Structural Connectivity of 18-Crown-6/H+/L-Tryptophan Non-Covalent Complexes in Gas Phase and in Solution: Delineating Host-Guest-Solvent Interactions in Solution from Gas Phase Structures

Young-Ho Oh, Han Bin Oh and Sungyul Lee



**Figure 1S. Structures of higher Gibbs free energy gas phase CR/TrpH+ complexes with naked –CO2H. Relative Gibbs free energy in kcal/mol.**

Cartesian Coordinates

**CR/TrpH+-G1**

C 0.5893110000 -3.1212320000 1.7750260000

C 2.0408720000 -3.3229020000 1.4240670000

O 2.4060540000 -2.4283470000 0.3863930000

C 3.7842100000 -2.5070290000 0.0493940000

C 4.0611210000 -1.6233480000 -1.1385330000

O 3.8458270000 -0.2791590000 -0.7664610000

C 3.9807090000 0.6158300000 -1.8527250000

C 3.8786810000 2.0250670000 -1.3331570000

O 2.5609700000 2.2729980000 -0.8617320000

C 2.4461480000 3.5441910000 -0.2458280000

C 1.0397590000 3.7637400000 0.2474110000

O 0.7681690000 2.8492750000 1.2886580000

C -0.4534390000 3.0947470000 1.9498990000

C -0.6055200000 2.0848920000 3.0572790000

O -0.6376560000 0.7811250000 2.5006250000

C -0.8589540000 -0.2192750000 3.4820140000

C -0.8525750000 -1.5803410000 2.8359280000

O 0.4395450000 -1.8304120000 2.3290520000

H -0.0384970000 -3.2331330000 0.8806260000

H 0.2944760000 -3.8888720000 2.5033590000

H 2.1943820000 -4.3580500000 1.0933710000

H 2.6626130000 -3.1425800000 2.3101720000

H 4.3939950000 -2.1934580000 0.9062010000

H 4.0443790000 -3.5423630000 -0.2045090000

H 3.4050270000 -1.8979400000 -1.9728290000

H 5.1044920000 -1.7719180000 -1.4508510000

H 3.2011330000 0.4225010000 -2.5989010000

H 4.9636350000 0.4940780000 -2.3287280000

H 4.5963860000 2.1685990000 -0.5156280000

H 4.1194910000 2.7292000000 -2.1395900000

H 3.1443790000 3.6143900000 0.5980880000

H 2.6959630000 4.3303950000 -0.9700270000

H 0.9603130000 4.7957600000 0.6150740000

H 0.3208520000 3.6385240000 -0.5741100000

H -1.2993020000 3.0216680000 1.2508650000

H -0.4623970000 4.1031550000 2.3853650000

H 0.2349220000 2.1685920000 3.7580940000

H -1.5366920000 2.2859170000 3.6024220000

H -1.8297420000 -0.0553600000 3.9679170000

H -0.0730920000 -0.1712420000 4.2463880000

H -1.6069100000 -1.6297210000 2.0368160000

H -1.1198260000 -2.3279090000 3.5955050000

O -0.2978970000 -2.4076590000 -1.5928900000

O 1.1950830000 -0.9810830000 -2.4537790000

N -3.7635250000 -0.0337570000 -3.0248850000

N 1.1343490000 0.0962170000 0.2933410000

C -2.0898150000 0.5269650000 -1.6474680000

C -0.7557640000 0.8951770000 -1.0928650000

C -3.2420390000 0.1937460000 -0.8567580000

C -0.0448620000 -0.3268870000 -0.4987940000

C -4.2726700000 -0.1517770000 -1.7530120000

C -2.4544780000 0.3747480000 -2.9542500000

C -3.4903810000 0.1729930000 0.5227290000

C -5.5423620000 -0.5253870000 -1.3099950000

C 0.3791780000 -1.2624430000 -1.6179310000

C -4.7453050000 -0.1984560000 0.9641920000

C -5.7597450000 -0.5461710000 0.0541350000

H -0.1062190000 1.3455740000 -1.8482520000

H -0.8759340000 1.6190960000 -0.2842990000

H -0.7110840000 -0.8564560000 0.1778550000

H -1.8755350000 0.5329040000 -3.8518210000

H -4.2778850000 -0.1820190000 -3.8747190000

H -2.7103410000 0.4545600000 1.2238990000

H -6.3308180000 -0.7871660000 -2.0060400000

H -4.9623020000 -0.2163790000 2.0261360000

H 0.7829000000 0.4889190000 1.1773290000

H 1.6951280000 0.8227840000 -0.1841570000

H -6.7348610000 -0.8307490000 0.4311320000

H -0.0302460000 -2.9275930000 -2.3614990000

H 1.7382040000 -0.7159060000 0.4966920000

**CR/TrpH+-G2**

C -1.6691330000 0.3889000000 -3.4834320000

C -2.4981400000 -0.8597260000 -3.3278350000

O -2.1332090000 -1.5212010000 -2.1296020000

C -2.9336340000 -2.6658880000 -1.8675380000

C -2.4030400000 -3.3829750000 -0.6543130000

O -2.5598880000 -2.5499480000 0.4736400000

