Supporting Information (53 pages)

Computational Investigation of the Thermochemistry of the CO_2 Capture Reaction by Ethylamine, Propylamine, and Butylamine in Aqueous Solution Considering the Full Conformational Space via Boltzmann Statistics

Joseph Schell,[§,†] Kaidi Yang,[†] and Rainer Glaser*[,§]

[§]Department of Chemistry, Missouri University of Science & Technology, Rolla, MO 65409

[†]Department of Chemistry, University of Missouri, Columbia, MO 65211

Email: GlaserR@umsystem.edu

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Theoretical Level Dependency

To ensure the accurate description of the structure at the carbamate N (planarity *vs.* pyramidalization), we collected in Table S1 the results of prior computational work as well as of some additional computations by us. We use the improper dihedral angle $\gamma = \angle(O_2C{-}N{-}C\cdots H)$ to characterize the N pyramidalization (Scheme S1). When $\gamma = \pm 180°$, the N atom is in the same plane with the two carbon atoms and the hydrogen atom. When $\gamma \neq \pm 180°$, then the smaller the $|\gamma|$ is, the more pronounced is the N pyramidalization.

Planar N occur in carbanions derived from alkylcarbamates such as compound **12** in Figure 2 reported in Ref. 1, and these carbanions of carbamate esters are very different from the carbamic acids and their corresponding carbamates in our paper. Calculated carbamates reported in the literature[2,3] are included in Table S1 and shown in Figure S1, and they all feature pyramidal N, just like all the carbamates and carbamic acid species calculated in our paper.

We also carried out additional calculations at the MP2 and B3LYP levels and all of these theoretical levels produced structures with pyramidal nitrogen (Table S1). We also optimized some structures beginning with initial trial structure with planar nitrogen, and all of these optimizations resulted in pyramidal N regardless of the various computational levels.

Thus, we are confident to say that the computational level we use in our current paper is treating the nitrogen lone pair correctly.

Scheme S1. Carbamate Structure and Definition of γ Dihedral.

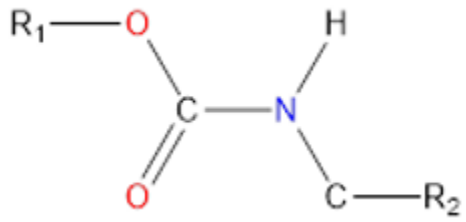


Table S1. Improper Dihedral Angle of Carbamates Computed with Various Theoretical Models

Compound	Theoretical Level	$\gamma = \angle(O_2C{-}N{-}C{-}H)$
	Calculation from Literature	
Compound **12** in Ref. 1	B3LYP/6-311+G*	-179.98
Compound "ES_C1" in Ref. 2	MP2/6-311+G**	173.76
Gly-carbamate, Ref. 3	CBS-QB3	137.67
β-ala carbamate, Ref. 3	CBS-QB3	-132.26
6-AHA carbamate, Ref. 3	CBS-QB3	131.40
	Calculation in Current Paper	
Ethylcarbamic acid	SMD(APFD/6-311G*)	161.11
Ethylcarbamate	SMD(APFD/6-311G*)	144.19
Butylcarbamic acid	SMD(APFD/6-311G*)	-160.94
Butylcarbamate	SMD(APFD/6-311G*)	-143.36
	Additional Calculations	
Ethylcarbamic acid	SMD(MP2/6-311+G*)	153.50
Ethylcarbamate	SMD(MP2/6-311+G*)	136.95
Butylcarbamic acid	SMD(MP2/6-311+G*)	-150.13
Butylcarbamate	SMD(MP2/6-311+G*)	-136.85
Ethylcarbamic acid	SMD(B3LYP/6-311+G*)	167.02
Ethylcarbamate	SMD(B3LYP/6-311+G*)	147.45
Ethylcarbamate, trial structure with planar N	MP2/6-311+G*	134.04
	B3LYP/6-311+G*	142.07
	APFD/6-311+G*	139.90

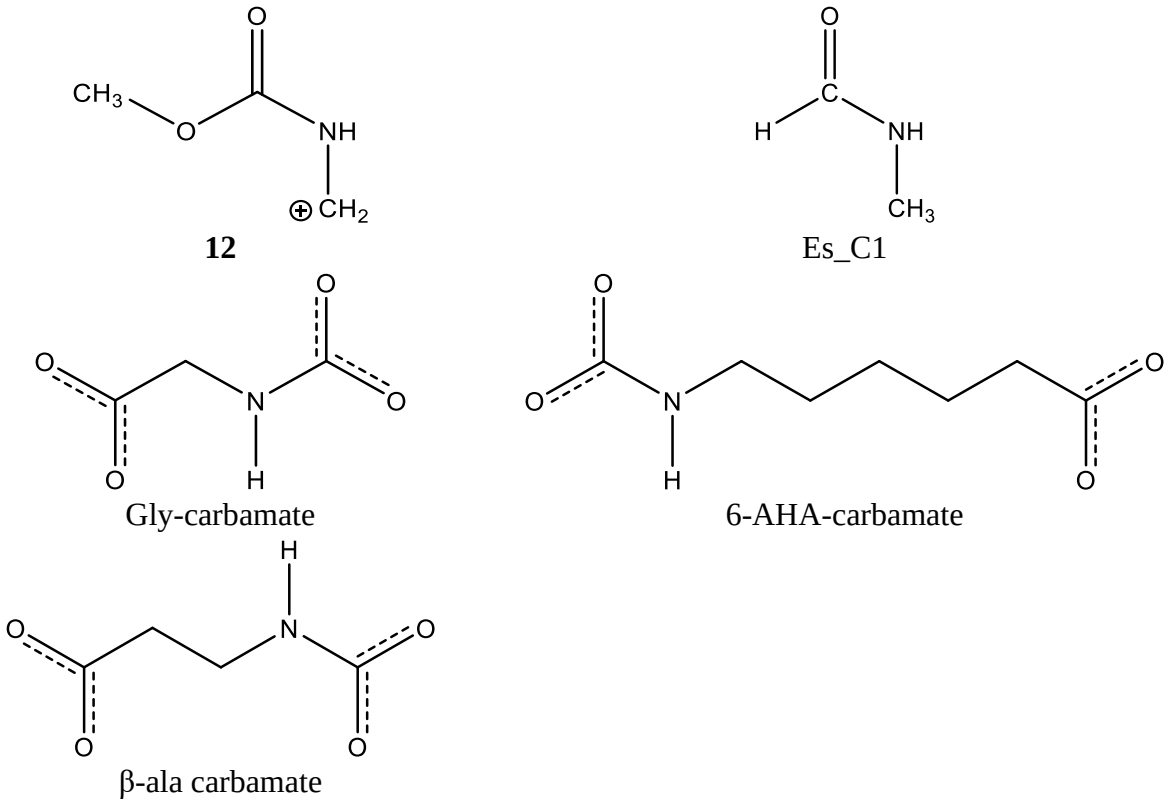


Figure S1. Calculated structure of carbamates.

References

(1) Wiberg, K. B. Dipole-Stabilized Carbanions: A Computational Study of N-Methylformamide Anion and Methyl N-Methylcarbamate Anion. *J. Org. Chem.* **2002**, *67*, 5365-5368.

(2) Wiberg, K. B.; Rush, D. J. Methyl Rotational Barriers in Amides and Thioamides. *J. Org. Chem.* **2002,** *67*, 826-830.

(3) Gupta, M.; Svendsen, H. F. Understanding Carbamate Formation Reaction Thermochemistry of Amino Acids as Solvents for Postcombustion CO_2 Capture. *J. Phys. Chem. B* **2019**, *123*, 8433-8447.

Table S2. Thermodynamic Properties and Relative Energies[a] of All Conformers of Alkyl Carbamic Acids

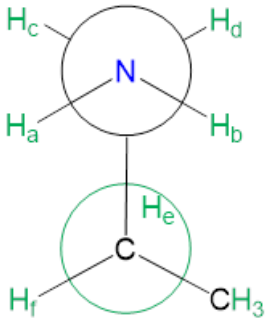
Species[b,c]	Energy	*VZPE*	*TE*	*S*	ΔE_{rel}	ΔG_{rel}	P_i[d]
CO_2	-188.486130	7.31	8.96	51.08		0.00	100.0
Methylcarbamic acid							
Me-2	-284.307332	50.08	53.73	75.54	0.00	0.00	64.8
Me-3	-284.305785	49.93	53.61	77.19	0.97	0.36	35.2
Ethylcarbamic acid							
Et-2t (2)	-323.599603	68.11	72.38	81.16	0.00	0.00	44.4
Et-2c (UBM)	-323.598561	68.12	72.43	81.13	0.65	0.71	-
Et-2c (TS) C_s	-323.598489	67.77	71.69	78.32	0.73	0.88	-
Et-2h	DNE						
Et-3t (2)	-323.597835	68.11	72.33	80.63	1.11	1.22	5.6
Et-3c (UBM) C_s	-323.596871	67.96	72.33	82.93	1.72	1.14	-
Et-3h	DNE						
Propylcarbamic acid							
Pr-2tg (2)	-362.888855	86.15	91.19	88.67	0.00	0.00	15.0
Pr-2tt (2)	-362.888645	86.13	91.21	88.48	0.13	0.21	10.5
Pr-2tq (2)	-362.889310	86.27	91.23	87.17	-0.29	0.20	10.7
Pr-2cg (2)	-362.887201	85.95	91.12	90.78	1.04	0.34	8.4
Pr-2ct (UBM)	DNE						
Pr-2ct (TS) C_s	-362.887182	85.72	90.48	85.98	1.05	1.15	-
Pr-2cq	**Pr-2cg'**						
Pr-2hg	DNE						
Pr-2ht (TS)	-362.880835	85.91	90.52	84.25	5.03	5.68	-
Pr-2hq	DNE						
Pr-2TS1 (TS)	-362.882353						
Pr-2TS2 (TS)	-362.882837						
Pr-2TS3 (TS)	-362.883438						
Pr-2TS4 (TS)	-362.881411						
Pr-3tg (2)	-362.887065	86.27	91.22	87.79	1.12	1.42	1.4
Pr-3tt (2)	-362.886908	86.01	91.08	88.31	1.22	1.22	1.9
Pr-3tq (2)	-362.887363	86.16	91.10	86.81	0.94	1.40	1.4
Pr-3cg (2)	-362.885624	85.99	91.10	89.31	2.03	1.75	0.8
Pr-3ct (UBM) C_s	-362.885646	86.01	91.20	90.42	1.97	1.45	-
Pr-3cq	**Pr-3cg'**						
Pr-3hg	DNE						
Pr-3ht	DNE						
Pr-3hq	DNE						
Pr-2TS1	-362.882353	86.16	90.69	83.79	4.07	5.04	
Pr-2TS2	-362.882837	86.03	90.62	84.79	3.77	4.36	
Pr-2TS3	-362.883438	86.03	90.62	84.60	3.39	4.04	
Pr-2TS4	-362.881411	85.99	90.68	86.79	4.67	4.72	

Butylcarbamic acid							
Bu-2tgg (2)	-402.177507	104.36	110.07	94.15	-0.15	0.65	2.8
Bu-2tgt (2)	-402.177630	104.25	110.05	95.33	-0.23	0.20	6.0
Bu-2tgq (2)	-402.175674	104.30	110.07	96.42	1.00	1.12	1.3
Bu-2ttg (2)	-402.176509	104.11	110.00	96.26	0.47	0.57	3.2
Bu-2ttt (2)	-402.177264	103.95	109.89	96.23	0.00	0.00	8.4
Bu-2ttq (2)	-402.176427	104.04	109.95	96.33	0.53	0.55	3.3
Bu-2tqg (2)	-402.175565	104.29	110.06	94.85	1.07	1.65	0.5
Bu-2tqt (2)	-402.178021	104.16	109.95	94.44	-0.48	0.12	6.8
Bu-2tqq (2)	-402.178203	104.33	110.05	93.74	-0.59	0.31	5.0
Bu-2cgg	DNE						
Bu-2cgt (2)	-402.175997	104.00	109.95	96.76	0.80	0.70	2.6
Bu-2cgq	DNE						
Bu-2ctg (2)	-402.175344	103.95	109.96	98.79	1.20	0.51	3.5
Bu-2ctt (UBM)	-402.175890	103.78	109.87	99.27	0.86	-0.06	-
Bu-2ctt (TS) C_s	-402.175885	104.85	109.74	89.94	0.83	1.11	-
Bu-2ctq	**Bu-2ctg'**						
Bu-2cqg	DNE						
Bu-2cqt	**Bu-2cgt'**						
Bu-2cqq	DNE						
Bu-2hgg	DNE						
Bu-2hgt	DNE						
Bu-2hgq	DNE						
Bu-2htg	DNE						
Bu-2htt	DNE						
Bu-2htq	DNE						
Bu-2hqg	DNE						
Bu-2hqt	DNE						
Bu-2hqq	DNE						
Bu-3tgg (2)	-402.175791	104.45	110.11	93.42	0.92	1.98	0.3
Bu-3tgt (2)	-402.175806	104.10	109.92	95.65	0.91	1.12	1.3
Bu-3tgq (2)	-402.174234	104.32	110.05	94.21	1.90	2.67	0.1
Bu-3ttg (2)	-402.174746	104.05	109.92	96.06	1.58	1.66	0.5
Bu-3ttt (2)	-402.175484	103.89	109.80	96.18	1.12	1.04	1.5
Bu-3ttq (2)	-402.174732	104.19	110.00	95.17	1.59	2.01	0.3
Bu-3tqg (2)	-402.173926	104.11	109.88	94.08	2.09	2.73	0.1
Bu-3tqt (2)	-402.176058	104.03	109.84	94.61	0.76	1.19	1.1
Bu-3tqq (2)	-402.175940	104.23	109.95	93.59	0.83	1.67	0.5
Bu-3cgg (2)	-402.174193	104.13	109.95	95.93	1.93	2.08	0.3
Bu-3cgt (2)	-402.174400	104.05	109.94	95.92	1.80	1.94	0.3
Bu-3cgq (2)	-402.172273	104.12	109.97	95.89	3.13	3.31	0.0
Bu-3ctg (2)	-402.173687	103.96	109.92	97.00	2.24	2.04	0.3
Bu-3ctt (UBM) C_s	-402.174294	103.79	109.87	98.36	1.83	1.17	-
Bu-3ctq	**Bu-3ctg'**						
Bu-3cqg	**Bu-3cgq'**						

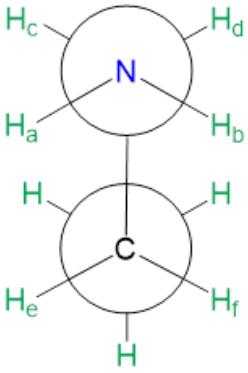
Bu-3cqt	**Bu-3cgt'**					
Bu-3cqq	**Bu-3cgg'**					
Bu-3hgg	DNE					
Bu-3hgt	DNE					
Bu-3hgq	DNE					
Bu-3htg	DNE					
Bu-3htt	DNE					
Bu-3htq	DNE					
Bu-3hqg	DNE					
Bu-3hqt	DNE					
Bu-3hqq	DNE					
Bu-2TS1	-402.171082	104.17	109.51	90.75	4.03	4.48
Bu-2TS2	-402.172505	104.02	109.40	91.14	3.13	3.36
Bu-2TS3	-402.171863	103.80	109.26	92.44	3.54	3.24
Bu-2TS4	-402.170421	103.94	109.45	93.64	4.44	3.98

a) E given in Hartrees, TE given in kcal/mol, S given in cal mol^{-1} K^{-1}, ΔG_{rel} given in kcal/mol.
b) A "(2)" behind the conformer descriptor indicates that the structure has an enantiomer that is included in the Boltzmann analysis.
c) Data refer to stationary minima except for: Unbound Minimum (UBM), Transition State (TS). If the trial structure listed in column 1 corresponds to the enantiomer of a previously listed trial structure, an appropriate indication is made in the energy column. If a trial structure listed in column 1 does not correspond to a minimum, DNE (does not exist) is reported in the energy column.
d) P_i is the percentage of molecules that exist as that conformer according to the Boltzmann statistics.
e) The slight preference of -0.065 kcal/mol for **Bu-2ctt** (C_1) over **Bu-2ttt** on the standard G surface is an artefact of the artificially large contribution $S(\nu_1)$ of its softest mode ν_1 to the total molecular entropy S. The true molecular entropy of **Bu-2ctt** (C_1) is best approximated by S - $S(\nu_1)$ and results in a more physically meaningful molecular Gibbs free energy $G''(\nu_1)$ = -402.04 of **Bu-2ctt**.

