

Oligoene and Cyanine Features of Tetracyano Quinoidal Oligothiophenes

Sergio Moles Quintero, José Luis Zafra, Keitaro Yamamoto,
Yoshio Aso, Yutaka Ie, Juan Casado

Supporting Information

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Part 1. Quantum Chemistry Calculations.

All geometry optimizations of the ground state of both neutral and charged species have been performed within the density functional theory (DFT) framework with B3LYP energy functional and the 6-31G** basis set using the Gaussian 16 software^{1,2,3}.

The computation of diradical index (γ_0) of **B2-6TQ** has been carried out with de restricted active space spin-flip (RAS-SF) method⁴. The diradical index has been quantified as the occupation of the Lowest Unoccupied Natural Orbital (LUNO). This calculation has been done with the Q-Chem program⁵.

Vertical transition energies were computed with the time-dependent version of DFT (TDDFT)^{6,7}.

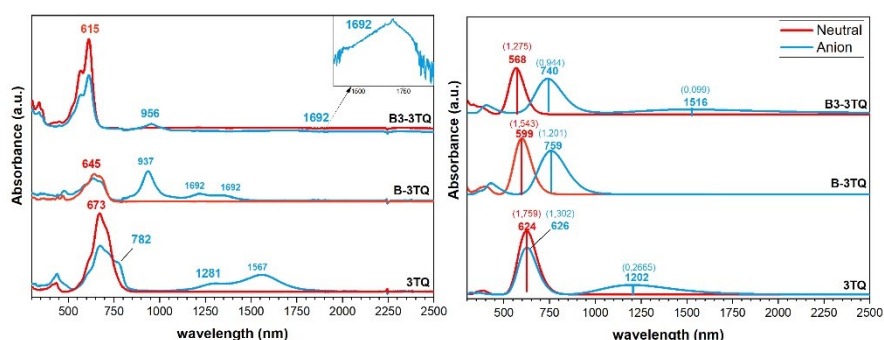


Figure S1. Left: UV-Vis-NIR electronic absorption spectra of neutrals (red lines) and anions (blue lines) of **B3-3TQ** (top), **B-3TQ** (middle) and **3TQ** (bottom). Right: Simulated UV-Vis-NIR spectra computed in neutrals (red lines) and anions (blue lines) of **B3-3TQ** (top), **B-3TQ** (middle) and **3TQ** (bottom). The oscillator strengths are indicated between brackets.

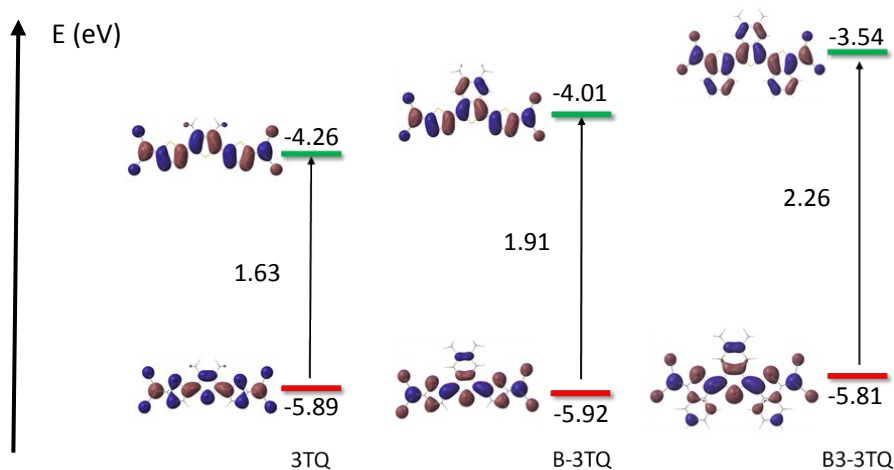


Figure S2. Frontier molecular orbitals and their energy in eV computed at the B3LYP/6-31G** level of theory. Highest Occupied Molecular Orbital, HOMO (red lines); Lowest Unoccupied Molecular Orbital, LUMO (green lines).

Part 2. UV-Vis-NIR and IR Spectroelectrochemistry.

Electrochemical experiments have been conducted in dichloromethane at room temperature by using 0.1 M tetrabutyl ammonium hexafluorophosphate, Bu_4NPF_6 , as the supporting electrolyte.

In situ IR and UV-Vis-NIR spectroelectrochemical studies were conducted on the VERTEX 70 FT-IR spectrometer and on the Varian Cary 5000 UV-Vis-NIR Spectrophotometer, respectively. A C3 epsilon potentiostat from BASi was used for the electrolysis using a thin layer cell from a demountable omni cell from Specac. In this cell a three electrodes system was coupled to conduct in situ spectroelectrochemistry. A Pt gauze was used as the working electrode, a Pt wire was used as the counter electrode, and an Ag wire was used as the pseudo-reference electrode. The spectra were collected at a constant potential electrolysis and the potentials were changed in interval of 15 mV. The electrochemical medium used was 0.1 Bu_4NPF_6 in fresh distilled dichloromethane, at room temperature with sample concentrations of 10^{-3} M.

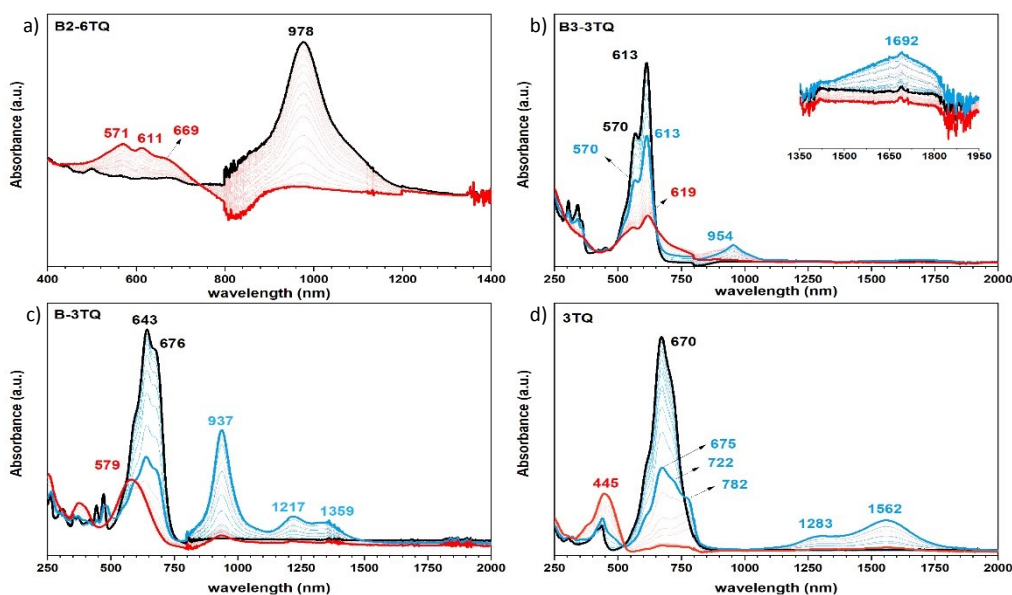


Figure S3. UV-Vis-NIR spectroelectrochemical reduction processes of **B2-6TQ** a), **B3-3TQ** b), **B-3TQ** c), **3TQ** d) and in 0.1 M Bu_4NPF_6 in dichloromethane at room temperature. Black lines correspond to the spectra of neutral species, blue lines correspond to the anionic species and red line correspond to the dianionic species. Dashed light colour lines correspond to the intermediate spectra between the former species.

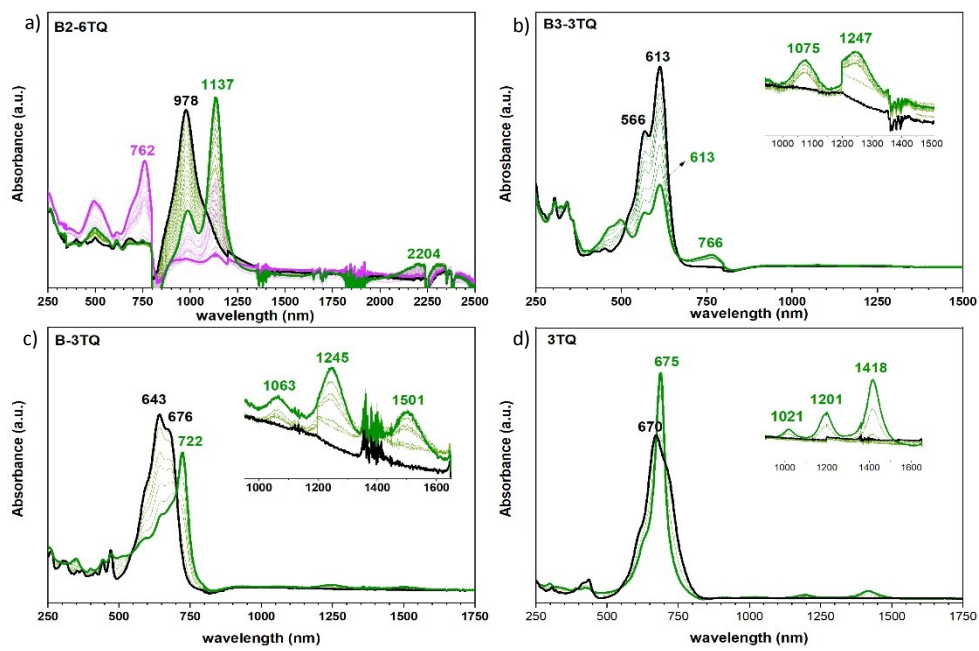


Figure
S4.
 UV-
 Vis-
 NIR

spectroelectrochemical oxidation processes of **B2-6TQ** a), **B3-3TQ** b), **B-3TQ** c) and **3TQ** d) in 0.1 M Bu_4NPF_6 in dichloromethane at room temperature. Black lines correspond to the spectra of neutral species, green lines correspond to the cationic species and pink line corresponds to the dicationic species. Dashed light colour lines correspond to the intermediate spectra between the former species.

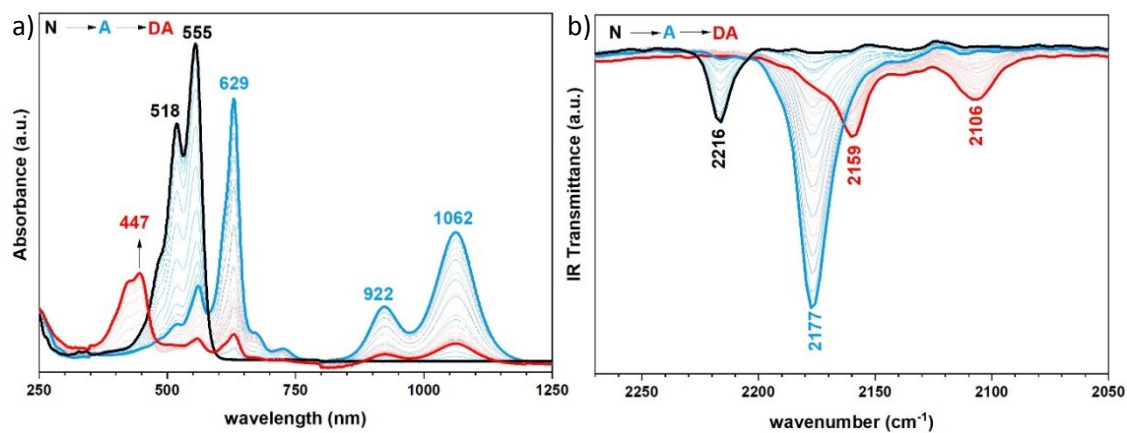
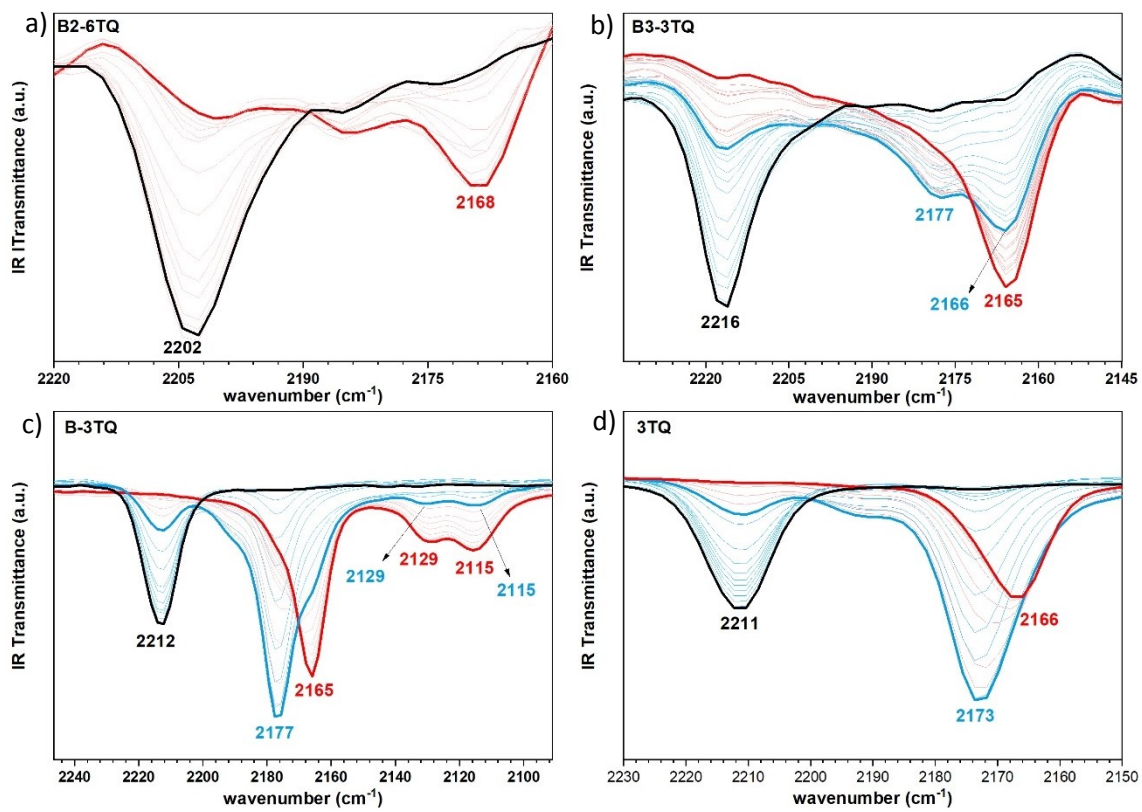


Figure S5. a) UV-Vis-NIR spectroelectrochemical reduction processes of **2TQ** in 0.1 M Bu_4NPF_6 in dichloromethane at room temperature. b) IR spectroelectrochemical reduction processes of **2TQ** in the same conditions. Black lines correspond to the spectra of neutral species, blue lines correspond to the anionic species and red line correspond of dianionic species. Dashed light colour lines correspond to the intermediate spectra between the former species.



and **3TQ d**) in 0.1 M Bu₄NPF₆ in dichloromethane at room temperature. Black lines correspond to the spectra of neutral species, blue lines correspond to the anionic species and red line correspond to the dianionic species. Dashed light colour lines correspond to the intermediate spectra between the former species.

Part 4. Deconvolution Fitting Parameters.

Table S1. Fitting parameters of **B2-6TQ** UV-Vis-NIR electronic absorption spectrum deconvolution.

Model	Gauss			
Equation	$y=y_0 + (A/(w*\sqrt{\pi/2})) * \exp(-2*((x-xc)/w)^2)$			
Plot	Peak1(B)	Peak2(B)	Peak3(B)	Peak4(B)
y0*	0,0116 ± 0	0,0116 ± 0	0,0116 ± 0	0,0116 ± 0
xc	890,94491 ± 5,75732	975,54256 ± 0,19466	1037,00309 ± 5,38497	1234,93076 ± 2,81074
w	145,07895 ± 6,32475	63,96035 ± 0,62563	149,79141 ± 5,12109	64,0343 ± 5,53716
A	3,34944 ± 0,32406	3,19777 ± 0,09841	4,65861 ± 0,35567	0,11892 ± 0,01323
y0	0,0116 ± 0	0,0116 ± 0	0,0116 ± 0	0,0116 ± 0
Reduced Chi-Sqr	2,19778E-7			
R-Square (COD)	0,99945			
Adj. R-Square	0,99943			

Part 5. Optimized Coordinates.