C -2.0012800000 -3.1136490000 1.6437000000

C -2.3084700000 -2.2153390000 2.8112440000

O -1.6104030000 -0.9849370000 2.6759390000

C -1.9335780000 -0.0771900000 3.7137440000

C -1.2367080000 1.2400600000 3.4956830000

O -1.7474380000 1.8416870000 2.3243130000

C -1.3452620000 3.1821070000 2.1614300000

C -1.9449040000 3.7062950000 0.8827250000

O -1.4530750000 2.9507420000 -0.2115810000

C -1.9367150000 3.4315000000 -1.4543880000

C -1.4307020000 2.5581610000 -2.5728350000

O -2.0085520000 1.2800800000 -2.4412100000

H -0.5984870000 0.1410010000 -3.4494950000

H -1.8876800000 0.8382840000 -4.4614830000

H -2.3247010000 -1.5206680000 -4.1866790000

H -3.5622520000 -0.5927000000 -3.3007370000

H -3.9744660000 -2.3594820000 -1.7028110000

H -2.9009750000 -3.3449800000 -2.7288280000

H -1.3457190000 -3.6343540000 -0.7982250000

H -2.9696040000 -4.3159600000 -0.5237670000

H -0.9182280000 -3.2304280000 1.5253800000

H -2.4447550000 -4.0995960000 1.8413230000

H -3.3880190000 -2.0232780000 2.8560400000

H -2.0018230000 -2.7119150000 3.7406170000

H -3.0184630000 0.0873870000 3.7412180000

H -1.6203490000 -0.4916920000 4.6808530000

H -1.4287160000 1.8786960000 4.3684950000

H -0.1506890000 1.0960820000 3.4118530000

H -0.2487890000 3.2601140000 2.1291340000

H -1.7005990000 3.7981580000 2.9988570000

H -3.0390240000 3.6298270000 0.9266800000

H -1.6743320000 4.7634770000 0.7641330000

H -1.5925450000 4.4614240000 -1.6156030000

H -3.0342320000 3.4267980000 -1.4569890000

H -0.3320370000 2.4985150000 -2.5413690000

H -1.7142470000 3.0136080000 -3.5316140000

O 1.3529190000 -1.2255650000 -1.9562650000

O 0.5292170000 -2.2370110000 -0.1356610000

N 4.3396070000 1.8482040000 -0.5837590000

N -1.2134360000 0.0448040000 0.0451570000

C 2.4934620000 0.9130910000 0.2753800000

C 1.0755870000 0.7119010000 0.7006390000

C 3.5576630000 -0.0547510000 0.3142220000

C 0.1931080000 0.1250030000 -0.4117910000

C 4.6986230000 0.5686620000 -0.2315830000

C 3.0191420000 2.0484310000 -0.2736810000

C 3.6548670000 -1.3786100000 0.7681410000

C 5.9250890000 -0.0884190000 -0.3429950000

C 0.6847890000 -1.2536440000 -0.8088040000

C 4.8655160000 -2.0321630000 0.6578690000

C 5.9898900000 -1.3922250000 0.1058550000

H 1.0190530000 0.0454710000 1.5678580000

H 0.6274740000 1.6657630000 0.9832840000

H 0.2143340000 0.7786830000 -1.2798710000

H 2.5463380000 3.0011560000 -0.4614920000

H 4.9581110000 2.5419260000 -0.9642950000

H 2.7955740000 -1.8828780000 1.1962930000

H 6.7944560000 0.4045390000 -0.7624780000

H 4.9581840000 -3.0536960000 1.0072910000

H -1.5688890000 1.0067500000 0.1285910000

H -1.3117750000 -0.4175670000 0.9659930000

H 6.9266570000 -1.9322910000 0.0365040000

H 1.7534980000 -2.0940410000 -2.0922970000

H -1.7790780000 -0.4711830000 -0.6473670000

**CR/TrpH+-G3**

C 4.0335400000 0.4076830000 -1.6565930000

C 3.9804820000 1.8304810000 -1.1615140000

O 2.6623480000 2.1597590000 -0.7480930000

C 2.5783410000 3.4631030000 -0.1935000000

C 1.1703930000 3.7382600000 0.2684420000

O 0.8533840000 2.8554710000 1.3250290000

C -0.3717980000 3.1562410000 1.9561810000

C -0.6356310000 2.1189570000 3.0177610000

O -0.7530400000 0.8423890000 2.4070860000

C -1.1630040000 -0.1697460000 3.3122970000

C -1.1696600000 -1.5038840000 2.6113050000

O 0.1605250000 -1.8323760000 2.2592620000

C 0.3128300000 -3.1474760000 1.7788670000

C 1.7829580000 -3.4101430000 1.5761760000

O 2.2670970000 -2.5775520000 0.5268860000

C 3.6868060000 -2.6397620000 0.3653270000

C 4.1059650000 -1.8066910000 -0.8212340000

O 3.7420220000 -0.4647680000 -0.5763350000

H 3.3224510000 0.2519200000 -2.4769160000

H 5.0469020000 0.2192350000 -2.0343040000

H 4.2916960000 2.5026080000 -1.9707690000

H 4.6719290000 1.9519340000 -0.3179470000