Scheme S2. Investigated Trial Conformations of Propylamine



Pr-1tg



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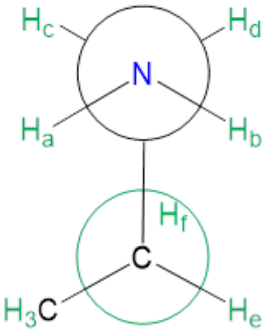

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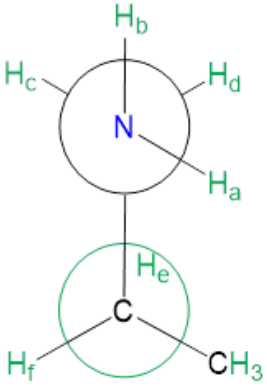

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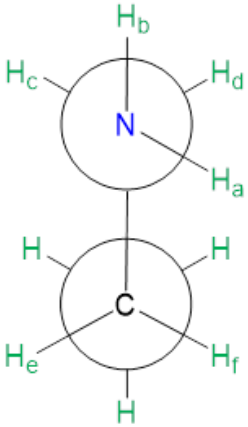

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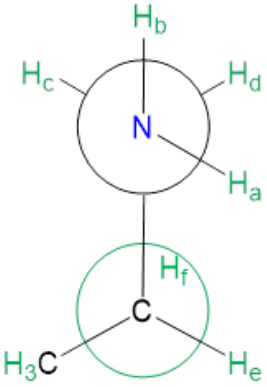
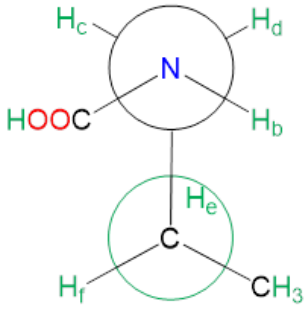


Pr-1gq

Scheme S3. Investigated Trial Structures of Propylcarbamic Acid



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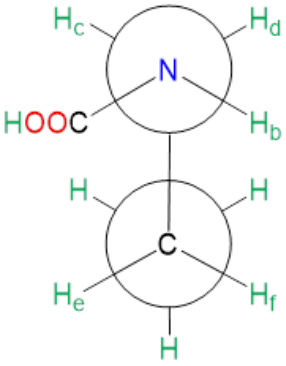

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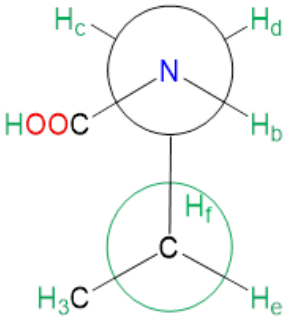

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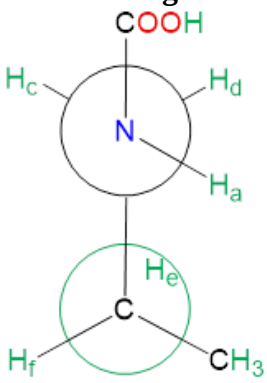

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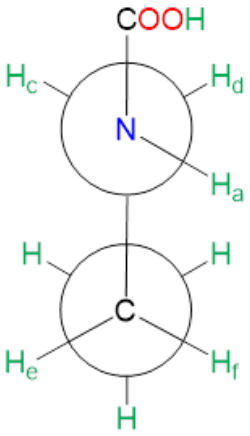

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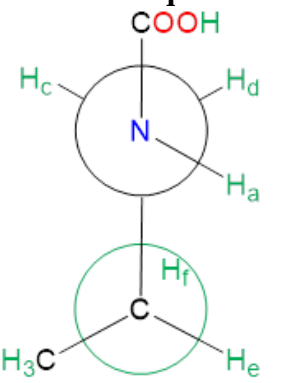

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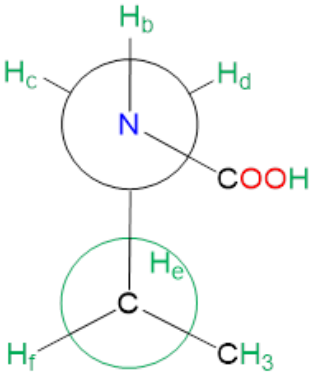

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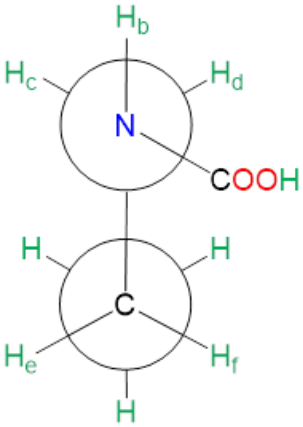

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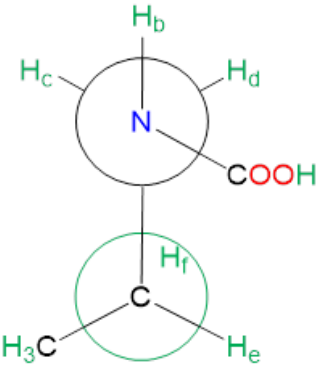
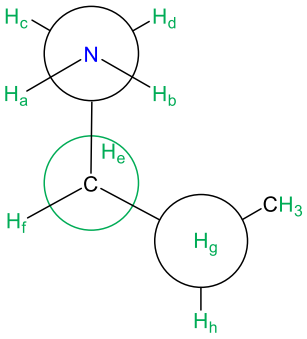
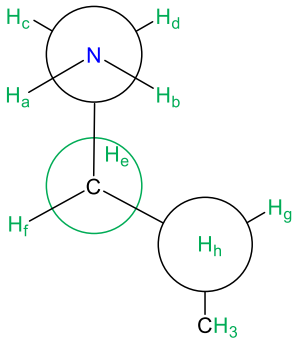


Pr-2hq

Scheme S4. Investigated Trial Conformations of Butylamine



Bu-1tgg



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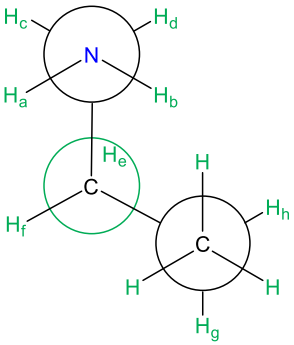

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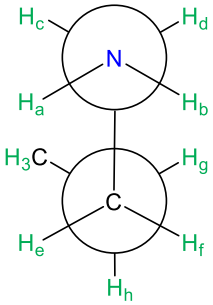

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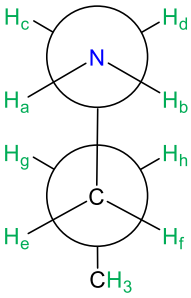

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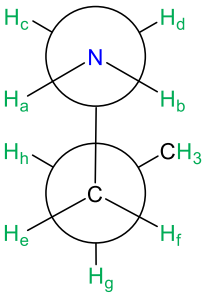

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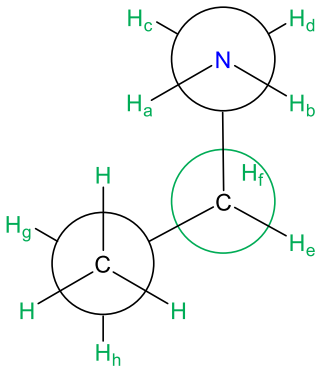
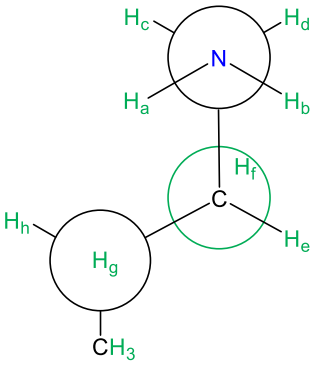


Bu-1tqg = Bu-1tgq'



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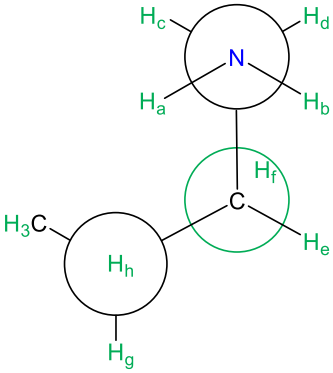

Bu-1tqq = Bu-1tgg'

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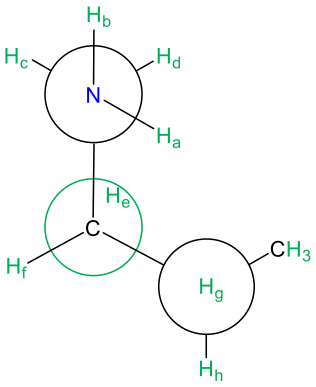
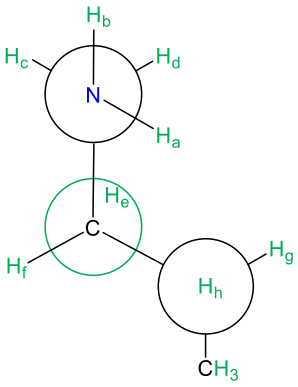


Bu-1ggg



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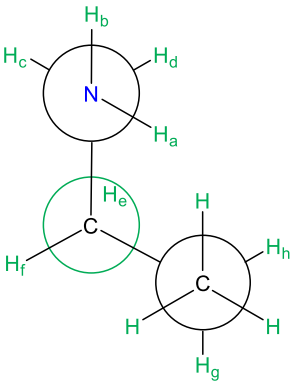

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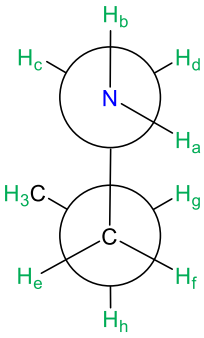

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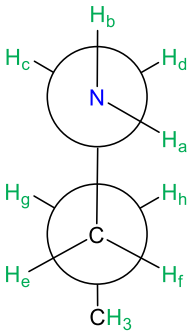

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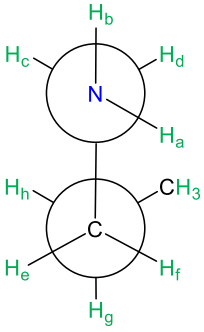

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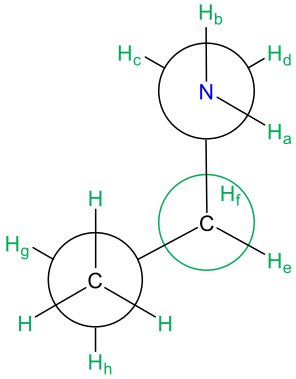

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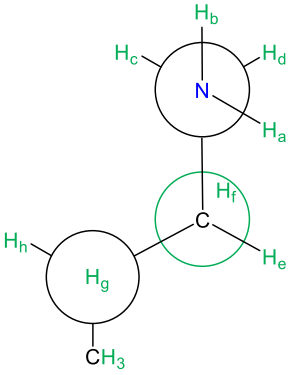
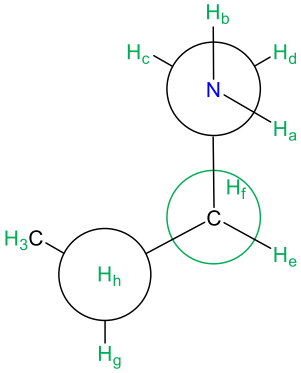
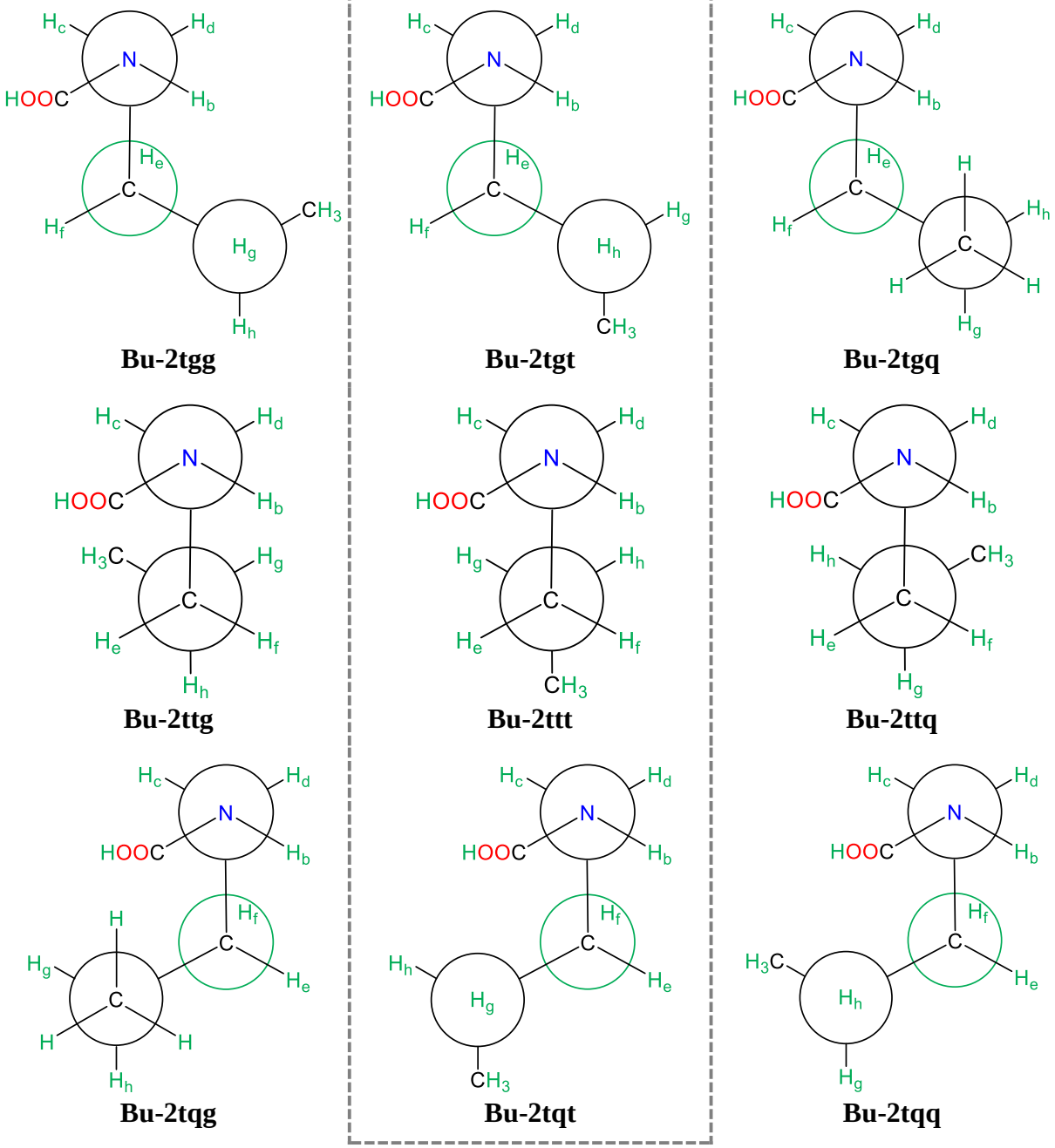


Bu-1gqt



Bu-1gqq

Scheme S5. Investigated Trial Conformations of Butylcarbamic Acids



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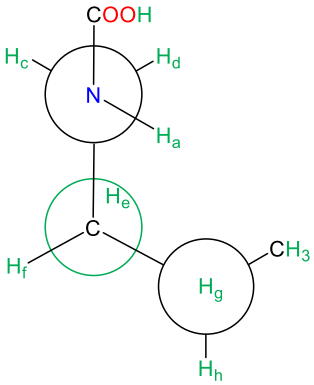
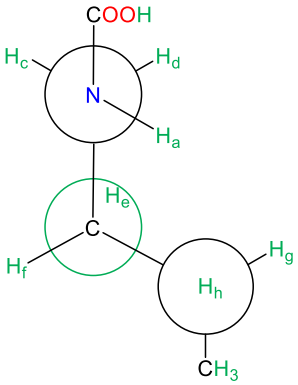
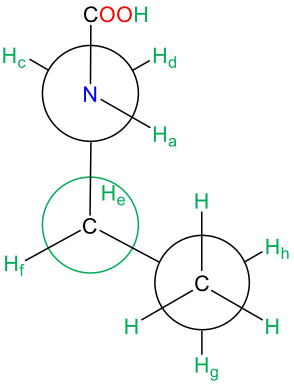


