7 (23.9) | 7.5 (16.3) | 2.7 (11.5) |
| H ⁺ K[N _e]-tggg.tt(-00/+00/-00/+00/-00/+00) | 18.4 (30.3) | 19.8 (28.0) | 11.9 (19.7) | 10.0 (17.7) |
| H ⁺ K[N _e]-tg.ggtt(-00/+00/-00/+00/-00/+00) | 18.6 (19.0) | 23.9 (20.7) | 27.8 (24.1) | 28.3 (24.6) |
| H ⁺ K[N _e]-tg.tgt(-00/+0+/-00/+0+/-00/--0) | 23.2 (20.8) | 28.5 (22.3) | 45.1 (38.4) | 44.1 (37.5) |
| H ⁺ K[N _α]-cg.ggg.g(-00/+0+/-00/-00/+00/--0) | 17.6 (26.4) | 16.1 (21.2) | 17.9 (22.6) | 10.0 (14.7) |
| H ⁺ K[N _α]-tg.gg.tg(-00/+00/-00/+00/-00/+00) | 18.4 (29.5) | 15.2 (22.7) | 12.9 (20.0) | 8.8 (15.9) |
| H ⁺ K[N _α]-cg.ggg.g(+0+/-00/-00/+00/-00/+00) | 20.5 (32.5) | 18.0 (26.3) | 18.8 (26.7) | 10.6 (18.5) |

^a Gibbs energies in parentheses. **Ground conformations in bold**. All values calculated at the level of theory indicated using the 6-311+G(2d,2p) basis set with conformations, zero-point energies, and thermal energies calculated at B3LYP/6-311+G(d,p) level of theory.

Table S4. Relative energies at 0 K (Gibbs energies at 298 K) in kJ/mol of the (Arg)H⁺(18C6) complexes.^a

| (Arg)H ⁺ (18C6) | B3LYP | B3P86 | M06 | MP2(full) |
|--|--------------------|--------------------|--------------------|------------------|
| H ⁺ R[N _o]-tcg.gg.t(-00/+0+/-00/-00/+0+/-00) | 0.0 (12.8) | 0.0 (11.2) | 1.4 (1.4) | 0.0 (1.9) |
| H ⁺ R[N _o]-cggg.tg(+00/-00/+0+/-00/-00/+0+) | 1.1 (0.0) | 2.6 (0.0) | 15.3 (1.5) | 24.4 (12.4) |
| H ⁺ R[N _o]-cgggtg(-00/+00/+0+/-00/-00/+00) | 2.7 (5.9) | 3.2 (4.8) | 9.6 (0.0) | 17.1 (9.4) |
| H ⁺ R[N _o]-tg.g.g.gg(+00/-00/+0+/-00/-00/+0+) | 3.4 (6.2) | 7.1 (8.4) | 18.2 (8.2) | 24.9 (16.8) |
| H ⁺ R[N _o]-ctg.ggg(-00/+00/-0/-00/+00/-0) | 4.7 (7.3) | 5.8 (6.8) | 18.4 (8.2) | 28.5 (20.2) |
| H ⁺ R[N _o]-cg.g.gtg(+00/-0/-00/+00/-00/+0+) | 5.1 (10.3) | 6.5 (9.2) | 17.3 (8.7) | 24.4 (17.7) |
| H ⁺ R[N _o]-cgggtg(+00/-00/+00/-00/+0+/-0+) | 10.3 (14.4) | 14.0 (16.5) | 22.8 (14.1) | 28.7 (21.8) |
| H ⁺ R[N _o]-tgtg.g.g(-00/+00/-0/-00/+00/-0) | 7.0 (5.8) | 9.8 (7.0) | 23.0 (9.0) | 29.6 (17.4) |
| H ⁺ R[N _o]-cg.g.gtg(-0/-00/+00/+00/-00/-0) | 6.9 (8.2) | 7.6 (7.4) | 15.8 (4.3) | 25.0 (15.4) |
| H ⁺ R[N _o]-cggg.tg(+00/-00/+00/-00/+0+/-0+) | 6.9 (8.2) | 7.6 (7.4) | 15.8 (4.3) | 25.0 (15.4) |
| H ⁺ R[N _o]-cg.g.gtg(-00/+0+/-0+/-00/-00/+00) | 7.4 (8.4) | 8.3 (7.7) | 15.2 (3.4) | 24.2 (14.2) |
| H ⁺ R[N _o]-cgggtg(-00/+0+/-00/-00/+00/-0) | 6.4 (9.4) | 7.2 (8.7) | 16.3 (6.5) | 23.9 (16.0) |
| H ⁺ R[N _o]-tcg.g.gg(-0/-00/-00/+00/-00/+00) | 9.6 (24.2) | 8.1 (21.1) | 0.0 (1.8) | 0.8 (4.4) |
| H ⁺ R[N _o]-tg.g.g.g(-00/+00/-0/-00/+00/-0) | 7.7 (7.9) | 9.9 (8.5) | 20.1 (7.5) | 25.9 (15.2) |
| H ⁺ R[N _o]-tcgg.gt(-0/-00/+0+/-0+/-00/-0) | 10.0 (21.0) | 10.7 (20.1) | 18.6 (16.9) | 15.6 (15.7) |
| H ⁺ R[N _o]-tcg.g.gg(-0/-00/+00/-0+/-00/-0) | 9.6 (23.3) | 9.4 (21.6) | 5.0 (6.0) | 5.7 (8.4) |
| H ⁺ R[N _o]-cg.g.gtg(-00/+00/-00/+00/-00/-0) | 8.0 (8.6) | 9.2 (8.2) | 19.5 (7.4) | 28.8 (18.5) |
| H ⁺ R[N _o]-tg.g.g.gg(-00/+0+/-0+/-00/-00/+00) | 8.5 (8.6) | 12.2 (10.8) | 21.0 (8.3) | 26.8 (16.0) |
| H ⁺ R[N _o]-ctg.ggg(+00/-00/+0+/-00/-00/+0+) | 8.1 (8.8) | 9.1 (8.2) | 23.8 (11.7) | 33.5 (23.3) |
| H ⁺ R[N _o]-ttg.gg.t(-00/+0+/-00/-00/-0) | 12.4 (21.6) | 12.9 (20.5) | 19.5 (15.9) | 19.2 (17.4) |
| H ⁺ R[N _o]-tcgg.gt(-0/-0+/-00/-00/+0+/-00) | 11.9 (25.0) | 10.5 (22.0) | 5.4 (5.7) | 5.0 (7.1) |
| H ⁺ R[N _o]-tcgg.gt(-00/-0/-00/+0+/-00/-0) | 12.0 (25.4) | 10.3 (22.2) | 3.6 (4.3) | 4.8 (7.4) |
| H ⁺ R[N _o]-tg.tg.tg(-0/-00/+00/-00/+00/-0) | 11.1 (10.7) | 13.0 (11.1) | 19.6 (6.4) | 24.9 13.5 |
| H ⁺ R[N _o]-tg.g.g.tg(+00/-00/+00/-0/-00/+0+) | 10.5 (13.2) | 13.1 (14.3) | 12.1 (2.0) | 19.2 (11.0) |
| H ⁺ R[N _o]-ctg.ggt(+00/-00/+0+/-00/-00/+0+) | 10.3 (8.7) | 12.1 (9.0) | 26.6 (12.3) | 37.0 (24.4) |
| H ⁺ R[N _o]-tcgg.gt(-00/+0+/-00/+0+/-00/-0) | 12.4 (25.7) | 10.2 (21.9) | 4.9 (5.4) | 4.0 (6.3) |
| H ⁺ R[N _o]-tg.g.g.gg(+00/-0/-0/-00/+00/-0) | 11.0 (13.1) | 14.6 (15.1) | 21.3 (10.6) | 28.7 (19.8) |
| H ⁺ R[N _o]-tg.g.gg.t(+00/-00/+0+/-00/-00/+0+) | 10.9 (14.0) | 13.7 (15.3) | 25.4 (15.8) | 30.9 (23.1) |
| H ⁺ R[N _o]-tgtg.gt(-0/-00/+00/-00/+00/-0) | 10.6 (6.8) | 14.4 (9.0) | 28.1 (11.6) | 33.8 (19.1) |
| H ⁺ R[N _o]-ctgg.tg(-00/+00/-0/-00/+00/-0) | 10.8 (12.3) | 12.1 (12.1) | 24.3 (13.1) | 33.6 (24.3) |
| H ⁺ R[N _o]-cgggtg(+00/-0/-0/-00/+00/-0) | 10.8 (10.9) | 12.5 (11.0) | 22.0 (9.4) | 30.1 (19.3) |
| H ⁺ R[N _o]-tgggtg(-00/+00/-00/+0+/-0+/-00) | 12.0 (17.2) | 13.7 (17.3) | 10.6 (3.0) | 16.6 (10.8) |
| H ⁺ R[N _o]-tcgg.gt(+0+/-0+/-00/-00/+0+/-0+) | 13.4 (25.9) | 12.3 (23.3) | 7.6 (7.4) | 8.8 (10.3) |
| H ⁺ R[N _o]-tg.tggg(+0+/-00/-00/+00/-00/+00) | 11.8 (12.8) | 13.3 (12.7) | 20.1 (8.2) | 27.0 (17.1) |
| H ⁺ R[N _o]-tcgg.gt(+0+/-00/-00/+00/+0+/-0+) | 14.3 (25.8) | 12.6 (22.5) | 3.9 (2.7) | 5.0 (5.6) |
| H ⁺ R[N _o]-tcgg.gt(-0/-00/+00/-0/-00/+00) | 14.0 (25.8) | 13.6 (23.8) | 8.9 (7.9) | 7.9 (8.7) |
| H ⁺ R[N _o]-tg.tggg(-0/-00/+00/-00/+00/-0) | 11.9 (10.4) | 14.5 (11.4) | 25.0 (10.7) | 33.4 (21.0) |
| H ⁺ R[N _o]-tgtg.g.g(+00/-00/+00/-00/+0+/-0+) | 11.9 (10.4) | 14.5 (14.4) | 25.0 (10.8) | 33.5 (21.0) |
| H ⁺ R[N _o]-cgggtg(+00/-00/+0+/-0+/-00/-00) | 11.7 (17.0) | 11.2 (15.0) | 14.9 (7.5) | 21.3 (15.8) |
| H ⁺ R[N _o]-tgtg.tg(+00/-00/+00/-00/+0+/-0+) | 12.5 (13.4) | 14.8 (14.2) | 22.3 (10.5) | 29.9 (19.9) |
| H ⁺ R[N _o]-tgtg.tg(+00/-00/+00/-00/+00/+0+) | 12.7 (12.8) | 15.1 (13.7) | 23.3 (10.7) | 31.8 (21.0) |
| H ⁺ R[N _o]-tg.tgg.t(-00/+0+/-0+/-00/-00/+00) | 12.0 (16.4) | 15.5 (18.4) | 25.0 (16.7) | 29.5 (23.0) |
| H ⁺ R[N _o]-tg.tg.tg(+00/-00/+00/-00/+0+/-0+) | 13.0 (14.7) | 14.6 (14.8) | 21.6 (10.6) | 27.5 (18.3) |

| | | | | |
|--|-------------|-------------|-------------|--------------------|
| H ⁺ R[N _ω]-cgggtg(+00/-00/+0+/-0+/-00/--+) | 11.5 (11.7) | 12.7 (11.4) | 19.4 (6.8) | 27.7 (17.0) |
| H ⁺ R[N _ω]-tg.tgtg(+00/-00/+00/-00/+0+/-0+) | 13.0 (14.4) | 15.4 (15.3) | 22.4 (11.1) | 31.3 (21.8) |
| H ⁺ R[N _ω]-tgtg.tg(--0/-00/+00/-00/+00/--0) | 13.0 (14.4) | 15.4 (15.3) | 22.4 (11.1) | 31.3 (21.8) |
| H ⁺ R[N _ω]-cg.g.gtg(-00/+00/+0+/-00/--0/-00) | 13.4 (17.5) | 13.2 (15.6) | 17.4 (8.7) | 26.7 (19.8) |
| H ⁺ R[N _ω]-tgggtg(-00/+00/-00/+00/--0/-00) | 13.1 (13.2) | 15.0 (13.6) | 15.8 (3.1) | 22.6 (11.8) |
| H ⁺ R[N _ω]-cgggtg(+00/+00/--0/-00/+00/+0+) | 12.1 (14.1) | 12.3 (12.8) | 19.9 (9.1) | 25.3 (16.3) |
| H ⁺ R[N _ω]-tgtgtg(+00/-00/+00/-00/+0+/-0+) | 13.4 (15.2) | 15.5 (15.6) | 23.5 (12.4) | 30.6 (21.5) |
| H ⁺ R[N _ω]-cg.g.g.tg(-00/+0+/-00/--0/--0/-00) | 12.1 (15.4) | 13.2 (14.9) | 19.0 (9.5) | 26.9 (19.2) |
| H ⁺ R[N _α]-g.g.g.gt(-00/+00/-00/+00/-00/+00) | 12.9 (23.0) | 9.8 (18.4) | 9.1 (6.4) | 5.6 (4.8) |
| H ⁺ R[N _α]-gggg.t(-00/+00/-00/+00/-00/+00) | 13.9 (23.2) | 10.2 (18.0) | 5.5 (2.0) | 1.6 (0.0) |
| H ⁺ R[N _α]-ggg.g.t(-00/+00/-00/+00/-00/+00) | 14.4 (17.2) | 13.1 (14.4) | 14.4 (4.5) | 14.4 (6.4) |

^a Gibbs energies in parentheses. **Ground conformations in bold.** All values calculated at the level of theory indicated using the 6-311+G(2d,2p) basis set with conformations, zero-point energies, and thermal energies calculated at B3LYP/6-311+G(d,p) level of theory.

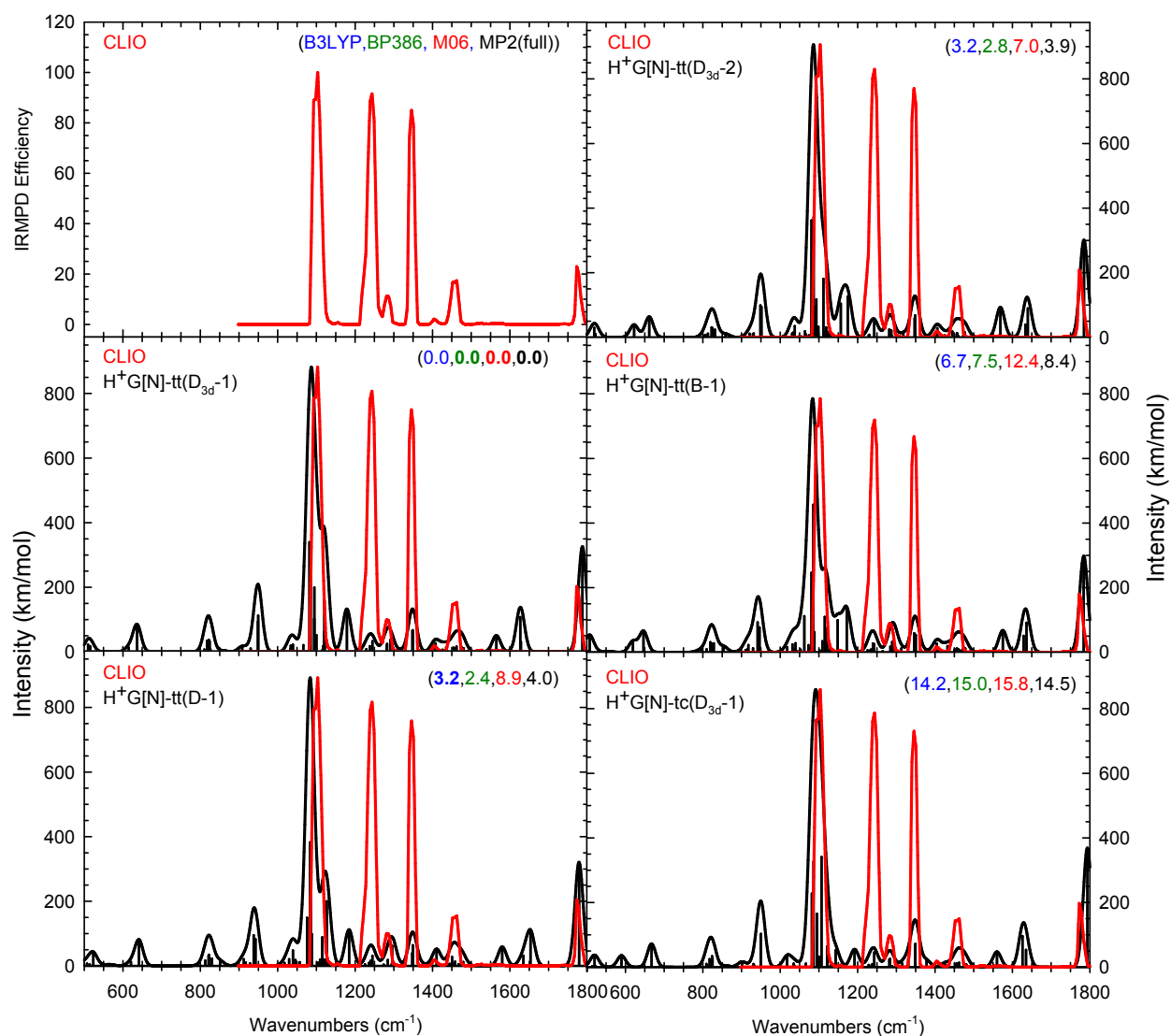


Figure S1. Comparison of the measured IRMPD actions spectrum of $(\text{Gly})\text{H}^+(\text{18C6})$ with the theoretical linear IR spectra for low-lying conformations of $(\text{Gly})\text{H}^+(\text{18C6})$ at 298 K. Relative energies in kJ/mol calculated at four levels of theory are given in parentheses in each panel. To facilitate comparison of the measured and computed spectra, the IRMPD spectrum is overlaid (in red) with the computed spectrum and normalized to match the intensity of the most intense feature.

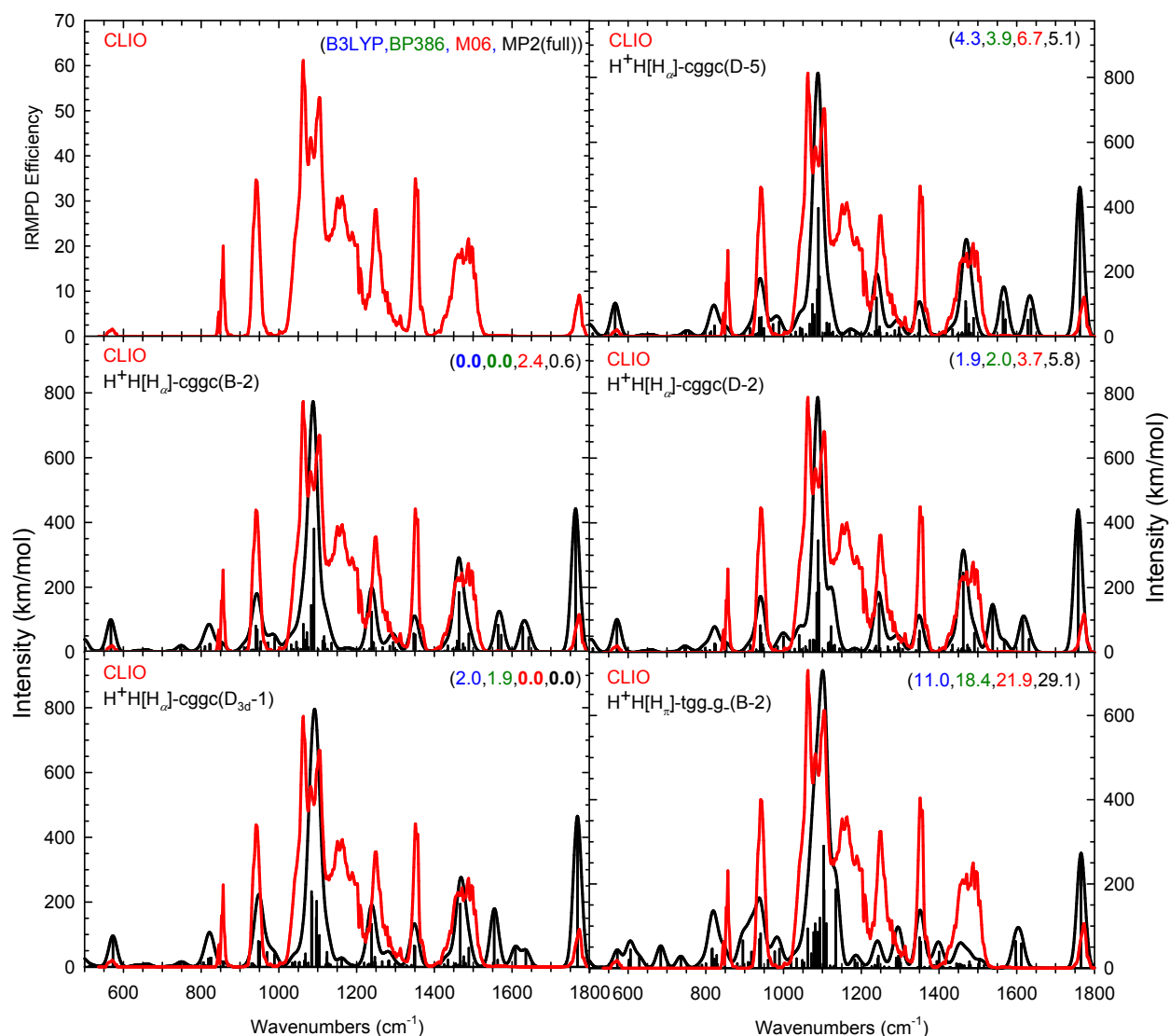


Figure S2. Comparison of the measured IRMPD actions spectrum of $(\text{His})\text{H}^+(18\text{C}6)$ with the theoretical linear IR spectra for low-lying conformations of $(\text{Gly})\text{H}^+(18\text{C}6)$ at 298 K. Relative energies in kJ/mol calculated at four levels of theory are given in parentheses in each panel. To facilitate comparison of the measured and computed spectra, the IRMPD spectrum is overlaid (in red) with the computed spectrum and normalized to match the intensity of the most intense feature.

Structures (Gly)H⁺-18C6H⁺G[N]-tt(-00/+00/-00/+00/-00/+00) #0

| | | | |
|---|-----------|-----------|-----------|
| N | -0.051338 | -0.000019 | 0.297683 |
| H | 0.475639 | 0.842463 | -0.002368 |
| C | -0.327437 | -0.000246 | 1.751617 |
| H | -0.962416 | 0.000091 | -0.185845 |
| H | 0.475576 | -0.842462 | -0.002609 |
| C | 0.940131 | -0.000226 | 2.582566 |
| H | -0.924327 | 0.876806 | 2.001526 |
| H | -0.924165 | -0.877475 | 2.001280 |
| O | 2.058928 | 0.000119 | 2.142706 |
| O | 0.627904 | -0.000627 | 3.886582 |
| H | 1.447975 | -0.000576 | 4.405781 |
| H | 1.014126 | 4.503598 | -0.711299 |
| C | 0.481224 | 3.564772 | -0.910484 |
| O | 1.274909 | 2.458699 | -0.475539 |
| C | -0.837849 | 3.581169 | -0.172923 |
| H | 0.300540 | 3.489669 | -1.989980 |
| C | 2.526348 | 2.382712 | -1.173606 |
| O | -1.572686 | 2.413819 | -0.522031 |
| H | -1.389678 | 4.484148 | -0.466988 |
| H | -0.673290 | 3.623546 | 0.913296 |
| C | 3.317523 | 1.188346 | -0.696360 |
| H | 2.338206 | 2.303441 | -2.251331 |
| H | 3.104678 | 3.295914 | -0.984914 |
| C | -2.914593 | 2.401963 | -0.052932 |
| O | 2.633004 | 0.000090 | -1.077147 |
| H | 4.310877 | 1.223305 | -1.165516 |
| H | 3.444636 | 1.220068 | 0.391779 |
| C | -3.613554 | 1.188887 | -0.622726 |
| H | -3.447570 | 3.302728 | -0.386298 |
| H | -2.940842 | 2.380863 | 1.046070 |
| C | 3.317524 | -1.188167 | -0.696354 |
| O | -2.982432 | 0.000025 | -0.140479 |
| H | -3.569799 | 1.213767 | -1.718726 |
| H | -4.667093 | 1.203543 | -0.314982 |
| C | 2.526389 | -2.382524 | -1.173682 |
| H | 4.310905 | -1.223092 | -1.165450 |
| H | 3.444570 | -1.219916 | 0.391793 |
| C | -3.613517 | -1.188762 | -0.622957 |
| O | 1.274940 | -2.458588 | -0.475630 |
| H | 2.338254 | -2.303186 | -2.251402 |
| H | 3.104734 | -3.295729 | -0.985044 |
| C | -2.914610 | -2.401928 | -0.053295 |
| H | -3.569674 | -1.213475 | -1.718958 |
| H | -4.667082 | -1.203466 | -0.315305 |
| C | 0.481287 | -3.564649 | -0.910667 |
| O | -1.572684 | -2.413759 | -0.522354 |
| H | -3.447595 | -3.302638 | -0.386794 |
| H | -2.940891 | -2.380962 | 1.045709 |
| C | -0.837845 | -3.581093 | -0.173213 |
| H | 0.300692 | -3.489518 | -1.990176 |
| H | 1.014176 | -4.503481 | -0.711469 |
| H | -1.389619 | -4.484085 | -0.467348 |
| H | -0.673377 | -3.623501 | 0.913020 |

H⁺G[N]-tt(+0+/-00/-00/+00/--0/-00) #34

| | | | |
|---|-----------|-----------|-----------|
| C | -2.385454 | -2.285082 | -1.393918 |
| C | -1.187783 | -3.133902 | -1.037179 |
| O | -0.000216 | -2.402336 | -1.322761 |
| C | 1.187224 | -3.134116 | -1.037197 |
| C | 2.385043 | -2.285503 | -1.393935 |
| O | 2.463374 | -1.160458 | -0.509552 |
| C | 3.561962 | -0.297065 | -0.801926 |
| C | 3.633506 | 0.800939 | 0.245783 |
| O | 2.472369 | 1.628728 | 0.297584 |
| C | 2.401630 | 2.632308 | -0.711904 |
| C | 1.193911 | 3.503326 | -0.452683 |
| O | 0.000288 | 2.732664 | -0.625963 |
| C | -1.193215 | 3.503539 | -0.452810 |
| C | -2.401067 | 2.632710 | -0.712053 |
| O | -2.472032 | 1.629203 | 0.297491 |
| C | -3.633335 | 0.801644 | 0.245714 |
| C | -3.562011 | -0.296417 | -0.801951 |
| O | -2.463574 | -1.159999 | -0.509563 |
| H | -3.296382 | -2.889033 | -1.297708 |
| H | -2.304903 | -1.935613 | -2.430821 |
| H | -1.222496 | -4.053689 | -1.637672 |
| H | -1.216701 | -3.409165 | 0.024152 |
| H | 1.221766 | -4.053904 | -1.637697 |
| H | 1.216104 | -3.409390 | 0.024132 |
| H | 2.304540 | -1.935994 | -2.430829 |
| H | 3.295863 | -2.889621 | -1.297754 |
| H | 3.451331 | 0.114533 | -1.813871 |
| H | 4.502056 | -0.864407 | -0.773493 |
| H | 4.530012 | 1.408556 | 0.067517 |
| H | 3.722482 | 0.351530 | 1.237143 |
| H | 2.325924 | 2.184183 | -1.710456 |
| H | 3.301110 | 3.261848 | -0.683517 |
| H | 1.198675 | 4.340146 | -1.162537 |
| H | 1.231626 | 3.909729 | 0.565734 |
| H | -1.197787 | 4.340316 | -1.162717 |
| H | -1.230929 | 3.910011 | 0.565580 |
| H | -2.325380 | 2.184512 | -1.710574 |
| H | -3.300442 | 3.262405 | -0.683755 |
| H | -4.529719 | 1.409434 | 0.067421 |
| H | -3.722405 | 0.352293 | 1.237092 |
| H | -3.451330 | 0.115114 | -1.813917 |
| H | -4.502208 | -0.863586 | -0.773471 |
| C | -0.000037 | 0.232712 | 1.917119 |
| C | -0.000164 | -1.098872 | 2.639225 |
| O | -0.000192 | -2.174213 | 2.097773 |
| O | -0.000240 | -0.909147 | 3.965694 |
| N | 0.000001 | 0.046265 | 0.449572 |
| H | 0.883176 | 0.808782 | 2.196033 |
| H | -0.883179 | 0.808921 | 2.195969 |
| H | -0.000319 | -1.774175 | 4.405745 |
| H | -0.840862 | -0.460994 | 0.121130 |
| H | 0.840779 | -0.461169 | 0.121188 |
| H | 0.000114 | 0.981714 | 0.005615 |

H⁺G[N]-tt(+00/-00/+00/-00/+00/-00) #85

| | | | |
|---|-----------|-----------|-----------|
| C | -3.658626 | 0.917225 | -0.091294 |
| C | -3.741490 | -0.486080 | -0.646360 |
| O | -2.709302 | -1.290540 | -0.082953 |
| C | -2.696210 | -2.614643 | -0.609635 |
| C | -1.490564 | -3.363270 | -0.087172 |
| O | -0.301938 | -2.735211 | -0.573649 |
| C | 0.879601 | -3.538547 | -0.473344 |
| C | 1.987121 | -2.871628 | -1.258040 |
| O | 2.263314 | -1.608337 | -0.672540 |
| C | 3.268177 | -0.870417 | -1.359874 |
| C | 3.471663 | 0.461895 | -0.674780 |
| O | 2.282478 | 1.250913 | -0.817503 |
| C | 2.421058 | 2.594792 | -0.349119 |
| C | 1.247614 | 3.410848 | -0.842923 |
| O | 0.038810 | 2.923683 | -0.261105 |
| C | -1.123314 | 3.518627 | -0.827852 |
| C | -2.360088 | 2.922495 | -0.195862 |
| O | -2.437180 | 1.529785 | -0.513862 |
| H | -3.715300 | 0.902879 | 1.005230 |
| H | -4.512210 | 1.493219 | -0.470201 |
| H | -3.641192 | -0.459542 | -1.739368 |
| H | -4.727914 | -0.903145 | -0.401096 |
| H | -2.658510 | -2.580443 | -1.706167 |
| H | -3.606824 | -3.152183 | -0.311283 |
| H | -1.541135 | -4.397129 | -0.449961 |
| H | -1.488482 | -3.386754 | 1.010526 |
| H | 0.689227 | -4.532748 | -0.895350 |
| H | 1.169466 | -3.655929 | 0.578513 |
| H | 1.680336 | -2.748306 | -2.305695 |
| H | 2.877944 | -3.514983 | -1.232982 |
| H | 2.972754 | -0.715381 | -2.406406 |
| H | 4.219602 | -1.420115 | -1.347623 |
| H | 4.311458 | 0.979281 | -1.155118 |
| H | 3.696990 | 0.317870 | 0.386217 |
| H | 3.342582 | 3.035809 | -0.749039 |
| H | 2.479632 | 2.607284 | 0.746099 |
| H | 1.187732 | 3.341532 | -1.936669 |
| H | 1.401605 | 4.463674 | -0.569943 |
| H | -1.141223 | 3.349045 | -1.912599 |
| H | -1.126742 | 4.602904 | -0.649511 |
| H | -3.242114 | 3.442168 | -0.590671 |
| H | -2.341527 | 3.060997 | 0.893559 |
| C | -0.377510 | 0.144067 | 1.713303 |
| C | 0.848332 | -0.050508 | 2.584775 |
| O | 1.981990 | 0.129508 | 2.226871 |
| O | 0.484288 | -0.397988 | 3.828367 |
| N | -0.069534 | 0.032576 | 0.267803 |
| H | -0.750905 | 1.151815 | 1.906801 |
| H | -1.163929 | -0.563830 | 1.966276 |
| H | 1.278797 | -0.442892 | 4.384451 |
| H | -0.829084 | 0.507437 | -0.245394 |
| H | -0.039587 | -0.955781 | -0.040652 |
| H | 0.831023 | 0.481578 | 0.003480 |

H⁺G[N]-tt(+0+/-00/-00/+0+/-00/-00) #3053

| | | | |
|---|-----------|-----------|-----------|
| C | 2.537920 | -2.116540 | -1.046735 |
| C | 3.313898 | -0.819622 | -1.044964 |
| O | 2.903654 | -0.025686 | 0.068898 |
| C | 3.513883 | 1.260958 | 0.134799 |
| C | 2.781838 | 2.316661 | -0.675344 |
| O | 1.463983 | 2.488987 | -0.145299 |
| C | 0.756575 | 3.571399 | -0.757954 |
| C | -0.593694 | 3.728579 | -0.098716 |
| O | -1.361571 | 2.557110 | -0.345357 |
| C | -2.693830 | 2.630304 | 0.149212 |
| C | -3.445537 | 1.390325 | -0.274916 |
| O | -2.898166 | 0.245643 | 0.387992 |
| C | -3.574089 | -0.985383 | 0.090338 |
| C | -3.027271 | -1.668139 | -1.150737 |
| O | -1.665679 | -1.979173 | -0.900857 |
| C | -1.009941 | -2.650354 | -1.969300 |
| C | 0.386104 | -3.029230 | -1.529909 |
| O | 1.160829 | -1.842696 | -1.316645 |
| H | 2.636848 | -2.627862 | -0.081648 |
| H | 2.946493 | -2.767407 | -1.830241 |
| H | 3.139235 | -0.288746 | -1.988834 |
| H | 4.385668 | -1.045523 | -0.966606 |
| H | 3.513055 | 1.549228 | 1.188937 |
| H | 4.558467 | 1.212333 | -0.197218 |
| H | 2.721168 | 2.040962 | -1.736214 |
| H | 3.336305 | 3.261717 | -0.603210 |
| H | 1.325507 | 4.501808 | -0.636828 |
| H | 0.631572 | 3.375592 | -1.830350 |
| H | -1.091512 | 4.611250 | -0.522940 |
| H | -0.474900 | 3.889502 | 0.981745 |
| H | -2.693584 | 2.720197 | 1.244253 |
| H | -3.206598 | 3.508910 | -0.265615 |
| H | -3.379568 | 1.275581 | -1.363108 |
| H | -4.501168 | 1.501470 | 0.002356 |
| H | -3.418681 | -1.631695 | 0.956219 |
| H | -4.649665 | -0.807087 | -0.017813 |
| H | -3.607956 | -2.582876 | -1.337930 |
| H | -3.119016 | -1.025277 | -2.037767 |
| H | -0.969873 | -2.005576 | -2.857927 |
| H | -1.552425 | -3.568615 | -2.233633 |
| H | 0.852732 | -3.633126 | -2.318420 |
| H | 0.346666 | -3.615703 | -0.605752 |
| C | 0.332668 | -0.027758 | 2.012163 |
| C | 0.366992 | -1.457042 | 2.519943 |
| O | 0.420976 | -2.432730 | 1.819201 |
| O | 0.367917 | -1.471988 | 3.860102 |
| N | 0.011666 | 0.031765 | 0.566978 |
| H | 1.321138 | 0.404445 | 2.169901 |
| H | -0.392625 | 0.559137 | 2.574597 |
| H | 0.442236 | -2.391198 | 4.162737 |
| H | 0.383769 | 0.912493 | 0.174919 |
| H | 0.436850 | -0.750963 | 0.031601 |
| H | -1.010446 | 0.013988 | 0.404374 |

H⁺G[N]-tt(+0+/+00/-00/+0+/+00/-00) #57

| | | | |
|---|-----------|-----------|-----------|
| C | 2.461581 | -2.198816 | -1.049610 |
| C | 3.287661 | -0.933101 | -1.032415 |
| O | 2.901495 | -0.132819 | 0.085438 |
| C | 3.560918 | 1.128726 | 0.165806 |
| C | 2.877165 | 2.218042 | -0.642016 |
| O | 1.561794 | 2.436613 | -0.122902 |
| C | 0.899344 | 3.544079 | -0.741584 |
| C | -0.450896 | 3.750217 | -0.096146 |
| O | -1.259129 | 2.607870 | -0.350428 |
| C | -2.592082 | 2.731043 | 0.132226 |
| C | -3.382769 | 1.514367 | -0.288782 |
| O | -2.876850 | 0.356514 | 0.384092 |
| C | -3.595970 | -0.852419 | 0.098115 |
| C | -3.085454 | -1.558733 | -1.145651 |
| O | -1.731753 | -1.910735 | -0.908617 |
| C | -1.101822 | -2.592294 | -1.985830 |
| C | 0.280299 | -3.025628 | -1.552470 |
| O | 1.097731 | -1.870366 | -1.326312 |
| H | 2.533683 | -2.720789 | -0.087793 |
| H | 2.850197 | -2.859195 | -1.835308 |
| H | 3.140437 | -0.388468 | -1.973155 |
| H | 4.349170 | -1.201577 | -0.949055 |
| H | 4.605357 | 1.041917 | -0.158787 |
| H | 3.563154 | 1.408972 | 1.222089 |
| H | 2.815944 | 1.953065 | -1.705548 |
| H | 3.466367 | 3.140733 | -0.557294 |
| H | 0.778318 | 3.353199 | -1.815307 |
| H | 1.500042 | 4.453406 | -0.614198 |
| H | -0.911366 | 4.650553 | -0.525429 |
| H | -0.337600 | 3.907239 | 0.985495 |
| H | -3.070627 | 3.623668 | -0.293465 |
| H | -2.597706 | 2.829244 | 1.226540 |
| H | -3.315079 | 1.390724 | -1.375859 |
| H | -4.435452 | 1.662449 | -0.017685 |
| H | -4.666283 | -0.639250 | 0.001243 |
| H | -3.451998 | -1.500043 | 0.964996 |
| H | -3.167833 | -0.918895 | -2.035780 |
| H | -3.696768 | -2.455803 | -1.320696 |
| H | -1.039747 | -1.938583 | -2.866634 |
| H | -1.676379 | -3.487827 | -2.260139 |
| H | 0.724863 | -3.636913 | -2.347997 |
| H | 0.220021 | -3.620552 | -0.634917 |
| C | 0.328381 | -0.058629 | 2.012982 |
| C | 0.280663 | -1.492775 | 2.505412 |
| O | 0.294008 | -2.462923 | 1.795148 |
| O | 0.262704 | -1.521564 | 3.845413 |
| N | 0.017064 | 0.035169 | 0.567391 |
| H | 1.339614 | 0.314096 | 2.178044 |
| H | -0.364314 | 0.562713 | 2.579410 |
| H | 0.287021 | -2.446516 | 4.138567 |
| H | 0.429329 | 0.904057 | 0.188821 |
| H | -1.004387 | 0.064803 | 0.400426 |
| H | 0.410469 | -0.757804 | 0.022813 |

H⁺G[N]-tt(++0/+00/--0/-00/+0+/+0+) #183

| | | | |
|---|-----------|-----------|-----------|
| C | -3.333103 | 1.676079 | 0.185148 |
| C | -3.429049 | 0.423774 | -0.671861 |
| O | -2.643444 | -0.601211 | -0.057270 |
| C | -2.797637 | -1.922251 | -0.597980 |
| C | -2.027822 | -2.127558 | -1.899015 |
| O | -0.628311 | -1.901459 | -1.761722 |
| C | 0.132153 | -3.028223 | -1.325878 |
| C | 1.600605 | -2.716478 | -1.507616 |
| O | 2.007088 | -1.700656 | -0.581547 |
| C | 3.322101 | -1.206357 | -0.835071 |
| C | 3.706017 | -0.209357 | 0.246530 |
| O | 2.824028 | 0.907831 | 0.346190 |
| C | 3.008808 | 1.915475 | -0.644891 |
| C | 2.051402 | 3.054188 | -0.373746 |
| O | 0.706124 | 2.604255 | -0.566732 |
| C | -0.263539 | 3.652901 | -0.471369 |
| C | -1.639141 | 3.097724 | -0.764273 |
| O | -2.007506 | 2.199004 | 0.278800 |
| H | -3.635919 | 1.436095 | 1.206492 |
| H | -4.020159 | 2.437049 | -0.205262 |
| H | -3.085367 | 0.615878 | -1.695494 |
| H | -4.478974 | 0.107138 | -0.718609 |
| H | -3.861661 | -2.134105 | -0.760872 |
| H | -2.431183 | -2.591295 | 0.181875 |
| H | -2.369563 | -1.428289 | -2.665969 |
| H | -2.224073 | -3.142400 | -2.270230 |
| H | -0.109879 | -3.906262 | -1.939501 |
| H | -0.077878 | -3.266514 | -0.276592 |
| H | 1.778543 | -2.371720 | -2.533300 |
| H | 2.190305 | -3.625189 | -1.333271 |
| H | 3.358754 | -0.755096 | -1.835082 |
| H | 4.045843 | -2.032315 | -0.815061 |
| H | 4.736126 | 0.127400 | 0.071921 |
| H | 3.673505 | -0.698991 | 1.222200 |
| H | 2.828090 | 1.517627 | -1.650881 |
| H | 4.036236 | 2.301631 | -0.604187 |
| H | 2.269087 | 3.873122 | -1.070703 |
| H | 2.179447 | 3.425231 | 0.650794 |
| H | -0.031105 | 4.435632 | -1.204299 |
| H | -0.240792 | 4.095579 | 0.532183 |
| H | -1.634364 | 2.593374 | -1.739201 |
| H | -2.350312 | 3.933144 | -0.811598 |
| C | 0.138276 | 0.143718 | 2.045617 |
| C | -0.196238 | -1.187912 | 2.687452 |
| O | -0.514246 | -2.178814 | 2.080489 |
| O | -0.090361 | -1.107575 | 4.019601 |
| N | 0.038208 | 0.052394 | 0.574346 |
| H | 1.149022 | 0.449935 | 2.317438 |
| H | -0.555694 | 0.906922 | 2.401430 |
| H | -0.314470 | -1.969749 | 4.404879 |
| H | 0.249946 | 0.976682 | 0.157521 |
| H | -0.921358 | -0.219962 | 0.283998 |
| H | 0.716422 | -0.622655 | 0.178204 |

H⁺G[N]-tt(+00/-00/+00/--0/-00/+0+) #150

| | | | |
|---|-----------|-----------|-----------|
| C | 0.686021 | -3.179709 | -1.165419 |
| C | 2.033866 | -2.565778 | -1.465600 |
| O | 2.333722 | -1.578096 | -0.483398 |
| C | 3.548435 | -0.885704 | -0.732614 |
| C | 3.732537 | 0.157610 | 0.353462 |
| O | 2.690740 | 1.142504 | 0.374941 |
| C | 2.887979 | 2.250378 | -0.510856 |
| C | 1.855511 | 3.310725 | -0.205294 |
| O | 0.561832 | 2.791984 | -0.490810 |
| C | -0.484757 | 3.721594 | -0.236116 |
| C | -1.809165 | 3.095302 | -0.605691 |
| O | -2.084545 | 2.004113 | 0.280632 |
| C | -3.406746 | 1.459906 | 0.164870 |
| C | -3.535883 | 0.450115 | -0.961042 |
| O | -2.641685 | -0.618265 | -0.690917 |
| C | -2.624452 | -1.620682 | -1.702180 |
| C | -1.651942 | -2.710131 | -1.313484 |
| O | -0.323989 | -2.177079 | -1.299510 |
| H | 0.664676 | -3.600289 | -0.153181 |
| H | 0.504919 | -3.989512 | -1.883684 |
| H | 2.021102 | -2.109167 | -2.464156 |
| H | 2.796917 | -3.356199 | -1.455479 |
| H | 3.523846 | -0.423528 | -1.729517 |
| H | 4.403149 | -1.577042 | -0.706206 |
| H | 4.707376 | 0.645378 | 0.240720 |
| H | 3.707601 | -0.327979 | 1.331447 |
| H | 2.799529 | 1.930841 | -1.555864 |
| H | 3.888427 | 2.672631 | -0.356698 |
| H | 2.060170 | 4.194506 | -0.825286 |
| H | 1.922282 | 3.607170 | 0.850204 |
| H | -0.345104 | 4.628404 | -0.840828 |
| H | -0.487302 | 4.012246 | 0.823147 |
| H | -1.780329 | 2.751667 | -1.646180 |
| H | -2.597335 | 3.852001 | -0.508727 |
| H | -4.134823 | 2.268053 | 0.031205 |
| H | -3.611560 | 0.969779 | 1.118735 |
| H | -3.304970 | 0.904048 | -1.935065 |
| H | -4.574491 | 0.091014 | -0.998353 |
| H | -2.332192 | -1.179252 | -2.664509 |
| H | -3.623357 | -2.064449 | -1.814349 |
| H | -1.717359 | -3.515730 | -2.056050 |
| H | -1.901734 | -3.116178 | -0.327600 |
| C | 0.066627 | -0.108171 | 2.096186 |
| C | -0.510345 | -1.428987 | 2.569397 |
| O | -0.768640 | -2.360945 | 1.854399 |
| O | -0.658538 | -1.417110 | 3.900090 |
| N | 0.018304 | 0.023300 | 0.617952 |
| H | 1.104943 | -0.052058 | 2.427040 |
| H | -0.469655 | 0.722461 | 2.554151 |
| H | -0.987613 | -2.283845 | 4.187502 |
| H | 0.899355 | 0.454296 | 0.292672 |
| H | -0.766206 | 0.636506 | 0.336093 |
| H | -0.095690 | -0.884511 | 0.126029 |

H⁺G[N]-tt(+00/-00/+00/--0/-00/+0+) #197

| | | | |
|---|-----------|-----------|-----------|
| C | -2.640055 | -1.604876 | -1.696952 |
| C | -1.682279 | -2.702577 | -1.295250 |
| O | -0.347858 | -2.185640 | -1.285940 |
| C | 0.651616 | -3.198016 | -1.147648 |
| C | 2.004408 | -2.599360 | -1.456202 |
| O | 2.315975 | -1.606484 | -0.482824 |
| C | 3.534928 | -0.925600 | -0.742782 |
| C | 3.739065 | 0.116173 | 0.341187 |
| O | 2.708890 | 1.113289 | 0.369928 |
| C | 2.916039 | 2.222334 | -0.511731 |
| C | 1.892473 | 3.290221 | -0.202397 |
| O | 0.594347 | 2.784079 | -0.490714 |
| C | -0.443576 | 3.724248 | -0.239318 |
| C | -1.773191 | 3.113010 | -0.615438 |
| O | -2.066157 | 2.024493 | 0.268709 |
| C | -3.394813 | 1.497595 | 0.145786 |
| C | -3.528711 | 0.483292 | -0.975635 |
| O | -2.648521 | -0.593709 | -0.694168 |
| H | -3.644024 | -2.037054 | -1.809024 |
| H | -2.338332 | -1.175242 | -2.661663 |
| H | -1.756969 | -3.515418 | -2.028963 |
| H | -1.938072 | -3.094181 | -0.305113 |
| H | 0.460017 | -4.010708 | -1.859825 |
| H | 0.629216 | -3.611531 | -0.132532 |
| H | 1.993206 | -2.150722 | -2.458401 |
| H | 2.760237 | -3.396606 | -1.441659 |
| H | 3.505826 | -0.463258 | -1.739464 |
| H | 4.383231 | -1.624978 | -0.723625 |
| H | 4.718711 | 0.592315 | 0.220636 |
| H | 3.715856 | -0.368546 | 1.319672 |
| H | 2.825312 | 1.907339 | -1.558011 |
| H | 3.919935 | 2.635773 | -0.355868 |
| H | 2.105160 | 4.174817 | -0.818473 |
| H | 1.961077 | 3.581512 | 0.854404 |
| H | -0.291578 | 4.630097 | -0.842487 |
| H | -0.447663 | 4.014074 | 0.820148 |
| H | -1.743305 | 2.769887 | -1.656126 |
| H | -2.553001 | 3.878720 | -0.521828 |
| H | -4.110783 | 2.314634 | 0.001394 |
| H | -3.614183 | 1.015953 | 1.100750 |
| H | -3.286713 | 0.929161 | -1.950631 |
| H | -4.571138 | 0.135983 | -1.017180 |
| C | 0.072444 | -0.098899 | 2.090470 |
| C | -0.529235 | -1.403143 | 2.578685 |
| O | -0.803196 | -2.338948 | 1.874526 |
| O | -0.678458 | -1.372966 | 3.908966 |
| N | 0.017535 | 0.020704 | 0.611576 |
| H | 1.114043 | -0.062458 | 2.413706 |
| H | -0.442771 | 0.747261 | 2.544042 |
| H | -1.022342 | -2.230623 | 4.206187 |
| H | -0.765456 | 0.634896 | 0.327973 |
| H | -0.101954 | -0.890219 | 0.126782 |
| H | 0.898875 | 0.444880 | 0.279637 |

H⁺G[N]-tt(--0/-00/+00/-00/+0+/-00) #308

| | | | |
|---|-----------|-----------|-----------|
| C | -2.612554 | 2.396970 | -0.848338 |
| C | -3.454168 | 1.631806 | 0.159787 |
| O | -3.011899 | 0.287854 | 0.350649 |
| C | -3.650448 | -0.671780 | -0.488866 |
| C | -3.087913 | -2.043777 | -0.195061 |
| O | -1.720371 | -2.090025 | -0.607352 |
| C | -1.155544 | -3.406180 | -0.625175 |
| C | 0.118143 | -3.378460 | -1.439247 |
| O | 1.037802 | -2.490492 | -0.823406 |
| C | 2.249792 | -2.342979 | -1.554106 |
| C | 3.134284 | -1.325968 | -0.870161 |
| O | 2.498427 | -0.040996 | -0.918674 |
| C | 3.367068 | 1.042502 | -0.582581 |
| C | 2.663983 | 2.348573 | -0.874080 |
| O | 1.572364 | 2.508067 | 0.032498 |
| C | 0.793471 | 3.685015 | -0.176133 |
| C | -0.437921 | 3.429882 | -1.029442 |
| O | -1.280115 | 2.501462 | -0.336067 |
| H | -3.039326 | 3.399774 | -0.976777 |
| H | -2.602830 | 1.902227 | -1.828472 |
| H | -4.505083 | 1.652965 | -0.152515 |
| H | -3.380721 | 2.123187 | 1.132710 |
| H | -3.493816 | -0.432646 | -1.548457 |
| H | -4.730646 | -0.682744 | -0.291509 |
| H | -3.668406 | -2.787508 | -0.755068 |
| H | -3.174711 | -2.272758 | 0.874949 |
| H | -1.859049 | -4.107519 | -1.089823 |
| H | -0.954665 | -3.743765 | 0.399321 |
| H | -0.102116 | -3.047255 | -2.463432 |
| H | 0.531951 | -4.395746 | -1.487863 |
| H | 2.031946 | -2.019660 | -2.581132 |
| H | 2.786030 | -3.301195 | -1.600687 |
| H | 4.091001 | -1.281458 | -1.405192 |
| H | 3.318078 | -1.608636 | 0.170863 |
| H | 4.277831 | 0.990208 | -1.192532 |
| H | 3.653336 | 0.986967 | 0.474981 |
| H | 2.311409 | 2.350393 | -1.913391 |
| H | 3.377991 | 3.172920 | -0.747192 |
| H | 1.397197 | 4.476163 | -0.636066 |
| H | 0.478531 | 4.032708 | 0.810934 |
| H | -0.171184 | 3.031344 | -2.017013 |
| H | -0.972544 | 4.377020 | -1.174884 |
| C | -0.141548 | 0.204467 | 1.938679 |
| C | 0.894573 | -0.613505 | 2.683782 |
| O | 1.899212 | -1.058750 | 2.194643 |
| O | 0.554275 | -0.730479 | 3.975290 |
| N | -0.027066 | 0.042064 | 0.469904 |
| H | 0.029138 | 1.254801 | 2.183230 |
| H | -1.152414 | -0.053269 | 2.249551 |
| H | 1.262370 | -1.201781 | 4.442925 |
| H | -0.465290 | 0.870086 | 0.030247 |
| H | -0.525436 | -0.798237 | 0.129037 |
| H | 0.956012 | -0.013559 | 0.138940 |

H⁺G[N]-tt(+00/-00/+00/--0/+00/+0+) #48

| | | | |
|---|-----------|-----------|-----------|
| C | 3.609022 | -0.953431 | -0.534287 |
| C | 3.744635 | 0.157774 | 0.490583 |
| O | 2.709172 | 1.142598 | 0.402302 |
| C | 2.950029 | 2.196440 | -0.535812 |
| C | 1.887163 | 3.255486 | -0.352563 |
| O | 0.618404 | 2.687235 | -0.653391 |
| C | -0.458781 | 3.608862 | -0.511576 |
| C | -1.755307 | 2.923955 | -0.876841 |
| O | -2.050735 | 1.914560 | 0.091090 |
| C | -3.350421 | 1.318722 | -0.033796 |
| C | -3.435810 | 0.281873 | -1.141057 |
| O | -2.532938 | -0.772018 | -0.836577 |
| C | -2.484094 | -1.796499 | -1.815715 |
| C | -1.546653 | -2.878765 | -1.329807 |
| O | -0.234669 | -2.324980 | -1.178018 |
| C | 0.789701 | -3.302166 | -0.982152 |
| C | 2.138506 | -2.674941 | -1.250814 |
| O | 2.390456 | -1.649600 | -0.295154 |
| H | 4.467000 | -1.633466 | -0.434273 |
| H | 3.617720 | -0.552791 | -1.557292 |
| H | 4.726956 | 0.633311 | 0.388593 |
| H | 3.677027 | -0.262662 | 1.496333 |
| H | 2.925049 | 1.813682 | -1.563026 |
| H | 3.935504 | 2.641202 | -0.350743 |
| H | 2.102235 | 4.097149 | -1.025296 |
| H | 1.901766 | 3.627432 | 0.680784 |
| H | -0.313107 | 4.467092 | -1.181798 |
| H | -0.507072 | 3.981203 | 0.520409 |
| H | -1.673962 | 2.491314 | -1.880897 |
| H | -2.559172 | 3.670926 | -0.883434 |
| H | -4.101054 | 2.100183 | -0.201327 |
| H | -3.542180 | 0.841888 | 0.926703 |
| H | -3.196326 | 0.714345 | -2.122683 |
| H | -4.467615 | -0.095061 | -1.186695 |
| H | -2.131143 | -1.393353 | -2.775085 |
| H | -3.479296 | -2.236398 | -1.971101 |
| H | -1.523749 | -3.690150 | -2.067480 |
| H | -1.897339 | -3.286311 | -0.373306 |
| H | 0.650224 | -4.134224 | -1.683208 |
| H | 0.743477 | -3.705100 | 0.038215 |
| H | 2.153752 | -2.254105 | -2.264834 |
| H | 2.911278 | -3.453514 | -1.187949 |
| C | 0.329395 | -0.447951 | 2.000546 |
| C | -0.923468 | -0.795241 | 2.780902 |
| O | -2.043087 | -0.509713 | 2.450843 |
| O | -0.595678 | -1.440329 | 3.910815 |
| N | 0.024996 | 0.006880 | 0.623129 |
| H | 1.005899 | -1.299794 | 1.948764 |
| H | 0.849107 | 0.355336 | 2.527140 |
| H | -1.404510 | -1.606288 | 4.421078 |
| H | -0.776117 | 0.668305 | 0.568277 |
| H | -0.181191 | -0.786922 | -0.009176 |
| H | 0.860975 | 0.491869 | 0.260465 |

H⁺G[N]-tt(--0/-00/+00/-00/+0+/-00) #151

| | | | |
|---|-----------|-----------|-----------|
| C | 3.447912 | 1.647064 | 0.162705 |
| C | 2.603396 | 2.406920 | -0.846970 |
| O | 1.269934 | 2.506026 | -0.336288 |
| C | 0.423486 | 3.426063 | -1.035775 |
| C | -0.809583 | 3.680668 | -0.185032 |
| O | -1.581906 | 2.500375 | 0.029954 |
| C | -2.680508 | 2.336894 | -0.867662 |
| C | -3.373040 | 1.025396 | -0.575687 |
| O | -2.499897 | -0.051786 | -0.919893 |
| C | -3.129078 | -1.339964 | -0.874188 |
| C | -2.237437 | -2.352083 | -1.555997 |
| O | -1.026280 | -2.494040 | -0.822475 |
| C | -0.102992 | -3.380314 | -1.435597 |
| C | 1.170939 | -3.401143 | -0.621616 |
| O | 1.729720 | -2.082407 | -0.605896 |
| C | 3.097910 | -2.029627 | -0.195976 |
| C | 3.653304 | -0.654770 | -0.489754 |
| O | 3.013741 | 0.300568 | 0.353651 |
| H | 3.370045 | 2.138220 | 1.135383 |
| H | 4.499152 | 1.674637 | -0.148111 |
| H | 2.596839 | 1.910794 | -1.826420 |
| H | 3.025554 | 3.411524 | -0.976525 |
| H | 0.158845 | 3.019128 | -2.020460 |
| H | 0.953652 | 4.374725 | -1.187467 |
| H | -1.417014 | 4.465172 | -0.651247 |
| H | -0.497677 | 4.037311 | 0.799859 |
| H | -2.337106 | 2.345631 | -1.910035 |
| H | -3.398915 | 3.155936 | -0.731331 |
| H | -4.286978 | 0.969607 | -1.180597 |
| H | -3.653119 | 0.964700 | 0.483224 |
| H | -4.084331 | -1.300083 | -1.412326 |
| H | -3.315204 | -1.624396 | 0.165999 |
| H | -2.018685 | -2.027664 | -2.582498 |
| H | -2.768766 | -3.312938 | -1.604276 |
| H | 0.116261 | -3.051099 | -2.460650 |
| H | -0.512996 | -4.399227 | -1.481449 |
| H | 1.877478 | -4.099931 | -1.085549 |
| H | 0.972109 | -3.738319 | 0.403361 |
| H | 3.680943 | -2.770063 | -0.757633 |
| H | 3.187779 | -2.259023 | 0.873706 |
| H | 3.491240 | -0.414765 | -1.548323 |
| H | 4.734299 | -0.661258 | -0.296651 |
| C | 0.141926 | 0.205647 | 1.937862 |
| C | -0.892451 | -0.614046 | 2.683428 |
| O | -1.895171 | -1.062997 | 2.193701 |
| O | -0.553425 | -0.727845 | 3.975496 |
| N | 0.027532 | 0.041135 | 0.469334 |
| H | 1.153545 | -0.049099 | 2.248827 |
| H | -0.031175 | 1.255851 | 2.181438 |
| H | -1.260619 | -1.200632 | 4.443038 |
| H | 0.531923 | -0.795927 | 0.129119 |
| H | 0.458964 | 0.872077 | 0.028655 |
| H | -0.955210 | -0.022231 | 0.139164 |