H 3.2672030000 3.5502440000 0.6563700000

H 2.8595430000 4.2061890000 -0.9500750000

H 0.4612870000 3.6127470000 -0.5609620000

H 1.1170600000 4.7810480000 0.6091830000

H -1.1936680000 3.1674950000 1.2262520000

H -0.3292880000 4.1458540000 2.4311420000

H 0.1835850000 2.1070010000 3.7475440000

H -1.5668750000 2.3711740000 3.5401080000

H -0.4775940000 -0.2061920000 4.1682340000

H -2.1738400000 0.0484980000 3.6803420000

H -1.5812230000 -2.2552360000 3.2982860000

H -1.8130120000 -1.4674460000 1.7210750000

H -0.2393780000 -3.2889030000 0.8366760000

H -0.0765080000 -3.8751190000 2.5035920000

H 2.3262960000 -3.1842370000 2.5004600000

H 1.9432260000 -4.4630820000 1.3168510000

H 3.9948540000 -3.6795830000 0.2071830000

H 4.1614360000 -2.2631860000 1.2785590000

H 3.6325810000 -2.1739480000 -1.7389660000

H 5.1949930000 -1.8969730000 -0.9333880000

O 1.2155430000 -2.0395050000 -1.9167420000

O 0.8295260000 -0.1375730000 -2.9603590000

N -3.6891120000 -0.2748410000 -3.0258070000

N 1.0875340000 0.1149270000 0.3354890000

C -2.1249190000 0.4709470000 -1.6081220000

C -0.8330400000 0.9268170000 -1.0118250000

C -3.3129960000 0.1631980000 -0.8603910000

C 0.0684160000 -0.2613330000 -0.6832480000

C -4.2735240000 -0.3018560000 -1.7823790000

C -2.4019450000 0.1883210000 -2.9158880000

C -3.6563580000 0.2639330000 0.4951750000

C -5.5555130000 -0.6849720000 -1.3855980000

C 0.7495060000 -0.7926460000 -1.9622040000

C -4.9236480000 -0.1166180000 0.8917990000

C -5.8624320000 -0.5906330000 -0.0418700000

H -0.2894690000 1.5957030000 -1.6815740000

H -1.0379240000 1.4599680000 -0.0826870000

H -0.5245030000 -1.0639820000 -0.2389450000

H -1.7656940000 0.2782240000 -3.7828100000

H -4.1377460000 -0.5316210000 -3.8870460000

H -2.9377320000 0.6482190000 1.2120820000

H -6.2870430000 -1.0393010000 -2.1026000000

H -5.2110470000 -0.0392020000 1.9342850000

H 1.6792540000 -0.6862960000 0.5794910000

H 0.5904440000 0.4282790000 1.1843680000

H -6.8500790000 -0.8782130000 0.2984130000

H 1.3379240000 -2.3603520000 -1.0051620000

H 1.6931450000 0.8860730000 -0.0017750000

**CR/TrpH+-G4**

C 4.1851210000 -1.3175940000 -0.7341770000

C 4.6241310000 0.1172070000 -0.5995280000

O 3.5272040000 0.9930530000 -0.8002530000

C 3.9011370000 2.3572750000 -0.7360450000

C 2.6628550000 3.2132400000 -0.7956650000

O 1.8868880000 2.9454950000 0.3544130000

C 0.7882040000 3.8105860000 0.5141740000

C 0.0292600000 3.3977310000 1.7501480000

O -0.5047630000 2.1013540000 1.5532570000

C -1.3404200000 1.6666640000 2.6122320000

C -1.9300530000 0.3200260000 2.2789280000

O -0.8841750000 -0.6297400000 2.2025500000

C -1.3373090000 -1.9513930000 2.0089130000

C -0.1711250000 -2.8841640000 2.2129730000

O 0.8265180000 -2.6601310000 1.2190320000

C 2.0807650000 -3.2458560000 1.5755050000

C 3.0957270000 -3.0215750000 0.4829200000

O 3.2727440000 -1.6314290000 0.3077800000

H 3.7199250000 -1.4907300000 -1.7115750000

H 5.0784540000 -1.9505560000 -0.6537100000

H 5.3984970000 0.3178900000 -1.3507480000

H 5.0520900000 0.2836570000 0.3976670000

H 4.4361460000 2.5559060000 0.2014370000

H 4.5601260000 2.6057610000 -1.5773630000

H 2.0903860000 2.9912120000 -1.7079190000

H 2.9613460000 4.2694890000 -0.8257290000

H 0.1293260000 3.7647020000 -0.3654360000

H 1.1249580000 4.8498450000 0.6309750000

H 0.6982000000 3.4049910000 2.6199750000

H -0.7835980000 4.1135580000 1.9299500000

H -0.7624070000 1.6045570000 3.5432150000

H -2.1589200000 2.3839760000 2.7558230000

H -2.6349750000 0.0453100000 3.0756260000

H -2.4787010000 0.3636920000 1.3315820000

H -1.7871130000 -2.0737120000 1.0119980000

H -2.1094650000 -2.2085880000 2.7469690000

H 0.2624250000 -2.6967890000 3.2016980000

H -0.5109710000 -3.9255970000 2.1687650000