All Cartesian coordinates corresponding to the optimized energy structures are shown below:

Neutrals

1TQ:

C	-1.25706900	-0.27795500	-0.00000900
S	0.00001800	0.96360500	0.00025000
C	1.25706300	-0.27793100	0.00005900
C	0.67742600	-1.60235900	-0.00009800
C	-0.67737300	-1.60237800	-0.00017000
C	2.60090400	0.01674300	-0.00005300
C	-2.60085300	0.01670100	-0.00000400
C	-3.07231900	1.36318100	0.00004400
N	-3.43399000	2.46981500	0.00023000
C	-3.57004400	-1.03242500	-0.00013300
N	-4.34432300	-1.90161500	-0.00019000
C	3.07221600	1.36318200	-0.00021200
N	3.43403800	2.46977500	-0.00049300
C	3.56987900	-1.03253000	0.00016600
N	4.34436800	-1.90154000	0.00032100
H	1.30019300	-2.48902600	-0.00026300
H	-1.30010100	-2.48907000	-0.00034600

2TQ:

C	3.19501000	0.23811700	0.00010800
S	1.97234100	-1.02952300	-0.00000200
C	0.66440600	0.17597300	0.00009600
C	1.21989500	1.50031800	0.00016200
C	2.57979500	1.53903500	0.00010200
C	-0.66435600	-0.17601100	0.00003400
C	-1.21991100	-1.50032300	-0.00013800
C	-2.57981500	-1.53899400	-0.00014600
C	-3.19499700	-0.23807100	-0.00000700
S	-1.97228900	1.02952700	0.00022500
C	-4.55143800	0.02804000	-0.00004100
C	4.55133400	-0.02796600	0.00003200
C	5.49292700	1.04267500	-0.00039900
N	6.24273200	1.93402200	-0.00045400
C	-5.04486100	1.36407400	-0.00000300
N	-5.41507400	2.46875900	0.00000800
C	5.04478600	-1.36406900	0.00021400
N	5.41492100	-2.46876100	0.00025000
C	-5.49283800	-1.04271500	-0.00013700
N	-6.24262900	-1.93409700	-0.00018400
H	0.59163000	2.38405200	0.00038500
H	3.17615000	2.44333200	0.00000900
H	-0.59170700	-2.38411300	-0.00027200
H	-3.17617600	-2.44329200	-0.00029300

3TQ:

S	-4.01429000	0.82462600	-0.00036200
C	-5.12788800	-0.53757300	-0.00020300
C	-4.40858500	-1.77619700	0.00058400
C	-3.05432100	-1.61862000	0.00102400
C	-2.59876600	-0.25901400	0.00067700
C	-1.27402400	0.14706300	0.00076400
C	-6.50549300	-0.37631100	-0.00078200
S	0.00000200	-1.07979800	-0.00006800
C	1.27402100	0.14706700	0.00046200
C	0.69263400	1.46760300	0.00093300
C	-0.69263600	1.46759400	0.00128500
C	2.59876400	-0.25900700	0.00043000
C	3.05432100	-1.61861200	0.00094700
C	4.40858300	-1.77619400	0.00062400
C	5.12789200	-0.53757200	-0.00020200
S	4.01429800	0.82463100	-0.00049100
C	6.50549300	-0.37631400	-0.00069200
C	-1.55206100	2.70092200	0.00237100
C	1.55200700	2.70097000	0.00109600
C	-7.09947600	0.91662900	-0.00146300
N	-7.55199200	1.99089900	-0.00200000
C	7.35792100	-1.51736400	-0.00032600
N	8.03230400	-2.46780200	0.00002100
C	7.09949100	0.91662500	-0.00155000
N	7.55201900	1.99089000	-0.00225600
C	-7.35791100	-1.51736600	-0.00071300
N	-8.03228400	-2.46781100	-0.00054700
H	-4.92236700	-2.72962600	0.00086600
H	-2.36150300	-2.45251400	0.00174100

H	2.36150000	-2.45250400	0.00168700
H	4.92236100	-2.72962500	0.00099600
H	-0.95726700	3.61322500	0.00479700
H	-2.19806600	2.73583400	-0.88137900
H	-2.20020300	2.73268600	0.88464000
H	2.19909600	2.73441300	-0.88189500
H	0.95713600	3.61322900	0.00102200
H	2.19904300	2.73433300	0.88413200

4TQ:

C	7.09848900	-0.24952800	-0.00010700
C	6.50756100	-1.55386500	-0.00058400
C	5.14019000	-1.53611800	-0.00056700
C	4.56539500	-0.23161900	-0.00007700
S	5.85207000	0.99402000	0.00035100
C	3.22317700	0.11103200	0.00004500
S	1.93047600	-1.10103400	-0.00024800
C	0.67699900	0.15237600	0.00009300
C	1.28528400	1.43918100	0.00038900
C	2.65539100	1.41895200	0.00038900
C	-0.67700000	-0.15237900	0.00009100
C	-1.28528500	-1.43918300	0.00031700
C	-2.65539300	-1.41895300	0.00033900
C	-3.22317700	-0.11103300	0.00007900
S	-1.93047600	1.10103200	-0.00015900
C	-4.56539600	0.23162000	-0.00001300
S	-5.85207100	-0.99401900	0.00045100
C	-7.09848900	0.24953000	-0.00007200
C	-6.50756100	1.55386700	-0.00052500
C	-5.14019000	1.53611900	-0.00049000
C	-8.45501700	-0.04823100	-0.00006100
C	8.45501600	0.04823200	-0.00004200
C	-9.41558000	1.00268000	-0.00053700
N	-10.18044700	1.88221300	-0.00083100
C	-8.91805300	-1.39285300	0.00036600
N	-9.26303100	-2.50654700	0.00082400
C	8.91805700	1.39285400	0.00036700
N	9.26303900	2.50654600	0.00081300
C	9.41558100	-1.00267800	-0.00042600
N	10.18044400	-1.88221400	-0.00064800
H	7.11697100	-2.44919900	-0.00096400
H	4.52919000	-2.43211000	-0.00090700
H	0.69878300	2.35093600	0.00065200
H	3.27091000	2.31112900	0.00064300
H	-0.69878500	-2.35093900	0.00051200
H	-3.27091300	-2.31113000	0.00054300
H	-7.11697100	2.44920200	-0.00091700
H	-4.52919000	2.43211200	-0.00082000

5TQ:

C	-9.07411600	-0.21870000	-0.00002600
S	-7.81156700	1.00808500	-0.00002100
C	-6.54899600	-0.22675400	-0.00000800
C	-7.12170200	-1.51169300	-0.00002400
C	-8.50593700	-1.51623100	-0.00003400

C	-5.17756400	0.12496800	0.00000900
C	-4.60644900	1.40177600	0.00002600
C	-3.20944100	1.39794100	0.00003900
C	-2.64525400	0.12189500	0.00002900
S	-3.91002200	-1.10123000	0.00001400
C	-1.26536100	-0.24170200	0.00003400
S	0.00000000	0.98136800	0.00002600
C	1.26536100	-0.24170200	0.00003100
C	0.70046200	-1.51471000	0.00004700
C	-0.70046200	-1.51471000	0.00005000
C	2.64525400	0.12189500	0.00002300
C	3.20944100	1.39794100	0.00001500
C	4.60644900	1.40177600	0.00000600
C	5.17756400	0.12496800	0.00000700
S	3.91002200	-1.10123000	0.00002200
C	6.54899600	-0.22675400	-0.00000200
S	7.81156700	1.00808500	-0.00002400
C	9.07411600	-0.21870000	-0.00001300
C	8.50593700	-1.51623100	-0.00000500
C	7.12170200	-1.51169300	0.00000200
C	10.43747700	0.10875900	-0.00001700
C	-10.43747700	0.10875900	-0.00002800
C	11.41442400	-0.92329200	-0.00001100
N	12.19483100	-1.79006000	-0.00000900
C	-10.87704200	1.45825700	-0.00002400
N	-11.20773000	2.57717900	-0.00001900
C	10.87704200	1.45825700	-0.00003000
N	11.20772900	2.57717900	-0.00003800
C	-11.41442400	-0.92329200	-0.00003600
N	-12.19483100	-1.79006000	-0.00004400
H	-6.52173100	-2.41479300	-0.00002400
H	-9.12042100	-2.40819800	-0.00004300
H	-5.20158500	2.30775300	0.00002900
H	-2.61125100	2.30190800	0.00005400
H	1.29632800	-2.42023100	0.00005600
H	-1.29632800	-2.42023100	0.00006200
H	2.61125100	2.30190800	0.00001500
H	5.20158500	2.30775300	-0.00000100
H	9.12042100	-2.40819800	0.00000000
H	6.52173100	-2.41479300	0.00001200

6TQ:

S	9.78122100	-0.98378600	0.00269200
C	11.03378500	0.25328700	0.00119800
C	10.45522800	1.54470900	-0.00112500
C	9.06955000	1.52834100	-0.00165600
C	8.50875500	0.23986500	0.00020400
C	7.13836800	-0.12570800	0.00024700
C	12.40083200	-0.06410300	0.00226300
S	5.86096600	1.08982000	-0.00234200
C	4.60671800	-0.14231400	-0.00074700
C	5.17906100	-1.41200300	0.00160400
C	6.57867400	-1.40493000	0.00215400
C	3.22076000	0.21404600	-0.00183200
C	2.64673600	1.47877400	-0.00412600
C	1.24150600	1.46587700	-0.00476900
C	0.69113800	0.19133700	-0.00298100

S	1.96581400	-1.01904700	-0.00009600
C	-0.69113800	-0.19133300	-0.00318800
S	-1.96581500	1.01904800	0.00032500
C	-3.22076000	-0.21404300	-0.00238400
C	-2.64673600	-1.47877000	-0.00542600
C	-1.24150500	-1.46587200	-0.00587300
C	-4.60671900	0.14231600	-0.00126700
C	-5.17906200	1.41200500	0.00063700
C	-6.57867500	1.40493100	0.00129100
C	-7.13836800	0.12570900	-0.00009200
S	-5.86096500	-1.08981900	-0.00216200
C	-8.50875500	-0.23986600	0.00003400
S	-9.78122100	0.98378500	0.00250700
C	-11.03378500	-0.25328900	0.00125200
C	-10.45522700	-1.54471100	-0.00098000
C	-9.06954900	-1.52834200	-0.00163100
C	-12.40083200	0.06410000	0.00239700
C	-13.36964100	-0.97521100	0.00132200
N	-14.14348300	-1.84799600	0.00040700
C	13.36964100	0.97520700	0.00097400
N	14.14348400	1.84799200	-0.00010900
C	12.85115500	-1.40974300	0.00462700
N	13.19140900	-2.52592200	0.00658800
C	-12.85115500	1.40974000	0.00462300
N	-13.19141100	2.52591800	0.00645200
H	11.06188700	2.44202500	-0.00233100
H	8.46183300	2.42622000	-0.00334500
H	4.58786900	-2.32051500	0.00290100
H	7.18071100	-2.30637500	0.00391900
H	3.23390600	2.39001200	-0.00549800
H	0.63781400	2.36619000	-0.00690000
H	-3.23390600	-2.39000600	-0.00755500
H	-0.63781400	-2.36618400	-0.00853500
H	-4.58787100	2.32051800	0.00140900
H	-7.18071300	2.30637600	0.00265700
H	-11.06188600	-2.44202800	-0.00204800
H	-8.46183100	-2.42622100	-0.00330200

7TQ:

S	-11.73384000	1.02029500	0.00040900
C	-12.99659300	-0.20642800	0.00007200
C	-12.42864800	-1.50202200	-0.00030000
C	-11.04236000	-1.49686000	-0.00032600
C	-10.47132300	-0.21346500	0.00001000
C	-9.09740400	0.14162800	0.00006100
C	-14.36140800	0.12249400	0.00017500
S	-7.83011000	-1.08451500	-0.00024700
C	-6.56564600	0.13656800	-0.00001700
C	-7.12666400	1.41045800	0.00029300
C	-8.52718300	1.41528000	0.00034300
C	-5.18173000	-0.23289300	-0.00014900
C	-4.61865200	-1.50099700	-0.00039900
C	-3.21177200	-1.49945700	-0.00044300
C	-2.65205700	-0.23055500	-0.00022600
S	-3.91636200	0.98958200	-0.00002800
C	-1.26468900	0.14321100	-0.00018400
S	0.00000000	-1.07765600	0.00004200

C	1.26468900	0.14321100	-0.00007800
C	0.70425000	1.41039100	-0.00024100
C	-0.70425000	1.41039100	-0.00030000
C	2.65205600	-0.23055600	0.00000000
C	3.21177100	-1.49945800	0.00024900
C	4.61865100	-1.50099700	0.00026900
C	5.18173000	-0.23289400	0.00003100
S	3.91636100	0.98958100	-0.00025700
C	6.56564500	0.13656700	-0.00001200
S	7.83011000	-1.08451600	0.00026100
C	9.09740400	0.14162800	0.00003700
C	8.52718300	1.41528000	-0.00023300
C	7.12666400	1.41045700	-0.00026000
C	10.47132300	-0.21346500	0.00013500
C	11.04236100	-1.49686100	0.00044200
C	12.42864800	-1.50202200	0.00045400
C	12.99659300	-0.20642800	0.00016000
S	11.73384000	1.02029500	-0.00014000
C	14.36140700	0.12249400	0.00008700
C	15.33873100	-0.90866700	0.00026800
N	16.11982900	-1.77504400	0.00039400
C	14.80084600	1.47160900	-0.00027700
N	15.13253700	2.59042400	-0.00060200
C	-14.80084700	1.47160800	0.00049000
N	-15.13253500	2.59042500	0.00074200
C	-15.33873200	-0.90866700	-0.00016800
N	-16.11982600	-1.77504700	-0.00049400
H	-13.04254800	-2.39440300	-0.00054400
H	-10.44178100	-2.39952500	-0.00059800
H	-6.52756700	2.31375300	0.00047900
H	-9.12156700	2.32182000	0.00056400
H	-5.21312700	-2.40754600	-0.00053200
H	-2.61521300	-2.40448200	-0.00063000
H	1.29939000	2.31645000	-0.00033100
H	-1.29938900	2.31645000	-0.00046000
H	2.61521200	-2.40448200	0.00042900
H	5.21312600	-2.40754600	0.00046100
H	9.12156700	2.32181900	-0.00040400
H	6.52756700	2.31375200	-0.00045600
H	10.44178200	-2.39952600	0.00065000
H	13.04254800	-2.39440300	0.00066700

B3-6TQ:

S	-9.96159500	0.09778200	-0.00029300
C	-10.90293300	-1.38903600	-0.00009300
C	-10.03786300	-2.52511600	0.00015100
C	-8.70896800	-2.20053700	0.00017300
C	-8.42517400	-0.80089600	-0.00004500
C	-7.16520600	-0.21864000	-0.00008200
C	-12.29429200	-1.39203400	-0.00017300
S	-5.73804200	-1.26067500	0.00008900
C	-4.60215200	0.09589500	-0.00003400
C	-5.33306300	1.33498400	-0.00019700
C	-6.74963400	1.16460000	-0.00023100
C	-3.23482500	-0.17763900	-0.00001700

C	-2.63308300	-1.46633400	0.00006300
C	-1.25658000	-1.46255000	0.00009200
C	-0.67696200	-0.17313700	0.00001800
S	-1.95564200	1.05162200	-0.00007000
C	0.67696200	0.17313500	0.00003800
S	1.95564200	-1.05162300	0.00007600
C	3.23482500	0.17763800	0.00011700
C	2.63308300	1.46633200	0.00009800
C	1.25658000	1.46254800	0.00006600
C	4.60215200	-0.09589600	0.00017500
C	5.33306300	-1.33498500	0.00010900
C	6.74963500	-1.16460200	0.00012900
C	7.16520600	0.21863900	0.00022600
S	5.73804200	1.26067300	0.00028000
C	8.42517400	0.80089600	0.00028900
S	9.96159600	-0.09778100	0.00016200
C	10.90293200	1.38903800	0.00032500
C	10.03786100	2.52511700	0.00046600
C	8.70896700	2.20053700	0.00044400
C	12.29429200	1.39203800	0.00031100
C	-4.80637400	2.64226000	-0.00030600
C	-5.63159600	3.75891000	-0.00046000
C	-7.04495300	3.58823600	-0.00050100
C	-7.57545600	2.30475400	-0.00038300
C	4.80637500	-2.64226200	0.00004300
C	5.63159700	-3.75891100	-0.00001800
C	7.04495400	-3.58823700	-0.00000500
C	7.57545700	-2.30475600	0.00007100
C	-5.02898500	5.14117600	-0.00058500
C	-7.96343200	4.78414400	-0.00067000
C	5.02898600	-5.14117700	-0.00009900
C	7.96343300	-4.78414600	-0.00007400
C	13.00317500	2.62603000	0.00044500
N	13.55832400	3.65132400	0.00054000
C	-13.00317700	-2.62602600	-0.00000500
N	-13.55832700	-3.65132000	0.00012400
C	13.03619700	0.17943700	0.00018100
N	13.61213300	-0.83473900	0.00008600
C	-13.03619700	-0.17943200	-0.00040200
N	-13.61213200	0.83474400	-0.00058000
H	-10.42900000	-3.53495700	0.00030600
H	-7.91913900	-2.94344800	0.00035500
H	-3.22338600	-2.37518000	0.00009600
H	-0.65643500	-2.36527200	0.00014800
H	3.22338600	2.37517800	0.00010500
H	0.65643500	2.36527000	0.00004400
H	10.42899700	3.53495800	0.00058400
H	7.91913700	2.94344800	0.00054800
H	-3.73532300	2.80059400	-0.00026200
H	-8.65314900	2.20211500	-0.00039900
H	3.73532300	-2.80059600	0.00004700
H	8.65315000	-2.20211600	0.00009600
H	-5.34305700	5.71561000	0.87868400
H	-3.93748000	5.09739400	-0.00046600
H	-5.34287300	5.71536200	-0.88008400
H	-7.79873800	5.41720200	-0.88048100
H	-9.01173300	4.47774900	-0.00063700
H	-7.79875300	5.41744800	0.87896500