H⁺G[N]-tt(+00/--0/-00/-00/+00/-00) #206

| | | | |
|---|-----------|-----------|-----------|
| C | -3.459260 | 1.142211 | -0.813989 |
| C | -3.489868 | -0.307301 | -0.382880 |
| O | -2.326506 | -0.957455 | -0.898833 |
| C | -2.414245 | -2.386765 | -0.943346 |
| C | -1.196885 | -2.920741 | -1.664693 |
| O | -0.046773 | -2.639632 | -0.877416 |
| C | 1.178707 | -3.093855 | -1.428628 |
| C | 2.248593 | -2.909400 | -0.368038 |
| O | 2.414363 | -1.538598 | 0.026932 |
| C | 3.454567 | -0.817727 | -0.641603 |
| C | 3.788054 | 0.417286 | 0.177694 |
| O | 2.709429 | 1.349969 | 0.257709 |
| C | 2.724226 | 2.372639 | -0.734951 |
| C | 1.624708 | 3.363179 | -0.430595 |
| O | 0.350889 | 2.741275 | -0.626119 |
| C | -0.748603 | 3.613301 | -0.342708 |
| C | -2.025071 | 3.028103 | -0.900567 |
| O | -2.310954 | 1.787750 | -0.264285 |
| H | -4.376408 | 1.644114 | -0.477338 |
| H | -3.419781 | 1.190219 | -1.909386 |
| H | -4.395182 | -0.771524 | -0.792876 |
| H | -3.522143 | -0.402439 | 0.709495 |
| H | -3.316059 | -2.682749 | -1.493397 |
| H | -2.462824 | -2.790934 | 0.073370 |
| H | -1.108726 | -2.453057 | -2.654793 |
| H | -1.310436 | -4.004888 | -1.801894 |
| H | 1.418130 | -2.539485 | -2.347914 |
| H | 1.120622 | -4.161578 | -1.684755 |
| H | 3.202421 | -3.316722 | -0.719339 |
| H | 1.953135 | -3.448982 | 0.533980 |
| H | 3.148241 | -0.551292 | -1.661612 |
| H | 4.353041 | -1.443652 | -0.708910 |
| H | 4.681752 | 0.898707 | -0.237336 |
| H | 4.010043 | 0.113703 | 1.203254 |
| H | 2.581071 | 1.952958 | -1.739521 |
| H | 3.685807 | 2.902253 | -0.717178 |
| H | 1.719532 | 4.224238 | -1.104110 |
| H | 1.717898 | 3.717300 | 0.603828 |
| H | -0.580381 | 4.587973 | -0.817288 |
| H | -0.830228 | 3.771994 | 0.740593 |
| H | -1.918992 | 2.875280 | -1.982585 |
| H | -2.840534 | 3.745656 | -0.733234 |
| C | -0.099364 | 0.412332 | 1.888530 |
| C | -0.705495 | -0.717399 | 2.697699 |
| O | -1.337754 | -1.628998 | 2.231603 |
| O | -0.475647 | -0.532140 | 4.004822 |
| N | 0.008604 | 0.059600 | 0.453871 |
| H | 0.885943 | 0.683178 | 2.264302 |
| H | -0.755945 | 1.279656 | 1.982202 |
| H | -0.918471 | -1.237724 | 4.503152 |
| H | 0.799711 | -0.587018 | 0.284798 |
| H | 0.176581 | 0.932730 | -0.074108 |
| H | -0.854792 | -0.377664 | 0.074648 |

H⁺G[N]-tt(+00/--0/--0/-00/+00/-00) #255

| | | | |
|---|-----------|-----------|-----------|
| C | -2.442018 | -2.357646 | -0.952232 |
| C | -1.226501 | -2.911793 | -1.661349 |
| O | -0.078049 | -2.641495 | -0.867762 |
| C | 1.143449 | -3.122449 | -1.405161 |
| C | 2.209559 | -2.940644 | -0.340306 |
| O | 2.395879 | -1.568064 | 0.037943 |
| C | 3.431180 | -0.863973 | -0.655915 |
| C | 3.799610 | 0.368476 | 0.151709 |
| O | 2.734196 | 1.314730 | 0.250277 |
| C | 2.757603 | 2.350208 | -0.728958 |
| C | 1.668220 | 3.347452 | -0.411045 |
| O | 0.387961 | 2.741450 | -0.614570 |
| C | -0.702173 | 3.625013 | -0.331187 |
| C | -1.982835 | 3.057253 | -0.897263 |
| O | -2.284905 | 1.816516 | -0.269220 |
| C | -3.437144 | 1.186400 | -0.828598 |
| C | -3.490571 | -0.263206 | -0.400382 |
| O | -2.333396 | -0.929822 | -0.909372 |
| H | -2.506781 | -2.758854 | 0.064750 |
| H | -3.342943 | -2.641281 | -1.510265 |
| H | -1.124868 | -2.451440 | -2.653666 |
| H | -1.353795 | -3.995101 | -1.793070 |
| H | 1.397168 | -2.584620 | -2.330386 |
| H | 1.069915 | -4.192449 | -1.647389 |
| H | 3.158978 | -3.368454 | -0.679279 |
| H | 1.899417 | -3.462323 | 0.567247 |
| H | 3.105633 | -0.594879 | -1.669224 |
| H | 4.318740 | -1.503044 | -0.741779 |
| H | 4.689968 | 0.836561 | -0.284889 |
| H | 4.040383 | 0.065407 | 1.173242 |
| H | 2.609270 | 1.944952 | -1.738710 |
| H | 3.724256 | 2.870243 | -0.705420 |
| H | 1.771884 | 4.216105 | -1.073393 |
| H | 1.765203 | 3.687600 | 0.627732 |
| H | -0.520653 | 4.599836 | -0.800596 |
| H | -0.786098 | 3.780148 | 0.752442 |
| H | -1.873715 | 2.909411 | -1.979686 |
| H | -2.791291 | 3.782531 | -0.729393 |
| H | -3.388929 | 1.236012 | -1.923617 |
| H | -4.350277 | 1.699501 | -0.497914 |
| H | -4.399650 | -0.713572 | -0.817537 |
| H | -3.531725 | -0.359978 | 0.691544 |
| C | -0.101668 | 0.414218 | 1.885157 |
| C | -0.726099 | -0.706783 | 2.692631 |
| O | -1.370446 | -1.608957 | 2.224817 |
| O | -0.496887 | -0.525126 | 4.000385 |
| N | 0.009771 | 0.058346 | 0.451436 |
| H | 0.884820 | 0.673466 | 2.266011 |
| H | -0.748555 | 1.289301 | 1.973959 |
| H | -0.951444 | -1.224172 | 4.497395 |
| H | 0.188634 | 0.929175 | -0.076597 |
| H | -0.855971 | -0.371292 | 0.068627 |
| H | 0.795529 | -0.596234 | 0.287227 |

H⁺G[N]-tt(+0+//+0/+00/-00/+00/-00) #386

| | | | |
|---|-----------|-----------|-----------|
| C | 2.460503 | 2.759216 | -0.047441 |
| C | 1.465943 | 3.102271 | -1.152341 |
| O | 0.141199 | 2.624613 | -0.877687 |
| C | -0.753044 | 3.533057 | -0.223475 |
| C | -2.175780 | 3.081816 | -0.482154 |
| O | -2.383366 | 1.792135 | 0.087479 |
| C | -3.599492 | 1.183159 | -0.340523 |
| C | -3.642193 | -0.262466 | 0.107430 |
| O | -2.571272 | -0.975645 | -0.515459 |
| C | -2.714686 | -2.400512 | -0.528974 |
| C | -1.623450 | -2.983461 | -1.401307 |
| O | -0.364421 | -2.669051 | -0.824515 |
| C | 0.748459 | -3.118571 | -1.589324 |
| C | 2.032663 | -2.718925 | -0.895663 |
| O | 2.152812 | -1.288667 | -0.905922 |
| C | 3.416849 | -0.811340 | -0.437748 |
| C | 3.504523 | 0.681373 | -0.673048 |
| O | 2.569035 | 1.353108 | 0.173903 |
| H | 2.141118 | 3.193743 | 0.903802 |
| H | 3.439021 | 3.191975 | -0.293203 |
| H | 1.759719 | 2.631784 | -2.093343 |
| H | 1.450421 | 4.186676 | -1.311583 |
| H | -0.627805 | 4.541537 | -0.634164 |
| H | -0.548415 | 3.573154 | 0.853867 |
| H | -2.349963 | 3.042298 | -1.564754 |
| H | -2.869774 | 3.812808 | -0.044841 |
| H | -3.668300 | 1.224875 | -1.434924 |
| H | -4.463921 | 1.713489 | 0.082087 |
| H | -4.605349 | -0.689018 | -0.198019 |
| H | -3.568298 | -0.340196 | 1.200249 |
| H | -3.692609 | -2.672393 | -0.944363 |
| H | -2.644805 | -2.799045 | 0.491064 |
| H | -1.694190 | -2.566871 | -2.415319 |
| H | -1.761354 | -4.071972 | -1.464473 |
| H | 0.714166 | -2.684873 | -2.598003 |
| H | 0.729066 | -4.213242 | -1.683562 |
| H | 2.877360 | -3.159342 | -1.439700 |
| H | 2.040041 | -3.082493 | 0.136826 |
| H | 4.226576 | -1.300562 | -0.993694 |
| H | 3.537323 | -1.043156 | 0.627579 |
| H | 3.298549 | 0.894022 | -1.728962 |
| H | 4.523384 | 1.019205 | -0.442461 |
| C | -0.006765 | 0.324914 | 1.798484 |
| C | 0.404309 | -0.887894 | 2.610983 |
| O | 0.998323 | -1.838310 | 2.174883 |
| O | 0.052969 | -0.728401 | 3.896074 |
| N | -0.023391 | 0.038980 | 0.346990 |
| H | 0.735240 | 1.102419 | 1.988821 |
| H | -0.981882 | 0.697712 | 2.105973 |
| H | 0.385028 | -1.484876 | 4.405720 |
| H | 0.001531 | 0.934500 | -0.173080 |
| H | -0.882919 | -0.459130 | 0.056366 |
| H | 0.795508 | -0.519950 | 0.037744 |

H⁺G[N]-tt(-00/+00/-00/+00/-00/+00) #19_6

| | | | |
|---|-----------|-----------|-----------|
| N | 0.051156 | 0.018659 | 0.314586 |
| H | -0.523069 | -0.759593 | -0.060412 |
| C | 0.389101 | -0.179047 | 1.747700 |
| H | 0.945411 | 0.032361 | -0.199497 |
| H | -0.434962 | 0.914366 | 0.125853 |
| C | -0.778167 | -0.343466 | 2.703108 |
| H | 1.020556 | -1.058752 | 1.837214 |
| H | 0.973791 | 0.679110 | 2.083795 |
| O | -0.663930 | -0.886808 | 3.765507 |
| O | -1.918184 | 0.224096 | 2.258217 |
| H | -2.587541 | 0.113939 | 2.953423 |
| H | -3.387903 | -2.909419 | -1.141071 |
| C | -2.724478 | -2.045939 | -1.276448 |
| O | -1.501421 | -2.264557 | -0.562051 |
| C | -3.416201 | -0.807123 | -0.758348 |
| H | -2.508956 | -1.934807 | -2.346063 |
| C | -0.812936 | -3.433244 | -1.020960 |
| O | -2.613121 | 0.328765 | -1.049659 |
| H | -4.393778 | -0.723727 | -1.253323 |
| H | -3.585162 | -0.887773 | 0.323372 |
| C | 0.509828 | -3.577276 | -0.304583 |
| H | -0.640513 | -3.357351 | -2.101467 |
| H | -1.426304 | -4.322090 | -0.826025 |
| C | -3.207549 | 1.559935 | -0.657129 |
| O | 1.336839 | -2.470569 | -0.646010 |
| H | 0.974747 | -4.518924 | -0.625891 |
| H | 0.360643 | -3.627695 | 0.783253 |
| C | -2.298546 | 2.696098 | -1.062199 |
| H | -4.176527 | 1.694172 | -1.157607 |
| H | -3.372800 | 1.573379 | 0.427418 |
| C | 2.689791 | -2.597107 | -0.225654 |
| O | -1.069797 | 2.626795 | -0.330009 |
| H | -2.088983 | 2.644097 | -2.137740 |
| H | -2.800809 | 3.648640 | -0.850077 |
| C | 3.473098 | -1.417086 | -0.754121 |
| H | 3.131774 | -3.519736 | -0.625423 |
| H | 2.752613 | -2.640161 | 0.870992 |
| C | -0.171326 | 3.681406 | -0.684417 |
| O | 2.966016 | -0.208813 | -0.182221 |
| H | 3.392366 | -1.372923 | -1.847470 |
| H | 4.530397 | -1.542042 | -0.487105 |
| C | 1.138214 | 3.524728 | 0.053167 |
| H | 0.010922 | 3.663444 | -1.766016 |
| H | -0.616785 | 4.649644 | -0.421702 |
| C | 3.699598 | 0.946353 | -0.595160 |
| O | 1.770827 | 2.326642 | -0.382238 |
| H | 1.768272 | 4.395225 | -0.173532 |
| H | 0.971618 | 3.501635 | 1.139536 |
| C | 3.113743 | 2.175679 | 0.061317 |
| H | 3.651347 | 1.047044 | -1.686711 |
| H | 4.752115 | 0.847643 | -0.299826 |
| H | 3.714833 | 3.048850 | -0.225881 |
| H | 3.151747 | 2.082957 | 1.155955 |

H⁺G[N]-tt(+00/-00/+0/+0/+0/+00/-00) #166

| | | | |
|---|-----------|-----------|-----------|
| C | 1.132999 | 3.398562 | -0.404081 |
| C | -0.305550 | 3.631665 | -0.817128 |
| O | -1.144828 | 2.649463 | -0.217819 |
| C | -2.473973 | 2.655522 | -0.740797 |
| C | -3.219533 | 1.420132 | -0.282187 |
| O | -2.570486 | 0.263174 | -0.815497 |
| C | -3.340567 | -0.944558 | -0.728943 |
| C | -2.605987 | -2.044951 | -1.463174 |
| O | -1.390714 | -2.340050 | -0.781910 |
| C | -0.590577 | -3.311217 | -1.439883 |
| C | 0.673961 | -3.531563 | -0.638509 |
| O | 1.415016 | -2.306125 | -0.591362 |
| C | 2.745618 | -2.440623 | -0.085587 |
| C | 3.515684 | -1.166102 | -0.357067 |
| O | 2.958164 | -0.104191 | 0.416054 |
| C | 3.550990 | 1.176844 | 0.200845 |
| C | 2.966809 | 1.903098 | -1.007028 |
| O | 1.553276 | 2.119173 | -0.893745 |
| H | 1.237227 | 3.449782 | 0.687318 |
| H | 1.752367 | 4.188515 | -0.844090 |
| H | -0.382267 | 3.570716 | -1.910148 |
| H | -0.607093 | 4.641166 | -0.504535 |
| H | -2.437475 | 2.671120 | -1.837234 |
| H | -3.014126 | 3.548640 | -0.398639 |
| H | -4.248471 | 1.479770 | -0.658094 |
| H | -3.257931 | 1.359497 | 0.812444 |
| H | -4.316040 | -0.790986 | -1.206617 |
| H | -3.490698 | -1.215763 | 0.320420 |
| H | -2.393698 | -1.730807 | -2.493987 |
| H | -3.248664 | -2.935484 | -1.498527 |
| H | -0.337109 | -2.972435 | -2.453745 |
| H | -1.127129 | -4.267184 | -1.520419 |
| H | 1.273718 | -4.309348 | -1.126735 |
| H | 0.432381 | -3.864676 | 0.378640 |
| H | 3.253414 | -3.269500 | -0.594214 |
| H | 2.725699 | -2.656953 | 0.990341 |
| H | 3.469404 | -0.938372 | -1.428741 |
| H | 4.566872 | -1.319842 | -0.079087 |
| H | 4.638176 | 1.084818 | 0.077487 |
| H | 3.370839 | 1.748740 | 1.114704 |
| H | 3.108052 | 1.315557 | -1.917182 |
| H | 3.485712 | 2.858464 | -1.145151 |
| C | 0.172290 | 0.339724 | 1.788592 |
| C | -0.869782 | -0.348794 | 2.647537 |
| O | -1.923384 | -0.770471 | 2.248041 |
| O | -0.471461 | -0.377765 | 3.927991 |
| N | 0.006425 | 0.033210 | 0.349332 |
| H | 1.179568 | 0.066049 | 2.096168 |
| H | 0.045475 | 1.415489 | 1.927484 |
| H | -1.180914 | -0.764175 | 4.466210 |
| H | 0.530694 | 0.737451 | -0.199404 |
| H | -0.983498 | 0.068279 | 0.032597 |
| H | 0.391599 | -0.893083 | 0.097852 |

H⁺G[N]-tt(+0+/+00/-0/-00/+00/-00) #271

| | | | |
|---|-----------|-----------|-----------|
| C | -1.591365 | 3.120762 | -1.140053 |
| C | -2.681200 | 2.189303 | -0.661802 |
| O | -2.317593 | 0.843335 | -0.983036 |
| C | -3.412943 | -0.075992 | -0.903210 |
| C | -2.948488 | -1.447342 | -1.336982 |
| O | -2.050940 | -1.965357 | -0.357559 |
| C | -1.594411 | -3.292950 | -0.596636 |
| C | -0.248292 | -3.326370 | -1.297356 |
| O | 0.715204 | -2.682291 | -0.455892 |
| C | 2.066330 | -2.855561 | -0.889622 |
| C | 3.000540 | -2.327545 | 0.184786 |
| O | 2.885380 | -0.919824 | 0.391528 |
| C | 3.736127 | -0.126108 | -0.431614 |
| C | 3.545418 | 1.329475 | -0.074322 |
| O | 2.232425 | 1.745659 | -0.460374 |
| C | 1.992267 | 3.141193 | -0.249173 |
| C | 0.733342 | 3.550717 | -0.977347 |
| O | -0.378413 | 2.844325 | -0.442250 |
| H | -1.903071 | 4.159280 | -0.963036 |
| H | -1.437912 | 2.984688 | -2.218486 |
| H | -3.613596 | 2.456533 | -1.174598 |
| H | -2.839807 | 2.283526 | 0.418722 |
| H | -4.214855 | 0.255469 | -1.575126 |
| H | -3.796288 | -0.114196 | 0.121598 |
| H | -2.465498 | -1.383630 | -2.321139 |
| H | -3.825878 | -2.101888 | -1.423947 |
| H | -2.325036 | -3.860781 | -1.185113 |
| H | -1.501848 | -3.772515 | 0.381152 |
| H | -0.287790 | -2.823624 | -2.272886 |
| H | 0.044076 | -4.371361 | -1.462801 |
| H | 2.223251 | -2.343431 | -1.848468 |
| H | 2.271744 | -3.923525 | -1.039652 |
| H | 4.033417 | -2.595680 | -0.068809 |
| H | 2.754174 | -2.799805 | 1.138547 |
| H | 3.510914 | -0.276821 | -1.495223 |
| H | 4.786299 | -0.396758 | -0.258999 |
| H | 4.293087 | 1.929041 | -0.608416 |
| H | 3.688592 | 1.475169 | 1.004050 |
| H | 2.831565 | 3.726377 | -0.644651 |
| H | 1.906275 | 3.348902 | 0.825466 |
| H | 0.837221 | 3.331436 | -2.048430 |
| H | 0.595693 | 4.634886 | -0.860743 |
| C | 0.214300 | 0.176804 | 1.916171 |
| C | -1.108981 | 0.052336 | 2.648793 |
| O | -2.186131 | 0.255660 | 2.154602 |
| O | -0.901476 | -0.258997 | 3.935578 |
| N | 0.052329 | 0.036499 | 0.447528 |
| H | 0.939175 | -0.551014 | 2.272960 |
| H | 0.607799 | 1.172604 | 2.130558 |
| H | -1.755773 | -0.266160 | 4.396558 |
| H | 0.166378 | -0.948138 | 0.152222 |
| H | 0.781894 | 0.600365 | -0.020466 |
| H | -0.874016 | 0.363142 | 0.105905 |

H⁺G[N]-tt(+00/-00/+0+/++0/+00/-00) #5

| | | | |
|---|-----------|-----------|-----------|
| C | 3.551011 | 1.176260 | 0.200806 |
| C | 2.967070 | 1.902640 | -1.007109 |
| O | 1.553576 | 2.119001 | -0.893926 |
| C | 1.133588 | 3.398393 | -0.404031 |
| C | -0.304966 | 3.631789 | -0.816891 |
| O | -1.144334 | 2.649673 | -0.217569 |
| C | -2.473504 | 2.655916 | -0.740466 |
| C | -3.219206 | 1.420621 | -0.281834 |
| O | -2.570435 | 0.263586 | -0.815305 |
| C | -3.340768 | -0.943997 | -0.728859 |
| C | -2.606404 | -2.044465 | -1.463195 |
| O | -1.391167 | -2.339839 | -0.781977 |
| C | -0.591186 | -3.311065 | -1.440055 |
| C | 0.673354 | -3.531661 | -0.638747 |
| O | 1.414630 | -2.306362 | -0.591613 |
| C | 2.745211 | -2.441091 | -0.085836 |
| C | 3.515451 | -1.166655 | -0.357215 |
| O | 2.957980 | -0.104704 | 0.415885 |
| H | 3.370806 | 1.748143 | 1.114662 |
| H | 4.638202 | 1.084099 | 0.077594 |
| H | 3.108258 | 1.315078 | -1.917259 |
| H | 3.486183 | 2.857900 | -1.145195 |
| H | 1.753041 | 4.188302 | -0.843999 |
| H | 1.237949 | 3.449438 | 0.687365 |
| H | -0.381810 | 3.570938 | -1.909907 |
| H | -0.606311 | 4.641310 | -0.504177 |
| H | -2.437065 | 2.671512 | -1.836905 |
| H | -3.013525 | 3.549100 | -0.398271 |
| H | -4.248185 | 1.480461 | -0.657597 |
| H | -3.257473 | 1.359922 | 0.812799 |
| H | -4.316210 | -0.790177 | -1.206515 |
| H | -3.490947 | -1.215273 | 0.320480 |
| H | -2.394074 | -1.730275 | -2.493986 |
| H | -3.249236 | -2.934883 | -1.498608 |
| H | -0.337695 | -2.972231 | -2.453893 |
| H | -1.127877 | -4.266949 | -1.520658 |
| H | 1.272946 | -4.309540 | -1.127024 |
| H | 0.431770 | -3.864753 | 0.378407 |
| H | 3.252893 | -3.270003 | -0.594519 |
| H | 2.725241 | -2.657501 | 0.990075 |
| H | 3.469294 | -0.938881 | -1.428885 |
| H | 4.566595 | -1.320524 | -0.079147 |
| C | 0.172342 | 0.339750 | 1.788546 |
| C | -0.869701 | -0.348716 | 2.647567 |
| O | -1.923270 | -0.770517 | 2.248115 |
| O | -0.471395 | -0.377485 | 3.928032 |
| N | 0.006497 | 0.033095 | 0.349313 |
| H | 1.179625 | 0.066132 | 2.096162 |
| H | 0.045484 | 1.415526 | 1.927318 |
| H | -1.180828 | -0.763874 | 4.466291 |
| H | -0.983428 | 0.068108 | 0.032572 |
| H | 0.391697 | -0.893205 | 0.097884 |
| H | 0.530759 | 0.737304 | -0.199465 |

H⁺G[N]-tt(+0+/+00/-00/+00/--0/-00) #66

| | | | |
|---|-----------|-----------|-----------|
| C | -1.193048 | 3.462275 | -0.558651 |
| C | -2.402061 | 2.581962 | -0.777250 |
| O | -2.461864 | 1.613963 | 0.267313 |
| C | -3.623739 | 0.786547 | 0.262342 |
| C | -3.576974 | -0.334630 | -0.761701 |
| O | -2.469820 | -1.192691 | -0.479782 |
| C | -2.385641 | -2.301722 | -1.380984 |
| C | -1.188549 | -3.155645 | -1.034030 |
| O | -0.000140 | -2.413381 | -1.279630 |
| C | 1.188296 | -3.155657 | -1.034195 |
| C | 2.385342 | -2.301712 | -1.381256 |
| O | 2.469628 | -1.192728 | -0.480005 |
| C | 3.576867 | -0.334773 | -0.761913 |
| C | 3.623708 | 0.786423 | 0.262100 |
| O | 2.461871 | 1.613893 | 0.267098 |
| C | 2.402036 | 2.581811 | -0.777535 |
| C | 1.193101 | 3.462220 | -0.558871 |
| O | -0.000006 | 2.685142 | -0.707236 |
| H | -1.225458 | 3.908353 | 0.443124 |
| H | -1.201596 | 4.270558 | -1.300751 |
| H | -2.334220 | 2.098983 | -1.759976 |
| H | -3.302079 | 3.211094 | -0.762788 |
| H | -4.524302 | 1.389907 | 0.090213 |
| H | -3.690192 | 0.361739 | 1.266261 |
| H | -3.490216 | 0.055673 | -1.784186 |
| H | -4.515284 | -0.902035 | -0.699391 |
| H | -2.299761 | -1.936300 | -2.411964 |
| H | -3.295131 | -2.910537 | -1.301309 |
| H | -1.211781 | -4.058919 | -1.659301 |
| H | -1.234351 | -3.463909 | 0.018710 |
| H | 1.211454 | -4.058908 | -1.659502 |
| H | 1.234221 | -3.463954 | 0.018529 |
| H | 2.299323 | -1.936234 | -2.412203 |
| H | 3.294849 | -2.910518 | -1.301722 |
| H | 3.490193 | 0.055500 | -1.784418 |
| H | 4.515125 | -0.902257 | -0.699550 |
| H | 4.524296 | 1.389735 | 0.089932 |
| H | 3.690176 | 0.361637 | 1.266028 |
| H | 2.334054 | 2.098760 | -1.760216 |
| H | 3.302100 | 3.210880 | -0.763213 |
| H | 1.201589 | 4.270436 | -1.301045 |
| H | 1.225661 | 3.908384 | 0.442862 |
| C | 0.000161 | 0.354274 | 1.935551 |
| C | 0.000306 | -0.839349 | 2.868880 |
| O | 0.000686 | -0.721299 | 4.061351 |
| O | -0.000062 | -2.027294 | 2.223326 |
| N | -0.000010 | 0.042564 | 0.483314 |
| H | 0.882316 | 0.957209 | 2.151465 |
| H | -0.881986 | 0.957151 | 2.151682 |
| H | 0.000035 | -2.723956 | 2.899830 |
| H | 0.841487 | -0.479354 | 0.184900 |
| H | -0.000096 | 0.945361 | -0.024700 |
| H | -0.841539 | -0.479411 | 0.185097 |

H⁺G[N]-tt(-00/+00/--0/-0/--0/--0) #1108

| | | | |
|---|-----------|-----------|-----------|
| C | -1.675760 | -2.832391 | -1.269775 |
| C | -2.762394 | -1.781946 | -1.315337 |
| O | -2.625375 | -0.921791 | -0.176188 |
| C | -3.671435 | 0.041748 | 0.002051 |
| C | -3.290359 | 1.423874 | -0.495569 |
| O | -2.238238 | 1.923624 | 0.329295 |
| C | -1.800686 | 3.245925 | 0.017609 |
| C | -0.785628 | 3.273326 | -1.119037 |
| O | 0.388844 | 2.507368 | -0.817041 |
| C | 1.507558 | 3.243887 | -0.307980 |
| C | 2.749886 | 2.389802 | -0.434818 |
| O | 2.629401 | 1.258353 | 0.424063 |
| C | 3.664743 | 0.284744 | 0.279126 |
| C | 3.437483 | -0.677489 | -0.875519 |
| O | 2.241043 | -1.421025 | -0.644527 |
| C | 1.968209 | -2.383042 | -1.670374 |
| C | 0.681313 | -3.113351 | -1.362681 |
| O | -0.413552 | -2.209055 | -1.482522 |
| H | -1.869910 | -3.577416 | -2.053926 |
| H | -1.689536 | -3.338701 | -0.296246 |
| H | -3.739210 | -2.278635 | -1.282029 |
| H | -2.691654 | -1.204244 | -2.244995 |
| H | -3.877985 | 0.087284 | 1.074060 |
| H | -4.581724 | -0.292078 | -0.506640 |
| H | -4.166948 | 2.082564 | -0.424453 |
| H | -2.980853 | 1.380558 | -1.548018 |
| H | -1.355862 | 3.638463 | 0.935433 |
| H | -2.655088 | 3.886137 | -0.239052 |
| H | -0.514558 | 4.310381 | -1.347027 |
| H | -1.207416 | 2.834864 | -2.026601 |
| H | 1.343101 | 3.527739 | 0.738849 |
| H | 1.648940 | 4.157226 | -0.897379 |
| H | 3.626849 | 2.987133 | -0.150819 |
| H | 2.863974 | 2.078504 | -1.479823 |
| H | 3.687063 | -0.272946 | 1.217956 |
| H | 4.638956 | 0.773686 | 0.154348 |
| H | 4.295893 | -1.360216 | -0.934518 |
| H | 3.365083 | -0.147022 | -1.834161 |
| H | 2.788931 | -3.109769 | -1.717682 |
| H | 1.891781 | -1.876907 | -2.640863 |
| H | 0.714136 | -3.532557 | -0.349252 |
| H | 0.572589 | -3.939041 | -2.079415 |
| C | 0.053698 | 0.121395 | 1.992499 |
| C | -0.010519 | -1.227427 | 2.682342 |
| O | -0.053316 | -2.286112 | 2.111568 |
| O | -0.007190 | -1.072490 | 4.013718 |
| N | 0.001302 | -0.043937 | 0.524856 |
| H | -0.785946 | 0.741524 | 2.309164 |
| H | 0.980257 | 0.631113 | 2.259405 |
| H | -0.043653 | -1.948359 | 4.430170 |
| H | 0.091925 | 0.876851 | 0.060982 |
| H | -0.900806 | -0.459633 | 0.229214 |
| H | 0.772963 | -0.634253 | 0.167169 |

H⁺G[N]-tt(--0/-00/+00/-00/+00/-00) #164

| | | | |
|---|-----------|-----------|-----------|
| C | 2.245287 | 2.711122 | -0.758285 |
| C | 1.047404 | 3.551477 | -0.372454 |
| O | -0.153767 | 2.799156 | -0.580159 |
| C | -1.343212 | 3.513532 | -0.229637 |
| C | -2.555410 | 2.746264 | -0.707516 |
| O | -2.626808 | 1.488677 | -0.040806 |
| C | -3.727127 | 0.695270 | -0.478801 |
| C | -3.618829 | -0.699779 | 0.097753 |
| O | -2.445984 | -1.328141 | -0.424945 |
| C | -2.396411 | -2.751103 | -0.271868 |
| C | -1.276427 | -3.285652 | -1.137828 |
| O | -0.045386 | -2.738127 | -0.688211 |
| C | 1.058218 | -3.069285 | -1.524543 |
| C | 2.309376 | -2.381553 | -1.022065 |
| O | 2.144850 | -0.958890 | -1.132469 |
| C | 3.343392 | -0.177305 | -1.220233 |
| C | 3.484597 | 0.767965 | -0.032030 |
| O | 2.356669 | 1.625728 | 0.157431 |
| H | 3.145054 | 3.339706 | -0.714689 |
| H | 2.124535 | 2.352629 | -1.787812 |
| H | 1.026580 | 4.454627 | -0.995052 |
| H | 1.123156 | 3.856067 | 0.679227 |
| H | -1.341704 | 4.498123 | -0.713578 |
| H | -1.382812 | 3.664582 | 0.856927 |
| H | -2.492970 | 2.589872 | -1.792486 |
| H | -3.453022 | 3.343834 | -0.496945 |
| H | -3.733095 | 0.635859 | -1.574805 |
| H | -4.674672 | 1.144877 | -0.151662 |
| H | -4.509951 | -1.267323 | -0.196958 |
| H | -3.581481 | -0.669904 | 1.194726 |
| H | -3.344559 | -3.195195 | -0.597989 |
| H | -2.233472 | -3.014733 | 0.780991 |
| H | -1.455470 | -3.007072 | -2.185081 |
| H | -1.262711 | -4.382549 | -1.069880 |
| H | 0.850974 | -2.757731 | -2.557171 |
| H | 1.228945 | -4.155169 | -1.517971 |
| H | 3.150119 | -2.707531 | -1.644281 |
| H | 2.505032 | -2.651313 | 0.020217 |
| H | 3.305739 | 0.374158 | -2.164862 |
| H | 4.226258 | -0.824220 | -1.251876 |
| H | 4.400919 | 1.362200 | -0.151751 |
| H | 3.565689 | 0.192681 | 0.891683 |
| C | -0.069305 | 0.315826 | 1.812026 |
| C | 0.668715 | -0.771880 | 2.568861 |
| O | 1.521658 | -1.477013 | 2.097433 |
| O | 0.276445 | -0.798649 | 3.851050 |
| N | -0.059827 | 0.082746 | 0.349565 |
| H | 0.453234 | 1.253279 | 2.012860 |
| H | -1.095452 | 0.416311 | 2.159309 |
| H | 0.814610 | -1.450689 | 4.328138 |
| H | -0.166029 | 0.996915 | -0.121458 |
| H | -0.843392 | -0.524279 | 0.050469 |
| H | 0.825727 | -0.338524 | 0.009942 |

H⁺G[N]-tt(+00/-00/+00/-0/-/--0/-00) #265

| | | | |
|---|-----------|-----------|-----------|
| C | 2.699992 | 2.155319 | -0.972709 |
| C | 1.726637 | 3.195520 | -0.464010 |
| O | 0.388957 | 2.704643 | -0.618711 |
| C | -0.620998 | 3.656353 | -0.269649 |
| C | -1.969528 | 3.162282 | -0.743499 |
| O | -2.316311 | 1.963849 | -0.055291 |
| C | -3.551219 | 1.408752 | -0.500211 |
| C | -3.772099 | 0.064184 | 0.156168 |
| O | -2.765317 | -0.846835 | -0.293838 |
| C | -2.986937 | -2.210790 | 0.082573 |
| C | -2.034532 | -3.099188 | -0.687314 |
| O | -0.695061 | -2.780369 | -0.333750 |
| C | 0.270723 | -3.463907 | -1.131493 |
| C | 1.649376 | -2.894570 | -0.870269 |
| O | 1.655128 | -1.518697 | -1.273510 |
| C | 2.924011 | -0.941031 | -1.605985 |
| C | 3.488159 | -0.070472 | -0.487635 |
| O | 2.622519 | 1.011260 | -0.130804 |
| H | 3.713398 | 2.579030 | -0.950017 |
| H | 2.455335 | 1.903702 | -2.012376 |
| H | 1.848607 | 4.117606 | -1.045365 |
| H | 1.925991 | 3.418445 | 0.591741 |
| H | -0.411324 | 4.615041 | -0.759888 |
| H | -0.626268 | 3.820718 | 0.815756 |
| H | -1.937150 | 2.976995 | -1.825200 |
| H | -2.716941 | 3.944074 | -0.549942 |
| H | -3.536112 | 1.286193 | -1.591047 |
| H | -4.385369 | 2.073996 | -0.238498 |
| H | -4.763688 | -0.307845 | -0.129367 |
| H | -3.742323 | 0.157445 | 1.249882 |
| H | -4.015873 | -2.501087 | -0.162251 |
| H | -2.844185 | -2.333320 | 1.164391 |
| H | -2.184939 | -2.951294 | -1.764932 |
| H | -2.260047 | -4.148314 | -0.449588 |
| H | 0.021714 | -3.345468 | -2.193831 |
| H | 0.272994 | -4.536123 | -0.891257 |
| H | 2.373833 | -3.463234 | -1.464567 |
| H | 1.913712 | -2.978731 | 0.188630 |
| H | 2.762135 | -0.352428 | -2.513164 |
| H | 3.649319 | -1.726147 | -1.848071 |
| H | 4.471877 | 0.312442 | -0.791434 |
| H | 3.612317 | -0.656912 | 0.422608 |
| C | -0.215977 | 0.120013 | 1.821760 |
| C | 0.995005 | -0.472083 | 2.517824 |
| O | 1.798871 | -1.204138 | 2.004026 |
| O | 1.012014 | -0.099330 | 3.804728 |
| N | -0.117344 | 0.045063 | 0.344018 |
| H | -0.364085 | 1.153047 | 2.130070 |
| H | -1.088374 | -0.446066 | 2.153185 |
| H | 1.760375 | -0.531909 | 4.246202 |
| H | 0.109354 | 0.975704 | -0.048311 |
| H | -1.024224 | -0.262657 | -0.046459 |
| H | 0.609260 | -0.613708 | 0.008886 |

H⁺G[N]-tt(-00/+0+/-00/-0/-00) #2811

| | | | |
|---|-----------|-----------|-----------|
| C | -1.095996 | 3.286285 | -0.950376 |
| C | -2.396397 | 2.884328 | -0.291489 |
| O | -2.402285 | 1.475255 | -0.022333 |
| C | -3.705664 | 0.886460 | -0.050765 |
| C | -3.690112 | -0.447769 | 0.683869 |
| O | -2.649575 | -1.333191 | 0.287388 |
| C | -2.766674 | -1.858806 | -1.031542 |
| C | -1.686436 | -2.897221 | -1.247727 |
| O | -0.395259 | -2.301751 | -1.085569 |
| C | 0.628262 | -2.867691 | -1.914400 |
| C | 1.988739 | -2.443472 | -1.410219 |
| O | 2.083799 | -1.023658 | -1.440276 |
| C | 3.351246 | -0.547753 | -1.000611 |
| C | 3.319635 | 0.961532 | -0.947426 |
| O | 2.448738 | 1.383436 | 0.112588 |
| C | 2.346159 | 2.803821 | 0.267641 |
| C | 1.248509 | 3.409592 | -0.586126 |
| O | -0.007413 | 2.939406 | -0.105461 |
| H | -1.119722 | 4.370674 | -1.127881 |
| H | -0.990766 | 2.783229 | -1.921944 |
| H | -3.216375 | 3.141144 | -0.971798 |
| H | -2.540647 | 3.429508 | 0.648262 |
| H | -4.430837 | 1.535325 | 0.456088 |
| H | -4.028431 | 0.776780 | -1.093534 |
| H | -4.672570 | -0.924556 | 0.562090 |
| H | -3.532284 | -0.276552 | 1.750880 |
| H | -3.747947 | -2.334499 | -1.167335 |
| H | -2.660377 | -1.060493 | -1.776387 |
| H | -1.794190 | -3.292750 | -2.264149 |
| H | -1.796488 | -3.725582 | -0.538491 |
| H | 0.575505 | -3.962689 | -1.882550 |
| H | 0.476497 | -2.537912 | -2.949172 |
| H | 2.752212 | -2.894417 | -2.060205 |
| H | 2.144813 | -2.804741 | -0.387063 |
| H | 3.585329 | -0.953649 | -0.009103 |
| H | 4.139355 | -0.858481 | -1.700866 |
| H | 4.331760 | 1.336161 | -0.752365 |
| H | 2.975761 | 1.361055 | -1.908630 |
| H | 3.305661 | 3.277429 | 0.032137 |
| H | 2.129885 | 2.984624 | 1.322967 |
| H | 1.377243 | 3.132496 | -1.641353 |
| H | 1.296089 | 4.505360 | -0.516449 |
| C | -0.123484 | -0.290605 | 2.072388 |
| C | 0.990764 | -1.177687 | 2.591508 |
| O | 1.829562 | -1.701540 | 1.906246 |
| O | 0.898484 | -1.303307 | 3.922133 |
| N | 0.007361 | -0.048817 | 0.619006 |
| H | -0.113944 | 0.662981 | 2.601652 |
| H | -1.080865 | -0.777207 | 2.260528 |
| H | 1.608720 | -1.887573 | 4.232267 |
| H | -0.770121 | 0.559844 | 0.312127 |
| H | 0.904020 | 0.418955 | 0.382990 |
| H | -0.058517 | -0.926031 | 0.068186 |

H⁺G[N]-tt(-0/-00/+00/-00/+0+/-00) #127

| | | | |
|---|-----------|-----------|-----------|
| C | -0.032194 | 3.647875 | -0.282803 |
| C | -1.460100 | 3.427413 | -0.727402 |
| O | -1.981847 | 2.249175 | -0.119761 |
| C | -3.256248 | 1.889430 | -0.643019 |
| C | -3.694492 | 0.564913 | -0.063648 |
| O | -2.781028 | -0.459300 | -0.469499 |
| C | -3.291443 | -1.783327 | -0.283331 |
| C | -2.277252 | -2.787057 | -0.780064 |
| O | -1.136048 | -2.747865 | 0.071069 |
| C | -0.116272 | -3.694813 | -0.254220 |
| C | 0.872907 | -3.182991 | -1.287852 |
| O | 1.566526 | -2.065650 | -0.735195 |
| C | 2.687333 | -1.622039 | -1.504729 |
| C | 3.471140 | -0.609070 | -0.686394 |
| O | 2.740019 | 0.584918 | -0.418194 |
| C | 2.883589 | 1.631580 | -1.366716 |
| C | 2.168246 | 2.846454 | -0.819796 |
| O | 0.771485 | 2.548241 | -0.718059 |
| H | 0.030564 | 3.753736 | 0.807972 |
| H | 0.328508 | 4.579329 | -0.735551 |
| H | -1.490000 | 3.326342 | -1.820124 |
| H | -2.062652 | 4.301893 | -0.445003 |
| H | -3.201093 | 1.811711 | -1.736784 |
| H | -4.005349 | 2.652269 | -0.389114 |
| H | -4.699219 | 0.337962 | -0.440718 |
| H | -3.743119 | 0.612945 | 1.031958 |
| H | -4.221922 | -1.901417 | -0.852526 |
| H | -3.508284 | -1.960963 | 0.777835 |
| H | -2.006661 | -2.555459 | -1.818366 |
| H | -2.731586 | -3.786675 | -0.757416 |
| H | -0.562910 | -4.632045 | -0.608275 |
| H | 0.414806 | -3.899882 | 0.677412 |
| H | 0.372500 | -2.895574 | -2.222750 |
| H | 1.584074 | -3.987010 | -1.519453 |
| H | 2.344908 | -1.197520 | -2.458423 |
| H | 3.341304 | -2.475209 | -1.728325 |
| H | 4.411197 | -0.378031 | -1.202558 |
| H | 3.704468 | -1.041659 | 0.287806 |
| H | 2.456897 | 1.353647 | -2.339971 |
| H | 3.943753 | 1.879719 | -1.512201 |
| H | 2.316549 | 3.696321 | -1.497389 |
| H | 2.572371 | 3.105787 | 0.166501 |
| C | -0.347180 | 0.066352 | 1.923124 |
| C | 0.899106 | -0.158158 | 2.760335 |
| O | 1.911265 | -0.667719 | 2.363396 |
| O | 0.686004 | 0.254374 | 4.020248 |
| N | -0.060745 | 0.001884 | 0.470366 |
| H | -0.811608 | 1.023113 | 2.155486 |
| H | -1.056392 | -0.727333 | 2.167598 |
| H | 1.470064 | 0.044453 | 4.552514 |
| H | 0.360659 | 0.878157 | 0.114243 |
| H | -0.957648 | -0.142959 | -0.023856 |
| H | 0.577173 | -0.777612 | 0.223975 |

H⁺G[N]-tt(-00/+00/--0/-0/-0/-0) #1145

| | | | |
|---|-----------|-----------|-----------|
| C | -2.271548 | 2.790680 | 0.308327 |
| C | -1.396544 | 3.268764 | -0.845064 |
| O | -0.072963 | 2.738045 | -0.777258 |
| C | 0.886998 | 3.580239 | -0.150762 |
| C | 2.254118 | 2.959365 | -0.321065 |
| O | 2.304038 | 1.721276 | 0.398620 |
| C | 3.585261 | 1.071438 | 0.386018 |
| C | 3.593579 | -0.163134 | -0.494470 |
| O | 2.736106 | -1.135789 | 0.098217 |
| C | 2.712895 | -2.407987 | -0.549803 |
| C | 1.709584 | -2.494089 | -1.686428 |
| O | 0.393693 | -2.297701 | -1.167049 |
| C | -0.637158 | -2.596047 | -2.119023 |
| C | -1.992431 | -2.354855 | -1.496327 |
| O | -2.157664 | -0.956676 | -1.291640 |
| C | -3.390027 | -0.613952 | -0.668309 |
| C | -3.469511 | 0.891366 | -0.565106 |
| O | -2.440349 | 1.367867 | 0.315587 |
| H | -3.250051 | 3.284663 | 0.264136 |
| H | -1.816989 | 3.045840 | 1.268832 |
| H | -1.375423 | 4.365757 | -0.853872 |
| H | -1.808912 | 2.939568 | -1.801439 |
| H | 0.666711 | 3.711273 | 0.917655 |
| H | 0.893853 | 4.571589 | -0.623131 |
| H | 3.010496 | 3.647043 | 0.075895 |
| H | 2.453563 | 2.789223 | -1.385839 |
| H | 3.814454 | 0.785934 | 1.415967 |
| H | 4.357646 | 1.767882 | 0.045708 |
| H | 4.619508 | -0.552160 | -0.552586 |
| H | 3.263430 | 0.088815 | -1.510986 |
| H | 2.445797 | -3.133872 | 0.221434 |
| H | 3.710531 | -2.664709 | -0.926894 |
| H | 1.785890 | -3.491325 | -2.139886 |
| H | 1.916602 | -1.752889 | -2.469995 |
| H | -0.558982 | -3.648370 | -2.419001 |
| H | -0.514315 | -1.966881 | -3.009246 |
| H | -2.074158 | -2.891597 | -0.543716 |
| H | -2.764406 | -2.734685 | -2.180254 |
| H | -3.454027 | -1.074824 | 0.324292 |
| H | -4.238587 | -0.965407 | -1.272033 |
| H | -4.449185 | 1.181182 | -0.166269 |
| H | -3.350442 | 1.330516 | -1.561133 |
| C | 0.276209 | -0.427270 | 2.046615 |
| C | -0.723238 | -1.450714 | 2.545697 |
| O | -1.603172 | -1.935448 | 1.883256 |
| O | -0.481917 | -1.742097 | 3.831008 |
| N | 0.022101 | -0.055835 | 0.636182 |
| H | 0.227394 | 0.464751 | 2.672839 |
| H | 1.285738 | -0.833650 | 2.119169 |
| H | -1.127975 | -2.401884 | 4.129736 |
| H | -0.910856 | 0.378470 | 0.491815 |
| H | 0.092826 | -0.874217 | 0.002363 |
| H | 0.743847 | 0.626170 | 0.345444 |

H⁺G[N]-tt(-00/+0+/-0+/-0+/-0+/-0) #1335

| | | | |
|---|-----------|-----------|-----------|
| C | 2.392309 | -1.953249 | -1.590709 |
| C | 1.182884 | -2.857279 | -1.600781 |
| O | -0.000050 | -2.065144 | -1.618643 |
| C | -1.182982 | -2.857282 | -1.600667 |
| C | -2.392411 | -1.953258 | -1.590661 |
| O | -2.447627 | -1.254851 | -0.341407 |
| C | -3.646229 | -0.502587 | -0.123166 |
| C | -3.511336 | 0.950006 | -0.536224 |
| O | -2.567575 | 1.569335 | 0.334588 |
| C | -2.360762 | 2.961372 | 0.103734 |
| C | -1.202281 | 3.237142 | -0.838176 |
| O | 0.000091 | 2.758009 | -0.228601 |
| C | 1.202504 | 3.237029 | -0.838185 |
| C | 2.360956 | 2.961208 | 0.103744 |
| O | 2.567664 | 1.569159 | 0.334633 |
| C | 3.511458 | 0.949763 | -0.536095 |
| C | 3.646214 | -0.502841 | -0.123028 |
| O | 2.447583 | -1.255028 | -0.341354 |
| H | 2.343286 | -1.246334 | -2.428249 |
| H | 3.293317 | -2.568021 | -1.704297 |
| H | 1.192249 | -3.501417 | -0.712497 |
| H | 1.226910 | -3.494374 | -2.495278 |
| H | -1.192314 | -3.501328 | -0.712316 |
| H | -1.227035 | -3.494468 | -2.495098 |
| H | -3.293419 | -2.568059 | -1.704108 |
| H | -2.343443 | -1.246462 | -2.428305 |
| H | -3.856363 | -0.555332 | 0.947537 |
| H | -4.482988 | -0.964685 | -0.658044 |
| H | -4.489711 | 1.440974 | -0.442080 |
| H | -3.190789 | 1.028598 | -1.583948 |
| H | -2.143895 | 3.408325 | 1.076752 |
| H | -3.271079 | 3.429225 | -0.289931 |
| H | -1.129337 | 4.320132 | -1.000481 |
| H | -1.348314 | 2.756396 | -1.814719 |
| H | 1.129638 | 4.320018 | -1.000538 |
| H | 1.348511 | 2.756231 | -1.814706 |
| H | 2.144111 | 3.408204 | 1.076748 |
| H | 3.271310 | 3.428985 | -0.289925 |
| H | 4.489861 | 1.440660 | -0.441864 |
| H | 3.191011 | 1.028386 | -1.583848 |
| H | 3.856255 | -0.555600 | 0.947693 |
| H | 4.482985 | -0.965000 | -0.657836 |
| C | -0.000035 | -0.011794 | 2.122126 |
| C | -0.000117 | -1.416665 | 2.695354 |
| O | -0.000143 | -2.422977 | 2.037085 |
| O | -0.000122 | -1.371952 | 4.035226 |
| N | -0.000017 | -0.054139 | 0.642786 |
| H | -0.884233 | 0.528638 | 2.462663 |
| H | 0.884207 | 0.528549 | 2.462692 |
| H | -0.000162 | -2.279977 | 4.377767 |
| H | -0.840626 | -0.539543 | 0.276751 |
| H | 0.840570 | -0.539590 | 0.276772 |
| H | 0.000015 | 0.914049 | 0.277383 |

H⁺G[N]-tt(+00/+00/--0/-00/++0/+0+) #1197

| | | | |
|---|-----------|-----------|-----------|
| C | -2.968412 | -1.667049 | -0.686913 |
| C | -3.618170 | -0.307363 | -0.540909 |
| O | -2.922243 | 0.442104 | 0.456163 |
| C | -3.242811 | 1.833905 | 0.490291 |
| C | -2.396409 | 2.665894 | -0.458828 |
| O | -1.034336 | 2.656437 | -0.017095 |
| C | -0.157339 | 3.367799 | -0.897533 |
| C | 1.206541 | 3.521424 | -0.253512 |
| O | 1.716530 | 2.238924 | 0.107279 |
| C | 3.117545 | 2.054825 | -0.070717 |
| C | 3.523009 | 0.789305 | 0.669831 |
| O | 2.761406 | -0.357897 | 0.278704 |
| C | 3.282908 | -1.091050 | -0.838576 |
| C | 2.267076 | -2.123831 | -1.275805 |
| O | 1.149582 | -1.439680 | -1.836227 |
| C | 0.192857 | -2.257311 | -2.506389 |
| C | -0.974264 | -2.672042 | -1.624038 |
| O | -1.643223 | -1.479700 | -1.186741 |
| H | -3.555392 | -2.265456 | -1.394345 |
| H | -2.946546 | -2.195687 | 0.274781 |
| H | -4.668833 | -0.435108 | -0.249151 |
| H | -3.585578 | 0.209149 | -1.507425 |
| H | -3.070243 | 2.165971 | 1.516767 |
| H | -4.303386 | 1.991725 | 0.260721 |
| H | -2.772720 | 3.697277 | -0.461977 |
| H | -2.457477 | 2.279376 | -1.484683 |
| H | -0.564393 | 4.365802 | -1.104462 |
| H | -0.073191 | 2.823085 | -1.846949 |
| H | 1.142104 | 4.151169 | 0.641569 |
| H | 1.865574 | 4.016975 | -0.976124 |
| H | 3.684015 | 2.894809 | 0.353327 |
| H | 3.352089 | 1.992311 | -1.141537 |
| H | 3.338818 | 0.920354 | 1.738561 |
| H | 4.593971 | 0.602903 | 0.531262 |
| H | 4.211494 | -1.592316 | -0.539586 |
| H | 3.496406 | -0.415015 | -1.673768 |
| H | 1.964870 | -2.743297 | -0.422329 |
| H | 2.734833 | -2.771337 | -2.029463 |
| H | 0.669414 | -3.155447 | -2.918489 |
| H | -0.186563 | -1.660151 | -3.339022 |
| H | -0.646987 | -3.251860 | -0.754405 |
| H | -1.662558 | -3.285246 | -2.219330 |
| C | -0.267487 | -0.244883 | 2.080844 |
| C | -0.031597 | -1.701095 | 2.427021 |
| O | 0.118202 | -2.580597 | 1.616956 |
| O | -0.039110 | -1.877017 | 3.753792 |
| N | -0.034492 | 0.001911 | 0.642993 |
| H | -1.302581 | 0.007421 | 2.316899 |
| H | 0.386511 | 0.394545 | 2.674031 |
| H | 0.081720 | -2.820592 | 3.946717 |
| H | 0.963277 | -0.132054 | 0.392082 |
| H | -0.290863 | 0.976532 | 0.409746 |
| H | -0.611496 | -0.610977 | 0.034382 |

H⁺G[N]-tt(-0/-00/+0+/+00/+00/--0) #492

| | | | |
|---|-----------|-----------|-----------|
| C | 3.592844 | 0.986587 | 0.542300 |
| C | 3.023651 | 2.125519 | -0.292252 |
| O | 1.619420 | 2.253825 | -0.039703 |
| C | 1.063823 | 3.549007 | -0.312576 |
| C | -0.350157 | 3.416934 | -0.838740 |
| O | -1.148421 | 2.712506 | 0.104650 |
| C | -2.527527 | 2.655898 | -0.251963 |
| C | -3.218095 | 1.646516 | 0.647297 |
| O | -2.768012 | 0.305457 | 0.407102 |
| C | -3.520617 | -0.410650 | -0.584525 |
| C | -2.742484 | -1.627431 | -1.035763 |
| O | -1.587257 | -1.174702 | -1.737501 |
| C | -0.868660 | -2.167080 | -2.465031 |
| C | 0.256535 | -2.813608 | -1.670984 |
| O | 1.176562 | -1.782390 | -1.283820 |
| C | 2.490856 | -2.228560 | -0.945391 |
| C | 3.382518 | -1.015191 | -0.787409 |
| O | 2.938441 | -0.263660 | 0.341607 |
| H | 3.468279 | 1.221049 | 1.602239 |
| H | 4.668729 | 0.900162 | 0.342452 |
| H | 3.184946 | 1.967380 | -1.365596 |
| H | 3.546936 | 3.044685 | -0.002348 |
| H | 1.661881 | 4.064533 | -1.071735 |
| H | 1.080962 | 4.143417 | 0.607560 |
| H | -0.350598 | 2.883018 | -1.799184 |
| H | -0.749184 | 4.426956 | -1.007943 |
| H | -2.633118 | 2.367635 | -1.306529 |
| H | -2.994517 | 3.641898 | -0.120365 |
| H | -4.303575 | 1.709497 | 0.516718 |
| H | -2.991116 | 1.868388 | 1.692464 |
| H | -3.713988 | 0.233142 | -1.449379 |
| H | -4.479198 | -0.723183 | -0.153329 |
| H | -3.385636 | -2.220017 | -1.700233 |
| H | -2.464965 | -2.246977 | -0.174882 |
| H | -0.441933 | -1.654295 | -3.330131 |
| H | -1.546801 | -2.948950 | -2.829793 |
| H | 0.764266 | -3.540955 | -2.316800 |
| H | -0.112304 | -3.332647 | -0.779573 |
| H | 2.889137 | -2.860752 | -1.748445 |
| H | 2.471941 | -2.816903 | -0.019004 |
| H | 3.335696 | -0.411845 | -1.701656 |
| H | 4.419353 | -1.343639 | -0.636629 |
| C | 0.267308 | -0.320634 | 2.069114 |
| C | -0.282601 | -1.685127 | 2.431963 |
| O | -0.668663 | -2.501859 | 1.634270 |
| O | -0.253401 | -1.866367 | 3.757498 |
| N | 0.037721 | -0.014407 | 0.642020 |
| H | 1.341390 | -0.319500 | 2.259959 |
| H | -0.194615 | 0.448232 | 2.688783 |
| H | -0.579492 | -2.757762 | 3.960520 |
| H | 0.518521 | 0.868352 | 0.392181 |
| H | -0.973739 | 0.096371 | 0.437910 |
| H | 0.424970 | -0.741995 | 0.009590 |

H⁺G[N]-tt(-0/-00/+0+/-00/-0/-0) #44

| | | | |
|---|-----------|-----------|-----------|
| C | 2.962546 | 2.317145 | 0.196482 |
| C | 1.940661 | 2.891218 | -0.771564 |
| O | 0.634837 | 2.735399 | -0.204426 |
| C | -0.414987 | 3.381001 | -0.934237 |
| C | -1.647283 | 3.436852 | -0.047582 |
| O | -2.116091 | 2.139849 | 0.322685 |
| C | -3.239563 | 1.654542 | -0.410700 |
| C | -3.679933 | 0.345498 | 0.216918 |
| O | -2.693590 | -0.685529 | 0.059323 |
| C | -3.024066 | -1.691929 | -0.909218 |
| C | -1.835521 | -2.601292 | -1.124077 |
| O | -0.810994 | -1.849915 | -1.769087 |
| C | 0.284431 | -2.607075 | -2.276339 |
| C | 1.439788 | -2.730570 | -1.295689 |
| O | 1.898942 | -1.405829 | -0.990177 |
| C | 3.224187 | -1.316050 | -0.465872 |
| C | 3.657556 | 0.132586 | -0.521979 |
| O | 2.839121 | 0.903257 | 0.358786 |
| H | 2.810964 | 2.760599 | 1.183460 |
| H | 3.971489 | 2.582038 | -0.140360 |
| H | 1.989547 | 2.393003 | -1.748637 |
| H | 2.150414 | 3.958240 | -0.919793 |
| H | -0.611877 | 2.837741 | -1.867960 |
| H | -0.114781 | 4.405191 | -1.189394 |
| H | -2.434134 | 4.006193 | -0.555329 |
| H | -1.396397 | 3.956653 | 0.880478 |
| H | -2.985603 | 1.508650 | -1.469431 |
| H | -4.068426 | 2.372756 | -0.350015 |
| H | -4.630498 | 0.028501 | -0.222764 |
| H | -3.832594 | 0.489170 | 1.289598 |
| H | -3.299948 | -1.221827 | -1.860044 |
| H | -3.873064 | -2.282271 | -0.543973 |
| H | -2.153867 | -3.436919 | -1.761817 |
| H | -1.487008 | -3.006385 | -0.166381 |
| H | 0.630122 | -2.077936 | -3.167433 |
| H | -0.042856 | -3.610015 | -2.578041 |
| H | 2.245579 | -3.301642 | -1.773602 |
| H | 1.145192 | -3.242218 | -0.373098 |
| H | 3.911103 | -1.914396 | -1.076668 |
| H | 3.259595 | -1.695796 | 0.563358 |
| H | 3.562310 | 0.493525 | -1.553162 |
| H | 4.710354 | 0.210362 | -0.220374 |
| C | 0.196154 | -0.001582 | 2.053145 |
| C | 0.132348 | -1.427983 | 2.558904 |
| O | 0.106077 | -2.403968 | 1.851992 |
| O | 0.132456 | -1.453840 | 3.896733 |
| N | 0.004610 | 0.051914 | 0.588024 |
| H | 1.175665 | 0.415129 | 2.293959 |
| H | -0.566433 | 0.607270 | 2.539364 |
| H | 0.117762 | -2.377870 | 4.193515 |
| H | 0.681047 | -0.545301 | 0.073348 |
| H | 0.157931 | 1.025183 | 0.267362 |
| H | -0.957841 | -0.230586 | 0.321876 |

H⁺G[N]-tt(-00/+00/-+/-+00/-0/-0) #724

| | | | |
|---|-----------|-----------|-----------|
| C | -3.661770 | 1.014516 | 0.191627 |
| C | -2.916178 | 1.976580 | -0.715445 |
| O | -1.670665 | 2.336191 | -0.109414 |
| C | -1.035044 | 3.448083 | -0.751715 |
| C | 0.309948 | 3.701173 | -0.109202 |
| O | 1.150642 | 2.587765 | -0.380091 |
| C | 2.479194 | 2.712258 | 0.113002 |
| C | 3.285799 | 1.536726 | -0.392974 |
| O | 2.748713 | 0.327996 | 0.152489 |
| C | 3.340295 | -0.881814 | -0.350653 |
| C | 2.808299 | -1.267122 | -1.727815 |
| O | 1.394740 | -1.448146 | -1.743079 |
| C | 0.941974 | -2.782688 | -1.521149 |
| C | -0.534274 | -2.845039 | -1.842672 |
| O | -1.284609 | -2.124175 | -0.855518 |
| C | -2.659076 | -1.958086 | -1.206315 |
| C | -3.421722 | -1.423905 | -0.007201 |
| O | -2.909781 | -0.171672 | 0.450711 |
| H | -4.625915 | 0.773249 | -0.268985 |
| H | -3.856997 | 1.499942 | 1.152965 |
| H | -3.534376 | 2.873420 | -0.853926 |
| H | -2.730553 | 1.531596 | -1.701936 |
| H | -1.663516 | 4.341049 | -0.646835 |
| H | -0.900999 | 3.236013 | -1.819645 |
| H | 0.195596 | 3.847135 | 0.974114 |
| H | 0.736619 | 4.620162 | -0.533852 |
| H | 2.481579 | 2.738367 | 1.211747 |
| H | 2.941903 | 3.639553 | -0.251106 |
| H | 4.331256 | 1.648653 | -0.079547 |
| H | 3.246194 | 1.518050 | -1.487098 |
| H | 3.096505 | -1.647733 | 0.385947 |
| H | 4.431362 | -0.773702 | -0.390427 |
| H | 3.322978 | -2.176404 | -2.064375 |
| H | 3.019953 | -0.483698 | -2.459489 |
| H | 1.119120 | -3.094540 | -0.485087 |
| H | 1.467334 | -3.476219 | -2.191224 |
| H | -0.862887 | -3.891752 | -1.852675 |
| H | -0.711766 | -2.409606 | -2.833373 |
| H | -3.092032 | -2.926346 | -1.491909 |
| H | -2.742243 | -1.279546 | -2.065986 |
| H | -3.329870 | -2.129904 | 0.823204 |
| H | -4.483445 | -1.342242 | -0.264403 |
| C | -0.210330 | -0.104762 | 2.073044 |
| C | 0.507352 | -1.329597 | 2.602507 |
| O | 1.126674 | -2.109734 | 1.925274 |
| O | 0.352317 | -1.423611 | 3.929111 |
| N | -0.034518 | 0.026343 | 0.610468 |
| H | -1.276286 | -0.175299 | 2.291326 |
| H | 0.179881 | 0.785181 | 2.569155 |
| H | 0.816948 | -2.215294 | 4.244301 |
| H | -0.426682 | -0.787150 | 0.101687 |
| H | 0.965855 | 0.134399 | 0.349263 |
| H | -0.544936 | 0.863406 | 0.278807 |