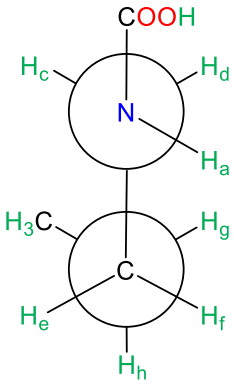
Bu-2cgg



Bu-2cgt



Bu-2cgq



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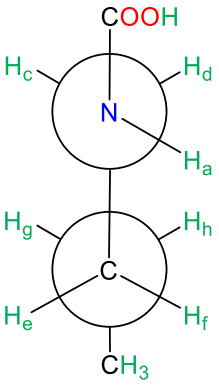
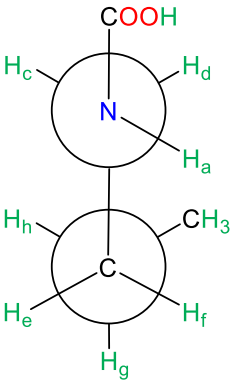
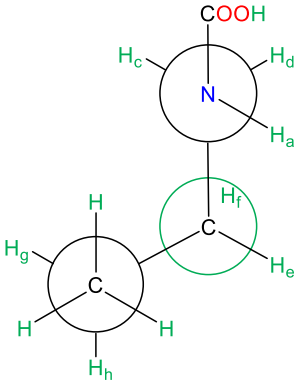


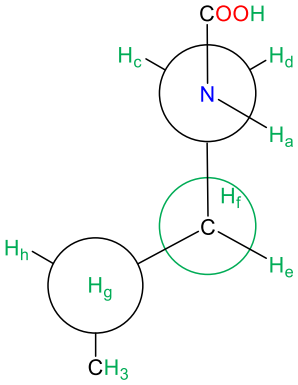
Bu-2ctt



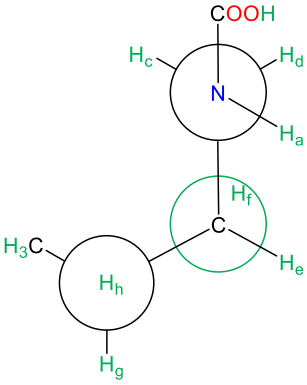
Bu-2ctq



Bu-2cqg



Bu-2cqt



Bu-2cqq

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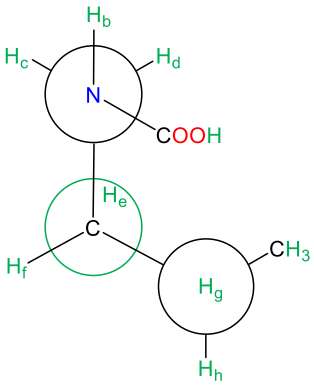
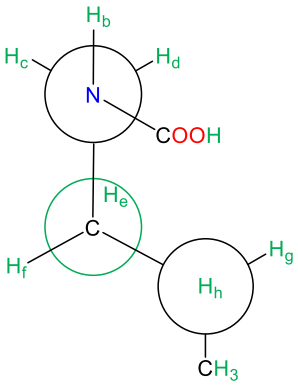
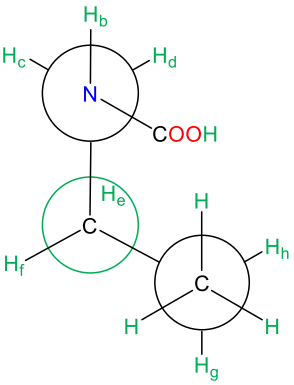


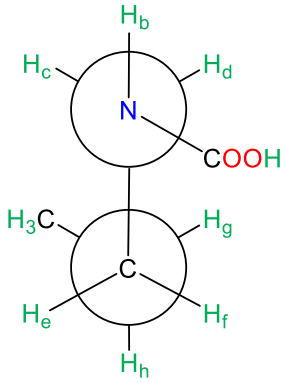
Bu-2hgg



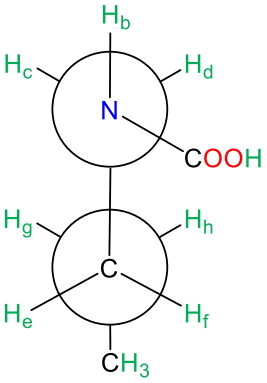
Bu-2hgt



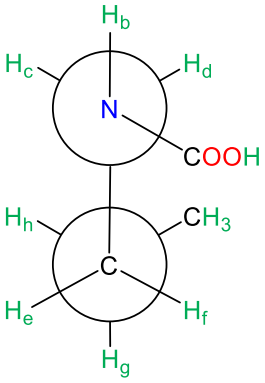
Bu-2hgq



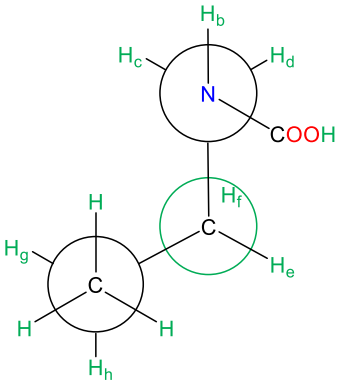
Bu-2htg



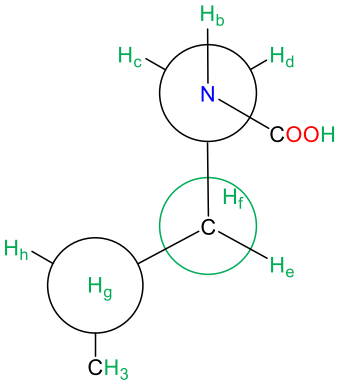
Bu-2htt



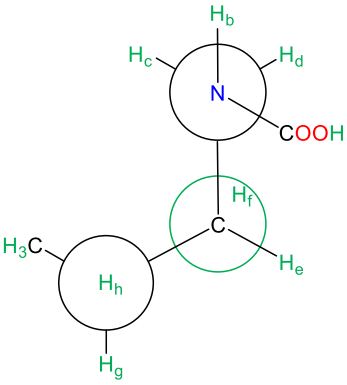
Bu-2htq



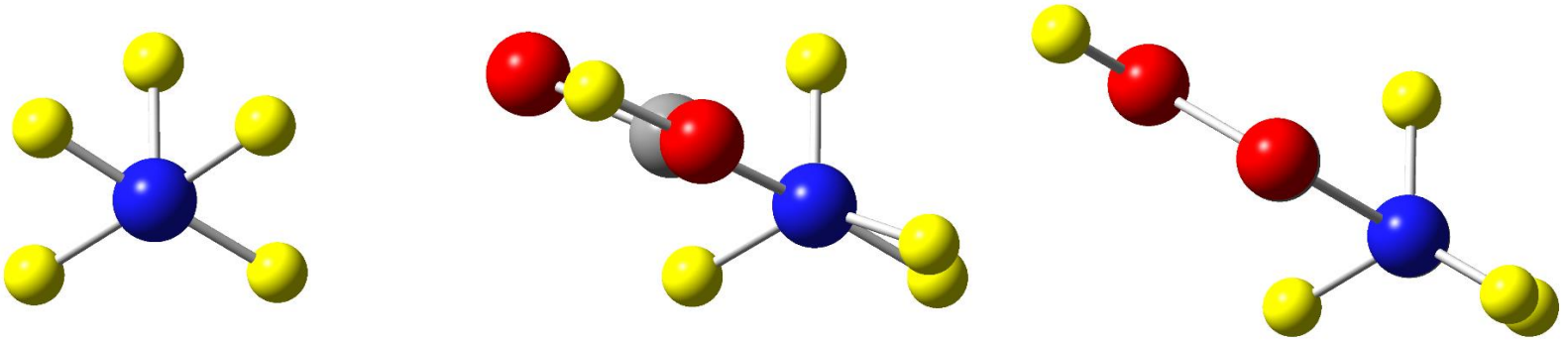
Bu-2hqg



Bu-2hqt

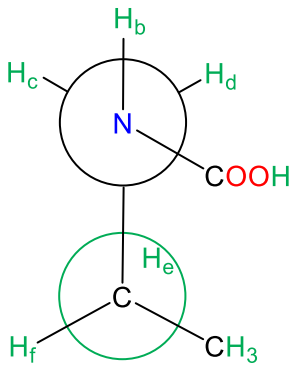


Bu-2hqq

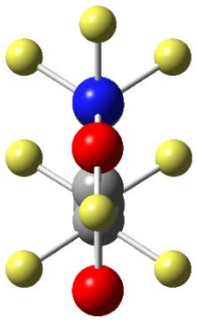


Me-1 **Me-2** **Me-3**, ΔE_{rel} = 0.97

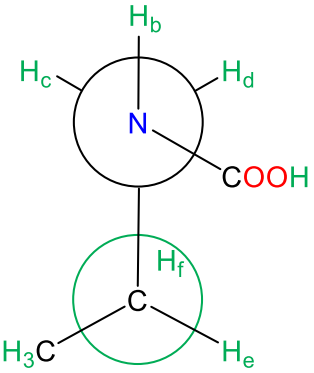
Figure S2. The optimized C_s symmetric structures of methylamine **Me-1** and methylcarbamic acids **Me-2** and **Me-3** are minima.



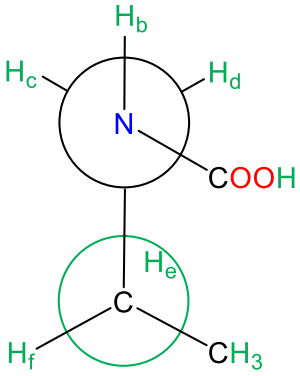
Pr-2hg turns into **Pr-2tg**



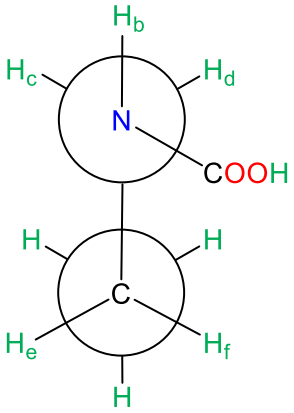
Pr-2ht (TS; ν = **i**103 cm^{-1})



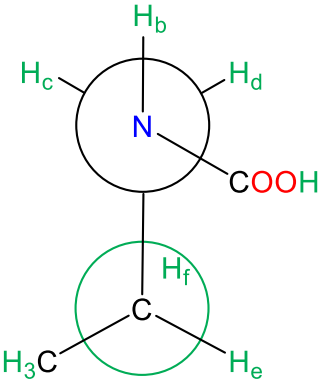
Pr-2hq turns into **Pr-2tg**



Pr-3hg



Pr-3ht



Pr-3hq

Figure S3. Newman projections of trial structures of propylcarbamic acids. **Pr-2h** trial structures contain *trans* amides and **Pr-3h** trial structures contain *cis* amides (Scheme 2). Only the optimization of **Pr-2ht** led to a stationary structure.

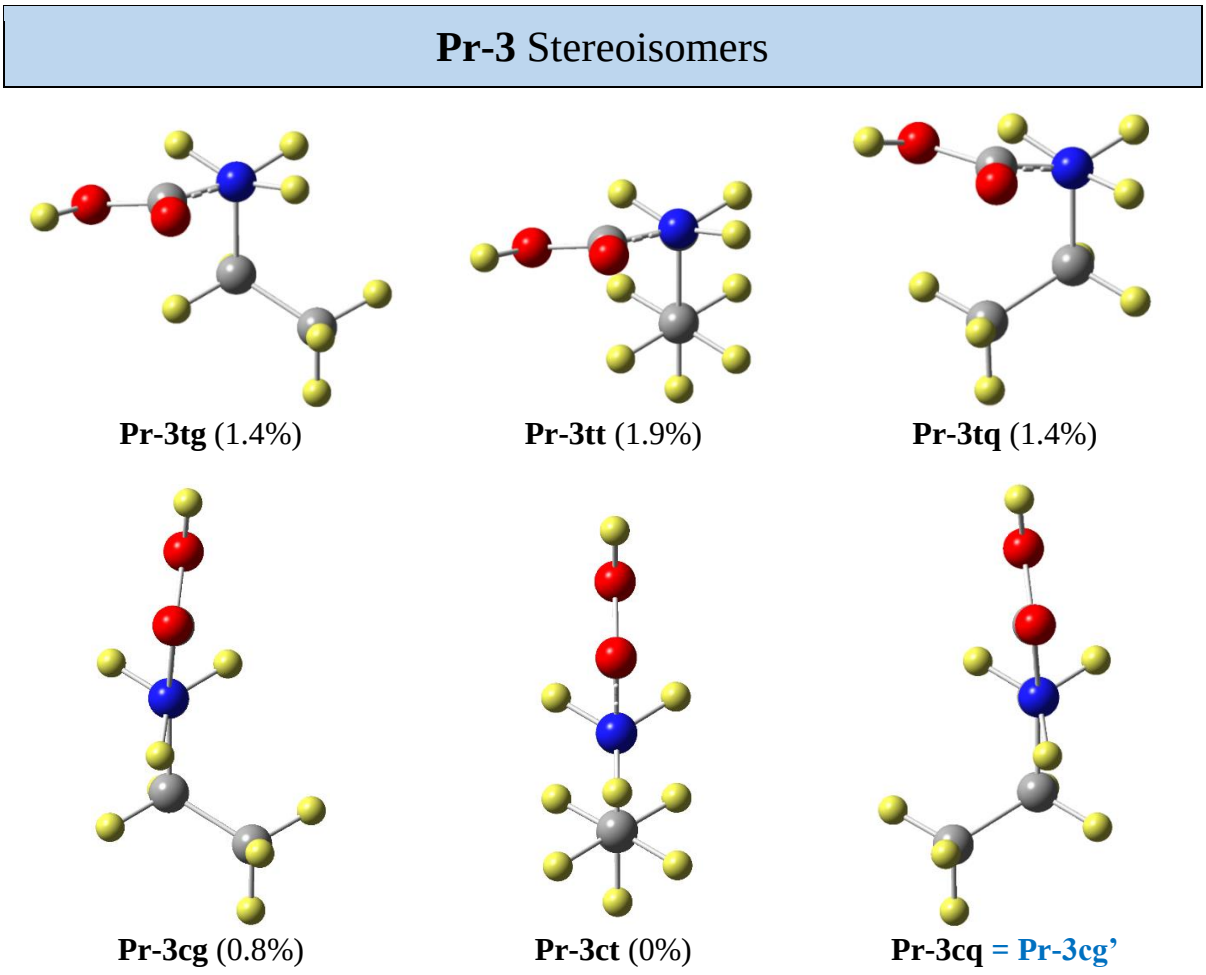


Figure S4. Optimized structures of propylcarbamic acid **Pr-3**. The number in parentheses is the population percentage in the Boltzmann analysis at 298 K for a single unique enantiomeric conformer.

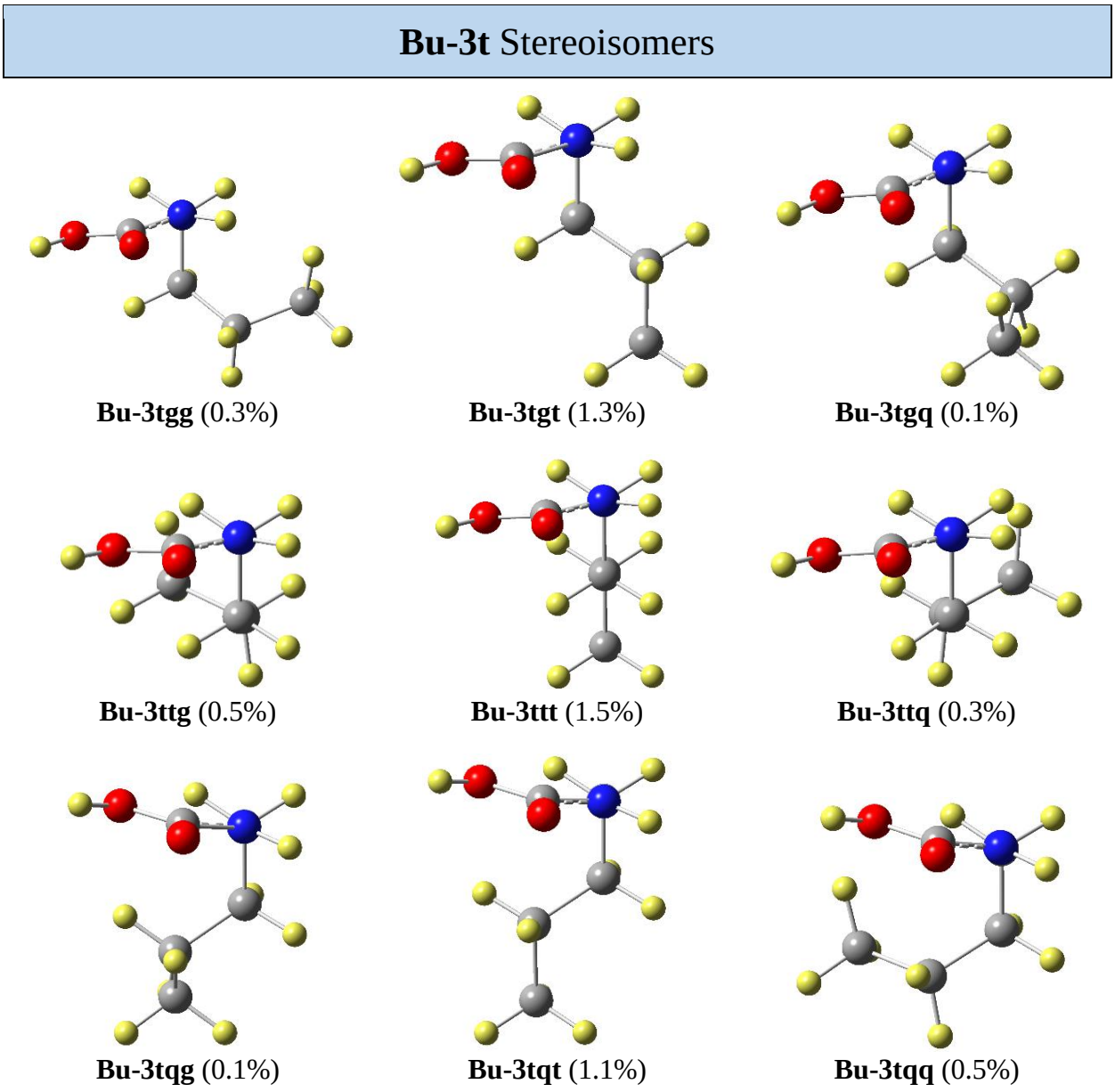


Figure S5. Optimized structures of the **Bu-3t** type (top) and **Bu-3c** type (bottom) conformers of butylcarbamic acid.