H	5.34302200	-5.71556900	0.87921100
H	3.93748100	-5.09739600	-0.00002700
H	5.34291000	-5.71540600	-0.87955700
H	7.79877700	-5.41724800	-0.87985900
H	9.01173400	-4.47775000	-0.00001200
H	7.79871700	-5.41740400	0.87958700

B2-2TQ:

C	3.21946600	0.33305300	0.07130900
S	1.77270500	1.32149800	-0.02765100
C	0.68219300	-0.08024000	-0.18634300
C	1.48805600	-1.30387500	-0.22537000
C	2.88324300	-1.07593300	-0.05725900
C	-0.68214700	0.08048700	-0.18621900
C	-1.48811900	1.30405500	-0.22516200
C	-2.88330500	1.07595300	-0.05722900
C	-3.21938500	-0.33305700	0.07136800
S	-1.77251300	-1.32134600	-0.02728100
C	-4.44214800	-0.95401000	0.24139300
C	4.44228600	0.95391400	0.24135000
C	-1.04252000	2.61905900	-0.43904500
C	-1.95003100	3.67380800	-0.43641200
C	-3.31429100	3.44531800	-0.23227500
C	-3.78645000	2.15098100	-0.05200800
C	1.04233100	-2.61878300	-0.43957400
C	1.94970800	-3.67364600	-0.43688600
C	3.31394900	-3.44534800	-0.23241000
C	3.78624700	-2.15108600	-0.05196000
C	-5.68079700	-0.25738200	0.34601300
N	-6.70560100	0.29001400	0.43370500
C	-4.51411100	-2.37811600	0.32229000
N	-4.54325000	-3.54116200	0.38200400
C	4.51439500	2.37801100	0.32197100
N	4.54365800	3.54105900	0.38160000
C	5.68081600	0.25711300	0.34638500
N	6.70545500	-0.29054400	0.43437200
H	-0.00242000	2.83819500	-0.63393700
H	-1.58745400	4.68321700	-0.60206700
H	-4.01212000	4.27600700	-0.22902700
H	-4.84592700	1.98033600	0.08252900
H	0.00225100	-2.83769700	-0.63483300
H	1.58705500	-4.68298800	-0.60278500
H	4.01166500	-4.27613100	-0.22907300
H	4.84572200	-1.98060000	0.08277400

B3-3TQ:

S	3.94899800	0.93382000	-0.00015200
C	5.22077100	-0.26853800	-0.00042800
C	4.65184700	-1.60463800	-0.00043000
C	3.22586400	-1.60861400	-0.00033100
C	2.63109400	-0.26958800	-0.00013700
C	1.31161400	0.12696500	0.00018100
C	6.54047000	0.15081500	-0.00060700

S	0.00013900	-1.06787000	0.00071200
C	-1.31149400	0.12679100	0.00091900
C	-0.71286100	1.46337700	0.00086100
C	0.71280300	1.46348600	0.00034600
C	-2.63096000	-0.26981200	0.00089500
C	-3.22580700	-1.60881800	0.00124300
C	-4.65179200	-1.60474300	0.00039900
C	-5.22063100	-0.26860900	-0.00049300
S	-3.94879100	0.93367100	0.00008000
C	-6.54030600	0.15081700	-0.00159600
C	-1.37825800	2.69401100	0.00138300
C	-0.70534500	3.92132700	0.00120500
C	0.70486200	3.92144300	0.00046200
C	1.37798500	2.69424000	0.00009200
C	-1.55687000	5.17191700	0.00183500
C	1.55617800	5.17217500	0.00009900
C	5.37434000	-2.80940900	-0.00060900
C	4.69542300	-4.02016000	-0.00072500
C	3.29713200	-4.03593100	-0.00071100
C	2.56785700	-2.85193200	-0.00053000
C	-2.56790800	-2.85219600	0.00234000
C	-3.29727700	-4.03613700	0.00244500
C	-4.69556500	-4.02026000	0.00148000
C	-5.37438200	-2.80945600	0.00048100
C	-6.84271200	1.54587000	-0.00223500
N	-7.05877800	2.69096000	-0.00276600
C	7.65796900	-0.73193700	-0.00083100
N	8.58825000	-1.43413300	-0.00100100
C	-7.65785000	-0.73187800	-0.00214900
N	-8.58816200	-1.43403200	-0.00260000
C	6.84295000	1.54585200	-0.00056100
N	7.05907400	2.69093000	-0.00054700
H	-2.45768000	2.73798100	0.00207100
H	2.45739300	2.73841100	-0.00039400
H	-0.97448700	6.09204200	0.00229300
H	-2.20847000	5.19386200	-0.87838200
H	-2.20843000	5.19297400	0.88209800
H	0.97364000	6.09220300	-0.00008300
H	2.20783300	5.19400200	0.88027800
H	2.20767600	5.19356900	-0.88020200
H	6.45583300	-2.80080200	-0.00069100
H	5.25352900	-4.95050900	-0.00087700
H	2.76644300	-4.98297100	-0.00088000
H	1.49067400	-2.91722100	-0.00064000
H	-1.49073600	-2.91758800	0.00320100
H	-2.76666300	-4.98321900	0.00329400
H	-5.25374400	-4.95056500	0.00154700
H	-6.45587400	-2.80076100	-0.00021200

B4-4TQ:

C	7.15819100	0.20383900	0.03869800
C	6.66530000	-1.13911300	-0.21428100
C	5.24827100	-1.19591300	-0.35462100
C	4.58375300	0.08985700	-0.16577400
S	5.82848000	1.34443500	0.08669600
C	3.24126800	0.38841200	-0.08566300

S	2.01886200	-0.89508300	0.01990600
C	0.65091200	0.22505900	0.21498200
C	1.16803100	1.58793600	0.25077800
C	2.57147200	1.68299400	0.02208700
C	-0.65089500	-0.22512400	0.21502700
C	-1.16803100	-1.58799500	0.25089600
C	-2.57149600	-1.68304900	0.02232600
C	-3.24127800	-0.38845400	-0.08546600
S	-2.01884100	0.89501800	0.02002100
C	-4.58374800	-0.08984300	-0.16566600
S	-5.82852200	-1.34442100	0.08653600
C	-7.15821100	-0.20380400	0.03860100
C	-6.66528300	1.13915500	-0.21426900
C	-5.24823800	1.19595400	-0.35449100
C	-8.44986700	-0.66849500	0.22509500
C	8.44983900	0.66852800	0.22525500
C	-7.44254300	2.30233100	-0.34564300
C	-6.82634500	3.51208900	-0.63728800
C	-5.44003900	3.56774700	-0.82052100
C	-4.65560700	2.42767000	-0.68718300
C	-0.43377000	-2.76127100	0.50104100
C	-1.05006100	-4.00473300	0.43433800
C	-2.40601000	-4.10282600	0.10961100
C	-3.16230700	-2.95425100	-0.08920900
C	0.43379500	2.76122800	0.50093700
C	1.05008300	4.00468400	0.43409800
C	2.40599400	4.10276900	0.10919700
C	3.16227100	2.95418500	-0.08963200
C	7.44257100	-2.30227800	-0.34569100
C	6.82639200	-3.51201000	-0.63748900
C	5.44010000	-3.56765600	-0.82085400
C	4.65566000	-2.42758900	-0.68749000
C	-9.60374300	0.16584700	0.21641000
N	-10.56204400	0.82944800	0.21343700
C	-8.68264900	-2.05959800	0.44299800
N	-8.84429400	-3.20067000	0.61587800
C	9.60371400	-0.16581400	0.21653700
N	10.56200300	-0.82943200	0.21356100
C	8.68261300	2.05961500	0.44326100
N	8.84426200	3.20068000	0.61618500
H	-8.51732100	2.26145600	-0.23131900
H	-7.42721000	4.40955200	-0.74066200
H	-4.96609800	4.50932600	-1.08014100
H	-3.59440000	2.50212100	-0.87848800
H	0.61038200	-2.71196700	0.77728800
H	-0.47002300	-4.90072600	0.63103000
H	-2.87983300	-5.07529400	0.02496300
H	-4.20632900	-3.06469400	-0.34622400
H	-0.61033300	2.71194300	0.77728400
H	0.47006800	4.90068700	0.63081400
H	2.87979000	5.07523900	0.02441200
H	4.20625600	3.06457800	-0.34683300
H	8.51734200	-2.26141400	-0.23129200
H	7.42726700	-4.40946300	-0.74089800
H	4.96619100	-4.50921100	-1.08061600
H	3.59447000	-2.50199500	-0.87892600

B5-5TQ:

C	-8.96674500	0.45444800	-0.15222100
S	-7.63795200	1.59552200	-0.23289100
C	-6.39326200	0.35179400	0.07545300
C	-7.05998800	-0.92510600	0.30222500
C	-8.47215900	-0.87438300	0.15154900
C	-5.05012500	0.64947400	-0.00136900
C	-4.37941900	1.93986100	-0.14325300
C	-2.97274500	1.83840700	-0.35114900
C	-2.45550400	0.47880900	-0.26805100
S	-3.82610200	-0.63576100	-0.05174600
C	-1.15252500	0.03024300	-0.24141700
S	0.21359200	1.15613700	-0.06706700
C	1.43869200	-0.12678500	0.06679000
C	0.76711800	-1.41986100	0.00653200
C	-0.63582800	-1.33336600	-0.23150000
C	2.78405700	0.16856100	0.11290000
C	3.45605300	1.45366800	0.24501100
C	4.86309400	1.39772200	0.05316500
C	5.38333500	0.04640100	-0.13005900
S	4.01914500	-1.08967300	-0.13506600
C	6.68517800	-0.40100500	-0.20711700
S	8.05763900	0.68044300	0.16013200
C	9.25033700	-0.59728200	0.04834600
C	8.61512800	-1.85265600	-0.31044600
C	7.20387800	-1.73643200	-0.47660300
C	10.58294600	-0.29785500	0.28901300
C	-6.47857700	-2.14739100	0.67995500
C	-7.24427300	-3.29889000	0.85593700
C	-8.64749900	-3.25000100	0.65870600
C	-9.24025100	-2.03767800	0.32063000
C	2.86612300	2.69192500	0.55193400
C	3.60639400	3.87097800	0.58754200
C	4.99094800	3.82881300	0.29445500
C	5.59214300	2.59892100	0.04015200
C	-4.97218900	3.21359500	-0.07898400
C	-4.21425200	4.35624900	-0.30299200
C	-2.85370700	4.24915100	-0.60582900
C	-2.23581700	3.00505300	-0.62629600
C	1.35550600	-2.68681200	0.17312600
C	0.60031800	-3.84178400	0.01052300
C	-0.75263700	-3.75607400	-0.33085400
C	-1.36776900	-2.51547600	-0.44596000
C	9.25869400	-3.08563600	-0.51414500
C	8.51710300	-4.19310600	-0.90201300
C	7.13740800	-4.07643700	-1.10963200
C	6.48387600	-2.86694700	-0.90628000
C	-9.49840500	-4.48330200	0.83138200
C	-6.57377900	-4.58643500	1.26439000
C	2.92985100	5.17531600	0.92715100
C	5.81686400	5.09053700	0.27243700
C	-10.25917200	0.91024700	-0.36425600
C	10.96522600	1.03805500	0.61279100
N	11.24916300	2.13841800	0.87191600
C	11.63503000	-1.25528600	0.23622900
N	12.51252100	-2.02199900	0.19890300
C	-11.41031900	0.07318600	-0.33297700

N	-12.36644500	-0.59365000	-0.31222300
C	-10.49469400	2.29138000	-0.63378800
N	-10.66089300	3.42476600	-0.84905700
H	-5.41728700	-2.21257400	0.87808900
H	-10.31466300	-1.99965300	0.19669000
H	1.81444800	2.74823800	0.79927200
H	6.64928400	2.59818300	-0.18826400
H	-6.01977000	3.33013200	0.16054300
H	-4.68970200	5.33046300	-0.25465600
H	-2.27142700	5.13938300	-0.82175200
H	-1.18791300	2.94757400	-0.88626000
H	2.39520800	-2.78076400	0.45451000
H	1.07050100	-4.81136500	0.14060700
H	-1.33174100	-4.65859600	-0.49880200
H	-2.41047200	-2.47573700	-0.72937600
H	10.32826400	-3.17579100	-0.38042000
H	9.01473000	-5.14405700	-1.06110500
H	6.56631100	-4.93724700	-1.44379200
H	5.42561300	-2.80531500	-1.11776800
H	-9.19401700	-5.28095000	0.14344500
H	-9.41500900	-4.89181400	1.84545300
H	-10.55160200	-4.26327500	0.64440800
H	-6.97841200	-4.96636500	2.20966500
H	-6.73117000	-5.37291000	0.51688600
H	-5.49701600	-4.45157000	1.38978200
H	3.38606300	5.64706500	1.80519300
H	3.01208500	5.89591800	0.10484200
H	1.86838800	5.02775700	1.13940900
H	5.43458700	5.80839600	-0.46276400
H	5.80220800	5.59661300	1.24491100
H	6.85897200	4.87797800	0.02390800

B6-6TQ:

S	9.21513800	-0.91138000	-1.26763800
C	10.27666700	0.29479500	-1.96271600
C	9.85076100	1.62717800	-1.57459100
C	8.69260000	1.62360200	-0.74271800
C	8.15711700	0.29341500	-0.48120900
C	7.00219500	-0.09128100	0.16666800
C	11.34168400	-0.11790100	-2.75037900
S	5.77009300	1.09514300	0.63709800
C	4.57698800	-0.13038200	1.13622100
C	5.20042900	-1.44354000	1.04131300
C	6.52255600	-1.42454000	0.52047400
C	3.28423700	0.22047800	1.45769100
C	2.69701300	1.53771500	1.68376300
C	1.27824700	1.52441900	1.82067300
C	0.68332300	0.19622500	1.71338500
S	1.99381200	-0.99861800	1.55977400
C	-0.64081000	-0.17955400	1.65169100
S	-1.93406200	1.02085800	1.41502400
C	-3.20991700	-0.19367900	1.17434900
C	-2.64532000	-1.51574600	1.42693400
C	-1.24172900	-1.50899000	1.67694100
C	-4.47025200	0.16116900	0.74473900
C	-5.07264300	1.47687300	0.58128600