H⁺G[N]-tt(+0+/+00/-0/-0/-0/-00) #10857

| | | | |
|---|-----------|-----------|-----------|
| C | -1.688204 | -2.599202 | -1.592488 |
| C | -2.815682 | -1.692585 | -1.149719 |
| O | -2.341298 | -0.341947 | -1.075347 |
| C | -3.359256 | 0.601626 | -0.727379 |
| C | -2.833282 | 2.002800 | -0.947123 |
| O | -1.770566 | 2.264627 | -0.027631 |
| C | -1.054384 | 3.472930 | -0.279924 |
| C | 0.055254 | 3.283547 | -1.307779 |
| O | 1.032850 | 2.320716 | -0.883790 |
| C | 2.231503 | 2.852155 | -0.306346 |
| C | 3.283293 | 1.765069 | -0.290646 |
| O | 2.853941 | 0.715105 | 0.572770 |
| C | 3.688392 | -0.444075 | 0.558931 |
| C | 3.326992 | -1.433547 | -0.536077 |
| O | 2.030495 | -1.974343 | -0.274136 |
| C | 1.606563 | -2.934399 | -1.248332 |
| C | 0.339356 | -3.605045 | -0.748920 |
| O | -0.722309 | -2.676779 | -0.547588 |
| H | -2.104056 | -3.594857 | -1.795727 |
| H | -1.239899 | -2.215522 | -2.518794 |
| H | -3.629582 | -1.751707 | -1.883305 |
| H | -3.189421 | -2.009809 | -0.170372 |
| H | -4.236910 | 0.455224 | -1.369423 |
| H | -3.662076 | 0.456134 | 0.316210 |
| H | -3.648471 | 2.720680 | -0.786993 |
| H | -2.485513 | 2.099090 | -1.982589 |
| H | -1.734406 | 4.266037 | -0.617364 |
| H | -0.635219 | 3.786670 | 0.679918 |
| H | 0.537556 | 4.245566 | -1.513678 |
| H | -0.351957 | 2.907281 | -2.249097 |
| H | 2.043964 | 3.217440 | 0.710976 |
| H | 2.598455 | 3.687449 | -0.913811 |
| H | 3.434703 | 1.396303 | -1.312459 |
| H | 4.230709 | 2.187583 | 0.070290 |
| H | 4.742188 | -0.158242 | 0.455278 |
| H | 3.565395 | -0.922534 | 1.533312 |
| H | 4.070266 | -2.242022 | -0.540515 |
| H | 3.341790 | -0.957852 | -1.525861 |
| H | 2.385163 | -3.696484 | -1.384138 |
| H | 1.443216 | -2.435353 | -2.213093 |
| H | 0.045833 | -4.394317 | -1.451027 |
| H | 0.536395 | -4.070457 | 0.220387 |
| C | -0.055276 | 0.322889 | 1.957950 |
| C | -1.112128 | -0.502467 | 2.668301 |
| O | -2.043748 | -1.033735 | 2.123788 |
| O | -0.888506 | -0.511859 | 3.989951 |
| N | 0.001840 | 0.003197 | 0.513350 |
| H | -0.338309 | 1.371073 | 2.069898 |
| H | 0.927559 | 0.185376 | 2.403295 |
| H | -1.611220 | -0.992234 | 4.424944 |
| H | 0.592305 | -0.821002 | 0.319807 |
| H | 0.410521 | 0.801510 | -0.004039 |
| H | -0.937590 | -0.175876 | 0.107690 |

H⁺G[N]-tt(-0/-00/-0/-00/+00/-0) #1242

| | | | |
|---|-----------|-----------|-----------|
| C | 2.110549 | 2.915528 | -0.465974 |
| C | 2.982264 | 1.735465 | -0.830458 |
| O | 2.795396 | 0.714754 | 0.143623 |
| C | 3.539248 | -0.483429 | -0.071393 |
| C | 3.072428 | -1.303294 | -1.268512 |
| O | 1.656453 | -1.461484 | -1.206513 |
| C | 1.159147 | -2.530885 | -2.013396 |
| C | -0.347769 | -2.428498 | -2.118680 |
| O | -0.901514 | -2.532158 | -0.814074 |
| C | -2.304139 | -2.756231 | -0.746637 |
| C | -3.127751 | -1.481252 | -0.828773 |
| O | -2.786088 | -0.644978 | 0.283545 |
| C | -3.649542 | 0.478558 | 0.492178 |
| C | -3.303678 | 1.678472 | -0.370750 |
| O | -2.002161 | 2.132654 | -0.018186 |
| C | -1.557035 | 3.231554 | -0.805872 |
| C | -0.167870 | 3.631497 | -0.365451 |
| O | 0.733575 | 2.546831 | -0.599322 |
| H | 2.335365 | 3.749018 | -1.143211 |
| H | 2.317597 | 3.239537 | 0.562138 |
| H | 4.032035 | 2.058940 | -0.848541 |
| H | 2.710288 | 1.379269 | -1.830892 |
| H | 3.407704 | -1.067435 | 0.840974 |
| H | 4.608750 | -0.260868 | -0.185426 |
| H | 3.574154 | -2.278437 | -1.221078 |
| H | 3.345060 | -0.835700 | -2.223454 |
| H | 1.442775 | -3.490526 | -1.565458 |
| H | 1.586784 | -2.471581 | -3.022822 |
| H | -0.707226 | -3.247716 | -2.756335 |
| H | -0.625796 | -1.477772 | -2.594572 |
| H | -2.482706 | -3.237435 | 0.217107 |
| H | -2.627938 | -3.443057 | -1.539603 |
| H | -4.191937 | -1.744275 | -0.777643 |
| H | -2.952667 | -0.953037 | -1.774302 |
| H | -3.545541 | 0.744746 | 1.546135 |
| H | -4.691372 | 0.187005 | 0.316661 |
| H | -4.047936 | 2.467469 | -0.192006 |
| H | -3.337764 | 1.424015 | -1.439245 |
| H | -2.229186 | 4.091478 | -0.680441 |
| H | -1.547479 | 2.954010 | -1.868531 |
| H | -0.163354 | 3.902442 | 0.698302 |
| H | 0.144497 | 4.508928 | -0.945499 |
| C | 0.289537 | 0.250387 | 2.095456 |
| C | 0.572789 | -1.036737 | 2.847145 |
| O | 0.887811 | -2.071399 | 2.322705 |
| O | 0.465405 | -0.841744 | 4.169142 |
| N | 0.011213 | -0.018524 | 0.665240 |
| H | -0.548641 | 0.787080 | 2.537116 |
| H | 1.179815 | 0.878599 | 2.159201 |
| H | 0.704142 | -1.664312 | 4.626000 |
| H | 0.158126 | 0.851110 | 0.125640 |
| H | -0.965636 | -0.332603 | 0.519096 |
| H | 0.639512 | -0.735851 | 0.263360 |

H⁺G[N]-tt(-00/+0/+0/+0/+00/--0) #1783

| | | | |
|---|-----------|-----------|-----------|
| C | 2.935881 | 2.120685 | -0.339303 |
| C | 1.933120 | 3.204399 | -0.017060 |
| O | 0.630997 | 2.765616 | -0.388976 |
| C | -0.372501 | 3.758384 | -0.208888 |
| C | -1.714874 | 3.171572 | -0.582058 |
| O | -2.020678 | 2.108589 | 0.328224 |
| C | -3.363761 | 1.606697 | 0.257019 |
| C | -3.495873 | 0.386509 | -0.635972 |
| O | -2.757850 | -0.676560 | -0.042241 |
| C | -2.803733 | -1.921823 | -0.743607 |
| C | -1.887994 | -1.953746 | -1.960966 |
| O | -0.525057 | -1.684357 | -1.611934 |
| C | 0.380605 | -2.794970 | -1.689374 |
| C | 1.789357 | -2.275110 | -1.873690 |
| O | 2.172161 | -1.517929 | -0.731136 |
| C | 3.462346 | -0.937635 | -0.837661 |
| C | 3.682877 | -0.056517 | 0.380005 |
| O | 2.706603 | 0.986509 | 0.504832 |
| H | 3.946842 | 2.507866 | -0.161560 |
| H | 2.847861 | 1.841286 | -1.395201 |
| H | 2.205524 | 4.108472 | -0.578864 |
| H | 1.962983 | 3.443797 | 1.054484 |
| H | -0.171648 | 4.627659 | -0.850163 |
| H | -0.391065 | 4.096819 | 0.835776 |
| H | -1.692742 | 2.801953 | -1.614446 |
| H | -2.478090 | 3.955096 | -0.506040 |
| H | -4.040025 | 2.394868 | -0.090516 |
| H | -3.647796 | 1.340950 | 1.277856 |
| H | -3.129904 | 0.608875 | -1.646611 |
| H | -4.558323 | 0.115160 | -0.712395 |
| H | -3.832732 | -2.147400 | -1.055089 |
| H | -2.490025 | -2.674925 | -0.019191 |
| H | -2.183703 | -1.198380 | -2.695090 |
| H | -1.977241 | -2.932568 | -2.444464 |
| H | 0.131190 | -3.418595 | -2.555382 |
| H | 0.310671 | -3.399286 | -0.779765 |
| H | 1.841768 | -1.647136 | -2.773358 |
| H | 2.465178 | -3.131399 | -2.008464 |
| H | 3.543572 | -0.360481 | -1.769270 |
| H | 4.241941 | -1.712861 | -0.858915 |
| H | 4.690938 | 0.373469 | 0.353862 |
| H | 3.591442 | -0.655950 | 1.287813 |
| C | -0.277281 | -0.266435 | 2.126598 |
| C | -0.175791 | -1.751932 | 2.416264 |
| O | -0.209240 | -2.617639 | 1.581669 |
| O | -0.088976 | -1.961914 | 3.736155 |
| N | -0.021061 | 0.040656 | 0.699031 |
| H | 0.414869 | 0.294291 | 2.753734 |
| H | -1.291787 | 0.047439 | 2.377481 |
| H | -0.083486 | -2.918236 | 3.902213 |
| H | -0.597939 | 0.853132 | 0.422952 |
| H | -0.270957 | -0.739268 | 0.063156 |
| H | 0.972169 | 0.281786 | 0.531663 |

Structures (His)H⁺-18C6H⁺H[Na]-cggc(-00/+00/--0/-00/-00/--0) 695

| | | | |
|---|-----------|-----------|-----------|
| C | -0.121408 | -2.435791 | 2.835191 |
| C | -0.870243 | -1.202335 | 3.284493 |
| O | -0.190293 | -0.035023 | 2.815610 |
| C | -0.635671 | 1.170728 | 3.437051 |
| C | 0.285655 | 2.304710 | 3.051501 |
| O | 0.185882 | 2.536858 | 1.652369 |
| C | 1.029192 | 3.591429 | 1.196820 |
| C | 0.929517 | 3.672404 | -0.315044 |
| O | 1.453516 | 2.514690 | -0.969484 |
| C | 2.846990 | 2.601214 | -1.302548 |
| C | 3.289606 | 1.318443 | -1.965307 |
| O | 3.279773 | 0.268791 | -1.004466 |
| C | 3.694158 | -0.977976 | -1.555782 |
| C | 3.591432 | -2.050018 | -0.497181 |
| O | 2.214364 | -2.292779 | -0.190366 |
| C | 2.020682 | -3.373959 | 0.715724 |
| C | 0.531895 | -3.637469 | 0.865455 |
| O | -0.191603 | -2.536393 | 1.417663 |
| H | -0.581449 | -3.319064 | 3.299793 |
| H | 0.918882 | -2.369568 | 3.176039 |
| H | -0.904962 | -1.194836 | 4.381314 |
| H | -1.900658 | -1.218404 | 2.906024 |
| H | -0.614890 | 1.056308 | 4.528461 |
| H | -1.667797 | 1.395145 | 3.135935 |
| H | 1.320039 | 2.052035 | 3.320308 |
| H | -0.006205 | 3.203433 | 3.612884 |
| H | 2.065195 | 3.406532 | 1.511403 |
| H | 0.709345 | 4.549140 | 1.631850 |
| H | 1.443726 | 4.572532 | -0.670338 |
| H | -0.120242 | 3.748838 | -0.608061 |
| H | 3.444994 | 2.780062 | -0.401046 |
| H | 2.998852 | 3.436043 | -1.997646 |
| H | 4.305681 | 1.464726 | -2.359053 |
| H | 2.622499 | 1.072185 | -2.799925 |
| H | 4.739833 | -0.914762 | -1.889098 |
| H | 3.063942 | -1.237400 | -2.413770 |
| H | 4.127373 | -1.745489 | 0.411103 |
| H | 4.048088 | -2.971588 | -0.880012 |
| H | 2.491833 | -3.145648 | 1.681463 |
| H | 2.494522 | -4.283453 | 0.321173 |
| H | 0.382387 | -4.537916 | 1.474932 |
| H | 0.096835 | -3.819122 | -0.119486 |
| C | -4.439927 | 0.916852 | -0.166916 |
| C | -3.342652 | 0.442189 | -0.837097 |
| N | -3.741972 | -0.536735 | -1.724265 |
| C | -5.048300 | -0.653292 | -1.603530 |
| N | -5.514690 | 0.211280 | -0.670058 |
| C | -1.902556 | 0.855531 | -0.740256 |
| C | -0.918577 | -0.335621 | -0.863360 |
| H | -1.341504 | -1.217094 | -0.377450 |

| | | | |
|---|-----------|-----------|-----------|
| C | -0.552532 | -0.695191 | -2.323459 |
| O | -1.541483 | -1.089560 | -3.099670 |
| O | 0.592576 | -0.619716 | -2.702583 |
| N | 0.352240 | -0.032277 | -0.140100 |
| H | -4.555283 | 1.674700 | 0.589288 |
| H | -5.679936 | -1.331536 | -2.154826 |
| H | -6.479318 | 0.320458 | -0.394441 |
| H | -1.733700 | 1.354264 | 0.216618 |
| H | -1.668925 | 1.593810 | -1.516041 |
| H | 1.041273 | -0.795054 | -0.265238 |
| H | 0.175539 | 0.058107 | 0.872636 |
| H | 0.792264 | 0.843497 | -0.478432 |
| H | -2.442697 | -1.022789 | -2.652531 |

H⁺H[Na]-cggc(--0/-00/+0/+00/-00/+00) 293

| | | | |
|---|-----------|-----------|-----------|
| C | 1.629979 | -3.266490 | 1.529691 |
| C | 0.139421 | -3.218797 | 1.819320 |
| O | -0.358369 | -1.908114 | 2.088550 |
| C | -0.071397 | -1.420804 | 3.394569 |
| C | -0.696900 | -0.055615 | 3.563132 |
| O | -0.068625 | 0.873066 | 2.675669 |
| C | -0.408727 | 2.232191 | 2.955353 |
| C | 0.350822 | 3.143388 | 2.018765 |
| O | -0.111427 | 2.915544 | 0.691910 |
| C | 0.412647 | 3.797802 | -0.298630 |
| C | 1.857773 | 3.527526 | -0.679225 |
| O | 1.986936 | 2.206831 | -1.195942 |
| C | 3.322668 | 1.930473 | -1.639107 |
| C | 3.444907 | 0.493422 | -2.084501 |
| O | 3.311100 | -0.357213 | -0.951353 |
| C | 3.501920 | -1.732193 | -1.268919 |
| C | 3.287949 | -2.554944 | -0.021435 |
| O | 1.913462 | -2.480709 | 0.376675 |
| H | 1.911019 | -4.313626 | 1.350374 |
| H | 2.221507 | -2.907572 | 2.382843 |
| H | -0.085769 | -3.892357 | 2.656637 |
| H | -0.410773 | -3.571680 | 0.944512 |
| H | 1.010186 | -1.347781 | 3.560452 |
| H | -0.491875 | -2.097048 | 4.151921 |
| H | -0.552852 | 0.269085 | 4.601527 |
| H | -1.774502 | -0.099515 | 3.359479 |
| H | -0.136785 | 2.475935 | 3.990524 |
| H | -1.489593 | 2.383724 | 2.836431 |
| H | 1.425656 | 2.942853 | 2.103253 |
| H | 0.168377 | 4.186233 | 2.312668 |
| H | 0.323403 | 4.840821 | 0.033761 |
| H | -0.225913 | 3.666028 | -1.174485 |
| H | 2.531843 | 3.658339 | 0.178087 |
| H | 2.150670 | 4.262474 | -1.442274 |
| H | 4.026801 | 2.128385 | -0.821132 |
| H | 3.570111 | 2.590217 | -2.480689 |
| H | 4.435378 | 0.362221 | -2.543546 |

| | | | |
|---|-----------|-----------|-----------|
| H | 2.680702 | 0.250864 | -2.831511 |
| H | 4.527901 | -1.900689 | -1.626257 |
| H | 2.800484 | -2.040337 | -2.051780 |
| H | 3.927493 | -2.188014 | 0.791572 |
| H | 3.552091 | -3.599349 | -0.230774 |
| C | -4.464395 | 0.860164 | -0.383284 |
| C | -3.359403 | 0.258452 | -0.926151 |
| N | -3.743411 | -0.906866 | -1.559351 |
| C | -5.048419 | -1.010390 | -1.412599 |
| N | -5.528193 | 0.041654 | -0.706174 |
| C | -1.925773 | 0.705254 | -0.926896 |
| C | -0.930825 | -0.473917 | -0.785094 |
| H | -1.356095 | -1.228001 | -0.120627 |
| C | -0.565399 | -1.130424 | -2.135776 |
| O | 0.570704 | -1.088257 | -2.547736 |
| O | -1.544070 | -1.723716 | -2.786510 |
| N | 0.340936 | -0.032350 | -0.133239 |
| H | -4.590687 | 1.770725 | 0.177357 |
| H | -5.669661 | -1.807235 | -1.789382 |
| H | -6.494617 | 0.198338 | -0.461591 |
| H | -1.762143 | 1.407008 | -0.107628 |
| H | -1.703685 | 1.253590 | -1.849951 |
| H | 0.152373 | 0.322822 | 0.818271 |
| H | 0.839015 | 0.706264 | -0.656758 |
| H | 0.991316 | -0.832491 | -0.039694 |
| H | -2.445482 | -1.577346 | -2.355641 |

H⁺H[N α]-cggc(-00/+00/-00/+00/-00/+00) 400

| | | | |
|---|-----------|-----------|-----------|
| C | -1.041336 | 2.761459 | 2.451050 |
| C | -0.809707 | 3.515683 | 1.162065 |
| O | 0.375619 | 3.023707 | 0.558496 |
| C | 0.751697 | 3.703496 | -0.634711 |
| C | 2.186446 | 3.363473 | -0.963595 |
| O | 2.322119 | 1.972692 | -1.243595 |
| C | 3.694225 | 1.612417 | -1.456746 |
| C | 3.832038 | 0.123730 | -1.661665 |
| O | 3.500519 | -0.543814 | -0.448459 |
| C | 3.653800 | -1.955538 | -0.532751 |
| C | 3.253117 | -2.566665 | 0.788143 |
| O | 1.851260 | -2.366428 | 1.019289 |
| C | 1.430288 | -2.917522 | 2.265518 |
| C | -0.041551 | -2.651347 | 2.483564 |
| O | -0.240326 | -1.246116 | 2.583926 |
| C | -1.531793 | -0.857092 | 3.028111 |
| C | -1.499640 | 0.618613 | 3.354250 |
| O | -1.242244 | 1.374974 | 2.169824 |
| H | -1.924151 | 3.175294 | 2.956618 |
| H | -0.174180 | 2.881876 | 3.112235 |
| H | -0.710567 | 4.585378 | 1.393512 |
| H | -1.669545 | 3.398635 | 0.486041 |
| H | 0.680852 | 4.790512 | -0.494255 |
| H | 0.083647 | 3.424685 | -1.461829 |

| | | | |
|---|-----------|-----------|-----------|
| H | 2.827676 | 3.634390 | -0.115093 |
| H | 2.500542 | 3.953331 | -1.835753 |
| H | 4.287985 | 1.925829 | -0.589053 |
| H | 4.073430 | 2.132569 | -2.346057 |
| H | 4.875879 | -0.085694 | -1.936822 |
| H | 3.180929 | -0.219761 | -2.471852 |
| H | 4.704410 | -2.214785 | -0.728224 |
| H | 3.038113 | -2.356477 | -1.345250 |
| H | 3.824732 | -2.108892 | 1.605045 |
| H | 3.469304 | -3.642422 | 0.768108 |
| H | 2.009746 | -2.472550 | 3.084448 |
| H | 1.600592 | -4.002462 | 2.269445 |
| H | -0.351874 | -3.149324 | 3.412155 |
| H | -0.636884 | -3.070741 | 1.659759 |
| H | -1.809783 | -1.408290 | 3.936867 |
| H | -2.289287 | -1.068573 | 2.259330 |
| H | -0.712256 | 0.809981 | 4.093825 |
| H | -2.463780 | 0.917696 | 3.786990 |
| C | -4.313417 | 0.537679 | -1.018773 |
| C | -3.114101 | -0.057508 | -1.312558 |
| N | -3.349048 | -1.312465 | -1.836882 |
| C | -4.655898 | -1.476231 | -1.870335 |
| N | -5.280332 | -0.376688 | -1.384226 |
| C | -1.718444 | 0.480227 | -1.160771 |
| C | -0.681980 | -0.607776 | -0.787983 |
| H | -1.142357 | -1.321445 | -0.102624 |
| C | -0.126639 | -1.380074 | -2.008702 |
| O | -0.983272 | -2.121426 | -2.678261 |
| O | 1.041306 | -1.291754 | -2.303620 |
| N | 0.474440 | -0.011607 | -0.048096 |
| H | -4.562378 | 1.498545 | -0.601651 |
| H | -5.178399 | -2.349155 | -2.227895 |
| H | -6.278563 | -0.248926 | -1.307511 |
| H | -1.723035 | 1.228711 | -0.368482 |
| H | -1.400536 | 0.981539 | -2.082152 |
| H | 1.095630 | -0.762128 | 0.308623 |
| H | 0.130976 | 0.524141 | 0.761639 |
| H | 1.062472 | 0.614915 | -0.626089 |
| H | -1.937215 | -1.987890 | -2.375079 |

H⁺H[N α]-cggc(+00/-00/+00/--0/-00/+0+) 6092

| | | | |
|---|-----------|-----------|-----------|
| C | 2.919259 | 2.346796 | -1.535495 |
| C | 3.423426 | 0.998226 | -1.993156 |
| O | 3.299926 | 0.057944 | -0.931453 |
| C | 3.744694 | -1.241950 | -1.307504 |
| C | 3.451846 | -2.214997 | -0.188918 |
| O | 2.033356 | -2.384921 | -0.083200 |
| C | 1.597776 | -3.463657 | 0.744371 |
| C | 1.379762 | -3.053976 | 2.187865 |
| O | 0.343390 | -2.078167 | 2.228257 |
| C | 0.089444 | -1.592531 | 3.538214 |
| C | -0.902170 | -0.454259 | 3.470245 |

| | | | | | | |
|---|-----------|-----------|-----------|--|-----------|---------------------|
| O | -0.320840 | 0.635000 | 2.748863 | | | |
| C | -0.934659 | 1.896412 | 3.009829 | H ⁺ H[Na]-cggc(+0+/-00/-00/+0+/-00/-00) | 3671 | |
| C | -0.070701 | 2.998751 | 2.442133 | C | 3.983793 | -0.154149 -1.347279 |
| O | -0.024568 | 2.877968 | 1.027094 | C | 3.484503 | -1.579537 -1.411039 |
| C | 0.817754 | 3.845594 | 0.408302 | O | 2.636535 | -1.842474 -0.287355 |
| C | 0.879803 | 3.551553 | -1.078911 | C | 2.215204 | -3.205533 -0.224698 |
| O | 1.494340 | 2.297897 | -1.379264 | C | 1.504203 | -3.448919 1.086424 |
| H | 3.171336 | 3.096036 | -2.295997 | O | 0.270411 | -2.728232 1.099973 |
| H | 3.401230 | 2.627724 | -0.591479 | C | -0.433711 | -2.786648 2.335149 |
| H | 4.478070 | 1.103273 | -2.285446 | C | 0.016005 | -1.733776 3.332856 |
| H | 2.848240 | 0.659491 | -2.862905 | O | -0.266850 | -0.431775 2.811445 |
| H | 4.828073 | -1.232046 | -1.494155 | C | 0.074489 | 0.607208 3.730703 |
| H | 3.230198 | -1.565052 | -2.219776 | C | -0.295931 | 1.950207 3.145725 |
| H | 3.917147 | -3.178983 | -0.427782 | O | 0.491103 | 2.177792 1.985503 |
| H | 3.869876 | -1.846681 | 0.755976 | C | 0.338593 | 3.477387 1.428296 |
| H | 0.654695 | -3.815210 | 0.318777 | C | 1.351563 | 3.659242 0.322019 |
| H | 2.316766 | -4.289671 | 0.700124 | O | 1.048910 | 2.777244 -0.760126 |
| H | 2.299249 | -2.641055 | 2.625324 | C | 1.958836 | 2.881702 -1.865126 |
| H | 1.095922 | -3.940741 | 2.772882 | C | 3.240430 | 2.093007 -1.655692 |
| H | 1.021922 | -1.238573 | 3.998091 | O | 2.883960 | 0.730322 -1.516178 |
| H | -0.325134 | -2.390102 | 4.171271 | H | 4.717358 | -0.008876 -2.152643 |
| H | -1.832760 | -0.777128 | 2.985341 | H | 4.483130 | 0.037056 -0.387194 |
| H | -1.140224 | -0.140049 | 4.494044 | H | 4.348173 | -2.257042 -1.384074 |
| H | -1.941572 | 1.931544 | 2.571734 | H | 2.927292 | -1.741960 -2.339064 |
| H | -1.029521 | 2.048386 | 4.092581 | H | 3.089514 | -3.868162 -0.273154 |
| H | -0.496412 | 3.969676 | 2.732780 | H | 1.557370 | -3.434337 -1.071488 |
| H | 0.941725 | 2.927570 | 2.861538 | H | 2.149555 | -3.131718 1.914724 |
| H | 0.412987 | 4.856898 | 0.558258 | H | 1.305773 | -4.523928 1.191957 |
| H | 1.819354 | 3.814472 | 0.858370 | H | -0.336464 | -3.779505 2.792690 |
| H | 1.407595 | 4.363437 | -1.592621 | H | -1.489568 | -2.632407 2.097731 |
| H | -0.134112 | 3.501863 | -1.482706 | H | 1.089176 | -1.819811 3.547137 |
| C | -4.508204 | 0.586872 | -0.345839 | H | -0.529697 | -1.881672 4.274783 |
| C | -3.367635 | 0.075143 | -0.907922 | H | 1.150489 | 0.577916 3.944529 |
| N | -3.682158 | -1.073687 | -1.605872 | H | -0.470764 | 0.464794 4.672998 |
| C | -4.980605 | -1.254777 | -1.478906 | H | -0.103212 | 2.725934 3.899707 |
| N | -5.523086 | -0.269689 | -0.722798 | H | -1.366919 | 1.976179 2.897800 |
| C | -1.960261 | 0.598708 | -0.874268 | H | 0.516670 | 4.244109 2.194908 |
| C | -0.897783 | -0.528269 | -0.824471 | H | -0.680584 | 3.614359 1.040071 |
| H | -1.274859 | -1.362970 | -0.229486 | H | 2.355077 | 3.461866 0.715826 |
| C | -0.497345 | -1.049679 | -2.227986 | H | 1.313372 | 4.698633 -0.029482 |
| O | -1.442978 | -1.658921 | -2.917123 | H | 2.190813 | 3.935121 -2.061645 |
| O | 0.625776 | -0.894441 | -2.641602 | H | 1.426707 | 2.478418 -2.728345 |
| N | 0.347186 | -0.055950 | -0.149655 | H | 3.792420 | 2.442424 -0.771098 |
| H | -4.689988 | 1.459623 | 0.258100 | H | 3.889488 | 2.240459 -2.531425 |
| H | -5.554443 | -2.062686 | -1.904260 | C | -4.464556 | 0.984084 -0.054971 |
| H | -6.498577 | -0.178737 | -0.480791 | C | -3.419590 | 0.459816 -0.770435 |
| H | -1.832583 | 1.245837 | -0.004575 | N | -3.902826 | -0.490987 -1.644580 |
| H | -1.771196 | 1.227796 | -1.751647 | C | -5.207146 | -0.545417 -1.472358 |
| H | 0.156767 | 0.216686 | 0.827139 | N | -5.592043 | 0.336023 -0.517664 |
| H | 1.050150 | -0.820246 | -0.139777 | C | -1.959465 | 0.803402 -0.729288 |
| H | 0.775125 | 0.752034 | -0.640558 | C | -1.017160 | -0.425014 -0.740033 |
| H | -2.342260 | -1.609747 | -2.468149 | H | -1.433550 | -1.216777 -0.114413 |

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|---|-----------|-----------|-----------|
| C | -0.724620 | -1.064102 | -2.124998 |
| O | 0.415786 | -1.312193 | -2.440105 |
| O | -1.753276 | -1.350118 | -2.891933 |
| N | 0.295570 | -0.054236 | -0.123944 |
| H | -4.512436 | 1.740106 | 0.710204 |
| H | -5.892230 | -1.189589 | -2.000136 |
| H | -6.538328 | 0.491187 | -0.203101 |
| H | -1.765458 | 1.369168 | 0.184296 |
| H | -1.700117 | 1.465035 | -1.563119 |
| H | 0.217483 | -0.065325 | 0.904169 |
| H | 0.618044 | 0.885362 | -0.410110 |
| H | 1.041222 | -0.724595 | -0.391554 |
| H | -2.649971 | -1.110315 | -2.489499 |

H⁺H[Na]-cggc(+00/-00/+0+/-00/-00/+0+) 7638

| | | | |
|---|-----------|-----------|-----------|
| C | 3.374676 | -2.118454 | -0.964420 |
| C | 2.944729 | -2.789035 | 0.318712 |
| O | 1.537857 | -2.582799 | 0.500484 |
| C | 0.967918 | -3.261552 | 1.620613 |
| C | 1.003153 | -2.436282 | 2.892287 |
| O | 0.191129 | -1.280811 | 2.706090 |
| C | 0.235285 | -0.390840 | 3.812260 |
| C | -0.620496 | 0.820189 | 3.523010 |
| O | -0.077936 | 1.536493 | 2.410323 |
| C | -0.547794 | 2.882096 | 2.318853 |
| C | 0.211602 | 3.606042 | 1.231035 |
| O | -0.118536 | 3.020994 | -0.023156 |
| C | 0.490692 | 3.636270 | -1.156879 |
| C | 1.954624 | 3.278001 | -1.343936 |
| O | 2.084265 | 1.872828 | -1.532221 |
| C | 3.440915 | 1.479943 | -1.774757 |
| C | 3.526752 | -0.006845 | -2.021400 |
| O | 3.252808 | -0.708110 | -0.812224 |
| H | 2.747621 | -2.463941 | -1.794139 |
| H | 4.419515 | -2.389792 | -1.172695 |
| H | 3.506830 | -2.378047 | 1.166064 |
| H | 3.148896 | -3.864417 | 0.248166 |
| H | 1.480254 | -4.216176 | 1.786589 |
| H | -0.069550 | -3.479523 | 1.355332 |
| H | 2.031280 | -2.136825 | 3.137871 |
| H | 0.619962 | -3.042112 | 3.726010 |
| H | 1.270260 | -0.076445 | 4.003266 |
| H | -0.146758 | -0.883095 | 4.718011 |
| H | -0.623107 | 1.461991 | 4.412951 |
| H | -1.655532 | 0.521942 | 3.311126 |
| H | -0.378825 | 3.398653 | 3.272434 |
| H | -1.625222 | 2.897026 | 2.106604 |
| H | 1.287450 | 3.536380 | 1.431400 |
| H | -0.074715 | 4.666961 | 1.242869 |
| H | 0.394624 | 4.728604 | -1.097655 |
| H | -0.080672 | 3.292443 | -2.021600 |
| H | 2.561193 | 3.597970 | -0.485868 |

| | | | |
|---|-----------|-----------|-----------|
| H | 2.327926 | 3.812905 | -2.228595 |
| H | 4.063537 | 1.757119 | -0.914371 |
| H | 3.817255 | 2.006517 | -2.661330 |
| H | 4.544697 | -0.236257 | -2.367635 |
| H | 2.815275 | -0.307689 | -2.798474 |
| C | -4.541599 | 0.623595 | -0.365718 |
| C | -3.417553 | 0.003687 | -0.845640 |
| N | -3.753722 | -1.256749 | -1.298541 |
| C | -5.049105 | -1.399442 | -1.106305 |
| N | -5.568501 | -0.281745 | -0.543400 |
| C | -2.008032 | 0.513120 | -0.946380 |
| C | -0.956242 | -0.596858 | -0.699245 |
| H | -1.336946 | -1.295979 | 0.048056 |
| C | -0.594741 | -1.376855 | -1.986507 |
| O | -1.554137 | -2.107386 | -2.517413 |
| O | 0.513898 | -1.295993 | -2.459445 |
| N | 0.313361 | -0.044138 | -0.136704 |
| H | -4.704328 | 1.598330 | 0.061840 |
| H | -5.636332 | -2.269995 | -1.351695 |
| H | -6.537022 | -0.137739 | -0.299235 |
| H | -1.855156 | 1.319080 | -0.228076 |
| H | -1.837707 | 0.955519 | -1.934670 |
| H | 0.141560 | 0.479953 | 0.736219 |
| H | 0.816026 | 0.580700 | -0.788816 |
| H | 0.949885 | -0.832649 | 0.082482 |
| H | -2.443639 | -1.965395 | -2.064928 |

H⁺H[Na]-cggc(+00/-00/+00/-0/-00/+0+) 13344

| | | | |
|---|-----------|-----------|-----------|
| C | -3.506548 | 0.900974 | -1.896560 |
| C | -3.923129 | -0.504197 | -1.529094 |
| O | -2.763887 | -1.311147 | -1.358036 |
| C | -3.045819 | -2.675225 | -1.109078 |
| C | -1.722845 | -3.393463 | -0.905696 |
| O | -0.949489 | -2.864062 | 0.180155 |
| C | -1.419499 | -3.251505 | 1.473312 |
| C | -0.447125 | -2.788203 | 2.532825 |
| O | -0.458624 | -1.366935 | 2.594271 |
| C | 0.345204 | -0.839000 | 3.640449 |
| C | 0.229309 | 0.668123 | 3.631694 |
| O | 0.762293 | 1.163276 | 2.400963 |
| C | 0.906829 | 2.586628 | 2.337885 |
| C | -0.378293 | 3.314806 | 1.986854 |
| O | -0.807932 | 2.882590 | 0.705899 |
| C | -2.040567 | 3.475564 | 0.299784 |
| C | -2.496239 | 2.867522 | -1.006404 |
| O | -2.798123 | 1.488097 | -0.800006 |
| H | -4.410323 | 1.488586 | -2.106092 |
| H | -2.870685 | 0.889429 | -2.786622 |
| H | -4.549109 | -0.904047 | -2.339094 |
| H | -4.517359 | -0.497538 | -0.604742 |
| H | -3.563547 | -3.132946 | -1.964998 |
| H | -3.702242 | -2.780093 | -0.233302 |

H⁺H[N_α]-cggc(-0/-00/-00/-00/-00/--0) 11

| | | | |
|---|-----------|-----------|-----------|
| C | -0.825708 | 1.623003 | 3.163278 |
| C | 0.147803 | 2.677836 | 2.685795 |
| O | 0.123639 | 2.727162 | 1.263668 |
| C | 1.034521 | 3.675300 | 0.710188 |
| C | 0.979344 | 3.573300 | -0.803617 |
| O | 1.475139 | 2.319796 | -1.285018 |
| C | 2.846389 | 2.341591 | -1.715138 |
| C | 3.351467 | 0.927212 | -1.893342 |
| O | 3.443227 | 0.324588 | -0.605064 |
| C | 4.155777 | -0.908086 | -0.548683 |
| C | 3.289764 | -2.132346 | -0.799683 |
| O | 2.279870 | -2.166947 | 0.218349 |
| C | 1.548479 | -3.387840 | 0.318161 |
| C | 0.880354 | -3.427399 | 1.676871 |
| O | -0.033520 | -2.336264 | 1.801467 |
| C | -0.361625 | -2.036778 | 3.152082 |
| C | -1.161204 | -0.753820 | 3.222764 |
| O | -0.366341 | 0.336568 | 2.745481 |
| H | -1.828656 | 1.819785 | 2.761130 |
| H | -0.881319 | 1.659504 | 4.258646 |
| H | 1.159067 | 2.438735 | 3.040253 |
| H | -0.145647 | 3.648590 | 3.108992 |
| H | 2.051208 | 3.477882 | 1.075552 |
| H | 0.752829 | 4.693439 | 1.014573 |
| H | 1.542019 | 4.400400 | -1.248917 |
| H | -0.057591 | 3.656318 | -1.138593 |
| H | 3.464771 | 2.855586 | -0.970813 |
| H | 2.914644 | 2.879271 | -2.668498 |
| H | 4.344003 | 0.975479 | -2.362204 |
| H | 2.680875 | 0.360369 | -2.549212 |
| H | 4.569453 | -0.965601 | 0.460678 |
| H | 4.989711 | -0.904960 | -1.262594 |
| H | 3.920487 | -3.027788 | -0.723557 |
| H | 2.820647 | -2.111357 | -1.787820 |
| H | 2.227582 | -4.245988 | 0.240900 |
| H | 0.815153 | -3.464384 | -0.494595 |
| H | 1.650382 | -3.350940 | 2.454011 |
| H | 0.353380 | -4.382934 | 1.801322 |
| H | 0.557077 | -1.924282 | 3.742075 |
| H | -0.958264 | -2.846635 | 3.595939 |
| H | -1.438661 | -0.581523 | 4.270040 |
| H | -2.084578 | -0.832165 | 2.633857 |
| C | -4.391589 | 0.952423 | -0.423322 |
| C | -3.285269 | 0.356411 | -0.970399 |
| N | -3.679214 | -0.751960 | -1.692614 |
| C | -4.990540 | -0.828020 | -1.594577 |
| N | -5.465384 | 0.187798 | -0.833957 |
| C | -1.840876 | 0.759227 | -0.902428 |
| C | -0.874719 | -0.445018 | -0.759368 |
| H | -1.330117 | -1.215639 | -0.133391 |

| | | | |
|---|-----------|-----------|-----------|
| C | -0.476510 | -1.095190 | -2.104873 |
| O | -1.450938 | -1.578586 | -2.844400 |
| O | 0.688059 | -1.162943 | -2.429201 |
| N | 0.375599 | -0.026348 | -0.061336 |
| H | -4.513406 | 1.829307 | 0.189648 |
| H | -5.619512 | -1.579996 | -2.043842 |
| H | -6.435210 | 0.356438 | -0.611446 |
| H | -1.692281 | 1.429755 | -0.053745 |
| H | -1.568165 | 1.331763 | -1.796368 |
| H | 0.167134 | 0.213061 | 0.921420 |
| H | 0.816886 | 0.796655 | -0.512187 |
| H | 1.080159 | -0.790144 | -0.040867 |
| H | -2.369294 | -1.402269 | -2.459542 |

H⁺H[N_α]-cggc(-00/+00/-00/+00/+00/--0) 1225

| | | | |
|---|-----------|-----------|-----------|
| C | 3.399083 | 1.287668 | -1.857921 |
| C | 2.912146 | 2.572917 | -1.232944 |
| O | 1.505699 | 2.476446 | -0.958231 |
| C | 0.940148 | 3.655648 | -0.378193 |
| C | 0.918131 | 3.610786 | 1.137759 |
| O | -0.013914 | 2.613024 | 1.547386 |
| C | 0.001131 | 2.372663 | 2.948165 |
| C | -1.088772 | 1.383167 | 3.297982 |
| O | -0.882377 | 0.145386 | 2.607727 |
| C | -1.157586 | -1.012034 | 3.400930 |
| C | -0.965471 | -2.257281 | 2.563785 |
| O | 0.360303 | -2.259435 | 2.066364 |
| C | 0.742519 | -3.453057 | 1.394727 |
| C | 2.192221 | -3.324450 | 0.988564 |
| O | 2.333497 | -2.285120 | 0.022906 |
| C | 3.702308 | -2.051588 | -0.327477 |
| C | 3.791184 | -1.002686 | -1.408999 |
| O | 3.361898 | 0.251150 | -0.884756 |
| H | 4.429368 | 1.443007 | -2.209455 |
| H | 2.772469 | 1.022353 | -2.717494 |
| H | 3.084244 | 3.399262 | -1.933250 |
| H | 3.467832 | 2.772840 | -0.308869 |
| H | -0.082603 | 3.734315 | -0.754726 |
| H | 1.490870 | 4.541111 | -0.713996 |
| H | 0.616254 | 4.592904 | 1.528407 |
| H | 1.916594 | 3.380392 | 1.533600 |
| H | -0.180629 | 3.304759 | 3.502226 |
| H | 0.980825 | 1.978454 | 3.251507 |
| H | -2.073336 | 1.784941 | 3.031354 |
| H | -1.067974 | 1.221258 | 4.381239 |
| H | -2.190766 | -0.986039 | 3.771102 |
| H | -0.477256 | -1.034569 | 4.260844 |
| H | -1.691079 | -2.283729 | 1.736703 |
| H | -1.151309 | -3.135769 | 3.197842 |
| H | 0.109790 | -3.621134 | 0.511336 |
| H | 0.634552 | -4.320876 | 2.059743 |
| H | 2.533658 | -4.277664 | 0.563315 |

| | | | |
|---|-----------|-----------|-----------|
| H | 2.802389 | -3.100630 | 1.873009 |
| H | 4.148892 | -2.982342 | -0.700717 |
| H | 4.257986 | -1.730502 | 0.562793 |
| H | 3.168231 | -1.284606 | -2.264322 |
| H | 4.837714 | -0.935531 | -1.739270 |
| C | -4.401703 | 0.798748 | -0.510990 |
| C | -3.248271 | 0.307612 | -1.064719 |
| N | -3.562767 | -0.727933 | -1.921907 |
| C | -4.873267 | -0.860925 | -1.897699 |
| N | -5.423289 | 0.046489 | -1.055155 |
| C | -1.827586 | 0.756621 | -0.878985 |
| C | -0.812170 | -0.413826 | -0.901328 |
| H | -1.260163 | -1.290063 | -0.428200 |
| C | -0.347111 | -0.806599 | -2.324290 |
| O | -1.273199 | -1.269716 | -3.138539 |
| O | 0.812646 | -0.690914 | -2.640613 |
| N | 0.397094 | -0.061513 | -0.096986 |
| H | -4.586354 | 1.595185 | 0.189674 |
| H | -5.450042 | -1.579852 | -2.457488 |
| H | -6.408279 | 0.154744 | -0.863864 |
| H | -1.734960 | 1.278323 | 0.074999 |
| H | -1.553480 | 1.478030 | -1.657175 |
| H | 0.125201 | 0.071951 | 0.889467 |
| H | 0.844890 | 0.809654 | -0.440523 |
| H | 1.113074 | -0.810574 | -0.131685 |
| H | -2.201889 | -1.215784 | -2.747955 |

H⁺H[N α]-cggc(-00/+00/--0/-00/+00/--0) 415

| | | | |
|---|-----------|-----------|-----------|
| C | 0.934951 | -3.251327 | 1.946295 |
| C | -0.015770 | -2.463838 | 2.817365 |
| O | 0.337482 | -1.087183 | 2.757453 |
| C | -0.387902 | -0.270491 | 3.664868 |
| C | 0.164270 | 1.134791 | 3.612762 |
| O | -0.098227 | 1.717477 | 2.333794 |
| C | 0.387800 | 3.061022 | 2.240302 |
| C | -0.000341 | 3.645655 | 0.893711 |
| O | 0.592415 | 2.960693 | -0.202742 |
| C | 1.884946 | 3.449114 | -0.567916 |
| C | 2.479389 | 2.560408 | -1.635490 |
| O | 2.772003 | 1.281466 | -1.071614 |
| C | 3.535683 | 0.452008 | -1.951963 |
| C | 3.901044 | -0.835592 | -1.248992 |
| O | 2.719557 | -1.591227 | -1.006670 |
| C | 2.953175 | -2.892437 | -0.496306 |
| C | 1.603488 | -3.570549 | -0.340056 |
| O | 0.742789 | -2.882727 | 0.579577 |
| H | 0.731450 | -4.322743 | 2.071142 |
| H | 1.966291 | -3.053095 | 2.260744 |
| H | 0.065336 | -2.834181 | 3.848677 |
| H | -1.052008 | -2.609710 | 2.481700 |
| H | -0.280096 | -0.648756 | 4.691104 |
| H | -1.458550 | -0.271948 | 3.414671 |

| | | | |
|---|-----------|-----------|-----------|
| H | 1.245284 | 1.116320 | 3.799964 |
| H | -0.313451 | 1.735751 | 4.397658 |
| H | 1.476596 | 3.068064 | 2.378505 |
| H | -0.058922 | 3.671590 | 3.036776 |
| H | 0.261471 | 4.711302 | 0.877260 |
| H | -1.082369 | 3.568593 | 0.762221 |
| H | 2.553119 | 3.468011 | 0.301956 |
| H | 1.796192 | 4.470963 | -0.960517 |
| H | 3.403874 | 3.028066 | -1.999859 |
| H | 1.787286 | 2.448714 | -2.478189 |
| H | 4.461513 | 0.971009 | -2.234346 |
| H | 2.956722 | 0.237340 | -2.856343 |
| H | 4.417661 | -0.624063 | -0.302652 |
| H | 4.585232 | -1.401152 | -1.896668 |
| H | 3.491829 | -2.841218 | 0.460991 |
| H | 3.566483 | -3.481399 | -1.193756 |
| H | 1.736181 | -4.612126 | -0.025648 |
| H | 1.083892 | -3.564501 | -1.300026 |
| C | -4.596291 | 0.368922 | 0.204317 |
| C | -3.481887 | 0.177228 | -0.570353 |
| N | -3.807053 | -0.637423 | -1.636366 |
| C | -5.086487 | -0.928941 | -1.520077 |
| N | -5.606072 | -0.337597 | -0.417500 |
| C | -2.093688 | 0.728363 | -0.403737 |
| C | -0.993880 | -0.271759 | -0.843588 |
| H | -1.310852 | -1.285720 | -0.593001 |
| C | -0.691529 | -0.206794 | -2.364422 |
| O | -1.657964 | -0.584422 | -3.172551 |
| O | 0.386157 | 0.175306 | -2.755664 |
| N | 0.297170 | -0.035863 | -0.119701 |
| H | -4.762690 | 0.931509 | 1.107275 |
| H | -5.661080 | -1.547445 | -2.190990 |
| H | -6.564324 | -0.402289 | -0.107621 |
| H | -1.939302 | 0.980823 | 0.647044 |
| H | -1.978014 | 1.660015 | -0.967477 |
| H | 0.182268 | 0.538813 | 0.727717 |
| H | 0.993299 | 0.433280 | -0.729706 |
| H | 0.703879 | -0.941585 | 0.161049 |
| H | -2.528035 | -0.751795 | -2.687684 |

H⁺H[N α]-cggc(+00/+00/+00/+00/-00/+00) 6554

| | | | |
|---|-----------|-----------|-----------|
| C | 3.546022 | 1.715288 | -1.447821 |
| C | 3.661091 | 0.258999 | -1.827131 |
| O | 3.389877 | -0.544481 | -0.684314 |
| C | 3.524594 | -1.937922 | -0.945890 |
| C | 3.215577 | -2.702363 | 0.318190 |
| O | 1.839492 | -2.523255 | 0.677830 |
| C | 1.506726 | -3.213223 | 1.880966 |
| C | 0.087832 | -2.890356 | 2.288877 |
| O | 0.015872 | -1.505526 | 2.601783 |
| C | -1.240798 | -1.072206 | 3.092300 |
| C | -1.113808 | 0.375984 | 3.511869 |

| | | | | | |
|---|-----------|-----------|-----------|---|-------------------------------|
| O | -0.683423 | 1.159982 | 2.396770 | | |
| C | -0.663933 | 2.565241 | 2.663233 | H ⁺ H[Na]-cggc(++0/+00/-00/+00/-00/+0+) 62 | |
| C | 0.308416 | 3.249601 | 1.727539 | C | -0.584200 2.814318 2.507587 |
| O | -0.098365 | 3.009303 | 0.386216 | C | -0.349586 3.553153 1.209528 |
| C | 0.579766 | 3.778559 | -0.604595 | O | 0.732168 2.943054 0.525013 |
| C | 2.045366 | 3.426383 | -0.792191 | C | 1.134434 3.629203 -0.655992 |
| O | 2.181387 | 2.059063 | -1.166492 | C | 2.373556 2.962432 -1.208386 |
| H | 3.908751 | 2.330723 | -2.281052 | O | 2.049157 1.641475 -1.642005 |
| H | 4.164115 | 1.922829 | -0.565147 | C | 3.142421 0.913746 -2.229457 |
| H | 4.686412 | 0.079643 | -2.181564 | C | 4.135991 0.388971 -1.196306 |
| H | 2.964262 | 0.014230 | -2.636124 | O | 3.549853 -0.492284 -0.244642 |
| H | 4.556131 | -2.170809 | -1.246771 | C | 3.554611 -1.872123 -0.608570 |
| H | 2.848064 | -2.237586 | -1.753280 | C | 3.121422 -2.682967 0.591080 |
| H | 3.853352 | -2.349850 | 1.138426 | O | 1.746233 -2.420874 0.904342 |
| H | 3.416368 | -3.768496 | 0.151200 | C | 1.348028 -3.018739 2.136712 |
| H | 2.193801 | -2.915532 | 2.683164 | C | -0.080948 -2.642945 2.460124 |
| H | 1.600293 | -4.296783 | 1.728572 | O | -0.150241 -1.231897 2.621895 |
| H | -0.175087 | -3.498386 | 3.165390 | C | -1.381478 -0.742879 3.131009 |
| H | -0.613491 | -3.142507 | 1.480086 | C | -1.212191 0.727004 3.444256 |
| H | -1.548819 | -1.664625 | 3.965365 | O | -0.961187 1.460051 2.241905 |
| H | -2.017235 | -1.182642 | 2.320443 | H | -1.379852 3.321385 3.069542 |
| H | -0.383344 | 0.468796 | 4.324655 | H | 0.331048 2.828540 3.112079 |
| H | -2.087827 | 0.730362 | 3.873823 | H | -0.117857 4.601461 1.444799 |
| H | -0.337432 | 2.748284 | 3.694225 | H | -1.256592 3.543246 0.587147 |
| H | -1.673894 | 2.975496 | 2.540833 | H | 1.371415 4.677043 -0.425967 |
| H | 1.320160 | 2.863824 | 1.904461 | H | 0.327162 3.615695 -1.401436 |
| H | 0.306960 | 4.327044 | 1.944597 | H | 3.147031 2.940296 -0.433001 |
| H | 0.506466 | 4.849338 | -0.369503 | H | 2.746259 3.547750 -2.058973 |
| H | 0.036244 | 3.597198 | -1.533834 | H | 3.667128 1.558556 -2.946241 |
| H | 2.626394 | 3.622035 | 0.119193 | H | 2.676881 0.093888 -2.774490 |
| H | 2.448275 | 4.075379 | -1.582358 | H | 4.566673 1.210395 -0.618514 |
| C | -4.395963 | 0.749580 | -0.677051 | H | 4.962089 -0.103638 -1.726767 |
| C | -3.247247 | 0.140768 | -1.110578 | H | 4.571923 -2.187151 -0.879139 |
| N | -3.570337 | -1.060307 | -1.711071 | H | 2.889920 -2.058202 -1.457589 |
| C | -4.881336 | -1.177554 | -1.652231 | H | 3.744535 -2.423052 1.455312 |
| N | -5.423348 | -0.100766 | -1.033733 | H | 3.248426 -3.750858 0.371967 |
| C | -1.824425 | 0.615352 | -1.036550 | H | 2.008468 -2.677196 2.943570 |
| C | -0.819441 | -0.540322 | -0.804359 | H | 1.423276 -4.112091 2.065250 |
| H | -1.278988 | -1.293506 | -0.161396 | H | -0.374653 -3.152783 3.387774 |
| C | -0.364021 | -1.222904 | -2.114578 | H | -0.760505 -2.976873 1.662525 |
| O | -1.290654 | -1.865305 | -2.794170 | H | -1.654690 -1.267736 4.056819 |
| O | 0.788483 | -1.152867 | -2.470475 | H | -2.193701 -0.894872 2.404894 |
| N | 0.398074 | -0.059001 | -0.079980 | H | -0.370105 0.853798 4.135385 |
| H | -4.573261 | 1.684869 | -0.173885 | H | -2.121682 1.106120 3.928758 |
| H | -5.464000 | -2.001065 | -2.033353 | C | -4.405916 0.723400 -0.779051 |
| H | -6.407025 | 0.053388 | -0.869018 | C | -3.250238 0.094253 -1.163019 |
| H | -1.722089 | 1.340654 | -0.228756 | N | -3.566337 -1.121057 -1.735771 |
| H | -1.555363 | 1.142355 | -1.959255 | C | -4.879178 -1.228114 -1.709902 |
| H | 0.945455 | 0.633560 | -0.618900 | N | -5.429416 -0.129692 -1.138917 |
| H | 1.032843 | -0.849931 | 0.135134 | C | -1.826221 0.562202 -1.055968 |
| H | 0.121452 | 0.373786 | 0.816475 | C | -0.827464 -0.580494 -0.745395 |
| H | -2.216535 | -1.730297 | -2.415533 | H | -1.295739 -1.286752 -0.056947 |

| | | | |
|---|-----------|-----------|-----------|
| C | -0.353214 | -1.359737 | -1.996725 |
| O | 0.814313 | -1.351695 | -2.310810 |
| O | -1.270789 | -2.019545 | -2.668936 |
| N | 0.382895 | -0.047192 | -0.051256 |
| H | -4.590710 | 1.671806 | -0.303955 |
| H | -5.456911 | -2.059104 | -2.082107 |
| H | -6.416009 | 0.035672 | -1.004991 |
| H | -1.765806 | 1.294379 | -0.249523 |
| H | -1.519560 | 1.069083 | -1.977860 |
| H | 0.984410 | -0.825004 | 0.279091 |
| H | 0.107743 | 0.501145 | 0.776553 |
| H | 0.963983 | 0.558836 | -0.666599 |
| H | -2.209035 | -1.838588 | -2.339026 |

H⁺H[Na]-cggc(+00/-0/-00/+00/-00/+0+) 70

| | | | |
|---|-----------|-----------|-----------|
| C | 0.719276 | 3.349862 | -1.669262 |
| C | 2.101840 | 2.871269 | -2.043535 |
| O | 2.187441 | 1.453709 | -1.938160 |
| C | 3.526284 | 0.994765 | -2.163762 |
| C | 3.630694 | -0.490341 | -1.922926 |
| O | 3.396062 | -0.753374 | -0.542766 |
| C | 3.577126 | -2.122109 | -0.205264 |
| C | 3.200830 | -2.319563 | 1.243376 |
| O | 1.786516 | -2.124035 | 1.395445 |
| C | 1.281286 | -2.411663 | 2.702279 |
| C | 1.060517 | -1.161839 | 3.531307 |
| O | 0.022895 | -0.399394 | 2.921190 |
| C | -0.377203 | 0.735413 | 3.677315 |
| C | -1.550906 | 1.384714 | 2.968259 |
| O | -1.207917 | 1.916153 | 1.684190 |
| C | -0.772244 | 3.278330 | 1.704147 |
| C | -0.594679 | 3.752298 | 0.280474 |
| O | 0.464033 | 3.014739 | -0.309050 |
| H | -0.042970 | 2.901035 | -2.321472 |
| H | 0.685827 | 4.438584 | -1.809465 |
| H | 2.838831 | 3.335898 | -1.375866 |
| H | 2.321885 | 3.186944 | -3.072925 |
| H | 4.208764 | 1.529204 | -1.490981 |
| H | 3.818550 | 1.211189 | -3.199859 |
| H | 4.645549 | -0.807793 | -2.203033 |
| H | 2.909959 | -1.038718 | -2.537739 |
| H | 4.629502 | -2.412347 | -0.337924 |
| H | 2.953946 | -2.757638 | -0.844813 |
| H | 3.752396 | -1.614490 | 1.877280 |
| H | 3.458613 | -3.342104 | 1.544109 |
| H | 1.962160 | -3.087186 | 3.230698 |
| H | 0.327895 | -2.930022 | 2.569434 |
| H | 1.980930 | -0.565673 | 3.600859 |
| H | 0.766059 | -1.455938 | 4.548805 |
| H | 0.461152 | 1.437369 | 3.789150 |
| H | -0.696744 | 0.431334 | 4.684544 |
| H | -1.977301 | 2.171364 | 3.601598 |

| | | | |
|---|-----------|-----------|-----------|
| H | -2.322593 | 0.631960 | 2.791796 |
| H | 0.175206 | 3.376068 | 2.247595 |
| H | -1.526000 | 3.902624 | 2.200751 |
| H | -0.359886 | 4.825875 | 0.286122 |
| H | -1.528936 | 3.612451 | -0.282095 |
| C | -4.485487 | 0.236282 | -0.779706 |
| C | -3.314045 | -0.422300 | -1.049001 |
| N | -3.585174 | -1.758992 | -1.259304 |
| C | -4.887061 | -1.911998 | -1.129565 |
| N | -5.473609 | -0.725432 | -0.840216 |
| C | -1.915224 | 0.118110 | -1.147926 |
| C | -0.847467 | -0.853256 | -0.587336 |
| H | -1.246541 | -1.353430 | 0.297862 |
| C | -0.376132 | -1.926868 | -1.598929 |
| O | -1.279805 | -2.785485 | -2.017974 |
| O | 0.776801 | -1.952429 | -1.960283 |
| N | 0.362604 | -0.103274 | -0.124165 |
| H | -4.702287 | 1.268241 | -0.562221 |
| H | -5.432056 | -2.836768 | -1.232540 |
| H | -6.460936 | -0.573305 | -0.696895 |
| H | -1.865982 | 1.045235 | -0.575105 |
| H | -1.673148 | 0.361382 | -2.188996 |
| H | 0.081260 | 0.639685 | 0.530193 |
| H | 0.906817 | 0.327729 | -0.890953 |
| H | 1.004931 | -0.750766 | 0.372765 |
| H | -2.214243 | -2.559817 | -1.705281 |