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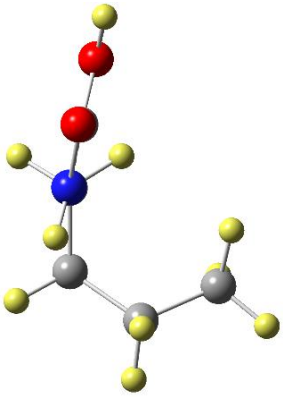
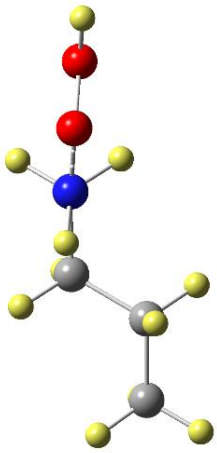
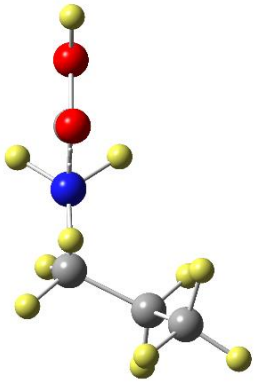
Bu-3c Stereoisomers



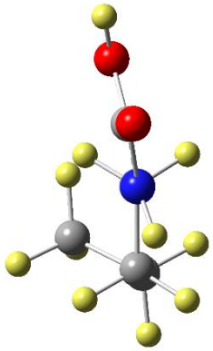
Bu-3cgg (0.3%)



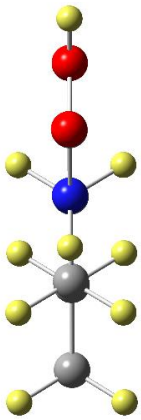
Bu-3cgt (0.3%)



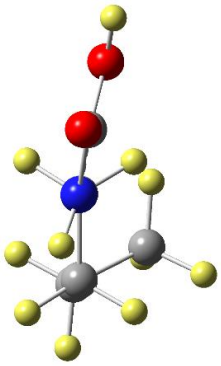
Bu-3cgq (0.0%)



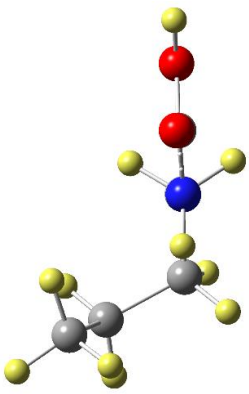
Bu-3ctg (0.3%)



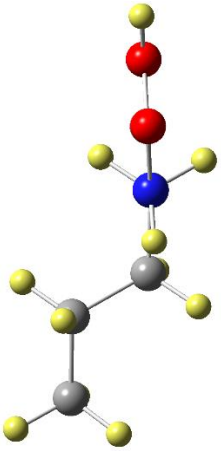
Bu-3ctt (0%)



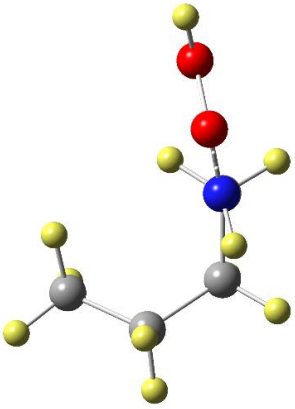
Bu-3ctq = **Bu-3ctg'**



Bu-3cqg = **Bu-3cgq'**



Bu-3cqt = **Bu-3cgt'**



Bu-3cqq = **Bu-3cgg'**

Cartesian Coordinates of Stationary Structures

Methylamine

Me-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.702107	0.000001	0.016811
2	1	0	-1.059765	-0.000051	1.055781
3	1	0	-1.122852	-0.878822	-0.477526
4	7	0	0.752919	-0.000000	-0.132518
5	1	0	1.123835	0.804777	0.362976
6	1	0	-1.122839	0.878874	-0.477442
7	1	0	1.123835	-0.804780	0.362969

Rotational constants (GHZ): 102.9635476 22.8543454 22.0407258
Standard basis: 6-311G(d) (5D, 7F)

Methylcarbamic acid

Me-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.906648	0.009284	0.012758
2	1	0	2.067967	0.532454	0.959206
3	1	0	2.011483	0.727539	-0.802519
4	7	0	0.610412	-0.630677	-0.030412
5	1	0	0.538649	-1.633244	0.033158
6	6	0	-0.515203	0.095101	-0.004770
7	8	0	-1.620235	-0.691469	0.009344
8	8	0	-0.569881	1.320095	-0.002425
9	1	0	-2.393018	-0.113063	0.018416
10	1	0	2.674294	-0.754266	-0.098655

Rotational constants (GHZ): 10.7807065 4.1370060 3.0475601
Standard basis: 6-311G(d) (5D, 7F)

Me-3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.863659	0.063102	0.000001
2	1	0	1.958310	0.692424	0.887338
3	1	0	1.958302	0.692442	-0.887324
4	7	0	0.612744	-0.668713	-0.000002
5	1	0	0.625337	-1.675267	0.000002
6	6	0	-0.603118	-0.103450	-0.000000
7	8	0	-1.668949	-0.712665	0.000001
8	8	0	-0.535347	1.248208	-0.000000
9	1	0	2.679652	-0.657351	-0.000010
10	1	0	-1.439686	1.586491	0.000001

```
---------------------------------------------------------------------
Rotational constants (GHZ):    10.5825220    4.2428753    3.0873337
Standard basis: 6-311G(d) (5D, 7F)
```

Ethylamine

Et-1t

```
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0        1.223833   -0.263003   -0.000001
     2          1           0        1.265135   -0.908120   -0.885063
     3          1           0        1.265199   -0.908001    0.885142
     4          1           0        2.124606    0.361578   -0.000076
     5          6           0       -0.044845    0.577737    0.000002
     6          1           0       -0.051783    1.237272    0.874401
     7          1           0       -0.051788    1.237237   -0.874421
     8          7           0       -1.294555   -0.185040    0.000005
     9          1           0       -1.281720   -0.806523   -0.804648
    10          1           0       -1.281688   -0.806565    0.804625
---------------------------------------------------------------------
Rotational constants (GHZ):    31.7459469    8.8820290    7.9004911
Standard basis: 6-311G(d) (5D, 7F)
```

Et-1g

```
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0        1.241916   -0.234128   -0.024646
     2          1           0        1.322603   -0.763160   -0.979637
     3          1           0        1.291817   -0.981229    0.775770
     4          1           0        2.114295    0.418387    0.078401
     5          6           0       -0.050017    0.556367    0.050117
     6          1           0       -0.079683    1.115409    0.998188
     7          1           0       -0.070162    1.304841   -0.748872
     8          7           0       -1.206503   -0.326623   -0.127591
     9          1           0       -1.231846   -0.969515    0.659388
    10          1           0       -2.052897    0.228195   -0.042928
---------------------------------------------------------------------
Rotational constants (GHZ):    32.8647823    8.9519539    7.8678750
Standard basis: 6-311G(d) (5D, 7F)
```

Ethylcarbamic acid

Et-2t

```
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -2.148877    0.208940   -0.656255
     2          1           0       -2.263347   -0.621738   -1.358926
     3          1           0       -1.610503    1.014766   -1.163474
     4          1           0       -3.147530    0.576873   -0.401906
```

5	6	0	-1.408449	-0.233651	0.594808
6	1	0	-1.309335	0.595362	1.298172
7	1	0	-1.956015	-1.023891	1.112112
8	7	0	-0.075966	-0.743608	0.318797
9	1	0	0.013481	-1.693538	-0.009442
10	6	0	0.944239	0.093866	0.066471
11	8	0	2.034115	-0.573860	-0.386036
12	1	0	2.735773	0.072755	-0.533245
13	8	0	0.934355	1.307577	0.235409

Rotational constants (GHZ): 7.3818557 2.2853258 2.0366357
Standard basis: 6-311G(d) (5D, 7F)

Et-2c, C_s (TS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.275555	1.307367	-0.000000
2	1	0	2.091277	1.922035	0.886324
3	1	0	2.091277	1.922035	-0.886324
4	1	0	3.331146	1.025995	-0.000000
5	6	0	1.405021	0.068012	0.000000
6	1	0	1.615483	-0.548766	-0.879609
7	1	0	1.615483	-0.548766	0.879609
8	7	0	-0.000000	0.440662	-0.000000
9	1	0	-0.256557	1.415889	-0.000000
10	6	0	-0.966561	-0.484604	0.000000
11	8	0	-2.202539	0.076013	-0.000000
12	1	0	-2.850488	-0.640023	0.000000
13	8	0	-0.787675	-1.698224	0.000000

Rotational constants (GHZ): 9.1263440 2.0056163 1.6785996
Standard basis: 6-311G(d) (5D, 7F)

Et-2c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.596762	-0.284886	-0.134216
2	1	0	2.588362	-0.698060	-1.146866
3	1	0	2.732573	-1.110934	0.571185
4	1	0	3.464269	0.373406	-0.044690
5	6	0	1.323665	0.482690	0.157251
6	1	0	1.375201	0.943717	1.150454
7	1	0	1.186562	1.291403	-0.564488
8	7	0	0.174400	-0.402518	0.077102
9	1	0	0.311310	-1.393567	0.206116
10	6	0	-1.078024	0.064196	-0.006538
11	8	0	-1.984441	-0.946126	-0.011145
12	1	0	-2.863667	-0.552883	-0.072202
13	8	0	-1.399287	1.245194	-0.081130

Rotational constants (GHZ): 9.0289617 2.0063353 1.6860476
Standard basis: 6-311G(d) (5D, 7F)

Et-3t

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.109728	0.263797	0.634855
2	1	0	2.261706	-0.531027	1.371133
3	1	0	1.549481	1.071085	1.114308
4	1	0	3.091981	0.655100	0.352817
5	6	0	1.375383	-0.259742	-0.588745
6	1	0	1.251299	0.528145	-1.333404
7	1	0	1.947259	-1.056694	-1.068158
8	7	0	0.062912	-0.812375	-0.282883
9	1	0	0.013455	-1.770627	0.027295
10	6	0	-1.030567	-0.081954	0.001139
11	8	0	-2.086732	-0.535349	0.430443
12	8	0	-0.861577	1.232664	-0.266723
13	1	0	-1.696362	1.679519	-0.077061

Rotational constants (GHZ): 7.2697842 2.3441519 2.0682107
Standard basis: 6-311G(d) (5D, 7F)

Et-3c, C_s (UBM)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.347203	1.142183	-0.000000
2	1	0	2.221093	1.771119	0.886446
3	1	0	2.221093	1.771119	-0.886446
4	1	0	3.371835	0.763162	0.000000
5	6	0	1.364645	-0.010904	0.000000
6	1	0	1.518033	-0.642239	-0.880319
7	1	0	1.518033	-0.642239	0.880319
8	7	0	-0.000000	0.499386	-0.000000
9	1	0	-0.146943	1.496856	-0.000000
10	6	0	-1.108360	-0.254049	-0.000000
11	8	0	-2.258882	0.174797	-0.000000
12	8	0	-0.823858	-1.577343	0.000000
13	1	0	-1.662161	-2.056487	0.000000

Rotational constants (GHZ): 9.0982827 2.0314919 1.6957482
Standard basis: 6-311G(d) (5D, 7F)

Propylamine

Pr-1tg

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.651530	0.646237	-0.295934
2	1	0	0.566207	0.688921	-1.390661
3	6	0	-0.750621	0.579263	0.308297
4	1	0	-0.674017	0.579905	1.401784
5	1	0	-1.302782	1.486917	0.042249
6	7	0	-1.568013	-0.572677	-0.080648

7	1	0	-1.588985	-0.617607	-1.096157
8	1	0	-1.091593	-1.421216	0.209584
9	6	0	1.537610	-0.525174	0.109649
10	1	0	1.634899	-0.586890	1.199506
11	1	0	1.133545	-1.480994	-0.239080
12	1	0	2.545341	-0.431540	-0.306672
13	1	0	1.122366	1.589286	0.011908

Rotational constants (GHZ): 13.7040086 4.9629138 4.2013760
Standard basis: 6-311G(d) (5D, 7F)

Pr-1tt

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.526939	0.523850	0.000003
2	1	0	-0.409459	1.172469	-0.878685
3	1	0	-0.409462	1.172463	0.878695
4	6	0	0.590299	-0.513398	0.000000
5	1	0	0.482394	-1.164580	0.874996
6	1	0	0.482387	-1.164584	-0.874992
7	7	0	1.952305	0.024067	-0.000004
8	1	0	2.047278	0.637729	-0.804928
9	6	0	-1.911118	-0.112206	-0.000001
10	1	0	-2.705819	0.640018	0.000010
11	1	0	-2.057101	-0.744571	-0.882568
12	1	0	-2.057097	-0.744593	0.882550
13	1	0	2.047292	0.637706	0.804936

Rotational constants (GHZ): 24.7575866 3.7222873 3.5039008
Standard basis: 6-311G(d) (5D, 7F)

Pr-1gg

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.666554	0.650819	-0.278488
2	1	0	0.607080	0.725496	-1.371941
3	6	0	-0.742655	0.573686	0.289275
4	1	0	-0.682178	0.562307	1.390041
5	1	0	-1.289426	1.483092	0.019834
6	7	0	-1.484216	-0.570063	-0.250376
7	1	0	-1.076628	-1.421926	0.123382
8	1	0	-2.427055	-0.545089	0.125367
9	6	0	1.542711	-0.534328	0.113040
10	1	0	1.589449	-0.648455	1.201996
11	1	0	1.168980	-1.475860	-0.302011
12	1	0	2.567898	-0.410585	-0.249404
13	1	0	1.131738	1.580400	0.072403

Rotational constants (GHZ): 13.9897947 4.9919944 4.1924602
Standard basis: 6-311G(d) (5D, 7F)

Pr-1gt

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.542862	0.523555	-0.061433
2	1	0	-0.454259	1.088008	-0.998037
3	1	0	-0.428335	1.254907	0.750478
4	6	0	0.590397	-0.484560	0.015709
5	1	0	0.482108	-1.073620	0.940639
6	1	0	0.498587	-1.195231	-0.813345
7	7	0	1.894181	0.175441	-0.092384
8	1	0	2.017694	0.760191	0.729707
9	6	0	-1.911643	-0.137430	0.029513
10	1	0	-2.720428	0.597132	-0.029408
11	1	0	-2.059978	-0.855925	-0.783968
12	1	0	-2.030238	-0.681691	0.972616
13	1	0	2.620224	-0.531251	-0.024734

Rotational constants (GHZ): 25.3104730 3.7455343 3.5064021
Standard basis: 6-311G(d) (5D, 7F)

Pr-1gq

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.661429	0.611349	-0.313043
2	6	0	0.727146	0.563766	0.308633
3	1	0	1.261814	1.493686	0.059664
4	1	0	0.633307	0.544437	1.400611
5	7	0	1.461657	-0.635790	-0.104521
6	1	0	1.636576	-0.565710	-1.103277
7	1	0	2.379169	-0.618655	0.329514
8	1	0	-1.121937	1.573652	-0.057245
9	6	0	-1.571132	-0.527253	0.130802
10	1	0	-1.711085	-0.516783	1.217660
11	1	0	-2.561558	-0.453000	-0.329317
12	1	0	-1.153480	-1.501014	-0.136707
13	1	0	-0.561920	0.606750	-1.407607