C	-6.33944300	1.46226000	-0.06301800
C	-6.84228100	0.12329500	-0.35386100
S	-5.61868600	-1.06100400	0.14455100
C	-8.06620300	-0.27879600	-0.84640300
S	-9.42316200	0.87121900	-1.00326700
C	-10.57605600	-0.36453700	-1.46163100
C	-9.92542600	-1.65995200	-1.53770900
C	-8.53578200	-1.60603100	-1.22242700
C	-11.89502600	-0.00278900	-1.69467600
C	4.65973600	-2.66893700	1.46558400
C	5.37224100	-3.86148500	1.37015900
C	6.68979200	-3.84250800	0.85280400
C	7.24261000	-2.62903200	0.45259600
C	-4.54610300	2.70970500	1.00320400
C	-5.19156500	3.91505800	0.74080100
C	-6.40678500	3.90661400	0.01405400
C	-6.95779300	2.68690400	-0.36835700
C	3.39070700	2.75061900	1.84061200
C	2.70310500	3.92945300	2.10026600
C	1.31159500	3.91722600	2.23198300
C	0.60659900	2.72685300	2.10529500
C	10.47473300	2.83733400	-1.92522700
C	9.97114900	4.03671000	-1.44181800
C	8.85635200	4.03898400	-0.59435100
C	8.22296100	2.85318500	-0.24384800
C	-3.35142000	-2.72925400	1.50672500
C	-2.68651200	-3.91588700	1.79040000
C	-1.30910400	-3.91086900	2.02691600
C	-0.59531100	-2.71952400	1.98388900
C	-10.52873900	-2.87717500	-1.89937000
C	-9.76094600	-4.03117400	-1.97138900
C	-8.38725200	-3.97810100	-1.70498500
C	-7.77561700	-2.78514200	-1.33948800
C	7.50198600	-5.10966500	0.75488800
C	4.74747700	-5.15179700	1.83841900
C	-4.58886100	5.21237700	1.21835800
C	-7.10954300	5.19460000	-0.33532600
C	-12.29193000	1.36167500	-1.56853200
N	-12.58759400	2.48408200	-1.46121800
C	12.26176100	0.77156600	-3.37343800
N	13.02759500	1.48068100	-3.89312100
C	11.56460600	-1.50919100	-2.97353300
N	11.72514000	-2.65228300	-3.13573600
C	-12.91839600	-0.92136100	-2.06195200
N	-13.77284000	-1.65531500	-2.36302600
H	3.67734400	-2.70359700	1.91706600
H	8.27066900	-2.63632100	0.11686100
H	-3.62509600	2.74359500	1.56951600
H	-7.88040800	2.71129300	-0.93213100
H	4.47090800	2.77685300	1.80334100
H	3.25514400	4.85590700	2.22274300
H	0.77691700	4.83467500	2.45693200
H	-0.46162400	2.73611400	2.27089700
H	11.34887900	2.83985900	-2.56228100
H	10.45352400	4.97026000	-1.71208900
H	8.48056700	4.97736200	-0.19805400
H	7.38464900	2.89376900	0.43700400
H	-4.42661300	-2.75094100	1.39507000

H	-3.24806600	-4.84263500	1.85257400
H	-0.79422300	-4.83468300	2.27121500
H	0.45670100	-2.73598700	2.23193100
H	-11.58445800	-2.91930600	-2.13109500
H	-10.22674600	-4.96992300	-2.25256200
H	-7.78440700	-4.87680400	-1.79312100
H	-6.70613500	-2.77548800	-1.18280600
H	7.63045200	-5.58361800	1.73520900
H	7.01381900	-5.84858700	0.10858900
H	8.49485400	-4.91315100	0.34434300
H	5.33827700	-5.62010000	2.63433500
H	3.73811400	-4.98670900	2.22252100
H	4.68169900	-5.88262400	1.02381400
H	-5.27589800	5.75545700	1.87774800
H	-3.66142900	5.03918100	1.76928000
H	-4.36179200	5.88185400	0.38028800
H	-6.47077500	5.85053300	-0.93847000
H	-8.02512300	5.00582600	-0.90017800
H	-7.38270000	5.75951500	0.56376300

B7-7TQ:

S	11.58214900	0.70952300	-0.49457700
C	12.76605800	-0.54812900	-0.78195200
C	12.10553600	-1.80425500	-1.08642900
C	10.68299200	-1.70443300	-1.07320400
C	10.18672100	-0.38279600	-0.71387900
C	8.89870000	0.04533700	-0.46730200
C	14.11556200	-0.23503900	-0.70201400
S	7.55799200	-1.10844900	-0.32550900
C	6.34815200	0.12813200	0.09787400
C	7.01636100	1.41899200	0.16895000
C	8.38991600	1.38566800	-0.19554200
C	5.01042800	-0.18516300	0.21315700
C	4.35227100	-1.48658200	0.21508500
C	2.92911400	-1.41602600	0.15699400
C	2.39834600	-0.06143200	0.23409600
S	3.76327500	1.08140700	0.25581900
C	1.09621800	0.36864900	0.37902400
S	-0.22285700	-0.76838300	0.74183300
C	-1.45285300	0.50063900	0.95261800
C	-0.81853500	1.79878000	0.75588900
C	0.55603300	1.72258100	0.38372200
C	-2.77713200	0.18299900	1.16538300
C	-3.39548200	-1.10286700	1.46208700
C	-4.81648100	-1.08470200	1.43838800
C	-5.38978300	0.22093400	1.13025400
S	-4.06579300	1.39994000	0.99536300
C	-6.69774500	0.58222500	0.88847700
S	-7.95953900	-0.64634900	0.62096000
C	-9.20073100	0.52564900	0.14370800
C	-8.66320400	1.87319600	0.32084400
C	-7.29431500	1.90037200	0.71903700
C	6.45469700	2.64465500	0.56740100
C	7.18047100	3.83242900	0.53273000
C	8.51919400	3.81403900	0.07154300
C	9.09826600	2.59689200	-0.27643100
C	-2.74069400	-2.29319900	1.82148600

C	-3.44168900	-3.45736600	2.12614600
C	-4.85651000	-3.43991000	2.09939100
C	-5.51445000	-2.25766200	1.77023100
C	4.97280400	-2.74718700	0.28640800
C	4.21812900	-3.91080000	0.20292600
C	2.83171000	-3.83919200	0.03723800
C	2.19108700	-2.60640500	0.01983600
C	12.73269900	-3.02418500	-1.39479600
C	11.96148900	-4.13407100	-1.71040900
C	10.56510300	-4.03273500	-1.74169500
C	9.92812400	-2.83707700	-1.43315200
C	-1.41478800	3.06325000	0.91224800
C	-0.70205500	4.22076700	0.62570200
C	0.61510300	4.14002400	0.16390000
C	1.24052100	2.90505600	0.04687600
C	-9.36896800	3.08351700	0.19858800
C	-8.73483300	4.29688600	0.43208600
C	-7.39150800	4.32396800	0.81877000
C	-6.68073200	3.14080400	0.97260000
C	9.32145700	5.08729700	-0.02930300
C	6.53582700	5.12206700	0.97533000
C	-2.69227100	-4.70992600	2.50712500
C	-5.65107400	-4.67360000	2.44915800
C	-10.41726400	0.11709500	-0.36201100
C	-11.00305700	-1.21489300	-0.44103700
C	-12.22716500	-1.26597600	-1.17060500
C	-12.65393200	0.03337700	-1.65740400
S	-11.51143400	1.26985100	-1.17669600
C	-13.77119700	0.39693800	-2.39525500
C	-10.52111100	-2.40204200	0.14204900
C	-11.20868300	-3.59671100	-0.03143800
C	-12.39045500	-3.64504700	-0.78111800
C	-12.90561700	-2.48529500	-1.34277300
C	14.52032200	1.09872000	-0.39831200
N	14.82280100	2.19714100	-0.15177000
C	15.16352100	-1.17613900	-0.90656100
N	16.03852300	-1.92931900	-1.06965300
C	-13.98180400	1.76427900	-2.74329700
N	-14.13219000	2.88860100	-3.01155100
C	-14.75897400	-0.52277100	-2.84735600
N	-15.58047000	-1.25741200	-3.22801000
H	5.44057700	2.68263400	0.94222000
H	10.11924200	2.61366100	-0.63303400
H	-1.66302700	-2.31520500	1.91334600
H	-6.59530600	-2.25372800	1.81662400
H	6.04090100	-2.82965800	0.43289000
H	4.71308200	-4.87523000	0.25786500
H	2.24703700	-4.74756500	-0.06933400
H	1.12040200	-2.57768700	-0.12801900
H	13.81159000	-3.10176500	-1.39712700
H	12.44619300	-5.07474500	-1.95019000
H	9.96670800	-4.89497100	-2.01984900
H	8.85104300	-2.78623000	-1.50912500
H	-2.42903500	3.15409900	1.27521100
H	-1.17931700	5.18777400	0.74930900
H	1.15731000	5.04227800	-0.10092800
H	2.25160000	2.86771700	-0.33431300
H	-10.42306600	3.09213700	-0.04076200

H	-9.29538100	5.22080100	0.33405700
H	-6.90272200	5.27138100	1.02326800
H	-5.66137000	3.18926100	1.32901300
H	8.84413500	5.81150000	-0.69998700
H	9.42027900	5.57795500	0.94618900
H	10.32776300	4.89272900	-0.40683900
H	7.09169900	5.58691000	1.79791600
H	6.50671700	5.85615700	0.16132900
H	5.51067400	4.95635900	1.31476100
H	-2.96688400	-5.05549000	3.51075600
H	-2.91348200	-5.53451200	1.81896700
H	-1.61251900	-4.54402700	2.49452100
H	-5.42364200	-5.02790300	3.46149100
H	-6.72513700	-4.48024500	2.39648400
H	-5.42635500	-5.50249400	1.76739800
H	-9.62990400	-2.39924400	0.75341100
H	-10.82276400	-4.50169000	0.42786700
H	-12.91511900	-4.58550300	-0.91353400
H	-13.83029100	-2.52479100	-1.90255400

Anions:

2TQ:

C	3.22165100	0.26598200	0.00017800
S	1.99156400	-0.99769700	-0.00031600
C	0.67625600	0.19665400	0.00023500
C	1.22012400	1.48970700	0.00074100
C	2.61032400	1.53490900	0.00070600
C	-0.67621900	-0.19678100	0.00015600
C	-1.22024900	-1.48975000	0.00014200
C	-2.61041300	-1.53483600	0.00002900
C	-3.22161600	-0.26583800	-0.00002400
S	-1.99151000	0.99769100	0.00005700
C	-4.60403200	0.03106300	-0.00012600
C	4.60402700	-0.03104800	0.00003900
C	5.55043600	1.02426200	0.00018500
N	6.31303000	1.91046800	0.00004200
C	-5.08495600	1.36238900	-0.00072300
N	-5.46683800	2.46778000	-0.00123600
C	5.08489600	-1.36238200	-0.00029800
N	5.46682700	-2.46775700	-0.00084100
C	-5.55036200	-1.02431300	0.00036600
N	-6.31297200	-1.91050300	0.00090000
H	0.59411300	2.37566600	0.00118000
H	3.19507500	2.44677300	0.00107800
H	-0.59429800	-2.37575700	0.00019300
H	-3.19529300	-2.44661200	0.00000100

3TQ:

S	-4.03732700	0.79877300	-0.00017800
C	-5.16400200	-0.55245100	-0.00010800

C	-4.45696900	-1.77022500	0.00022100
C	-3.07735800	-1.61480200	0.00038100
C	-2.62319900	-0.28458500	0.00018900
C	-1.27594800	0.14984000	0.00017200
C	-6.56499600	-0.36063000	-0.00034000
S	-0.00001500	-1.07088200	-0.00015300
C	1.27594100	0.14980900	0.00014800
C	0.70675400	1.44216600	0.00036800
C	-0.70673100	1.44218300	0.00041700
C	2.62318600	-0.28461600	0.00014900
C	3.07735600	-1.61483100	0.00039300
C	4.45696400	-1.77024100	0.00032000
C	5.16398700	-0.55245800	-0.00003600
S	4.03730500	0.79875600	-0.00021500
C	6.56497500	-0.36062900	-0.00022800
C	-1.55619900	2.68615100	0.00090600
C	1.55627900	2.68609100	0.00046400
C	-7.14191400	0.93181400	-0.00056300
N	-7.59919200	2.00820800	-0.00078000
C	7.42795100	-1.48482300	-0.00020200
N	8.11887700	-2.42795000	-0.00012400
C	7.14189000	0.93181900	-0.00044200
N	7.59920000	2.00820000	-0.00063100
C	-7.42795800	-1.48483200	-0.00031100
N	-8.11885400	-2.42798100	0.00019100
H	-4.96696800	-2.72579400	0.00036100
H	-2.39078800	-2.45456700	0.00066800
H	2.39078600	-2.45459600	0.00070000
H	4.96697600	-2.72580300	0.00051400
H	-0.95185100	3.59358000	0.00139100
H	-2.20631300	2.72934300	-0.87990200
H	-2.20642100	2.72848400	0.88167600
H	2.20643900	2.72882000	-0.88033700
H	0.95199100	3.59355700	0.00045000
H	2.20647600	2.72878900	0.88123500

4TQ:

C	7.14195200	-0.26881600	0.00001400
C	6.55289500	-1.55020300	-0.00001900
C	5.16328400	-1.52635200	0.00005600
C	4.59947900	-0.24387000	0.00015400
S	5.89193600	0.97263600	0.00016600
C	3.23774300	0.12932400	0.00022900
S	1.94416400	-1.07793200	0.00023600
C	0.68774800	0.16846600	0.00006300
C	1.28357500	1.43280800	0.00017800
C	2.67881400	1.41408000	0.00030900
C	-0.68774700	-0.16847300	-0.00014200
C	-1.28357400	-1.43281400	-0.00057000
C	-2.67881400	-1.41408600	-0.00057700
C	-3.23774100	-0.12932900	-0.00021900
S	-1.94416200	1.07792600	0.00011600
C	-4.59947900	0.24386700	-0.00015300
S	-5.89193800	-0.97263700	-0.00025900
C	-7.14195200	0.26881900	0.00002400

C	-6.55289300	1.55020500	0.00010600
C	-5.16328000	1.52635100	-0.00001200
C	-8.51742100	-0.05030500	0.00010000
C	8.51741800	0.05030900	-0.00007900
C	-9.48014000	0.99044000	0.00005000
N	-10.25387700	1.86646500	-0.00001700
C	-8.97295200	-1.39076900	0.00021600
N	-9.32841700	-2.50455800	0.00036700
C	8.97294700	1.39077300	-0.00038200
N	9.32840400	2.50456400	-0.00057700
C	9.48014000	-0.99043300	0.00010200
N	10.25388600	-1.86644900	0.00025000
H	7.15312800	-2.45169400	-0.00010200
H	4.55300200	-2.42352000	0.00002200
H	0.69952200	2.34652100	0.00014100
H	3.29000800	2.30938500	0.00038600
H	-0.69952200	-2.34652800	-0.00086400
H	-3.29000800	-2.30939100	-0.00088600
H	-7.15312400	2.45169800	0.00025800
H	-4.55299700	2.42351800	0.00004000

5TQ:

C	9.10464700	-0.22644500	0.00026700
S	7.83862500	0.99845100	0.00001000
C	6.56325700	-0.23460400	-0.00010000
C	7.14272500	-1.50937800	-0.00002000
C	8.53283600	-1.51543000	0.00018300
C	5.19530600	0.12160300	-0.00025300
C	4.62025600	1.39795300	-0.00034800
C	3.22316900	1.39668600	-0.00042500
C	2.64706900	0.12609900	-0.00039700
S	3.91908700	-1.10236000	-0.00037300
C	1.27317200	-0.23370700	-0.00039800
S	0.00000000	0.99157900	-0.00041500
C	-1.27317200	-0.23370700	-0.00038600
C	-0.69962000	-1.50543600	-0.00038500
C	0.69961900	-1.50543600	-0.00039100
C	-2.64706900	0.12609900	-0.00037100
C	-3.22316900	1.39668600	-0.00038600
C	-4.62025700	1.39795200	-0.00030600
C	-5.19530700	0.12160300	-0.00022800
S	-3.91908700	-1.10236100	-0.00034400
C	-6.56325700	-0.23460400	-0.00009000
S	-7.83862500	0.99845100	0.00002200
C	-9.10464600	-0.22644500	0.00025900
C	-8.53283600	-1.51543000	0.00016300
C	-7.14272500	-1.50937800	-0.00003000
C	-10.47576300	0.11084100	0.00049800
C	10.47576400	0.11084100	0.00050800
C	-11.45200700	-0.91718200	0.00067900
N	-12.23663900	-1.78337700	0.00081500
C	10.91302300	1.45736900	0.00056200
N	11.25226600	2.57613900	0.00060900
C	-10.91302200	1.45736900	0.00056400
N	-11.25226600	2.57613800	0.00062500
C	11.45200700	-0.91718200	0.00070500

N	12.23663900	-1.78337700	0.00086200
H	6.54423900	-2.41447000	-0.00009800
H	9.14470800	-2.40903400	0.00028100
H	5.21864700	2.30175200	-0.00034400
H	2.62702900	2.30267500	-0.00048900
H	-1.29656000	-2.41053800	-0.00037800
H	1.29656000	-2.41053800	-0.00039000
H	-2.62703000	2.30267400	-0.00044100
H	-5.21864800	2.30175100	-0.00029300
H	-9.14470800	-2.40903400	0.00024600
H	-6.54423900	-2.41447000	-0.00011500

6TQ:

S	9.80742500	0.97497600	-0.00010700
C	11.06432000	-0.25922600	0.00035100
C	10.48350000	-1.54347000	0.00094400
C	9.09268200	-1.52683300	0.00111400
C	8.52402300	-0.24818800	0.00066700
C	7.15708300	0.11984800	0.00086000
C	12.43820700	0.06875600	0.00006200
S	5.87244000	-1.09399000	-0.00157400
C	4.61080400	0.14315400	0.00056200
C	5.19416700	1.40804700	0.00258900
C	6.59306500	1.39940200	0.00277000
C	3.23124000	-0.20897600	0.00012200
C	2.64983200	-1.47444800	-0.00045000
C	1.24746200	-1.46204200	-0.00097300
C	0.68773200	-0.18847800	-0.00083000
S	1.96924200	1.02534400	0.00030800
C	-0.68772900	0.18844000	-0.00141700
S	-1.96924000	-1.02538100	0.00096300
C	-3.23123900	0.20893900	-0.00128200
C	-2.64982800	1.47440800	-0.00368600
C	-1.24745900	1.46200200	-0.00376500
C	-4.61080200	-0.14318200	-0.00054000
C	-5.19417700	-1.40807100	0.00089700
C	-6.59307400	-1.39941700	0.00136100
C	-7.15708500	-0.11985700	0.00025900
S	-5.87243200	1.09397400	-0.00140400
C	-8.52402000	0.24818800	0.00035300
S	-9.80743500	-0.97496300	-0.00042200
C	-11.06431700	0.25925000	0.00057500
C	-10.48348300	1.54349100	0.00122100
C	-9.09266700	1.52684000	0.00109500
C	-12.43820600	-0.06871100	0.00059400
C	-13.40731300	0.96593000	0.00162300
N	-14.18570300	1.83772700	0.00231100
C	13.40732900	-0.96587100	0.00030300
N	14.18572700	-1.83766200	0.00038800
C	12.88426000	1.41232700	-0.00052100
N	13.23008800	2.52909000	-0.00093900
C	-12.88428400	-1.41227500	-0.00047100
N	-13.23013600	-2.52903000	-0.00132900

H	11.08844800	-2.44175800	0.00132100
H	8.48752400	-2.42745900	0.00172900
H	4.60494200	2.31857900	0.00423600
H	7.19777700	2.29892400	0.00459600
H	3.23877000	-2.38464800	-0.00045700
H	0.64360100	-2.36265800	-0.00159100
H	-3.23876400	2.38460800	-0.00547800
H	-0.64359800	2.36261700	-0.00568500
H	-4.60496300	-2.31861100	0.00164700
H	-7.19779200	-2.29893500	0.00261300
H	-11.08842300	2.44178500	0.00182200
H	-8.48749700	2.42745800	0.00165300

7TQ:

S	11.76286900	1.00886300	0.00367300
C	13.02834600	-0.21653500	0.00233100
C	12.45715500	-1.50418400	0.00029500
C	11.06527600	-1.49698200	-0.00017200
C	10.48911100	-0.22276200	0.00149700
C	9.11779000	0.13711000	0.00157500
C	14.40033800	0.12210400	0.00326800
S	7.84303500	-1.08610700	-0.00163300
C	6.57298200	0.14055000	0.00046900
C	7.14458800	1.40874100	0.00328800
C	8.54538800	1.41110700	0.00390800
C	5.19362600	-0.22501600	-0.00071800
C	4.62415200	-1.49356900	-0.00088500
C	3.21912500	-1.49151900	-0.00207600
C	2.65219400	-0.22417800	-0.00285200
S	3.92303600	0.99863000	-0.00232400
C	1.27027400	0.14570600	-0.00395000
S	-0.00000400	-1.07706400	-0.00067600
C	-1.27027900	0.14570600	-0.00493100
C	-0.70312600	1.41279700	-0.00797100
C	0.70312800	1.41279700	-0.00742500
C	-2.65219700	-0.22417300	-0.00480200
C	-3.21913100	-1.49151400	-0.00686800
C	-4.62415200	-1.49356600	-0.00663700
C	-5.19363200	-0.22501300	-0.00438200
S	-3.92303700	0.99863100	-0.00155000
C	-6.57298000	0.14054400	-0.00401500
S	-7.84302700	-1.08611200	0.00142200
C	-9.11779100	0.13709100	-0.00160300
C	-8.54539400	1.41109300	-0.00616500
C	-7.14460300	1.40873200	-0.00752000
C	-10.48909800	-0.22277100	0.00065500
C	-11.06528100	-1.49698800	0.00259500
C	-12.45714400	-1.50418100	0.00446800
C	-13.02834300	-0.21652300	0.00405500
S	-11.76285800	1.00886300	0.00129500
C	-14.40031800	0.12210000	0.00556100
C	-15.37696100	-0.90508800	0.00799900
N	-16.16158000	-1.77128500	0.00999900
C	-14.83586900	1.46885300	0.00468800
N	-15.17284300	2.58833200	0.00393900
C	14.83587600	1.46885200	0.00545500
N	15.17282100	2.58834100	0.00726000

C	15.37697400	-0.90508600	0.00200000
N	16.16155800	-1.77131900	0.00090700
H	13.06815600	-2.39836200	-0.00074300
H	10.46629000	-2.40169700	-0.00160700
H	6.54853500	2.31482500	0.00512000
H	9.14286400	2.31542700	0.00617400
H	5.21974600	-2.39935800	0.00000200
H	2.62250500	-2.39699600	-0.00243200
H	-1.29899200	2.31858500	-0.01110600
H	1.29899700	2.31858500	-0.00999200
H	-2.62250500	-2.39698500	-0.00926200
H	-5.21975300	-2.39934900	-0.00886100
H	-9.14288300	2.31540300	-0.00894000
H	-6.54854800	2.31480800	-0.01157700
H	-10.46630100	-2.40170900	0.00238700
H	-13.06815000	-2.39835500	0.00598000

B2-2TQ:

C	3.24240400	0.30979700	0.12021300
S	1.78856100	1.28458600	0.15255900
C	0.69742600	-0.08818100	-0.13069100
C	1.48647400	-1.27934600	-0.25332200
C	2.90056500	-1.06322500	-0.09885800
C	-0.69746800	0.08823100	-0.13082600
C	-1.48651500	1.27939700	-0.25339600
C	-2.90061700	1.06324200	-0.09901100
C	-3.24244200	-0.30977100	0.12010500
S	-1.78858200	-1.28455600	0.15236200
C	-4.49517300	-0.93747200	0.29132600
C	4.49516500	0.93738600	0.29135400
C	-1.03454000	2.59147000	-0.54621900
C	-1.93206800	3.63686100	-0.63469000
C	-3.31486400	3.42456200	-0.44375000
C	-3.79596700	2.15615400	-0.18880900
C	1.03450800	-2.59139400	-0.54627000
C	1.93204100	-3.63679300	-0.63469700
C	3.31481100	-3.42453300	-0.44357900
C	3.79590600	-2.15612900	-0.18856100
C	-5.73073900	-0.24352900	0.28295300
N	-6.76338000	0.30555700	0.28034600
C	-4.57604800	-2.34190800	0.48391700
N	-4.63143800	-3.49926000	0.63844500
C	4.57618200	2.34183200	0.48408300
N	4.63171900	3.49918200	0.63854500
C	5.73071900	0.24341300	0.28273000
N	6.76337700	-0.30563700	0.27980000
H	0.01513800	2.78276100	-0.72666500
H	-1.56557200	4.63404500	-0.86150800
H	-4.00585400	4.25962900	-0.51059400
H	-4.85900300	1.99630900	-0.06275000
H	-0.01515300	-2.78265700	-0.72684000
H	1.56554700	-4.63395100	-0.86163300
H	4.00580000	-4.25960500	-0.51034500
H	4.85893500	-1.99630500	-0.06237900

B3-3TQ:

S	3.94445800	0.89420200	-0.20908700
C	5.21601000	-0.29957900	-0.07299500
C	4.65506400	-1.57221500	0.27930500
C	3.22759200	-1.53594300	0.44261600
C	2.64235100	-0.25030600	0.19076200
C	1.29690200	0.14212500	0.14337400
C	6.55145000	0.09006900	-0.29805800
S	0.00002100	-1.05314500	-0.00052300
C	-1.29692000	0.14214300	-0.14377200
C	-0.70993800	1.45405600	-0.09820200
C	0.70991000	1.45402800	0.09821300
C	-2.64236300	-0.25030600	-0.19113500
C	-3.22759900	-1.53603000	-0.44262300
C	-4.65505800	-1.57229900	-0.27917900
C	-5.21602800	-0.29955900	0.07269400
S	-3.94450700	0.89431000	0.20830300
C	-6.55147000	0.09014000	0.29763700
C	-1.36430600	2.69367400	-0.24701800
C	-0.69821700	3.90886600	-0.13962600
C	0.69819700	3.90880900	0.14068400
C	1.36428100	2.69357600	0.24758000
C	-1.51726900	5.16974200	-0.33101300
C	1.51739700	5.16959300	0.33212000
C	5.35988800	-2.78152500	0.48224600
C	4.67977100	-3.92328000	0.85907200
C	3.28456500	-3.88380200	1.06301300
C	2.56943400	-2.71843000	0.86397800
C	-2.56945500	-2.71865500	-0.86361500
C	-3.28455000	-3.88415900	-1.06203000
C	-4.67971300	-3.92363900	-0.85783000
C	-5.35983900	-2.78174500	-0.48143900
C	-6.85986600	1.43578500	0.63057700
N	-7.09735100	2.53643400	0.89804600
C	7.65546200	-0.79473500	-0.21255900
N	8.57519700	-1.49933700	-0.14941900
C	-7.65551800	-0.79460400	0.21197800
N	-8.57528300	-1.49915400	0.14869800
C	6.85986600	1.43568900	-0.63107700
N	7.09737400	2.53631800	-0.89860700
H	-2.42391600	2.71791100	-0.47111100
H	2.42389700	2.71768300	0.47168700
H	-0.97040300	6.08141600	-0.08962900
H	-1.86032100	5.25973400	-1.36874300
H	-2.41237200	5.14800600	0.29928300
H	0.96915200	6.08163600	0.09534700
H	1.86456800	5.25691500	1.36868500
H	2.41001500	5.15000700	-0.30179700
H	6.43352200	-2.81167400	0.34891600
H	5.22512200	-4.84934000	1.01383200
H	2.76228800	-4.77842700	1.39055600
H	1.50578100	-2.71181700	1.06306600
H	-1.50585500	-2.71207600	-1.06296900
H	-2.76227100	-4.77888600	-1.38929300
H	-5.22503000	-4.84980900	-1.01205500

H -6.43345400 -2.81188600 -0.34795500

B4-4TQ:

C 7.18414000 0.17155000 0.05866600
C 6.68332000 -1.09169900 -0.41038300
C 5.25378200 -1.11907700 -0.54031800
C 4.60633400 0.10202800 -0.14854500
S 5.85538200 1.27342100 0.33795600
C 3.24424300 0.40829400 -0.03414600
S 2.02111400 -0.86795800 0.00080400
C 0.66127800 0.23247700 0.28127000
C 1.17210000 1.57105100 0.37678300
C 2.58809600 1.67567200 0.16010900
C -0.66127400 -0.23246300 0.28124800
C -1.17209800 -1.57103800 0.37674000
C -2.58809200 -1.67565400 0.16004700
C -3.24423500 -0.40827600 -0.03421000
S -2.02110100 0.86797200 0.00074200
C -4.60632900 -0.10201800 -0.14860300
S -5.85535700 -1.27343100 0.33789600
C -7.18412900 -0.17156300 0.05866600
C -6.68333200 1.09168700 -0.41040400
C -5.25379800 1.11907900 -0.54037600
C -8.49914300 -0.60730500 0.29674300
C 8.49916500 0.60729000 0.29669100
C -7.44804300 2.23118300 -0.74681800
C -6.82179300 3.36796900 -1.22248700
C -5.42318400 3.38704500 -1.39292300
C -4.65028300 2.28889800 -1.06394800
C -0.43833100 -2.74420800 0.67850800
C -1.05902000 -3.97862400 0.68409800
C -2.42985400 -4.09029300 0.37953500
C -3.18316300 -2.95931400 0.12783900
C 0.43832500 2.74421900 0.67854400
C 1.05901000 3.97863600 0.68414400
C 2.42984700 4.09031000 0.37959500
C 3.18316200 2.95933400 0.12790500
C 7.44800900 -2.23120500 -0.74681100
C 6.82173400 -3.36798800 -1.22245300
C 5.42311900 -3.38705300 -1.39284700
C 4.65023900 -2.28889500 -1.06386000
C -9.64657100 0.20395500 0.10306200
N -10.60740400 0.85186100 -0.04819500
C -8.74486500 -1.92960300 0.75678200
N -8.93234700 -3.02003500 1.13131100
C 9.64658400 -0.20397300 0.10296800
N 10.60741300 -0.85187700 -0.04832200
C 8.74490700 1.92958900 0.75671600
N 8.93241000 3.02003100 1.13120400
H -8.52469500 2.21341300 -0.63906100
H -7.41277600 4.24156000 -1.47979200
H -4.94158900 4.27299400 -1.79718600
H -3.58347400 2.32386700 -1.24065300
H 0.61141900 -2.67951800 0.93399600
H -0.48217600 -4.86748800 0.92219800
H -2.90307200 -5.06705100 0.35066800
H -4.23212100 -3.07108800 -0.11314300

H	-0.61142900	2.67952500	0.93401700
H	0.48216000	4.86749800	0.92223800
H	2.90306100	5.06707000	0.35073100
H	4.23212000	3.07111300	-0.11307000
H	8.52466500	-2.21344500	-0.63908500
H	7.41270100	-4.24158700	-1.47977000
H	4.94150400	-4.27300000	-1.79708700
H	3.58342400	-2.32385400	-1.24053100

B5-5TQ:

C	-8.99354800	0.39509800	-0.28341200
S	-7.66310400	1.48699900	-0.59737000
C	-6.41935100	0.34419400	-0.02933400
C	-7.07509500	-0.85605200	0.41678600
C	-8.49642800	-0.83860300	0.26218300
C	-5.05833100	0.64383000	-0.13781100
C	-4.39740800	1.89845500	-0.40641300
C	-2.97777800	1.78147100	-0.58363900
C	-2.46735800	0.45340300	-0.38269300
S	-3.83378200	-0.62898000	-0.05544100
C	-1.14645600	-0.00632200	-0.31928400
S	0.20894300	1.11428100	-0.10796700
C	1.43220700	-0.15793600	0.04516900
C	0.77629000	-1.43503900	-0.04510800
C	-0.63504400	-1.35080300	-0.29555700
C	2.79479600	0.15160800	0.13157700
C	3.44678400	1.40380900	0.39728900
C	4.86766300	1.37299800	0.23301200
C	5.39233800	0.07100100	-0.09478700
S	4.03822500	-1.05645900	-0.24386300
C	6.71559500	-0.36818700	-0.21163700
S	8.06532800	0.60499400	0.42278200
C	9.27809800	-0.60049100	0.05906300
C	8.66258500	-1.74744800	-0.55318300
C	7.24379600	-1.60619700	-0.71691900
C	10.62190500	-0.33783000	0.37281900
C	-6.48874000	-1.99653500	1.01185500
C	-7.24755200	-3.09178100	1.39669300
C	-8.65912500	-3.08461500	1.19819900
C	-9.25706200	-1.96250900	0.64823100
C	2.84312000	2.61258700	0.81447400
C	3.57560600	3.77507300	0.99114100
C	4.97725800	3.76656700	0.73359500
C	5.59119400	2.57902100	0.37030500
C	-4.99404100	3.17855000	-0.47583400
C	-4.23647600	4.29253100	-0.78819700
C	-2.86019200	4.16276700	-1.05285600
C	-2.23846200	2.93247800	-0.94826000
C	1.36780600	-2.71135600	0.11115500
C	0.61801200	-3.86009600	-0.06059100
C	-0.74454400	-3.77609000	-0.40566200
C	-1.36298200	-2.54450100	-0.51560700
C	9.31439800	-2.92149000	-0.99124800
C	8.58839600	-3.92932800	-1.59853100
C	7.20248200	-3.77949700	-1.80031700
C	6.53852600	-2.64362900	-1.37407000