H⁺H[Na]-cggc(++0/+00/-+0/-00/+0+/-+0+) 288

| | | | |
|---|-----------|-----------|-----------|
| C | -0.037730 | 1.688571 | 3.307963 |
| C | 0.687607 | 2.712410 | 2.463923 |
| O | 0.081555 | 2.759748 | 1.175910 |
| C | 0.605242 | 3.755290 | 0.296209 |
| C | 1.873270 | 3.329242 | -0.426318 |
| O | 1.573673 | 2.205391 | -1.253529 |
| C | 2.610105 | 1.814078 | -2.170498 |
| C | 3.790191 | 1.126067 | -1.490710 |
| O | 3.425672 | -0.059055 | -0.792793 |
| C | 3.442875 | -1.250044 | -1.581207 |
| C | 3.244657 | -2.436181 | -0.666422 |
| O | 1.907979 | -2.446358 | -0.150428 |
| C | 1.697527 | -3.469826 | 0.817454 |
| C | 0.235240 | -3.485596 | 1.232843 |
| O | -0.229386 | -2.252531 | 1.780586 |
| C | 0.187826 | -1.994792 | 3.117032 |
| C | -0.376994 | -0.665390 | 3.564426 |
| O | 0.194898 | 0.382624 | 2.776968 |
| H | -1.113694 | 1.906036 | 3.324535 |
| H | 0.342078 | 1.741460 | 4.336425 |
| H | 1.749112 | 2.443951 | 2.393884 |
| H | 0.610421 | 3.692186 | 2.954867 |
| H | 0.797690 | 4.686652 | 0.844299 |
| H | -0.179948 | 3.947985 | -0.437632 |

| | | | | | | | |
|--|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | 2.670386 | 3.087162 | 0.286440 | O | 3.403305 | -0.179492 | -0.905795 |
| H | 2.218737 | 4.166265 | -1.047755 | C | 3.676212 | -1.550268 | -1.167559 |
| H | 2.966144 | 2.696579 | -2.717477 | C | 3.488648 | -2.330561 | 0.110996 |
| H | 2.120892 | 1.142078 | -2.875743 | O | 2.100188 | -2.347948 | 0.469547 |
| H | 4.249854 | 1.784258 | -0.749118 | C | 1.843598 | -3.103299 | 1.649899 |
| H | 4.553169 | 0.911843 | -2.251297 | C | 0.347131 | -3.311788 | 1.795604 |
| H | 4.419053 | -1.358792 | -2.073348 | O | -0.394314 | -2.100866 | 1.942424 |
| H | 2.660313 | -1.228770 | -2.346389 | H | -0.734490 | -2.326998 | 3.977860 |
| H | 3.958423 | -2.386784 | 0.165248 | H | 0.575297 | -1.199101 | 3.558378 |
| H | 3.423472 | -3.360519 | -1.230451 | H | -1.586796 | -0.103190 | 4.316398 |
| H | 2.362712 | -3.310698 | 1.676584 | H | -2.376119 | -0.783233 | 2.880959 |
| H | 1.940641 | -4.451998 | 0.388776 | H | 0.412853 | 1.646714 | 3.651298 |
| H | 0.075258 | -4.306733 | 1.944182 | H | -1.280524 | 2.075976 | 4.002269 |
| H | -0.389629 | -3.672520 | 0.356974 | H | -0.230467 | 3.916468 | 2.821198 |
| H | 1.281490 | -1.964713 | 3.190846 | H | -1.466069 | 3.173980 | 1.778660 |
| H | -0.183345 | -2.781579 | 3.788509 | H | 0.583637 | 4.735990 | 0.707490 |
| H | -0.123311 | -0.515629 | 4.621499 | H | -0.227484 | 3.648276 | -0.439420 |
| H | -1.470059 | -0.657226 | 3.465499 | H | 2.750767 | 3.670465 | 0.279492 |
| C | -4.535355 | 0.934942 | 0.053623 | H | 2.037158 | 4.376624 | -1.190219 |
| C | -3.472881 | 0.434891 | -0.652551 | H | 4.077380 | 2.328340 | -0.896070 |
| N | -3.916124 | -0.575381 | -1.482837 | H | 3.460414 | 2.733172 | -2.517986 |
| C | -5.215084 | -0.685133 | -1.292974 | H | 4.459691 | 0.533758 | -2.549631 |
| N | -5.633874 | 0.213646 | -0.369601 | H | 2.704460 | 0.346761 | -2.785579 |
| C | -2.029410 | 0.847638 | -0.639763 | H | 4.715802 | -1.674602 | -1.503615 |
| C | -1.059470 | -0.353907 | -0.774955 | H | 3.006663 | -1.930900 | -1.946580 |
| H | -1.471294 | -1.214375 | -0.244322 | H | 4.074903 | -1.877720 | 0.920687 |
| C | -0.773909 | -0.748787 | -2.242656 | H | 3.835859 | -3.360446 | -0.040150 |
| O | -1.796714 | -1.180571 | -2.948658 | H | 2.271640 | -2.593956 | 2.524410 |
| O | 0.346224 | -0.658360 | -2.692368 | H | 2.320296 | -4.090272 | 1.574518 |
| N | 0.250303 | -0.050187 | -0.129198 | H | 0.155584 | -3.980722 | 2.644609 |
| H | -4.611784 | 1.718466 | 0.788244 | H | -0.038949 | -3.789292 | 0.892617 |
| H | -5.873543 | -1.381722 | -1.787005 | C | -4.421864 | 0.821343 | -0.599274 |
| H | -6.583306 | 0.333838 | -0.049474 | C | -3.279022 | 0.274215 | -1.121723 |
| H | -1.808969 | 1.377051 | 0.289067 | N | -3.612526 | -0.825392 | -1.885464 |
| H | -1.832489 | 1.559834 | -1.449192 | C | -4.923440 | -0.943752 | -1.836796 |
| H | 0.131195 | 0.143262 | 0.878194 | N | -5.456029 | 0.036768 | -1.068261 |
| H | 0.719259 | 0.768984 | -0.563786 | C | -1.851808 | 0.721508 | -0.979026 |
| H | 0.890316 | -0.860767 | -0.202311 | C | -0.849608 | -0.453636 | -0.861981 |
| H | -2.674840 | -1.099534 | -2.455340 | H | -1.290969 | -1.247506 | -0.256121 |
| H ⁺ H[N α]-cggc(--0/--0/-00/+00/-00/+00) 95 | | | | | | | |
| C | -0.418040 | -1.558594 | 3.258193 | C | -0.399888 | -1.047798 | -2.217193 |
| C | -1.424671 | -0.425034 | 3.282582 | O | 0.767477 | -1.024409 | -2.531479 |
| O | -1.021604 | 0.690187 | 2.474202 | O | -1.334831 | -1.578104 | -2.974917 |
| C | -0.569620 | 1.837236 | 3.202109 | N | 0.375185 | -0.016527 | -0.119619 |
| C | -0.487933 | 3.011224 | 2.253776 | H | -4.591785 | 1.672222 | 0.038223 |
| O | 0.504999 | 2.736464 | 1.277789 | H | -5.512192 | -1.702297 | -2.327486 |
| C | 0.612364 | 3.731380 | 0.264671 | H | -6.437720 | 0.169630 | -0.875626 |
| C | 1.934838 | 3.572896 | -0.447783 | H | -1.771816 | 1.326453 | -0.074289 |
| O | 2.015867 | 2.301877 | -1.086932 | H | -1.566085 | 1.360036 | -1.822902 |
| C | 3.317814 | 2.080073 | -1.647290 | H | 1.032749 | -0.807958 | 0.005733 |
| C | 3.477152 | 0.639549 | -2.067355 | H | 0.095154 | 0.319562 | 0.813924 |
| | | | | H | 0.902798 | 0.739829 | -0.588780 |
| | | | | H | -2.267927 | -1.439831 | -2.610677 |

H⁺H[N_α]-cggc(--0/-00/-00/--0/-0/--0) 313

| | | | |
|---|-----------|-----------|-----------|
| C | 2.146628 | -3.130494 | 0.924209 |
| C | 0.798160 | -3.411599 | 1.567370 |
| O | 0.110572 | -2.226714 | 1.973877 |
| C | 0.444868 | -1.771048 | 3.279748 |
| C | -0.349414 | -0.523632 | 3.591489 |
| O | 0.101532 | 0.549259 | 2.760534 |
| C | -0.403106 | 1.827501 | 3.149731 |
| C | 0.396415 | 2.914236 | 2.467888 |
| O | 0.208140 | 2.832253 | 1.061381 |
| C | 0.995844 | 3.773166 | 0.336769 |
| C | 0.850733 | 3.486259 | -1.146163 |
| O | 1.375900 | 2.208406 | -1.511945 |
| C | 2.759096 | 2.215414 | -1.892179 |
| C | 3.247518 | 0.795732 | -2.069753 |
| O | 3.321789 | 0.174845 | -0.785911 |
| C | 3.963831 | -1.096819 | -0.771579 |
| C | 3.036225 | -2.244638 | -1.156808 |
| O | 1.919109 | -2.377194 | -0.265620 |
| H | 2.622778 | -4.087495 | 0.673453 |
| H | 2.811590 | -2.590348 | 1.610120 |
| H | 0.931948 | -4.089273 | 2.419809 |
| H | 0.150864 | -3.903431 | 0.838425 |
| H | 1.516444 | -1.548122 | 3.359842 |
| H | 0.195923 | -2.541439 | 4.022610 |
| H | -0.193559 | -0.262786 | 4.645978 |
| H | -1.420537 | -0.704643 | 3.433519 |
| H | -0.303712 | 1.952236 | 4.235480 |
| H | -1.467958 | 1.909602 | 2.893430 |
| H | 1.460429 | 2.798261 | 2.713301 |
| H | 0.060477 | 3.890347 | 2.845955 |
| H | 2.046728 | 3.697994 | 0.646764 |
| H | 0.654323 | 4.797664 | 0.543004 |
| H | 1.337886 | 4.278099 | -1.726230 |
| H | -0.207860 | 3.476970 | -1.416354 |
| H | 3.362636 | 2.716695 | -1.126845 |
| H | 2.867494 | 2.756468 | -2.840242 |
| H | 4.245664 | 0.830134 | -2.527584 |
| H | 2.571115 | 0.248732 | -2.735540 |
| H | 4.339694 | -1.228345 | 0.246284 |
| H | 4.831124 | -1.099107 | -1.446313 |
| H | 3.602785 | -3.183546 | -1.183777 |
| H | 2.595711 | -2.080103 | -2.140482 |
| C | -4.553986 | 0.784284 | -0.002517 |
| C | -3.486294 | 0.237455 | -0.665069 |
| N | -3.909262 | -0.872457 | -1.368326 |
| C | -5.201533 | -0.996889 | -1.146050 |
| N | -5.635559 | -0.011408 | -0.323372 |
| C | -2.055949 | 0.689787 | -0.725349 |
| C | -1.047385 | -0.486961 | -0.734550 |
| H | -1.417758 | -1.294726 | -0.099456 |

| | | | |
|---|-----------|-----------|-----------|
| C | -0.764112 | -1.052933 | -2.148467 |
| O | 0.351906 | -1.007257 | -2.611883 |
| O | -1.786499 | -1.577793 | -2.790955 |
| N | 0.260958 | -0.065649 | -0.156926 |
| H | -4.645338 | 1.644221 | 0.639042 |
| H | -5.844919 | -1.763734 | -1.547179 |
| H | -6.583944 | 0.116979 | -0.003267 |
| H | -1.841341 | 1.330272 | 0.132479 |
| H | -1.893427 | 1.306916 | -1.616428 |
| H | 0.679448 | 0.731329 | -0.672579 |
| H | 0.931983 | -0.857938 | -0.201290 |
| H | 0.165170 | 0.203773 | 0.834798 |
| H | -2.659648 | -1.464436 | -2.298506 |

H⁺H[N_α]-cggc(-00/+00/--0/--0/-00/--0) 1522

| | | | |
|---|-----------|-----------|-----------|
| C | -0.969452 | -1.114869 | 3.564834 |
| C | -0.810438 | 0.389631 | 3.483812 |
| O | 0.345985 | 0.694361 | 2.699136 |
| C | 0.858209 | 2.020739 | 2.860216 |
| C | 0.114717 | 3.072265 | 2.055132 |
| O | 0.303048 | 2.792362 | 0.673095 |
| C | -0.294827 | 3.731161 | -0.221255 |
| C | -1.772325 | 3.481560 | -0.467738 |
| O | -1.936038 | 2.201923 | -1.070459 |
| C | -3.280606 | 1.952415 | -1.496837 |
| C | -3.361236 | 0.610701 | -2.184610 |
| O | -3.140811 | -0.416806 | -1.224575 |
| C | -3.192888 | -1.720552 | -1.793071 |
| C | -2.928407 | -2.735860 | -0.706762 |
| O | -1.556400 | -2.645612 | -0.300937 |
| C | -1.191300 | -3.507063 | 0.774914 |
| C | -1.553922 | -2.951177 | 2.144545 |
| O | -1.014935 | -1.638234 | 2.244809 |
| H | -1.898830 | -1.335039 | 4.107410 |
| H | -0.132659 | -1.562601 | 4.116960 |
| H | -0.695361 | 0.791613 | 4.498246 |
| H | -1.706478 | 0.834664 | 3.033800 |
| H | 1.896676 | 1.980345 | 2.525677 |
| H | 0.848102 | 2.298755 | 3.921172 |
| H | 0.529145 | 4.059951 | 2.302897 |
| H | -0.951705 | 3.083228 | 2.315863 |
| H | 0.248019 | 3.633721 | -1.163787 |
| H | -0.155483 | 4.755208 | 0.148132 |
| H | -2.146806 | 4.265010 | -1.141012 |
| H | -2.354907 | 3.537566 | 0.462363 |
| H | -3.589527 | 2.734474 | -2.202055 |
| H | -3.954429 | 1.976434 | -0.630611 |
| H | -2.613871 | 0.547440 | -2.983400 |
| H | -4.362225 | 0.508090 | -2.627887 |
| H | -2.447698 | -1.815605 | -2.591556 |
| H | -4.189379 | -1.911595 | -2.216509 |
| H | -3.124936 | -3.743802 | -1.092925 |

| | | | |
|---|-----------|-----------|-----------|
| H | -3.593180 | -2.546541 | 0.143573 |
| H | -0.107273 | -3.622513 | 0.707428 |
| H | -1.644823 | -4.497597 | 0.645452 |
| H | -1.123233 | -3.613147 | 2.908719 |
| H | -2.640075 | -2.919673 | 2.301987 |
| C | 4.489003 | -0.967072 | 0.588754 |
| C | 3.478638 | -0.801977 | -0.322207 |
| N | 4.001694 | -0.288602 | -1.491321 |
| C | 5.297688 | -0.149213 | -1.302687 |
| N | 5.637733 | -0.551217 | -0.053949 |
| C | 2.015185 | -1.113339 | -0.200202 |
| C | 1.104649 | -0.042518 | -0.852431 |
| H | 1.527236 | 0.949204 | -0.675863 |
| C | 0.874031 | -0.222993 | -2.372958 |
| O | -0.248230 | -0.356160 | -2.802460 |
| O | 1.940161 | -0.203052 | -3.144511 |
| N | -0.233611 | -0.046693 | -0.190652 |
| H | 4.498631 | -1.335969 | 1.600344 |
| H | 6.007850 | 0.229010 | -2.020664 |
| H | 6.568773 | -0.547996 | 0.335372 |
| H | 1.759009 | -1.183268 | 0.859614 |
| H | 1.797626 | -2.091229 | -0.644945 |
| H | -0.118813 | 0.138663 | 0.816684 |
| H | -0.730399 | -0.950928 | -0.300675 |
| H | -0.848248 | 0.687824 | -0.582750 |
| H | 2.806001 | -0.149410 | -2.627078 |

H⁺H[N_α]-cggc(++0/+0+/-00/-00/+0+) 1548

| | | | |
|---|-----------|-----------|-----------|
| C | 3.883203 | -0.589392 | -1.671985 |
| C | 2.732318 | -0.721045 | -2.665468 |
| O | 1.713251 | 0.277115 | -2.480860 |
| C | 2.068246 | 1.578473 | -2.946618 |
| C | 0.931243 | 2.537705 | -2.681204 |
| O | 0.747409 | 2.649230 | -1.274312 |
| C | -0.161749 | 3.668573 | -0.892251 |
| C | -0.268340 | 3.682537 | 0.615362 |
| O | -0.864087 | 2.456762 | 1.054379 |
| C | -1.160153 | 2.410023 | 2.455674 |
| C | -0.005078 | 1.896845 | 3.295906 |
| O | 0.234071 | 0.542909 | 2.938845 |
| C | 1.284301 | -0.072852 | 3.678972 |
| C | 1.391574 | -1.518822 | 3.235151 |
| O | 1.798791 | -1.636772 | 1.868894 |
| C | 3.181515 | -1.973029 | 1.684681 |
| C | 3.502718 | -2.030792 | 0.209708 |
| O | 3.466912 | -0.705411 | -0.315195 |
| H | 4.365492 | 0.387257 | -1.758193 |
| H | 4.640841 | -1.346831 | -1.913508 |
| H | 2.221106 | -1.674835 | -2.543176 |
| H | 3.123190 | -0.660018 | -3.689531 |
| H | 2.265566 | 1.543244 | -4.026131 |
| H | 2.967993 | 1.942395 | -2.438957 |

| | | | |
|---|-----------|-----------|-----------|
| H | 0.007140 | 2.185224 | -3.160217 |
| H | 1.189448 | 3.514330 | -3.113210 |
| H | -1.151046 | 3.493061 | -1.338887 |
| H | 0.194475 | 4.651276 | -1.232288 |
| H | -0.896822 | 4.528025 | 0.922498 |
| H | 0.727790 | 3.809527 | 1.055245 |
| H | -2.010698 | 1.733368 | 2.564281 |
| H | -1.464164 | 3.402142 | 2.808990 |
| H | -0.279814 | 1.972291 | 4.358032 |
| H | 0.900816 | 2.499536 | 3.140465 |
| H | 1.060226 | -0.041336 | 4.754791 |
| H | 2.230003 | 0.459961 | 3.509038 |
| H | 0.413789 | -2.000255 | 3.322743 |
| H | 2.089753 | -2.053485 | 3.887455 |
| H | 3.374681 | -2.955662 | 2.132062 |
| H | 3.820756 | -1.227946 | 2.173323 |
| H | 2.785812 | -2.679512 | -0.304407 |
| H | 4.510952 | -2.452656 | 0.095522 |
| C | -4.594082 | 0.280460 | -0.643057 |
| C | -3.475315 | -0.506955 | -0.725321 |
| N | -3.831971 | -1.822779 | -0.511506 |
| C | -5.133763 | -1.840368 | -0.311093 |
| N | -5.637827 | -0.584883 | -0.384201 |
| C | -2.053280 | -0.122058 | -1.018944 |
| C | -1.016899 | -0.930978 | -0.199383 |
| H | -1.404639 | -1.095744 | 0.808912 |
| C | -0.645750 | -2.303161 | -0.815721 |
| O | 0.495691 | -2.530783 | -1.144883 |
| O | -1.615689 | -3.181345 | -0.942700 |
| N | 0.246095 | -0.148723 | -0.044238 |
| H | -4.741594 | 1.341966 | -0.746894 |
| H | -5.735080 | -2.713530 | -0.114119 |
| H | -6.607481 | -0.329421 | -0.270226 |
| H | -1.925645 | 0.934969 | -0.777956 |
| H | -1.838622 | -0.238998 | -2.087297 |
| H | 0.040347 | 0.773162 | 0.367773 |
| H | 0.741569 | 0.000419 | -0.946646 |
| H | 0.899981 | -0.646679 | 0.590140 |
| H | -2.525244 | -2.805190 | -0.709800 |

H⁺H[N_α]-cggc(++0/+0+/-00/-00/+0+) 3544

| | | | |
|---|-----------|-----------|-----------|
| C | -0.197239 | 3.558681 | 1.156193 |
| C | -0.060659 | 3.783014 | -0.332141 |
| O | 0.831450 | 2.813651 | -0.857485 |
| C | 1.026477 | 2.910303 | -2.263922 |
| C | 2.155608 | 1.988058 | -2.661360 |
| O | 1.783605 | 0.636268 | -2.396496 |
| C | 2.807219 | -0.331224 | -2.688225 |
| C | 3.910542 | -0.366700 | -1.634956 |
| O | 3.435486 | -0.701434 | -0.334819 |
| C | 3.455996 | -2.094298 | -0.029175 |
| C | 3.088693 | -2.270781 | 1.425429 |

| | | | | | |
|---|-----------|-----------|-----------|--|-------------------------------|
| O | 1.703434 | -1.949590 | 1.616539 | | |
| C | 1.254288 | -2.034839 | 2.972089 | H ⁺ H[Na]-cggc(++0/+0/+00/--0/-00/+0+) 16 | |
| C | 1.170034 | -0.673874 | 3.635616 | C | 3.456230 -2.093483 -0.032373 |
| O | 0.159530 | 0.080975 | 2.973206 | C | 3.089631 -2.271634 1.422208 |
| C | -0.051137 | 1.372056 | 3.526886 | O | 1.704329 -1.951148 1.614220 |
| C | -1.171657 | 2.041877 | 2.752700 | C | 1.255855 -2.037623 2.969902 |
| O | -0.839237 | 2.299096 | 1.382991 | C | 1.172171 -0.677281 3.634786 |
| H | -0.805341 | 4.364462 | 1.586402 | O | 0.161337 0.078299 2.973710 |
| H | 0.793321 | 3.579163 | 1.625752 | C | -0.048639 1.369011 3.528499 |
| H | 0.326028 | 4.797336 | -0.504900 | C | -1.169660 2.039574 2.755686 |
| H | -1.044701 | 3.707594 | -0.816720 | O | -0.838265 2.297717 1.385899 |
| H | 1.298465 | 3.937060 | -2.544746 | C | -0.196432 3.557462 1.159478 |
| H | 0.102763 | 2.643324 | -2.796106 | C | -0.061324 3.782987 -0.328808 |
| H | 3.055169 | 2.261869 | -2.099624 | O | 0.830445 2.814196 -0.855794 |
| H | 2.361441 | 2.111244 | -3.732812 | C | 1.023724 2.911720 -2.262409 |
| H | 3.246138 | -0.115410 | -3.671047 | C | 2.152811 1.990239 -2.661754 |
| H | 2.288542 | -1.287354 | -2.741086 | O | 1.781899 0.638138 -2.396930 |
| H | 4.390601 | 0.610125 | -1.538344 | C | 2.806017 -0.328578 -2.689487 |
| H | 4.682362 | -1.076346 | -1.961497 | C | 3.909561 -0.363998 -1.636452 |
| H | 4.467174 | -2.497326 | -0.179182 | O | 3.435050 -0.700294 -0.336514 |
| H | 2.754814 | -2.648560 | -0.662011 | H | 2.754962 -2.647323 -0.665481 |
| H | 3.717186 | -1.621837 | 2.047042 | H | 4.467492 -2.495955 -0.183276 |
| H | 3.259222 | -3.314756 | 1.715404 | H | 3.718143 -1.623091 2.044218 |
| H | 1.915674 | -2.687738 | 3.551125 | H | 3.260659 -3.315841 1.711055 |
| H | 0.261720 | -2.492673 | 2.953250 | H | 1.917400 -2.691223 3.547966 |
| H | 2.134002 | -0.149944 | 3.577826 | H | 0.263190 -2.495242 2.951091 |
| H | 0.912877 | -0.804253 | 4.696473 | H | 2.136160 -0.153404 3.576878 |
| H | 0.874322 | 1.963002 | 3.481402 | H | 0.915664 -0.808613 4.695683 |
| H | -0.348447 | 1.294595 | 4.582778 | H | 0.876889 1.959826 3.482673 |
| H | -1.460246 | 2.974628 | 3.250979 | H | -0.345104 1.290848 4.584576 |
| H | -2.040629 | 1.380343 | 2.735783 | H | -1.457695 2.972019 3.254855 |
| C | -4.581982 | 0.424958 | -0.640082 | H | -2.038758 1.378200 2.738986 |
| C | -3.467723 | -0.350543 | -0.828324 | H | 0.794581 3.577544 1.628094 |
| N | -3.834118 | -1.680988 | -0.807695 | H | -0.804087 4.362919 1.590922 |
| C | -5.137310 | -1.717544 | -0.619011 | H | 0.324998 4.797511 -0.501182 |
| N | -5.632854 | -0.460981 | -0.513984 | H | -1.045834 3.707747 -0.812463 |
| C | -2.041287 | 0.062854 | -1.054356 | H | 1.294869 3.938760 -2.543011 |
| C | -1.016594 | -0.872067 | -0.364457 | H | 0.099482 2.644598 -2.793605 |
| H | -1.412003 | -1.187085 | 0.604198 | H | 3.053002 2.264303 -2.101151 |
| C | -0.652997 | -2.134701 | -1.185426 | H | 2.357120 2.113972 -3.733432 |
| O | -1.628280 | -2.977664 | -1.443940 | H | 3.244573 -0.111943 -3.672285 |
| O | 0.486505 | -2.314051 | -1.549155 | H | 2.287912 -1.284997 -2.742802 |
| N | 0.252103 | -0.136011 | -0.083001 | H | 4.388737 0.613179 -1.539042 |
| H | -4.722055 | 1.491463 | -0.592181 | H | 4.681977 -1.072662 -1.963725 |
| H | -5.745489 | -2.605523 | -0.552538 | C | -4.582105 0.425515 -0.638479 |
| H | -6.601572 | -0.217570 | -0.369747 | C | -3.467917 -0.349892 -0.827519 |
| H | -1.906174 | 1.069503 | -0.653561 | N | -3.834357 -1.680340 -0.807761 |
| H | -1.822355 | 0.109371 | -2.127201 | C | -5.137507 -1.716983 -0.618818 |
| H | 0.762362 | 0.135980 | -0.947160 | N | -5.632981 -0.460476 -0.512791 |
| H | 0.889682 | -0.731104 | 0.479954 | C | -2.041517 0.063604 -1.053587 |
| H | 0.052065 | 0.718272 | 0.457136 | C | -1.016696 -0.871920 -0.364696 |
| H | -2.534395 | -2.635388 | -1.153861 | H | -1.411873 -1.187715 0.603799 |

| | | | |
|---|-----------|-----------|-----------|
| C | -0.653380 | -2.133914 | -1.186784 |
| O | -1.628758 | -2.976667 | -1.445638 |
| O | 0.486002 | -2.312998 | -1.551016 |
| N | 0.252110 | -0.136156 | -0.083004 |
| H | -4.722132 | 1.491989 | -0.589795 |
| H | -5.745707 | -2.604986 | -0.552847 |
| H | -6.601659 | -0.217134 | -0.368170 |
| H | -1.906236 | 1.069944 | -0.652066 |
| H | -1.822857 | 0.110937 | -2.126453 |
| H | 0.889989 | -0.731841 | 0.478982 |
| H | 0.052335 | 0.717525 | 0.458180 |
| H | 0.761930 | 0.136773 | -0.947123 |
| H | -2.534766 | -2.634588 | -1.155012 |

H⁺H[N_α]-cggc(++0/+00/--0/-00/+00/--+) 9660

| | | | |
|---|-----------|-----------|-----------|
| C | -1.709971 | -2.869005 | 1.844636 |
| C | -1.391986 | -3.499919 | 0.501280 |
| O | -1.312442 | -2.543398 | -0.560611 |
| C | -2.364232 | -2.543883 | -1.540864 |
| C | -3.605898 | -1.785328 | -1.084269 |
| O | -3.344287 | -0.420818 | -0.772755 |
| C | -3.468879 | 0.478119 | -1.876834 |
| C | -3.345150 | 1.897432 | -1.371333 |
| O | -1.993839 | 2.170179 | -0.983725 |
| C | -1.819484 | 3.474862 | -0.438798 |
| C | -0.339176 | 3.731131 | -0.205562 |
| O | 0.266385 | 2.820038 | 0.712558 |
| C | 0.039927 | 3.117240 | 2.086035 |
| C | 0.626231 | 2.011055 | 2.935149 |
| O | -0.095130 | 0.801636 | 2.688021 |
| C | 0.135331 | -0.230761 | 3.648159 |
| C | -0.887935 | -1.325891 | 3.447921 |
| O | -0.676363 | -1.949614 | 2.187077 |
| H | -1.774981 | -3.667638 | 2.598172 |
| H | -2.674494 | -2.345940 | 1.816100 |
| H | -2.147572 | -4.259512 | 0.274764 |
| H | -0.419398 | -3.997493 | 0.556059 |
| H | -2.633360 | -3.576460 | -1.793759 |
| H | -1.926296 | -2.076144 | -2.423278 |
| H | -4.018103 | -2.232220 | -0.175442 |
| H | -4.374675 | -1.865992 | -1.864849 |
| H | -4.459888 | 0.365549 | -2.337195 |
| H | -2.701784 | 0.282796 | -2.633615 |
| H | -4.014153 | 2.048210 | -0.514822 |
| H | -3.638085 | 2.588228 | -2.172357 |
| H | -2.400219 | 3.572164 | 0.488187 |
| H | -2.190642 | 4.230322 | -1.145121 |
| H | -0.201676 | 4.766376 | 0.132489 |
| H | 0.201496 | 3.609041 | -1.146454 |
| H | -1.032146 | 3.202323 | 2.299605 |
| H | 0.523277 | 4.067360 | 2.352693 |
| H | 0.531672 | 2.291374 | 3.991714 |

| | | | |
|---|-----------|-----------|-----------|
| H | 1.691352 | 1.872660 | 2.708054 |
| H | 0.025616 | 0.172938 | 4.662576 |
| H | 1.153845 | -0.628477 | 3.545527 |
| H | -1.896768 | -0.894695 | 3.492772 |
| H | -0.790574 | -2.060227 | 4.259836 |
| C | 4.496000 | -1.044456 | 0.490947 |
| C | 3.468804 | -0.764324 | -0.371990 |
| N | 3.976554 | -0.135079 | -1.490646 |
| C | 5.278883 | -0.038605 | -1.318667 |
| N | 5.638268 | -0.579389 | -0.129479 |
| C | 2.002972 | -1.067075 | -0.254056 |
| C | 1.099970 | 0.057844 | -0.822172 |
| H | 1.541262 | 1.032140 | -0.601479 |
| C | 0.852827 | -0.048768 | -2.347005 |
| O | 1.907730 | 0.044029 | -3.127892 |
| O | -0.269960 | -0.198421 | -2.773073 |
| N | -0.231261 | 0.032161 | -0.152767 |
| H | 4.522438 | -1.525962 | 1.453711 |
| H | 5.980343 | 0.403511 | -2.008125 |
| H | 6.577438 | -0.633758 | 0.235757 |
| H | 1.751816 | -1.220191 | 0.797818 |
| H | 1.765318 | -2.007935 | -0.762525 |
| H | -0.145281 | 0.234200 | 0.856127 |
| H | -0.689447 | -0.893742 | -0.266331 |
| H | -0.863035 | 0.751856 | -0.545961 |
| H | 2.775607 | 0.084443 | -2.612660 |

H⁺H[N_α]-cggc(+00/-+0/-00/--0/-00/-0+) 19

| | | | |
|---|-----------|-----------|-----------|
| C | -0.441315 | -1.309850 | 3.355023 |
| C | -0.488862 | -2.685280 | 2.723763 |
| O | -0.720477 | -2.541462 | 1.328933 |
| C | -1.281089 | -3.687827 | 0.699186 |
| C | -1.117622 | -3.526964 | -0.804849 |
| O | -1.604787 | -2.282927 | -1.299420 |
| C | -3.021230 | -2.219845 | -1.503037 |
| C | -3.374165 | -0.886062 | -2.118004 |
| O | -3.192382 | 0.141182 | -1.148617 |
| C | -3.459059 | 1.436065 | -1.676059 |
| C | -3.177158 | 2.474001 | -0.615294 |
| O | -1.765717 | 2.521913 | -0.371128 |
| C | -1.326500 | 3.592280 | 0.466030 |
| C | -1.243814 | 3.204910 | 1.930313 |
| O | -0.264934 | 2.179605 | 2.066702 |
| C | -0.053033 | 1.769169 | 3.408904 |
| C | 0.966051 | 0.643117 | 3.415042 |
| O | 0.552939 | -0.521510 | 2.695547 |
| H | -0.195076 | -1.413712 | 4.419693 |
| H | -1.424638 | -0.831704 | 3.271279 |
| H | -1.299713 | -3.252085 | 3.200393 |
| H | 0.452879 | -3.223772 | 2.893328 |
| H | -2.335080 | -3.791817 | 0.989048 |
| H | -0.756540 | -4.603429 | 1.005664 |

H⁺H[N_α]-cggc(++0/0+0/+00/-00/+0+/-+00) 1592

| | | | |
|---|-----------|-----------|-----------|
| C | 3.048348 | -2.654517 | -0.264769 |
| C | 3.394666 | -1.632356 | -1.322948 |
| O | 3.325686 | -0.331012 | -0.738845 |
| C | 3.766083 | 0.724384 | -1.587717 |
| C | 2.661063 | 1.283225 | -2.478764 |
| O | 1.579332 | 1.870815 | -1.737166 |
| C | 1.822095 | 3.179775 | -1.224597 |
| C | 0.510881 | 3.747233 | -0.705923 |
| O | -0.040398 | 3.007182 | 0.383908 |
| C | 0.472675 | 3.357660 | 1.664347 |
| C | -0.227484 | 2.529373 | 2.717418 |
| O | 0.158062 | 1.160797 | 2.579335 |
| C | -0.315782 | 0.316089 | 3.632446 |
| C | 0.552354 | -0.918498 | 3.716218 |
| O | 0.434143 | -1.667793 | 2.515196 |
| C | 1.307845 | -2.791678 | 2.472509 |
| C | 1.211319 | -3.424100 | 1.097396 |
| O | 1.656988 | -2.548663 | 0.059592 |
| H | 3.664521 | -2.486340 | 0.626443 |
| H | 3.253277 | -3.659645 | -0.653529 |
| H | 2.702490 | -1.723414 | -2.166825 |
| H | 4.416101 | -1.830702 | -1.675268 |
| H | 4.594705 | 0.387628 | -2.225326 |
| H | 4.160849 | 1.499558 | -0.925925 |
| H | 2.200118 | 0.492474 | -3.070554 |
| H | 3.083570 | 2.030089 | -3.162958 |
| H | 2.190029 | 3.830952 | -2.028774 |
| H | 2.583427 | 3.156406 | -0.435191 |
| H | -0.235256 | 3.710899 | -1.502269 |
| H | 0.656744 | 4.797127 | -0.421122 |
| H | 0.285228 | 4.420946 | 1.868344 |
| H | 1.554032 | 3.180660 | 1.721904 |
| H | -1.316209 | 2.633326 | 2.619987 |
| H | 0.066044 | 2.896702 | 3.709062 |
| H | -1.364282 | 0.044200 | 3.455160 |
| H | -0.255663 | 0.845790 | 4.591006 |
| H | 0.231567 | -1.519375 | 4.579333 |
| H | 1.598030 | -0.621625 | 3.873206 |
| H | 1.019743 | -3.531432 | 3.233138 |
| H | 2.337557 | -2.472516 | 2.683504 |
| H | 0.168391 | -3.663098 | 0.875410 |
| H | 1.782203 | -4.359308 | 1.077792 |
| C | -4.610698 | 0.683164 | 0.011614 |
| C | -3.533216 | 0.115561 | -0.616526 |
| N | -3.928453 | -1.062755 | -1.218423 |
| C | -5.214111 | -1.206741 | -0.970021 |
| N | -5.670094 | -0.169143 | -0.227393 |
| C | -2.118193 | 0.604913 | -0.730844 |
| C | -1.082259 | -0.546468 | -0.677653 |
| H | -1.437557 | -1.323833 | 0.002444 |

| | | | |
|---|-----------|-----------|-----------|
| C | -0.806062 | -1.176792 | -2.065282 |
| O | 0.287137 | -1.081566 | -2.572696 |
| O | -1.813208 | -1.802272 | -2.638212 |
| N | 0.226046 | -0.073735 | -0.139104 |
| H | -4.721795 | 1.590490 | 0.580651 |
| H | -5.837596 | -2.023445 | -1.297365 |
| H | -6.618767 | -0.042715 | 0.092630 |
| H | -1.906911 | 1.311580 | 0.073064 |
| H | -1.984757 | 1.163342 | -1.664214 |
| H | 0.670845 | 0.631955 | -0.758522 |
| H | 0.876955 | -0.878005 | -0.061414 |
| H | 0.128991 | 0.341083 | 0.801276 |
| H | -2.678212 | -1.691576 | -2.130980 |

H⁺H[N_α]-cggc(+0+/-+00/-00/+00/-00/+00) 181

| | | | |
|---|-----------|-----------|-----------|
| C | 0.752721 | 3.064257 | 2.114175 |
| C | 1.013471 | 3.622355 | 0.726215 |
| O | 0.164314 | 3.087282 | -0.281827 |
| C | -1.110264 | 3.718585 | -0.383531 |
| C | -1.823993 | 3.211422 | -1.617420 |
| O | -2.125463 | 1.817660 | -1.500449 |
| C | -3.451178 | 1.476779 | -1.934215 |
| C | -3.625645 | -0.022378 | -1.962594 |
| O | -3.463965 | -0.539863 | -0.647946 |
| C | -3.653967 | -1.949175 | -0.584346 |
| C | -3.379438 | -2.413371 | 0.825051 |
| O | -1.996740 | -2.216766 | 1.150145 |
| C | -1.699931 | -2.632677 | 2.480456 |
| C | -0.264311 | -2.304562 | 2.819564 |
| O | -0.104115 | -0.891677 | 2.774473 |
| C | 1.097744 | -0.404840 | 3.350667 |
| C | 1.005105 | 1.101533 | 3.425157 |
| O | 0.959380 | 1.650115 | 2.105066 |
| H | -0.265581 | 3.287178 | 2.458763 |
| H | 1.453540 | 3.540865 | 2.813152 |
| H | 2.034540 | 3.374433 | 0.425826 |
| H | 0.931020 | 4.716684 | 0.760184 |
| H | -0.980960 | 4.806123 | -0.475216 |
| H | -1.720632 | 3.516163 | 0.505995 |
| H | -1.206607 | 3.374657 | -2.507901 |
| H | -2.748757 | 3.787370 | -1.730998 |
| H | -3.622537 | 1.864441 | -2.946048 |
| H | -4.179711 | 1.933661 | -1.253411 |
| H | -4.636878 | -0.238037 | -2.337845 |
| H | -2.897725 | -0.482273 | -2.639138 |
| H | -2.986523 | -2.453453 | -1.290876 |
| H | -4.692903 | -2.205842 | -0.837268 |
| H | -4.001919 | -1.854803 | 1.535354 |
| H | -3.626612 | -3.479726 | 0.906584 |
| H | -1.854462 | -3.715767 | 2.578394 |
| H | -2.366766 | -2.121972 | 3.186913 |
| H | -0.048145 | -2.684137 | 3.827230 |

| | | | |
|---|-----------|-----------|-----------|
| H | 0.424463 | -2.796145 | 2.117689 |
| H | 1.970826 | -0.709919 | 2.755511 |
| H | 1.226821 | -0.799292 | 4.367998 |
| H | 0.100495 | 1.383704 | 3.978161 |
| H | 1.878712 | 1.496513 | 3.959999 |
| C | 4.419862 | 0.382240 | -0.950561 |
| C | 3.235532 | -0.267283 | -1.182484 |
| N | 3.494625 | -1.597108 | -1.449507 |
| C | 4.801526 | -1.753131 | -1.389989 |
| N | 5.402743 | -0.576665 | -1.090713 |
| C | 1.833600 | 0.273463 | -1.202008 |
| C | 0.789992 | -0.745175 | -0.681148 |
| H | 1.230399 | -1.329535 | 0.128932 |
| C | 0.287898 | -1.713347 | -1.777418 |
| O | -0.863355 | -1.676606 | -2.141909 |
| O | 1.172763 | -2.553898 | -2.269805 |
| N | -0.396310 | -0.046556 | -0.094086 |
| H | 4.649732 | 1.407290 | -0.714743 |
| H | 5.340223 | -2.673145 | -1.551958 |
| H | 6.396218 | -0.428342 | -0.993015 |
| H | 1.557655 | 0.585351 | -2.215444 |
| H | 1.784959 | 1.168511 | -0.582989 |
| H | -1.072180 | -0.734488 | 0.286871 |
| H | -0.914015 | 0.540218 | -0.773911 |
| H | -0.088738 | 0.556272 | 0.683831 |
| H | 2.109768 | -2.368389 | -1.941896 |

H⁺H[N_α]-cggc(+0+/-00/-00/+0+/-00) 8251

| | | | |
|---|-----------|-----------|-----------|
| C | -0.084586 | 3.501065 | 1.298881 |
| C | -0.226210 | 2.729210 | 2.590997 |
| O | -0.719673 | 1.412830 | 2.321527 |
| C | -0.890849 | 0.642462 | 3.513247 |
| C | -1.436626 | -0.732673 | 3.164239 |
| O | -0.576640 | -1.511604 | 2.338719 |
| C | 0.525599 | -2.109436 | 3.019307 |
| C | 1.294065 | -2.991033 | 2.058600 |
| O | 1.836392 | -2.204625 | 0.996206 |
| C | 3.092350 | -2.682643 | 0.493238 |
| C | 3.480670 | -1.912778 | -0.748988 |
| O | 3.626959 | -0.536727 | -0.409180 |
| C | 4.114610 | 0.290479 | -1.457754 |
| C | 3.026682 | 0.782247 | -2.411090 |
| O | 1.994427 | 1.543621 | -1.760535 |
| C | 2.373614 | 2.864128 | -1.374987 |
| C | 1.199639 | 3.550143 | -0.713549 |
| O | 0.894984 | 2.863906 | 0.496066 |
| H | 0.218949 | 4.529808 | 1.538734 |
| H | -1.048597 | 3.549963 | 0.771288 |
| H | -0.923989 | 3.258756 | 3.252691 |
| H | 0.747684 | 2.664314 | 3.091871 |
| H | -1.607513 | 1.141449 | 4.180016 |
| H | 0.065524 | 0.571603 | 4.047018 |

| | | | |
|---|-----------|-----------|-----------|
| H | -2.368755 | -0.623087 | 2.605095 |
| H | -1.662776 | -1.268081 | 4.096072 |
| H | 0.161932 | -2.726104 | 3.853015 |
| H | 1.197706 | -1.341746 | 3.421730 |
| H | 0.645989 | -3.773150 | 1.645349 |
| H | 2.103022 | -3.473853 | 2.619142 |
| H | 3.011759 | -3.745682 | 0.233892 |
| H | 3.855111 | -2.563722 | 1.271983 |
| H | 2.722802 | -2.048984 | -1.526121 |
| H | 4.435776 | -2.318067 | -1.113108 |
| H | 4.876133 | -0.237112 | -2.049079 |
| H | 4.612106 | 1.129660 | -0.966210 |
| H | 2.506901 | -0.054039 | -2.876732 |
| H | 3.486321 | 1.390062 | -3.201472 |
| H | 2.671930 | 3.437285 | -2.262676 |
| H | 3.215232 | 2.839730 | -0.674606 |
| H | 0.327897 | 3.553145 | -1.382748 |
| H | 1.473803 | 4.592932 | -0.503213 |
| C | -4.479502 | 0.828906 | -0.641809 |
| C | -3.362202 | 0.172199 | -1.087912 |
| N | -3.740495 | -1.022534 | -1.665443 |
| C | -5.053123 | -1.091491 | -1.581094 |
| N | -5.543802 | 0.012752 | -0.968185 |
| C | -1.920492 | 0.591774 | -1.039423 |
| C | -0.949582 | -0.578526 | -0.741955 |
| H | -1.403384 | -1.255149 | -0.015087 |
| C | -0.541024 | -1.398455 | -1.988616 |
| O | 0.622641 | -1.468321 | -2.314547 |
| O | -1.502205 | -2.010090 | -2.643781 |
| N | 0.300272 | -0.067248 | -0.104059 |
| H | -4.614095 | 1.774728 | -0.145077 |
| H | -5.671773 | -1.899040 | -1.938837 |
| H | -6.517801 | 0.204495 | -0.786300 |
| H | -1.807008 | 1.338679 | -0.251264 |
| H | -1.631959 | 1.073079 | -1.980830 |
| H | 0.897830 | -0.854440 | 0.214569 |
| H | 0.069196 | 0.492631 | 0.729839 |
| H | 0.874382 | 0.519844 | -0.742018 |
| H | -2.425441 | -1.786070 | -2.296881 |

H⁺H[N_α]-cggc(+0+/-00/-00/+0+/-00) 136

| | | | |
|---|-----------|-----------|-----------|
| C | -0.033350 | -2.299345 | 2.911435 |
| C | -0.945706 | -1.141410 | 3.277561 |
| O | -0.377203 | 0.074760 | 2.787233 |
| C | -1.003442 | 1.250363 | 3.306026 |
| C | -0.164436 | 2.454021 | 2.919177 |
| O | -0.114239 | 2.657886 | 1.508494 |
| C | -1.058744 | 3.601956 | 1.005686 |
| C | -0.887031 | 3.690454 | -0.498810 |
| O | -1.298163 | 2.497128 | -1.172490 |
| C | -2.641725 | 2.537555 | -1.674890 |
| C | -2.970138 | 1.231562 | -2.357392 |

| | | | | | |
|---|-----------|-----------|-----------|---|-------------------------------|
| O | -3.061750 | 0.201800 | -1.379031 | | |
| C | -3.387166 | -1.062187 | -1.950076 | H ⁺ H[Na]-cggc(-0/--0/-00/+00/-00/+00) | 12883 |
| C | -3.414106 | -2.107046 | -0.860416 | C | 3.665079 0.019769 -1.706725 |
| O | -2.090987 | -2.300115 | -0.351516 | C | 3.448186 1.506935 -1.864961 |
| C | -1.992253 | -3.370366 | 0.580535 | O | 2.095206 1.865811 -1.551044 |
| C | -0.529186 | -3.600389 | 0.917525 | C | 1.934153 3.276844 -1.429289 |
| O | 0.117666 | -2.471280 | 1.503496 | C | 0.543518 3.608714 -0.936730 |
| H | -0.418414 | -3.214437 | 3.376354 | O | 0.365772 3.024520 0.348171 |
| H | 0.963161 | -2.106779 | 3.319544 | C | -0.750437 3.509429 1.074415 |
| H | -1.026415 | -1.095794 | 4.372125 | C | -0.760320 2.842856 2.431349 |
| H | -1.954375 | -1.275537 | 2.866107 | O | -0.928846 1.430020 2.282844 |
| H | -1.056342 | 1.189590 | 4.401167 | C | -0.911790 0.759207 3.546157 |
| H | -2.028192 | 1.334927 | 2.919379 | C | -0.940464 -0.739246 3.348638 |
| H | 0.864298 | 2.292619 | 3.251179 | O | 0.250955 -1.135051 2.685633 |
| H | -0.548491 | 3.346087 | 3.427923 | C | 0.477387 -2.540310 2.668097 |
| H | -0.871842 | 4.589991 | 1.448585 | C | 1.808176 -2.806203 2.000269 |
| H | -2.084625 | 3.302339 | 1.258273 | O | 1.727123 -2.412319 0.630015 |
| H | -1.444879 | 4.550966 | -0.883656 | C | 2.902834 -2.681517 -0.153792 |
| H | 0.169301 | 3.841227 | -0.734140 | C | 3.982051 -1.619035 0.028941 |
| H | -2.728680 | 3.353371 | -2.402828 | O | 3.542616 -0.312739 -0.322882 |
| H | -3.349350 | 2.719205 | -0.856818 | H | 4.680654 -0.208754 -2.058687 |
| H | -3.930910 | 1.345860 | -2.879458 | H | 2.947370 -0.540086 -2.312522 |
| H | -2.198259 | 0.983751 | -3.095597 | H | 3.672695 1.795905 -2.899986 |
| H | -2.646000 | -1.332552 | -2.710649 | H | 4.127109 2.047090 -1.194303 |
| H | -4.379832 | -1.020887 | -2.420603 | H | 2.095639 3.762312 -2.401601 |
| H | -4.085691 | -1.799007 | -0.048306 | H | 2.672075 3.670045 -0.719025 |
| H | -3.786583 | -3.049409 | -1.281980 | H | -0.220314 3.239307 -1.635723 |
| H | -2.393922 | -4.292925 | 0.138243 | H | 0.449627 4.701646 -0.881027 |
| H | -2.584365 | -3.148072 | 1.479605 | H | -1.687835 3.306630 0.535638 |
| H | -0.442637 | -4.475671 | 1.573125 | H | -0.678263 4.596615 1.218360 |
| H | 0.020066 | -3.813176 | -0.002372 | H | -1.581401 3.256759 3.031844 |
| C | 4.542089 | 0.821715 | 0.421097 | H | 0.185520 3.047611 2.947807 |
| C | 3.543273 | 0.396768 | -0.414944 | H | -1.784491 1.062201 4.140106 |
| N | 4.047374 | -0.558499 | -1.274438 | H | -0.004124 1.035689 4.096622 |
| C | 5.321269 | -0.708874 | -0.975555 | H | -1.825329 -1.039495 2.768589 |
| N | 5.665121 | 0.111298 | 0.046952 | H | -1.009090 -1.213760 4.337323 |
| C | 2.110263 | 0.833609 | -0.503244 | H | -0.328402 -3.055132 2.126237 |
| C | 1.133190 | -0.344149 | -0.745395 | H | 0.507925 -2.935011 3.692885 |
| H | 1.474332 | -1.223871 | -0.195639 | H | 2.033093 -3.878452 2.063832 |
| C | 0.948557 | -0.722388 | -2.234932 | H | 2.596594 -2.251424 2.521740 |
| O | -0.148642 | -0.673301 | -2.742089 | H | 2.556680 -2.711108 -1.186803 |
| O | 2.025069 | -1.103269 | -2.888860 | H | 3.303594 -3.668562 0.108286 |
| N | -0.218455 | -0.016846 | -0.200199 | H | 4.864746 -1.906460 -0.558844 |
| H | 4.559879 | 1.545034 | 1.218450 | H | 4.291900 -1.557492 1.075154 |
| H | 6.012848 | -1.381122 | -1.457884 | C | -4.482160 0.423475 -0.597345 |
| H | 6.582413 | 0.188441 | 0.460354 | C | -3.311319 -0.128590 -1.047997 |
| H | 1.990276 | 1.571575 | -1.304890 | N | -3.578922 -1.361180 -1.607502 |
| H | 1.828864 | 1.339200 | 0.422601 | C | -4.878219 -1.554213 -1.508851 |
| H | -0.889724 | -0.777489 | -0.400871 | N | -5.466286 -0.494291 -0.903624 |
| H | -0.607505 | 0.852824 | -0.609359 | C | -1.916511 0.429191 -1.018019 |
| H | -0.180351 | 0.092761 | 0.825486 | C | -0.833711 -0.636308 -0.720982 |
| H | 2.871497 | -1.024672 | -2.341871 | H | -1.223516 -1.348562 0.009495 |

C -0.360686 -1.431698 -1.962957
 O -1.267109 -2.139875 -2.598945
 O 0.799823 -1.393287 -2.300554
 N 0.371513 -0.014156 -0.091925
 H -4.701875 1.357017 -0.107942
 H -5.420123 -2.421381 -1.851215
 H -6.452329 -0.394569 -0.712764
 H -1.867802 1.186175 -0.235037
 H -1.685379 0.926903 -1.966785
 H 0.900293 0.611255 -0.726309
 H 1.021313 -0.766638 0.211626
 H 0.104856 0.528296 0.743042
 H -2.204471 -1.999603 -2.245884

H⁺H[Na]-cggc(++0/+00/--0/--0/-00/+0+) 2568

C -1.691328 3.356303 1.059334
 C -0.198875 3.501772 1.299202
 O 0.451510 2.289179 1.678514
 C 0.343446 1.940243 3.054587
 C 1.239863 0.741525 3.305486
 O 0.784407 -0.448385 2.645372
 C 0.042074 -1.351075 3.474007
 C -0.163612 -2.648551 2.725543
 O -0.986142 -2.396945 1.597661
 C -1.223929 -3.542161 0.785601
 C -2.278180 -3.198256 -0.241366
 O -1.777712 -2.192669 -1.122632
 C -2.696429 -1.778818 -2.149200
 C -3.894041 -1.000732 -1.609393
 O -3.513781 0.119385 -0.818130
 C -3.495187 1.371582 -1.500807
 C -3.267625 2.465514 -0.484342
 O -1.917083 2.429706 -0.000191
 H -2.087799 4.343630 0.785801
 H -2.220455 3.024864 1.963173
 H -0.030151 4.278440 2.056453
 H 0.285025 3.819888 0.373312
 H -0.695621 1.711375 3.326277
 H 0.683848 2.774758 3.683905
 H 1.325423 0.563850 4.382796
 H 2.236852 0.954010 2.912355
 H -0.928433 -0.917492 3.744234
 H 0.603361 -1.555363 4.393888
 H -0.640890 -3.375525 3.397752
 H 0.807166 -3.059160 2.413254
 H -1.592591 -4.376347 1.398147
 H -0.293715 -3.861604 0.295610
 H -3.176669 -2.847371 0.276203
 H -2.531311 -4.099632 -0.814963
 H -3.052379 -2.659486 -2.700216
 H -2.105332 -1.159212 -2.822084
 H -4.517508 -1.631758 -0.970729

H -4.515802 -0.692081 -2.459596
 H -4.466715 1.552403 -1.981000
 H -2.712381 1.393537 -2.265856
 H -3.962802 2.338624 0.354547
 H -3.453306 3.440282 -0.952892
 C 4.510088 -1.065011 -0.190675
 C 3.417146 -0.578441 -0.859255
 N 3.833971 0.349258 -1.791851
 C 5.145928 0.423477 -1.700430
 N 5.598891 -0.420061 -0.741908
 C 1.965769 -0.935214 -0.709404
 C 1.016270 0.280444 -0.857143
 H 1.468291 1.152907 -0.380663
 C 0.655490 0.637360 -2.318453
 O 1.644622 0.983042 -3.111503
 O -0.498658 0.604169 -2.682756
 N -0.259124 0.022078 -0.123364
 H 4.612435 -1.791263 0.597642
 H 5.789719 1.056375 -2.290151
 H 6.564210 -0.552786 -0.479226
 H 1.817839 -1.363192 0.284385
 H 1.683873 -1.705919 -1.435786
 H -0.048457 -0.182180 0.864999
 H -0.795550 -0.779798 -0.512451
 H -0.879250 0.851858 -0.148163
 H 2.554416 0.874820 -2.681527

H⁺H[Na]-cggc(+0+/-00/+00/--0/-00/+00) 1043

C 0.882762 2.987476 1.980570
 C 1.266127 3.236537 0.527771
 O 0.282740 2.847888 -0.420586
 C -0.916917 3.616440 -0.402014
 C -1.804595 3.178818 -1.547119
 O -2.142815 1.798843 -1.401004
 C -3.429633 1.447175 -1.927076
 C -3.513677 -0.048534 -2.126611
 O -3.315264 -0.704625 -0.878535
 C -3.346519 -2.122439 -0.996665
 C -3.022420 -2.735785 0.344717
 O -1.639736 -2.509343 0.659868
 C -1.242230 -3.005437 1.940276
 C -1.429439 -1.985709 3.047843
 O -0.506361 -0.917489 2.846102
 C -0.770750 0.207013 3.672933
 C 0.329929 1.231014 3.508922
 O 0.430800 1.641343 2.140162
 H 1.772061 3.171391 2.597901
 H 0.096921 3.675004 2.318073
 H 1.518843 4.300224 0.413599
 H 2.154965 2.652985 0.277737
 H -1.451068 3.474560 0.545494
 H -0.686218 4.684839 -0.517806

H⁺H[N α]-cggc(-0/-00/+0/+00/+00/--0) 7309

| | | | |
|---|-----------|-----------|-----------|
| C | -0.406977 | -0.265486 | 3.729482 |
| C | -1.348122 | -1.332852 | 3.212436 |
| O | -0.738487 | -2.031734 | 2.133958 |
| C | -1.508245 | -3.145297 | 1.681791 |
| C | -0.978308 | -3.590818 | 0.330723 |
| O | -1.233987 | -2.626657 | -0.696534 |
| C | -2.483053 | -2.806571 | -1.386308 |
| C | -2.921824 | -1.501617 | -2.012601 |
| O | -3.227482 | -0.592028 | -0.957835 |
| C | -3.929299 | 0.586531 | -1.341969 |
| C | -3.029975 | 1.730391 | -1.783090 |
| O | -2.181793 | 2.082514 | -0.680830 |
| C | -1.562043 | 3.363196 | -0.789157 |
| C | -0.909417 | 3.694232 | 0.535670 |
| O | 0.164896 | 2.780787 | 0.761987 |
| C | 0.755024 | 2.840077 | 2.055317 |
| C | 0.015583 | 2.028002 | 3.108391 |
| O | -0.069493 | 0.661997 | 2.688478 |
| H | 0.514235 | -0.716851 | 4.114823 |
| H | -0.906471 | 0.255978 | 4.553213 |
| H | -1.575749 | -2.020025 | 4.039883 |
| H | -2.289503 | -0.878003 | 2.874961 |
| H | -2.565776 | -2.862348 | 1.600450 |
| H | -1.429878 | -3.973514 | 2.399974 |
| H | -1.414406 | -4.558523 | 0.060640 |
| H | 0.105685 | -3.716263 | 0.382743 |
| H | -3.252840 | -3.142650 | -0.683618 |
| H | -2.356382 | -3.568583 | -2.164465 |
| H | -3.816824 | -1.697500 | -2.619068 |
| H | -2.138166 | -1.101881 | -2.665456 |
| H | -4.492412 | 0.897133 | -0.458867 |
| H | -4.644537 | 0.364270 | -2.144792 |
| H | -3.665130 | 2.585763 | -2.048113 |
| H | -2.416080 | 1.464604 | -2.649362 |
| H | -2.317091 | 4.127946 | -1.011542 |
| H | -0.820790 | 3.365193 | -1.598301 |
| H | -1.657337 | 3.622777 | 1.334267 |
| H | -0.525944 | 4.722834 | 0.506260 |
| H | 1.767120 | 2.443087 | 1.941856 |
| H | 0.839152 | 3.878748 | 2.400914 |
| H | -0.994451 | 2.417457 | 3.287138 |
| H | 0.578970 | 2.101505 | 4.047415 |
| C | 4.462620 | -1.100967 | 0.529469 |
| C | 3.475599 | -0.748280 | -0.353346 |
| N | 4.033358 | -0.034477 | -1.394251 |
| C | 5.326685 | 0.043123 | -1.157486 |
| N | 5.631789 | -0.592999 | -0.000556 |
| C | 2.006661 | -1.052543 | -0.326794 |
| C | 1.117917 | 0.145197 | -0.746194 |
| H | 1.537341 | 1.076054 | -0.359536 |

| | | | |
|---|-----------|-----------|-----------|
| C | 0.922413 | 0.324094 | -2.271309 |
| O | -0.195930 | 0.384884 | -2.733809 |
| O | 2.003572 | 0.435575 | -3.009073 |
| N | -0.233209 | 0.007369 | -0.130372 |
| H | 4.444315 | -1.656846 | 1.451491 |
| H | 6.058457 | 0.536522 | -1.777090 |
| H | 6.553758 | -0.681160 | 0.400262 |
| H | 1.725779 | -1.349144 | 0.686613 |
| H | 1.785718 | -1.907641 | -0.975486 |
| H | -0.887159 | 0.740562 | -0.462651 |
| H | -0.173413 | 0.116011 | 0.894705 |
| H | -0.659382 | -0.914051 | -0.340918 |
| H | 2.863810 | 0.344106 | -2.482980 |