Rotational constants (GHZ): 14.1394691 4.8752562 4.2054208
Standard basis: 6-311G(d) (5D, 7F)

Propylcarbamic acid

Pr-2tg

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.844393	-0.718500	0.802321
2	1	0	0.474806	-1.745784	0.818138
3	1	0	1.379395	-0.555500	1.741278
4	7	0	-0.306520	0.169506	0.806712
5	1	0	-0.185465	1.109283	1.152902
6	6	0	-1.343386	-0.044661	-0.022157
7	8	0	-2.195289	1.010049	-0.032943
8	1	0	-2.933539	0.786897	-0.613470

9	8	0	-1.541411	-1.062210	-0.675211
10	6	0	1.776684	-0.502138	-0.384699
11	1	0	2.575635	-1.251232	-0.328249
12	1	0	1.226051	-0.704733	-1.310926
13	6	0	2.373838	0.897980	-0.420716
14	1	0	1.598938	1.664171	-0.523524
15	1	0	2.932590	1.113949	0.496578
16	1	0	3.061645	1.017606	-1.262968

Rotational constants (GHZ): 4.8808500 1.5396500 1.4152767
Standard basis: 6-311G(d) (5D, 7F)

Pr-2tt

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.655573	-0.051673	0.562189
2	1	0	1.668959	-0.853951	1.309716
3	1	0	1.181788	0.814802	1.038126
4	6	0	0.805311	-0.488653	-0.623751
5	1	0	0.774020	0.302452	-1.376992
6	1	0	1.242445	-1.367436	-1.103880
7	7	0	-0.562084	-0.821705	-0.268833
8	1	0	-0.760376	-1.741380	0.094720
9	6	0	-1.473662	0.140861	-0.053601
10	8	0	-2.629186	-0.369116	0.439987
11	1	0	-3.252064	0.360625	0.548196
12	8	0	-1.323651	1.334911	-0.286442
13	6	0	3.073953	0.293030	0.131030
14	1	0	3.687048	0.606456	0.980837
15	1	0	3.568756	-0.566694	-0.333364
16	1	0	3.079659	1.109304	-0.599088

Rotational constants (GHZ): 6.7737657 1.2715039 1.1794833
Standard basis: 6-311G(d) (5D, 7F)

Pr-2tq

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.938740	-1.004626	0.519511
2	1	0	-0.795834	-0.592813	1.520219
3	1	0	-1.202476	-2.058444	0.639920
4	7	0	0.341792	-0.939326	-0.162023
5	1	0	0.425634	-1.402016	-1.055274
6	6	0	1.248759	0.012219	0.117300
7	8	0	2.251876	0.017801	-0.796175
8	1	0	2.884259	0.698314	-0.533873
9	8	0	1.226545	0.775366	1.075465
10	6	0	-2.050508	-0.262079	-0.213634
11	1	0	-2.984312	-0.430262	0.336531
12	1	0	-2.191227	-0.716220	-1.202789
13	6	0	-1.790314	1.231600	-0.358321
14	1	0	-1.655983	1.709186	0.617301
15	1	0	-0.890896	1.429449	-0.949816
16	1	0	-2.624255	1.730066	-0.861518

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---------------------------------------------------------------------
Rotational constants (GHZ):    4.5461310    1.6773507    1.5392468
Standard basis: 6-311G(d) (5D, 7F)
```

Pr-2cg

```
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -0.777500    0.859197   -0.259641
     2          1           0       -0.685140    1.314991    0.730477
     3          1           0       -0.597491    1.650317   -0.996651
     4          6           0       -2.169981    0.277781   -0.440867
     5          7           0        0.237414   -0.172680   -0.384742
     6          1           0        0.007576   -1.037769   -0.849752
     7          6           0        1.493779    0.016087    0.035811
     8          8           0        1.920435    1.029544    0.579447
     9          8           0        2.271897   -1.069406   -0.206720
    10          1           0        3.158651   -0.874213    0.120774
    11          1           0       -2.878953    1.112679   -0.435878
    12          1           0       -2.245934   -0.180108   -1.435494
    13          6           0       -2.548168   -0.732037    0.635260
    14          1           0       -3.574587   -1.086178    0.502134
    15          1           0       -1.896814   -1.610962    0.618906
    16          1           0       -2.476645   -0.287268    1.633485
---------------------------------------------------------------------
Rotational constants (GHZ):    5.7839582    1.3281907    1.2029345
Standard basis: 6-311G(d) (5D, 7F)
```

Pr-2ct, C_s (TS)

```
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -3.286916   -0.233912   -0.000000
     2          1           0       -4.168774    0.412714   -0.000027
     3          1           0       -3.348876   -0.877843    0.883323
     4          1           0       -3.348867   -0.877905   -0.883279
     5          6           0       -2.002182    0.581774   -0.000022
     6          1           0       -1.971642    1.236383   -0.879669
     7          1           0       -1.971659    1.236455    0.879572
     8          6           0       -0.778499   -0.316286    0.000026
     9          1           0       -0.788911   -0.968579   -0.880061
    10          1           0       -0.788933   -0.968513    0.880162
    11          7           0        0.438393    0.476037    0.000005
    12          1           0        0.377390    1.482471    0.000041
    13          6           0        1.645555   -0.100771   -0.000002
    14          8           0        2.644293    0.818039    0.000001
    15          8           0        1.854519   -1.309633   -0.000013
    16          1           0        3.483282    0.340486   -0.000005
---------------------------------------------------------------------
Rotational constants (GHZ):    8.2782997    1.1184494    1.0036952
Standard basis: 6-311G(d) (5D, 7F)
```

Pr-2ht (TS)

```
---------------------------------------------------------------------
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.856369	0.905763	-0.000000
2	1	0	-1.175845	1.479198	0.877289
3	1	0	-1.175845	1.479198	-0.877290
4	6	0	-1.575625	-0.434375	0.000000
5	7	0	0.604851	0.886512	0.000000
6	1	0	1.048255	1.792655	-0.000001
7	6	0	1.440277	-0.160182	0.000000
8	8	0	1.166418	-1.354015	-0.000000
9	8	0	2.734654	0.274602	0.000000
10	1	0	3.299683	-0.507843	0.000000
11	1	0	-1.286081	-1.018838	-0.877739
12	1	0	-1.286081	-1.018838	0.877740
13	6	0	-3.081563	-0.202407	0.000000
14	1	0	-3.626502	-1.150634	-0.000000
15	1	0	-3.400219	0.361011	0.883344
16	1	0	-3.400219	0.361012	-0.883343

Rotational constants (GHZ): 7.1495131 1.3222099 1.1393801
Standard basis: 6-311G(d) (5D, 7F)

Pr-3tg

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.804950	-0.667227	0.848949
2	1	0	0.401943	-1.677788	0.932310
3	1	0	1.364409	-0.472030	1.767402
4	7	0	-0.309276	0.272100	0.832751
5	1	0	-0.128665	1.214571	1.143287
6	6	0	-1.381214	0.166433	0.023835
7	8	0	-2.208192	1.052413	-0.164803
8	8	0	-1.484900	-1.054506	-0.546869
9	6	0	1.724327	-0.548680	-0.361674
10	1	0	2.498254	-1.320799	-0.273905
11	1	0	1.155562	-0.781738	-1.269301
12	6	0	2.368739	0.825518	-0.482148
13	1	0	1.619164	1.611673	-0.616782
14	1	0	2.948189	1.071265	0.414550
15	1	0	3.047477	0.874538	-1.338686
16	1	0	-2.297480	-1.063924	-1.068528

Rotational constants (GHZ): 4.8139612 1.5714746 1.4456099
Standard basis: 6-311G(d) (5D, 7F)

Pr-3tt

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.616125	-0.059057	0.560979
2	1	0	1.648542	-0.863183	1.305964
3	1	0	1.125024	0.794962	1.041264
4	6	0	0.775306	-0.514106	-0.624995
5	1	0	0.735850	0.267383	-1.386761

6	1	0	1.229174	-1.388972	-1.096852
7	7	0	-0.586663	-0.882641	-0.269883
8	1	0	-0.749178	-1.815200	0.077629
9	6	0	-1.566680	-0.006947	0.017756
10	8	0	-2.657368	-0.304299	0.494547
11	8	0	-1.239414	1.264415	-0.306367
12	6	0	3.026124	0.318232	0.129274
13	1	0	3.633284	0.640751	0.979961
14	1	0	3.538988	-0.528169	-0.339917
15	1	0	3.013046	1.138112	-0.596705
16	1	0	-1.999088	1.823140	-0.098918

Rotational constants (GHZ): 6.5650074 1.3055900 1.2059649
Standard basis: 6-311G(d) (5D, 7F)

Pr-3tq

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.909541	-0.976405	0.571758
2	1	0	-0.732932	-0.518787	1.545443
3	1	0	-1.187469	-2.017477	0.755411
4	7	0	0.348314	-0.982586	-0.161120
5	1	0	0.368747	-1.499575	-1.027978
6	6	0	1.320648	-0.056678	-0.065683
7	8	0	2.257712	0.052111	-0.850989
8	8	0	1.196279	0.736589	1.021983
9	6	0	-2.031344	-0.257597	-0.169825
10	1	0	-2.951104	-0.380181	0.414963
11	1	0	-2.206567	-0.764959	-1.127081
12	6	0	-1.755522	1.221120	-0.406117
13	1	0	-1.597432	1.752662	0.537492
14	1	0	-0.865637	1.373269	-1.025126
15	1	0	-2.593095	1.700507	-0.921562
16	1	0	1.949920	1.340396	1.027539

Rotational constants (GHZ): 4.4657776 1.7074608 1.5702559
Standard basis: 6-311G(d) (5D, 7F)

Pr-3cg

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.719237	-0.821462	-0.182545
2	1	0	0.658549	-1.244980	0.824757
3	1	0	0.445611	-1.614941	-0.885430
4	6	0	2.134836	-0.342178	-0.458382
5	7	0	-0.227262	0.280036	-0.296908
6	1	0	0.099367	1.168720	-0.644044
7	6	0	-1.536810	0.209254	-0.022593
8	8	0	-1.901582	-1.020051	0.410665
9	8	0	-2.337932	1.132550	-0.139308
10	1	0	2.782562	-1.225198	-0.475063
11	1	0	2.181268	0.089789	-1.466126
12	6	0	2.652028	0.656462	0.570087
13	1	0	3.691682	0.928655	0.366053

14	1	0	2.071282	1.583897	0.576021
15	1	0	2.610636	0.235857	1.580347
16	1	0	-2.849751	-0.994492	0.591593

Rotational constants (GHZ): 6.0465384 1.3179936 1.1761314
Standard basis: 6-311G(d) (5D, 7F)

Pr-3ct (UBM)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.356338	-2.263484	-0.000000
2	1	0	-3.446571	-2.348098	-0.000000
3	1	0	-1.983555	-2.792159	0.883323
4	1	0	-1.983555	-2.792159	-0.883323
5	6	0	-1.914064	-0.807357	-0.000000
6	1	0	-2.317116	-0.290850	-0.879757
7	1	0	-2.317116	-0.290850	0.879757
8	6	0	-0.400550	-0.690893	-0.000000
9	1	0	0.013717	-1.192117	-0.880847
10	1	0	0.013717	-1.192117	0.880847
11	7	0	-0.000000	0.708431	0.000000
12	1	0	-0.714580	1.419624	0.000000
13	6	0	1.265434	1.149605	0.000000
14	8	0	1.608290	2.328480	0.000000
15	8	0	2.157401	0.131029	-0.000000
16	1	0	3.042637	0.516410	-0.000000

Rotational constants (GHZ): 8.1886647 1.1340072 1.0148557
Standard basis: 6-311G(d) (5D, 7F)

Pr-2TS1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.955083	-1.157720	-0.184904
2	1	0	-0.691553	-1.759317	0.685636
3	1	0	-1.342688	-1.850187	-0.933324
4	7	0	0.285674	-0.623885	-0.718809
5	1	0	0.299136	-0.312502	-1.678388
6	6	0	1.211531	-0.094688	0.100916
7	8	0	2.174887	0.557009	-0.594482
8	1	0	2.820398	0.893486	0.039614
9	8	0	1.228031	-0.195415	1.321815
10	6	0	-2.036066	-0.109645	0.191031
11	1	0	-2.942090	-0.315744	-0.388601
12	1	0	-2.313227	-0.249509	1.241115
13	6	0	-1.629988	1.343380	-0.026161
14	1	0	-0.774228	1.626043	0.593964
15	1	0	-1.365310	1.542970	-1.068664
16	1	0	-2.455861	2.011238	0.236360

Rotational constants (GHZ): 4.3939077 1.7266219 1.6341493
Standard basis: 6-311G(d) (5D, 7F)

Pr-2TS2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.800315	-0.132542	0.841419
2	1	0	-0.574040	0.621152	1.598144
3	1	0	-1.353236	-0.924956	1.349622
4	7	0	0.457075	-0.719513	0.412106
5	1	0	0.483056	-1.692874	0.150231
6	6	0	1.468861	0.064756	0.008198
7	8	0	2.489734	-0.659875	-0.512252
8	1	0	3.191781	-0.044027	-0.757116
9	8	0	1.504452	1.286531	0.105030
10	6	0	-1.646061	0.470311	-0.297102
11	1	0	-1.770146	1.546348	-0.136142
12	1	0	-1.095938	0.369135	-1.238945
13	6	0	-3.011158	-0.193409	-0.424100
14	1	0	-2.911135	-1.264999	-0.627602
15	1	0	-3.590601	-0.086859	0.499191
16	1	0	-3.600711	0.245725	-1.234840

Rotational constants (GHZ): 6.3465858 1.2930914 1.2146983
Standard basis: 6-311G(d) (5D, 7F)

Pr-2TS3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.798478	-0.928384	-0.572995
2	1	0	0.876847	-0.294904	-1.459752
3	1	0	1.050823	-1.940347	-0.892400
4	7	0	-0.599426	-0.957569	-0.178975
5	1	0	-0.947357	-1.768372	0.309813
6	6	0	-1.313437	0.175118	-0.074859
7	8	0	-2.523093	-0.051477	0.494594
8	1	0	-3.001050	0.786879	0.518332
9	8	0	-0.960482	1.284465	-0.458321
10	6	0	1.764288	-0.436807	0.523156
11	1	0	1.200057	-0.293364	1.451138
12	1	0	2.503126	-1.216658	0.737698
13	6	0	2.480639	0.855509	0.149577
14	1	0	3.070678	0.729831	-0.764512
15	1	0	1.766450	1.664800	-0.027076
16	1	0	3.165196	1.178596	0.940137

Rotational constants (GHZ): 5.1713451 1.5531620 1.3381129
Standard basis: 6-311G(d) (5D, 7F)

Pr-2TS4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.763444	0.536309	0.031475
2	1	0	-0.483511	1.418661	0.609257

3	1	0	-0.929312	0.877806	-0.997476
4	6	0	-2.040533	-0.111037	0.586923
5	1	0	-1.815837	-1.124478	0.938097
6	7	0	0.361343	-0.383387	0.064453
7	1	0	0.185036	-1.373265	-0.018416
8	6	0	1.626960	0.044939	-0.031063
9	8	0	1.987190	1.216902	-0.061042
10	8	0	2.501718	-0.992277	-0.074944
11	1	0	3.392644	-0.623775	-0.122910
12	1	0	-2.375625	0.438449	1.472240
13	6	0	-3.164072	-0.167407	-0.440014
14	1	0	-2.862949	-0.741914	-1.322396
15	1	0	-4.061701	-0.637269	-0.026644
16	1	0	-3.442875	0.835669	-0.778965

Rotational constants (GHZ): 7.5209497 1.1366865 1.0425266
Standard basis: 6-311G(d) (5D, 7F)

Butylamine

Bu-1tgg

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.061151	1.053792	0.016690
2	1	0	-0.511372	1.718672	-0.733569
3	6	0	-1.161039	0.175220	0.614399
4	1	0	-0.766491	-0.399830	1.457983
5	1	0	-1.940553	0.820052	1.034029
6	7	0	-1.800731	-0.767528	-0.306726
7	1	0	-2.092301	-0.253532	-1.134306
8	1	0	-1.096264	-1.419088	-0.640104
9	6	0	1.090862	0.280103	-0.624938
10	1	0	0.715455	-0.300010	-1.477661
11	1	0	1.803876	0.997593	-1.049123
12	1	0	0.334876	1.706467	0.807514
13	6	0	1.818468	-0.647037	0.342301
14	1	0	1.172282	-1.455733	0.698005
15	1	0	2.688976	-1.113347	-0.129840
16	1	0	2.173797	-0.101012	1.223441

Rotational constants (GHZ): 7.8282898 3.0334986 2.7411101
Standard basis: 6-311G(d) (5D, 7F)