H 1.9566030000 -4.3229400000 1.7385750000

H 2.4291000000 -2.7865890000 2.5080890000

H 2.7742890000 -3.4891460000 -0.4543830000

H 4.0377740000 -3.4922300000 0.7959900000

O 0.8335210000 -2.5801710000 -1.5357290000

O 1.5302880000 -0.8762360000 -2.7667110000

N -3.8864430000 1.8943640000 -0.5198130000

N 1.0096330000 0.1595320000 0.1605320000

C -1.9789760000 0.9992410000 -1.2921370000

C -0.5541160000 0.7984710000 -1.7028740000

C -2.9859680000 -0.0295710000 -1.2434500000

C 0.1107510000 -0.3438540000 -0.9097030000

C -4.1652530000 0.5671760000 -0.7510240000

C -2.5777170000 2.1443940000 -0.8590020000

C -2.9984940000 -1.3970620000 -1.5624240000

C -5.3418750000 -0.1575200000 -0.5553320000

C 0.9095290000 -1.2807550000 -1.8284850000

C -4.1594450000 -2.1186160000 -1.3663900000

C -5.3196820000 -1.5033440000 -0.8638230000

H -0.4908930000 0.5548530000 -2.7656310000

H 0.0215360000 1.7183150000 -1.5726740000

H -0.6587900000 -0.9117150000 -0.3925830000

H -2.1650110000 3.1349310000 -0.7483690000

H -4.5609490000 2.5920380000 -0.2603340000

H -2.1234350000 -1.8832940000 -1.9827380000

H -6.2422040000 0.3166540000 -0.1819040000

H -4.1869530000 -3.1716290000 -1.6201960000

H 1.2663130000 -0.6187480000 0.7751690000

H 0.5199680000 0.8765040000 0.7248150000

H -6.2173890000 -2.0946390000 -0.7287740000

H 0.5345630000 -2.7096170000 -0.6175650000

H 1.8893500000 0.5596050000 -0.2148200000

**CR/TrpH+-GS1**

C 2.8164950000 2.4260260000 -2.0873410000

C 2.2479380000 3.4712850000 -1.1661520000

O 1.1421820000 2.9391130000 -0.4497190000

C 0.6233240000 3.8685860000 0.4853720000

C -0.5154500000 3.2552400000 1.2566650000

O -0.0159390000 2.1957760000 2.0437800000

C -0.9537750000 1.6884300000 2.9670490000

C -0.2986630000 0.5746340000 3.7412590000

O 0.0828110000 -0.4595790000 2.8488140000

C 0.6340640000 -1.5751990000 3.5272410000

C 1.0341000000 -2.6322310000 2.5312850000

O 2.0864390000 -2.1302080000 1.7385760000

C 2.6054540000 -3.0671580000 0.8185500000

C 3.8240550000 -2.4672950000 0.1655690000

O 3.4405990000 -1.3478040000 -0.6148960000

C 4.5516390000 -0.6700930000 -1.1865320000

C 4.0583670000 0.4300960000 -2.0890410000

O 3.3875540000 1.3933390000 -1.3073320000

H 2.0327930000 2.0189090000 -2.7360530000

H 3.5848810000 2.8999600000 -2.7137870000

H 1.9213030000 4.3356710000 -1.7580710000

H 3.0202530000 3.8014190000 -0.4598520000

H 1.4123590000 4.1746110000 1.1842740000

H 0.2598500000 4.7605200000 -0.0412970000

H -1.2935020000 2.8923920000 0.5704380000

H -0.9591780000 4.0315590000 1.8946400000

H -1.8516460000 1.3181280000 2.4511820000

H -1.2684480000 2.4719610000 3.6697540000

H 0.5857000000 0.9563880000 4.2676350000

H -1.0079100000 0.1880300000 4.4839990000

H 1.5137970000 -1.2655380000 4.1059890000

H -0.1082060000 -1.9953980000 4.2179530000

H 1.3569360000 -3.5282720000 3.0787480000

H 0.1707390000 -2.9107600000 1.9082250000

H 1.8539130000 -3.3210500000 0.0576790000

H 2.9007760000 -3.9911000000 1.3338880000

H 4.5393720000 -2.1582440000 0.9381700000

H 4.3025740000 -3.2204180000 -0.4734040000

H 5.1530900000 -1.3753710000 -1.7737950000

H 5.1803610000 -0.2529820000 -0.3897860000

H 3.3849440000 0.0203690000 -2.8515240000

H 4.9231290000 0.8810720000 -2.5961280000

O 0.6080130000 -2.2720920000 -2.1021490000

O 0.9289340000 -0.1247460000 -2.6408540000

N -3.8026340000 -2.3155440000 -1.3243430000

N 1.2096420000 0.1687130000 0.2509210000

C -2.3586260000 -0.6972860000 -0.7591890000

C -1.1478890000 0.1002560000 -0.3992870000

C -3.6936030000 -0.1688330000 -0.6936810000

C 0.1746570000 -0.6569830000 -0.4189750000

C -4.5715050000 -1.2091350000 -1.0553840000

C -2.4759610000 -2.0029180000 -1.1444950000

C -4.2172740000 1.0858900000 -0.3556260000

C -5.9552500000 -1.0311440000 -1.0922330000