H⁺H[N π]-tg.g.g.(+00/-00/+0/+00/-00/+0+) sc12214

| | | | |
|---|-----------|-----------|-----------|
| C | -1.075465 | 2.586998 | 2.194269 |
| C | -1.361660 | 1.191931 | 2.702596 |
| O | -0.207860 | 0.379189 | 2.528389 |
| C | -0.340610 | -0.904182 | 3.127324 |
| C | 0.978470 | -1.642330 | 3.078690 |
| O | 1.241754 | -2.117667 | 1.762483 |
| C | 2.475965 | -2.808791 | 1.673490 |
| C | 2.647687 | -3.351693 | 0.266111 |
| O | 2.758562 | -2.330833 | -0.735253 |
| C | 4.069940 | -1.771305 | -0.879997 |
| C | 4.014999 | -0.531588 | -1.743644 |
| O | 3.373578 | 0.513237 | -1.029101 |
| C | 3.462460 | 1.774766 | -1.683361 |
| C | 2.981929 | 2.875186 | -0.763579 |
| O | 1.567714 | 2.820882 | -0.625369 |
| C | 1.052500 | 3.855203 | 0.200890 |
| C | -0.465486 | 3.782101 | 0.201734 |
| O | -0.980976 | 2.577398 | 0.768839 |
| H | -0.140852 | 2.944100 | 2.641402 |
| H | -1.886767 | 3.259354 | 2.505152 |
| H | -2.225247 | 0.758144 | 2.179796 |
| H | -1.616525 | 1.261590 | 3.770273 |
| H | -0.631147 | -0.792798 | 4.182042 |
| H | -1.121459 | -1.488755 | 2.622116 |
| H | 0.929863 | -2.491596 | 3.775562 |
| H | 1.784136 | -0.973258 | 3.409865 |
| H | 2.494118 | -3.660540 | 2.370819 |
| H | 3.306280 | -2.142217 | 1.946715 |
| H | 1.771486 | -3.944115 | -0.005011 |
| H | 3.526506 | -4.005618 | 0.225690 |
| H | 4.725723 | -2.514868 | -1.349885 |
| H | 4.482084 | -1.506507 | 0.099008 |
| H | 5.046752 | -0.246079 | -1.994638 |
| H | 3.489076 | -0.743221 | -2.686151 |
| H | 2.869683 | 1.772007 | -2.608401 |
| H | 4.508780 | 1.982082 | -1.949040 |

| | | | |
|---|-----------|-----------|-----------|
| H | 3.467169 | 2.774830 | 0.216832 |
| H | 3.278007 | 3.842367 | -1.194998 |
| H | 1.458113 | 3.765214 | 1.218323 |
| H | 1.350055 | 4.840634 | -0.188214 |
| H | -0.824476 | 3.810202 | -0.829618 |
| H | -0.871365 | 4.656633 | 0.726385 |
| C | -0.689618 | -1.507076 | -2.047406 |
| C | -1.715214 | -0.617544 | -1.901261 |
| N | -1.246251 | 0.352708 | -1.026123 |
| C | -0.000207 | 0.065091 | -0.651667 |
| N | 0.360248 | -1.054138 | -1.268939 |
| C | -3.081608 | -0.582362 | -2.509222 |
| C | -4.213587 | -0.294102 | -1.490669 |
| H | -5.165602 | -0.427072 | -2.023223 |
| C | -4.235121 | -1.314841 | -0.358214 |
| O | -4.203771 | -1.040444 | 0.814900 |
| O | -4.316013 | -2.573042 | -0.829206 |
| N | -4.056555 | 1.048070 | -0.924600 |
| H | -0.623266 | -2.406381 | -2.634714 |
| H | 0.597388 | 0.645018 | 0.027517 |
| H | 1.273913 | -1.513315 | -1.115512 |
| H | -3.128916 | 0.198878 | -3.275496 |
| H | -3.267590 | -1.532756 | -3.010932 |
| H | -4.492903 | 1.097912 | -0.008629 |
| H | -4.493361 | 1.743475 | -1.520060 |
| H | -1.800909 | 1.124718 | -0.655284 |
| H | -4.366995 | -3.177086 | -0.072010 |

H⁺H[N π]-tg.tg(+00/-00/+0+/-00/-00/+0+) sc5117

| | | | |
|---|-----------|-----------|-----------|
| C | -3.879989 | -1.466061 | -1.896792 |
| C | -3.468485 | -2.741761 | -1.183823 |
| O | -2.878850 | -2.520415 | 0.104630 |
| C | -3.815295 | -2.298017 | 1.165911 |
| C | -3.089667 | -1.829289 | 2.406531 |
| O | -2.608202 | -0.510730 | 2.199255 |
| C | -2.084287 | 0.086049 | 3.380815 |
| C | -1.834571 | 1.560294 | 3.154054 |
| O | -0.705363 | 1.749429 | 2.310572 |
| C | -0.412430 | 3.120769 | 2.085889 |
| C | 0.846815 | 3.231592 | 1.242925 |
| O | 0.709550 | 2.681957 | -0.067924 |
| C | 0.107493 | 3.564608 | -1.015363 |
| C | -0.225859 | 2.809710 | -2.282452 |
| O | -1.303496 | 1.919009 | -2.034120 |
| C | -1.773616 | 1.272507 | -3.210559 |
| C | -3.032676 | 0.490395 | -2.910915 |
| O | -2.726972 | -0.689497 | -2.176303 |
| H | -4.594296 | -0.885404 | -1.296104 |
| H | -4.390579 | -1.749643 | -2.829919 |
| H | -2.710789 | -3.260804 | -1.774163 |
| H | -4.335637 | -3.404862 | -1.083566 |
| H | -4.549774 | -1.540759 | 0.874016 |

| | | | |
|---|-----------|-----------|-----------|
| H | -4.341250 | -3.236249 | 1.382371 |
| H | -2.265054 | -2.514948 | 2.650984 |
| H | -3.800174 | -1.850213 | 3.245423 |
| H | -1.153747 | -0.412311 | 3.685831 |
| H | -2.809052 | -0.015473 | 4.201127 |
| H | -2.726565 | 2.019971 | 2.707089 |
| H | -1.656232 | 2.036146 | 4.129330 |
| H | -1.264162 | 3.614419 | 1.597274 |
| H | -0.234594 | 3.636864 | 3.041525 |
| H | 1.650470 | 2.669984 | 1.724481 |
| H | 1.155005 | 4.283536 | 1.186042 |
| H | 0.802709 | 4.381327 | -1.252894 |
| H | -0.812415 | 4.000744 | -0.609712 |
| H | -0.506028 | 3.538896 | -3.056435 |
| H | 0.656863 | 2.261662 | -2.643049 |
| H | -1.003447 | 0.602645 | -3.617794 |
| H | -2.010966 | 2.023401 | -3.977829 |
| H | -3.731615 | 1.121789 | -2.345793 |
| H | -3.509288 | 0.220585 | -3.864461 |
| C | 0.877780 | -2.297433 | -0.233653 |
| C | 1.892887 | -1.397455 | -0.389898 |
| N | 1.302113 | -0.146362 | -0.282368 |
| C | -0.006751 | -0.276161 | -0.065253 |
| N | -0.284690 | -1.574207 | -0.034701 |
| C | 3.347352 | -1.597534 | -0.670338 |
| C | 4.273849 | -0.759527 | 0.246238 |
| H | 4.027561 | -0.986198 | 1.287004 |
| C | 5.727317 | -1.186141 | 0.007302 |
| O | 6.536396 | -0.528210 | -0.592218 |
| O | 5.981119 | -2.401721 | 0.531040 |
| N | 4.060935 | 0.667907 | 0.007096 |
| H | 0.888337 | -3.373376 | -0.253675 |
| H | -0.701347 | 0.532305 | 0.070830 |
| H | -1.244851 | -1.942600 | 0.076312 |
| H | 3.578619 | -2.658077 | -0.559240 |
| H | 3.563960 | -1.330228 | -1.711803 |
| H | 4.444058 | 1.212072 | 0.774519 |
| H | 4.589540 | 0.950990 | -0.816485 |
| H | 1.809958 | 0.737628 | -0.291314 |
| H | 6.903619 | -2.633024 | 0.336739 |

H⁺H[N π]-tg.g.g(-00/-00/-00/-00/+00/-0) sc13838

| | | | |
|---|-----------|-----------|-----------|
| C | 3.940661 | -1.304730 | -1.821888 |
| C | 4.370768 | 0.079718 | -1.364344 |
| O | 3.240272 | 0.930868 | -1.283908 |
| C | 3.583771 | 2.259144 | -0.902866 |
| C | 2.346078 | 3.124076 | -0.812912 |
| O | 1.588139 | 2.773190 | 0.336849 |
| C | 0.505731 | 3.657833 | 0.586343 |
| C | -0.157652 | 3.291259 | 1.895671 |
| O | -0.817511 | 2.034139 | 1.776293 |
| C | -1.292554 | 1.530543 | 3.025575 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | -1.689736 | 0.078318 | 2.879391 | H | -4.509923 | -2.835347 | -1.300368 |
| O | -0.517679 | -0.699630 | 2.680327 | | | | |
| C | -0.782933 | -2.069005 | 2.426234 | H ⁺ H[N π]-tg.tg(+00/-00/+00/--0/-00/+0+) sc241 | | | |
| C | 0.517600 | -2.840348 | 2.369757 | C | -1.092010 | -1.733095 | 3.112743 |
| O | 1.319716 | -2.369639 | 1.291707 | C | -0.529387 | -0.374848 | 3.469430 |
| C | 2.480842 | -3.155650 | 1.065842 | O | 0.453208 | 0.011428 | 2.514548 |
| C | 3.507849 | -2.333507 | 0.319476 | C | 1.157123 | 1.202204 | 2.841284 |
| O | 2.995644 | -1.957304 | -0.964736 | C | 0.404244 | 2.490069 | 2.546319 |
| H | 4.830814 | -1.936636 | -1.932874 | O | 0.188088 | 2.609343 | 1.144935 |
| H | 3.449526 | -1.234809 | -2.794234 | C | -0.563996 | 3.768661 | 0.796585 |
| H | 5.094779 | 0.461659 | -2.100338 | C | -1.000929 | 3.678810 | -0.648097 |
| H | 4.887016 | 0.038928 | -0.395061 | O | -1.949759 | 2.628856 | -0.778949 |
| H | 4.097514 | 2.255314 | 0.067863 | C | -2.528751 | 2.543286 | -2.075727 |
| H | 4.262677 | 2.696843 | -1.648900 | C | -3.688059 | 1.572851 | -2.056349 |
| H | 2.666344 | 4.173779 | -0.744742 | O | -3.216257 | 0.235673 | -1.933214 |
| H | 1.741825 | 3.013116 | -1.724560 | C | -4.274076 | -0.705935 | -1.862165 |
| H | -0.223100 | 3.620053 | -0.237212 | C | -3.699298 | -2.110629 | -1.810573 |
| H | 0.869154 | 4.693081 | 0.660397 | O | -2.884134 | -2.371072 | -0.661152 |
| H | -0.878957 | 4.076352 | 2.163728 | C | -3.604842 | -2.595689 | 0.556436 |
| H | 0.602944 | 3.238885 | 2.684688 | C | -2.631222 | -2.835673 | 1.687708 |
| H | -2.159711 | 2.114748 | 3.363448 | O | -1.948826 | -1.627683 | 1.982060 |
| H | -0.503588 | 1.614846 | 3.783007 | H | -1.659871 | -2.108733 | 3.976266 |
| H | -2.208743 | -0.238896 | 3.795602 | H | -0.272017 | -2.436078 | 2.911283 |
| H | -2.388329 | -0.049711 | 2.041060 | H | -0.071272 | -0.440399 | 4.466995 |
| H | -1.333284 | -2.182113 | 1.481240 | H | -1.348855 | 0.353179 | 3.515134 |
| H | -1.401956 | -2.498578 | 3.227676 | H | 2.073562 | 1.180677 | 2.246727 |
| H | 0.280622 | -3.905612 | 2.236108 | H | 1.443485 | 1.199631 | 3.902617 |
| H | 1.063129 | -2.724746 | 3.315658 | H | 1.005566 | 3.334887 | 2.914179 |
| H | 2.223661 | -4.062565 | 0.501425 | H | -0.558287 | 2.515948 | 3.074423 |
| H | 2.933296 | -3.463721 | 2.018507 | H | 0.043694 | 4.673362 | 0.937786 |
| H | 4.418647 | -2.931339 | 0.185915 | H | -1.451607 | 3.845838 | 1.437515 |
| H | 3.752043 | -1.441900 | 0.906137 | H | -0.133677 | 3.502583 | -1.301257 |
| C | -0.486441 | -0.965537 | -2.242835 | H | -1.450896 | 4.638228 | -0.939826 |
| C | -1.495624 | -0.086055 | -1.971636 | H | -1.779646 | 2.224704 | -2.814084 |
| N | -1.119494 | 0.563980 | -0.803376 | H | -2.909585 | 3.527998 | -2.381100 |
| C | 0.056311 | 0.097061 | -0.379772 | H | -4.254696 | 1.684240 | -2.992012 |
| N | 0.457726 | -0.826541 | -1.243128 | H | -4.355369 | 1.818969 | -1.219495 |
| C | -2.765601 | 0.219098 | -2.701532 | H | -4.914834 | -0.638221 | -2.754580 |
| C | -4.011018 | 0.305868 | -1.783612 | H | -4.908290 | -0.499246 | -0.988774 |
| H | -4.886010 | 0.414353 | -2.439166 | H | -3.050316 | -2.270987 | -2.673644 |
| C | -4.239560 | -0.988261 | -1.010167 | H | -4.516044 | -2.841220 | -1.855977 |
| O | -4.351777 | -1.061330 | 0.187585 | H | -4.246446 | -3.477603 | 0.436338 |
| O | -4.322196 | -2.047949 | -1.834926 | H | -4.232013 | -1.731036 | 0.796312 |
| N | -3.868798 | 1.414344 | -0.833611 | H | -1.920478 | -3.629327 | 1.415083 |
| H | -0.368505 | -1.664853 | -3.052262 | H | -3.199565 | -3.179835 | 2.564114 |
| H | 0.566649 | 0.415382 | 0.510946 | C | 0.797712 | -1.884440 | -1.225322 |
| H | 1.353244 | -1.332052 | -1.137177 | C | 1.810857 | -0.971229 | -1.176278 |
| H | -2.923567 | -0.540816 | -3.467810 | N | 1.230125 | 0.207695 | -0.731069 |
| H | -2.676323 | 1.180330 | -3.219402 | C | -0.071312 | 0.019020 | -0.504407 |
| H | -4.182233 | 2.284888 | -1.249948 | N | -0.354423 | -1.239606 | -0.813929 |
| H | -4.433373 | 1.241482 | -0.006592 | C | 3.257616 | -1.076107 | -1.538364 |
| H | -1.710122 | 1.229472 | -0.305842 | C | 4.200854 | -0.439102 | -0.487420 |

| | | | |
|---|-----------|-----------|-----------|
| H | 3.999904 | -0.901334 | 0.482788 |
| C | 5.654150 | -0.752131 | -0.862314 |
| O | 6.427301 | 0.054471 | -1.307593 |
| O | 5.952517 | -2.049158 | -0.651622 |
| N | 3.947280 | 1.000979 | -0.386567 |
| H | 0.801723 | -2.918973 | -1.521655 |
| H | -0.762387 | 0.764574 | -0.147804 |
| H | -1.297617 | -1.652029 | -0.714605 |
| H | 3.435885 | -0.584351 | -2.502683 |
| H | 3.509258 | -2.129673 | -1.667897 |
| H | 4.404602 | 1.474706 | -1.164320 |
| H | 4.389772 | 1.373720 | 0.448810 |
| H | 1.783561 | 1.031540 | -0.497701 |
| H | 6.872749 | -2.200231 | -0.921051 |

H⁺H[N π]-tg.g.g(+00/-00/+0+/-+00/-00/+0+) sc329

| | | | |
|---|-----------|-----------|-----------|
| C | -0.578183 | -2.986924 | 1.734125 |
| C | -1.978523 | -3.229554 | 1.211581 |
| O | -2.105560 | -2.797668 | -0.149366 |
| C | -3.449743 | -2.762573 | -0.642923 |
| C | -4.210042 | -1.506692 | -0.253360 |
| O | -3.584493 | -0.374833 | -0.841295 |
| C | -4.312215 | 0.829997 | -0.629236 |
| C | -3.574772 | 1.995620 | -1.248604 |
| O | -2.405442 | 2.285149 | -0.485956 |
| C | -1.747389 | 3.475393 | -0.899127 |
| C | -0.719756 | 3.880999 | 0.133105 |
| O | 0.415948 | 3.007809 | 0.100116 |
| C | 1.319934 | 3.198303 | 1.196799 |
| C | 0.981085 | 2.350108 | 2.412476 |
| O | 1.217107 | 0.967241 | 2.133197 |
| C | 0.805870 | 0.105104 | 3.205815 |
| C | 0.783871 | -1.344503 | 2.771077 |
| O | -0.379307 | -1.602441 | 1.985846 |
| H | 0.172264 | -3.369774 | 1.028209 |
| H | -0.472650 | -3.557687 | 2.667999 |
| H | -2.690341 | -2.692961 | 1.846998 |
| H | -2.200159 | -4.303116 | 1.265679 |
| H | -3.999732 | -3.646021 | -0.296952 |
| H | -3.372869 | -2.816833 | -1.730912 |
| H | -4.256769 | -1.387936 | 0.838015 |
| H | -5.242466 | -1.607772 | -0.619685 |
| H | -4.448202 | 1.009448 | 0.445798 |
| H | -5.305522 | 0.755029 | -1.093899 |
| H | -4.242362 | 2.868260 | -1.251655 |
| H | -3.309701 | 1.764383 | -2.289258 |
| H | -2.473719 | 4.295389 | -0.988521 |
| H | -1.275907 | 3.340980 | -1.883419 |
| H | -1.186161 | 3.858628 | 1.124192 |
| H | -0.389636 | 4.906887 | -0.074850 |
| H | 1.328462 | 4.253552 | 1.492891 |
| H | 2.315334 | 2.951205 | 0.825827 |

| | | | |
|---|-----------|-----------|-----------|
| H | -0.068955 | 2.486145 | 2.698558 |
| H | 1.606265 | 2.676626 | 3.255736 |
| H | -0.195441 | 0.398033 | 3.541364 |
| H | 1.501436 | 0.217668 | 4.047582 |
| H | 0.756035 | -1.960781 | 3.681441 |
| H | 1.696260 | -1.600215 | 2.218821 |
| C | 1.050894 | -1.447706 | -2.118351 |
| C | 1.628688 | -0.211085 | -2.043585 |
| N | 0.707162 | 0.593097 | -1.380915 |
| C | -0.367694 | -0.121120 | -1.052931 |
| N | -0.183181 | -1.358470 | -1.501905 |
| C | 3.012158 | 0.246826 | -2.383594 |
| C | 4.084354 | -0.495856 | -1.526296 |
| H | 5.011603 | 0.092218 | -1.582488 |
| C | 3.652282 | -0.501821 | -0.061925 |
| O | 3.588342 | -1.492253 | 0.625324 |
| O | 3.301928 | 0.722657 | 0.357570 |
| N | 4.240523 | -1.868193 | -1.985198 |
| H | 1.440016 | -2.363675 | -2.524960 |
| H | -1.235820 | 0.242170 | -0.529081 |
| H | -0.833516 | -2.109118 | -1.244267 |
| H | 3.090614 | 1.323428 | -2.224394 |
| H | 3.234409 | 0.053081 | -3.434788 |
| H | 4.463549 | -2.483268 | -1.209224 |
| H | 4.966860 | -1.948907 | -2.686718 |
| H | 0.818186 | 1.558875 | -1.058698 |
| H | 2.774015 | 0.658648 | 1.187011 |

H⁺H[N π]-tg.g.g(-00/+00/--0/-00/+00/--0) sc283

| | | | |
|---|-----------|-----------|-----------|
| C | -1.006066 | 3.250873 | 1.311785 |
| C | -0.699331 | 2.297948 | 2.453961 |
| O | -0.938484 | 0.956128 | 2.044480 |
| C | -0.728095 | 0.026042 | 3.105658 |
| C | -0.794565 | -1.400688 | 2.606159 |
| O | 0.406136 | -1.727691 | 1.906994 |
| C | 0.553176 | -3.117016 | 1.664671 |
| C | 1.931986 | -3.393171 | 1.104519 |
| O | 2.023252 | -2.938368 | -0.253154 |
| C | 3.345269 | -2.937771 | -0.806505 |
| C | 4.179741 | -1.733371 | -0.406685 |
| O | 3.588450 | -0.549788 | -0.923427 |
| C | 4.404086 | 0.599730 | -0.717545 |
| C | 3.727326 | 1.832230 | -1.273800 |
| O | 2.630037 | 2.199980 | -0.442295 |
| C | 2.060291 | 3.457643 | -0.787614 |
| C | 1.069510 | 3.880216 | 0.273619 |
| O | -0.123766 | 3.097008 | 0.191231 |
| H | -0.966626 | 4.282726 | 1.680309 |
| H | -2.010656 | 3.063482 | 0.929638 |
| H | -1.349375 | 2.560244 | 3.302718 |
| H | 0.341547 | 2.404567 | 2.790156 |
| H | -1.500085 | 0.165975 | 3.875759 |

| | | | |
|---|-----------|-----------|-----------|
| H | 0.252085 | 0.199931 | 3.568677 |
| H | -1.673498 | -1.546362 | 1.965354 |
| H | -0.899919 | -2.057465 | 3.481455 |
| H | -0.221862 | -3.483003 | 0.975294 |
| H | 0.451681 | -3.680531 | 2.603652 |
| H | 2.126102 | -4.472598 | 1.130156 |
| H | 2.676196 | -2.885675 | 1.726179 |
| H | 3.214565 | -2.946962 | -1.890435 |
| H | 3.868186 | -3.857374 | -0.518315 |
| H | 5.188742 | -1.871254 | -0.823251 |
| H | 4.281609 | -1.659909 | 0.684957 |
| H | 5.367799 | 0.468637 | -1.229777 |
| H | 4.601139 | 0.740609 | 0.353737 |
| H | 3.387691 | 1.645416 | -2.301759 |
| H | 4.462634 | 2.648187 | -1.300380 |
| H | 1.572205 | 3.407252 | -1.771432 |
| H | 2.847761 | 4.222105 | -0.843747 |
| H | 0.819188 | 4.939290 | 0.128310 |
| H | 1.534858 | 3.764947 | 1.258860 |
| C | -1.053719 | -1.323482 | -1.893982 |
| C | -1.654967 | -0.096339 | -1.865942 |
| N | -0.742151 | 0.749247 | -1.249852 |
| C | 0.347864 | 0.067065 | -0.902897 |
| N | 0.184097 | -1.190204 | -1.296113 |
| C | -3.020188 | 0.335488 | -2.287799 |
| C | -4.042453 | 0.375791 | -1.111046 |
| H | -4.974741 | 0.765147 | -1.526427 |
| C | -4.319055 | -1.049222 | -0.621524 |
| O | -3.889359 | -1.523055 | 0.400681 |
| O | -5.084125 | -1.736138 | -1.494405 |
| N | -3.582896 | 1.265164 | -0.055750 |
| H | -1.404822 | -2.262415 | -2.285428 |
| H | 1.213370 | 0.476000 | -0.407758 |
| H | 0.855186 | -1.931853 | -1.036921 |
| H | -3.386475 | -0.337340 | -3.065178 |
| H | -2.978615 | 1.340576 | -2.712900 |
| H | -2.954796 | 0.780409 | 0.583453 |
| H | -4.368613 | 1.589393 | 0.498308 |
| H | -0.855396 | 1.728614 | -0.983905 |
| H | -5.232413 | -2.626604 | -1.138398 |

Structures (Lys)H⁺-18C6H⁺K[Ne]-ctggtt(-00/+00/-00/+00/-00/+00) 389

| | | | |
|---|-----------|-----------|-----------|
| C | -1.211123 | -1.682179 | 2.507865 |
| C | -0.126718 | -2.726927 | 2.387374 |
| O | 0.531609 | -2.624281 | 1.116481 |
| C | 1.570715 | -3.593566 | 0.969182 |
| C | 2.293239 | -3.390212 | -0.343107 |
| O | 2.962201 | -2.135361 | -0.311217 |
| C | 3.811164 | -1.898527 | -1.425580 |
| C | 4.535433 | -0.587792 | -1.217023 |
| O | 3.594341 | 0.488155 | -1.213686 |
| C | 4.213808 | 1.763887 | -1.036795 |
| C | 3.158324 | 2.846420 | -1.046634 |
| O | 2.309109 | 2.665528 | 0.078310 |
| C | 1.325385 | 3.679742 | 0.237212 |
| C | 0.612963 | 3.470652 | 1.554108 |
| O | -0.131966 | 2.251955 | 1.527478 |
| C | -0.751087 | 1.970324 | 2.790788 |
| C | -1.522584 | 0.673686 | 2.719672 |
| O | -0.606296 | -0.390854 | 2.484332 |
| H | -1.952722 | -1.776972 | 1.706611 |
| H | -1.729628 | -1.840367 | 3.463947 |
| H | -0.578062 | -3.722357 | 2.486231 |
| H | 0.611495 | -2.596159 | 3.188326 |
| H | 2.283029 | -3.502934 | 1.798838 |
| H | 1.141257 | -4.603847 | 0.988918 |
| H | 1.585461 | -3.428275 | -1.183595 |
| H | 3.016292 | -4.207272 | -0.472161 |
| H | 3.227910 | -1.868463 | -2.357106 |
| H | 4.556999 | -2.700089 | -1.518509 |
| H | 5.079265 | -0.609594 | -0.264341 |
| H | 5.260203 | -0.445679 | -2.029292 |
| H | 4.759781 | 1.784196 | -0.085287 |
| H | 4.925855 | 1.948817 | -1.851699 |
| H | 3.657179 | 3.824277 | -0.999375 |
| H | 2.578236 | 2.805469 | -1.979668 |
| H | 0.609393 | 3.656724 | -0.597059 |
| H | 1.796538 | 4.672210 | 0.251020 |
| H | 1.348411 | 3.438484 | 2.367691 |
| H | -0.065248 | 4.315557 | 1.732541 |
| H | -1.441168 | 2.783236 | 3.050219 |
| H | 0.021897 | 1.905760 | 3.566550 |
| H | -2.286786 | 0.713651 | 1.935026 |
| H | -2.037150 | 0.528814 | 3.679942 |
| C | -1.984254 | -0.340915 | -2.587634 |
| C | -1.257455 | -0.338270 | -1.232966 |
| C | 0.215873 | 0.025818 | -1.378241 |
| N | 0.925177 | 0.026838 | -0.061193 |
| C | -3.390585 | -0.970673 | -2.576269 |
| C | -4.497966 | -0.218625 | -1.809234 |
| H | -5.418000 | -0.798290 | -1.932155 |
| C | -4.243334 | -0.222619 | -0.285568 |

| | | | |
|---|-----------|-----------|-----------|
| O | -3.958582 | -1.218494 | 0.332455 |
| O | -4.363630 | 0.977274 | 0.293320 |
| N | -4.748585 | 1.162777 | -2.260935 |
| H | -1.388842 | -0.913344 | -3.307963 |
| H | -2.016807 | 0.680176 | -2.989869 |
| H | -1.726309 | 0.369211 | -0.544394 |
| H | -1.339073 | -1.326908 | -0.773386 |
| H | 0.735741 | -0.686441 | -2.021122 |
| H | 0.344358 | 1.018516 | -1.813996 |
| H | 0.823623 | -0.882926 | 0.420995 |
| H | 0.562454 | 0.764562 | 0.566301 |
| H | -3.729716 | -1.080462 | -3.610823 |
| H | -3.328671 | -1.977988 | -2.156812 |
| H | -4.605628 | 1.589968 | -0.443325 |
| H | -5.631857 | 1.255038 | -2.747913 |
| H | -4.019961 | 1.512996 | -2.872457 |
| H | 1.929028 | 0.200688 | -0.218632 |

H⁺K[Ne]-tg.tttt(-00/+00/-00/+00/-00/+00) 0

| | | | |
|---|-----------|-----------|-----------|
| O | -0.822236 | 0.624645 | 2.890536 |
| C | -0.123391 | -0.430093 | 3.539154 |
| C | -0.917451 | -1.708085 | 3.395155 |
| C | -0.222809 | 1.902673 | 3.059309 |
| C | -1.113516 | 2.949510 | 2.430625 |
| O | -1.184460 | 2.749116 | 1.015739 |
| C | -2.018473 | 3.716539 | 0.371594 |
| C | -2.135092 | 3.405030 | -1.103069 |
| O | -2.824800 | 2.171705 | -1.259154 |
| C | -3.141199 | 1.845987 | -2.606509 |
| C | -3.955891 | 0.572384 | -2.620512 |
| O | -3.161426 | -0.511959 | -2.134408 |
| C | -3.864403 | -1.756876 | -2.133600 |
| C | -2.956398 | -2.854779 | -1.627422 |
| O | -2.635696 | -2.592600 | -0.267357 |
| O | -0.989705 | -2.091079 | 2.018623 |
| C | -1.738871 | -3.295179 | 1.829393 |
| C | -1.858370 | -3.607649 | 0.355205 |
| H | 0.879894 | -0.549521 | 3.107503 |
| H | -0.008142 | -0.212553 | 4.609999 |
| H | -0.426056 | -2.500488 | 3.974519 |
| H | -1.930300 | -1.563838 | 3.791235 |
| H | 0.776070 | 1.922874 | 2.602050 |
| H | -0.112359 | 2.136712 | 4.127189 |
| H | -0.701147 | 3.944295 | 2.643735 |
| H | -2.120229 | 2.889619 | 2.862403 |
| H | -1.585904 | 4.717983 | 0.494664 |
| H | -3.015419 | 3.709036 | 0.829262 |
| H | -1.139574 | 3.352749 | -1.566549 |
| H | -2.690730 | 4.220280 | -1.586494 |
| H | -2.224245 | 1.719090 | -3.199226 |
| H | -3.734909 | 2.647786 | -3.066650 |
| H | -4.278917 | 0.365121 | -3.648972 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | -4.847363 | 0.692054 | -1.992233 | C | -4.555837 | -1.156838 | -0.417497 |
| H | -4.188174 | -2.001708 | -3.153497 | O | -3.289016 | -1.771569 | -0.617381 |
| H | -4.752520 | -1.682052 | -1.493748 | H | -3.402085 | -2.939948 | 1.092900 |
| H | -2.043314 | -2.907390 | -2.236901 | H | -3.887921 | -3.753070 | -0.408265 |
| H | -3.482316 | -3.814990 | -1.719915 | H | -1.545649 | -3.588288 | -1.261227 |
| H | -1.233023 | -4.128494 | 2.334073 | H | -1.691690 | -4.586539 | 0.194454 |
| H | -2.739524 | -3.179502 | 2.263902 | H | -0.270061 | -4.046084 | 1.938503 |
| H | -0.863444 | -3.671555 | -0.107834 | H | -1.419347 | -2.757443 | 2.379490 |
| H | -2.345749 | -4.586235 | 0.246440 | H | 1.531865 | -2.323942 | 1.672114 |
| O | 6.588882 | 1.464732 | -0.743015 | H | 0.853613 | -2.413488 | 3.313474 |
| C | 6.363422 | 0.134878 | -0.638061 | H | 2.230849 | -0.096466 | 2.256970 |
| H | 7.404937 | 1.667331 | -0.258907 | H | 1.356853 | -0.045935 | 3.806948 |
| C | 5.072701 | -0.285335 | -1.346174 | H | 1.560885 | 2.206698 | 2.966034 |
| O | 7.088993 | -0.611278 | -0.031844 | H | -0.152289 | 1.717580 | 2.903764 |
| N | 5.044568 | -1.702453 | -1.685409 | H | 1.030137 | 3.245614 | -0.330019 |
| H | 4.998534 | 0.298368 | -2.268505 | H | 1.356098 | 3.790721 | 1.324361 |
| C | 3.872119 | 0.076965 | -0.441912 | H | -0.732446 | 4.762984 | 0.556154 |
| H | 5.641909 | -1.894567 | -2.482808 | H | -1.110358 | 3.599213 | 1.840083 |
| H | 5.416339 | -2.247493 | -0.911342 | H | -3.089195 | 4.353287 | -0.269769 |
| H | 3.916157 | -0.560389 | 0.449929 | H | -3.278890 | 3.173878 | 1.051117 |
| H | 3.975608 | 1.112142 | -0.101830 | H | -3.379871 | 2.511595 | -1.939486 |
| C | 2.528303 | -0.114807 | -1.150918 | H | -4.786101 | 2.746742 | -0.876211 |
| H | 2.454002 | 0.598734 | -1.981051 | H | -4.335101 | 0.083135 | -2.168061 |
| H | 2.508540 | -1.115535 | -1.591747 | H | -5.588536 | 0.608631 | -1.020932 |
| C | 1.331675 | 0.067499 | -0.208754 | H | -5.355514 | -1.779918 | -0.841913 |
| H | 1.401440 | -0.654337 | 0.612198 | H | -4.750526 | -1.031557 | 0.656072 |
| H | 1.353125 | 1.067788 | 0.237863 | C | 2.028533 | -0.120569 | -1.804871 |
| C | 0.009437 | -0.131228 | -0.940713 | C | 0.727287 | -0.770781 | -2.294393 |
| H | -0.112208 | 0.601723 | -1.739827 | C | -0.547379 | 0.005242 | -1.967207 |
| H | -0.040972 | -1.123021 | -1.392582 | N | -0.856879 | 0.021032 | -0.500734 |
| N | -1.180070 | 0.000648 | -0.041040 | C | 3.242351 | -1.033561 | -2.033571 |
| H | -2.038253 | -0.145168 | -0.595110 | C | 4.558763 | -0.515625 | -1.427247 |
| H | -1.161491 | -0.701924 | 0.716093 | H | 5.315322 | -1.297362 | -1.550864 |
| H | -1.228935 | 0.938850 | 0.388087 | C | 4.424998 | -0.341696 | 0.103095 |
| H+K[Ne]-ctgtg(+00/-00/+00/--0/+00/+0+) 2088 | | | | | | | |
| C | -3.173241 | -3.037419 | 0.022938 | O | 3.825235 | -1.122238 | 0.803264 |
| C | -1.764894 | -3.562935 | -0.191431 | O | 5.034187 | 0.740278 | 0.588355 |
| O | -0.754726 | -2.741011 | 0.400687 | N | 5.107053 | 0.721431 | -2.009382 |
| C | -0.521225 | -2.987919 | 1.794675 | H | 2.159944 | 0.839332 | -2.321574 |
| C | 0.633294 | -2.138246 | 2.272301 | H | 1.952254 | 0.105935 | -0.737487 |
| O | 0.262886 | -0.764640 | 2.191922 | H | 0.643263 | -1.778978 | -1.874348 |
| C | 1.261053 | 0.107590 | 2.722571 | H | 0.762495 | -0.892808 | -3.382141 |
| C | 0.841812 | 1.537707 | 2.477935 | H | -1.405591 | -0.456737 | -2.456242 |
| O | 0.833993 | 1.796819 | 1.065642 | H | -0.486447 | 1.045285 | -2.293677 |
| C | 0.693590 | 3.172286 | 0.706496 | H | -0.837191 | -0.935931 | -0.105961 |
| C | -0.728978 | 3.694169 | 0.814387 | H | -1.804713 | 0.401890 | -0.353015 |
| O | -1.555461 | 2.961109 | -0.081941 | H | 3.037890 | -2.008281 | -1.583589 |
| C | -2.932120 | 3.304116 | 0.017309 | H | 3.396963 | -1.201906 | -3.104757 |
| C | -3.738819 | 2.420209 | -0.905780 | H | 5.415739 | 1.197919 | -0.197048 |
| O | -3.641216 | 1.063610 | -0.467074 | H | 5.806343 | 0.536797 | -2.718312 |
| C | -4.577149 | 0.190263 | -1.102354 | H | 4.390482 | 1.307887 | -2.423439 |
| | | | | H | -0.202007 | 0.607485 | 0.044779 |

H⁺K[Ne]-cgggt(-00/+00/--0/-00/+00/--0) 739

| | | | |
|---|-----------|-----------|-----------|
| C | -3.760328 | -0.529498 | -2.124823 |
| C | -3.132243 | 0.685918 | -2.768700 |
| O | -2.461645 | 1.461728 | -1.774668 |
| C | -1.971561 | 2.711899 | -2.268582 |
| C | -1.466736 | 3.545705 | -1.112868 |
| O | -0.372159 | 2.877866 | -0.505344 |
| C | 0.225021 | 3.608251 | 0.560837 |
| C | 1.335370 | 2.765036 | 1.160599 |
| O | 0.854951 | 1.549858 | 1.759918 |
| C | 0.371040 | 1.681537 | 3.095884 |
| C | 0.017442 | 0.312100 | 3.629467 |
| O | -1.083859 | -0.203003 | 2.889056 |
| C | -1.498276 | -1.493579 | 3.311539 |
| C | -2.741684 | -1.888444 | 2.549100 |
| O | -2.438841 | -2.044973 | 1.159989 |
| C | -3.579225 | -2.440398 | 0.396326 |
| C | -3.184539 | -2.606397 | -1.061276 |
| O | -2.729511 | -1.404365 | -1.675330 |
| H | -4.400123 | -0.210780 | -1.292786 |
| H | -4.387962 | -1.039244 | -2.868672 |
| H | -3.924702 | 1.286143 | -3.234335 |
| H | -2.426552 | 0.378718 | -3.551507 |
| H | -1.165523 | 2.538309 | -2.992919 |
| H | -2.781407 | 3.255015 | -2.772353 |
| H | -2.271506 | 3.704521 | -0.381499 |
| H | -1.156073 | 4.526563 | -1.499833 |
| H | -0.536186 | 3.868301 | 1.310008 |
| H | 0.659658 | 4.545645 | 0.185314 |
| H | 2.031612 | 2.452252 | 0.381446 |
| H | 1.884557 | 3.352419 | 1.905587 |
| H | 1.152267 | 2.120355 | 3.729558 |
| H | -0.512171 | 2.330798 | 3.131935 |
| H | 0.882861 | -0.359250 | 3.543912 |
| H | -0.245990 | 0.400312 | 4.692694 |
| H | -1.736927 | -1.489656 | 4.384501 |
| H | -0.697894 | -2.228462 | 3.145252 |
| H | -3.122643 | -2.835552 | 2.953155 |
| H | -3.515083 | -1.120218 | 2.675674 |
| H | -4.378657 | -1.696689 | 0.512695 |
| H | -3.961448 | -3.401560 | 0.767011 |
| H | -4.034883 | -3.025467 | -1.615184 |
| H | -2.355112 | -3.313689 | -1.134017 |
| C | 2.275301 | -2.546883 | -1.159145 |
| C | 1.350183 | -1.710491 | -0.253737 |
| C | 0.430364 | -0.771742 | -1.032329 |
| N | -0.554646 | -0.098753 | -0.127355 |
| C | 3.279920 | -1.796382 | -2.054717 |
| C | 4.447411 | -1.069964 | -1.355584 |
| H | 5.091218 | -0.671961 | -2.147248 |
| C | 3.988816 | 0.191536 | -0.592698 |
| O | 3.171399 | 0.965554 | -1.033971 |

| | | | |
|---|-----------|-----------|-----------|
| O | 4.593614 | 0.374388 | 0.580242 |
| N | 5.291571 | -1.891036 | -0.471936 |
| H | 1.650834 | -3.159134 | -1.819145 |
| H | 2.803915 | -3.270405 | -0.527327 |
| H | 0.736353 | -2.408007 | 0.327746 |
| H | 1.927685 | -1.129539 | 0.472097 |
| H | 0.999637 | 0.017977 | -1.521251 |
| H | -0.151260 | -1.314046 | -1.779136 |
| H | -0.079165 | 0.484129 | 0.586372 |
| H | -1.158799 | -0.778742 | 0.357005 |
| H | 3.720331 | -2.523419 | -2.743961 |
| H | 2.761256 | -1.062597 | -2.675916 |
| H | 5.194919 | -0.401886 | 0.683045 |
| H | 4.802096 | -2.699001 | -0.103089 |
| H | 6.130202 | -2.220273 | -0.934572 |
| H | -1.177051 | 0.521017 | -0.670099 |

H⁺K[Ne]-cgg.g.tt(+00/-00/+0+/-00/-00/+0+) 1158

| | | | |
|---|-----------|-----------|-----------|
| C | 3.745910 | 2.535519 | -0.607584 |
| C | 4.192918 | 1.356238 | -1.441384 |
| O | 3.711140 | 0.147550 | -0.849206 |
| C | 4.274092 | -1.035075 | -1.422676 |
| C | 3.839889 | -2.240149 | -0.618874 |
| O | 2.438288 | -2.429280 | -0.785226 |
| C | 1.896521 | -3.555518 | -0.097505 |
| C | 1.597472 | -3.294887 | 1.369307 |
| O | 0.602783 | -2.277168 | 1.479238 |
| C | 0.203090 | -2.037663 | 2.835580 |
| C | -0.867426 | -0.972833 | 2.885449 |
| O | -0.309845 | 0.263775 | 2.443874 |
| C | -1.210742 | 1.361042 | 2.566000 |
| C | -0.522421 | 2.613514 | 2.075122 |
| O | -0.271506 | 2.497954 | 0.667067 |
| C | 0.294150 | 3.664723 | 0.061687 |
| C | 1.810504 | 3.704040 | 0.130407 |
| O | 2.326853 | 2.624288 | -0.639410 |
| H | 4.197246 | 3.449065 | -1.019317 |
| H | 4.094903 | 2.415174 | 0.426917 |
| H | 5.289777 | 1.343160 | -1.472683 |
| H | 3.818727 | 1.448211 | -2.469192 |
| H | 5.369415 | -0.970335 | -1.399398 |
| H | 3.954673 | -1.139849 | -2.467539 |
| H | 4.096048 | -2.085678 | 0.436583 |
| H | 4.385377 | -3.122006 | -0.981908 |
| H | 2.572185 | -4.416831 | -0.178314 |
| H | 0.968635 | -3.805384 | -0.616642 |
| H | 2.500167 | -2.993708 | 1.917718 |
| H | 1.228910 | -4.226687 | 1.819559 |
| H | 1.074804 | -1.725084 | 3.424550 |
| H | -0.196386 | -2.964138 | 3.266919 |
| H | -1.209834 | -0.883703 | 3.926090 |
| H | -1.730435 | -1.247590 | 2.267080 |

H⁺K[Ne]-cggg.tt(-00/+00/--0/-00/+00/--0) 5206

| | | | |
|---|-----------|-----------|-----------|
| C | 0.066921 | 3.384039 | 1.248671 |
| C | 1.249750 | 2.467005 | 1.501153 |
| O | 0.855409 | 1.126156 | 1.832851 |
| C | 0.546756 | 0.899161 | 3.207855 |
| C | 0.315533 | -0.580375 | 3.417259 |
| O | -0.847650 | -0.973067 | 2.696307 |
| C | -1.136763 | -2.359889 | 2.798903 |
| C | -2.450995 | -2.647754 | 2.110790 |
| O | -2.332430 | -2.419906 | 0.703696 |
| C | -3.546039 | -2.693689 | 0.002071 |
| C | -3.346984 | -2.432092 | -1.481344 |
| O | -3.035485 | -1.076641 | -1.791347 |
| C | -4.155552 | -0.198635 | -1.857660 |
| C | -3.676602 | 1.184733 | -2.236878 |
| O | -2.892404 | 1.728511 | -1.173294 |
| C | -2.490500 | 3.082449 | -1.403115 |
| C | -1.836649 | 3.635961 | -0.157035 |
| O | -0.646634 | 2.909108 | 0.110734 |
| H | 0.440683 | 4.401867 | 1.067620 |
| H | -0.602602 | 3.422971 | 2.119525 |
| H | 1.870271 | 2.879881 | 2.304776 |
| H | 1.867920 | 2.380159 | 0.606342 |
| H | -0.346427 | 1.460629 | 3.507989 |
| H | 1.388698 | 1.220932 | 3.833617 |
| H | 0.182585 | -0.774387 | 4.490685 |
| H | 1.189651 | -1.147270 | 3.069551 |
| H | -0.330603 | -2.954699 | 2.346684 |
| H | -1.227254 | -2.657190 | 3.853230 |
| H | -3.237383 | -2.004472 | 2.525683 |
| H | -2.726290 | -3.694811 | 2.292950 |
| H | -4.358148 | -2.078657 | 0.412002 |
| H | -3.825620 | -3.747672 | 0.136953 |
| H | -4.244855 | -2.755730 | -2.023955 |
| H | -2.503449 | -3.023877 | -1.844041 |
| H | -4.680751 | -0.151730 | -0.895584 |
| H | -4.863692 | -0.548555 | -2.621291 |
| H | -4.550834 | 1.824081 | -2.415549 |
| H | -3.085024 | 1.140838 | -3.160451 |
| H | -3.369882 | 3.693926 | -1.642647 |
| H | -1.795188 | 3.127812 | -2.251077 |
| H | -2.527153 | 3.562393 | 0.694605 |
| H | -1.611258 | 4.698554 | -0.325167 |
| C | 2.312725 | -1.390127 | -2.145483 |
| C | 1.344967 | -1.186352 | -0.965120 |
| C | 0.165737 | -0.305994 | -1.364694 |
| N | -0.763791 | -0.062862 | -0.217536 |
| C | 3.730099 | -1.831404 | -1.729436 |
| C | 4.756585 | -0.688160 | -1.546383 |
| H | 4.882185 | -0.183955 | -2.510139 |
| C | 4.242701 | 0.383769 | -0.566279 |
| O | 3.414442 | 1.210786 | -0.865985 |

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|---|-----------|-----------|-----------|
| O | 4.764924 | 0.299731 | 0.660310 |
| N | 6.018950 | -1.234218 | -1.022429 |
| H | 1.893414 | -2.141160 | -2.821450 |
| H | 2.383863 | -0.463166 | -2.722003 |
| H | 0.985664 | -2.160446 | -0.612503 |
| H | 1.857137 | -0.710928 | -0.125891 |
| H | 0.525551 | 0.671537 | -1.688975 |
| H | -0.425236 | -0.746567 | -2.168615 |
| H | -1.504096 | 0.600506 | -0.496152 |
| H | -1.233486 | -0.923240 | 0.099976 |
| H | 4.144513 | -2.491852 | -2.497538 |
| H | 3.687425 | -2.419841 | -0.805000 |
| H | 5.457400 | -0.400046 | 0.599961 |
| H | 6.828831 | -0.733703 | -1.373669 |
| H | 6.139017 | -2.214685 | -1.251013 |
| H | -0.253216 | 0.348829 | 0.584489 |

H⁺K[Ne]-ctgg.g.t(+0+/-00/-00/+0+/-00) 3671

| | | | |
|---|-----------|-----------|-----------|
| C | -4.323025 | -1.169372 | -0.929719 |
| C | -4.286481 | 0.208168 | -1.548941 |
| O | -3.503262 | 1.067364 | -0.730677 |
| C | -3.519534 | 2.424524 | -1.153730 |
| C | -2.717825 | 3.251774 | -0.176073 |
| O | -1.340820 | 2.874805 | -0.258810 |
| C | -0.467267 | 3.634022 | 0.585987 |
| C | -0.359536 | 3.081228 | 1.995922 |
| O | 0.239752 | 1.796173 | 1.933441 |
| C | 0.364079 | 1.167701 | 3.206138 |
| C | 0.989984 | -0.196812 | 3.035114 |
| O | 0.107315 | -1.025501 | 2.270737 |
| C | 0.507228 | -2.402752 | 2.255366 |
| C | -0.572195 | -3.230363 | 1.597126 |
| O | -0.633481 | -2.906143 | 0.209571 |
| C | -1.594001 | -3.642796 | -0.536633 |
| C | -3.001734 | -3.081812 | -0.431375 |
| O | -3.017689 | -1.749383 | -0.949653 |
| H | -4.687036 | -1.105453 | 0.103735 |
| H | -5.016203 | -1.797825 | -1.504068 |
| H | -5.316813 | 0.583611 | -1.621433 |
| H | -3.869808 | 0.159646 | -2.564729 |
| H | -4.550043 | 2.805678 | -1.176789 |
| H | -3.097124 | 2.518371 | -2.163854 |
| H | -2.824425 | 4.313516 | -0.432734 |
| H | -3.102366 | 3.096575 | 0.838766 |
| H | -0.796833 | 4.678984 | 0.622346 |
| H | 0.515037 | 3.603612 | 0.110613 |
| H | -1.347214 | 3.018144 | 2.474437 |
| H | 0.257658 | 3.766437 | 2.595611 |
| H | -0.625117 | 1.072073 | 3.674213 |
| H | 1.003001 | 1.769826 | 3.866912 |
| H | 1.962400 | -0.126119 | 2.536691 |
| H | 1.138888 | -0.636395 | 4.030048 |

| | | | | | | | |
|--|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | 1.457449 | -2.507307 | 1.723713 | C | -2.059611 | -3.579471 | 0.320207 |
| H | 0.632771 | -2.754720 | 3.287749 | H | 0.777024 | -0.672124 | 3.133836 |
| H | -1.534737 | -3.038455 | 2.088088 | H | -0.118379 | -0.296928 | 4.622845 |
| H | -0.325828 | -4.293847 | 1.720895 | H | -0.643492 | -2.557270 | 3.971136 |
| H | -1.604596 | -4.696057 | -0.226396 | H | -2.093369 | -1.543580 | 3.761301 |
| H | -1.264946 | -3.602143 | -1.577710 | H | 0.807405 | 1.803485 | 2.636301 |
| H | -3.356374 | -3.078187 | 0.607641 | H | -0.091622 | 2.056066 | 4.148980 |
| H | -3.680973 | -3.716761 | -1.016352 | H | -0.563916 | 3.897742 | 2.664990 |
| C | 2.388106 | 0.650750 | -2.679459 | H | -2.038757 | 2.917488 | 2.860429 |
| C | 1.355214 | 0.871840 | -1.557768 | H | -1.393426 | 4.723664 | 0.514973 |
| C | 0.333140 | -0.259073 | -1.458148 | H | -2.870881 | 3.774328 | 0.815767 |
| N | -0.660219 | -0.020975 | -0.359140 | H | -0.968834 | 3.355196 | -1.548695 |
| C | 3.371315 | -0.526817 | -2.528768 | H | -2.480084 | 4.290147 | -1.590166 |
| C | 4.443705 | -0.408148 | -1.426149 | H | -2.092266 | 1.778271 | -3.212502 |
| H | 5.081798 | -1.294662 | -1.507106 | H | -3.560105 | 2.776024 | -3.103159 |
| C | 3.844057 | -0.517041 | -0.008542 | H | -4.198986 | 0.525005 | -3.711468 |
| O | 2.983827 | -1.314339 | 0.284044 | H | -4.784047 | 0.869036 | -2.063923 |
| O | 4.371467 | 0.327131 | 0.878038 | H | -4.227922 | -1.847040 | -3.230930 |
| N | 5.319203 | 0.773848 | -1.491180 | H | -4.812941 | -1.508917 | -1.582049 |
| H | 1.851327 | 0.508241 | -3.624084 | H | -2.148060 | -2.855689 | -2.272316 |
| H | 2.943814 | 1.585743 | -2.816998 | H | -3.638853 | -3.698623 | -1.793379 |
| H | 0.822742 | 1.805076 | -1.769098 | H | -1.503748 | -4.136584 | 2.309892 |
| H | 1.842368 | 1.009394 | -0.589296 | H | -2.955856 | -3.108905 | 2.211541 |
| H | -0.232122 | -0.343762 | -2.389081 | H | -1.060211 | -3.694989 | -0.122935 |
| H | 0.801139 | -1.218360 | -1.244738 | H | -2.595445 | -4.530925 | 0.198858 |
| H | -0.270933 | -0.268340 | 0.568360 | O | 7.420502 | -0.547683 | -0.711780 |
| H | -0.970223 | 0.962814 | -0.323151 | C | 6.351372 | 0.268761 | -0.582607 |
| H | 3.899269 | -0.648612 | -3.479497 | H | 8.175814 | -0.106343 | -0.292429 |
| H | 2.828008 | -1.459115 | -2.358696 | C | 5.087594 | -0.290133 | -1.259375 |
| H | 5.033780 | 0.854087 | 0.368543 | O | 6.405344 | 1.332219 | -0.017163 |
| H | 4.890061 | 1.552594 | -1.978923 | N | 5.131126 | -1.681975 | -1.690740 |
| H | 6.204172 | 0.575093 | -1.941790 | H | 4.972609 | 0.327564 | -2.159752 |
| H | -1.493103 | -0.614478 | -0.495211 | C | 3.867336 | -0.034779 | -0.356109 |
| H ⁺ K[Ne]-tttttt(-00/+00/-00/+00/-00/+00) 4.3 | | | | | | | |
| O | -0.859694 | 0.587601 | 2.894375 | H | 5.838261 | -1.823599 | -2.403641 |
| C | -0.226246 | -0.503662 | 3.549063 | H | 5.374649 | -2.293091 | -0.916943 |
| C | -1.081615 | -1.738998 | 3.384968 | H | 3.916942 | -0.724557 | 0.496877 |
| C | -0.197843 | 1.832802 | 3.078405 | H | 3.943717 | 0.976002 | 0.051211 |
| C | -1.024535 | 2.926561 | 2.442324 | C | 2.537185 | -0.216283 | -1.091711 |
| O | -1.086816 | 2.735220 | 1.025790 | H | 2.481557 | 0.509226 | -1.913200 |
| C | -1.866459 | 3.742882 | 0.375747 | H | 2.513822 | -1.209021 | -1.550575 |
| C | -1.969538 | 3.447970 | -1.103227 | C | 1.326805 | -0.031142 | -0.168085 |
| O | -2.709637 | 2.247067 | -1.281543 | H | 1.368764 | -0.765334 | 0.644035 |
| C | -3.013795 | 1.944583 | -2.636898 | H | 1.359965 | 0.961992 | 0.293144 |
| C | -3.886999 | 0.710940 | -2.675552 | C | 0.013277 | -0.190774 | -0.924275 |
| O | -3.154471 | -0.412648 | -2.181204 | H | -0.066236 | 0.539922 | -1.730841 |
| C | -3.915441 | -1.622572 | -2.202824 | H | -0.065165 | -1.183575 | -1.370023 |
| C | -3.071423 | -2.764269 | -1.683224 | N | -1.187242 | -0.006290 | -0.048898 |
| O | -2.769791 | -2.524108 | -0.314732 | H | -2.040062 | -0.110756 | -0.620230 |
| O | -1.145970 | -2.114455 | 2.005797 | H | -1.217355 | -0.709595 | 0.707083 |
| C | -1.953891 | -3.276444 | 1.797413 | H | -1.200476 | 0.932611 | 0.381629 |

H⁺K[Ne]-tgggtt(-00/+00/-00/+00/-00/+00) 213

| | | | |
|---|-----------|-----------|-----------|
| C | -1.374903 | 1.538851 | 2.453247 |
| C | -1.185078 | 0.211227 | 3.152352 |
| O | -0.909150 | -0.801826 | 2.188303 |
| C | -0.597194 | -2.061952 | 2.772635 |
| C | -0.198648 | -3.044438 | 1.693118 |
| O | 1.035948 | -2.623264 | 1.101458 |
| C | 1.625818 | -3.586700 | 0.225141 |
| C | 3.045669 | -3.169825 | -0.090755 |
| O | 3.038496 | -1.945667 | -0.818855 |
| C | 4.345753 | -1.434783 | -1.059033 |
| C | 4.252956 | -0.095569 | -1.755986 |
| O | 3.656246 | 0.860637 | -0.876314 |
| C | 3.677655 | 2.199555 | -1.378414 |
| C | 3.183453 | 3.145017 | -0.306333 |
| O | 1.812106 | 2.881368 | -0.029990 |
| C | 1.296962 | 3.676683 | 1.033878 |
| C | -0.125349 | 3.264743 | 1.343470 |
| O | -0.131843 | 1.929029 | 1.852664 |
| H | -2.163808 | 1.476556 | 1.695073 |
| H | -1.669962 | 2.286097 | 3.200770 |
| H | -2.101070 | -0.030303 | 3.709308 |
| H | -0.355517 | 0.282876 | 3.868199 |
| H | 0.224916 | -1.950337 | 3.491997 |
| H | -1.469786 | -2.462353 | 3.307653 |
| H | -0.982899 | -3.119735 | 0.929754 |
| H | -0.066791 | -4.032247 | 2.152125 |
| H | 1.033854 | -3.677609 | -0.694995 |
| H | 1.651563 | -4.568432 | 0.714355 |
| H | 3.609986 | -3.048115 | 0.843232 |
| H | 3.524134 | -3.963132 | -0.681826 |
| H | 4.886441 | -1.320782 | -0.110124 |
| H | 4.914251 | -2.124820 | -1.698055 |
| H | 5.265893 | 0.230054 | -2.024731 |
| H | 3.663619 | -0.181195 | -2.678428 |
| H | 3.052679 | 2.276822 | -2.277760 |
| H | 4.704346 | 2.478084 | -1.647693 |
| H | 3.783054 | 3.017222 | 0.604748 |
| H | 3.311415 | 4.177492 | -0.660318 |
| H | 1.304527 | 4.739087 | 0.752854 |
| H | 1.919391 | 3.552450 | 1.929798 |
| H | -0.756145 | 3.334687 | 0.448128 |
| H | -0.527605 | 3.951247 | 2.099075 |
| C | -2.010834 | -0.223408 | -2.437412 |
| C | -1.132739 | -0.516094 | -1.214544 |
| C | 0.255043 | 0.103383 | -1.337188 |
| N | 1.003403 | 0.043493 | -0.041415 |
| C | -3.339592 | -0.995740 | -2.488687 |
| C | -4.313659 | -0.840779 | -1.286805 |
| H | -5.277379 | -1.224406 | -1.629524 |
| C | -4.510672 | 0.640284 | -0.963740 |
| O | -3.981172 | 1.228340 | -0.047734 |

| | | | |
|---|-----------|-----------|-----------|
| O | -5.324343 | 1.247348 | -1.848090 |
| N | -3.908665 | -1.632245 | -0.125756 |
| H | -1.458274 | -0.468273 | -3.352314 |
| H | -2.205172 | 0.854832 | -2.487067 |
| H | -1.606826 | -0.124562 | -0.313675 |
| H | -1.040470 | -1.597701 | -1.075576 |
| H | 0.858533 | -0.419306 | -2.080863 |
| H | 0.200619 | 1.156700 | -1.617500 |
| H | 1.977901 | 0.346983 | -0.192426 |
| H | 1.020254 | -0.914662 | 0.345343 |
| H | -3.144396 | -2.068258 | -2.573480 |
| H | -3.871189 | -0.692436 | -3.394894 |
| H | -5.394279 | 2.184535 | -1.606788 |
| H | -4.718567 | -1.863582 | 0.439616 |
| H | -3.274980 | -1.111006 | 0.471937 |
| H | 0.576422 | 0.668360 | 0.663068 |

H⁺K[Ne]-ctg.ggt(+00/-00/+00/-00/+00/-00) 1433

| | | | |
|---|-----------|-----------|-----------|
| C | -0.378763 | 3.358982 | 1.744254 |
| C | 0.839670 | 2.530294 | 2.077144 |
| O | 0.441961 | 1.162668 | 2.264623 |
| C | 1.403670 | 0.378642 | 2.976561 |
| C | 0.814767 | -0.985726 | 3.252036 |
| O | 0.657035 | -1.683159 | 2.017008 |
| C | 0.100271 | -2.988260 | 2.136240 |
| C | -1.409834 | -3.012812 | 1.971006 |
| O | -1.736348 | -2.621441 | 0.633998 |
| C | -3.105412 | -2.837546 | 0.287476 |
| C | -3.286361 | -2.548387 | -1.193226 |
| O | -3.061181 | -1.181747 | -1.532770 |
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| O | -3.020854 | 1.630548 | -0.861661 |
| C | -2.719146 | 3.011130 | -1.084807 |
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| O | -0.927512 | 2.938882 | 0.498208 |
| H | -0.082725 | 4.416209 | 1.691124 |
| H | -1.132158 | 3.251462 | 2.536407 |
| H | 1.270501 | 2.916716 | 3.009414 |
| H | 1.594611 | 2.590168 | 1.287827 |
| H | 1.633180 | 0.861269 | 3.935599 |
| H | 2.330911 | 0.291225 | 2.399434 |
| H | -0.149679 | -0.874200 | 3.764661 |
| H | 1.496073 | -1.540599 | 3.910992 |
| H | 0.363442 | -3.436656 | 3.102261 |
| H | 0.553870 | -3.595422 | 1.348762 |
| H | -1.903426 | -2.344130 | 2.688770 |
| H | -1.769351 | -4.034159 | 2.154123 |
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| H | -2.558885 | -3.131310 | -1.762888 |

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H 4.928438 -0.549869 0.214642
H 5.935987 -1.048751 -2.136873
H 4.607546 -1.938847 -1.780086
H -1.014030 -0.922438 0.047216

H⁺K[Ne]-tgtttg(+0+/-+00/-0/-00/+00/-00) 2021

C -0.504882 -2.696815 2.153841
C 0.480248 -1.669403 2.662841
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C -0.209096 3.472747 0.633014
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C -2.804263 -3.404633 0.066999
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H 4.557857 -0.608106 1.208963
H 4.735946 0.990966 1.387252
H -0.858147 -0.912797 0.002988