Bu-1tgt

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.013661	0.706233	0.229058
2	1	0	-0.035680	0.674022	1.328205
3	6	0	1.430037	0.554196	-0.246019
4	1	0	1.461399	0.618735	-1.339736
5	1	0	2.022696	1.397817	0.123513
6	7	0	2.115252	-0.680155	0.147604
7	1	0	2.030004	-0.780909	1.155799

8	1	0	1.606651	-1.469992	-0.237869
9	6	0	-0.960367	-0.350276	-0.330175
10	1	0	-0.377120	1.703919	-0.054773
11	1	0	-0.913437	-0.330578	-1.427544
12	1	0	-0.621019	-1.349560	-0.030099
13	6	0	-2.398443	-0.147951	0.129140
14	1	0	-2.783594	0.827333	-0.188100
15	1	0	-3.067597	-0.913856	-0.275962
16	1	0	-2.474463	-0.189051	1.221314

Rotational constants (GHZ): 12.1000538 2.3301842 2.1509525
Standard basis: 6-311G(d) (5D, 7F)

Bu-1tgq

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.045232	1.026455	0.359006
2	1	0	0.157544	0.825367	1.434197
3	6	0	1.246676	0.421332	-0.377379
4	1	0	1.021413	0.351153	-1.447969
5	1	0	2.095206	1.108637	-0.296668
6	7	0	1.717115	-0.893999	0.072722
7	1	0	1.898293	-0.835665	1.071058
8	1	0	0.960061	-1.562614	-0.015373
9	6	0	-1.329102	0.553736	-0.117009
10	1	0	-2.096876	1.086031	0.459009
11	1	0	0.084671	2.118794	0.252076
12	1	0	-1.469834	0.867194	-1.160290
13	6	0	-1.580789	-0.947219	-0.008035
14	1	0	-0.979565	-1.519359	-0.721443
15	1	0	-1.354483	-1.321793	0.996189
16	1	0	-2.628335	-1.185576	-0.219332

Rotational constants (GHZ): 7.2578351 3.3748046 2.5898156
Standard basis: 6-311G(d) (5D, 7F)

Bu-1ttg

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.082958	0.687409	0.267517
2	1	0	-0.098462	0.581813	1.361956
3	6	0	-1.006600	-0.361539	-0.343599
4	1	0	-0.965429	-0.288147	-1.436683
5	1	0	-0.657013	-1.367959	-0.094880
6	7	0	-2.410085	-0.266561	0.066402
7	1	0	-2.445211	-0.341119	1.079743
8	1	0	-2.731157	0.677486	-0.132573
9	6	0	1.359098	0.619754	-0.234787
10	1	0	-0.499658	1.680469	0.049445
11	1	0	1.366229	0.726887	-1.327949
12	1	0	1.913387	1.482604	0.154540
13	6	0	2.087660	-0.661504	0.158661
14	1	0	1.640187	-1.547762	-0.300830
15	1	0	3.137979	-0.633921	-0.148640

16	1	0	2.066539	-0.809148	1.244313

Rotational constants (GHZ): 12.0538594 2.3223902 2.1441949
Standard basis: 6-311G(d) (5D, 7F)

Bu-1ttt

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.024677	-0.321997	-0.000085
2	1	0	-0.029054	-0.982362	-0.879088
3	6	0	-1.299495	0.512481	-0.000185
4	1	0	-1.304692	1.172467	0.874679
5	1	0	-1.304756	1.172183	-0.875276
6	7	0	-2.551225	-0.248420	0.000073
7	1	0	-2.539023	-0.870163	-0.804268
8	1	0	-2.539204	-0.869470	0.804957
9	6	0	1.244092	0.523315	0.000148
10	1	0	-0.029185	-0.982375	0.878917
11	1	0	1.239147	1.184958	-0.876214
12	1	0	1.239058	1.184456	0.876876
13	6	0	2.512640	-0.319844	-0.000025
14	1	0	2.558093	-0.966986	-0.882741
15	1	0	3.414910	0.300099	0.000272
16	1	0	2.557923	-0.967592	0.882260

Rotational constants (GHZ): 17.8339283 1.9619279 1.8656713
Standard basis: 6-311G(d) (5D, 7F)

Bu-1ggg

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.039127	1.072448	0.010837
2	1	0	-0.457799	1.746110	-0.748027
3	6	0	-1.159626	0.210513	0.575743
4	1	0	-0.784836	-0.357632	1.440892
5	1	0	-1.947484	0.864859	0.962508
6	7	0	-1.752034	-0.648156	-0.454113
7	1	0	-1.064126	-1.346585	-0.720845
8	1	0	-2.510512	-1.175451	-0.032749
9	6	0	1.123784	0.287804	-0.601494
10	1	0	0.782038	-0.243783	-1.498778
11	1	0	1.877465	1.001922	-0.955221
12	1	0	0.343878	1.711131	0.817994
13	6	0	1.773082	-0.700984	0.360490
14	1	0	1.088094	-1.507839	0.639910
15	1	0	2.657051	-1.167861	-0.085258
16	1	0	2.091781	-0.206466	1.284911

Rotational constants (GHZ): 7.7995923 3.0830108 2.7594957
Standard basis: 6-311G(d) (5D, 7F)

Bu-1ggt

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.025921	0.709725	-0.215030
2	1	0	0.053415	0.730873	-1.313016
3	6	0	-1.414837	0.550362	0.243749
4	1	0	-1.444959	0.587701	1.345053
5	1	0	-2.000879	1.405170	-0.108847
6	7	0	-2.028035	-0.665613	-0.300054
7	1	0	-1.600640	-1.469631	0.149458
8	1	0	-3.000523	-0.690120	-0.009440
9	6	0	0.962372	-0.381420	0.296154
10	1	0	0.396315	1.686443	0.124102
11	1	0	0.888708	-0.436842	1.390810
12	1	0	0.639079	-1.359654	-0.081022
13	6	0	2.409767	-0.140668	-0.112920
14	1	0	2.780501	0.811930	0.281197
15	1	0	3.073984	-0.929889	0.253486
16	1	0	2.511897	-0.104674	-1.203120

Rotational constants (GHZ): 12.4063893 2.3390784 2.1495987
Standard basis: 6-311G(d) (5D, 7F)

Bu-1ggq

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.018990	1.031917	-0.356757
2	1	0	-0.117965	0.842244	-1.433971
3	6	0	-1.233862	0.437482	0.351457
4	1	0	-1.010664	0.345438	1.427037
5	1	0	-2.070992	1.138376	0.274425
6	7	0	-1.679277	-0.825193	-0.251949
7	1	0	-0.963369	-1.529431	-0.109599
8	1	0	-2.484901	-1.158483	0.269067
9	6	0	1.340514	0.534313	0.138510
10	1	0	2.125602	1.064762	-0.415204
11	1	0	-0.042860	2.122166	-0.236771
12	1	0	1.464675	0.829356	1.189005
13	6	0	1.570199	-0.968133	0.010491
14	1	0	0.925657	-1.540450	0.685515
15	1	0	1.380296	-1.318497	-1.009978
16	1	0	2.602291	-1.232602	0.261916

Rotational constants (GHZ): 7.3495406 3.3833782 2.5926779
Standard basis: 6-311G(d) (5D, 7F)

Bu-1gtg

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.070147	0.709255	-0.260842
2	1	0	0.069977	0.673824	-1.358627
3	6	0	0.994465	-0.374593	0.269425
4	1	0	0.920583	-0.399787	1.368977

5	1	0	0.663571	-1.355845	-0.084105
6	7	0	2.364087	-0.167094	-0.208177
7	1	0	2.712509	0.695275	0.201642
8	1	0	2.954494	-0.899600	0.173735
9	6	0	-1.361889	0.608189	0.261326
10	1	0	0.485665	1.688659	0.014752
11	1	0	-1.355644	0.685973	1.356777
12	1	0	-1.931283	1.474208	-0.097742
13	6	0	-2.079185	-0.671633	-0.155738
14	1	0	-1.620775	-1.562051	0.284820
15	1	0	-3.128408	-0.660782	0.156182
16	1	0	-2.060528	-0.797519	-1.244202

Rotational constants (GHZ): 12.1670638 2.3487425 2.1483453
Standard basis: 6-311G(d) (5D, 7F)

Bu-1gtt

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.014838	-0.331268	-0.041889
2	1	0	-0.002070	-0.922328	-0.967251
3	6	0	-1.292780	0.486539	0.007514
4	1	0	-1.290292	1.101343	0.921736
5	1	0	-1.307413	1.187666	-0.834392
6	7	0	-2.474482	-0.374355	-0.097561
7	1	0	-2.506225	-0.963052	0.730451
8	1	0	-3.304063	0.208392	-0.038275
9	6	0	1.242732	0.525676	0.041678
10	1	0	-0.017457	-1.056322	0.784931
11	1	0	1.239947	1.254296	-0.779763
12	1	0	1.222290	1.114720	0.967947
13	6	0	2.519553	-0.303004	-0.011488
14	1	0	2.580590	-0.877701	-0.942108
15	1	0	3.414997	0.323861	0.047422
16	1	0	2.563064	-1.018048	0.817339

Rotational constants (GHZ): 18.1577279 1.9721858 1.8701954
Standard basis: 6-311G(d) (5D, 7F)

Bu-1gtq

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.068484	0.717934	-0.235920
2	1	0	-0.463540	1.708152	0.024411
3	6	0	-1.008590	-0.333474	0.329411
4	1	0	-0.660918	-1.336958	0.045065
5	1	0	-0.977018	-0.293308	1.424365
6	7	0	-2.388786	-0.077298	-0.096865
7	1	0	-2.426532	-0.183573	-1.107199
8	1	0	-2.979698	-0.819118	0.266342
9	6	0	1.372352	0.594738	0.257668
10	1	0	-0.083433	0.660583	-1.334234
11	1	0	1.943791	1.457736	-0.105449
12	1	0	1.386318	0.665083	1.353592

13	6	0	2.072311	-0.687462	-0.182239
14	1	0	3.126662	-0.686642	0.112345
15	1	0	1.614870	-1.578792	0.256742
16	1	0	2.035466	-0.802501	-1.271445

Rotational constants (GHZ): 12.1168669 2.3274569 2.1521146
Standard basis: 6-311G(d) (5D, 7F)

Bu-1gqg

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.056387	-0.988429	0.389401
2	6	0	1.373266	-0.447798	-0.151033
3	1	0	2.195607	-0.949915	0.383513
4	1	0	1.472108	-0.736515	-1.204370
5	7	0	1.466921	1.013085	-0.071921
6	1	0	1.335705	1.285265	0.898424
7	1	0	2.415339	1.289472	-0.306369
8	1	0	-0.029731	-0.732677	1.455751
9	1	0	0.121931	-2.083040	0.352287
10	6	0	-1.207532	-0.534029	-0.348244
11	1	0	-1.992872	-1.285587	-0.198287
12	1	0	-1.009068	-0.522804	-1.428497
13	6	0	-1.743138	0.823995	0.094449
14	1	0	-1.011761	1.614650	-0.082056
15	1	0	-2.662969	1.085838	-0.439691
16	1	0	-1.976632	0.821290	1.165296

Rotational constants (GHZ): 7.3934615 3.3511068 2.5935635
Standard basis: 6-311G(d) (5D, 7F)

Bu-1gqt

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.023895	0.672261	0.254882
2	6	0	-1.412123	0.550156	-0.232163
3	1	0	-1.993611	1.402479	0.152486
4	1	0	-1.432529	0.632018	-1.325055
5	7	0	-1.997872	-0.742392	0.137243
6	1	0	-2.063826	-0.776072	1.150908
7	1	0	-2.957147	-0.768980	-0.194013
8	1	0	0.043171	0.552600	1.348287
9	1	0	0.374497	1.694289	0.059205
10	6	0	0.988012	-0.321654	-0.383645
11	1	0	0.977015	-0.181346	-1.473068
12	1	0	0.630758	-1.341479	-0.206023
13	6	0	2.409861	-0.171851	0.141032
14	1	0	3.094888	-0.885806	-0.327527
15	1	0	2.801471	0.833577	-0.049735
16	1	0	2.452547	-0.338005	1.223206

Rotational constants (GHZ): 12.2863766 2.3177677 2.1588576
Standard basis: 6-311G(d) (5D, 7F)

Bu-1gqq

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.032054	1.016793	0.107410
2	6	0	1.133006	0.103367	0.629328
3	1	0	1.861679	0.717675	1.181067
4	1	0	0.719820	-0.602332	1.357421
5	7	0	1.748903	-0.668738	-0.452921
6	1	0	2.187514	-0.014145	-1.094853
7	1	0	2.509684	-1.218925	-0.067171
8	1	0	0.481726	1.755773	-0.570801
9	1	0	-0.369499	1.589355	0.954220
10	6	0	-1.115169	0.305925	-0.610575
11	1	0	-0.728366	-0.210358	-1.496150
12	1	0	-1.816539	1.062848	-0.983561
13	6	0	-1.865446	-0.686025	0.270855
14	1	0	-2.737132	-1.099734	-0.246293
15	1	0	-1.234213	-1.530334	0.564159
16	1	0	-2.223661	-0.209014	1.190298

Rotational constants (GHZ): 8.1179320 2.9343404 2.7046253
Standard basis: 6-311G(d) (5D, 7F)

Butylcarbamic acid

Bu-2tgg

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.191010	-1.036934	0.401189
2	1	0	0.543966	-1.402363	1.206992
3	6	0	0.357531	-0.884019	-0.869084
4	1	0	0.992983	-0.683739	-1.733408
5	1	0	-0.179410	-1.810521	-1.082566
6	7	0	-0.613365	0.196523	-0.798336
7	1	0	-0.284015	1.133881	-0.977222
8	6	0	1.884726	0.248470	0.849131
9	1	0	1.127796	0.993227	1.126318
10	1	0	2.445702	0.039865	1.767821
11	1	0	1.937946	-1.820786	0.221275
12	6	0	2.822866	0.837394	-0.198190
13	1	0	2.282949	1.175464	-1.088564
14	1	0	3.367041	1.701393	0.195551
15	1	0	3.564795	0.100716	-0.525922
16	6	0	-1.706149	0.083241	-0.021417
17	8	0	-2.327123	1.277801	0.138279
18	8	0	-2.133261	-0.955638	0.467145
19	1	0	-3.123032	1.130980	0.664913

Rotational constants (GHZ): 3.7244710 1.1161351 1.0175108
Standard basis: 6-311G(d) (5D, 7F)

Bu-2tgt

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.251684	-0.737807	0.341224
2	1	0	0.869297	-0.310116	1.276749
3	6	0	0.086104	-1.306930	-0.458523
4	1	0	0.443011	-1.750998	-1.391076
5	1	0	-0.413607	-2.099400	0.102083
6	7	0	-0.915336	-0.314032	-0.812231
7	1	0	-0.740182	0.282501	-1.606665
8	6	0	2.052838	0.311480	-0.420043
9	1	0	1.909551	-1.568700	0.626930
10	1	0	2.421831	-0.125624	-1.357476
11	1	0	1.394226	1.139874	-0.709114
12	6	0	3.220524	0.851200	0.394762
13	1	0	3.916723	0.051132	0.668926
14	1	0	3.787594	1.606552	-0.158309
15	1	0	2.873241	1.314936	1.324454
16	6	0	-1.794389	0.130482	0.102663
17	8	0	-1.995800	-0.367100	1.204150
18	8	0	-2.482999	1.206532	-0.351442
19	1	0	-3.124515	1.452061	0.326951

Rotational constants (GHZ): 3.7271450 0.9716919 0.9214439
Standard basis: 6-311G(d) (5D, 7F)

Bu-2tgq

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.338827	-1.004893	-0.416763
2	1	0	-0.760175	-0.818156	-1.329954
3	6	0	-0.369835	-1.176183	0.750769
4	1	0	-0.912641	-1.224202	1.697843
5	1	0	0.171196	-2.119611	0.647666
6	7	0	0.619002	-0.115557	0.878153
7	1	0	0.364674	0.718026	1.384970
8	6	0	-2.402360	0.078556	-0.245347
9	1	0	-3.080210	0.021662	-1.106076
10	1	0	-1.840976	-1.968644	-0.567859
11	1	0	-3.016988	-0.153935	0.634346
12	6	0	-1.869625	1.505252	-0.132848
13	1	0	-1.407133	1.702124	0.838243
14	1	0	-1.120298	1.715796	-0.903720
15	1	0	-2.677835	2.234387	-0.249000
16	6	0	1.600024	0.012420	-0.031581
17	8	0	2.235500	1.204423	0.086911
18	8	0	1.924246	-0.830756	-0.859388
19	1	0	2.953150	1.221199	-0.559084