C	-9.50089600	-4.27256500	1.59623400
C	-6.57354500	-4.28321100	2.03228300
C	2.88766000	5.03868900	1.44666000
C	5.79192900	5.03021300	0.86459700
C	-10.30419000	0.81030800	-0.56892700
C	10.98887100	0.89669300	0.97482600
N	11.27447900	1.91730000	1.46578100
C	11.68330700	-1.24549600	0.12309400
N	12.57469200	-1.97556400	-0.07179300
C	-11.45147100	0.00342200	-0.35416500
N	-12.41142900	-0.64153100	-0.18680200
C	-10.54719700	2.10521700	-1.10348600
N	-10.73268300	3.17287800	-1.53907100
H	-5.42437400	-2.01914600	1.20751900
H	-10.33216600	-1.95159800	0.52005900
H	1.78256500	2.63754500	1.03171500
H	6.65504200	2.59774800	0.17049200
H	-6.04804000	3.30487500	-0.26659100
H	-4.71143200	5.26754800	-0.83741100
H	-2.27813300	5.03428100	-1.33795600
H	-1.18321200	2.85318000	-1.17476800
H	2.40933600	-2.79893400	0.39186900
H	1.08769300	-4.83108900	0.06573200
H	-1.31738500	-4.68184500	-0.58138100
H	-2.40684400	-2.50206500	-0.79828400
H	10.38279200	-3.03108400	-0.85857300
H	9.09264400	-4.83027300	-1.93404700
H	6.64388800	-4.56186700	-2.30640300
H	5.48058500	-2.54505100	-1.57745700
H	-9.19846700	-5.18217300	1.06231900
H	-9.41323800	-4.49389800	2.66732000
H	-10.55641200	-4.09307100	1.37813100
H	-6.96917500	-4.48358100	3.03553500
H	-6.73269100	-5.19618400	1.44529500
H	-5.49587800	-4.12635100	2.12191300
H	3.31084800	5.41365400	2.38668300
H	2.99529900	5.84557500	0.71120100
H	1.81934200	4.87074400	1.60400500
H	5.43115400	5.81776600	0.19127400
H	5.74353300	5.43998000	1.88107600
H	6.84345400	4.84614400	0.63139500

B6-6TQ:

S	9.78947000	-0.99449500	-0.17972300
C	11.05347000	0.11012400	-0.66512100
C	10.53444000	1.45093100	-0.73399400
C	9.14453500	1.53729300	-0.38927200
C	8.54150200	0.27047100	-0.06159700
C	7.21408200	-0.05677000	0.23140500
C	12.34107200	-0.38931700	-0.91277500
S	5.90486900	1.08541600	-0.08396100
C	4.61066000	-0.02449900	0.40357300
C	5.21165300	-1.25936800	0.83066700
C	6.63920000	-1.28159500	0.73887100
C	3.26451500	0.33136500	0.26916300

C	2.65817400	1.62059000	0.04700600
C	1.24380900	1.56668700	-0.19122600
C	0.68037700	0.24693900	-0.08810400
S	1.99329700	-0.89974700	0.23265300
C	-0.65594500	-0.16702700	-0.11132700
S	-1.98209400	0.99105800	0.09425800
C	-3.25346500	-0.24158100	0.12393000
C	-2.63674800	-1.53756500	-0.00098400
C	-1.21349500	-1.49183100	-0.18021400
C	-4.60568300	0.11157100	0.16437600
C	-5.22679700	1.37550900	0.45410900
C	-6.63772500	1.40356000	0.22380600
C	-7.19152800	0.13419900	-0.18309600
S	-5.87181900	-1.03524700	-0.31677200
C	-8.52042600	-0.24977000	-0.38106600
S	-9.86556100	0.75458800	0.21503000
C	-11.10023200	-0.39316500	-0.24781100
C	-10.49572700	-1.54402000	-0.86651800
C	-9.06699500	-1.45175800	-0.95377700
C	-12.44659300	-0.09097100	0.00722500
C	4.55336100	-2.38556100	1.37458000
C	5.24598900	-3.51030500	1.79371300
C	6.66616200	-3.53443700	1.69836500
C	7.32892300	-2.42763800	1.19168700
C	-4.60228000	2.54277100	0.94932700
C	-5.30189400	3.72366700	1.14131900
C	-6.68821000	3.77720500	0.81948800
C	-7.32470100	2.62789500	0.37809900
C	3.29899300	2.88098600	0.07451100
C	2.59249500	4.03763700	-0.19980700
C	1.22503300	3.97392900	-0.52607000
C	0.55979500	2.76183100	-0.51803400
C	11.25572900	2.61393900	-1.08124700
C	10.62711200	3.84555600	-1.07268300
C	9.27278400	3.94325400	-0.70200200
C	8.54187200	2.81783100	-0.36570600
C	-3.27833200	-2.79646900	0.06408100
C	-2.56082200	-3.96307500	-0.12868100
C	-1.18166500	-3.91158200	-0.40385500
C	-0.51665000	-2.69918000	-0.42355300
C	-11.16699400	-2.67722500	-1.37505900
C	-10.44799800	-3.69316400	-1.97819500
C	-9.04972100	-3.59023800	-2.10453500
C	-8.36726700	-2.49389700	-1.60795200
C	7.44991600	-4.73679000	2.16488900
C	4.49586800	-4.68701800	2.36813700
C	-4.59259800	4.94142700	1.68104000
C	-7.46442700	5.06307600	0.96639200
C	-12.79894400	1.13805000	0.62983600
N	-13.07112300	2.15342900	1.13846200
C	13.43705300	0.41548800	-1.31900100
N	14.35511000	1.05607000	-1.65335500
C	12.61218600	-1.77669100	-0.75768200
N	12.81781400	-2.91814400	-0.62152100
C	-13.52612200	-0.95075900	-0.32332800
N	-14.43197500	-1.64068500	-0.58496700
H	3.47929800	-2.37008900	1.50722300
H	8.41054500	-2.45143600	1.17916400

H	-3.55323500	2.52031300	1.21647700
H	-8.37642000	2.69431500	0.13057400
H	4.34754600	2.95277200	0.33145100
H	3.10101800	4.99673600	-0.17248000
H	0.68499900	4.88033900	-0.78329400
H	-0.48689800	2.73356500	-0.79116400
H	12.30191300	2.54437700	-1.34879700
H	11.18408800	4.73775900	-1.34116800
H	8.79048500	4.91625800	-0.67378000
H	7.51123300	2.93442000	-0.06047900
H	-4.33449100	-2.85979200	0.29128100
H	-3.06888100	-4.92116300	-0.07270500
H	-0.63142900	-4.82796400	-0.59592100
H	0.54064700	-2.68195000	-0.65364000
H	-12.24407300	-2.74986600	-1.30024000
H	-10.96710100	-4.56307900	-2.36830400
H	-8.49451800	-4.37723700	-2.60704900
H	-7.29751000	-2.43005200	-1.75491100
H	7.27367300	-4.95091900	3.22635800
H	7.16900000	-5.64132900	1.61147000
H	8.52318900	-4.58425600	2.02807700
H	4.81274900	-4.90804000	3.39474600
H	3.41949300	-4.49909300	2.38309300
H	4.66921300	-5.59908700	1.78382100
H	-5.04786800	5.29394600	2.61465900
H	-3.53984200	4.72768200	1.88162000
H	-4.63594800	5.78030500	0.97542300
H	-7.04441200	5.86415000	0.34547700
H	-8.50907300	4.92735600	0.67618500
H	-7.45143000	5.42812200	2.00079400

B7-7TQ:

S	11.72532200	0.61796200	0.01350500
C	12.91573500	-0.58892400	-0.41358500
C	12.26412200	-1.75761900	-0.94786600
C	10.83707000	-1.63171200	-1.00156200
C	10.33767300	-0.38319800	-0.48407200
C	9.02684800	0.04581500	-0.27099100
C	14.27486100	-0.31055200	-0.21256800
S	7.67337000	-1.09174900	-0.31368100
C	6.45078600	0.11250200	0.14272700
C	7.11403000	1.37212800	0.35557400
C	8.51754600	1.34990400	0.08755000
C	5.09089000	-0.20328300	0.15278000
C	4.43560300	-1.48746000	0.09347700
C	3.01026700	-1.40867500	-0.04690500
C	2.48937400	-0.06654900	-0.00905900
S	3.85228400	1.06214900	0.11506300
C	1.16731600	0.38336300	0.04076100
S	-0.16622500	-0.71853600	0.42383300
C	-1.40456900	0.54774700	0.45959400
C	-0.76995200	1.81424100	0.18924900
C	0.63552000	1.71690700	-0.08234900
C	-2.75507900	0.23064900	0.63426800
C	-3.37592500	-0.98429300	1.09598200

C	-4.80538500	-0.96730800	1.04573100
C	-5.36213700	0.26194900	0.53530800
S	-4.03192100	1.37043800	0.17417700
C	-6.68819000	0.60765000	0.25906700
S	-7.95040500	-0.63365800	0.14248600
C	-9.22062800	0.48498700	-0.36455500
C	-8.65480500	1.81251100	-0.45049200
C	-7.27300200	1.88152400	-0.07195800
C	6.53474400	2.57812300	0.80918900
C	7.27067000	3.74766600	0.92466100
C	8.64756700	3.74716400	0.56432200
C	9.24071700	2.55986100	0.16308500
C	-2.73368600	-2.12046300	1.63700100
C	-3.44430200	-3.21838400	2.09679500
C	-4.86651900	-3.19981700	2.04993000
C	-5.51341800	-2.08319500	1.54350800
C	5.04527000	-2.75929100	0.18781200
C	4.29218500	-3.91297500	0.05850400
C	2.90853400	-3.83321700	-0.17984800
C	2.27527700	-2.60395200	-0.22583100
C	12.89182600	-2.93527600	-1.40708100
C	12.13018000	-3.96482500	-1.93048900
C	10.73267000	-3.83145400	-2.02469900
C	10.09270400	-2.68971800	-1.57449700
C	-1.37649700	3.09159100	0.19620700
C	-0.64645500	4.22106400	-0.12717200
C	0.70960000	4.11264000	-0.48442700
C	1.34218600	2.88280700	-0.45897300
C	-9.30726100	2.98747600	-0.88740100
C	-8.64922400	4.20420100	-0.87835200
C	-7.32079700	4.28571500	-0.42462500
C	-6.64057800	3.14635700	-0.03511500
C	9.46186300	5.01615500	0.62708700
C	6.60857500	5.00903600	1.42230000
C	-2.71008300	-4.40702600	2.66757900
C	-5.66902800	-4.36702000	2.57099900
C	-10.53542400	0.05061500	-0.54315200
C	-11.07026100	-1.28410500	-0.63185300
C	-12.50217900	-1.33822500	-0.67841100
C	-13.11869600	-0.03628800	-0.65854700
S	-11.89149800	1.20606900	-0.57269200
C	-14.46916400	0.33722500	-0.70131500
C	-10.35129500	-2.49974200	-0.71800200
C	-11.02438900	-3.70650100	-0.79749300
C	-12.43064500	-3.75399600	-0.80036800
C	-13.16461300	-2.58226900	-0.75178200
C	14.67640800	0.94285300	0.32699800
N	14.98820200	1.97830900	0.76738500
C	15.32211500	-1.21816300	-0.51982900
N	16.20175300	-1.94704700	-0.76376500
C	-14.83337500	1.71209300	-0.68011000
N	-15.11539800	2.84501200	-0.66516200
C	-15.54360600	-0.58804100	-0.76723200
N	-16.44497500	-1.32911900	-0.82112900
H	5.49349900	2.59827300	1.10497800
H	10.28643900	2.58556300	-0.11510300
H	-1.65622600	-2.13468500	1.73760900
H	-6.59521800	-2.06748300	1.57313000

H	6.10522400	-2.84379200	0.38836900
H	4.77645700	-4.88175400	0.13599700
H	2.32847200	-4.74025100	-0.32213300
H	1.21275500	-2.56641000	-0.42699700
H	13.96836500	-3.03261500	-1.35744800
H	12.61578900	-4.86932400	-2.28313800
H	10.14326600	-4.63057700	-2.46520200
H	9.02133500	-2.60568800	-1.69665400
H	-2.41628100	3.19927900	0.47470200
H	-1.12959200	5.19351900	-0.11514100
H	1.26659100	4.99665400	-0.78019400
H	2.38017300	2.81915500	-0.75778500
H	-10.32425100	2.94791800	-1.25382900
H	-9.16586300	5.09638000	-1.21812200
H	-6.81842900	5.24781000	-0.38658900
H	-5.62270000	3.23639900	0.31954500
H	9.04614100	5.79751100	-0.02113900
H	9.48748500	5.43104400	1.64223000
H	10.49397200	4.83732900	0.31620300
H	7.09860700	5.39337400	2.32519000
H	6.65482000	5.81111600	0.67538400
H	5.55650100	4.83449300	1.66063800
H	-2.99687300	-4.60047100	3.70856100
H	-2.92917800	-5.32411700	2.10677700
H	-1.62879300	-4.25104600	2.64258800
H	-5.45739100	-4.56702600	3.62863500
H	-6.74166600	-4.18100400	2.47515100
H	-5.43997800	-5.29099300	2.02559800
H	-9.27037300	-2.49803700	-0.75620000
H	-10.45367800	-4.62814400	-0.86791000
H	-12.94308500	-4.70922300	-0.85731300
H	-14.24563300	-2.62207800	-0.77761800

Cations:

2TQ:

C	3.17741400	0.25409800	0.00000300
S	1.95830100	-1.01158600	0.00007500
C	0.67851300	0.18571400	-0.00007000
C	1.20841300	1.50939400	-0.00019400
C	2.57895800	1.55101100	-0.00016200
C	-0.67852500	-0.18577900	-0.00004500
C	-1.20843300	-1.50942600	-0.00000300
C	-2.57901300	-1.55098900	0.00003000
C	-3.17737100	-0.25410300	0.00000600
S	-1.95831000	1.01154400	-0.00008900
C	-4.54237300	0.03054100	0.00004700
C	4.54232400	-0.03050600	0.00006800
C	5.49476400	1.02516000	0.00022300
N	6.25713200	1.90657200	0.00037400
C	-5.01693100	1.37044800	-0.00001800
N	-5.36752300	2.48205200	-0.00007100
C	5.01694500	-1.37042100	-0.00013800

N	5.36760800	-2.48199700	-0.00028200
C	-5.49476900	-1.02510900	0.00012100
N	-6.25710400	-1.90655800	0.00019200
H	0.58055900	2.39326000	-0.00035800
H	3.17200100	2.45834000	-0.00018300
H	-0.58061700	-2.39331700	0.00000800
H	-3.17208900	-2.45829800	0.00006800

3TQ:

S	-3.98962700	0.81153200	-0.00002900
C	-5.10673300	-0.54857400	-0.00003200
C	-4.40134400	-1.78888300	0.00006300
C	-3.04119000	-1.63258600	0.00007400
C	-2.60291700	-0.27199000	0.00006800
C	-1.25851700	0.15048400	0.00009000
C	-6.48617400	-0.37291600	-0.00009600
S	0.00001000	-1.07072600	0.00005500
C	1.25850900	0.15049700	0.00004000
C	0.70104800	1.46525100	0.00005400
C	-0.70107400	1.46523800	0.00010800
C	2.60292400	-0.27197200	0.00001100
C	3.04118400	-1.63256100	0.00000500
C	4.40134800	-1.78887000	0.00000400
C	5.10673200	-0.54857200	-0.00003700
S	3.98964400	0.81153900	-0.00004200
C	6.48619400	-0.37291400	-0.00005900
C	-1.55506200	2.70016200	0.00017400
C	1.55504200	2.70017000	0.00002100
C	-7.06435400	0.92698100	-0.00012200
N	-7.49747900	2.00871100	-0.00015600
C	7.35212600	-1.50245100	-0.00003900
N	8.03779800	-2.44420400	-0.00001700
C	7.06436000	0.92697700	-0.00006400
N	7.49747500	2.00871300	-0.00007900
C	-7.35213100	-1.50244300	-0.00004900
N	-8.03782500	-2.44417900	-0.00001700
H	-4.91573400	-2.74260000	0.00008200
H	-2.34945800	-2.46677300	0.00012000
H	2.34945100	-2.46674700	0.00003000
H	4.91572500	-2.74259400	0.00000400
H	-0.95779700	3.61010100	0.00024200
H	-2.19940900	2.73793200	-0.88508100
H	-2.19941200	2.73782300	0.88543300
H	2.19933100	2.73788100	-0.88528200
H	0.95779500	3.61012000	0.00004800
H	2.19944000	2.73786900	0.88524100

4TQ:

C	7.07999000	-0.25650300	0.00009600
C	6.49110600	-1.55769400	-0.00021800
C	5.11971500	-1.53232400	-0.00032000
C	4.56769500	-0.22067600	-0.00011100