H⁺K[Ne]-cg.g.gtt(-00/+0/+00/-00/+00/-0) 102

| | | | | | | | |
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| C | 4.139325 | 1.103219 | -1.723247 | H | -1.750568 | -0.798165 | -3.483830 |
| O | 3.261506 | 1.634361 | -0.728986 | H | -2.220636 | 0.706870 | -2.720138 |
| C | 2.954212 | 3.019116 | -0.918194 | H | -0.954977 | -1.746666 | -1.408551 |
| C | 2.283350 | 3.558654 | 0.324405 | H | -1.731101 | -0.511316 | -0.440195 |
| O | 1.044365 | 2.893916 | 0.526476 | H | -0.233542 | 1.232731 | -1.501271 |
| C | 0.396921 | 3.292518 | 1.732701 | H | 0.658000 | -0.077349 | -2.297386 |
| C | -0.813947 | 2.423637 | 1.982785 | H | 1.149497 | -0.964240 | -0.059840 |
| O | -0.382119 | 1.068723 | 2.182324 | H | 0.374383 | 0.348281 | 0.630245 |
| C | -1.355550 | 0.244100 | 2.830782 | H | -3.578513 | -1.844717 | -1.788705 |
| C | -0.760641 | -1.125235 | 3.067424 | H | -4.015478 | -1.191904 | -3.357854 |
| O | -0.564188 | -1.769139 | 1.809711 | H | -5.306031 | -0.599593 | 0.329478 |
| C | -0.037365 | -3.089844 | 1.884644 | H | -6.690272 | -0.038181 | -1.594145 |
| C | 1.476412 | -3.138357 | 1.765488 | H | -6.017024 | -1.437744 | -2.116203 |
| O | 1.853873 | -2.684309 | 0.462241 | H | 1.732548 | 0.578371 | -0.313816 |
| C | 3.232794 | -2.898332 | 0.155449 | | | | |
| C | 3.478280 | -2.520184 | -1.295471 | H ⁺ K[Ne]-cggtag(+00/-00/+0+/-00/-00) 2151 | | | |
| O | 3.296836 | -1.129536 | -1.556208 | C | 4.274380 | -1.003967 | -1.316516 |
| H | 4.842080 | -0.393667 | -0.358021 | C | 4.003520 | -2.217477 | -0.456960 |
| H | 5.258785 | -0.682505 | -2.064631 | O | 2.597794 | -2.373458 | -0.247174 |
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| H | 2.305949 | 3.143588 | -1.795200 | O | 0.361908 | -2.379373 | 1.525401 |
| H | 3.878793 | 3.584430 | -1.090670 | C | -1.006657 | -2.433394 | 1.922971 |
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| H | 2.938340 | 3.406724 | 1.193092 | O | -1.172963 | -0.024420 | 1.812073 |
| H | 0.074119 | 4.340587 | 1.661663 | C | -1.595698 | 1.183793 | 2.448766 |
| H | 1.096605 | 3.203086 | 2.574488 | C | -1.309080 | 2.373136 | 1.562329 |
| H | -1.528693 | 2.468535 | 1.154852 | O | 0.096912 | 2.482528 | 1.369549 |
| H | -1.312977 | 2.787362 | 2.889650 | C | 0.504849 | 3.668911 | 0.705534 |
| H | -2.263809 | 0.171561 | 2.222474 | C | 2.014215 | 3.678029 | 0.621265 |
| H | -1.621085 | 0.685526 | 3.800190 | O | 2.452696 | 2.590206 | -0.196121 |
| H | -1.455541 | -1.710611 | 3.684391 | C | 3.874765 | 2.528642 | -0.315138 |
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| C | -2.171875 | -0.375299 | -2.566730 | H | 0.288253 | -3.697594 | -0.080307 |
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| C | 0.028102 | 0.175449 | -1.442551 | H | -1.659270 | -2.562846 | 1.052123 |
| N | 0.871956 | 0.016515 | -0.215926 | H | -0.731478 | -1.055935 | 3.552714 |
| C | -3.601024 | -0.922451 | -2.381400 | H | -2.411596 | -1.222448 | 2.964286 |
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| H | -4.732509 | 0.915572 | -2.407387 | H | -2.673574 | 1.137329 | 2.644579 |
| C | -4.100675 | 0.611882 | -0.403131 | H | -1.701133 | 3.273109 | 2.055260 |
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| H | 0.176370 | 4.557056 | 1.263056 | H | -1.260018 | -3.708018 | -0.189966 |
| H | 2.346763 | 4.629441 | 0.185934 | H | -2.593519 | -4.406193 | 0.755755 |
| H | 2.443718 | 3.584943 | 1.626582 | H | -3.437820 | -3.826767 | -1.424064 |
| H | 4.326350 | 2.390660 | 0.675373 | H | -4.167635 | -2.740046 | -0.215637 |
| H | 4.254539 | 3.465646 | -0.743395 | H | -0.186951 | -3.062439 | 1.995413 |
| H | 5.349991 | 1.406090 | -1.372503 | H | -1.583341 | -3.765668 | 2.841390 |
| H | 3.780603 | 1.491712 | -2.203333 | H | -0.600210 | -2.077021 | 4.257321 |
| C | -1.735453 | -1.140264 | -1.699258 | H | -2.201816 | -1.518540 | 3.713108 |
| C | -0.304187 | -0.899099 | -2.208236 | H | 0.112509 | 0.235840 | 4.609039 |
| C | 0.435178 | 0.292268 | -1.596670 | H | -1.538625 | 0.717358 | 4.142948 |
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| C | -4.206555 | -0.355552 | -1.742870 | H | 0.414775 | 3.365833 | 0.986984 |
| H | -4.501351 | -1.389013 | -1.952874 | H | -0.471422 | 4.212918 | 2.274646 |
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| O | -3.938988 | -1.033149 | 0.569463 | H | -2.612978 | 3.838597 | 1.052564 |
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| H | -1.756816 | -1.130579 | -0.608895 | H | -1.659515 | 2.125526 | -3.072288 |
| H | -2.042030 | -2.147580 | -1.998552 | H | -3.374015 | 2.467520 | -3.397696 |
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| H | 1.499034 | -0.788737 | -0.131448 | O | 6.941613 | 0.496213 | -1.274121 |
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| H | -2.467556 | 0.893176 | -1.999999 | H | 7.536691 | 1.118686 | -0.828055 |
| H | -2.781524 | -0.203251 | -3.336455 | C | 4.820630 | -0.581640 | -1.173461 |
| H | -4.961093 | 1.496029 | -0.646230 | O | 5.581209 | 1.119935 | 0.405604 |
| H | -6.051079 | 0.295347 | -2.442212 | N | 5.276533 | -1.955041 | -0.923723 |
| H | -4.790357 | 0.905215 | -3.290358 | H | 4.823042 | -0.437646 | -2.258757 |
| H | 1.485642 | 0.865197 | 0.089284 | C | 3.403064 | -0.376838 | -0.628975 |
| H ⁺ K[Ne]-ttttgt(-00/+00/-00/+00/-00/+00) 4 | | | | H | 6.138468 | -2.155372 | -1.419522 |
| O | -2.048834 | -2.471251 | 1.283324 | H | 5.444967 | -2.111390 | 0.066059 |
| C | -2.218346 | -3.480869 | 0.297040 | H | 3.406882 | -0.613386 | 0.441784 |
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| C | -1.202480 | -2.854477 | 2.359686 | C | 2.360539 | -1.236376 | -1.353792 |
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| C | 0.026091 | 1.748750 | 3.098882 | H | 0.337558 | -1.974016 | -1.187880 |
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| C | -0.551662 | 3.431751 | 1.506215 | C | 0.296737 | 0.106892 | -0.667639 |
| C | -1.645168 | 3.818134 | 0.536110 | H | 0.888022 | 0.853612 | -0.137961 |
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| C | -3.656531 | -1.385661 | -2.402912 | H ⁺ K[Ne]-tg.g.ttg.(+00/-00/+00/--0/-00/+00) 776 | | | |
| C | -3.110430 | -0.140040 | -3.063027 | C | -2.510279 | -3.297143 | -0.615222 |

| | | | | | | | |
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| C | -3.802177 | -2.500780 | -0.567883 | H | 1.930524 | -0.254090 | -0.220523 |
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| C | -0.279810 | -2.621571 | 2.279353 | | | | |
| C | -1.526162 | -3.118774 | 1.583387 | H ⁺ K[Ne]-ctg.tg.g.(-00/+0/+00/-00/+0/+00) 6333 | | | |
| O | -1.470160 | -2.749203 | 0.201003 | C | -1.089260 | 2.761345 | 1.525499 |
| H | -2.708124 | -4.335704 | -0.324819 | C | 0.317527 | 3.290565 | 1.737185 |
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| H | -4.557235 | -3.018174 | -1.177151 | C | 3.270072 | 2.815610 | -0.427148 |
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| H | -5.050095 | -0.260090 | 0.005210 | C | 4.244224 | 0.824186 | -1.318386 |
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| H | -4.066530 | 3.539043 | -1.046527 | C | 3.102629 | -2.703811 | -1.308769 |
| H | -2.572015 | 3.107982 | -1.909594 | C | 2.788015 | -3.165548 | 0.103793 |
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| H | -2.855672 | 3.463906 | 1.121218 | C | 1.058514 | -3.226720 | 1.738359 |
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| H | 1.729161 | 3.113880 | 2.098216 | C | -1.304505 | 0.761934 | 2.849225 |
| H | -0.202382 | 1.205373 | 3.283782 | O | -1.173951 | 1.334655 | 1.539599 |
| H | 1.564280 | 1.298642 | 3.487166 | H | -1.448815 | 3.079667 | 0.544263 |
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| H | 0.615738 | -3.003207 | 1.771518 | H | 2.913030 | 2.908664 | 1.688423 |
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| O | 5.043045 | 1.350385 | -0.558625 | H | 2.816170 | -4.263665 | 0.122498 |
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| H | -0.662068 | -3.200239 | 2.988070 |
| H | -1.031654 | -2.937829 | 1.266746 |
| H | -1.709824 | -1.135543 | 3.727904 |
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| H | -2.191109 | 1.181779 | 3.340300 |
| C | -2.070356 | 1.085622 | -1.922384 |
| C | -0.591850 | 0.967458 | -2.336233 |
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| H | -5.310100 | -0.082771 | 0.170724 |
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| H | 1.466213 | 0.590513 | -0.370106 |

H⁺K[Ne]-cggg.tt(+0+/+00/-00/+00/--0/-00) 116

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| C | 4.579857 | -1.155329 | -0.878229 |
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| C | 3.666006 | 2.404677 | -1.193321 |
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| O | 1.653728 | 2.879637 | 0.047068 |
| C | 1.037339 | 3.558608 | 1.143704 |
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| O | -0.694027 | 1.825380 | 1.405952 |
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| H | 4.989527 | -1.041591 | 0.133530 |
| H | 4.034845 | 0.101731 | -2.543052 |
| H | 5.516057 | 0.585636 | -1.684970 |
| H | 4.673516 | 2.796712 | -1.389589 |
| H | 3.093842 | 2.455815 | -2.130619 |
| H | 3.074700 | 4.314757 | -0.428576 |
| H | 3.564003 | 3.139176 | 0.816904 |
| H | 1.134546 | 4.645051 | 1.012129 |
| H | 1.547004 | 3.285849 | 2.077265 |
| H | -0.922844 | 3.815298 | 1.970738 |
| H | -0.901659 | 3.457004 | 0.235929 |
| H | 0.326137 | 1.508391 | 3.201303 |
| H | -1.376808 | 2.004725 | 3.359019 |
| H | -1.196061 | -0.340371 | 3.885879 |
| H | -2.090814 | -0.173752 | 2.353186 |
| H | -1.373003 | -2.456820 | 1.654341 |
| H | -0.666718 | -2.543089 | 3.289465 |
| H | 1.601750 | -2.818720 | 2.294883 |
| H | 0.476201 | -4.147632 | 1.922237 |
| H | 1.614044 | -3.692369 | -1.332808 |
| H | 1.909143 | -4.640400 | 0.134019 |
| H | 3.994038 | -3.677128 | -0.628808 |
| H | 3.561063 | -2.877123 | 0.895964 |
| C | -2.311878 | -0.169502 | -2.526353 |
| C | -1.307557 | 0.413503 | -1.519581 |
| C | 0.015866 | -0.345446 | -1.546632 |
| N | 0.899166 | 0.005670 | -0.387440 |
| C | -3.741202 | 0.392217 | -2.385379 |
| C | -4.702992 | -0.409542 | -1.475495 |
| H | -4.790041 | -1.424463 | -1.877170 |
| C | -4.149773 | -0.557210 | -0.046073 |
| O | -3.293694 | -1.354091 | 0.257622 |
| O | -4.672702 | 0.300641 | 0.834513 |
| N | -5.997476 | 0.287465 | -1.398984 |
| H | -2.340765 | -1.258491 | -2.421352 |
| H | -1.959238 | 0.033046 | -3.542720 |
| H | -1.711645 | 0.366382 | -0.509201 |
| H | -1.135884 | 1.472689 | -1.742610 |
| H | -0.154924 | -1.419186 | -1.472248 |
| H | 0.579984 | -0.147806 | -2.460749 |
| H | 1.793222 | -0.503936 | -0.459655 |
| H | 0.456012 | -0.275507 | 0.506806 |
| H | -3.706979 | 1.430645 | -2.035121 |
| H | -4.213654 | 0.414836 | -3.372578 |
| H | -5.393076 | 0.767376 | 0.348596 |
| H | -6.774488 | -0.357273 | -1.296138 |
| H | -6.176183 | 0.857430 | -2.218261 |
| H | 1.107440 | 1.013126 | -0.322654 |

H⁺K[Ne]-ttg.ttg(+00/-00/+00/--0/-00/+0+) 125

| | | | |
|---|----------|----------|-----------|
| C | 3.469978 | 2.750357 | -0.814278 |
| C | 2.616071 | 3.475456 | 0.200234 |

| | | | | | | | |
|--|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | 0.596503 | -3.950423 | 2.490188 | H | 2.448919 | -2.993210 | -2.065038 |
| H | -1.091054 | -2.458881 | 3.415031 | H | 2.238706 | -4.426964 | -1.029552 |
| H | -1.656601 | -1.968172 | 1.793898 | H | 4.294012 | -2.245522 | -0.818185 |
| H | -0.299861 | -0.128921 | 3.829991 | H | 4.208453 | -3.612902 | 0.310046 |
| H | -2.061421 | -0.258008 | 3.569141 | H | 5.270615 | -1.762613 | 1.468950 |
| C | -2.242985 | 0.381250 | -2.689438 | H | 3.673588 | -2.050205 | 2.179778 |
| C | -1.273711 | 0.736052 | -1.541041 | H | 4.741421 | 0.166220 | -0.690524 |
| C | -0.147875 | -0.285583 | -1.429109 | H | 5.724625 | 0.357985 | 0.783102 |
| N | 0.739369 | -0.027292 | -0.249637 | H | 4.229764 | 2.206300 | 1.532089 |
| C | -3.703339 | 0.798606 | -2.432854 | H | 5.050137 | 2.545101 | -0.011556 |
| C | -4.585100 | -0.254654 | -1.718688 | H | 3.244608 | 4.102202 | -0.566643 |
| H | -4.657751 | -1.134194 | -2.366727 | H | 2.394311 | 3.713396 | 0.948613 |
| C | -3.951489 | -0.746247 | -0.402054 | H | 0.900803 | 4.533255 | -0.889507 |
| O | -3.053980 | -1.553860 | -0.356681 | H | 1.354409 | 3.114160 | -1.864347 |
| O | -4.464059 | -0.179216 | 0.694569 | H | -1.774832 | 2.525283 | 0.108655 |
| N | -5.898750 | 0.333435 | -1.408667 | H | -1.307718 | 3.871824 | -0.937828 |
| H | -2.213082 | -0.696403 | -2.877065 | H | -0.664183 | 2.218632 | -2.733225 |
| H | -1.898631 | 0.859026 | -3.610464 | H | -2.371888 | 2.109788 | -2.232697 |
| H | -0.866792 | 1.741597 | -1.692163 | H | -0.596233 | -0.124632 | -3.405101 |
| H | -1.804169 | 0.753824 | -0.586880 | H | -2.340993 | -0.194503 | -3.036396 |
| H | -0.576503 | -1.278012 | -1.286898 | H | -1.340000 | -2.423317 | -2.936298 |
| H | 0.490757 | -0.302697 | -2.313264 | H | -1.950619 | -1.939078 | -1.338330 |
| H | 0.179296 | 0.152419 | 0.601993 | C | -2.031863 | -0.403069 | 1.737487 |
| H | 1.376704 | 0.770533 | -0.388223 | C | -0.812702 | 0.196055 | 2.450332 |
| H | -3.733715 | 1.733375 | -1.860402 | C | 0.543784 | -0.357507 | 2.020858 |
| H | -4.194070 | 1.005112 | -3.389273 | N | 0.938219 | -0.002867 | 0.615046 |
| H | -5.228714 | 0.356044 | 0.374209 | C | -3.344245 | 0.215569 | 2.246979 |
| H | -6.647117 | -0.350155 | -1.460062 | C | -4.599075 | -0.188503 | 1.451998 |
| H | -6.135069 | 1.096615 | -2.032979 | H | -5.443536 | 0.384387 | 1.846168 |
| H | 1.327935 | -0.857547 | -0.076391 | C | -4.458995 | 0.261585 | -0.021530 |
| H ⁺ K[Ne]-cgg.ttg(+00/-00/+00/--0/-00/+0+) 2358 | | | | O | -4.132023 | 1.378980 | -0.336214 |
| C | 0.469179 | -3.253583 | -1.280935 | O | -4.722127 | -0.697066 | -0.914393 |
| C | 1.971138 | -3.367666 | -1.149943 | N | -4.937124 | -1.623840 | 1.497850 |
| O | 2.413267 | -2.614655 | -0.026648 | H | -2.031406 | -1.490603 | 1.889439 |
| C | 3.828541 | -2.600172 | 0.111903 | H | -1.946098 | -0.227757 | 0.661045 |
| C | 4.191713 | -1.705034 | 1.282562 | H | -0.895025 | 0.018573 | 3.528391 |
| O | 3.795830 | -0.341959 | 1.100749 | H | -0.810023 | 1.284678 | 2.324801 |
| C | 4.716988 | 0.467858 | 0.363309 | H | 1.327384 | 0.045323 | 2.663698 |
| C | 4.292603 | 1.914619 | 0.474848 | H | 0.581696 | -1.445755 | 2.094541 |
| O | 3.030575 | 2.075573 | -0.159048 | H | 0.708308 | 0.978544 | 0.371776 |
| C | 2.533679 | 3.407980 | -0.097345 | H | 0.509122 | -0.608956 | -0.101672 |
| C | 1.220581 | 3.484545 | -0.841321 | H | -3.267789 | 1.304540 | 2.193945 |
| O | 0.233400 | 2.716828 | -0.148099 | H | -3.502116 | -0.040018 | 3.300252 |
| C | -1.094644 | 2.826094 | -0.687672 | H | -4.971611 | -1.484423 | -0.372928 |
| C | -1.336774 | 1.954386 | -1.905293 | H | -5.786357 | -1.803667 | 2.019557 |
| O | -1.136214 | 0.592713 | -1.537176 | H | -4.198828 | -2.187393 | 1.903410 |
| C | -1.334812 | -0.313237 | -2.613860 | H | 1.961349 | -0.111984 | 0.534170 |
| C | -1.190916 | -1.727981 | -2.100792 | H ⁺ K[Ne]-ctgtgg(--0/-00/+0+/-00/-00/+00) 2960 | | | |
| O | 0.120561 | -1.897050 | -1.554193 | C | -3.057681 | 3.033496 | -0.083382 |
| H | 0.145252 | -3.898150 | -2.107788 | C | -1.967173 | 3.381630 | 0.903421 |
| H | -0.027131 | -3.600144 | -0.364421 | O | -0.716993 | 2.950482 | 0.374957 |

| | | | | | | | |
|---|-----------|-----------|-----------|--|-----------|-----------|-----------|
| C | 0.422205 | 3.313335 | 1.150129 | H | 0.090321 | 1.976283 | -1.893870 |
| C | 0.660742 | 2.428458 | 2.361509 | H | 0.585306 | 1.086138 | -3.319472 |
| O | 0.908039 | 1.086914 | 1.946716 | H | -1.009547 | -0.358442 | -2.376878 |
| C | 1.164916 | 0.221803 | 3.061814 | H | 0.489347 | -1.047590 | -1.744015 |
| C | 1.344253 | -1.202807 | 2.597283 | H | -1.061486 | -0.932434 | -0.039253 |
| O | 0.105211 | -1.673433 | 2.070780 | H | -0.003482 | 0.295266 | 0.345069 |
| C | 0.151986 | -3.033304 | 1.652198 | H | 2.420500 | -0.808384 | -2.697195 |
| C | -1.244345 | -3.468160 | 1.274864 | H | 3.232365 | 0.515450 | -3.510873 |
| O | -1.686992 | -2.737837 | 0.124720 | H | 5.390705 | -0.058206 | 0.175503 |
| C | -3.024252 | -3.059080 | -0.253607 | H | 5.939911 | 0.874570 | -2.240040 |
| C | -3.361075 | -2.360188 | -1.559984 | H | 4.788251 | 1.702952 | -1.418512 |
| O | -3.291184 | -0.937807 | -1.490652 | H | -1.477186 | 0.650066 | -0.333359 |
| C | -4.426503 | -0.305029 | -0.910648 | | | | |
| C | -4.258423 | 1.194005 | -1.009610 | H ⁺ K[Ne]-cg.g.g.tg.(--0/-00/-00/--0/-0/--0) 3404 | | | |
| O | -3.167676 | 1.612635 | -0.185607 | C | -1.297202 | -3.422703 | 0.916183 |
| H | -4.007004 | 3.454436 | 0.272536 | C | -1.842751 | -3.602799 | -0.490459 |
| H | -2.832547 | 3.466847 | -1.066349 | O | -2.423497 | -2.416648 | -1.030367 |
| H | -1.960372 | 4.469894 | 1.053935 | C | -3.788348 | -2.207372 | -0.682123 |
| H | -2.176452 | 2.900503 | 1.866832 | C | -4.279798 | -0.941515 | -1.346132 |
| H | 0.341229 | 4.356319 | 1.484449 | O | -3.639933 | 0.189932 | -0.752163 |
| H | 1.276166 | 3.242817 | 0.473399 | C | -4.121950 | 1.439274 | -1.251393 |
| H | -0.195896 | 2.451706 | 3.048662 | C | -3.635144 | 2.560047 | -0.362022 |
| H | 1.531233 | 2.819207 | 2.907337 | O | -2.216511 | 2.635957 | -0.424822 |
| H | 2.078645 | 0.548125 | 3.574896 | C | -1.672922 | 3.633487 | 0.431865 |
| H | 0.327506 | 0.281890 | 3.768667 | C | -0.158605 | 3.517940 | 0.419194 |
| H | 2.133548 | -1.279713 | 1.842426 | O | 0.315683 | 2.270643 | 0.933383 |
| H | 1.639964 | -1.809126 | 3.465388 | C | 0.419166 | 2.216454 | 2.363487 |
| H | 0.502011 | -3.674282 | 2.473557 | C | 0.773262 | 0.813218 | 2.797866 |
| H | 0.844293 | -3.151014 | 0.809432 | O | -0.348929 | -0.035919 | 2.548705 |
| H | -1.930436 | -3.287480 | 2.111928 | C | -0.222683 | -1.356725 | 3.067752 |
| H | -1.241802 | -4.542038 | 1.048634 | C | 0.487258 | -2.310222 | 2.112605 |
| H | -3.120701 | -4.142614 | -0.407244 | O | -0.220399 | -2.486361 | 0.872719 |
| H | -3.716271 | -2.773757 | 0.550040 | H | -0.929399 | -4.392160 | 1.278475 |
| H | -4.357652 | -2.680070 | -1.891574 | H | -2.082864 | -3.082629 | 1.602278 |
| H | -2.639392 | -2.656488 | -2.324239 | H | -2.570978 | -4.423773 | -0.495222 |
| H | -4.546881 | -0.592024 | 0.141520 | H | -1.023819 | -3.870759 | -1.161575 |
| H | -5.337785 | -0.592214 | -1.453275 | H | -3.912534 | -2.120530 | 0.404838 |
| H | -5.184171 | 1.675229 | -0.668588 | H | -4.399591 | -3.049941 | -1.033472 |
| H | -4.077741 | 1.487849 | -2.051458 | H | -5.365736 | -0.865940 | -1.204715 |
| C | 2.088765 | 1.125173 | -1.767764 | H | -4.072482 | -0.974655 | -2.423601 |
| C | 0.619146 | 1.078356 | -2.225138 | H | -5.219462 | 1.443201 | -1.247554 |
| C | -0.144362 | -0.160163 | -1.746411 | H | -3.781397 | 1.589619 | -2.284209 |
| N | -0.692274 | -0.019572 | -0.354007 | H | -3.956574 | 2.378927 | 0.672395 |
| C | 2.974819 | 0.116729 | -2.524620 | H | -4.086838 | 3.502087 | -0.703668 |
| C | 4.267014 | -0.278701 | -1.793013 | H | -2.068634 | 3.510382 | 1.448851 |
| H | 4.783147 | -1.032635 | -2.397034 | H | -1.956190 | 4.636915 | 0.082470 |
| C | 3.930093 | -1.002991 | -0.470162 | H | 0.278405 | 4.350542 | 0.983276 |
| O | 2.996905 | -1.763022 | -0.352532 | H | 0.203909 | 3.580132 | -0.609307 |
| O | 4.758779 | -0.724512 | 0.535560 | H | -0.528219 | 2.513010 | 2.826944 |
| N | 5.233597 | 0.796838 | -1.518264 | H | 1.205353 | 2.907176 | 2.693292 |
| H | 2.467203 | 2.141726 | -1.919035 | H | 0.993443 | 0.834660 | 3.874209 |
| H | 2.136452 | 0.937646 | -0.688875 | H | 1.664255 | 0.460828 | 2.267344 |

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| H | -1.241037 | -1.697178 | 3.271904 |
| H | 0.317275 | -1.346396 | 4.024197 |
| H | 0.623463 | -3.284539 | 2.598926 |
| H | 1.468063 | -1.923816 | 1.835271 |
| C | 2.117806 | 0.882680 | -1.831694 |
| C | 1.225953 | -0.319244 | -2.171415 |
| C | -0.269927 | -0.066894 | -1.986221 |
| N | -0.691603 | -0.008013 | -0.549331 |
| C | 3.610673 | 0.673018 | -2.127025 |
| C | 4.330147 | -0.469944 | -1.372210 |
| H | 3.893264 | -1.429121 | -1.665671 |
| C | 4.113415 | -0.343094 | 0.146274 |
| O | 3.068130 | -0.634183 | 0.684329 |
| O | 5.154957 | 0.139697 | 0.816875 |
| N | 5.774240 | -0.409696 | -1.648776 |
| H | 1.986869 | 1.165079 | -0.784872 |
| H | 1.791234 | 1.742220 | -2.429148 |
| H | 1.514460 | -1.189771 | -1.574918 |
| H | 1.372312 | -0.594915 | -3.222106 |
| H | -0.853439 | -0.871638 | -2.432911 |
| H | -0.574867 | 0.875500 | -2.446211 |
| H | -0.276028 | 0.781258 | -0.025627 |
| H | -0.470870 | -0.889010 | -0.051267 |
| H | 3.744385 | 0.477402 | -3.197664 |
| H | 4.144460 | 1.605506 | -1.911031 |
| H | 5.878445 | 0.223543 | 0.151056 |
| H | 6.196422 | -1.329630 | -1.714208 |
| H | 5.986373 | 0.092543 | -2.503367 |
| H | -1.715992 | 0.111241 | -0.503120 |

H⁺K[Ne]-tg.g.tgg.(+0+/+00/-00/+00/-0/-00) 357

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|---|-----------|-----------|-----------|
| C | -1.632780 | 3.578755 | 0.647519 |
| C | -2.781231 | 3.335629 | -0.305581 |
| O | -3.138020 | 1.950344 | -0.283602 |
| C | -4.275440 | 1.650816 | -1.096979 |
| C | -4.611485 | 0.181092 | -0.977760 |
| O | -3.552765 | -0.580384 | -1.550911 |
| C | -3.785903 | -1.983644 | -1.636062 |
| C | -3.558106 | -2.731025 | -0.333184 |
| O | -2.196385 | -2.587021 | 0.072605 |
| C | -1.899988 | -3.317388 | 1.266446 |
| C | -0.474933 | -3.051597 | 1.693902 |
| O | -0.350801 | -1.681862 | 2.049045 |
| C | 0.905121 | -1.353176 | 2.638475 |
| C | 0.885462 | 0.103612 | 3.039642 |
| O | 0.804901 | 0.931451 | 1.875067 |
| C | 0.808608 | 2.324719 | 2.187915 |
| C | 0.717744 | 3.134605 | 0.905254 |
| O | -0.476475 | 2.906519 | 0.159073 |
| H | -1.446870 | 4.660042 | 0.704664 |
| H | -1.905607 | 3.222863 | 1.648929 |
| H | -2.498135 | 3.632692 | -1.323200 |

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| H | -3.639571 | 3.942871 | 0.009211 |
| H | -5.136696 | 2.241749 | -0.759568 |
| H | -4.066139 | 1.905960 | -2.143433 |
| H | -5.549835 | -0.009269 | -1.516291 |
| H | -4.761151 | -0.078307 | 0.077820 |
| H | -3.091957 | -2.354690 | -2.393499 |
| H | -4.807275 | -2.183258 | -1.985871 |
| H | -4.220505 | -2.365541 | 0.462715 |
| H | -3.789444 | -3.792316 | -0.498179 |
| H | -2.587797 | -3.014200 | 2.065773 |
| H | -2.028787 | -4.392134 | 1.084114 |
| H | -0.246128 | -3.695689 | 2.554444 |
| H | 0.225195 | -3.306366 | 0.886104 |
| H | 1.730360 | -1.550142 | 1.941815 |
| H | 1.068249 | -1.957912 | 3.541715 |
| H | 0.027408 | 0.302627 | 3.694410 |
| H | 1.804946 | 0.333192 | 3.593736 |
| H | 1.742752 | 2.591059 | 2.701066 |
| H | -0.022034 | 2.553432 | 2.868946 |
| H | 1.540963 | 2.860235 | 0.242655 |
| H | 0.819982 | 4.200050 | 1.149436 |
| C | 2.110980 | -0.392547 | -1.282226 |
| C | 0.822886 | -0.811111 | -2.001634 |
| C | -0.354278 | 0.135809 | -1.781177 |
| N | -0.923177 | 0.055806 | -0.395276 |
| C | 3.255431 | -1.388898 | -1.492305 |
| C | 4.520574 | -1.074449 | -0.656600 |
| H | 5.256029 | -1.850228 | -0.882636 |
| C | 5.119187 | 0.261431 | -1.099167 |
| O | 5.043592 | 1.289751 | -0.470745 |
| O | 5.718202 | 0.174846 | -2.303431 |
| N | 4.228946 | -1.092272 | 0.778802 |
| H | 1.927233 | -0.288006 | -0.209393 |
| H | 2.407797 | 0.600033 | -1.642325 |
| H | 1.004450 | -0.852498 | -3.080864 |
| H | 0.532773 | -1.826878 | -1.706624 |
| H | -0.065008 | 1.176104 | -1.938296 |
| H | -1.179948 | -0.095473 | -2.453491 |
| H | -1.294289 | -0.884711 | -0.190045 |
| H | -1.712615 | 0.718403 | -0.318152 |
| H | 3.528208 | -1.438326 | -2.551082 |
| H | 2.929997 | -2.390188 | -1.193922 |
| H | 6.061201 | 1.052512 | -2.534603 |
| H | 5.035826 | -1.426605 | 1.294927 |
| H | 4.064680 | -0.140470 | 1.097464 |
| H | -0.247727 | 0.309700 | 0.341170 |

H⁺K[Ne]-cg.gttg.(--0/-00/+0/+00/-00/+00) 2636

| | | | |
|---|-----------|----------|-----------|
| C | -0.806664 | 3.267260 | -1.455896 |
| C | -2.008194 | 3.513141 | -0.572345 |
| O | -2.623262 | 2.261564 | -0.252753 |
| C | -3.837845 | 2.401391 | 0.486651 |

H -0.756617 3.692151 -0.510557
H -1.450966 3.315125 2.449448
H -0.059780 4.242043 1.836447
C 2.274709 -0.245368 -2.588415
C 1.429952 -0.264803 -1.304545
C -0.026051 0.104582 -1.566335
N -0.839917 0.043165 -0.310983
C 3.669053 -0.888138 -2.459113
C 4.709123 -0.159261 -1.583239
H 5.630596 -0.747710 -1.630134
C 4.318130 -0.177818 -0.088545
O 3.972673 -1.177781 0.490988
O 4.393771 1.015179 0.511529
N 5.013355 1.224877 -1.992297
H 2.350215 0.782631 -2.966547
H 1.743547 -0.800088 -3.370035
H 1.468568 -1.261660 -0.857332
H 1.836836 0.427802 -0.563145
H -0.487693 -0.584502 -2.275815
H -0.123725 1.114900 -1.968744
H -1.833054 0.212266 -0.534855
H -0.540481 0.749596 0.382136
H 4.100568 -0.985850 -3.459929
H 3.560094 -1.901120 -2.063403
H 4.705882 1.632667 -0.194440
H 4.347150 1.589712 -2.663603
H 5.938385 1.313479 -2.395115
H -0.755118 -0.889687 0.129437

H⁺K[Ne]-cgggtg(-0/-0/-0/-00/+00/-0) 5348

C -2.996834 -3.008914 -0.128376
C -3.814447 -2.099438 -1.016803
O -3.556539 -0.736662 -0.672543
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O -2.901839 2.032197 -0.933944
C -2.679661 3.305691 -0.339100
C -1.195510 3.621899 -0.404624
O -0.394382 2.706757 0.347553
C -0.281984 3.019350 1.742872
C 0.405216 1.882209 2.463083
O -0.464161 0.747940 2.446893
C -0.037117 -0.344486 3.255534
C 0.966388 -1.256737 2.557800
O 0.424233 -1.892182 1.385836
C -0.332438 -3.076624 1.636428
C -0.736234 -3.689713 0.305829
O -1.618110 -2.865550 -0.455310
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H -3.183730 -2.755814 0.922879
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H -5.421407 -0.114174 -1.338509
H -4.071212 0.213122 -2.449808
H -4.496407 1.521207 0.288984
H -4.942239 2.244700 -1.276123
H -3.235646 4.085030 -0.880035
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H -1.021674 4.648598 -0.061463
H -0.851344 3.549518 -1.438800
H -1.273749 3.182091 2.179232
H 0.310330 3.935410 1.860868
H 0.592651 2.195872 3.499360
H 1.364813 1.654158 1.988001
H -0.945204 -0.892856 3.518565
H 0.408938 0.019949 4.191153
H 1.317525 -2.022400 3.260883
H 1.829937 -0.688921 2.209920
H -1.214655 -2.853680 2.249445
H 0.285272 -3.800180 2.185224
H -1.186901 -4.674721 0.482151
H 0.154273 -3.829392 -0.310671
C 2.122605 -0.993449 -1.774866
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C -0.279072 -0.097221 -1.974936
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O 3.059811 0.612747 0.684150
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H 1.991591 -1.217484 -0.713918
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H -0.550165 0.932567 -0.151997
H 3.743851 -0.624076 -3.156046
H 4.161731 -1.685347 -1.819307
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H 5.971758 -0.154608 -2.496706
H 6.150590 1.307886 -1.776119
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H⁺K[Ne]-tg.g.ttg.(-00/+00/-0/-00/+00/-0) 1555

C -1.218263 -1.213872 2.409883
C -0.984035 0.216216 2.839776
O -0.949688 1.053957 1.688062
C -0.730810 2.429330 1.985347
C -0.561545 3.185010 0.679356

| | | | | | | | |
|---|-----------|-----------|-----------|--|-----------|-----------|-----------|
| O | 0.641467 | 2.832703 | -0.021725 | H | 1.320576 | -0.047751 | -2.674236 |
| C | 1.792801 | 3.581660 | 0.377946 | H | 0.433776 | -1.444748 | -2.058027 |
| C | 2.990292 | 3.140878 | -0.431724 | H | 0.406011 | -0.531533 | 0.105810 |
| O | 3.312410 | 1.798268 | -0.088632 | H | 0.872161 | 0.988887 | -0.412458 |
| C | 4.485194 | 1.310664 | -0.727480 | H | -3.675457 | 0.083620 | -2.903980 |
| C | 4.774413 | -0.084687 | -0.224487 | H | -3.112761 | 1.646174 | -2.316324 |
| O | 3.731149 | -0.971483 | -0.636983 | H | -5.727154 | -2.277519 | -0.992981 |
| C | 3.971555 | -2.328419 | -0.256855 | H | -3.376675 | 1.097661 | 0.773376 |
| C | 2.874329 | -3.212171 | -0.826034 | H | -4.834439 | 1.825365 | 0.693061 |
| O | 1.576882 | -2.905215 | -0.322659 | H | 1.929749 | -0.303087 | -0.489973 |
| C | 1.262685 | -3.510398 | 0.928704 | | | | |
| C | -0.113684 | -3.063790 | 1.367518 | H ⁺ K[Ne]-tg.g.ttt(+0+/-00/-00/+0+/-00/-00) | 10625 | | |
| O | -0.095236 | -1.660865 | 1.638470 | C | 1.094485 | -0.340500 | 2.848984 |
| H | -2.143205 | -1.300813 | 1.828411 | C | 0.563077 | 1.062469 | 3.031924 |
| H | -1.314202 | -1.835026 | 3.309686 | O | 0.456454 | 1.699994 | 1.762614 |
| H | -0.037010 | 0.295952 | 3.390175 | C | -0.037066 | 3.030120 | 1.834216 |
| H | -1.799265 | 0.520244 | 3.510961 | C | -0.171418 | 3.567416 | 0.420365 |
| H | 0.155008 | 2.538989 | 2.625932 | O | -1.159660 | 2.874358 | -0.352055 |
| H | -1.591216 | 2.844960 | 2.528711 | C | -2.481305 | 3.411763 | -0.238627 |
| H | -0.575721 | 4.263677 | 0.872161 | C | -3.422432 | 2.627758 | -1.123763 |
| H | -1.394041 | 2.948523 | 0.014597 | O | -3.553637 | 1.308712 | -0.609058 |
| H | 1.998729 | 3.435810 | 1.444894 | C | -4.483591 | 0.506560 | -1.326192 |
| H | 1.614716 | 4.649638 | 0.199481 | C | -4.602322 | -0.836572 | -0.644162 |
| H | 3.833245 | 3.807165 | -0.201932 | O | -3.362249 | -1.540115 | -0.746827 |
| H | 2.773873 | 3.221841 | -1.505968 | C | -3.410010 | -2.838503 | -0.150807 |
| H | 5.345325 | 1.953022 | -0.493044 | C | -2.097216 | -3.558593 | -0.407322 |
| H | 4.353446 | 1.302183 | -1.818458 | O | -0.973580 | -2.924196 | 0.196409 |
| H | 4.850460 | -0.081231 | 0.870236 | C | -0.740138 | -3.282355 | 1.555628 |
| H | 5.732603 | -0.422441 | -0.639684 | C | 0.453965 | -2.512090 | 2.072550 |
| H | 4.023181 | -2.403111 | 0.837308 | O | 0.131225 | -1.119363 | 2.126396 |
| H | 4.936085 | -2.662249 | -0.662581 | H | 1.251936 | -0.783943 | 3.840630 |
| H | 3.125091 | -4.263377 | -0.634466 | H | 2.052511 | -0.328497 | 2.317432 |
| H | 2.821649 | -3.071192 | -1.908010 | H | -0.419678 | 1.033522 | 3.521896 |
| H | 1.995660 | -3.231165 | 1.695585 | H | 1.254940 | 1.617492 | 3.680783 |
| H | 1.266481 | -4.604488 | 0.827940 | H | 0.659833 | 3.671242 | 2.394052 |
| H | -0.381849 | -3.614930 | 2.277736 | H | -1.002713 | 3.050801 | 2.358742 |
| H | -0.859471 | -3.293237 | 0.596154 | H | 0.774754 | 3.436941 | -0.108960 |
| C | -1.994583 | -0.037032 | -1.534169 | H | -0.401265 | 4.638549 | 0.449352 |
| C | -0.796335 | 0.318840 | -2.420443 | H | -2.830431 | 3.367429 | 0.799821 |
| C | 0.509335 | -0.358220 | -2.014011 | H | -2.477778 | 4.460319 | -0.562030 |
| N | 0.943737 | -0.023366 | -0.614366 | H | -3.040771 | 2.602566 | -2.153795 |
| C | -3.299711 | 0.609618 | -2.021402 | H | -4.397930 | 3.133647 | -1.132532 |
| C | -4.410967 | 0.671628 | -0.946087 | H | -4.155913 | 0.376829 | -2.367009 |
| H | -5.304444 | 1.079850 | -1.423617 | H | -5.473361 | 0.983638 | -1.336358 |
| C | -4.749967 | -0.743576 | -0.472775 | H | -5.398095 | -1.415331 | -1.130635 |
| O | -4.322741 | -1.258731 | 0.534542 | H | -4.867986 | -0.698662 | 0.411743 |
| O | -5.564392 | -1.384032 | -1.334521 | H | -4.224506 | -3.422929 | -0.599822 |
| N | -4.022963 | 1.563536 | 0.142816 | H | -3.614626 | -2.745500 | 0.923982 |
| H | -2.109907 | -1.126990 | -1.496808 | H | -2.184869 | -4.597907 | -0.065782 |
| H | -1.789041 | 0.289534 | -0.512058 | H | -1.898416 | -3.573498 | -1.481515 |
| H | -0.995157 | 0.028046 | -3.457762 | H | -0.528061 | -4.357722 | 1.629577 |
| H | -0.655265 | 1.405658 | -2.429807 | H | -1.615788 | -3.058324 | 2.177900 |

| | | | |
|---|-----------|-----------|-----------|
| H | 1.326963 | -2.674800 | 1.428672 |
| H | 0.693835 | -2.874461 | 3.080262 |
| C | 2.327836 | -0.396969 | -2.623326 |
| C | 1.448883 | 0.101486 | -1.469709 |
| C | 0.019736 | -0.413011 | -1.604285 |
| N | -0.827759 | -0.040249 | -0.426354 |
| C | 3.792268 | 0.062840 | -2.571043 |
| C | 4.612568 | -0.424544 | -1.348972 |
| H | 5.662577 | -0.163747 | -1.565712 |
| C | 4.331215 | 0.338437 | -0.062926 |
| O | 4.126930 | -0.163037 | 1.017731 |
| O | 4.398526 | 1.675772 | -0.239877 |
| N | 4.414572 | -1.849754 | -1.106366 |
| H | 1.906204 | -0.055732 | -3.575927 |
| H | 2.302320 | -1.489734 | -2.637366 |
| H | 1.853323 | -0.252267 | -0.517957 |
| H | 1.450534 | 1.196238 | -1.435794 |
| H | -0.468018 | -0.011410 | -2.494913 |
| H | 0.006819 | -1.501021 | -1.661441 |
| H | -1.762949 | -0.469145 | -0.504881 |
| H | -0.414975 | -0.384352 | 0.458126 |
| H | 4.295733 | -0.317709 | -3.465503 |
| H | 3.861058 | 1.152261 | -2.623881 |
| H | 4.297095 | 2.088967 | 0.630796 |
| H | 4.772056 | -2.114136 | -0.194605 |
| H | 4.893027 | -2.403443 | -1.808423 |
| H | -0.948344 | 0.982580 | -0.347770 |

H⁺K[Ne]-cgg.gtt(+0/+00/--0/-00/+00/-00) 11557

| | | | |
|---|-----------|-----------|-----------|
| C | 0.915320 | -3.049874 | 2.171639 |
| C | 1.478930 | -3.515467 | 0.848056 |
| O | 2.272594 | -2.467326 | 0.283706 |
| C | 3.140530 | -2.889586 | -0.769103 |
| C | 4.089490 | -1.763664 | -1.113284 |
| O | 3.354612 | -0.695709 | -1.704851 |
| C | 4.139964 | 0.440092 | -2.064585 |
| C | 4.191032 | 1.498940 | -0.975092 |
| O | 2.872148 | 2.017297 | -0.785353 |
| C | 2.801142 | 3.181522 | 0.043895 |
| C | 1.405596 | 3.772905 | -0.073579 |
| O | 0.389696 | 2.907567 | 0.428474 |
| C | 0.014715 | 3.151573 | 1.783986 |
| C | -1.030895 | 2.143761 | 2.204683 |
| O | -0.434133 | 0.843666 | 2.252794 |
| C | -1.262790 | -0.151566 | 2.875107 |
| C | -0.425237 | -1.373137 | 3.173209 |
| O | 0.054019 | -1.941918 | 1.957714 |
| H | 0.367207 | -3.882007 | 2.636342 |
| H | 1.738876 | -2.765395 | 2.840905 |
| H | 2.102027 | -4.401205 | 1.023418 |
| H | 0.672681 | -3.793520 | 0.157026 |
| H | 3.727197 | -3.756897 | -0.440493 |

| | | | |
|---|-----------|-----------|-----------|
| H | 2.558493 | -3.180194 | -1.653424 |
| H | 4.841433 | -2.139408 | -1.820422 |
| H | 4.606037 | -1.431089 | -0.203581 |
| H | 5.161643 | 0.137799 | -2.324693 |
| H | 3.676289 | 0.868297 | -2.956352 |
| H | 4.863590 | 2.305237 | -1.295820 |
| H | 4.575805 | 1.088859 | -0.031618 |
| H | 3.532297 | 3.924807 | -0.299714 |
| H | 3.041571 | 2.919749 | 1.083000 |
| H | 1.179530 | 3.943370 | -1.129162 |
| H | 1.379443 | 4.741988 | 0.439139 |
| H | -0.408000 | 4.160793 | 1.878573 |
| H | 0.884955 | 3.076225 | 2.448866 |
| H | -1.396067 | 2.417305 | 3.202779 |
| H | -1.881286 | 2.149173 | 1.512590 |
| H | -1.649900 | 0.239050 | 3.824658 |
| H | -2.115546 | -0.398438 | 2.234020 |
| H | -1.045831 | -2.099902 | 3.715422 |
| H | 0.424045 | -1.097744 | 3.813356 |
| C | -2.296023 | -0.694273 | -2.397340 |
| C | -1.320001 | -0.793195 | -1.213526 |
| C | -0.078958 | 0.068173 | -1.420243 |
| N | 0.829130 | 0.037538 | -0.231947 |
| C | -3.646637 | -1.402751 | -2.150305 |
| C | -4.747730 | -0.560210 | -1.466266 |
| H | -5.594107 | -1.226323 | -1.273801 |
| C | -4.274838 | -0.062897 | -0.086854 |
| O | -4.080221 | -0.795581 | 0.850493 |
| O | -4.045983 | 1.257045 | -0.030481 |
| N | -5.138713 | 0.604756 | -2.282939 |
| H | -1.826170 | -1.140908 | -3.279538 |
| H | -2.464422 | 0.358808 | -2.650326 |
| H | -1.032308 | -1.839946 | -1.069023 |
| H | -1.807721 | -0.485629 | -0.287797 |
| H | 0.509323 | -0.257772 | -2.279979 |
| H | -0.354868 | 1.113278 | -1.568080 |
| H | 0.332581 | 0.306378 | 0.637190 |
| H | 1.253369 | -0.891216 | -0.080678 |
| H | -3.488763 | -2.299919 | -1.546232 |
| H | -4.061503 | -1.744139 | -3.104066 |
| H | -4.322361 | 1.600712 | -0.914420 |
| H | -4.895220 | 0.490072 | -3.260383 |
| H | -6.137352 | 0.778218 | -2.237336 |
| H | 1.596591 | 0.713071 | -0.378503 |

H⁺K[Ne]-ctg.ttg(-00/+00/--0/-00/+0+/-00) 483

| | | | |
|---|----------|----------|-----------|
| C | 4.424848 | 0.194088 | -1.952287 |
| C | 4.556362 | 1.364639 | -0.992491 |
| O | 3.262240 | 1.902651 | -0.718690 |
| C | 3.312874 | 3.082337 | 0.088234 |
| C | 1.909650 | 3.583831 | 0.339092 |
| O | 1.218242 | 2.619416 | 1.118746 |

| | | | | | | | |
|---|-----------|-----------|-----------|--|-----------|-----------|-----------|
| C | -0.104168 | 3.002994 | 1.478221 | H | 0.460136 | 1.010188 | -2.194039 |
| C | -0.668621 | 1.980678 | 2.437199 | H | 0.273812 | 0.301024 | 0.257794 |
| O | -0.783431 | 0.714166 | 1.789857 | H | 1.785164 | 0.659376 | -0.352024 |
| C | -1.295042 | -0.297509 | 2.662272 | H | -3.436938 | -0.817397 | -3.012535 |
| C | -1.568650 | -1.566256 | 1.875320 | H | -3.411104 | -1.536775 | -1.410016 |
| O | -0.425913 | -2.105772 | 1.208240 | H | -6.678334 | 0.217790 | -0.565853 |
| C | 0.465778 | -2.840713 | 2.036645 | H | -6.016395 | 0.196411 | -3.152413 |
| C | 1.536677 | -3.456378 | 1.165351 | H | -5.906926 | -1.229044 | -2.349372 |
| O | 2.326460 | -2.416146 | 0.582109 | H | 1.329361 | -0.920610 | -0.125799 |
| C | 3.429169 | -2.907427 | -0.182023 | | | | |
| C | 4.339312 | -1.759750 | -0.556399 | H ⁺ K[Ne]-cgttgt(-00/+00/-00/+00/-00/+00) 8.4 | | | |
| O | 3.647817 | -0.886804 | -1.444172 | O | -2.099855 | -2.528837 | 1.125438 |
| H | 3.917178 | 0.526495 | -2.860425 | C | -2.495288 | -3.397459 | 0.071780 |
| H | 5.428494 | -0.151740 | -2.232588 | C | -3.584895 | -2.728883 | -0.735235 |
| H | 5.187412 | 2.130167 | -1.464297 | C | -1.167868 | -3.105896 | 2.030802 |
| H | 5.040190 | 1.066558 | -0.052882 | C | -0.897360 | -2.126543 | 3.150226 |
| H | 3.804287 | 2.859291 | 1.043611 | O | -0.250973 | -0.958731 | 2.635926 |
| H | 3.889172 | 3.860629 | -0.428357 | C | 0.046933 | -0.004749 | 3.662241 |
| H | 1.390146 | 3.756813 | -0.614366 | C | 0.636106 | 1.248949 | 3.056788 |
| H | 1.967665 | 4.542698 | 0.872790 | O | -0.352552 | 1.874012 | 2.246816 |
| H | -0.737573 | 3.081998 | 0.583490 | C | 0.022212 | 3.153922 | 1.750520 |
| H | -0.097634 | 3.982004 | 1.976747 | C | -1.151431 | 3.747695 | 1.004491 |
| H | -0.011850 | 1.892920 | 3.312393 | O | -1.450678 | 2.945684 | -0.141911 |
| H | -1.658349 | 2.314554 | 2.773578 | C | -2.540409 | 3.460146 | -0.910166 |
| H | -0.581453 | -0.465716 | 3.480256 | C | -2.769446 | 2.581119 | -2.118855 |
| H | -2.245364 | 0.035516 | 3.096704 | O | -3.174939 | 1.290758 | -1.678478 |
| H | -2.003083 | -2.313418 | 2.552573 | O | -3.073577 | -1.558719 | -1.381331 |
| H | -2.299365 | -1.345260 | 1.099234 | C | -4.077766 | -0.872136 | -2.135031 |
| H | -0.072122 | -3.645670 | 2.556565 | C | -3.507492 | 0.394837 | -2.730734 |
| H | 0.930648 | -2.194818 | 2.792511 | H | -1.636103 | -3.641337 | -0.568638 |
| H | 2.174688 | -4.103182 | 1.781261 | H | -2.893243 | -4.337615 | 0.477933 |
| H | 1.077758 | -4.066761 | 0.377191 | H | -3.956029 | -3.435379 | -1.489062 |
| H | 3.066636 | -3.417017 | -1.083960 | H | -4.417997 | -2.452657 | -0.077257 |
| H | 4.002547 | -3.627707 | 0.415798 | H | -0.234147 | -3.361695 | 1.510743 |
| H | 5.234016 | -2.166358 | -1.047632 | H | -1.576822 | -4.028021 | 2.466363 |
| H | 4.654181 | -1.231629 | 0.352309 | H | -0.253356 | -2.608503 | 3.897221 |
| C | -2.051107 | 0.135461 | -1.663134 | H | -1.840650 | -1.844434 | 3.634100 |
| C | -0.835868 | -0.726020 | -2.036798 | H | 0.767645 | -0.436553 | 4.368409 |
| C | 0.510149 | -0.025182 | -1.850611 | H | -0.870316 | 0.246033 | 4.209003 |
| N | 0.989519 | 0.006945 | -0.427496 | H | 1.530788 | 1.012862 | 2.464124 |
| C | -3.381230 | -0.579591 | -1.944262 | H | 0.941400 | 1.916127 | 3.874360 |
| C | -4.642347 | 0.235768 | -1.590213 | H | 0.896749 | 3.072279 | 1.090461 |
| H | -4.486468 | 1.275889 | -1.900871 | H | 0.285908 | 3.824888 | 2.579354 |
| C | -4.892388 | 0.314018 | -0.064373 | H | -0.895429 | 4.766833 | 0.687623 |
| O | -4.004613 | 0.376135 | 0.753426 | H | -2.028096 | 3.796255 | 1.662456 |
| O | -6.179030 | 0.334804 | 0.275153 | H | -2.310270 | 4.478969 | -1.247832 |
| N | -5.883369 | -0.219490 | -2.238246 | H | -3.447906 | 3.494072 | -0.294252 |
| H | -2.013020 | 0.424793 | -0.611397 | H | -1.851899 | 2.511991 | -2.720127 |
| H | -2.020518 | 1.063209 | -2.249991 | H | -3.550847 | 3.037082 | -2.742099 |
| H | -0.841178 | -1.661127 | -1.466753 | H | -4.438463 | -1.519173 | -2.945117 |
| H | -0.903381 | -1.007287 | -3.093474 | H | -4.924372 | -0.624591 | -1.482953 |
| H | 1.297945 | -0.526526 | -2.411379 | H | -2.620810 | 0.168733 | -3.340308 |

| | | | |
|---|-----------|-----------|-----------|
| H | -4.265956 | 0.839850 | -3.389341 |
| O | 6.817680 | 0.139486 | -0.583539 |
| C | 5.525706 | 0.468122 | -0.577365 |
| H | 6.889695 | -0.658390 | -1.152350 |
| C | 4.635668 | -0.427389 | -1.478022 |
| O | 5.083880 | 1.397653 | 0.049335 |
| N | 5.382707 | -1.629390 | -1.874069 |
| H | 4.477780 | 0.170685 | -2.383310 |
| C | 3.279415 | -0.660978 | -0.797947 |
| H | 5.192267 | -2.423559 | -1.271339 |
| H | 5.213709 | -1.907354 | -2.832504 |
| H | 3.422642 | -1.346420 | 0.047923 |
| H | 2.983653 | 0.296694 | -0.365614 |
| C | 2.181362 | -1.203901 | -1.719854 |
| H | 2.105970 | -0.574703 | -2.616050 |
| H | 2.449628 | -2.204008 | -2.074104 |
| C | 0.805810 | -1.281579 | -1.031841 |
| H | 0.122785 | -1.886870 | -1.635703 |
| H | 0.913208 | -1.784904 | -0.065096 |
| C | 0.191191 | 0.100034 | -0.816794 |
| H | 0.880540 | 0.768350 | -0.302551 |
| H | -0.066440 | 0.564546 | -1.769973 |
| N | -1.055667 | 0.061824 | 0.007883 |
| H | -1.414582 | 1.024646 | 0.104031 |
| H | -1.791753 | -0.517302 | -0.427502 |
| H | -0.864747 | -0.306775 | 0.954213 |

H⁺K[Ne]-cgtttt(-00/+00/-00/+00/-00/+00) 13.1

| | | | |
|---|-----------|-----------|-----------|
| O | -0.743992 | 0.422899 | 2.895094 |
| C | -0.141255 | -0.721768 | 3.484448 |
| C | -1.050563 | -1.912250 | 3.283696 |
| C | -0.038235 | 1.635050 | 3.131605 |
| C | -0.843016 | 2.786316 | 2.573859 |
| O | -0.952724 | 2.668280 | 1.151384 |
| C | -1.712768 | 3.735900 | 0.577482 |
| C | -1.868766 | 3.523630 | -0.910962 |
| O | -2.651849 | 2.356546 | -1.128618 |
| C | -3.012392 | 2.139041 | -2.486399 |
| C | -3.933773 | 0.942481 | -2.558491 |
| O | -3.230706 | -0.233036 | -2.147316 |
| C | -4.042193 | -1.408988 | -2.200122 |
| C | -3.230043 | -2.607689 | -1.764931 |
| O | -2.870463 | -2.444211 | -0.399111 |
| O | -1.165782 | -2.217592 | 1.889398 |
| C | -2.030367 | -3.332302 | 1.650588 |
| C | -2.192346 | -3.559231 | 0.164817 |
| H | 0.845765 | -0.909933 | 3.040017 |
| H | -0.002739 | -0.570316 | 4.563772 |
| H | -0.632935 | -2.775465 | 3.817747 |
| H | -2.043766 | -1.694518 | 3.695194 |
| H | 0.957010 | 1.598507 | 2.668127 |
| H | 0.096457 | 1.796662 | 4.209873 |

| | | | |
|---|-----------|-----------|-----------|
| H | -0.342428 | 3.728965 | 2.829502 |
| H | -1.844936 | 2.790541 | 3.020570 |
| H | -1.200411 | 4.690595 | 0.753043 |
| H | -2.702485 | 3.778954 | 1.048571 |
| H | -0.885397 | 3.424841 | -1.392491 |
| H | -2.366607 | 4.405553 | -1.336610 |
| H | -2.117519 | 1.970756 | -3.102295 |
| H | -3.541583 | 3.013726 | -2.888666 |
| H | -4.286271 | 0.822575 | -3.591053 |
| H | -4.803248 | 1.101719 | -1.908750 |
| H | -4.397805 | -1.569904 | -3.226072 |
| H | -4.912979 | -1.289983 | -1.543520 |
| H | -2.332458 | -2.709175 | -2.391386 |
| H | -3.840274 | -3.511697 | -1.896466 |
| H | -1.604876 | -4.235012 | 2.107805 |
| H | -3.011568 | -3.142239 | 2.102668 |
| H | -1.212476 | -3.698675 | -0.314030 |
| H | -2.774924 | -4.478754 | 0.016448 |
| O | 6.285197 | 1.124735 | 0.344092 |
| C | 6.330053 | 0.246643 | -0.477239 |
| H | 5.060303 | -2.268617 | -1.467400 |
| C | 5.088678 | -0.193131 | -1.296232 |
| O | 7.451303 | -0.408332 | -0.788443 |
| N | 5.375689 | -1.457646 | -1.990088 |
| H | 4.982518 | 0.581720 | -2.064624 |
| C | 3.839024 | -0.179138 | -0.404550 |
| H | 4.980955 | -1.501794 | -2.920912 |
| H | 7.196663 | -1.074322 | -1.463087 |
| H | 3.905416 | -1.013733 | 0.306021 |
| H | 3.877278 | 0.735043 | 0.192820 |
| C | 2.512769 | -0.247569 | -1.168217 |
| H | 2.476326 | 0.567948 | -1.901414 |
| H | 2.447466 | -1.182045 | -1.738747 |
| C | 1.307516 | -0.135019 | -0.224757 |
| H | 1.334912 | -0.949546 | 0.506996 |
| H | 1.377700 | 0.802693 | 0.335986 |
| C | -0.021619 | -0.172685 | -0.969771 |
| H | -0.080590 | 0.626447 | -1.710530 |
| H | -0.156720 | -1.120189 | -1.494042 |
| N | -1.193230 | -0.005137 | -0.053962 |
| H | -2.063499 | -0.054141 | -0.606249 |
| H | -1.223744 | -0.747374 | 0.664253 |
| H | -1.165860 | 0.909597 | 0.426491 |