C 0.6210850000 -0.9622890000 -1.8405880000

C -5.5852500000 1.2668230000 -0.3887280000

C -6.4445050000 0.2155720000 -0.7549060000

H -1.0478860000 0.9754910000 -1.0523340000

H -1.2688080000 0.4767610000 0.6188290000

H 0.0948940000 -1.5839250000 0.1449300000

H -1.7142110000 -2.7473010000 -1.3170870000

H -4.1500860000 -3.2076330000 -1.6267490000

H -3.5601260000 1.9053310000 -0.0811450000

H -6.6225010000 -1.8372930000 -1.3743150000

H -6.0092160000 2.2309300000 -0.1342940000

H 2.1451680000 -0.2406350000 0.1014980000

H 0.9963070000 0.1731560000 1.2592300000

H -7.5139100000 0.3887630000 -0.7740020000

H 0.8538990000 -2.3899480000 -3.0288560000

H 1.2142470000 1.1482350000 -0.0853620000

**CR/TrpH+-GS2**

C 2.3580320000 3.3907950000 0.2667320000

C 1.2032210000 3.6400870000 1.1967680000

O 0.2037740000 2.6478740000 1.0126770000

C -0.8172240000 2.7540800000 1.9925270000

C -1.8012400000 1.6259810000 1.8554830000

O -1.1527560000 0.4086550000 2.1635350000

C -2.0552460000 -0.6666350000 2.3036440000

C -1.2644380000 -1.9159630000 2.5844730000

O -0.4184320000 -2.1935450000 1.4814290000

C 0.3041300000 -3.3966660000 1.6438160000

C 1.2337100000 -3.5883660000 0.4739670000

O 2.1973630000 -2.5642680000 0.5041180000

C 3.2341970000 -2.7133520000 -0.4422270000

C 4.3093130000 -1.7162490000 -0.0993880000

O 3.7876880000 -0.4053920000 -0.2171170000

C 4.6898840000 0.5742030000 0.2799630000

C 4.1838660000 1.9512050000 -0.0540680000

O 2.9672080000 2.1669420000 0.6247550000

H 2.0214950000 3.3523570000 -0.7754010000

H 3.0701970000 4.2207660000 0.3753970000

H 0.7804070000 4.6333330000 0.9984720000

H 1.5585700000 3.6116030000 2.2344030000

H -0.3689350000 2.7261240000 2.9937280000

H -1.3452210000 3.7092140000 1.8735840000

H -2.2246590000 1.5910230000 0.8455780000

H -2.6267750000 1.8066040000 2.5578160000

H -2.6542110000 -0.7891340000 1.3950120000

H -2.7389510000 -0.4862630000 3.1452050000

H -0.6592450000 -1.7833030000 3.4906650000

H -1.9568980000 -2.7525600000 2.7476150000

H 0.8920370000 -3.3646140000 2.5702440000

H -0.3883850000 -4.2475400000 1.7024630000

H 1.7115680000 -4.5740200000 0.5592510000

H 0.6728150000 -3.5704760000 -0.4735100000

H 2.8594390000 -2.5438500000 -1.4609330000

H 3.6611620000 -3.7241330000 -0.3946580000

H 4.6501980000 -1.8919070000 0.9288670000

H 5.1630930000 -1.8445900000 -0.7774330000

H 5.6764940000 0.4365300000 -0.1806560000

H 4.7936400000 0.4598890000 1.3664880000

H 4.0408430000 2.0474820000 -1.1360730000

H 4.9362970000 2.6864220000 0.2656660000

O 2.1644510000 -0.6197670000 -3.0861620000

O 2.0350380000 1.4496740000 -2.2421500000

N -3.4280800000 -1.9760380000 -0.7852850000

N 0.9201850000 0.0300610000 0.0863050000

C -1.9450210000 -0.3900410000 -1.3446800000

C -0.7128900000 0.3312080000 -1.7924470000

C -3.2366800000 0.2220450000 -1.1809630000

C 0.6198680000 -0.2749110000 -1.3357420000

C -4.1394110000 -0.7990280000 -0.8239140000

C -2.1180370000 -1.7238400000 -1.1129660000

C -3.7065210000 1.5381790000 -1.3016770000

C -5.4871700000 -0.5443200000 -0.5641710000

C 1.7028530000 0.2981310000 -2.2358240000

C -5.0379030000 1.7950610000 -1.0461440000

C -5.9190180000 0.7619050000 -0.6784340000

H -0.6967470000 0.3764110000 -2.8873990000

H -0.7338620000 1.3725350000 -1.4532500000

H 0.6218190000 -1.3593520000 -1.4344680000

H -1.4042580000 -2.5311690000 -1.1343680000

H -3.8155350000 -2.8856490000 -0.6095170000

H -3.0384430000 2.3409320000 -1.5961880000

H -6.1711530000 -1.3393260000 -0.2904330000

H -5.4184900000 2.8052480000 -1.1384110000

H 1.9161020000 -0.1622140000 0.2758670000

H 0.3526160000 -0.5738150000 0.7025280000

H -6.9597700000 0.9958960000 -0.4890100000

H 2.7852440000 -0.1848710000 -3.6849450000

H 0.7284470000 1.0158310000 0.3436210000