S	5.83970000	0.99410500	0.00020900
C	3.20878400	0.13533800	-0.00013100
S	1.92998900	-1.07540400	-0.00044000
C	0.68685100	0.16356200	-0.00022000
C	1.27079000	1.44862500	0.00002600
C	2.65237500	1.43374600	0.00004800
C	-0.68684300	-0.16361000	-0.00028300
C	-1.27080200	-1.44865100	-0.00022500
C	-2.65240300	-1.43374900	-0.00021800
C	-3.20876700	-0.13533700	-0.00023200
S	-1.92998100	1.07537900	-0.00045000
C	-4.56770900	0.22071500	-0.00014100
S	-5.83970200	-0.99407100	0.00018100
C	-7.07998800	0.25652900	0.00012000
C	-6.49113100	1.55770400	-0.00014700
C	-5.11971100	1.53234000	-0.00028700
C	-8.43784400	-0.04127500	0.00032000
C	8.43781400	0.04126800	0.00027000
C	-9.40075100	1.00722000	0.00010100
N	-10.16699200	1.88461800	-0.00011900
C	-8.89821000	-1.38724300	0.00065100
N	-9.23451400	-2.50289900	0.00091200
C	8.89822900	1.38723800	0.00050600
N	9.23457700	2.50287700	0.00068700
C	9.40073300	-1.00723400	0.00016400
N	10.16699500	-1.88461000	0.00007100
H	7.09495200	-2.45741200	-0.00031800
H	4.50340300	-2.42406700	-0.00057100
H	0.68266400	2.35903300	0.00019700
H	3.26114000	2.33065700	0.00023300
H	-0.68270200	-2.35907600	-0.00015700
H	-3.26117600	-2.33065400	-0.00015400
H	-7.09496500	2.45742900	-0.00020700
H	-4.50342200	2.42409800	-0.00050300

5TQ:

C	7.07999000	-0.25650300	0.00009600
C	6.49110600	-1.55769400	-0.00021800
C	5.11971500	-1.53232400	-0.00032000
C	4.56769500	-0.22067600	-0.00011100
S	5.83970000	0.99410500	0.00020900
C	3.20878400	0.13533800	-0.00013100
S	1.92998900	-1.07540400	-0.00044000
C	0.68685100	0.16356200	-0.00022000
C	1.27079000	1.44862500	0.00002600
C	2.65237500	1.43374600	0.00004800
C	-0.68684300	-0.16361000	-0.00028300
C	-1.27080200	-1.44865100	-0.00022500
C	-2.65240300	-1.43374900	-0.00021800
C	-3.20876700	-0.13533700	-0.00023200
S	-1.92998100	1.07537900	-0.00045000
C	-4.56770900	0.22071500	-0.00014100
S	-5.83970200	-0.99407100	0.00018100
C	-7.07998800	0.25652900	0.00012000
C	-6.49113100	1.55770400	-0.00014700

C	-5.11971100	1.53234000	-0.00028700
C	-8.43784400	-0.04127500	0.00032000
C	8.43781400	0.04126800	0.00027000
C	-9.40075100	1.00722000	0.00010100
N	-10.16699200	1.88461800	-0.00011900
C	-8.89821000	-1.38724300	0.00065100
N	-9.23451400	-2.50289900	0.00091200
C	8.89822900	1.38723800	0.00050600
N	9.23457700	2.50287700	0.00068700
C	9.40073300	-1.00723400	0.00016400
N	10.16699500	-1.88461000	0.00007100
H	7.09495200	-2.45741200	-0.00031800
H	4.50340300	-2.42406700	-0.00057100
H	0.68266400	2.35903300	0.00019700
H	3.26114000	2.33065700	0.00023300
H	-0.68270200	-2.35907600	-0.00015700
H	-3.26117600	-2.33065400	-0.00015400
H	-7.09496500	2.45742900	-0.00020700
H	-4.50342200	2.42409800	-0.00050300

6TQ:

S	9.73979700	0.99468400	-0.00033500
C	10.98993700	-0.24603100	-0.00007100
C	10.40939900	-1.54890600	0.00022700
C	9.03576700	-1.53329600	0.00029400
C	8.47261500	-0.22995700	0.00005300
C	7.11143300	0.11923300	0.00009000
C	12.34710600	0.06202400	-0.00015800
S	5.83711100	-1.10031900	-0.00003800
C	4.58480400	0.13078600	0.00014600
C	5.16040000	1.41533000	0.00027100
C	6.54547300	1.40997300	0.00022300
C	3.21027100	-0.20813000	0.00015600
C	2.62940200	-1.48560100	0.00047100
C	1.23992100	-1.47163000	0.00048600
C	0.68509800	-0.18265600	0.00010900
S	1.95837300	1.02786300	-0.00025900
C	-0.68507900	0.18268400	0.00000200
S	-1.95835200	-1.02785500	0.00043100
C	-3.21024600	0.20811700	-0.00001200
C	-2.62941100	1.48559300	-0.00043000
C	-1.23991800	1.47164000	-0.00041500
C	-4.58480300	-0.13082800	0.00005800
C	-5.16039100	-1.41534800	0.00018000
C	-6.54549500	-1.40997900	0.00016300
C	-7.11141700	-0.11925000	0.00008000
S	-5.83710500	1.10028700	-0.00005500
C	-8.47263600	0.22998300	0.00012700
S	-9.73980700	-0.99465300	-0.00051800
C	-10.98994100	0.24606100	0.00002800
C	-10.40942200	1.54891500	0.00064000
C	-9.03575900	1.53330100	0.00068800
C	-12.34713700	-0.06202500	-0.00015600
C	-13.31621400	0.98045700	0.00023700
N	-14.08704500	1.85410400	0.00059500
C	13.31618800	-0.98046800	0.00002000

N	14.08702800	-1.85410500	0.00019800
C	12.79845100	1.41053500	-0.00039700
N	13.12876700	2.52823000	-0.00057200
C	-12.79844800	-1.41053400	-0.00071700
N	-13.12873300	-2.52824100	-0.00115700
H	11.01931500	-2.44429300	0.00042700
H	8.42629200	-2.42978300	0.00054900
H	4.56649200	2.32195300	0.00043700
H	7.14795300	2.31107800	0.00035200
H	3.21745300	-2.39610900	0.00076000
H	0.63382800	-2.37018600	0.00074900
H	-3.21747200	2.39609300	-0.00076200
H	-0.63384400	2.37021000	-0.00072800
H	-4.56650400	-2.32198500	0.00026600
H	-7.14797200	-2.31108600	0.00027700
H	-11.01932300	2.44431200	0.00107200
H	-8.42629400	2.42979600	0.00117100

7TQ:

S	11.68632800	1.03368400	0.00068700
C	12.94858700	-0.19451000	0.00097900
C	12.38059500	-1.50149600	0.00111900
C	11.00554100	-1.49896300	0.00099000
C	10.42998500	-0.20305200	0.00074000
C	9.06467400	0.13504200	0.00061700
C	14.30387300	0.12737700	0.00099800
S	7.80123300	-1.09605100	-0.00078400
C	6.53704800	0.12349700	0.00006400
C	7.10039000	1.41141700	0.00125700
C	8.48718900	1.41892900	0.00153800
C	5.16447100	-0.23010000	-0.00050600
C	4.59560900	-1.51067300	-0.00158000
C	3.20389700	-1.50907300	-0.00179200
C	2.63824300	-0.22711400	-0.00097300
S	3.90070700	0.99451800	0.00010800
C	1.26303700	0.12829900	-0.00094900
S	0.00001300	-1.09448000	-0.00129300
C	-1.26300900	0.12828200	-0.00137100
C	-0.69636300	1.40855400	-0.00092100
C	0.69636900	1.40856000	-0.00063600
C	-2.63822800	-0.22714800	-0.00179500
C	-3.20388700	-1.50908900	-0.00296800
C	-4.59562200	-1.51067400	-0.00291300
C	-5.16444800	-0.23009900	-0.00176100
S	-3.90068700	0.99450000	-0.00078800
C	-6.53705600	0.12353400	-0.00140600
S	-7.80123300	-1.09601900	0.00036000
C	-9.06467600	0.13507600	-0.00038800
C	-8.48720500	1.41894600	-0.00181600
C	-7.10038200	1.41143700	-0.00234400
C	-10.43000900	-0.20304000	0.00045700
C	-11.00551800	-1.49896000	0.00173600
C	-12.38059500	-1.50152300	0.00232200
C	-12.94857900	-0.19454300	0.00152200
S	-11.68636200	1.03367400	0.00001500
C	-14.30385500	0.12737300	0.00183700

C	-15.28262400	-0.90569000	0.00306500
N	-16.06163400	-1.77224900	0.00409000
C	-14.74225800	1.47980300	0.00094300
N	-15.06281200	2.60050200	0.00020000
C	14.74223000	1.47981800	0.00110800
N	15.06275300	2.60052900	0.00122000
C	15.28260200	-0.90571500	0.00099900
N	16.06166500	-1.77223200	0.00098800
H	12.99868600	-2.39119700	0.00134300
H	10.40495700	-2.40145500	0.00117600
H	6.49836300	2.31267900	0.00196200
H	9.08110900	2.32567900	0.00255400
H	5.19154000	-2.41605500	-0.00212700
H	2.60604700	-2.41312800	-0.00256500
H	-1.29294800	2.31347800	-0.00086800
H	1.29294300	2.31349300	-0.00036400
H	-2.60606200	-2.41316000	-0.00392300
H	-5.19155100	-2.41605600	-0.00389800
H	-9.08111500	2.32570400	-0.00253900
H	-6.49837200	2.31271100	-0.00360900
H	-10.40489400	-2.40142300	0.00217400
H	-12.99868900	-2.39122100	0.00328500

B2-2TQ:

C	3.18683800	0.34318600	0.15055000
S	1.71574700	1.30936400	0.13731800
C	0.70247400	-0.07058200	-0.22510300
C	1.50040200	-1.26517800	-0.38703300
C	2.89471600	-1.04159800	-0.15743100
C	-0.70239000	0.07082700	-0.22508400
C	-1.50046400	1.26531500	-0.38693100
C	-2.89476800	1.04148000	-0.15748800
C	-3.18664200	-0.34330000	0.15054500
S	-1.71549900	-1.30925400	0.13746600
C	-4.38434800	-0.97725400	0.43975400
C	4.38450900	0.97711700	0.43967800
C	-1.06329200	2.54419900	-0.78599500
C	-1.98070500	3.58055100	-0.89075900
C	-3.34056100	3.36462000	-0.62018000
C	-3.80646300	2.10164100	-0.26696200
C	1.06300000	-2.54388600	-0.78638100
C	1.98020300	-3.58042800	-0.89116200
C	3.34002600	-3.36483000	-0.62024100
C	3.80616200	-2.10198300	-0.26680100
C	-5.63049500	-0.29331600	0.51346800
N	-6.65635600	0.25496600	0.57561200
C	-4.41129500	-2.38345900	0.68237700
N	-4.39363700	-3.53262900	0.87104800
C	4.41148000	2.38335100	0.68215200
N	4.39386900	3.53253200	0.87073600
C	5.63066900	0.29320500	0.51351800
N	6.65664700	-0.25482800	0.57583000
H	-0.02895500	2.73080300	-1.04355100
H	-1.64142000	4.56414200	-1.19738400

H	-4.04432300	4.18564500	-0.70629900
H	-4.86296500	1.95110100	-0.09041500
H	0.02865100	-2.73013500	-1.04414500
H	1.64078400	-4.56388300	-1.19807500
H	4.04361700	-4.18601300	-0.70626400
H	4.86264800	-1.95175500	-0.08994800

B3-3TQ:

S	3.89896000	0.89919400	-0.18468100
C	5.15719300	-0.32698200	-0.06566800
C	4.59132600	-1.59911900	0.34282900
C	3.17923200	-1.53324800	0.53907100
C	2.61692400	-0.22814600	0.23999300
C	1.27389100	0.17028600	0.16878100
C	6.45944600	0.03511600	-0.35202700
S	-0.00002500	-1.02813500	-0.00005100
C	-1.27388200	0.17032100	-0.16890400
C	-0.70629400	1.49419400	-0.10965900
C	0.70633200	1.49417700	0.10943100
C	-2.61694700	-0.22806800	-0.24000300
C	-3.17931600	-1.53310200	-0.53920900
C	-4.59139300	-1.59896800	-0.34283600
C	-5.15717100	-0.32689400	0.06593900
S	-3.89889700	0.89922800	0.18505600
C	-6.45940200	0.03514900	0.35250400
C	-1.36879600	2.72606600	-0.27766300
C	-0.69644800	3.93523200	-0.15790300
C	0.69654800	3.93522400	0.15745500
C	1.36886400	2.72604700	0.27733300
C	-1.43675800	5.23147800	-0.34811600
C	1.43692700	5.23146400	0.34742100
C	5.28337800	-2.79673600	0.57791900
C	4.58422100	-3.91189800	1.02797200
C	3.20610000	-3.83978000	1.27090900
C	2.50467600	-2.66332000	1.03836000
C	-2.50483400	-2.66311500	-1.03874900
C	-3.20632000	-3.83950800	-1.27143900
C	-4.58442900	-3.91161600	-1.02840000
C	-5.28351000	-2.79651500	-0.57808300
C	-6.76366300	1.38510600	0.70604900
N	-6.96990800	2.49618600	0.98712800
C	7.55254400	-0.87802200	-0.32052000
N	8.45401200	-1.61499500	-0.29841500
C	-7.55247500	-0.87801000	0.32092300
N	-8.45387300	-1.61506700	0.29875100
C	6.76372100	1.38514100	-0.70531700
N	6.96998500	2.49627100	-0.98618000
H	-2.42113200	2.75592700	-0.52765000
H	2.42119100	2.75591100	0.52735100
H	-0.99474300	5.82527700	-1.15598500
H	-2.48744800	5.06034000	-0.58934600
H	-1.39381000	5.84834100	0.55655900
H	0.99453900	5.82580000	1.15468000
H	2.48745400	5.06030200	0.58934200
H	1.39459600	5.84781000	-0.55764600

H	6.35237400	-2.86029900	0.42544300
H	5.11930200	-4.83704100	1.21375600
H	2.68082400	-4.70588400	1.65951500
H	1.45157100	-2.62372100	1.28311500
H	-1.45174700	-2.62350000	-1.28358000
H	-2.68111300	-4.70556600	-1.66023800
H	-5.11956100	-4.83670100	-1.21432400
H	-6.35250100	-2.86005800	-0.42554000

B4-4TQ:

C	7.12212500	0.17921200	0.09486500
C	6.63257800	-1.09257000	-0.40769000
C	5.22036000	-1.10132100	-0.60275300
C	4.57153800	0.14038200	-0.20303600
S	5.79129200	1.31324600	0.30200900
C	3.21439600	0.44207600	-0.10221700
S	2.00313900	-0.83956100	-0.11899100
C	0.66109200	0.24099500	0.19995300
C	1.14745600	1.59211500	0.33640800
C	2.55840500	1.71210500	0.13007400
C	-0.66108800	-0.24099800	0.19994700
C	-1.14748200	-1.59210500	0.33645500
C	-2.55841400	-1.71208500	0.13002600
C	-3.21437500	-0.44205200	-0.10231700
S	-2.00310400	0.83955600	-0.11911200
C	-4.57151400	-0.14035100	-0.20311500
S	-5.79124100	-1.31326000	0.30189600
C	-7.12209300	-0.17924400	0.09483100
C	-6.63257700	1.09257600	-0.40766900
C	-5.22036000	1.10136400	-0.60274800
C	-8.40019400	-0.59656200	0.40628700
C	8.40023900	0.59650600	0.40629000
C	-7.39971000	2.22300500	-0.72723600
C	-6.77482000	3.34509900	-1.26106900
C	-5.39597000	3.34214700	-1.50323600
C	-4.62128700	2.23208700	-1.18644700
C	-0.39761800	-2.73722200	0.68270300
C	-1.01069100	-3.97673500	0.73687200
C	-2.37750300	-4.10789600	0.43909900
C	-3.14653200	-2.99332900	0.14517400
C	0.39754200	2.73723800	0.68250700
C	1.01059300	3.97676300	0.73668400
C	2.37743900	4.10792400	0.43908300
C	3.14651200	2.99335500	0.14527100
C	7.39967700	-2.22300900	-0.72730500
C	6.77475500	-3.34505700	-1.26119800
C	5.39590900	-3.34205200	-1.50337700
C	4.62125500	-2.23198900	-1.18652500
C	-9.54834900	0.24157800	0.30461600
N	-10.49466700	0.91574800	0.22626300
C	-8.62339900	-1.93196200	0.86205100
N	-8.76449100	-3.02841900	1.22791000
C	9.54836700	-0.24166700	0.30458700
N	10.49465100	-0.91588100	0.22620200
C	8.62348200	1.93189600	0.86206300