H⁺K[Ne]-cggttg(-00/+0+/-00/-00/+0+/-00) 6338

| | | | |
|---|-----------|-----------|----------|
| C | -0.295718 | 1.641408 | 2.849847 |
| C | -0.755792 | 0.202935 | 2.880401 |
| O | 0.348306 | -0.638730 | 2.542934 |
| C | 0.133590 | -2.028144 | 2.770158 |
| C | -0.511137 | -2.735076 | 1.582353 |
| O | 0.281516 | -2.652004 | 0.384605 |
| C | 1.392202 | -3.547449 | 0.329289 |

| | | | | | | | |
|---|-----------|-----------|-----------|--|-----------|-----------|-----------|
| C | 2.053186 | -3.427265 | -1.034303 | H | 0.511337 | -0.910116 | -0.181105 |
| O | 2.607899 | -2.138288 | -1.291820 | H | 1.738287 | 0.164680 | -0.503920 |
| C | 3.908744 | -1.922233 | -0.754044 | H | -3.731033 | 1.017000 | -3.035163 |
| C | 4.403290 | -0.564276 | -1.199165 | H | -4.116342 | 1.904377 | -1.567943 |
| O | 3.608027 | 0.457356 | -0.593214 | H | -5.898020 | 0.195844 | 0.200343 |
| C | 4.045790 | 1.779066 | -0.918026 | H | -5.981508 | 0.547051 | -2.433239 |
| C | 3.233369 | 2.786183 | -0.135398 | H | -6.215137 | -0.990846 | -1.913311 |
| O | 1.883017 | 2.738966 | -0.585297 | H | 0.317253 | 0.739570 | 0.101177 |
| C | 1.003463 | 3.676156 | 0.029220 | | | | |
| C | 0.625863 | 3.333339 | 1.461458 | H ⁺ K[N _e]-ttgg.g.t(+00/-00/+00/-00/+00/-00) 1073 | | | |
| O | 0.007753 | 2.049616 | 1.509176 | C | -2.186160 | 3.534719 | 0.022523 |
| H | 0.599296 | 1.753783 | 3.474069 | C | -0.704138 | 3.738862 | 0.244775 |
| H | -1.088967 | 2.282078 | 3.256594 | O | -0.216577 | 2.735954 | 1.142714 |
| H | -1.600263 | 0.045191 | 2.201296 | C | 1.105156 | 2.990377 | 1.626603 |
| H | -1.095268 | -0.017884 | 3.901938 | C | 1.419896 | 2.037741 | 2.759557 |
| H | -0.496373 | -2.184631 | 3.656106 | O | 1.571926 | 0.699961 | 2.266193 |
| H | 1.116332 | -2.452101 | 2.991437 | C | 1.534151 | -0.286573 | 3.309317 |
| H | -1.466847 | -2.275326 | 1.330468 | C | 1.472719 | -1.676758 | 2.719186 |
| H | -0.688689 | -3.788838 | 1.833080 | O | 0.214536 | -1.853037 | 2.057213 |
| H | 2.107376 | -3.331160 | 1.131990 | C | -0.040020 | -3.205325 | 1.661399 |
| H | 1.041250 | -4.579971 | 0.459798 | C | -1.521718 | -3.392555 | 1.422195 |
| H | 1.305898 | -3.592637 | -1.813364 | O | -1.940971 | -2.602775 | 0.314729 |
| H | 2.824165 | -4.202687 | -1.130742 | C | -3.345200 | -2.657812 | 0.096300 |
| H | 4.603595 | -2.687666 | -1.125889 | C | -3.718737 | -1.706562 | -1.018513 |
| H | 3.898931 | -1.969180 | 0.342333 | O | -3.412081 | -0.371014 | -0.611111 |
| H | 4.350182 | -0.484057 | -2.292360 | C | -3.927412 | 0.639518 | -1.480099 |
| H | 5.450607 | -0.448001 | -0.891597 | C | -3.782785 | 1.991228 | -0.816988 |
| H | 3.937418 | 1.956884 | -1.995579 | O | -2.402943 | 2.307022 | -0.664100 |
| H | 5.104342 | 1.894010 | -0.651319 | H | -2.574064 | 4.376724 | -0.567644 |
| H | 3.654301 | 3.787315 | -0.302448 | H | -2.706527 | 3.522796 | 0.989379 |
| H | 3.302067 | 2.555327 | 0.934368 | H | -0.550486 | 4.733156 | 0.682575 |
| H | 0.107521 | 3.688466 | -0.595085 | H | -0.159374 | 3.692453 | -0.706707 |
| H | 1.440476 | 4.683854 | 0.012280 | H | 1.161918 | 4.014061 | 2.018287 |
| H | -0.066521 | 4.103364 | 1.830030 | H | 1.835101 | 2.892980 | 0.813813 |
| H | 1.505507 | 3.340788 | 2.118158 | H | 0.605288 | 2.064760 | 3.491977 |
| C | -2.103205 | 1.138686 | -1.620012 | H | 2.343793 | 2.360806 | 3.256771 |
| C | -1.236323 | -0.007330 | -2.159886 | H | 0.652830 | -0.109831 | 3.936516 |
| C | 0.265703 | 0.193668 | -1.965292 | H | 2.431057 | -0.202485 | 3.936723 |
| N | 0.713334 | 0.039511 | -0.543313 | H | 1.555503 | -2.394986 | 3.545360 |
| C | -3.599443 | 1.015260 | -1.946657 | H | 2.295191 | -1.848247 | 2.017939 |
| C | -4.342365 | -0.231176 | -1.410039 | H | 0.265002 | -3.889264 | 2.463109 |
| H | -3.914936 | -1.129752 | -1.864762 | H | 0.539429 | -3.451743 | 0.763646 |
| C | -4.137264 | -0.374143 | 0.108482 | H | -2.079623 | -3.101494 | 2.322211 |
| O | -3.096376 | -0.760166 | 0.593446 | H | -1.714883 | -4.456668 | 1.225640 |
| O | -5.181071 | -0.011158 | 0.846345 | H | -3.880969 | -2.379524 | 1.013708 |
| N | -5.782747 | -0.103151 | -1.681429 | H | -3.652063 | -3.674637 | -0.186549 |
| H | -1.756595 | 2.080379 | -2.061794 | H | -4.793947 | -1.799173 | -1.216695 |
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| H | -1.402703 | -0.109878 | -3.238368 | H | -4.992448 | 0.457353 | -1.671619 |
| H | -1.531429 | -0.957290 | -1.704658 | H | -3.398190 | 0.622110 | -2.441968 |
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 H 3.822198 1.830458 -2.037709
 H 3.563633 1.290413 -3.559262
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H⁺K[Ne]-tggg.tt(-00/+00/-00/+00/-00/+00) 6195

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 H 5.098748 0.368152 -3.405485
 H 4.008642 1.414691 -2.725933
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H⁺K[Ne]-tg.gggt(-00/+00/-00/+00/-00/+00) 9.1

O 3.144363 1.482952 -1.408340
 C 3.453284 2.813626 -0.986366
 C 2.189168 3.512677 -0.540518
 C 4.293815 0.767284 -1.866633
 C 3.888816 -0.624067 -2.297751
 O 3.413817 -1.335585 -1.162075
 C 3.101922 -2.699079 -1.416601
 C 2.770756 -3.377711 -0.107098

| | | | | | | | |
|---|-----------|-----------|-----------|--|-----------|-----------|-----------|
| O | 1.571853 | -2.826689 | 0.445527 | H | -5.541186 | -2.435584 | -0.524714 |
| C | 1.258531 | -3.387506 | 1.724547 | O | -5.850008 | 1.095503 | -1.703002 |
| C | -0.000671 | -2.758900 | 2.275294 | O | -4.111789 | 1.676451 | -0.401334 |
| O | 0.239940 | -1.379665 | 2.519075 | H | 0.631180 | 0.486754 | 0.800750 |
| C | -0.844156 | -0.707394 | 3.147680 | H | 1.220875 | -0.958295 | 0.192258 |
| C | -0.427208 | 0.711307 | 3.459403 | H | 1.878681 | 0.493141 | -0.313455 |
| O | -0.179372 | 1.428337 | 2.246510 | H | -4.446947 | 2.556912 | -0.635164 |
| O | 1.683066 | 2.852643 | 0.612538 | | | | |
| C | 0.536977 | 3.471538 | 1.182348 | H ⁺ K[Ne]-tgttgt(-00/+0+/-00/+0+/-00/-0) 1517 | | | |
| C | 0.208710 | 2.783679 | 2.487740 | C | -0.842807 | -2.174233 | 2.908875 |
| H | 4.175157 | 2.783661 | -0.160741 | C | -1.944016 | -2.894154 | 2.148786 |
| H | 3.897960 | 3.374131 | -1.818893 | O | -1.711958 | -2.726246 | 0.757385 |
| H | 2.429636 | 4.559579 | -0.309709 | C | -2.661728 | -3.381664 | -0.072389 |
| H | 1.443929 | 3.505097 | -1.348511 | C | -2.280205 | -3.128171 | -1.520344 |
| H | 5.039936 | 0.707726 | -1.064402 | O | -2.333179 | -1.745715 | -1.888926 |
| H | 4.741755 | 1.290917 | -2.721175 | C | -3.628920 | -1.287518 | -2.289238 |
| H | 4.765841 | -1.127015 | -2.727758 | C | -3.527587 | 0.124367 | -2.818096 |
| H | 3.112050 | -0.573030 | -3.073856 | O | -3.176746 | 1.000691 | -1.755044 |
| H | 3.963111 | -3.213097 | -1.865188 | C | -3.128889 | 2.368147 | -2.146496 |
| H | 2.258230 | -2.778693 | -2.116997 | C | -2.735616 | 3.204747 | -0.950759 |
| H | 3.599444 | -3.241078 | 0.598542 | O | -1.399299 | 2.862891 | -0.577890 |
| H | 2.636350 | -4.452781 | -0.283639 | C | -0.830297 | 3.659432 | 0.461629 |
| H | 2.092239 | -3.215919 | 2.416538 | C | -1.357009 | 3.316568 | 1.848750 |
| H | 1.104341 | -4.469916 | 1.626128 | O | -1.277414 | 1.906609 | 2.013121 |
| H | -0.265055 | -3.274015 | 3.209126 | C | -1.408743 | 1.457247 | 3.356601 |
| H | -0.834552 | -2.885735 | 1.570845 | C | -1.795401 | -0.006287 | 3.352815 |
| H | -1.110812 | -1.206311 | 4.089502 | O | -0.795383 | -0.764984 | 2.668718 |
| H | -1.729840 | -0.713436 | 2.497657 | H | 0.128108 | -2.559323 | 2.591949 |
| H | 0.479806 | 0.705817 | 4.076565 | H | -0.954486 | -2.367457 | 3.982867 |
| H | -1.230392 | 1.203216 | 4.023030 | H | -2.937478 | -2.508655 | 2.417770 |
| H | 0.735789 | 4.531938 | 1.389852 | H | -1.916002 | -3.958983 | 2.421239 |
| H | -0.316066 | 3.415001 | 0.491293 | H | -3.674886 | -3.015702 | 0.145303 |
| H | 1.085730 | 2.805906 | 3.146460 | H | -2.651399 | -4.465850 | 0.110114 |
| H | -0.611812 | 3.320985 | 2.980738 | H | -2.924710 | -3.718221 | -2.182288 |
| C | -2.260471 | -0.449482 | -2.081578 | H | -1.247566 | -3.444016 | -1.680986 |
| C | -3.600834 | -1.176346 | -1.883307 | H | -4.328744 | -1.316630 | -1.445722 |
| H | -1.777067 | -0.872572 | -2.969538 | H | -4.014630 | -1.936273 | -3.085647 |
| H | -2.438636 | 0.607292 | -2.307980 | H | -4.501277 | 0.407815 | -3.242005 |
| C | -1.300587 | -0.559295 | -0.887332 | H | -2.777867 | 0.174626 | -3.619449 |
| C | -4.509328 | -0.665961 | -0.731248 | H | -4.113547 | 2.698014 | -2.505937 |
| H | -3.409527 | -2.238468 | -1.688945 | H | -2.401166 | 2.507439 | -2.957181 |
| H | -4.178358 | -1.129548 | -2.811717 | H | -3.429616 | 3.018142 | -0.123027 |
| H | -1.741530 | -0.088454 | -0.004365 | H | -2.786571 | 4.267195 | -1.221130 |
| H | -1.132020 | -1.615537 | -0.648695 | H | -0.989072 | 4.725915 | 0.258265 |
| C | 0.036437 | 0.109337 | -1.187496 | H | 0.242536 | 3.462337 | 0.419057 |
| N | -5.731229 | -1.439707 | -0.538094 | H | -2.394287 | 3.649330 | 1.989938 |
| H | -3.946495 | -0.676760 | 0.205583 | H | -0.735507 | 3.838987 | 2.588731 |
| C | -4.926153 | 0.772392 | -1.004917 | H | -2.197339 | 2.016274 | 3.878204 |
| H | 0.521921 | -0.349887 | -2.050210 | H | -0.464148 | 1.606272 | 3.894963 |
| H | -0.098430 | 1.168883 | -1.410383 | H | -2.770208 | -0.129606 | 2.865204 |
| N | 1.000315 | 0.022439 | -0.045746 | H | -1.880104 | -0.351061 | 4.391323 |
| H | -6.397831 | -1.248122 | -1.280141 | C | 2.856178 | -1.124375 | -1.367455 |

| | | | |
|---|-----------|-----------|-----------|
| C | 1.421434 | -1.223968 | -0.823906 |
| C | 0.731115 | 0.135014 | -0.740585 |
| N | -0.670662 | 0.033569 | -0.221863 |
| C | 3.863270 | -0.512834 | -0.386248 |
| C | 5.237273 | -0.256707 | -1.049263 |
| H | 5.575900 | -1.187903 | -1.511990 |
| C | 6.242704 | 0.113992 | 0.042602 |
| O | 6.558116 | 1.241322 | 0.329606 |
| O | 6.719364 | -0.974820 | 0.686104 |
| N | 5.118668 | 0.767881 | -2.080487 |
| H | 3.193539 | -2.131814 | -1.632287 |
| H | 2.865261 | -0.540911 | -2.292923 |
| H | 1.423492 | -1.699336 | 0.163504 |
| H | 0.835349 | -1.872956 | -1.482646 |
| H | 0.674640 | 0.602424 | -1.725094 |
| H | 1.260301 | 0.817575 | -0.075277 |
| H | -0.691874 | -0.298378 | 0.755698 |
| H | -1.249083 | -0.606406 | -0.791809 |
| H | 3.992678 | -1.175388 | 0.475559 |
| H | 3.503331 | 0.447770 | 0.000417 |
| H | 7.327779 | -0.670453 | 1.377891 |
| H | 5.164909 | 1.689580 | -1.653038 |
| H | 5.892093 | 0.714916 | -2.734959 |
| H | -1.116909 | 0.964952 | -0.244419 |

H⁺K[N_e]-cg.ggg.g(-00/+0+/+00/-00/+00/--0) 1831bb

| | | | |
|---|-----------|-----------|-----------|
| C | -1.033821 | 0.428091 | 3.596546 |
| C | -1.125263 | 1.793176 | 2.954343 |
| O | 0.007139 | 1.995079 | 2.108807 |
| C | 0.260472 | 3.364492 | 1.787706 |
| C | 1.659214 | 3.489270 | 1.229715 |
| O | 1.741314 | 2.762351 | 0.013200 |
| C | 3.049083 | 2.751956 | -0.548358 |
| C | 3.023681 | 1.910175 | -1.810221 |
| O | 2.712229 | 0.538619 | -1.566306 |
| C | 3.838600 | -0.297515 | -1.278313 |
| C | 3.397375 | -1.742019 | -1.246017 |
| O | 2.606489 | -1.974393 | -0.083681 |
| C | 2.123434 | -3.311328 | -0.017247 |
| C | 1.233905 | -3.459816 | 1.194798 |
| O | 0.048480 | -2.676177 | 1.001432 |
| C | -0.983124 | -2.879676 | 1.967981 |
| C | -0.919484 | -1.890938 | 3.115701 |
| O | -1.142275 | -0.581396 | 2.600852 |
| H | -1.841725 | 0.325944 | 4.335079 |
| H | -0.074035 | 0.337092 | 4.121953 |
| H | -1.136542 | 2.548610 | 3.750019 |
| H | -2.056083 | 1.891703 | 2.379473 |
| H | 0.186411 | 3.979900 | 2.692982 |
| H | -0.478341 | 3.730435 | 1.062464 |
| H | 2.382821 | 3.096617 | 1.956931 |
| H | 1.882387 | 4.552495 | 1.061359 |

| | | | |
|---|-----------|-----------|-----------|
| H | 3.768048 | 2.352082 | 0.179969 |
| H | 3.363878 | 3.773496 | -0.806297 |
| H | 3.987083 | 1.992940 | -2.326917 |
| H | 2.248341 | 2.285892 | -2.481934 |
| H | 4.292221 | -0.021675 | -0.318460 |
| H | 4.589511 | -0.176267 | -2.069007 |
| H | 4.292117 | -2.380384 | -1.225428 |
| H | 2.817316 | -1.973539 | -2.146890 |
| H | 2.962514 | -4.015805 | 0.074633 |
| H | 1.558728 | -3.552847 | -0.925653 |
| H | 1.765290 | -3.137397 | 2.098579 |
| H | 0.958021 | -4.515385 | 1.305390 |
| H | -0.939869 | -3.901795 | 2.360541 |
| H | -1.932178 | -2.764076 | 1.438101 |
| H | 0.057399 | -1.935103 | 3.616357 |
| H | -1.690685 | -2.148280 | 3.856170 |
| C | -2.513849 | 1.401647 | -2.514802 |
| C | -3.835810 | 1.711684 | -1.788086 |
| C | -4.362228 | 0.683520 | -0.781289 |
| N | -4.413169 | -0.682676 | -1.353691 |
| C | -1.246700 | 1.265430 | -1.650163 |
| C | -1.041568 | -0.072783 | -0.909836 |
| H | -1.823563 | -0.245477 | -0.171068 |
| C | -0.960466 | -1.270703 | -1.879555 |
| O | 0.106885 | -1.655625 | -2.291260 |
| O | -2.109455 | -1.820328 | -2.232005 |
| N | 0.243014 | -0.031181 | -0.142941 |
| H | -2.335127 | 2.232723 | -3.203190 |
| H | -2.628381 | 0.523402 | -3.155275 |
| H | -4.603857 | 1.868395 | -2.554678 |
| H | -3.746242 | 2.669177 | -1.262592 |
| H | -5.349166 | 1.011439 | -0.434858 |
| H | -3.721708 | 0.643567 | 0.104558 |
| H | -2.929797 | -1.373444 | -1.840956 |
| H | -4.997388 | -0.688626 | -2.188317 |
| H | -1.218770 | 2.072380 | -0.910196 |
| H | -0.373942 | 1.409266 | -2.294187 |
| H | 0.231089 | 0.718000 | 0.566818 |
| H | 1.064689 | 0.112461 | -0.760148 |
| H | -4.862020 | -1.319268 | -0.699318 |
| H | 0.375461 | -0.934683 | 0.344682 |

H⁺K[N_e]-tg.gg.tg(-00/+00/-00/+00/-00/+00) 21bb

| | | | |
|---|----------|-----------|-----------|
| C | 1.222205 | 3.602454 | -1.210053 |
| C | 1.263104 | 2.696188 | -2.418959 |
| O | 1.965451 | 1.509453 | -2.069271 |
| C | 2.242036 | 0.644610 | -3.160922 |
| C | 3.162308 | -0.455454 | -2.684525 |
| O | 2.499279 | -1.264787 | -1.710888 |
| C | 3.362372 | -2.265461 | -1.167053 |
| C | 2.610701 | -3.088582 | -0.146940 |
| O | 2.222724 | -2.240112 | 0.924270 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 1.591633 | -2.922933 | 2.000602 | H | -0.209752 | -2.240571 | -1.384218 |
| C | 1.430504 | -1.974893 | 3.165960 | H | -1.049473 | -2.127204 | 0.159540 |
| O | 0.528342 | -0.920195 | 2.835365 | H | 0.577820 | 1.085957 | 0.067575 |
| C | 0.383793 | 0.013015 | 3.912834 | H | 1.255730 | -0.391661 | -0.328383 |
| C | -0.456976 | 1.189536 | 3.478988 | H | -5.897509 | 0.144521 | -1.505769 |
| O | 0.258100 | 1.922415 | 2.490270 | H | 0.275995 | -0.256328 | 1.016518 |
| C | -0.409960 | 3.107960 | 2.077190 | | | | |
| C | 0.421850 | 3.791713 | 1.018368 | | | | |
| O | 0.474675 | 2.982740 | -0.163356 | H ⁺ K[Ne]-cg.ggg.g.(+0+/+00/-00/+00/-00/+00) | | | |
| H | 0.751231 | 4.553848 | -1.490256 | l122bb | | | |
| H | 2.243852 | 3.807402 | -0.865903 | C | 4.079449 | 0.185334 | -1.144976 |
| H | 1.779257 | 3.221797 | -3.233921 | C | 3.707482 | -1.276951 | -1.114801 |
| H | 0.244807 | 2.458698 | -2.757498 | O | 3.037647 | -1.555245 | 0.112074 |
| H | 2.745168 | 1.193153 | -3.969179 | C | 2.621870 | -2.908491 | 0.222931 |
| H | 1.312612 | 0.221754 | -3.569502 | C | 1.931167 | -3.102116 | 1.552818 |
| H | 4.065037 | -0.012974 | -2.245066 | O | 0.789226 | -2.234944 | 1.645332 |
| H | 3.459584 | -1.073724 | -3.542086 | C | -0.060458 | -2.518513 | 2.759350 |
| H | 4.229315 | -1.787894 | -0.693365 | C | -0.667560 | -1.244581 | 3.304899 |
| H | 3.722526 | -2.925539 | -1.967336 | O | -1.497456 | -0.642961 | 2.312959 |
| H | 3.271867 | -3.888171 | 0.215045 | C | -2.268195 | 0.460603 | 2.779107 |
| H | 1.729825 | -3.559500 | -0.605244 | C | -1.488585 | 1.753402 | 2.948471 |
| H | 2.210252 | -3.769530 | 2.328963 | O | -0.962409 | 2.172314 | 1.689822 |
| H | 0.616251 | -3.319503 | 1.685495 | C | -0.357368 | 3.467040 | 1.762604 |
| H | 2.408013 | -1.555611 | 3.435945 | C | 0.216658 | 3.836153 | 0.414921 |
| H | 1.045910 | -2.537076 | 4.027891 | O | 1.257377 | 2.922282 | 0.107243 |
| H | 1.374826 | 0.362117 | 4.228391 | C | 1.953766 | 3.213433 | -1.099855 |
| H | -0.099417 | -0.482849 | 4.765038 | C | 3.217789 | 2.387200 | -1.148528 |
| H | -0.645207 | 1.820402 | 4.359507 | O | 2.902651 | 0.999526 | -1.206707 |
| H | -1.418760 | 0.853400 | 3.075810 | H | 4.706454 | 0.377548 | -2.025665 |
| H | -0.524051 | 3.797131 | 2.926382 | H | 4.653092 | 0.443777 | -0.245888 |
| H | -1.406086 | 2.867456 | 1.688121 | H | 4.630732 | -1.869631 | -1.185795 |
| H | 1.439630 | 3.963897 | 1.390171 | H | 3.061803 | -1.528004 | -1.962484 |
| H | -0.031397 | 4.761875 | 0.777431 | H | 3.488298 | -3.585300 | 0.187021 |
| C | -2.377569 | -2.156204 | -1.559111 | H | 1.950255 | -3.166668 | -0.603756 |
| C | -3.613319 | -2.201392 | -0.614489 | H | 2.615865 | -2.876962 | 2.379138 |
| C | -4.934024 | -1.667677 | -1.202230 | H | 1.611606 | -4.148251 | 1.632532 |
| N | -5.110574 | -0.205595 | -0.965000 | H | 0.520003 | -2.982708 | 3.565024 |
| C | -1.047572 | -1.761687 | -0.872607 | H | -0.844879 | -3.219867 | 2.451315 |
| C | -0.752039 | -0.241180 | -0.851085 | H | 0.133607 | -0.559927 | 3.610102 |
| H | -0.476857 | 0.094192 | -1.849569 | H | -1.265364 | -1.494118 | 4.192721 |
| C | -2.003292 | 0.509007 | -0.412491 | H | -2.748768 | 0.212791 | 3.735203 |
| O | -2.761545 | 0.802120 | -1.451666 | H | -3.055306 | 0.610586 | 2.036813 |
| O | -2.289709 | 0.683764 | 0.753830 | H | -0.672426 | 1.643029 | 3.674631 |
| N | 0.407809 | 0.064224 | 0.042170 | H | -2.176963 | 2.515771 | 3.339081 |
| H | -2.564441 | -1.479800 | -2.396084 | H | 0.440194 | 3.463112 | 2.516117 |
| H | -2.244548 | -3.147231 | -1.999557 | H | -1.108820 | 4.212294 | 2.054397 |
| H | -3.408647 | -1.661209 | 0.315172 | H | 0.605767 | 4.862514 | 0.467269 |
| H | -3.776465 | -3.239661 | -0.313076 | H | -0.565783 | 3.810800 | -0.356840 |
| H | -5.775138 | -2.221599 | -0.773548 | H | 2.233321 | 4.275126 | -1.132348 |
| H | -4.962746 | -1.831124 | -2.282476 | H | 1.317008 | 3.003991 | -1.970645 |
| H | -3.762129 | 0.614422 | -1.233317 | H | 3.822431 | 2.594297 | -0.256104 |
| H | -5.340610 | -0.040966 | 0.012868 | H | 3.799304 | 2.678624 | -2.034257 |
| | | | | C | -2.518083 | 0.622787 | -2.726457 |

| | | | |
|---|-----------|-----------|-----------|
| C | -3.934950 | 0.657391 | -2.123603 |
| C | -4.293162 | -0.389571 | -1.064489 |
| N | -3.995324 | -1.769815 | -1.514505 |
| C | -1.334194 | 0.832888 | -1.761825 |
| C | -0.885023 | -0.380641 | -0.920265 |
| H | -1.649170 | -0.680684 | -0.205635 |
| C | -0.487863 | -1.577862 | -1.801949 |
| O | 0.660962 | -1.727326 | -2.148530 |
| O | -1.455840 | -2.398068 | -2.158863 |
| N | 0.307299 | 0.001823 | -0.094624 |
| H | -2.472205 | 1.433926 | -3.458888 |
| H | -2.372364 | -0.290914 | -3.308426 |
| H | -4.648000 | 0.570328 | -2.951827 |
| H | -4.116916 | 1.643255 | -1.681208 |
| H | -5.351455 | -0.272041 | -0.804334 |
| H | -3.726606 | -0.218267 | -0.145231 |
| H | -4.327009 | -2.441039 | -0.825620 |
| H | -2.385452 | -2.127366 | -1.846497 |
| H | -1.565563 | 1.649818 | -1.070636 |
| H | -0.467773 | 1.147154 | -2.352784 |
| H | 1.141202 | 0.226841 | -0.663842 |
| H | 0.573096 | -0.775769 | 0.539546 |
| H | -4.507023 | -1.975786 | -2.371049 |
| H | 0.086282 | 0.824002 | 0.485990 |

Strutture (Arg)H⁺-18C6H⁺R[N_ω]-tcg-gg-t(-00/+0+/-00/-00/+0+/-00) 60

| | | | |
|---|-----------|-----------|-----------|
| C | 3.719425 | 1.218404 | -2.188534 |
| C | 4.636046 | 0.584174 | -1.122807 |
| C | 4.347417 | -0.867668 | -0.682776 |
| H | 5.235612 | -1.202924 | -0.123006 |
| C | 3.202859 | -1.049050 | 0.320141 |
| O | 2.555508 | -2.070823 | 0.390892 |
| O | 3.028954 | 0.000149 | 1.125415 |
| N | 4.060015 | -1.742790 | -1.831807 |
| C | 2.222626 | 1.275831 | -1.874116 |
| N | 1.645874 | -0.069819 | -1.964979 |
| C | 0.385631 | -0.399656 | -1.669706 |
| N | -0.062802 | -1.624141 | -1.997101 |
| N | -0.451844 | 0.471333 | -1.106501 |
| H | 3.854701 | 0.716605 | -3.151925 |
| H | 4.061404 | 2.246240 | -2.338112 |
| H | 4.652408 | 1.206604 | -0.226283 |
| H | 5.655274 | 0.605562 | -1.522644 |
| H | 4.857105 | -1.779072 | -2.460094 |
| H | 3.883321 | -2.687900 | -1.502476 |
| H | 1.720273 | 1.929560 | -2.594545 |
| H | 2.059858 | 1.695085 | -0.878093 |
| H | 2.299384 | -0.820662 | -2.212089 |
| H | -0.856593 | -2.015438 | -1.484286 |
| H | -0.113634 | 1.256456 | -0.556834 |
| H | -1.424556 | 0.213562 | -0.960902 |
| H | 2.224240 | -0.115442 | 1.691716 |
| H | 0.575984 | -2.269656 | -2.432817 |
| C | 0.627121 | 1.644332 | 2.999808 |
| C | 1.141730 | 2.606866 | 1.941071 |
| O | 0.280699 | 2.738818 | 0.807307 |
| C | -0.719536 | 3.750027 | 0.965046 |
| C | -1.650768 | 3.746719 | -0.224844 |
| O | -2.448432 | 2.575625 | -0.182849 |
| C | -3.409711 | 2.505829 | -1.226294 |
| C | -4.288696 | 1.296251 | -1.011433 |
| O | -3.553415 | 0.098461 | -1.257433 |
| C | -4.339728 | -1.066122 | -1.032581 |
| C | -3.566451 | -2.297707 | -1.464883 |
| O | -2.395502 | -2.541663 | -0.682470 |
| C | -2.626661 | -3.239748 | 0.545912 |
| C | -1.357150 | -3.291895 | 1.365474 |
| O | -1.092226 | -2.010611 | 1.910813 |
| C | 0.004093 | -2.011588 | 2.815181 |
| C | 0.134865 | -0.645756 | 3.450620 |
| O | 0.712596 | 0.294667 | 2.532458 |
| H | -0.415113 | 1.870077 | 3.254680 |
| H | 1.232161 | 1.763298 | 3.910000 |
| H | 2.106829 | 2.264916 | 1.564439 |
| H | 1.296392 | 3.587704 | 2.407130 |
| H | -0.235065 | 4.732402 | 1.042098 |

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| H | -2.913755 | 2.446669 | -2.205131 |
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| H | -5.144160 | 1.351273 | -1.698708 |
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| H | 0.929872 | -2.292745 | 2.298098 |
| H | -0.174912 | -2.740479 | 3.619985 |
| H | 0.768849 | -0.717130 | 4.344319 |
| H | -0.856364 | -0.290372 | 3.753352 |

H⁺R[N_ω]-cggg.tg(+00/-00/+0+/-00/-00/+0+) 1134

| | | | |
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| C | -3.369596 | 1.206081 | -1.251569 |
| C | -4.895020 | 1.245134 | -1.017193 |
| C | -5.637109 | -0.110421 | -1.096152 |
| H | -5.430885 | -0.555864 | -2.074887 |
| C | -5.112479 | -1.113870 | -0.049860 |
| O | -4.015273 | -1.628001 | -0.120205 |
| O | -5.946086 | -1.358763 | 0.947933 |
| N | -7.078714 | 0.080598 | -0.870156 |
| C | -2.544730 | 1.164104 | 0.047048 |
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| H | -7.647486 | -0.481486 | -1.493896 |
| H | -2.897429 | 0.373079 | 0.711675 |
| H | -2.671572 | 2.104010 | 0.588746 |
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| H | 1.368077 | 0.693956 | -0.671636 |
| H | -2.162938 | -1.386056 | -0.325325 |
| H | -0.656910 | -2.139930 | -0.750048 |
| H | -6.768553 | -0.855126 | 0.727544 |
| H | 1.330949 | -1.035020 | -0.631953 |
| C | 3.999150 | 1.417896 | -2.016013 |
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| C | 3.223408 | -2.177576 | -2.401493 |

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| C | 3.024514 | -3.214412 | -1.319219 | N | 0.845064 | 1.236863 | -1.057787 |
| O | 1.801674 | -2.959361 | -0.618684 | H | 2.896585 | -0.554048 | 0.469682 |
| C | 1.649905 | -3.730427 | 0.581204 | H | 2.875560 | -2.296850 | 0.359769 |
| C | 2.266013 | -3.071509 | 1.802151 | H | 4.774560 | -2.288838 | -1.235485 |
| O | 1.534368 | -1.896565 | 2.101739 | H | 5.169076 | -1.564931 | 0.315181 |
| C | 2.016691 | -1.218525 | 3.252945 | H | 6.942939 | -1.233230 | -1.293587 |
| C | 1.187789 | 0.019435 | 3.512676 | H | 6.970009 | 0.053975 | -2.311228 |
| O | 1.520488 | 1.031770 | 2.571818 | H | 2.408396 | -0.505252 | -2.084600 |
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| C | 1.347429 | 3.296929 | 1.835439 | H | 0.220404 | -1.874242 | -0.602487 |
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| C | 1.584933 | 3.778464 | -0.508273 | H | 1.855152 | 1.285748 | -0.936475 |
| C | 2.947531 | 3.230704 | -0.896643 | H | 0.329401 | 2.103242 | -1.015332 |
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| H | 4.439102 | 2.129317 | -2.728130 | H | -1.750165 | -0.654046 | -0.691166 |
| H | 4.716042 | 1.256372 | -1.200661 | C | -4.569867 | -1.204967 | -1.403836 |
| H | 4.624304 | -0.133629 | -3.339866 | C | -4.343637 | 0.092364 | -2.148964 |
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| H | 4.070083 | -2.487392 | -3.030949 | C | -3.561556 | 2.318870 | -1.857897 |
| H | 2.330419 | -2.117860 | -3.039991 | C | -3.213311 | 3.328053 | -0.786106 |
| H | 3.874727 | -3.180558 | -0.628975 | O | -2.009756 | 2.945308 | -0.111365 |
| H | 2.983350 | -4.212252 | -1.774671 | C | -1.848975 | 3.619025 | 1.139985 |
| H | 2.079540 | -4.729032 | 0.440112 | C | -0.638533 | 3.091279 | 1.876872 |
| H | 0.575781 | -3.845280 | 0.742718 | O | -0.843625 | 1.725534 | 2.193405 |
| H | 3.325049 | -2.831165 | 1.628752 | C | 0.117173 | 1.205007 | 3.101962 |
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| H | 3.069584 | -0.934579 | 3.119260 | O | 0.293686 | -1.059090 | 2.299578 |
| H | 1.948491 | -1.876898 | 4.131615 | C | 0.068406 | -2.450705 | 2.474521 |
| H | 1.397162 | 0.373679 | 4.532765 | C | -1.220893 | -2.953233 | 1.843005 |
| H | 0.119386 | -0.229957 | 3.450417 | O | -1.084133 | -2.968167 | 0.417117 |
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| H | 2.440402 | 3.321734 | 1.893686 | O | -3.314302 | -1.808787 | -1.079054 |
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| H | 0.928814 | 3.764222 | -1.381368 | H | -3.591033 | -0.059027 | -2.935213 |
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| H | 3.410402 | 3.930740 | -1.607361 | H | -4.401054 | 2.715208 | -2.447069 |
| H ⁺ R[N _ω]-cgggtg(-00/+00/+0+/-00/-00/+00) 869 | | | | | | | |
| C | 3.093246 | -1.386600 | -0.207465 | H | -2.712259 | 2.168163 | -2.539587 |
| C | 4.578122 | -1.420266 | -0.595967 | H | -3.085589 | 4.318681 | -1.241573 |
| C | 5.144365 | -0.182487 | -1.335437 | H | -4.036433 | 3.380569 | -0.064007 |
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| N | 6.608279 | -0.285876 | -1.426822 | H | 1.133199 | 1.307537 | 2.697176 |
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| C | 0.148869 | 0.100452 | -0.891325 | H | 0.333534 | -0.548684 | 4.304925 |
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H⁺R[N ω]-tg.g.gg(+00/-00/+0+/-00/-00/+0+) 619

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H⁺R[N ω]-ctg.ggg.(-00/+00/--0/-00/+00/--0) 72

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| C | -1.264329 | 0.748651 | 3.457882 | N | -0.941652 | -1.241840 | -0.348820 |
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| C | -3.823448 | 0.964576 | -2.449135 | H | -7.387539 | 0.334128 | -1.965769 |
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| C | -1.527577 | -3.511810 | 1.279674 | H | 1.564519 | -0.853546 | -0.399396 |
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| H | 0.075041 | 2.742458 | 2.293430 | C | 0.891696 | 1.532164 | 3.092977 |
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| H | -4.215635 | 1.500760 | -3.324055 | O | 3.589214 | -0.110886 | -2.057835 |
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| H | -2.176927 | -3.192657 | 3.291695 | H | 0.806360 | -0.724522 | 4.424389 |
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| H ⁺ R[N _ω]-cg.g.gtg(+00/--0/-00/+00/-00/+0+) 2266 | | | | H | 0.676243 | 1.658892 | 4.164823 |
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H 1.641481 -3.992666 -0.442302
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H 1.820335 -4.295717 2.069046

H⁺R[N_ω]-cgggtg(+00/-00/+00/-00/+0+/-0+) 5345

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H⁺R[N_ω]-tgtg.g.g.(-00/+00/-0/-00/+00/--0) 255

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| H | 0.403663 | 2.013102 | -1.427307 | O | -3.864254 | 1.497368 | -0.168254 |
| H | 7.358082 | 0.243135 | 0.736230 | O | -5.838715 | 1.073049 | 0.760340 |
| H | -1.566607 | -0.686280 | -0.487988 | N | -6.852329 | -0.145997 | -1.275232 |
| C | -4.758761 | 0.151977 | -1.048129 | C | -2.351670 | -1.289752 | -0.250463 |
| C | -4.334330 | -1.232081 | -1.490192 | N | -0.909482 | -1.101696 | -0.410225 |
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| C | -2.988388 | -3.102909 | -0.891781 | N | 1.018803 | 0.149127 | -0.620228 |
| C | -2.172995 | -3.659844 | 0.252977 | N | -1.006905 | 1.233876 | -0.511514 |
| O | -0.906698 | -2.998791 | 0.326061 | H | -2.791905 | -2.043623 | -2.207971 |
| C | -0.191310 | -3.250446 | 1.542879 | H | -2.842199 | -0.298796 | -2.114893 |
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| O | -0.179560 | -1.021718 | 2.415272 | H | -4.919384 | -1.847768 | -0.520949 |
| C | -0.507948 | -0.108756 | 3.454044 | H | -7.391413 | 0.491365 | -1.851274 |
| C | -0.078234 | 1.290752 | 3.073685 | H | -7.124816 | -1.091955 | -1.516345 |
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| C | -0.659068 | 3.156889 | 1.734062 | H | -2.741794 | -0.576768 | 0.478906 |
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| O | -1.700656 | 2.989482 | -0.436166 | H | 1.505549 | 1.024209 | -0.443554 |
| C | -2.813687 | 3.279978 | -1.294322 | H | -2.014072 | 1.277923 | -0.379283 |
| C | -4.035406 | 2.422909 | -1.003189 | H | -0.508453 | 2.096393 | -0.665166 |
| O | -3.715116 | 1.076890 | -1.313324 | H | -6.638239 | 0.586291 | 0.439956 |
| H | -5.005332 | 0.144288 | 0.022509 | H | 1.582851 | -0.693643 | -0.664291 |
| H | -5.664209 | 0.429713 | -1.607005 | C | 4.209686 | -1.400545 | -1.882117 |
| H | -5.215430 | -1.887885 | -1.484088 | C | 3.862107 | -0.153487 | -2.665084 |
| H | -3.941251 | -1.190505 | -2.514416 | O | 3.645710 | 0.922983 | -1.765046 |
| H | -3.889827 | -3.720915 | -1.003158 | C | 3.198422 | 2.114172 | -2.393896 |
| H | -2.425156 | -3.156874 | -1.834378 | C | 3.105148 | 3.207846 | -1.353028 |
| H | -2.729304 | -3.517569 | 1.185556 | O | 2.063020 | 2.916413 | -0.415339 |
| H | -2.019227 | -4.736192 | 0.099075 | C | 2.206936 | 3.646377 | 0.805733 |
| H | 0.864059 | -3.085307 | 1.316260 | C | 1.151886 | 3.225699 | 1.803715 |
| H | -0.315799 | -4.299573 | 1.837296 | O | 1.345351 | 1.864959 | 2.145407 |
| H | -1.683244 | -2.378422 | 2.857734 | C | 0.550152 | 1.443216 | 3.245947 |
| H | -0.113838 | -2.719378 | 3.610194 | C | 0.841522 | -0.006383 | 3.566627 |
| H | 0.007570 | -0.396119 | 4.382321 | O | 0.170394 | -0.855532 | 2.638929 |
| H | -1.589426 | -0.118979 | 3.646831 | C | 0.358015 | -2.243083 | 2.878033 |
| H | -0.075881 | 1.915968 | 3.978516 | C | 1.494201 | -2.857433 | 2.075183 |
| H | 0.944937 | 1.269024 | 2.673216 | O | 1.116132 | -2.936103 | 0.695369 |
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| H | 0.319860 | 3.192390 | 1.232949 | C | 3.285773 | -3.105856 | -0.498177 |
| H | -2.713596 | 3.548249 | 1.299259 | O | 3.034654 | -1.937017 | -1.268178 |
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| H | -4.870126 | 2.777190 | -1.626609 | H | 3.908571 | 2.434169 | -3.169987 |
| | | | | H | 2.223215 | 1.951247 | -2.874905 |
| | | | | H | 2.905794 | 4.168841 | -1.844811 |
| | | | | H | 4.063060 | 3.279518 | -0.824963 |
| | | | | H | 3.202229 | 3.458330 | 1.226243 |
| H ⁺ R[N _ω]-cg.g.gtg(--0/-00/+00/+00/-00/--0) 4444 | | | | | | | |
| C | -3.120335 | -1.210612 | -1.580684 | | | | |
| C | -4.653674 | -1.278148 | -1.420222 | | | | |

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| H | 2.108119 | 4.723113 | 0.612295 |
| H | 1.253479 | 3.868049 | 2.691135 |
| H | 0.141887 | 3.383497 | 1.397499 |
| H | -0.518733 | 1.564571 | 3.023741 |
| H | 0.787572 | 2.052990 | 4.129871 |
| H | 0.483519 | -0.220091 | 4.583502 |
| H | 1.926894 | -0.169661 | 3.542146 |
| H | 0.540214 | -2.431228 | 3.944125 |
| H | -0.576658 | -2.743956 | 2.609542 |
| H | 1.687044 | -3.870827 | 2.453051 |
| H | 2.410157 | -2.266289 | 2.189543 |
| H | 2.159627 | -4.704842 | 0.384209 |
| H | 1.390299 | -3.952814 | -1.027143 |
| H | 3.885755 | -2.855495 | 0.387232 |
| H | 3.856832 | -3.835629 | -1.089735 |

H⁺R[N_ω]-cggg.tg.(+00/-00/+00/-00/+0+/-0+) 11955

| | | | |
|---|-----------|-----------|-----------|
| C | 3.120233 | -1.210549 | -1.580960 |
| C | 4.653580 | -1.278098 | -1.420581 |
| C | 5.402394 | 0.076072 | -1.395154 |
| H | 5.143954 | 0.626767 | -2.305595 |
| C | 4.951682 | 0.959795 | -0.215139 |
| O | 3.864226 | 1.497408 | -0.168558 |
| O | 5.838728 | 1.073090 | 0.759948 |
| N | 6.852250 | -0.145962 | -1.275666 |
| C | 2.351642 | -1.289711 | -0.250698 |
| N | 0.909444 | -1.101658 | -0.410376 |
| C | 0.303571 | 0.094151 | -0.497401 |
| N | 1.006851 | 1.233919 | -0.511582 |
| N | -1.018861 | 0.149167 | -0.620188 |
| H | 2.791764 | -2.043545 | -2.208245 |
| H | 2.842074 | -0.298721 | -2.115135 |
| H | 4.919333 | -1.847735 | -0.521331 |
| H | 5.069267 | -1.833136 | -2.266623 |
| H | 7.391315 | 0.491383 | -1.851744 |
| H | 7.124723 | -1.091927 | -1.516766 |
| H | 2.484690 | -2.281980 | 0.185323 |
| H | 2.741802 | -0.576736 | 0.478660 |
| H | 0.297114 | -1.855667 | -0.105661 |
| H | 0.508384 | 2.096440 | -0.665163 |
| H | -1.582913 | -0.693602 | -0.664223 |
| H | -1.505595 | 1.024239 | -0.443435 |
| H | 6.638239 | 0.586334 | 0.439527 |
| H | 2.014030 | 1.277963 | -0.379444 |
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| C | -3.862355 | -0.153333 | -2.664771 |
| O | -3.645891 | 0.923087 | -1.764690 |
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| C | -3.105292 | 3.207927 | -1.352582 |
| O | -2.063062 | 2.916434 | -0.415025 |
| C | -2.206845 | 3.646323 | 0.806108 |
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| O | -1.345132 | 1.864819 | 2.145587 |
| C | -0.549858 | 1.443019 | 3.246051 |
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| C | -3.285813 | -3.105834 | -0.498099 |
| O | -3.034770 | -1.936942 | -1.268044 |
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| H | -2.223520 | 1.951429 | -2.874635 |
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| H | -1.253200 | 3.867876 | 2.691426 |
| H | -0.141736 | 3.383400 | 1.397652 |
| H | -0.787218 | 2.052748 | 4.130022 |
| H | 0.519012 | 1.564384 | 3.023781 |
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| H | -0.483141 | -0.220357 | 4.583516 |
| H | -0.539892 | -2.431467 | 3.944022 |
| H | 0.576870 | -2.744134 | 2.609333 |
| H | -2.409972 | -2.266399 | 2.189598 |
| H | -1.686858 | -3.870961 | 2.452950 |
| H | -2.159581 | -4.704862 | 0.384099 |
| H | -1.390375 | -3.952743 | -1.027271 |
| H | -3.885730 | -2.855539 | 0.387373 |
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H⁺R[N_ω]-cg.g.tg(-00/+0+/-0+/-00/+00) 9813

| | | | |
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| H | -5.408373 | -0.194540 | 0.913063 |
| C | -4.771156 | -1.228006 | -0.829348 |
| O | -3.716347 | -1.680948 | -0.434640 |
| O | -5.407756 | -1.718334 | -1.881377 |
| N | -6.839183 | 0.059180 | -0.660696 |
| C | -2.269038 | 1.057059 | -1.284078 |
| N | -0.864381 | 0.924522 | -0.910476 |
| C | -0.211957 | -0.231321 | -0.708076 |
| N | 1.106782 | -0.216925 | -0.559255 |
| N | -0.853556 | -1.409293 | -0.705944 |
| H | -3.003513 | 0.608062 | 0.701630 |
| H | -2.967118 | 2.314200 | 0.312558 |
| H | -4.825609 | 1.525454 | -1.544040 |

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|---|-----------|-----------|-----------|--|-----------|-----------|-----------|
| H | -5.231789 | 2.084361 | 0.065673 | H | 1.398339 | 4.239254 | 1.750490 |
| H | -7.502424 | -0.378522 | -0.030347 | H ⁺ R[N _ω]-cgggtg(-00/+0/+00/-00/+00/--0) 581 | | | |
| H | -7.143257 | 1.012663 | -0.821434 | C | -3.257243 | 1.222917 | -0.048353 |
| H | -2.340596 | 1.882025 | -1.999200 | C | -4.743094 | 1.228650 | -0.436826 |
| H | -2.563708 | 0.157111 | -1.824156 | C | -5.267812 | 0.019886 | -1.250611 |
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| H | 1.656381 | 0.620087 | -0.724383 | C | -2.290983 | 1.241857 | -1.245262 |
| C | 1.916319 | 3.696782 | -0.723208 | N | -0.889022 | 1.073841 | -0.874389 |
| C | 3.284458 | 3.046221 | -0.849876 | C | -0.253187 | -0.110003 | -0.783952 |
| O | 3.133146 | 1.749060 | -1.411896 | N | -0.914492 | -1.265840 | -0.963400 |
| C | 4.372129 | 1.146095 | -1.796154 | N | 1.051782 | -0.137762 | -0.579055 |
| C | 4.119717 | -0.223225 | -2.388803 | H | -3.034088 | 0.361801 | 0.583504 |
| O | 3.821983 | -1.143836 | -1.349249 | H | -3.072478 | 2.109755 | 0.565754 |
| C | 3.427803 | -2.424219 | -1.818881 | H | -4.968446 | 2.127484 | -1.022740 |
| C | 3.219901 | -3.339691 | -0.632509 | H | -5.338331 | 1.297838 | 0.480350 |
| O | 2.088321 | -2.914413 | 0.135417 | H | -7.078387 | -0.202122 | -2.257883 |
| C | 2.087942 | -3.461220 | 1.456970 | H | -7.101087 | 1.005980 | -1.147032 |
| C | 0.953875 | -2.879836 | 2.271336 | H | -2.540121 | 0.457886 | -1.962002 |
| O | 1.152674 | -1.484871 | 2.418038 | H | -2.375641 | 2.191354 | -1.781425 |
| C | 0.276141 | -0.883529 | 3.360564 | H | -0.375876 | 1.867170 | -0.501505 |
| C | 0.535319 | 0.606371 | 3.426893 | H | -1.923864 | -1.346704 | -0.858334 |
| O | -0.095963 | 1.260983 | 2.328827 | H | 1.624785 | 0.698826 | -0.569703 |
| C | 0.055089 | 2.673213 | 2.328760 | H | 1.516123 | -1.020310 | -0.386377 |
| C | 1.253247 | 3.171598 | 1.535154 | H | -6.675284 | -1.410203 | -0.172519 |
| O | 1.005420 | 3.005726 | 0.134202 | H | -0.376227 | -2.118241 | -0.908776 |
| H | 2.042630 | 4.731284 | -0.378233 | C | 1.326131 | -3.039723 | 2.016405 |
| H | 1.438242 | 3.719169 | -1.704663 | C | 2.384392 | -3.423015 | 1.006704 |
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| H | 3.797754 | 2.982633 | 0.119217 | C | 3.002475 | -3.193192 | -1.306571 |
| H | 5.037244 | 1.058596 | -0.927765 | C | 4.164915 | -2.213364 | -1.347556 |
| H | 4.862980 | 1.776932 | -2.548899 | O | 3.655489 | -0.935569 | -1.691579 |
| H | 5.019342 | -0.544897 | -2.932777 | C | 4.637094 | 0.086121 | -1.769981 |
| H | 3.289437 | -0.166973 | -3.106221 | C | 3.972937 | 1.391776 | -2.152822 |
| H | 4.208498 | -2.860099 | -2.458886 | O | 3.197695 | 1.881675 | -1.057252 |
| H | 2.507736 | -2.346161 | -2.415764 | C | 2.632686 | 3.169022 | -1.279348 |
| H | 3.065503 | -4.367924 | -0.984525 | C | 2.161679 | 3.728830 | 0.044644 |
| H | 4.117298 | -3.318884 | -0.003263 | O | 1.075950 | 2.955364 | 0.563307 |
| H | 1.974878 | -4.552840 | 1.411574 | C | 0.919643 | 3.127549 | 1.974829 |
| H | 3.042569 | -3.230375 | 1.944991 | C | -0.278992 | 2.342987 | 2.483563 |
| H | 0.953669 | -3.379308 | 3.251581 | O | -0.171057 | 0.935225 | 2.360097 |
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| H | 1.618776 | 0.782615 | 3.426717 | H | 0.332580 | -3.356492 | 1.667372 |
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H⁺R[N_ω]-tcg.g.gg(--0/-00/-00/+00/-00/+00) 4321

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H⁺R[N_ω]-tg.g.g.g(-00/+00/--0/-00/+00/--0) 1154

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| H | -4.250518 | -1.571715 | -1.929187 | H ⁺ R[N _ω]-tcgg.gt(--0/-00/+0+/-00/--0) 2236 | | | |
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| O | 2.017127 | -2.914890 | -0.318612 | C | -0.466473 | -0.611679 | -1.605781 |
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| O | 3.024409 | 1.950867 | -1.052374 | H | 1.353552 | 0.199441 | -1.193606 |
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| H | 4.886461 | -2.448923 | -2.067896 | H | 0.015358 | 1.212661 | -0.786431 |
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| H | -0.309139 | -1.272031 | 3.054886 | O | -0.952749 | 0.588961 | 2.425838 |
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H⁺R[N_ω]-tcg.g.gg(--0/-00/+00/--+/-+00/--0) 9472

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H⁺R[N_ω]-cg.g.gtg(-00/+00/-00/+00/--0/-00) 11396

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H⁺R[N_ω]-tg.g.gg(-00/+0/+0/+00/-00/+00) 5534

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 C -4.795027 1.440208 -0.400246
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 H -6.200609 -0.007430 0.303926
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 O -3.907690 -1.970384 -0.376243
 O -5.346256 -1.064656 -1.843397
 N -4.455066 -0.109881 1.536596
 C -2.193474 1.756383 -0.067416
 N -1.842724 0.448823 0.477873
 C -0.803059 -0.315094 0.122851
 N -0.890307 -1.639283 0.345161
 N 0.286863 0.191073 -0.444741
 H -3.199905 0.968213 -1.804835
 H -3.464623 2.670768 -1.515092
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 H -4.654786 -1.027505 1.924569
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 H -1.337056 2.162250 -0.603459
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 H 1.020799 -0.425522 -0.781817
 H 0.546074 1.167361 -0.325001
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 O 1.046168 1.728785 2.409699
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 C 1.674738 -2.489941 2.713107
 C 2.281117 -3.335967 1.615535
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H⁺R[N_ω]-ttg.gg.t(-00/+0+/++0/--0/-00/--0) 5707

| | | | |
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| C | -4.369520 | -2.313405 | -1.010989 |
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| C | -4.282361 | 0.317219 | -0.862360 |
| H | -5.009980 | 1.140636 | -0.789032 |
| C | -3.290401 | 0.607206 | 0.271301 |
| O | -3.425791 | 0.195955 | 1.401254 |
| O | -2.292057 | 1.406168 | -0.118636 |
| N | -3.587499 | 0.320994 | -2.164829 |
| C | -3.016889 | -2.605647 | -0.353584 |
| N | -1.971710 | -1.752392 | -0.929856 |
| C | -0.696324 | -1.738420 | -0.536363 |
| N | 0.147699 | -0.828756 | -1.020837 |
| N | -0.229498 | -2.655673 | 0.325709 |
| H | -4.250983 | -2.388007 | -2.096689 |
| H | -5.046582 | -3.124264 | -0.729174 |
| H | -5.993443 | -0.933870 | -1.205219 |
| H | -5.350391 | -1.011294 | 0.421928 |
| H | -4.253362 | 0.171151 | -2.917687 |
| H | -3.150220 | 1.223220 | -2.325224 |
| H | -2.765174 | -3.657633 | -0.529687 |
| H | -3.080760 | -2.438233 | 0.727413 |
| H | -2.284422 | -1.057494 | -1.619778 |
| H | 1.148096 | -0.894117 | -0.860528 |
| H | -0.858569 | -3.321858 | 0.739567 |
| H | 0.672582 | -2.495414 | 0.775822 |
| H | -1.678862 | 1.594203 | 0.645197 |
| H | -0.164030 | -0.026984 | -1.546634 |
| C | 0.318206 | 3.709570 | 0.549459 |
| C | 0.244192 | 3.091750 | 1.928769 |
| O | -0.580949 | 1.926578 | 1.884855 |
| C | -0.779632 | 1.244511 | 3.127515 |
| C | 0.464804 | 0.584258 | 3.697660 |
| O | 1.042863 | -0.284227 | 2.735145 |
| C | 2.141874 | -1.030062 | 3.236737 |
| C | 3.108997 | -1.351288 | 2.118575 |
| O | 2.503963 | -2.225197 | 1.161527 |
| C | 3.415723 | -2.812566 | 0.230650 |
| C | 4.059360 | -1.832224 | -0.736660 |
| O | 3.053786 | -1.195936 | -1.514137 |
| C | 3.584983 | -0.317710 | -2.505780 |
| C | 2.451427 | 0.284287 | -3.322093 |
| O | 1.599763 | 1.159701 | -2.590178 |
| C | 2.120388 | 2.475886 | -2.419710 |
| C | 1.142732 | 3.324201 | -1.638154 |
| O | 1.094988 | 2.876078 | -0.294052 |
| H | 0.778415 | 4.705268 | 0.635075 |
| H | -0.693534 | 3.842114 | 0.140331 |
| H | -0.181158 | 3.819978 | 2.632451 |
| H | 1.253778 | 2.828160 | 2.259236 |
| H | -1.546210 | 0.499724 | 2.916330 |
| H | -1.177243 | 1.942714 | 3.876866 |

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| H | 0.153222 | 0.030735 | 4.596145 |
| H | 1.208197 | 1.328574 | 4.017256 |
| H | 1.789721 | -1.950644 | 3.722018 |
| H | 2.695834 | -0.446124 | 3.984854 |
| H | 3.993513 | -1.840031 | 2.549212 |
| H | 3.420539 | -0.418983 | 1.635445 |
| H | 2.831156 | -3.546680 | -0.327220 |
| H | 4.209358 | -3.344355 | 0.772091 |
| H | 4.740778 | -2.400122 | -1.386232 |
| H | 4.660337 | -1.079859 | -0.208322 |
| H | 4.240305 | -0.879964 | -3.185948 |
| H | 4.191659 | 0.461865 | -2.026288 |
| H | 1.813025 | -0.519743 | -3.694682 |
| H | 2.881103 | 0.804907 | -4.188709 |
| H | 2.284565 | 2.938218 | -3.403398 |
| H | 3.077793 | 2.453015 | -1.885497 |
| H | 0.145291 | 3.272761 | -2.097689 |
| H | 1.483297 | 4.369541 | -1.683784 |