**CR/TrpH+-GS3**

C -3.1768010000 -2.8265170000 0.9351010000

C -3.1685220000 -2.1846530000 2.2962470000

O -2.0818340000 -1.2723400000 2.4029670000

C -2.1174990000 -0.5517820000 3.6211490000

C -1.0083140000 0.4662020000 3.6665220000

O -1.2376140000 1.4460490000 2.6743120000

C -0.4376830000 2.5965960000 2.8274920000

C -0.7520630000 3.5486150000 1.7031200000

O -0.4303230000 2.9397420000 0.4634070000

C -0.6490830000 3.8124720000 -0.6303460000

C -0.4490250000 3.0657040000 -1.9234050000

O -1.4494410000 2.0800840000 -2.0218070000

C -1.4838010000 1.4119170000 -3.2653410000

C -2.7321630000 0.5701940000 -3.3198460000

O -2.6507000000 -0.4563590000 -2.3513390000

C -3.8227250000 -1.2596260000 -2.3046910000

C -3.6186120000 -2.3869500000 -1.3284450000

O -3.4942340000 -1.8449940000 -0.0295900000

H -2.2011520000 -3.2738820000 0.7134400000

H -3.9352320000 -3.6220820000 0.9358760000

H -3.0711700000 -2.9611850000 3.0653990000

H -4.1128680000 -1.6490890000 2.4546460000

H -3.0821590000 -0.0382460000 3.7225120000

H -2.0019720000 -1.2435120000 4.4659430000

H -0.0322740000 -0.0147660000 3.5119190000

H -1.0061420000 0.9254100000 4.6640940000

H 0.6310000000 2.3357690000 2.8194070000

H -0.6531560000 3.0931290000 3.7833650000

H -1.8184820000 3.8074960000 1.7234750000

H -0.1682290000 4.4686450000 1.8370010000

H -1.6733730000 4.2050370000 -0.5979660000

H 0.0485560000 4.6594150000 -0.5829730000

H -0.5215080000 3.7777240000 -2.7568680000

H 0.5546870000 2.6128200000 -1.9549220000

H -0.5927710000 0.7786300000 -3.3922960000

H -1.5075370000 2.1355270000 -4.0910150000

H -3.6077260000 1.2042160000 -3.1289520000

H -2.8294100000 0.1326060000 -4.3218530000

H -4.0230800000 -1.6770740000 -3.2993500000

H -4.6800060000 -0.6444820000 -2.0023530000

H -2.7181230000 -2.9505780000 -1.5937240000

H -4.4874530000 -3.0582770000 -1.3802990000

O 1.3975090000 -1.8345810000 -1.6992990000

O -0.5453310000 -2.4266850000 -0.8375560000

N 4.3847330000 1.3739380000 -0.4839130000

N -1.2068030000 0.0434090000 0.0441870000

C 2.5750490000 0.2927580000 0.2776520000

C 1.1761100000 0.0386240000 0.7465870000

C 3.6658380000 -0.6447820000 0.1865660000

C 0.1807310000 -0.1895180000 -0.4059400000

C 4.7814740000 0.0707790000 -0.2956360000

C 3.0670940000 1.5029960000 -0.1349330000

C 3.8022250000 -2.0124570000 0.4749470000

C 6.0227260000 -0.5352840000 -0.5022870000

C 0.2960070000 -1.5900290000 -0.9965660000

C 5.0263740000 -2.6124490000 0.2742460000

C 6.1258320000 -1.8794960000 -0.2111310000

H 1.1405280000 -0.8163710000 1.4288600000

H 0.8175620000 0.9076160000 1.2940460000

H 0.3752700000 0.5454680000 -1.1874200000

H 2.5675350000 2.4596100000 -0.1788310000

H 4.9782660000 2.1215550000 -0.7974270000

H 2.9611020000 -2.5894810000 0.8433200000

H 6.8721140000 0.0266080000 -0.8726410000

H 5.1494250000 -3.6665800000 0.4908580000

H -1.8729260000 -0.1508140000 -0.7250890000

H -1.2867760000 1.0305740000 0.3158170000

H 7.0735440000 -2.3834250000 -0.3578730000

H 2.0630640000 -1.1420840000 -1.5848950000

H -1.4778950000 -0.5345840000 0.8597300000

**CR/TrpH+-S1**

C 0.0536190000 -1.6872510000 -3.1703340000

C -1.4155490000 -2.0262540000 -3.1741540000

O -1.9956370000 -1.6121460000 -1.9455620000

C -3.4061490000 -1.8012380000 -1.9247580000

C -3.9384350000 -1.4400650000 -0.5614090000

O -3.7143410000 -0.0616630000 -0.3376160000

C -4.1316190000 0.3456660000 0.9533510000

C -4.0314320000 1.8467840000 1.0426350000

O -2.6663710000 2.2384230000 0.9626390000

C -2.5173490000 3.6489810000 0.9456450000

C -1.0576700000 4.0109150000 0.8327970000

O -0.5714850000 3.5778940000 -0.4243640000

C 0.7124580000 4.0860960000 -0.7279540000

C 1.0999280000 3.5984400000 -2.1011410000

O 1.1318060000 2.1779490000 -2.0976680000