N	8.76460400	3.02834800	1.22792500
H	-8.47055700	2.22780200	-0.57486300
H	-7.36827700	4.21786200	-1.51168200
H	-4.92523200	4.20836500	-1.95637900
H	-3.56829500	2.24432600	-1.43341400
H	0.65095700	-2.65705700	0.93613400
H	-0.43007400	-4.85204100	1.00809800
H	-2.84236700	-5.08801700	0.45122400
H	-4.19311700	-3.13258100	-0.08787200
H	-0.65106300	2.65708500	0.93581700
H	0.42992800	4.85207800	1.00777800
H	2.84230100	5.08804600	0.45126100
H	4.19312700	3.13262300	-0.08762300
H	8.47052500	-2.22784700	-0.57493000
H	7.36818600	-4.21782600	-1.51184800
H	4.92515200	-4.20822400	-1.95658800
H	3.56826400	-2.24416900	-1.43349500

B5-5TQ:

C	-8.85005400	0.52843600	-0.66175700
S	-7.47388200	1.61524200	-0.82045000
C	-6.32865600	0.43618000	-0.15592400
C	-7.05112600	-0.76162200	0.25218900
C	-8.43801700	-0.72368600	-0.05514200
C	-4.96502500	0.69561900	-0.15897100
C	-4.24850800	1.92631200	-0.43824100
C	-2.83121700	1.75615200	-0.51479900
C	-2.39352900	0.41140000	-0.21511500
S	-3.79270800	-0.60773000	0.07922400
C	-1.09297000	-0.09202400	-0.05963900
S	0.26184600	0.99037800	0.22807600
C	1.42758500	-0.30547300	0.45145500
C	0.75836800	-1.57626000	0.32075200
C	-0.63274900	-1.45773200	0.00412500
C	2.79032500	-0.01669500	0.61781200
C	3.42952000	1.22083400	0.99628700
C	4.85078400	1.18511400	0.89177900
C	5.36667100	-0.09065900	0.43312000
S	4.01456300	-1.21546400	0.22841400
C	6.65702600	-0.45760700	0.08176000
S	7.89815500	0.77745900	-0.19147400
C	9.08698800	-0.38598900	-0.76333400
C	8.54757900	-1.73414100	-0.70470400
C	7.21107000	-1.77483700	-0.21303100
C	10.32249600	0.07479800	-1.17242400
C	-6.54901600	-1.88110900	0.93597100
C	-7.36471300	-2.96470400	1.25994000
C	-8.73781300	-2.94133200	0.90286000
C	-9.25591700	-1.81653500	0.26226100
C	2.80940000	2.37875100	1.50657700
C	3.54472700	3.49809400	1.87319800
C	4.96319100	3.46643700	1.76012900
C	5.58684200	2.31430400	1.29170700
C	-4.79255100	3.21434600	-0.61264000
C	-3.96950200	4.28160700	-0.93847200
C	-2.58960800	4.09273600	-1.11081300

C	-2.02263200	2.84742700	-0.89798000
C	1.31622600	-2.86033900	0.50540400
C	0.54359000	-3.98957000	0.30345800
C	-0.79831300	-3.87308100	-0.10153000
C	-1.38380100	-2.62801900	-0.24490700
C	9.21563900	-2.92098300	-1.04468900
C	8.57220800	-4.14163300	-0.87610000
C	7.27559800	-4.19180200	-0.35110300
C	6.59845700	-3.02467300	-0.01671100
C	-9.64176700	-4.10089200	1.23086900
C	-6.78651300	-4.14441500	1.99816800
C	2.84623200	4.71756900	2.41686500
C	5.79235500	4.65347300	2.17445200
C	-10.08780700	0.95929200	-1.09600100
C	10.61803900	1.47077400	-1.10632200
N	10.82068900	2.61536900	-1.03408600
C	11.35433500	-0.77046300	-1.67396700
N	12.20700700	-1.44840900	-2.08615700
C	-11.26472600	0.15758300	-1.03944500
N	-12.23406000	-0.48691800	-0.99918000
C	-10.23660800	2.27132200	-1.64070700
N	-10.32035300	3.34797100	-2.07681300
H	-5.51810500	-1.91115900	1.26379300
H	-10.31065100	-1.79520000	0.02139600
H	1.73872800	2.39881400	1.66524500
H	6.66843700	2.29950700	1.27899700
H	-5.84950100	3.39836400	-0.47957000
H	-4.40339400	5.26668100	-1.07420300
H	-1.96162300	4.92533300	-1.40986200
H	-0.96064100	2.72006100	-1.05899600
H	2.34301200	-2.97444500	0.82608800
H	0.98050300	-4.97196500	0.44903200
H	-1.38219700	-4.76604300	-0.29880500
H	-2.41194800	-2.56533600	-0.57487600
H	10.22770300	-2.89663900	-1.42557600
H	9.08937600	-5.05898400	-1.13638200
H	6.79370600	-5.15107100	-0.19256400
H	5.61352100	-3.10075700	0.42353000
H	-9.28874400	-5.02625200	0.76138000
H	-9.67664700	-4.28726600	2.31043200
H	-10.66161000	-3.91702400	0.88800200
H	-7.30214600	-4.31004000	2.95071600
H	-6.89404500	-5.06795200	1.41792100
H	-5.72490300	-4.00075300	2.21109500
H	3.18842700	4.95693500	3.42991800
H	3.04870900	5.60004200	1.79939400
H	1.76433700	4.57281100	2.45325500
H	5.52914800	5.54335900	1.59139100
H	5.62905700	4.90697400	3.22812800
H	6.85825400	4.46406700	2.03412400

B6-6TQ:

S	9.12164500	-0.94548700	-1.32297100
C	10.15598900	0.24604700	-2.09776600
C	9.76280000	1.59015300	-1.70839200

C	8.65102000	1.60707100	-0.81819700
C	8.11710400	0.28064800	-0.52233800
C	6.97806100	-0.08690900	0.17066800
C	11.16616800	-0.19211200	-2.93144400
S	5.72912900	1.10594400	0.57481400
C	4.58609300	-0.09675700	1.16491900
C	5.20792300	-1.40309100	1.13932000
C	6.52350600	-1.40063300	0.59489700
C	3.27611600	0.26657700	1.48815300
C	2.71198100	1.56789100	1.76004100
C	1.28756400	1.55593300	1.89548100
C	0.70551400	0.24575200	1.73087200
S	1.98314200	-0.93125600	1.47645300
C	-0.64303400	-0.13741400	1.66288600
S	-1.88474100	1.03423100	1.25404400
C	-3.17510100	-0.16245700	1.15466100
C	-2.64494500	-1.45795900	1.51121000
C	-1.24109100	-1.44436100	1.78929300
C	-4.44612200	0.19070900	0.69238700
C	-5.05483600	1.49563500	0.54899400
C	-6.31932800	1.47035000	-0.10550000
C	-6.78509200	0.13152900	-0.42762800
S	-5.53606000	-1.03399500	0.04853100
C	-8.00403700	-0.29364800	-0.92484900
S	-9.38301300	0.82058600	-1.02501700
C	-10.51165800	-0.43992700	-1.50183700
C	-9.82438800	-1.71380300	-1.63356000
C	-8.43199400	-1.62520700	-1.34563400
C	-11.83770600	-0.10616500	-1.69483300
C	4.68284000	-2.60433800	1.65269400
C	5.40202600	-3.79210700	1.61333300
C	6.71340300	-3.79176400	1.06458300
C	7.25252700	-2.60230000	0.58355200
C	-4.55218800	2.72688800	1.01263900
C	-5.21845100	3.92313600	0.78026800
C	-6.43173700	3.90832000	0.03976500
C	-6.95937100	2.69143900	-0.38135700
C	3.41309000	2.77445300	1.97125000
C	2.72537200	3.93450500	2.28114600
C	1.32583300	3.92220600	2.41577900
C	0.61504100	2.74898000	2.23909600
C	10.37994400	2.78955900	-2.09793700
C	9.91383600	3.99672100	-1.59083100
C	8.84987700	4.01738900	-0.68189800
C	8.22382700	2.83859300	-0.29259200
C	-3.36651000	-2.66001800	1.67593000
C	-2.71468500	-3.81504700	2.07184100
C	-1.33553800	-3.80139200	2.34361800
C	-0.60860900	-2.63121900	2.21883100
C	-10.39278900	-2.93470200	-2.02946900
C	-9.58305600	-4.05649000	-2.16431900
C	-8.20663800	-3.96564400	-1.93011700
C	-7.62990800	-2.76468800	-1.53093400
C	7.53160200	-5.05618000	1.02836600
C	4.80618300	-5.05724700	2.17531300
C	-4.65320700	5.21928300	1.30167300
C	-7.15489700	5.19128500	-0.27712700
C	-12.26215100	1.24669800	-1.52207900

N	-12.56859000	2.36062400	-1.37422200
C	12.05178700	0.68042500	-3.62770000
N	12.78319700	1.37998500	-4.20433700
C	11.36253300	-1.59221400	-3.13445800
N	11.49228700	-2.74146400	-3.27241700
C	-12.84455000	-1.04505900	-2.06263800
N	-13.67930700	-1.80000400	-2.36273400
H	3.71143900	-2.61305300	2.13038100
H	8.27479600	-2.62267600	0.23053500
H	-3.63667900	2.75883200	1.58906200
H	-7.87856500	2.71592900	-0.95056200
H	4.49388700	2.79756200	1.93344400
H	3.27531100	4.85474200	2.44878300
H	0.80170600	4.83246100	2.68771600
H	-0.45376200	2.74888500	2.40684000
H	11.21998500	2.78286300	-2.77926500
H	10.39247200	4.92318100	-1.88978100
H	8.51229400	4.96139100	-0.26638600
H	7.43059500	2.88774000	0.44076700
H	-4.43906600	-2.68366000	1.53853300
H	-3.28134000	-4.73118200	2.20223600
H	-0.84283500	-4.70683500	2.68222000
H	0.43802500	-2.62859500	2.49267200
H	-11.45088100	-3.00865500	-2.24135900
H	-10.02188600	-4.99915100	-2.47355600
H	-7.57535200	-4.83688300	-2.07231700
H	-6.55680700	-2.72079200	-1.40532800
H	7.68131100	-5.46512100	2.03417700
H	7.03174000	-5.83549500	0.44178400
H	8.51416600	-4.88242900	0.58539000
H	5.42172000	-5.46575200	2.98463200
H	3.80370500	-4.88174100	2.57205300
H	4.73392000	-5.83781300	1.40941300
H	-5.35995600	5.72295300	1.97065400
H	-3.72663200	5.05368000	1.85598500
H	-4.43790400	5.91879700	0.48588500
H	-6.52036800	5.87562300	-0.85183100
H	-8.06151300	5.00535300	-0.85622900
H	-7.44387400	5.72153200	0.63758300

B7-7TQ:

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C	10.56158600	-1.75347800	-1.31223600
C	10.11663800	-0.45773800	-0.80505700
C	8.84228000	-0.00555200	-0.52360200
C	14.03237100	-0.48475800	-0.69895100
S	7.45798300	-1.11678300	-0.51024300
C	6.31301000	0.09787100	0.06335100
C	7.01223200	1.35148200	0.26581000
C	8.38506900	1.31161500	-0.10731200
C	4.95521700	-0.19538000	0.17493200
C	4.27271900	-1.46990100	0.12900200
C	2.84710100	-1.35692000	0.09772600

C	2.37242500	0.00385500	0.20287400
S	3.75013800	1.09421300	0.26608500
C	1.06411400	0.48811100	0.33941600
S	-0.24815800	-0.57698400	0.83092600
C	-1.44614200	0.70892200	0.92311200
C	-0.81834500	1.96417200	0.58867300
C	0.56187700	1.83630700	0.23075400
C	-2.79054400	0.41566700	1.18869100
C	-3.38326900	-0.77742500	1.74545400
C	-4.80898100	-0.77674200	1.71442800
C	-5.37727800	0.42502000	1.14513700
S	-4.06536900	1.53370500	0.72367400
C	-6.69748100	0.73461300	0.83187800
S	-7.91800000	-0.53336800	0.71191900
C	-9.16620000	0.54228200	0.05182900
C	-8.65166100	1.90515000	0.04245600
C	-7.29504100	2.00844200	0.47127900
C	6.48920400	2.54163200	0.80622200
C	7.25244300	3.69948700	0.90293600
C	8.59180300	3.68754700	0.43187000
C	9.13259200	2.50050800	-0.05481900
C	-2.71441300	-1.85835000	2.35518200
C	-3.40568800	-2.93377600	2.89501200
C	-4.82893000	-2.93610700	2.85830100
C	-5.49937600	-1.86258200	2.28596800
C	4.85712700	-2.75411000	0.14002600
C	4.06291800	-3.88394800	0.03309900
C	2.66980000	-3.76709400	-0.10017800
C	2.06603400	-2.52198000	-0.06309700
C	12.55736100	-3.11775800	-1.74050500
C	11.74366000	-4.14379000	-2.20626900
C	10.35619100	-3.97304300	-2.26223700
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C	-1.40554600	3.24833900	0.61605100
C	-0.67648900	4.35713200	0.22590900
C	0.65064700	4.21761800	-0.21716200
C	1.26596500	2.97867000	-0.21139500
C	-9.36386700	3.07835600	-0.26754200
C	-8.74439000	4.31778800	-0.18150600
C	-7.41417200	4.41905300	0.24494600
C	-6.69924800	3.27939900	0.58179400
C	9.43398800	4.93628600	0.47258100
C	6.65745300	4.95061600	1.49697100
C	-2.65338400	-4.06825300	3.54262900
C	-5.60786100	-4.07537000	3.46365100
C	-10.36046900	0.04155000	-0.42648700
C	-10.94004200	-1.29294700	-0.29488800
C	-12.11664100	-1.48565700	-1.07362700
C	-12.51528500	-0.29316000	-1.80366000
S	-11.40584900	1.02868300	-1.47336100
C	-13.57820300	-0.07365800	-2.65807700
C	-10.49548100	-2.34166000	0.52831200
C	-11.17120300	-3.55689300	0.53622100
C	-12.30190000	-3.75292700	-0.26438600
C	-12.78350300	-2.72121800	-1.06117200
C	14.47681800	0.79433200	-0.24481500
N	14.80100000	1.85012900	0.12531900
C	15.04665000	-1.44695800	-0.97400900

N	15.88845200	-2.22169800	-1.19358600
C	-13.76667900	1.21568000	-3.24274800
N	-13.89037400	2.28000700	-3.69952600
C	-14.52841700	-1.07447600	-3.01284000
N	-15.31328600	-1.88090000	-3.31404100
H	5.47814100	2.56882600	1.19110400
H	10.15292200	2.52627900	-0.41240600
H	-1.63652500	-1.84554200	2.45358900
H	-6.58091300	-1.86009200	2.32475500
H	5.92531900	-2.87431300	0.25811600
H	4.52534200	-4.86559600	0.04364400
H	2.06065500	-4.65601500	-0.22701800
H	0.99350200	-2.45525200	-0.18645900
H	13.63100700	-3.24835300	-1.72851400
H	12.19283400	-5.07075300	-2.54662200
H	9.72962200	-4.76468700	-2.66055800
H	8.69529800	-2.67725000	-1.93002700
H	-2.42193600	3.38178900	0.96105400
H	-1.13753500	5.33902800	0.25232500
H	1.19964000	5.08748400	-0.56264400
H	2.28102500	2.89474700	-0.57527000
H	-10.40992300	3.04232000	-0.53823300
H	-9.30837100	5.21308700	-0.42126000
H	-6.94697000	5.39377800	0.33928600
H	-5.69530300	3.38626500	0.96989600
H	8.97410500	5.74735100	-0.10359200
H	9.55086000	5.30452600	1.49835600
H	10.43149700	4.75753100	0.06632200
H	7.23120300	5.29235500	2.36581800
H	6.65784400	5.77568500	0.77536700
H	5.62689500	4.78579800	1.81954600
H	-2.93268000	-4.18650300	4.59577300
H	-2.86941800	-5.02339300	3.05018500
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H	-5.38016300	-4.19605900	4.52888200
H	-6.68394800	-3.91610400	3.36697700
H	-5.36316800	-5.02766000	2.97916400
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H	-10.81909500	-4.35712200	1.17933000
H	-12.81905100	-4.70648300	-0.25278900
H	-13.67346000	-2.87433800	-1.65647400

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