Rotational constants (GHZ): 3.2105739 1.2796342 1.0855154
Standard basis: 6-311G(d) (5D, 7F)

Bu-2ttg

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.147396	-0.610458	0.603215
2	1	0	-0.788265	0.175203	1.280271
3	6	0	-0.327204	-0.565536	-0.680732
4	1	0	-0.667397	-1.335272	-1.378060
5	1	0	-0.441982	0.394904	-1.185149
6	7	0	1.092532	-0.772046	-0.456984
7	1	0	1.430370	-1.713295	-0.324436
8	6	0	-2.646030	-0.441182	0.362508
9	1	0	-0.958917	-1.567651	1.104670
10	1	0	-2.995749	-1.228427	-0.318572
11	1	0	-3.173671	-0.606688	1.309323
12	6	0	-3.028456	0.927205	-0.192798
13	1	0	-2.625347	1.093658	-1.196132
14	1	0	-4.115147	1.039344	-0.259435
15	1	0	-2.652850	1.731554	0.449348
16	6	0	1.875555	0.231707	-0.028127
17	8	0	3.114184	-0.210355	0.302853
18	8	0	1.553851	1.412397	0.042062
19	1	0	3.638136	0.554241	0.573344

Rotational constants (GHZ): 4.8585971 0.9075817 0.8315880
Standard basis: 6-311G(d) (5D, 7F)

Bu-2ttt

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.170174	0.137801	-0.292508
2	1	0	-0.835894	-0.899825	-0.416188
3	6	0	-0.140232	0.895616	0.534104
4	1	0	-0.437898	1.939856	0.654374
5	1	0	-0.071452	0.467291	1.537082
6	7	0	1.190552	0.888689	-0.046332
7	1	0	1.416831	1.569592	-0.755234
8	6	0	-2.550015	0.162465	0.352880
9	1	0	-1.220537	0.573881	-1.298436
10	1	0	-2.485058	-0.259480	1.364300
11	1	0	-2.874050	1.203789	0.479473
12	6	0	-3.584997	-0.604238	-0.459483
13	1	0	-3.299538	-1.655617	-0.572934
14	1	0	-4.571770	-0.579718	0.013418
15	1	0	-3.690790	-0.183493	-1.465254
16	6	0	1.980637	-0.192994	0.048895
17	8	0	3.098280	-0.060599	-0.707794
18	8	0	1.763349	-1.181045	0.741168
19	1	0	3.631931	-0.855852	-0.586596

Rotational constants (GHZ): 5.2121052 0.8012106 0.7691289
Standard basis: 6-311G(d) (5D, 7F)

Bu-2ttq

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.112026	-0.209234	-0.639503

2	1	0	-0.512797	-1.047792	-1.013338
3	6	0	-0.358004	0.440820	0.515447
4	1	0	-0.868781	1.338211	0.867734
5	1	0	-0.302356	-0.247870	1.362508
6	7	0	0.995973	0.831867	0.165255
7	1	0	1.145520	1.720555	-0.287360
8	6	0	-2.499427	-0.708954	-0.242606
9	1	0	-1.196457	0.510167	-1.464446
10	1	0	-2.926126	-1.264571	-1.086149
11	1	0	-2.402113	-1.433401	0.576835
12	6	0	-3.461721	0.402234	0.164596
13	1	0	-4.465318	0.008955	0.354457
14	1	0	-3.138925	0.915025	1.075593
15	1	0	-3.547970	1.157420	-0.624591
16	6	0	1.979979	-0.078367	0.088346
17	8	0	3.114709	0.456123	-0.427500
18	8	0	1.905591	-1.246501	0.452674
19	1	0	3.788314	-0.235741	-0.437098

Rotational constants (GHZ): 5.8754652 0.8310251 0.7846619
Standard basis: 6-311G(d) (5D, 7F)

Bu-2tqg

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.841949	-0.856011	-0.274052
2	6	0	0.512147	-1.407191	0.233772
3	1	0	0.498471	-2.495199	0.117413
4	1	0	0.383830	-1.199500	1.297442
5	7	0	-0.644336	-0.865935	-0.456843
6	1	0	-0.680330	-0.953813	-1.461459
7	1	0	1.836856	-0.873779	-1.372462
8	1	0	2.623752	-1.561605	0.032612
9	6	0	2.226624	0.537501	0.222479
10	1	0	3.243103	0.749245	-0.132212
11	1	0	2.290855	0.520049	1.318463
12	6	0	1.305258	1.673127	-0.213536
13	1	0	1.110184	1.642321	-1.290732
14	1	0	0.342977	1.643685	0.302114
15	1	0	1.755478	2.645635	0.010809
16	6	0	-1.531069	-0.044673	0.120307
17	8	0	-1.581554	0.253142	1.309081
18	8	0	-2.416411	0.437274	-0.788885
19	1	0	-3.040561	1.004657	-0.319476

Rotational constants (GHZ): 3.1010956 1.3172362 1.1445139
Standard basis: 6-311G(d) (5D, 7F)

Bu-2tqt

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.446407	0.958366	-0.125639
2	6	0	-0.082053	1.493703	0.291619
3	1	0	-0.025774	2.569993	0.110167

4	1	0	0.081879	1.340004	1.359740
5	7	0	1.022640	0.864596	-0.410427
6	1	0	1.110469	1.032363	-1.401929
7	1	0	-1.596180	1.147956	-1.197161
8	1	0	-2.213214	1.543462	0.398575
9	6	0	-1.646445	-0.524934	0.164556
10	1	0	-1.475367	-0.713232	1.231860
11	1	0	-0.890623	-1.111381	-0.372295
12	6	0	-3.035883	-1.005369	-0.232802
13	1	0	-3.170444	-2.071993	-0.027322
14	1	0	-3.815521	-0.463450	0.313478
15	1	0	-3.218262	-0.850429	-1.301864
16	6	0	1.661698	-0.208205	0.085176
17	8	0	2.489364	-0.757832	-0.838673
18	8	0	1.561636	-0.649058	1.224089
19	1	0	2.941089	-1.501709	-0.421043

Rotational constants (GHZ): 3.3337986 1.1042710 0.9882404
Standard basis: 6-311G(d) (5D, 7F)

Bu-2tqq

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.564330	1.100153	0.207840
2	6	0	0.382566	1.213725	-0.750915
3	1	0	0.369290	2.206570	-1.208097
4	1	0	0.455868	0.492090	-1.565096
5	7	0	-0.896143	1.002648	-0.096899
6	1	0	-1.166910	1.653203	0.626133
7	1	0	1.440646	1.851492	0.998312
8	1	0	2.473666	1.378944	-0.340297
9	6	0	1.746081	-0.281137	0.834466
10	1	0	0.820684	-0.580445	1.343517
11	1	0	2.505144	-0.207932	1.622620
12	6	0	2.161150	-1.356437	-0.163039
13	1	0	2.330760	-2.316048	0.335593
14	1	0	1.399027	-1.521185	-0.928825
15	1	0	3.090703	-1.081869	-0.673905
16	6	0	-1.520917	-0.186456	-0.105087
17	8	0	-2.559770	-0.199536	0.768215
18	8	0	-1.245772	-1.147680	-0.813351
19	1	0	-3.000796	-1.054722	0.689831

Rotational constants (GHZ): 3.0975637 1.3206917 1.1237859
Standard basis: 6-311G(d) (5D, 7F)

Bu-2cgt

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.540701	0.685517	-0.492080
2	1	0	1.600397	0.304986	-1.520666
3	6	0	0.098926	1.030539	-0.162760
4	1	0	0.023679	1.395377	0.866924
5	1	0	-0.256663	1.836006	-0.814467

6	7	0	-0.761985	-0.130597	-0.314860
7	1	0	-0.391052	-0.975667	-0.721675
8	6	0	2.176384	-0.314159	0.469337
9	1	0	2.116952	1.617979	-0.479393
10	1	0	2.087964	0.069264	1.494111
11	1	0	1.622974	-1.260898	0.451188
12	6	0	3.638911	-0.576875	0.136636
13	1	0	4.228799	0.344835	0.185131
14	1	0	4.089630	-1.294121	0.829503
15	1	0	3.748502	-0.982573	-0.874978
16	6	0	-2.050048	-0.098070	0.045053
17	8	0	-2.669448	-1.282301	-0.191345
18	8	0	-2.627559	0.868442	0.532392
19	1	0	-3.590470	-1.191839	0.082850

Rotational constants (GHZ): 5.1444447 0.8114448 0.7443528
Standard basis: 6-311G(d) (5D, 7F)

Bu-2ctg

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.441760	-0.917402	-0.149895
2	1	0	1.372812	-0.984043	-1.243143
3	6	0	0.328200	-0.022133	0.367874
4	1	0	0.422024	0.103411	1.454277
5	1	0	0.388082	0.973358	-0.075055
6	7	0	-0.971037	-0.575694	0.034312
7	1	0	-1.075896	-1.577544	-0.023100
8	6	0	2.830998	-0.427548	0.252465
9	1	0	1.289736	-1.933792	0.236011
10	1	0	2.896686	-0.381032	1.347322
11	1	0	3.567873	-1.175684	-0.062353
12	6	0	3.202135	0.925977	-0.344268
13	1	0	2.566632	1.732319	0.033813
14	1	0	4.236886	1.193260	-0.108519
15	1	0	3.104812	0.915063	-1.435560
16	6	0	-2.075594	0.181670	-0.003207
17	8	0	-2.117671	1.397233	0.154413
18	8	0	-3.182214	-0.561851	-0.256864
19	1	0	-3.938310	0.038098	-0.282082

Rotational constants (GHZ): 5.4816480 0.7996850 0.7244333
Standard basis: 6-311G(d) (5D, 7F)

Bu-2ctt, C_s (TS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.485535	0.153523	-0.000000
2	1	0	-1.732930	-0.454857	0.879696
3	6	0	0.000000	0.460803	0.000000
4	1	0	0.263664	1.057571	-0.879918
5	1	0	0.263664	1.057571	0.879918
6	7	0	0.775055	-0.767402	0.000000
7	1	0	0.299857	-1.656799	0.000000

8	6	0	-2.329905	1.421526	-0.000000
9	1	0	-1.732930	-0.454857	-0.879696
10	1	0	-2.073329	2.028955	0.877249
11	1	0	-2.073329	2.028955	-0.877249
12	6	0	-3.822427	1.120206	-0.000000
13	1	0	-4.109535	0.538733	0.882688
14	1	0	-4.420408	2.036702	-0.000000
15	1	0	-4.109535	0.538733	-0.882688
16	6	0	2.112826	-0.747398	0.000000
17	8	0	2.807667	0.263654	0.000000
18	8	0	2.636310	-1.999392	0.000000
19	1	0	3.597864	-1.914952	0.000000

Rotational constants (GHZ): 7.4991681 0.6875392 0.6397511

Bu-2ctt, C_1 (UBM)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.439695	-0.377698	-0.032964
2	1	0	1.410222	-0.847921	-1.024009
3	6	0	0.164726	0.415634	0.185473
4	1	0	0.186834	0.906250	1.166398
5	1	0	0.075763	1.205764	-0.564827
6	7	0	-0.998979	-0.446469	0.083226
7	1	0	-0.893302	-1.434163	0.259301
8	6	0	2.682846	0.494812	0.087408
9	1	0	1.492998	-1.194718	0.699121
10	1	0	2.619879	1.318315	-0.635389
11	1	0	2.704837	0.962117	1.080178
12	6	0	3.965351	-0.294005	-0.139611
13	1	0	3.981972	-0.745107	-1.137566
14	1	0	4.852324	0.340701	-0.050069
15	1	0	4.065808	-1.105928	0.588716
16	6	0	-2.236887	0.052437	-0.028675
17	8	0	-2.521277	1.240139	-0.140549
18	8	0	-3.173697	-0.929413	-0.019171
19	1	0	-4.039070	-0.512915	-0.116460

Rotational constants (GHZ): 7.4192448 0.6878464 0.6418557
Standard basis: 6-311G(d) (5D, 7F)

Bu-3tgg

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.138443	1.053359	-0.367577
2	1	0	0.477999	1.423603	-1.159883
3	6	0	0.318930	0.829947	0.901259
4	1	0	0.970849	0.626830	1.752775
5	1	0	-0.248195	1.727873	1.152226
6	7	0	-0.604625	-0.294310	0.812647
7	1	0	-0.221483	-1.212887	0.979546
8	6	0	1.875550	-0.190986	-0.860181
9	1	0	1.144674	-0.952704	-1.160201
10	1	0	2.424867	0.068559	-1.772916
11	1	0	1.859014	1.855775	-0.162924

12	6	0	2.838843	-0.780322	0.163817
13	1	0	2.315877	-1.168029	1.044019
14	1	0	3.412352	-1.609939	-0.260990
15	1	0	3.554968	-0.028539	0.513886
16	6	0	-1.705938	-0.309763	0.036033
17	8	0	-2.344433	-1.315530	-0.255411
18	8	0	-2.075839	0.925688	-0.366850
19	1	0	-2.891336	0.834948	-0.876086

Rotational constants (GHZ): 3.7308242 1.1275547 1.0301224
Standard basis: 6-311G(d) (5D, 7F)

Bu-3tgt

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.205854	0.737016	0.350167
2	1	0	-0.819059	0.291110	1.275021
3	6	0	-0.045561	1.302515	-0.459989
4	1	0	-0.416571	1.771827	-1.374615
5	1	0	0.478716	2.077158	0.101689
6	7	0	0.926144	0.297054	-0.871748
7	1	0	0.701656	-0.260717	-1.681603
8	6	0	-2.032144	-0.291138	-0.413457
9	1	0	-1.848280	1.573289	0.654978
10	1	0	-2.401738	0.160569	-1.343700
11	1	0	-1.390628	-1.128259	-0.715344
12	6	0	-3.201602	-0.817999	0.407162
13	1	0	-3.881922	-0.008907	0.694312
14	1	0	-3.785947	-1.558969	-0.147373
15	1	0	-2.854096	-1.295767	1.329645
16	6	0	1.807471	-0.292320	-0.040568
17	8	0	1.937407	0.365294	1.133242
18	8	0	2.461245	-1.294943	-0.308559
19	1	0	2.611787	-0.091968	1.651874

Rotational constants (GHZ): 3.6732379 0.9925361 0.9412202
Standard basis: 6-311G(d) (5D, 7F)

Bu-3tgq

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.390802	-0.950502	-0.470692
2	1	0	-0.927769	-0.682837	-1.427947
3	6	0	-0.316975	-1.430019	0.501405
4	1	0	-0.784629	-1.805707	1.414604
5	1	0	0.241441	-2.262967	0.069104
6	7	0	0.631675	-0.406259	0.923551
7	1	0	0.353014	0.184460	1.692315
8	6	0	-2.243727	0.217679	0.035865
9	1	0	-3.223611	0.172920	-0.453914
10	1	0	-2.033255	-1.815616	-0.675720
11	1	0	-2.441495	0.087759	1.108458
12	6	0	-1.646239	1.599551	-0.221030
13	1	0	-0.709661	1.767138	0.315552

14	1	0	-1.439176	1.741538	-1.287369
15	1	0	-2.339233	2.390275	0.084796
16	6	0	1.527886	0.175474	0.103081
17	8	0	2.126943	1.218287	0.345257
18	8	0	1.735328	-0.535157	-1.026428
19	1	0	2.403639	-0.071279	-1.547147

Rotational constants (GHZ): 2.9390371 1.4156416 1.1788574
Standard basis: 6-311G(d) (5D, 7F)

Bu-3ttg

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.112695	-0.611158	-0.610313
2	1	0	0.743758	0.186468	-1.267356
3	6	0	0.295790	-0.612245	0.676504
4	1	0	0.642513	-1.406215	1.342848
5	1	0	0.410008	0.325750	1.220048
6	7	0	-1.125119	-0.833458	0.451769
7	1	0	-1.438548	-1.782473	0.316278
8	6	0	2.609955	-0.430875	-0.368462
9	1	0	0.934203	-1.557588	-1.135332
10	1	0	2.968414	-1.224876	0.300093
11	1	0	3.138010	-0.576764	-1.318248
12	6	0	2.979284	0.932921	0.206529
13	1	0	2.571441	1.082737	1.210568
14	1	0	4.064786	1.053101	0.278349
15	1	0	2.599199	1.742564	-0.426239
16	6	0	-1.982368	0.098919	-0.001909
17	8	0	-3.130633	-0.123940	-0.372619
18	8	0	-1.457514	1.345289	0.019978
19	1	0	-2.144908	1.955335	-0.276348

Rotational constants (GHZ): 4.7364845 0.9308943 0.8490390
Standard basis: 6-311G(d) (5D, 7F)