C 1.5483460000 1.6569480000 -3.3527080000

C 1.5243540000 0.1498530000 -3.3132460000

O 0.1881300000 -0.2774660000 -3.1387760000

H 0.5487900000 -2.1371740000 -2.2994150000

H 0.5126030000 -2.0920100000 -4.0810410000

H -1.5428810000 -3.1083110000 -3.2978530000

H -1.9106350000 -1.5151600000 -4.0087380000

H -3.8708410000 -1.1714360000 -2.6928280000

H -3.6411240000 -2.8503610000 -2.1396160000

H -3.4386210000 -2.0333510000 0.2121080000

H -5.0142910000 -1.6575740000 -0.5345560000

H -3.5032360000 -0.1308170000 1.7142630000

H -5.1772860000 0.0569570000 1.1212770000

H -4.5928720000 2.3063660000 0.2206570000

H -4.4552370000 2.1862690000 1.9951690000

H -3.0669080000 4.0692790000 0.0948740000

H -2.9232510000 4.0744440000 1.8715610000

H -0.9615700000 5.1003930000 0.9203140000

H -0.4806400000 3.5469690000 1.6436210000

H 1.4478590000 3.7535970000 0.0174060000

H 0.6997250000 5.1832390000 -0.7278400000

H 0.3711280000 3.9478310000 -2.8423470000

H 2.0879910000 3.9956430000 -2.3632540000

H 2.5677140000 1.9971480000 -3.5739240000

H 0.8782820000 2.0168850000 -4.1426690000

H 2.1627160000 -0.2252530000 -2.5005300000

H 1.9248300000 -0.2322010000 -4.2610190000

O 0.2981410000 -2.3767160000 0.2816760000

O -1.4084730000 -1.3334150000 1.2930490000

N 3.3017330000 -0.9891170000 3.0304750000

N -0.9423940000 0.7061110000 -0.7078060000

C 1.9145820000 0.1940430000 1.7270420000

C 0.7036610000 0.8327960000 1.1331090000

C 3.1991930000 0.1251770000 1.0855830000

C 0.1323890000 -0.0305820000 0.0000560000

C 4.0449570000 -0.6238610000 1.9302040000

C 2.0248620000 -0.4940370000 2.9032520000

C 3.7053810000 0.6475350000 -0.1147830000

C 5.3802830000 -0.8760970000 1.6054780000

C -0.4361450000 -1.3091520000 0.5893950000

C 5.0256930000 0.3979380000 -0.4402200000

C 5.8519680000 -0.3604020000 0.4123840000

H -0.0821230000 0.9902810000 1.8781180000

H 0.9615830000 1.8016460000 0.6972760000

H 0.9067140000 -0.2687860000 -0.7267220000

H 1.2849590000 -0.6690000000 3.6700140000

H 3.6473730000 -1.5036670000 3.8235660000

H 3.0708020000 1.2487720000 -0.7603820000

H 6.0239110000 -1.4501390000 2.2612000000

H 5.4425570000 0.7959000000 -1.3576850000

H -0.4949510000 1.4409540000 -1.2733920000

H -1.6071960000 1.1569670000 -0.0546970000

H 6.8826850000 -0.5362500000 0.1303720000

H -0.0714810000 -3.1453430000 0.7406560000

H -1.4656350000 0.0649270000 -1.3233150000

O -0.8664790000 -4.3852110000 1.5865630000

H -1.3894030000 -4.5725200000 0.7733250000

H -1.4515080000 -3.8196110000 2.1121280000

O -1.9287680000 -4.4232420000 -0.9276650000

H -1.7573850000 -3.4686490000 -1.0099310000

H -1.1876550000 -4.8227320000 -1.4056030000

O 2.9177030000 -2.4292570000 -1.0135970000

H 2.0843660000 -2.3714540000 -0.5182650000

H 3.3113950000 -1.5541900000 -0.8795750000

O -1.7542250000 1.6319060000 3.6006650000

H -2.0162310000 1.7293240000 2.6681700000

H -1.7462370000 0.6632120000 3.7433240000

O -1.7651150000 -1.1633380000 4.0640560000

H -2.7220370000 -1.2661520000 4.1625530000

H -1.6051680000 -1.4069720000 3.1360360000

**CR/TrpH+-S2**

C -1.6258730000 -0.2526000000 3.5108820000

C -2.0213170000 1.1992470000 3.4144970000

O -1.6064360000 1.7127770000 2.1584480000

C -2.0557270000 3.0472740000 1.9488870000

C -1.4971200000 3.5650120000 0.6484850000

O -2.0183140000 2.7875920000 -0.4115730000

C -1.5001070000 3.1880940000 -1.6669590000

C -2.2109370000 2.4245040000 -2.7542050000

O -1.8904880000 1.0421300000 -2.6570140000

C -2.5834580000 0.2716670000 -3.6256190000

C -2.2787020000 -1.1925180000 -3.4320890000

O -2.7901660000 -1.6047130000 -2.1779010000

C -2.8245870000 -3.0086710000 -2.0255670000

C -3.4224980000 -3.3198720000 -0.6768000000

O -2.6026330000 -2.7544810000 0.3360390000

C -3.0967170000 -3.0418920000 1.6358870000