H⁺R[N_ω]-tcgg.gt(--0/-0+/+00/-00/+0+/+00) 3651

| | | | |
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| C | 4.224810 | -1.696400 | -0.434951 |
| C | 4.426879 | -0.196952 | -0.756663 |
| H | 5.388669 | 0.089457 | -0.300614 |
| C | 3.424912 | 0.762098 | -0.110347 |
| O | 3.081088 | 1.802252 | -0.636216 |
| O | 3.007714 | 0.372124 | 1.091055 |
| N | 4.401551 | 0.057131 | -2.204764 |
| C | 1.719167 | -2.015183 | -1.143177 |
| N | 1.556148 | -0.719015 | -1.813074 |
| C | 0.508363 | 0.094426 | -1.660322 |
| N | -0.577119 | -0.278281 | -0.998452 |
| N | 0.548455 | 1.327519 | -2.229314 |
| H | 3.205263 | -3.515420 | -0.895483 |
| H | 3.459225 | -2.515466 | -2.302477 |
| H | 4.015284 | -1.786510 | 0.632402 |
| H | 5.187513 | -2.192073 | -0.597308 |
| H | 5.124683 | -0.479321 | -2.674288 |
| H | 4.579870 | 1.039953 | -2.389410 |
| H | 1.415078 | -1.924615 | -0.096025 |
| H | 1.069879 | -2.758912 | -1.616412 |
| H | 2.378814 | -0.362179 | -2.307124 |
| H | -0.685107 | -1.195142 | -0.570164 |
| H | -0.024628 | 2.021859 | -1.753142 |
| H | 1.478300 | 1.671728 | -2.429685 |
| H | 2.277301 | 0.956102 | 1.411558 |
| H | -1.364710 | 0.356254 | -0.898679 |
| C | -4.167269 | 0.973501 | -1.571069 |
| C | -4.586308 | -0.357041 | -0.986706 |
| O | -3.506126 | -1.269373 | -1.080952 |
| C | -3.770535 | -2.541603 | -0.514976 |
| C | -2.482825 | -3.346724 | -0.542125 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| O | -1.452473 | -2.752821 | 0.253210 | H | -3.663845 | 3.020522 | -1.588631 |
| C | -1.450613 | -3.113131 | 1.637203 | H | -3.856366 | 1.671195 | -2.677882 |
| C | -1.091686 | -1.927781 | 2.510539 | H | -4.137791 | 1.628878 | 0.387756 |
| O | 0.246224 | -1.524168 | 2.252359 | H | -5.431518 | 1.617642 | -0.786665 |
| C | 0.826882 | -0.704060 | 3.256813 | H | -4.533707 | -1.862231 | -1.864134 |
| C | 0.327728 | 0.734027 | 3.306525 | H | -5.265316 | -0.514604 | -2.446342 |
| O | 0.694093 | 1.455487 | 2.124250 | H | -1.478496 | 2.335898 | -2.272825 |
| C | 0.243560 | 2.815402 | 2.148903 | H | -1.663420 | 1.910858 | -0.563158 |
| C | 0.305484 | 3.433224 | 0.760571 | H | -2.502550 | -0.288360 | -2.190433 |
| O | -0.686319 | 2.946081 | -0.149077 | H | 0.479480 | 1.305598 | -0.840754 |
| C | -1.988063 | 3.503970 | 0.017956 | H | 0.229454 | -2.133369 | -1.240977 |
| C | -2.920409 | 2.931006 | -1.026344 | H | -1.313304 | -2.149310 | -1.922018 |
| O | -3.129407 | 1.545511 | -0.770819 | H | -2.059559 | -0.732358 | 1.609436 |
| H | -3.821008 | 0.844861 | -2.604548 | H | 1.396046 | -0.141175 | -1.064429 |
| H | -5.039952 | 1.639577 | -1.579647 | C | 0.337717 | -0.827699 | 3.065002 |
| H | -5.458014 | -0.727079 | -1.546079 | C | -0.089265 | 0.596186 | 3.352633 |
| H | -4.883883 | -0.224069 | 0.062986 | O | 0.039056 | 1.387281 | 2.181338 |
| H | -4.541328 | -3.074372 | -1.091894 | C | 0.228610 | 2.768394 | 2.440840 |
| H | -4.141880 | -2.432393 | 0.515013 | C | 0.131538 | 3.537579 | 1.130871 |
| H | -2.099341 | -3.379505 | -1.564065 | O | 0.996469 | 3.064182 | 0.101292 |
| H | -2.675154 | -4.375810 | -0.217994 | C | 2.359165 | 3.463834 | 0.254916 |
| H | -0.733183 | -3.926649 | 1.795239 | C | 3.203777 | 2.859058 | -0.842664 |
| H | -2.442922 | -3.465301 | 1.941161 | O | 3.330409 | 1.460332 | -0.626740 |
| H | -1.196834 | -2.237376 | 3.561101 | C | 4.218639 | 0.832274 | -1.539748 |
| H | -1.794253 | -1.105564 | 2.322018 | C | 4.291475 | -0.644498 | -1.225721 |
| H | 1.900932 | -0.720836 | 3.068266 | O | 3.037195 | -1.252480 | -1.538462 |
| H | 0.654006 | -1.144366 | 4.249657 | C | 3.027225 | -2.676505 | -1.472190 |
| H | 0.771664 | 1.215323 | 4.189393 | C | 2.700476 | -3.219745 | -0.092139 |
| H | -0.762639 | 0.770243 | 3.420490 | O | 1.362147 | -2.863398 | 0.256331 |
| H | 0.879566 | 3.403056 | 2.825176 | C | 0.993205 | -3.339982 | 1.548981 |
| H | -0.778129 | 2.846529 | 2.545195 | C | -0.387097 | -2.854913 | 1.961979 |
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| H | 0.211630 | 4.522462 | 0.860976 | H | 0.312259 | -1.398726 | 4.003431 |
| H | -1.945535 | 4.595191 | -0.102351 | H | 1.363058 | -0.819401 | 2.681805 |
| H | -2.382877 | 3.279455 | 1.015466 | H | 0.565649 | 0.974645 | 4.149920 |
| H | -2.507105 | 3.080564 | -2.033616 | H | -1.123068 | 0.629313 | 3.723618 |
| H | -3.874925 | 3.471546 | -0.970181 | H | 1.198194 | 2.925906 | 2.934277 |
| | | | | H | -0.549552 | 3.158972 | 3.113517 |
| | | | | H | 0.317208 | 4.602464 | 1.325895 |
| | | | | H | -0.880405 | 3.443690 | 0.733624 |
| | | | | H | 2.751864 | 3.142977 | 1.226195 |
| | | | | H | 2.427091 | 4.558708 | 0.195757 |
| | | | | H | 4.193369 | 3.337820 | -0.820537 |
| | | | | H | 2.752231 | 3.058662 | -1.824563 |
| | | | | H | 5.226457 | 1.263033 | -1.450270 |
| | | | | H | 3.874278 | 0.975314 | -2.573168 |
| | | | | H | 4.543118 | -0.786408 | -0.167411 |
| | | | | H | 5.082790 | -1.097611 | -1.837006 |
| | | | | H | 3.995486 | -3.079292 | -1.793936 |
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| | | | | H | 2.808251 | -4.313577 | -0.107548 |
| H ⁺ R[N _ω]-tcgg.gt(-00/--0/-00/+0+/-00/--0) 7677 | | | | | | | |
| C | -3.516502 | 1.940033 | -1.673268 | | | | |
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| H | -5.351074 | -0.544166 | 0.010738 | | | | |
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| O | -2.913364 | -2.067466 | -0.111241 | | | | |
| O | -2.845513 | -0.265014 | 1.224006 | | | | |
| N | -4.464744 | -0.850368 | -1.919653 | | | | |
| C | -2.011686 | 1.682532 | -1.574194 | | | | |
| N | -1.712155 | 0.281192 | -1.873462 | | | | |
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| N | 0.510929 | 0.347365 | -1.176114 | | | | |
| N | -0.435485 | -1.653154 | -1.844302 | | | | |

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H⁺R[N_ω]-tg.tg.tg.(--0/-00/+00/-00/+00/--0) 2928

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 H 5.145650 -0.799379 -1.065815
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H⁺R[N_ω]-tg.g.g.tg.(+00/-00/+00/--0/-00/+0+) 54

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| H | -4.600893 | -2.762366 | -1.975762 |
| H | -4.313547 | -2.510952 | -0.242003 |
| H | -2.138858 | -3.063876 | -2.332723 |
| H | -2.870070 | -4.323252 | -1.321112 |
| H | -1.599494 | -4.702720 | 0.740021 |
| H | -2.852627 | -3.526851 | 1.205675 |
| H | 0.148086 | -3.081180 | 1.577225 |
| H | -0.960097 | -3.698952 | 2.820352 |

H⁺R[N_ω]-tcgg.gt(-00/+0+/-00/+0+/-00) 3983

| | | | |
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| C | 3.425014 | -2.382812 | -1.245903 |
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| C | 4.534170 | -0.097440 | -0.508163 |
| H | 5.449802 | 0.195208 | 0.030955 |
| C | 3.449787 | 0.785383 | 0.114109 |
| O | 3.130798 | 1.853827 | -0.372080 |
| O | 2.924925 | 0.302954 | 1.235291 |
| N | 4.594073 | 0.246300 | -1.936827 |
| C | 1.944540 | -1.997421 | -1.206532 |
| N | 1.758093 | -0.638003 | -1.719976 |
| C | 0.637031 | 0.077497 | -1.595535 |
| N | -0.469874 | -0.432176 | -1.077133 |
| N | 0.619631 | 1.358753 | -2.047406 |
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| H | 3.486976 | -3.442889 | -0.984105 |
| H | 5.364091 | -2.068982 | -0.410122 |
| H | 4.080602 | -1.790154 | 0.741458 |
| H | 4.745029 | 1.244502 | -2.048372 |
| H | 5.364333 | -0.234797 | -2.390972 |
| H | 1.367019 | -2.705659 | -1.810122 |
| H | 1.569542 | -2.052922 | -0.180466 |
| H | 2.586492 | -0.193853 | -2.126492 |
| H | -1.331820 | 0.107989 | -1.095937 |
| H | 1.529509 | 1.777689 | -2.186215 |
| H | -0.020297 | 1.971465 | -1.546240 |
| H | 2.166465 | 0.881235 | 1.517802 |
| H | -0.511009 | -1.320675 | -0.584922 |
| C | 0.605786 | 3.047934 | 1.552233 |
| C | -0.758557 | 3.540220 | 1.101170 |
| O | -1.152604 | 2.945144 | -0.133994 |
| C | -2.453742 | 3.365255 | -0.542874 |
| C | -2.880519 | 2.598422 | -1.784006 |
| O | -2.999269 | 1.191528 | -1.597499 |
| C | -4.142853 | 0.772089 | -0.852643 |
| C | -4.400979 | -0.697139 | -1.113169 |
| O | -3.259733 | -1.438154 | -0.710834 |
| C | -3.467560 | -2.836479 | -0.613452 |
| C | -2.107727 | -3.527792 | -0.551015 |
| O | -1.185680 | -2.933871 | 0.362540 |
| C | -1.565294 | -3.025229 | 1.735807 |
| C | -0.534333 | -2.345124 | 2.608840 |

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| O | -0.607463 | -0.939580 | 2.421412 |
| C | 0.180501 | -0.207991 | 3.344895 |
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| O | 0.674706 | 1.655494 | 1.886271 |
| H | 1.342656 | 3.186769 | 0.760257 |
| H | 0.911773 | 3.650773 | 2.418078 |
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| H | -1.525318 | 3.340945 | 1.860999 |
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| H | 0.473231 | -2.716147 | 2.373040 |
| H | -0.751902 | -2.601966 | 3.656092 |
| H | 1.239629 | -0.490309 | 3.266090 |
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| H | 0.428057 | 1.837307 | 3.939233 |
| H | -1.062430 | 1.498887 | 3.022570 |

H⁺R[N_ω]-tg.g.gg(+00/--0/--0/-00/+00/--0) 622

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| C | 4.973346 | 1.095665 | 0.538586 |
| C | 5.221523 | -0.131336 | -0.377881 |
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| C | 4.775417 | -1.439475 | 0.260615 |
| O | 3.959200 | -2.201416 | -0.204870 |
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| N | 4.554002 | 0.008434 | -1.678308 |
| C | 2.390052 | 1.591596 | 0.299106 |
| N | 1.969219 | 0.443914 | -0.499452 |
| C | 0.920369 | -0.353171 | -0.259290 |
| N | -0.136320 | 0.069273 | 0.439586 |
| N | 0.956903 | -1.608954 | -0.724255 |
| H | 3.354640 | 0.407523 | 1.823456 |
| H | 3.697938 | 2.119069 | 1.900066 |
| H | 5.215949 | 1.987094 | -0.051920 |
| H | 5.719670 | 1.050485 | 1.335012 |
| H | 4.704919 | -0.816827 | -2.251645 |
| H | 4.940185 | 0.800892 | -2.182375 |
| H | 2.632537 | 2.413718 | -0.381917 |
| H | 1.554890 | 1.927357 | 0.911729 |
| H | 2.694250 | 0.103885 | -1.139682 |

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| H | -0.878048 | -0.584766 | 0.665851 | H | 6.199930 | -0.741893 | -0.272714 |
| H | 1.852568 | -2.031599 | -0.923939 | C | 4.486173 | -1.288804 | 0.754801 |
| H | 0.099161 | -2.157190 | -0.786097 | O | 3.775690 | -2.256483 | 0.602352 |
| H | 5.127288 | -2.526649 | 1.763498 | O | 4.859592 | -0.841070 | 1.964859 |
| H | -0.389803 | 1.054694 | 0.451299 | N | 4.567995 | -0.967405 | -1.645014 |
| C | -0.836765 | 3.787830 | -0.534755 | C | 2.428250 | 1.440590 | -0.240722 |
| C | -1.677950 | 3.237432 | -1.672393 | N | 2.010561 | 0.088774 | -0.621927 |
| O | -1.060741 | 2.055455 | -2.155031 | C | 0.909162 | -0.530606 | -0.170764 |
| C | -1.728090 | 1.452148 | -3.259602 | N | -0.104636 | 0.153663 | 0.344151 |
| C | -2.825024 | 0.475603 | -2.865029 | N | 0.859740 | -1.870701 | -0.235485 |
| O | -2.235411 | -0.743410 | -2.435460 | H | 3.968895 | 2.836550 | -0.680190 |
| C | -3.184624 | -1.704422 | -2.012432 | H | 3.764526 | 1.619194 | -1.912282 |
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| O | -1.544220 | -2.998400 | -0.704205 | H | 5.145833 | 1.301474 | 0.820028 |
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| C | -2.877013 | -3.010574 | 1.379251 | H | 4.667920 | -1.974653 | -1.729523 |
| O | -2.312787 | -1.790030 | 1.838855 | H | 2.447869 | 1.523338 | 0.853131 |
| C | -3.153574 | -1.126120 | 2.779905 | H | 1.706686 | 2.176660 | -0.604915 |
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| C | -1.931025 | 3.324808 | 1.548132 | H | 1.728932 | -2.385664 | -0.222369 |
| O | -0.877604 | 2.979781 | 0.646188 | H | 4.488887 | -1.436139 | 2.635101 |
| H | -1.154909 | 4.810219 | -0.298229 | H | -0.237657 | 1.147534 | 0.171047 |
| H | 0.207992 | 3.820460 | -0.851138 | C | -1.538518 | 3.662090 | -0.921304 |
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| H | -2.283522 | -4.710154 | 0.213957 | C | -2.251532 | -0.432219 | 3.372953 |
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| H | -3.097903 | -3.670892 | 2.231123 | O | -1.639631 | 1.688175 | 2.437972 |
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| H | -3.352904 | -1.791971 | 3.631140 | C | -0.807455 | 3.647960 | 1.363395 |
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| H | -0.936421 | 2.259091 | 3.129327 | H | -1.232007 | 4.702243 | -1.095201 |
| H | -2.604232 | 2.758367 | 3.493186 | H | -1.932062 | 3.490529 | -3.008096 |
| H | -2.902726 | 3.296880 | 1.040866 | H | -0.399656 | 2.746372 | -2.504775 |
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| H ⁺ R[N _ω]-tg.g.gg.t(+00/-00/+0+/-00/-00/+0+) | 185 | | | | | | |
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H⁺R[N_ω]-tgtg.gt(-0/-00/+00/-00/+00/--0) 544

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H⁺R[N_ω]-ctgg.tg(-00/+00/--0/-00/+00/--0) 2183

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| H | 1.529722 | -0.693542 | -0.584953 | | | | |
| H | -0.441020 | 2.033895 | -1.418040 | | | | |
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| C | 0.194019 | -0.208469 | 3.341107 | | | | |
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| O | 0.705214 | 1.801293 | 2.126984 | | | | |
| C | 1.365320 | 3.053734 | 2.064109 | | | | |
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| O | 1.616792 | 2.995665 | -0.388116 | | | | |
| C | 2.960511 | 3.382643 | -0.701725 | | | | |
| C | 3.554415 | 2.417537 | -1.702644 | | | | |
| O | 3.756078 | 1.159558 | -1.075368 | | | | |
| H | 3.739915 | 0.058331 | -2.838219 | | | | |
| H | 5.348529 | 0.536547 | -2.245698 | | | | |
| H | 4.930954 | -0.963547 | -0.218830 | | | | |
| H | 5.180691 | -1.763085 | -1.790639 | | | | |
| H | 3.718108 | -3.033390 | 0.472008 | | | | |
| H | 3.988580 | -3.704086 | -1.148072 | | | | |
| H | 2.002230 | -4.761427 | -0.267230 | | | | |
| H | 1.537761 | -3.676495 | -1.590111 | | | | |
| H | 2.082398 | -3.319543 | 1.985733 | | | | |
| H | 0.672409 | -4.384709 | 1.775765 | | | | |
| H | 0.128795 | -2.815769 | 3.474387 | | | | |
| H | -0.802297 | -2.327061 | 2.043557 | | | | |
| H | 0.169762 | -0.600550 | 4.368669 | | | | |
| H | -0.842330 | -0.041328 | 3.014791 | | | | |
| H | 2.016861 | 0.917999 | 3.474732 | | | | |
| H | 0.592800 | 1.707800 | 4.193972 | | | | |
| H | 2.449053 | 2.922602 | 2.195709 | | | | |
| H | 1.010890 | 3.719627 | 2.866081 | | | | |
| H | 1.402345 | 4.740429 | 0.726074 | | | | |
| H | -0.027477 | 3.706901 | 0.575247 | | | | |
| H | 3.577914 | 3.386793 | 0.203371 | | | | |
| H | 2.958565 | 4.393714 | -1.128591 | | | | |
| H | 4.510453 | 2.828411 | -2.058058 | | | | |
| H | 2.888341 | 2.311925 | -2.570832 | | | | |
| | | | | H ⁺ R[N _ω]-cgggtg(+00/--0/--0/-00/+00/--+) 2783 | | | |
| | | | | C | 3.170725 | -1.395753 | -0.076393 |
| | | | | C | 4.699843 | -1.466971 | -0.201665 |
| | | | | C | 5.403834 | -0.319055 | -0.967252 |
| | | | | H | 5.124602 | -0.363295 | -2.024487 |
| | | | | C | 4.934203 | 1.058453 | -0.460157 |
| | | | | O | 3.837450 | 1.510827 | -0.713086 |
| | | | | O | 5.814378 | 1.703715 | 0.289989 |
| | | | | N | 6.859421 | -0.418519 | -0.783775 |
| | | | | C | 2.430239 | -1.378607 | -1.422669 |
| | | | | N | 0.982356 | -1.237463 | -1.293532 |
| | | | | C | 0.325544 | -0.080276 | -1.079409 |
| | | | | N | 0.966739 | 1.089881 | -1.082698 |
| | | | | N | -0.997789 | -0.120983 | -0.934331 |
| | | | | H | 2.834953 | -2.264336 | 0.498086 |
| | | | | H | 2.883719 | -0.515686 | 0.502294 |
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| | | | | H | 4.987135 | -2.401599 | -0.697556 |
| | | | | H | 7.376359 | -0.189207 | -1.625556 |
| | | | | H | 7.153669 | -1.337670 | -0.474347 |
| | | | | H | 2.609195 | -2.308753 | -1.967935 |
| | | | | H | 2.796174 | -0.572019 | -2.060391 |
| | | | | H | 0.422382 | -2.074141 | -1.235201 |
| | | | | H | 0.460595 | 1.893080 | -0.710090 |
| | | | | H | -1.460140 | -1.003976 | -0.741551 |
| | | | | H | -1.531625 | 0.724785 | -0.765214 |
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| | | | | H | 1.981331 | 1.145003 | -1.076776 |
| | | | | C | -0.940707 | -0.068023 | 3.188069 |
| | | | | C | -0.069429 | -1.300418 | 3.003319 |
| | | | | O | -0.326158 | -2.034710 | 1.808725 |
| | | | | C | -1.367236 | -2.994032 | 1.920494 |
| | | | | C | -1.483221 | -3.734966 | 0.600876 |
| | | | | O | -2.027283 | -2.928329 | -0.451535 |
| | | | | C | -3.436722 | -3.107632 | -0.635631 |
| | | | | C | -3.963975 | -2.097220 | -1.627075 |
| | | | | O | -3.948041 | -0.808295 | -1.031827 |
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| | | | | C | -1.683120 | 3.833480 | -0.521403 |
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| | | | | C | -0.615252 | 3.245744 | 1.595956 |
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H⁺R[N_ω]-tgggtg(-00/+00/-00/+0+/-0+/-00) 1518

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H⁺R[N_ω]-tcgg.gt(+0+/-0+/-00/-00/+0+/-0+) 1260

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| H | 3.440557 | -2.542705 | -2.282707 | H | -0.742436 | 2.717837 | 2.593152 |
| H | 4.062470 | -1.820886 | 0.641374 | H | 1.335732 | 3.252569 | 0.419295 |
| H | 5.205975 | -2.239157 | -0.612288 | H | 0.248739 | 4.523663 | 1.012411 |
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| H | 1.532981 | 1.682358 | -2.320589 | O | -5.193955 | 1.987882 | -0.228358 |
| H | 2.354607 | 0.930947 | 1.444821 | O | -6.167854 | 0.010790 | 0.216218 |
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| C | -2.819498 | 3.024084 | -1.008507 | N | -0.500786 | -1.235656 | -1.337008 |
| O | -3.061034 | 1.635857 | -0.800108 | C | -0.005435 | 0.006080 | -1.214585 |
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| C | 0.608100 | 0.635028 | 3.333870 | H | -0.037333 | -1.942607 | -0.769396 |
| O | 0.837971 | 1.443248 | 2.165924 | H | -0.234437 | 1.962842 | -1.664129 |
| C | 0.291913 | 2.766513 | 2.234431 | H | 1.486483 | 1.097341 | -0.323874 |
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| O | -0.613563 | 2.975868 | -0.066916 | H | -6.694998 | 0.563954 | 0.814170 |
| H | -2.337816 | 3.301662 | 1.059310 | H | -1.691235 | 1.016105 | -1.891258 |
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| H | -3.645678 | 0.963808 | -2.680196 | C | 4.280711 | -0.456579 | -1.845580 |
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| H | -1.332573 | -0.036812 | 2.660744 | C | 2.039943 | 3.673414 | 0.966852 |
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| H | 0.567576 | -1.830215 | 3.452197 | C | -0.248406 | -2.899311 | 2.297310 |
| H | -1.173718 | -2.094741 | 3.612656 | O | 0.259038 | -1.575672 | 2.174202 |
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| H | 0.370758 | 4.164209 | 2.200500 | H | -0.539786 | 2.609952 | 2.886556 |
| H | -0.082919 | 3.556921 | 0.595916 | H | 1.302917 | 3.279904 | 0.532950 |
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| H | 2.144886 | 4.729407 | 0.682895 | H | -2.052304 | 4.349545 | 0.896735 |
| H ⁺ R[N _ω]-tcgg.gt(+0+/+00/-00/+00/+0+/+0+) 3896 | | | | H | -2.298295 | 2.671728 | 1.444126 |
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| H | 4.351233 | 1.120162 | -2.602552 | H ⁺ R[N _ω]-tcgg.gt(--0/-00/+00/--0/-00/+00) 4080 | | | |
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 H 4.104456 2.923654 -1.382329
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H⁺R[N_ω]-tg.tggg.(-0/-00/+00/-00/+00/--0) 590

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H⁺R[N_ω]-tgtg.g.g(+00/-00/+00/-00/+0+/-0+) 2041

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H⁺R[N_ω]-cgggtg(+00/-00/+0+/-0+/-00/-00) 2529

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| C | 4.796861 | 0.994996 | -0.812912 | H | -5.303186 | -1.206372 | -0.782825 |
| O | 3.681118 | 1.471736 | -0.819043 | H | -5.411814 | 1.253264 | -2.425406 |
| O | 5.834455 | 1.622709 | -0.281211 | H | -5.285575 | 1.122347 | -0.653772 |
| N | 6.569247 | -0.522626 | -1.548633 | H | -3.201907 | 2.432958 | -2.479338 |
| C | 2.100909 | -1.500538 | -1.171261 | H | -4.468144 | 3.284063 | -1.563151 |
| N | 0.719389 | -1.256314 | -0.765134 | H | -1.806893 | 4.031464 | -0.889375 |
| C | 0.127462 | -0.041821 | -0.753491 | H | -3.259622 | 4.385462 | 0.073642 |
| N | 0.807474 | 1.062996 | -1.100239 | H | -1.377782 | 4.545076 | 1.548062 |
| N | -1.161352 | 0.034409 | -0.459519 | H | -2.275712 | 3.066336 | 1.972189 |
| H | 2.953087 | -0.502605 | 0.545701 | H | 0.255603 | 3.411377 | 2.786215 |
| H | 2.927968 | -2.249560 | 0.669851 | H | 1.368699 | 2.492874 | 1.760213 |
| H | 4.747550 | -2.466543 | -0.993440 | H | -1.079377 | 1.164522 | 2.993904 |
| H | 5.217430 | -1.541256 | 0.423404 | H | 0.441688 | 1.363887 | 3.890606 |
| H | 6.885081 | -0.299446 | -2.486209 | | | | |
| H | 6.908547 | -1.448733 | -1.315301 | | | | |
| H | 2.342806 | -0.788724 | -1.961272 | H ⁺ R[N _ω]-tgtg.tg.(+00/-00/+00/-00/+0+/-0+) 309 | | | |
| H | 2.135068 | -2.492495 | -1.631486 | C | 3.092109 | -1.314189 | -1.354828 |
| H | 0.268008 | -1.939626 | -0.165028 | C | 4.577035 | -1.121632 | -0.998214 |
| H | 1.823576 | 1.082112 | -1.040451 | C | 4.979732 | 0.362305 | -0.842789 |
| H | -1.733526 | -0.800466 | -0.365122 | H | 4.843666 | 0.848876 | -1.813215 |
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| H | 6.612925 | 1.043729 | -0.464865 | O | 6.885071 | 0.737322 | 0.607887 |
| H | 0.359384 | 1.939381 | -0.861445 | O | 7.252348 | 0.140790 | -1.532791 |
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| O | -0.828376 | -2.463330 | 1.547788 | N | 0.789409 | -1.201943 | -0.359721 |
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| O | -2.987628 | -2.322932 | -0.357427 | N | 1.106130 | 1.096862 | -0.109271 |
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| C | -4.651170 | -1.201326 | -1.667112 | H | 2.738879 | -0.449507 | -1.923951 |
| O | -3.906508 | 0.004145 | -1.722557 | H | 5.208926 | -1.551439 | -1.777506 |
| C | -4.705701 | 1.167888 | -1.586048 | H | 4.819932 | -1.662720 | -0.075060 |
| C | -3.822486 | 2.396479 | -1.574917 | H | 4.360423 | 2.063469 | 0.096955 |
| O | -2.993140 | 2.385737 | -0.410582 | H | 4.440563 | 0.789578 | 1.075368 |
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| C | -1.653834 | 3.539800 | 1.201935 | H | 2.561240 | -0.919975 | 0.723462 |
| O | -0.478513 | 2.770882 | 0.956005 | H | 0.095826 | -1.936658 | -0.234939 |
| C | 0.336563 | 2.550321 | 2.112125 | H | -1.626804 | -0.516917 | -0.747750 |
| C | 0.007431 | 1.278214 | 2.883754 | H | 0.709387 | 2.017696 | -0.216985 |
| O | 0.577624 | 0.156153 | 2.215653 | H | 2.124659 | 1.015865 | -0.013951 |
| H | 1.418573 | -1.643082 | 2.587475 | H | 8.177585 | 0.183418 | -1.243095 |
| H | 0.756005 | -0.848846 | 4.021465 | H | -1.417093 | 1.144881 | -0.300574 |
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| H | -0.624549 | -2.694740 | 3.599881 | C | -2.284013 | -3.571845 | -0.809101 |
| H | -2.747447 | -3.052966 | 2.079023 | O | -1.482052 | -2.978639 | 0.214869 |
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| H | -2.999610 | -2.359352 | -2.439235 | C | -1.417006 | -0.580136 | 3.514587 |
| | | | | C | -0.992273 | 0.872183 | 3.502594 |

| | | | | | | | |
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| O | -1.566947 | 1.535701 | 2.384838 | H | 4.740967 | 1.209454 | -1.551089 |
| C | -1.210140 | 2.903201 | 2.298564 | H | 4.204561 | -2.399222 | -0.664574 |
| C | -2.079438 | 3.585018 | 1.266115 | H | 4.261375 | -1.444823 | -1.957346 |
| O | -1.835174 | 3.045437 | -0.035491 | H | 2.429022 | 0.362832 | -2.015781 |
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| C | -2.787904 | 2.657973 | -2.224235 | H | 0.125726 | 1.754091 | -0.778933 |
| O | -3.406226 | 1.442160 | -1.834062 | H | -1.722784 | 0.433548 | -0.692801 |
| C | -3.603034 | 0.531708 | -2.906182 | H | 2.006203 | -1.304666 | -0.756507 |
| C | -4.135216 | -0.776838 | -2.364803 | H | 0.539562 | -2.241797 | -0.635937 |
| O | -3.083789 | -1.506686 | -1.727045 | H | 8.113109 | -0.350659 | -0.029987 |
| H | -4.184474 | -2.604258 | -0.351237 | H | -1.530980 | -1.201976 | -0.142894 |
| H | -4.056358 | -3.326063 | -1.965570 | C | -0.814522 | 0.479670 | 3.642048 |
| H | -2.603158 | -4.575272 | -0.499530 | C | -0.558080 | -0.988905 | 3.384754 |
| H | -1.628118 | -3.673336 | -1.676171 | O | -1.555507 | -1.505948 | 2.516354 |
| H | -2.898354 | -2.493713 | 1.669214 | C | -1.486318 | -2.909456 | 2.341949 |
| H | -2.276672 | -4.159180 | 1.719984 | C | -2.648275 | -3.358819 | 1.484554 |
| H | -1.237640 | -3.058906 | 3.543695 | O | -2.502268 | -2.849963 | 0.158174 |
| H | 0.002438 | -3.220916 | 2.293328 | C | -3.632778 | -3.134691 | -0.671789 |
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| H | -2.490023 | -0.642998 | 3.291488 | O | -3.780627 | -0.997911 | -1.737916 |
| H | -1.335329 | 1.348149 | 4.432760 | C | -3.559123 | -0.180664 | -2.874865 |
| H | 0.104277 | 0.933836 | 3.471193 | C | -3.818883 | 1.267565 | -2.520951 |
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| H | -3.729355 | 3.675126 | -0.598058 | C | -0.379149 | 3.406409 | 1.422900 |
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| H | -3.371009 | 3.156388 | -3.012088 | O | -0.468627 | 1.254613 | 2.500532 |
| H | -1.780740 | 2.465201 | -2.621417 | H | -0.213768 | 0.798240 | 4.506773 |
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| H ⁺ R[N _ω]-tgtg.tg.(+00/-00/+00/-00/+00/+0+) 9068 | | | | | | | |
| C | 3.073657 | 1.289811 | -0.151512 | H | -1.550462 | -3.425278 | 3.311489 |
| C | 4.535019 | 0.955512 | -0.503744 | H | -3.586007 | -2.992660 | 1.919911 |
| C | 4.897793 | -0.525387 | -0.253601 | H | -2.679224 | -4.456678 | 1.462761 |
| H | 4.793180 | -0.718679 | 0.818175 | H | -4.554838 | -2.845830 | -0.153193 |
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| O | 6.729857 | -1.355106 | -1.606475 | H | -4.272799 | -2.782352 | -2.679344 |
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| N | 4.004514 | -1.448946 | -0.970291 | H | -4.236067 | -0.462460 | -3.694796 |
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| C | 0.197244 | -0.247541 | -0.720016 | H | -4.840633 | 1.387821 | -2.139943 |
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| N | 0.983686 | -1.338250 | -0.667721 | H | -3.968309 | 3.462463 | -1.303664 |
| H | 2.728103 | 0.630188 | 0.649520 | H | -2.511212 | 4.460021 | 0.325053 |
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| | | | | H | -1.888481 | 2.724884 | 2.835323 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | -0.291634 | 3.058447 | 3.518767 | H | 1.099663 | -2.952053 | 3.481113 |
| | | | | H | 0.132782 | -2.996386 | 1.988439 |
| H ⁺ R[N _ω]-tg.tgg.t(-00/+0+/-0+/-+00/-00/+00) 7969 | | | | H | 0.672678 | -0.420697 | 3.511572 |
| C | -3.089440 | -2.176170 | -2.256542 | H | -0.670978 | -1.506991 | 3.935247 |
| C | -3.865996 | -1.604662 | -1.045714 | H | -1.850569 | 0.411508 | 3.543322 |
| C | -4.282097 | -0.121679 | -1.217829 | H | -2.561310 | 0.425895 | 1.928244 |
| H | -4.871715 | -0.045963 | -2.135006 | H | 0.053095 | 1.852252 | 2.611875 |
| C | -5.186010 | 0.277459 | -0.051813 | H | -1.556791 | 2.604166 | 2.706564 |
| O | -4.822301 | 0.922387 | 0.901830 | H | -1.251088 | 4.119820 | 1.073787 |
| O | -6.433459 | -0.203968 | -0.192326 | H | -0.990364 | 3.556181 | -0.589600 |
| N | -3.118522 | 0.767330 | -1.326117 | H | 1.203337 | 3.653801 | 1.550992 |
| C | -1.581048 | -2.349718 | -2.050499 | H | 0.898856 | 4.892260 | 0.317565 |
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| N | 1.223602 | -1.908524 | -1.637045 | H | 4.606496 | 2.836230 | -1.664772 |
| N | 0.759102 | 0.219327 | -0.870385 | H | 3.041199 | 2.439215 | -2.417037 |
| H | -3.258350 | -1.552235 | -3.139983 | H | 5.369884 | 0.735804 | -2.027882 |
| H | -3.485465 | -3.163986 | -2.504108 | H | 3.909827 | -0.144653 | -2.517890 |
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| H | -2.860740 | 1.127177 | -0.406863 | H ⁺ R[N _ω]-tg.tg.tg.(+00/-00/+00/-00/+0+/-0+) 6186 | | | |
| H | -1.159011 | -2.781396 | -2.966329 | C | 3.016017 | -1.065737 | -1.690653 |
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| C | 2.735403 | -2.968425 | 1.437564 | N | 0.779977 | -1.140313 | -0.573857 |
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| C | -1.616668 | 0.478753 | 2.472839 | H | 2.860920 | -1.843911 | -2.443443 |
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| O | -0.950833 | 2.083247 | 0.795512 | H | 4.989584 | -0.619585 | -2.401285 |
| C | -0.661446 | 3.440451 | 0.445285 | H | 4.287437 | 1.813077 | -1.419768 |
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| O | 1.533345 | 3.049419 | -0.405821 | H | 2.305181 | -2.477564 | -0.200696 |
| C | 2.910292 | 3.385440 | -0.487693 | H | 2.587771 | -0.876695 | 0.445263 |
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| O | 3.670035 | 1.149308 | -0.904835 | H | -1.684069 | -0.541020 | -0.723669 |
| C | 4.467902 | 0.235851 | -1.651041 | H | 2.054053 | 1.144662 | -0.325520 |
| C | 4.905072 | -0.891889 | -0.741124 | H | 0.583392 | 2.070473 | -0.337727 |
| O | 3.772531 | -1.641511 | -0.300503 | H | 8.049775 | -0.380735 | -0.118003 |
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| H | 4.481527 | -1.748843 | 1.639804 | C | -3.520464 | -2.835351 | -0.983082 |
| H | 2.995449 | -3.637580 | 2.271581 | C | -2.247329 | -3.618544 | -0.709613 |
| H | 2.218449 | -3.573425 | 0.677972 | O | -1.359649 | -2.998530 | 0.223803 |

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| C | -1.732500 | -3.140242 | 1.599744 | N | -1.032154 | -0.128813 | -0.882905 |
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| C | -1.024216 | -0.602584 | 3.517232 | H | 2.737907 | -2.379251 | 0.845341 |
| C | -0.663191 | 0.866110 | 3.467733 | H | 4.801892 | -2.788366 | -0.453260 |
| O | -1.383415 | 1.507026 | 2.423732 | H | 5.069851 | -1.738217 | 0.928465 |
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| O | -1.949292 | 3.005754 | 0.046363 | H | 2.330475 | -2.764245 | -1.552491 |
| C | -2.946488 | 3.508129 | -0.850964 | H | 2.640507 | -1.084926 | -1.934110 |
| C | -3.080323 | 2.597961 | -2.051816 | H | 0.217032 | -2.204831 | -0.694451 |
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| C | -3.862634 | 0.442308 | -2.681961 | H | 2.024789 | 0.850241 | -1.216989 |
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| O | -3.181070 | -1.579684 | -1.558008 | H | 6.685723 | 0.729355 | 0.021893 |
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| H | -4.131425 | -3.421924 | -1.683818 | C | -4.798451 | 0.233419 | -1.266479 |
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| H | -2.511584 | -4.625273 | -0.361560 | O | -3.174270 | 1.980419 | -0.888555 |
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| H | -3.750057 | 3.079262 | -2.779011 | H | -5.675520 | -0.001646 | -1.886355 |
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| . | | | | H | -2.134181 | 3.246858 | -2.173330 |
| H ⁺ R[N _ω]-cgggtg(+00/-00/+0+/-+0+/-+00/-+/-) 5919 | | | | H | -2.323487 | 3.695591 | 0.843443 |
| C | 3.076789 | -1.616347 | 0.137296 | H | -1.550498 | 4.831971 | -0.288660 |
| C | 4.590504 | -1.788834 | -0.055461 | H | 0.165319 | 4.362803 | 1.321536 |
| C | 5.306395 | -0.776681 | -0.984167 | H | 1.278970 | 3.108965 | 0.754867 |
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| C | 4.948050 | 0.674127 | -0.607503 | H | 0.452574 | 2.887359 | 3.151678 |
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H⁺R[N_ω]-tgtg(+00/-00/+00/-00/+0+/-0+) 1349

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H⁺R[N_ω]-tgtg.tg(--0/-00/+00/-00/+00/--0) 2384

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| H | 0.055162 | 3.325314 | 3.068195 |
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| H | 2.628756 | 2.500092 | 1.914861 |
| H | 1.940610 | 4.141669 | 1.979339 |
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| H | 2.013179 | 4.267253 | -0.507570 |
| H | 4.771027 | 2.431360 | -1.174665 |
| H | 3.693427 | 3.238827 | -2.342812 |
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H⁺R[N ω]-tgggtg(-00/+00/-00/+00/--0/-00) 12333

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| H | 5.720729 | 0.367289 | -2.064968 |
| C | 4.868590 | 0.835413 | -0.205068 |
| O | 4.309411 | 1.821023 | 0.208920 |
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| N | 3.722466 | 1.095489 | -2.328053 |
| C | 1.806164 | -1.551655 | -1.954759 |
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| H | 3.828586 | 0.966589 | -3.330565 |
| H | 3.895466 | 2.079239 | -2.134380 |
| H | 1.718849 | -2.535605 | -2.420654 |
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| H | 5.828111 | 0.538802 | 1.393334 |
| H | 1.809964 | 1.004393 | -1.741005 |
| C | -4.230638 | -0.287492 | -1.968910 |
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| O | -3.122184 | -1.912279 | -0.577252 |
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| O | -0.773123 | -2.976170 | 0.712784 |
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| O | 0.544847 | -0.813506 | 2.260871 |
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| O | -0.505180 | 1.951951 | 2.045450 |

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| O | -4.063468 | 0.745914 | -1.012445 |
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| H | -3.121337 | 2.025271 | -2.350865 |
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H⁺R[N ω]-cgggtg(+00/+00/--0/-00/+00/+0+) 2865

| | | | |
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| C | 3.193847 | -1.281654 | 0.181387 |
| C | 4.699793 | -1.415748 | -0.087942 |
| C | 5.344913 | -0.359949 | -1.020207 |
| H | 4.944213 | -0.475573 | -2.031911 |
| C | 4.980029 | 1.069935 | -0.575417 |
| O | 3.872295 | 1.543770 | -0.726772 |
| O | 5.962836 | 1.738036 | 0.005103 |
| N | 6.808488 | -0.499802 | -0.996202 |
| C | 2.314501 | -1.411155 | -1.073236 |
| N | 0.904821 | -1.124101 | -0.829935 |
| C | 0.324328 | 0.076136 | -0.987625 |
| N | -0.995779 | 0.182428 | -0.915081 |
| N | 1.053915 | 1.167645 | -1.274544 |
| H | 2.906948 | -2.061881 | 0.893288 |
| H | 2.987404 | -0.327584 | 0.669899 |
| H | 4.912244 | -2.398193 | -0.525451 |
| H | 5.226223 | -1.382344 | 0.872337 |
| H | 7.111266 | -1.397348 | -0.635834 |
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| H | 2.660051 | -0.745206 | -1.865068 |

| | | | | | | | |
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| H | 2.378307 | -2.428319 | -1.470548 | C | -4.554004 | -1.369413 | -1.228875 |
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| H | -1.592630 | -0.628732 | -0.792143 | H | -4.653594 | -0.313262 | 0.661862 |
| H | 2.057047 | 1.222442 | -1.110502 | C | -6.376090 | 0.185231 | -0.464685 |
| H | 0.559318 | 2.030893 | -1.441032 | O | -6.860907 | 1.146406 | -1.003168 |
| H | 6.751688 | 1.145940 | -0.055029 | O | -7.098032 | -0.776592 | 0.146174 |
| H | -1.420810 | 1.092239 | -0.756030 | N | -4.060494 | 1.040433 | -0.803157 |
| C | -1.634484 | -2.999554 | 1.617007 | C | -2.219811 | -1.687559 | -0.176517 |
| C | -0.730304 | -2.293525 | 2.605414 | N | -0.793834 | -1.451451 | -0.389541 |
| O | -0.546264 | -0.946312 | 2.201901 | C | -0.228133 | -0.230082 | -0.478379 |
| C | -0.256546 | -0.055654 | 3.270915 | N | 1.094899 | -0.147036 | -0.553236 |
| C | 0.140566 | 1.298250 | 2.723838 | N | -0.977258 | 0.874891 | -0.525584 |
| O | -0.947107 | 1.885620 | 2.029405 | H | -2.660403 | -0.786382 | -2.082490 |
| C | -0.669103 | 3.196314 | 1.565692 | H | -2.924151 | -2.513700 | -2.048799 |
| C | -1.818695 | 3.679123 | 0.710842 | H | -5.009165 | -2.230755 | -0.733523 |
| O | -1.820658 | 2.992484 | -0.547132 | H | -5.043030 | -1.284583 | -2.205467 |
| C | -2.978818 | 3.253486 | -1.350790 | H | -4.288334 | 1.284424 | -1.765852 |
| C | -4.160840 | 2.368254 | -0.993045 | H | -4.336910 | 1.856343 | -0.261523 |
| O | -3.846808 | 1.027846 | -1.345273 | H | -2.566061 | -0.963957 | 0.563896 |
| C | -4.792718 | 0.084579 | -0.867490 | H | -2.322560 | -2.673270 | 0.282085 |
| C | -4.504278 | -1.289186 | -1.434284 | H | -0.171787 | -2.238033 | -0.505598 |
| O | -3.253387 | -1.796232 | -0.956582 | H | 1.558766 | 0.739276 | -0.728041 |
| C | -3.204096 | -3.216060 | -0.896100 | H | -0.513713 | 1.749657 | -0.292658 |
| C | -1.765066 | -3.680496 | -0.697407 | H | -1.998813 | 0.857210 | -0.587903 |
| O | -1.040040 | -2.984805 | 0.316448 | H | -8.038080 | -0.553095 | 0.057356 |
| H | -2.600698 | -2.486445 | 1.587373 | H | 1.675809 | -0.932780 | -0.274085 |
| H | -1.787400 | -4.036644 | 1.945985 | C | 1.658990 | -2.916875 | 2.150665 |
| H | 0.240402 | -2.804383 | 2.680564 | C | 2.708529 | -3.344126 | 1.149302 |
| H | -1.215452 | -2.346749 | 3.589762 | O | 2.447981 | -2.759546 | -0.129094 |
| H | 0.579270 | -0.435013 | 3.877222 | C | 3.490975 | -3.025353 | -1.074639 |
| H | -1.134340 | 0.045218 | 3.923530 | C | 3.435735 | -2.033313 | -2.215219 |
| H | 1.004179 | 1.192428 | 2.052101 | O | 3.764519 | -0.745719 | -1.718574 |
| H | 0.446370 | 1.933682 | 3.568686 | C | 3.847336 | 0.251297 | -2.726848 |
| H | -0.548441 | 3.887438 | 2.413127 | C | 4.055234 | 1.603602 | -2.081301 |
| H | 0.264811 | 3.214257 | 0.986042 | O | 2.831400 | 2.060818 | -1.499914 |
| H | -2.759271 | 3.507655 | 1.245764 | C | 2.948447 | 3.327317 | -0.862416 |
| H | -1.710689 | 4.756761 | 0.532267 | C | 1.560453 | 3.850850 | -0.531745 |
| H | -3.265248 | 4.308510 | -1.266975 | O | 0.820059 | 3.034048 | 0.377151 |
| H | -2.682850 | 3.061000 | -2.383983 | C | 1.194193 | 3.167313 | 1.752624 |
| H | -4.389893 | 2.436430 | 0.079431 | C | 0.163477 | 2.475202 | 2.632239 |
| H | -5.046777 | 2.712130 | -1.546900 | O | 0.205175 | 1.056145 | 2.576648 |
| H | -4.772077 | 0.051137 | 0.231027 | C | 1.073492 | 0.459088 | 3.534650 |
| H | -5.808329 | 0.368574 | -1.181058 | C | 0.978747 | -1.048482 | 3.445403 |
| H | -5.318285 | -1.954373 | -1.119442 | O | 1.728420 | -1.514643 | 2.331360 |
| H | -4.489206 | -1.255385 | -2.530140 | H | 1.860166 | -3.444061 | 3.094914 |
| H | -3.566351 | -3.664524 | -1.831326 | H | 0.653605 | -3.212698 | 1.814382 |
| H | -3.857164 | -3.571902 | -0.088002 | H | 2.705483 | -4.439777 | 1.069864 |
| H | -1.193705 | -3.518150 | -1.613613 | H | 3.696811 | -3.023965 | 1.500572 |
| H | -1.775464 | -4.758871 | -0.487203 | H | 3.386143 | -4.045112 | -1.467308 |
| | | | | H | 4.464358 | -2.942992 | -0.577695 |
| | | | | H | 2.436687 | -2.023855 | -2.674605 |
| | | | | H | 4.156344 | -2.349727 | -2.983150 |
| H ⁺ R[N _ω]-tgtgtg(+00/-00/+00/-00/+0/+0+) 6963 | | | | | | | |
| C | -3.054101 | -1.597101 | -1.465557 | | | | |

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| H | 2.930686 | 0.267899 | -3.332472 |
| H | 4.694693 | 0.043379 | -3.395648 |
| H | 4.382766 | 2.319568 | -2.846644 |
| H | 4.837095 | 1.532069 | -1.314584 |
| H | 3.428598 | 4.049490 | -1.537838 |
| H | 3.577797 | 3.242730 | 0.033881 |
| H | 0.964996 | 3.890634 | -1.446280 |
| H | 1.646995 | 4.870320 | -0.134106 |
| H | 1.222579 | 4.233565 | 2.016002 |
| H | 2.192049 | 2.746068 | 1.922374 |
| H | -0.836771 | 2.773565 | 2.307192 |
| H | 0.296247 | 2.822694 | 3.665636 |
| H | 0.775865 | 0.771200 | 4.545839 |
| H | 2.116065 | 0.763301 | 3.374454 |
| H | -0.075729 | -1.344777 | 3.357653 |
| H | 1.380269 | -1.485181 | 4.371357 |

H⁺R[N_ω]-cg.g.g.tg.(-00/+0+/-00/--0/--0/-00) 5800

| | | | |
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| C | -4.486173 | -1.772331 | -0.491969 |
| C | -5.151167 | -0.610854 | -1.271808 |
| H | -4.768765 | -0.594251 | -2.297091 |
| C | -4.781215 | 0.750609 | -0.653747 |
| O | -3.685299 | 1.254960 | -0.783957 |
| O | -5.745547 | 1.319915 | 0.053072 |
| N | -6.613175 | -0.761857 | -1.234955 |
| C | -2.117740 | -1.636403 | -1.508208 |
| N | -0.698717 | -1.406497 | -1.247549 |
| C | -0.124957 | -0.198058 | -1.074455 |
| N | 1.173763 | -0.131420 | -0.811742 |
| N | -0.829322 | 0.928869 | -1.241424 |
| H | -2.751275 | -0.789183 | 0.371403 |
| H | -2.678938 | -2.538762 | 0.363267 |
| H | -4.994690 | -1.861508 | 0.474305 |
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| H | -6.904238 | -1.707798 | -1.016416 |
| H | -7.055815 | -0.490557 | -2.106246 |
| H | -2.462012 | -0.863947 | -2.197862 |
| H | -2.195376 | -2.584339 | -2.046768 |
| H | -0.121059 | -2.203365 | -1.028257 |
| H | 1.623163 | 0.767470 | -0.653155 |
| H | -1.845569 | 0.913426 | -1.208878 |
| H | -0.408708 | 1.766732 | -0.847154 |
| H | -6.532986 | 0.734679 | -0.059819 |
| H | 1.726482 | -0.966111 | -0.631404 |
| C | 4.311821 | -2.274138 | -0.823630 |
| C | 4.415247 | -1.189615 | -1.871615 |
| O | 4.161738 | 0.069230 | -1.265780 |
| C | 4.050324 | 1.132172 | -2.199243 |
| C | 3.865173 | 2.438160 | -1.458589 |
| O | 2.665885 | 2.394352 | -0.685114 |
| C | 2.312893 | 3.647914 | -0.103402 |

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| C | 1.442922 | 3.425581 | 1.113388 |
| O | 0.218643 | 2.807438 | 0.730297 |
| C | -0.735706 | 2.670771 | 1.788474 |
| C | -0.452044 | 1.540864 | 2.766212 |
| O | -0.663097 | 0.286856 | 2.130057 |
| C | -0.501262 | -0.836028 | 2.990806 |
| C | 0.917138 | -1.380121 | 3.065679 |
| O | 1.229032 | -2.084246 | 1.869698 |
| C | 2.501422 | -2.714414 | 1.912548 |
| C | 2.740812 | -3.418088 | 0.590104 |
| O | 2.935737 | -2.503964 | -0.494850 |
| H | 4.874278 | -1.971638 | 0.067664 |
| H | 4.748766 | -3.200778 | -1.216677 |
| H | 5.425183 | -1.207955 | -2.305530 |
| H | 3.694976 | -1.383939 | -2.678616 |
| H | 3.201095 | 0.955138 | -2.874070 |
| H | 4.960633 | 1.209902 | -2.811374 |
| H | 3.813408 | 3.250796 | -2.195432 |
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| H | 1.793867 | 4.269735 | -0.843869 |
| H | 3.215846 | 4.180274 | 0.222003 |
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| H | 1.239293 | 4.398860 | 1.581354 |
| H | -0.799901 | 3.614224 | 2.346088 |
| H | -1.698275 | 2.496047 | 1.304309 |
| H | 0.568498 | 1.613605 | 3.165865 |
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| H | 0.982344 | -2.062849 | 3.926303 |
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| H | 3.291043 | -1.973374 | 2.102516 |
| H | 1.867852 | -4.028186 | 0.342523 |
| H | 3.602737 | -4.088272 | 0.678287 |

H⁺R[N_α]-g.g.g.gt(-00/+00/-00/+00/-00/+00) 116BB

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| C | -1.419350 | 0.797789 | -1.200919 |
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| H | -1.546008 | -1.576349 | 0.200082 | H | 0.377223 | 4.730116 | 1.077619 |
| H | 1.353276 | -0.673630 | 0.131435 | | | | |
| H | 0.181599 | 0.190546 | 0.953643 | H ⁺ R[N _a]-gggg.t(-00/+00/-00/+00/-00/+00) 160 | | | |
| H | -3.700915 | -2.640233 | -0.671941 | C | -1.828346 | -2.002593 | -0.451616 |
| H | -3.979587 | -2.599666 | -2.417214 | C | -1.065816 | -1.117163 | -1.474359 |
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| H | -5.303554 | 1.491091 | 0.381570 | H | -0.091830 | 0.766207 | -1.838987 |
| H | -6.226589 | -0.709268 | 0.778835 | C | -1.626236 | 1.085554 | -0.353507 |
| H | -6.031089 | -1.820293 | -0.520901 | O | -2.273648 | 1.806758 | -1.143014 |
| H | 1.111200 | 0.944878 | -0.200435 | O | -1.874269 | 0.855112 | 0.859683 |
| H | -3.626738 | 1.439674 | -0.194855 | N | 0.632933 | 0.060752 | -0.017913 |
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| C | 0.016219 | 1.585226 | 3.569414 | N | -3.929146 | -0.675614 | -0.211669 |
| O | 0.023672 | 0.285824 | 2.970951 | C | -4.914891 | -0.062859 | -0.866167 |
| C | 0.486371 | -0.715162 | 3.870761 | N | -4.930659 | 1.268615 | -0.903299 |
| C | 0.528875 | -2.061126 | 3.185065 | N | -5.869832 | -0.788533 | -1.488089 |
| O | 1.521988 | -2.038363 | 2.168755 | H | -1.534574 | -1.759704 | 0.572764 |
| C | 1.799729 | -3.311246 | 1.606054 | H | -1.539202 | -3.045559 | -0.611768 |
| C | 2.939090 | -3.167625 | 0.623732 | H | -1.715191 | -0.885021 | -2.323852 |
| O | 2.544206 | -2.318571 | -0.453443 | H | -0.228378 | -1.685886 | -1.887554 |
| C | 3.597741 | -2.129282 | -1.399678 | H | 0.363960 | -0.410513 | 0.857306 |
| C | 3.179460 | -1.131431 | -2.455259 | H | 1.001160 | 0.992296 | 0.245192 |
| O | 3.013111 | 0.137366 | -1.842966 | H | -3.758673 | -2.749090 | 0.147178 |
| C | 2.783741 | 1.203739 | -2.756681 | H | -3.683745 | -2.262915 | -1.550708 |
| C | 2.795306 | 2.507327 | -1.991972 | H | -3.348066 | -0.076126 | 0.392770 |
| O | 1.706292 | 2.540439 | -1.071985 | H | -4.004881 | 1.747573 | -0.868815 |
| C | 1.646221 | 3.766711 | -0.337210 | H | -6.062269 | -1.734222 | -1.200616 |
| C | 0.472089 | 3.737974 | 0.612346 | H | -6.535387 | -0.343350 | -2.098584 |
| O | 0.712492 | 2.748397 | 1.605778 | H | 1.399633 | -0.471378 | -0.452610 |
| H | -0.504815 | 3.587125 | 3.064508 | H | -5.743793 | 1.762757 | -1.234906 |
| H | -1.275837 | 2.354176 | 2.025837 | C | 1.415507 | -3.426131 | 1.351264 |
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| H | 1.007987 | 1.804328 | 3.984832 | O | 0.599697 | -1.503550 | 2.565436 |
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| H | -0.453653 | -2.306295 | 2.756487 | O | 0.789326 | 1.377163 | 2.809787 |
| H | 0.771184 | -2.824951 | 3.937262 | C | 0.293927 | 2.695927 | 2.607758 |
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| H | 2.099109 | -4.022251 | 2.388987 | O | 1.276507 | 2.880556 | 0.416735 |
| H | 3.211740 | -4.160726 | 0.241141 | C | 2.159589 | 3.565619 | -0.468008 |
| H | 3.813034 | -2.740135 | 1.131426 | C | 2.095085 | 2.940909 | -1.842835 |
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| H | 4.495158 | -1.762292 | -0.885893 | C | 2.715435 | 0.952501 | -3.010251 |
| H | 2.248726 | -1.454149 | -2.944120 | C | 3.410837 | -0.371634 | -2.793632 |
| H | 3.964812 | -1.089074 | -3.223138 | O | 2.586194 | -1.242909 | -2.017688 |
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| H | 3.578286 | 1.235495 | -3.515089 | C | 2.358834 | -3.323271 | -0.833571 |
| H | 2.706073 | 3.337982 | -2.704856 | O | 2.111882 | -2.645138 | 0.388909 |
| H | 3.744300 | 2.613608 | -1.450672 | H | 0.394771 | -3.641385 | 1.006191 |
| H | 1.524550 | 4.606180 | -1.034161 | H | 1.930033 | -4.384999 | 1.505652 |
| H | 2.580190 | 3.907555 | 0.221626 | H | 2.408663 | -2.430708 | 2.969411 |

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| H | 0.959755 | -3.353546 | 3.434260 | O | -2.244448 | -2.449316 | -0.881483 |
| H | 1.588194 | -0.648971 | 4.176340 | H | -3.160577 | -4.214350 | -0.274343 |
| H | -0.008081 | -1.349275 | 4.544327 | H | -4.022502 | -2.714516 | 0.150363 |
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| H | -0.697733 | 2.658873 | 2.142961 | C | -2.862928 | -2.402426 | -2.168014 |
| H | 2.273852 | 3.408847 | 2.158715 | C | -1.731338 | -1.712367 | 3.187171 |
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| H | 3.186567 | 3.516183 | -0.083373 | H | -2.902071 | -3.411768 | -2.600113 |
| H | 1.866692 | 4.621439 | -0.543395 | H | -3.889318 | -2.026564 | -2.071666 |
| H | 2.720729 | 3.531399 | -2.526557 | C | -1.944546 | -0.300943 | 3.683265 |
| H | 1.063885 | 2.956520 | -2.221728 | H | -0.661388 | -1.964917 | 3.190154 |
| H | 3.326846 | 1.556867 | -3.695227 | H | -2.244710 | -2.400174 | 3.873472 |
| H | 1.733809 | 0.800289 | -3.482159 | O | -2.170757 | -0.166080 | -2.605105 |
| H | 4.361903 | -0.202840 | -2.273161 | H | -1.034333 | -1.819233 | -3.157704 |
| H | 3.624176 | -0.831157 | -3.768342 | H | -2.520043 | -1.567114 | -4.098037 |
| H | 4.183647 | -2.242706 | -1.154539 | O | -1.180492 | 0.619950 | 2.913964 |
| H | 3.505611 | -3.009478 | -2.612579 | H | -1.642465 | -0.250130 | 4.739214 |
| H | 2.867902 | -4.279501 | -0.648279 | H | -3.010918 | -0.048062 | 3.618711 |
| H | 1.414607 | -3.539269 | -1.354306 | C | -1.632299 | 0.817432 | -3.481183 |
| | | | | C | -1.385286 | 1.971595 | 3.339195 |
| | | | | C | -1.953422 | 2.186096 | -2.925898 |
| H ⁺ R[N _a]-ggg.g.t(-00/+00/-00/+00/-00/+00) GS | | | | H | -0.545310 | 0.692251 | -3.583132 |
| N | -0.644214 | 0.070206 | 0.013898 | H | -2.083071 | 0.728281 | -4.479440 |
| H | -1.344862 | -0.678292 | -0.071778 | C | -0.689119 | 2.927155 | 2.400402 |
| C | 0.676889 | -0.364677 | -0.554481 | H | -0.983668 | 2.102200 | 4.353299 |
| H | -0.993868 | 0.896994 | -0.502316 | H | -2.460686 | 2.189212 | 3.359853 |
| H | 0.494105 | -0.604131 | -1.601639 | O | -1.284925 | 2.372056 | -1.681663 |
| C | 1.161752 | -1.625133 | 0.198521 | H | -1.623205 | 2.948297 | -3.644605 |
| C | 1.673523 | 0.822634 | -0.460055 | H | -3.037762 | 2.285727 | -2.786798 |
| H | 1.506994 | -1.330872 | 1.195921 | O | -1.354905 | 2.898406 | 1.142543 |
| H | 0.281856 | -2.255240 | 0.345405 | H | 0.362919 | 2.649857 | 2.273663 |
| C | 2.225911 | -2.505100 | -0.506632 | H | -0.742250 | 3.936251 | 2.835182 |
| O | 2.519051 | 0.889253 | -1.407361 | C | -1.538116 | 3.659898 | -1.109570 |
| O | 1.592145 | 1.542991 | 0.540235 | C | -0.792858 | 3.799352 | 0.196350 |
| H | 2.006640 | -3.549732 | -0.269633 | H | -1.197847 | 4.440378 | -1.802719 |
| H | 2.127233 | -2.423374 | -1.594383 | H | -2.616159 | 3.783071 | -0.945039 |
| C | 3.699010 | -2.292879 | -0.123082 | H | 0.272404 | 3.583996 | 0.056684 |
| H | -0.577271 | 0.342741 | 1.006726 | H | -0.900875 | 4.836460 | 0.547227 |
| H | 3.810867 | -2.325457 | 0.966344 | | | | |
| H | 4.288770 | -3.113908 | -0.545273 | | | | |
| N | 4.190096 | -1.009805 | -0.629629 | | | | |
| H | 3.532144 | -0.467409 | -1.217525 | | | | |
| C | 5.109279 | -0.237078 | -0.057043 | | | | |
| N | 5.092561 | 1.068536 | -0.331119 | | | | |
| N | 6.024896 | -0.758944 | 0.786043 | | | | |
| H | 4.229277 | 1.442497 | -0.752740 | | | | |
| H | 5.823704 | 1.685613 | -0.019374 | | | | |
| H | 6.213308 | -1.747833 | 0.781828 | | | | |
| H | 6.695279 | -0.165554 | 1.246764 | | | | |
| C | -3.030902 | -3.176344 | 0.061640 | | | | |
| C | -2.347777 | -3.174003 | 1.409642 | | | | |