Bu-3ttt

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.140573	-0.172167	-0.290211
2	1	0	0.797204	0.848025	-0.501062
3	6	0	0.108486	-0.879117	0.577592
4	1	0	0.415281	-1.910301	0.768099
5	1	0	0.028536	-0.391143	1.551179
6	7	0	-1.217297	-0.936560	-0.019618
7	1	0	-1.413702	-1.682948	-0.668576
8	6	0	2.510672	-0.128917	0.375000
9	1	0	1.211710	-0.685624	-1.257665
10	1	0	2.426936	0.378295	1.345012
11	1	0	2.840761	-1.152441	0.595864
12	6	0	3.552148	0.573796	-0.485499
13	1	0	3.259511	1.608098	-0.696074
14	1	0	4.530999	0.601318	0.003419
15	1	0	3.678421	0.066910	-1.448243

16	6	0	-2.070977	0.100030	-0.093350
17	8	0	-3.109778	0.110504	-0.746408
18	8	0	-1.682878	1.149458	0.666487
19	1	0	-2.358740	1.834280	0.583551

Rotational constants (GHZ): 5.0899615 0.8176056 0.7831203
Standard basis: 6-311G(d) (5D, 7F)

Bu-3ttq

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.084583	0.189218	0.647141
2	1	0	-0.477264	1.012823	1.039799
3	6	0	-0.334068	-0.456381	-0.512491
4	1	0	-0.859040	-1.341753	-0.874552
5	1	0	-0.267802	0.236303	-1.354610
6	7	0	1.010397	-0.888113	-0.160794
7	1	0	1.125272	-1.800322	0.252838
8	6	0	-2.461949	0.714271	0.247143
9	1	0	-1.186257	-0.541690	1.459931
10	1	0	-2.886071	1.265673	1.094703
11	1	0	-2.348511	1.447300	-0.562562
12	6	0	-3.438004	-0.377316	-0.180068
13	1	0	-4.434530	0.033205	-0.370623
14	1	0	-3.117566	-0.883170	-1.095767
15	1	0	-3.540097	-1.141202	0.598790
16	6	0	2.066501	-0.070792	-0.006322
17	8	0	3.157256	-0.408708	0.443574
18	8	0	1.817830	1.188472	-0.432589
19	1	0	2.631016	1.697502	-0.322690

Rotational constants (GHZ): 5.7844072 0.8453069 0.7956836
Standard basis: 6-311G(d) (5D, 7F)

Bu-3tqg

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.773524	-0.845192	-0.167010
2	6	0	0.431503	-1.547448	0.012257
3	1	0	0.490128	-2.557758	-0.402128
4	1	0	0.196529	-1.656941	1.071243
5	7	0	-0.692436	-0.882540	-0.630649
6	1	0	-0.683979	-0.836863	-1.638717
7	1	0	2.006752	-0.775645	-1.237962
8	1	0	2.529001	-1.515158	0.262032
9	6	0	1.895952	0.538083	0.481757
10	1	0	2.955518	0.725557	0.693222
11	1	0	1.395310	0.529130	1.457596
12	6	0	1.374312	1.697190	-0.363796
13	1	0	1.872608	1.721430	-1.339137
14	1	0	0.299804	1.648665	-0.552750
15	1	0	1.569328	2.656899	0.125943
16	6	0	-1.507410	0.019827	-0.058143
17	8	0	-1.391867	0.066367	1.287336

18	8	0	-2.303896	0.726529	-0.670374
19	1	0	-2.025128	0.720541	1.609120

Rotational constants (GHZ): 2.8253141 1.4689821 1.2358608
Standard basis: 6-311G(d) (5D, 7F)

Bu-3tqt

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.417750	0.969728	-0.074321
2	6	0	-0.040059	1.475132	0.336714
3	1	0	0.016641	2.558654	0.204294
4	1	0	0.148214	1.275803	1.391867
5	7	0	1.043059	0.884957	-0.436979
6	1	0	1.082747	1.117021	-1.418502
7	1	0	-1.586455	1.209024	-1.133009
8	1	0	-2.167817	1.538240	0.490777
9	6	0	-1.629112	-0.522489	0.153623
10	1	0	-1.450995	-0.757611	1.210428
11	1	0	-0.884918	-1.093866	-0.414919
12	6	0	-3.027270	-0.971443	-0.250134
13	1	0	-3.172083	-2.043896	-0.086280
14	1	0	-3.795931	-0.443374	0.324519
15	1	0	-3.217006	-0.771656	-1.310403
16	6	0	1.720089	-0.233843	-0.119855
17	8	0	2.464063	-0.839299	-0.885846
18	8	0	1.537555	-0.620462	1.162859
19	1	0	2.077862	-1.407458	1.307816

Rotational constants (GHZ): 3.2970621 1.1195674 1.0021511
Standard basis: 6-311G(d) (5D, 7F)

Bu-3tqq

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.515001	-1.121236	0.185239
2	6	0	-0.326943	-1.206893	-0.768998
3	1	0	-0.310220	-2.188207	-1.250271
4	1	0	-0.397877	-0.469578	-1.567672
5	7	0	0.951526	-1.028659	-0.095933
6	1	0	1.210748	-1.729648	0.582630
7	1	0	-1.384917	-1.883757	0.963726
8	1	0	-2.418431	-1.402856	-0.371286
9	6	0	-1.717685	0.248347	0.830746
10	1	0	-0.788195	0.569694	1.318075
11	1	0	-2.452860	0.148705	1.638349
12	6	0	-2.191292	1.318393	-0.146011
13	1	0	-2.340298	2.278827	0.357616
14	1	0	-1.474258	1.485124	-0.953921
15	1	0	-3.145111	1.035981	-0.605040
16	6	0	1.619372	0.130509	0.047102
17	8	0	2.570360	0.298140	0.805166
18	8	0	1.168506	1.108607	-0.768769
19	1	0	1.719106	1.887627	-0.620324

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---------------------------------------------------------------------
Rotational constants (GHZ):    3.0808642    1.3402986    1.1340464
Standard basis: 6-311G(d) (5D, 7F)
```

Bu-3cgg

```
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0        1.653517    1.078174   -0.218873
     2          1           0        1.563740    1.721695   -1.103456
     3          6           0        0.286041    0.938398    0.432163
     4          1           0        0.353253    0.341223    1.344249
     5          1           0       -0.087071    1.925928    0.724563
     6          7           0       -0.654171    0.304076   -0.480433
     7          1           0       -0.410690    0.234665   -1.456600
     8          6           0        2.319219   -0.242389   -0.608574
     9          1           0        1.725356   -0.750741   -1.378343
    10          1           0        3.280910   -0.012914   -1.082726
    11          1           0        2.297470    1.616218    0.486774
    12          6           0        2.545777   -1.183999    0.568226
    13          1           0        1.603912   -1.539083    0.997401
    14          1           0        3.114697   -2.068151    0.264564
    15          1           0        3.106323   -0.689443    1.369294
    16          6           0       -1.872483   -0.150191   -0.155810
    17          8           0       -2.146878    0.010970    1.159945
    18          8           0       -2.669813   -0.660510   -0.938072
    19          1           0       -3.027598   -0.351568    1.319543
---------------------------------------------------------------------
Rotational constants (GHZ):    3.8311692    0.9591827    0.9491099
Standard basis: 6-311G(d) (5D, 7F)
```

Bu-3cgt

```
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -1.519525    0.670799    0.501915
     2          1           0       -1.587956    0.269920    1.522213
     3          6           0       -0.067937    0.976885    0.175464
     4          1           0        0.013426    1.357063   -0.847606
     5          1           0        0.311819    1.757864    0.842022
     6          7           0        0.752766   -0.219287    0.310265
     7          1           0        0.334453   -1.057275    0.683992
     8          6           0       -2.190390   -0.286289   -0.478815
     9          1           0       -2.065349    1.621414    0.511670
    10          1           0       -2.097764    0.119682   -1.494480
    11          1           0       -1.664915   -1.249008   -0.488169
    12          6           0       -3.657638   -0.514744   -0.141699
    13          1           0       -4.220445    0.424801   -0.161134
    14          1           0       -4.134086   -1.199630   -0.849907
    15          1           0       -3.772051   -0.944049    0.859562
    16          6           0        2.056783   -0.303924    0.014001
    17          8           0        2.751357   -1.307697    0.147961
    18          8           0        2.548711    0.863812   -0.462793
    19          1           0        3.485194    0.728944   -0.656559
---------------------------------------------------------------------
Rotational constants (GHZ):    5.2713327    0.8097252    0.7441322
```

Standard basis: 6-311G(d) (5D, 7F)

Bu-3cgq

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.689804	-0.963717	-0.546323
2	1	0	-1.669292	-0.623094	-1.590264
3	6	0	-0.261307	-1.093377	-0.032721
4	1	0	-0.262761	-1.185934	1.058774
5	1	0	0.195859	-2.004291	-0.430141
6	7	0	0.557216	0.047838	-0.425659
7	1	0	0.129911	0.806088	-0.933502
8	6	0	-2.606496	-0.065399	0.284740
9	1	0	-3.619368	-0.137237	-0.130249
10	1	0	-2.119442	-1.971120	-0.568922
11	1	0	-2.669565	-0.470631	1.303023
12	6	0	-2.196706	1.402084	0.348106
13	1	0	-1.258135	1.543762	0.890868
14	1	0	-2.067754	1.824875	-0.654947
15	1	0	-2.957844	1.999820	0.859329
16	6	0	1.834814	0.237852	-0.068983
17	8	0	2.515388	1.218093	-0.359286
18	8	0	2.318766	-0.795612	0.659321
19	1	0	3.241643	-0.601620	0.866441

Rotational constants (GHZ): 3.8414397 1.0410868 0.8980494
Standard basis: 6-311G(d) (5D, 7F)

Bu-3ctg

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.443819	-0.930329	-0.058586
2	1	0	1.440253	-1.151525	-1.133668
3	6	0	0.297923	0.014847	0.261967
4	1	0	0.325565	0.290446	1.323099
5	1	0	0.384872	0.938012	-0.313996
6	7	0	-0.973563	-0.615891	-0.060781
7	1	0	-1.000827	-1.618658	-0.165723
8	6	0	2.805396	-0.372979	0.349968
9	1	0	1.272547	-1.883374	0.458300
10	1	0	2.808386	-0.178862	1.430396
11	1	0	3.561624	-1.148442	0.180814
12	6	0	3.205013	0.891881	-0.402317
13	1	0	2.549314	1.735973	-0.168777
14	1	0	4.225411	1.196856	-0.150255
15	1	0	3.166069	0.734648	-1.485930
16	6	0	-2.167568	-0.005314	-0.047960
17	8	0	-2.062620	1.320185	0.204339
18	8	0	-3.246648	-0.556234	-0.246855
19	1	0	-2.951619	1.695913	0.172898

Rotational constants (GHZ): 5.5330841 0.8010020 0.7274610
Standard basis: 6-311G(d) (5D, 7F)

Bu-3ctt, C_s (UBM)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.486071	0.103801	-0.000000
2	1	0	-1.733438	-0.504056	0.880060
3	6	0	0.000000	0.410517	0.000000
4	1	0	0.261296	1.005770	-0.880852
5	1	0	0.261296	1.005770	0.880852
6	7	0	0.770222	-0.824921	-0.000000
7	1	0	0.278607	-1.705235	-0.000000
8	6	0	-2.328825	1.372980	0.000000
9	1	0	-1.733438	-0.504056	-0.880060
10	1	0	-2.071165	1.980197	0.877105
11	1	0	-2.071165	1.980197	-0.877105
12	6	0	-3.821915	1.074472	0.000000
13	1	0	-4.110341	0.493893	0.882836
14	1	0	-4.417834	1.992338	0.000000
15	1	0	-4.110341	0.493893	-0.882836
16	6	0	2.108008	-0.903374	-0.000000
17	8	0	2.689089	0.319355	0.000000
18	8	0	2.758681	-1.944695	-0.000000
19	1	0	3.645627	0.188084	0.000000

Rotational constants (GHZ): 7.4789903 0.6938312 0.6450532
Standard basis: 6-311G(d) (5D, 7F)

Bu-2TS1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.432968	0.950024	0.157634
2	1	0	-1.703630	1.076998	1.212063
3	6	0	-0.040074	1.585658	-0.085430
4	1	0	-0.125311	2.438769	-0.759834
5	1	0	0.369597	1.970922	0.848748
6	7	0	0.968045	0.708081	-0.655505
7	1	0	0.918932	0.500329	-1.641630
8	6	0	-1.555144	-0.528064	-0.201455
9	1	0	-2.183196	1.509489	-0.413064
10	1	0	-1.284421	-0.681377	-1.252943
11	1	0	-0.840876	-1.116227	0.386768
12	6	0	-2.964403	-1.049571	0.046142
13	1	0	-3.701784	-0.503893	-0.552575
14	1	0	-3.052732	-2.110350	-0.208698
15	1	0	-3.250351	-0.938389	1.097744
16	6	0	1.617273	-0.181084	0.116768
17	8	0	1.609106	-0.206625	1.341619
18	8	0	2.332651	-1.057505	-0.629708
19	1	0	2.795300	-1.651574	-0.025289

Rotational constants (GHZ): 3.1909055 1.1619489 1.0292934
Standard basis: 6-311G(d) (5D, 7F)

Bu-2TS2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.232132	0.756134	-0.359076
2	1	0	-1.858368	1.588316	-0.702071
3	6	0	-0.052690	1.297040	0.469852
4	1	0	-0.086213	2.385065	0.537937
5	1	0	-0.106025	0.921523	1.494659
6	7	0	1.260160	0.957244	-0.052381
7	1	0	1.666758	1.549093	-0.760624
8	6	0	-2.100203	-0.242434	0.401138
9	1	0	-0.841166	0.280727	-1.266481
10	1	0	-1.475720	-1.077679	0.738818
11	1	0	-2.488135	0.235094	1.310469
12	6	0	-3.256323	-0.763860	-0.440392
13	1	0	-2.893210	-1.270573	-1.341312
14	1	0	-3.872114	-1.479168	0.113913
15	1	0	-3.911161	0.051902	-0.765993
16	6	0	1.747024	-0.288773	0.062994
17	8	0	1.265462	-1.186653	0.744572
18	8	0	2.886109	-0.448584	-0.655226
19	1	0	3.197611	-1.351753	-0.514514

Rotational constants (GHZ): 3.9718691 0.9832681
0.8829289
Standard basis: 6-311G(d) (5D, 7F)

Bu-2TS3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.165604	-0.200371	0.297239
2	1	0	-0.776474	-0.783570	-0.545698
3	6	0	-0.124287	0.859227	0.699824
4	1	0	-0.549361	1.861839	0.620595
5	1	0	0.177271	0.733056	1.741454
6	7	0	1.079227	0.860178	-0.113648
7	1	0	1.115870	1.438768	-0.938657
8	6	0	-2.510243	0.407217	-0.087612
9	1	0	-1.309094	-0.915551	1.115323
10	1	0	-2.892858	1.001435	0.752634
11	1	0	-2.360981	1.113766	-0.914836
12	6	0	-3.534790	-0.646413	-0.483311
13	1	0	-3.721011	-1.346813	0.338199
14	1	0	-4.494702	-0.197516	-0.757388
15	1	0	-3.188286	-1.233568	-1.340818
16	6	0	1.969609	-0.138496	-0.009923
17	8	0	1.955363	-1.018965	0.843416
18	8	0	2.930455	-0.055852	-0.962727
19	1	0	3.550393	-0.781542	-0.818088

Rotational constants (GHZ): 4.8543115 0.8109441 0.7961329
Standard basis: 6-311G(d) (5D, 7F)

Bu-2TS4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.478454	0.072464	0.559079
2	1	0	-1.355934	-0.982501	0.833547
3	6	0	-0.136198	0.652922	0.097342
4	1	0	-0.232426	1.072878	-0.911210
5	1	0	0.182955	1.472775	0.743597
6	7	0	0.914453	-0.352380	0.104706
7	1	0	0.663435	-1.325594	0.018985
8	6	0	-2.570200	0.186687	-0.499873
9	1	0	-1.806474	0.576313	1.474783
10	1	0	-2.700849	1.241811	-0.772609
11	1	0	-2.238440	-0.324204	-1.413248
12	6	0	-3.896642	-0.393334	-0.030733
13	1	0	-4.258844	0.120504	0.866405
14	1	0	-4.672339	-0.303576	-0.797504
15	1	0	-3.799435	-1.455809	0.217817
16	6	0	2.203894	-0.015316	-0.029608
17	8	0	3.002949	-1.109926	-0.104887
18	8	0	2.643138	1.129328	-0.068026
19	1	0	3.914086	-0.801699	-0.187444

Rotational constants (GHZ): 6.6548706 0.7061403 0.6647145
Standard basis: 6-311G(d) (5D, 7F)