C -2.2205400000 -2.3770850000 2.6669110000

O -2.3492340000 -0.9769700000 2.5320670000

H -0.5443830000 -0.3651430000 3.3509080000

H -1.8691780000 -0.6218820000 4.5149010000

H -1.5436170000 1.7649820000 4.2232060000

H -3.1094770000 1.2916010000 3.5128600000

H -3.1518840000 3.0630610000 1.9250410000

H -1.7112760000 3.6855720000 2.7711610000

H -0.4032920000 3.5082320000 0.6542130000

H -1.7967370000 4.6147630000 0.5310980000

H -0.4220460000 2.9964590000 -1.7029870000

H -1.6778390000 4.2600170000 -1.8241030000

H -3.2948370000 2.5558100000 -2.6545700000

H -1.8960410000 2.8068120000 -3.7325130000

H -3.6632110000 0.4355260000 -3.5247930000

H -2.2736940000 0.5755290000 -4.6326940000

H -2.7595350000 -1.7564790000 -4.2411780000

H -1.1972320000 -1.3755210000 -3.4797600000

H -1.8141020000 -3.4314440000 -2.1058850000

H -3.4467980000 -3.4637800000 -2.8064740000

H -4.4325030000 -2.8975610000 -0.6113230000

H -3.4860680000 -4.4068570000 -0.5461570000

H -3.0969950000 -4.1260530000 1.8014740000

H -4.1241860000 -2.6709970000 1.7332360000

H -1.1734850000 -2.6858910000 2.5329440000

H -2.5430990000 -2.6947750000 3.6665270000

O 1.5618350000 0.4813750000 1.6235430000

O 0.8167320000 1.6619630000 -0.1332650000

N 3.3770970000 -3.2789730000 0.1779190000

N -1.4843210000 0.0185270000 -0.0474690000

C 1.7655450000 -1.9049050000 -0.5607820000

C 0.4183320000 -1.3303210000 -0.8637900000

C 3.0390220000 -1.2556070000 -0.7390200000

C -0.1362100000 -0.4903480000 0.2984810000

C 4.0248150000 -2.1468360000 -0.2621350000

C 2.0245510000 -3.1286020000 -0.0068190000

C 3.4351620000 -0.0122920000 -1.2582080000

C 5.3868660000 -1.8353330000 -0.2837880000

C 0.7801090000 0.6873510000 0.5671830000

C 4.7817260000 0.2998080000 -1.2810370000

C 5.7475090000 -0.6034130000 -0.7947900000

H 0.4627960000 -0.6884250000 -1.7511630000

H -0.3066630000 -2.1245530000 -1.0543900000

H -0.2283780000 -1.1017450000 1.1931910000

H 1.3393600000 -3.9173070000 0.2665420000

H 3.8265550000 -4.1029030000 0.5415640000

H 2.7038910000 0.6885660000 -1.6463880000

H 6.1312940000 -2.5317900000 0.0831980000

H 5.1057840000 1.2510910000 -1.6848270000

H -2.1280550000 -0.7840250000 -0.0807830000

H -1.5060020000 0.4919240000 -0.9683140000

H 6.7944820000 -0.3284620000 -0.8285820000

H 2.2214160000 1.1902790000 1.6620670000

H -1.8008800000 0.6886870000 0.6702660000

O 3.1277490000 2.6113260000 1.7845300000

H 3.0111960000 2.9852880000 0.8990690000

H 2.3879640000 2.9957910000 2.3088620000

O 2.2410230000 3.1996910000 -1.9742810000

H 1.8784370000 2.7868810000 -1.1714540000

H 1.6885390000 3.9850000000 -2.0924990000

O 0.8348040000 1.2319340000 -3.5729910000

H -0.0288780000 1.1114680000 -3.1402730000

H 1.2764020000 1.9236640000 -3.0421850000

O 0.8661130000 3.0848320000 3.2886250000

H 0.2898320000 2.4842830000 2.7867520000

H 1.1274650000 2.5519240000 4.0534720000

O 1.5023610000 -2.0619770000 3.0757930000

H 1.6121790000 -1.1965890000 2.6486170000

H 1.1975110000 -2.6177080000 2.3451850000

**CR/TrpH+-S3**

C -4.1318530000 0.5805620000 -0.0345520000

C -4.2433340000 -0.2041720000 -1.3192000000

O -2.9505940000 -0.5937670000 -1.7653450000

C -3.0052890000 -1.4426050000 -2.9034310000

C -1.6075190000 -1.8402190000 -3.3089010000

O -1.0209430000 -2.5918350000 -2.2612620000

C 0.1961960000 -3.2046460000 -2.6399560000

C 0.7508080000 -3.9503060000 -1.4505040000

O 0.9945780000 -3.0234320000 -0.4001650000

C 1.6878700000 -3.5982080000 0.6978260000

C 1.7891840000 -2.5806650000 1.8073380000

O 0.4799350000 -2.2887840000 2.2673070000

C 0.4592140000 -1.5323640000 3.4598460000

C -0.9690480000 -1.4445490000 3.9372200000

O -1.7255970000 -0.6882110000 2.9949670000

C -3.1326590000 -0.7191930000 3.2527420000

C -3.8403460000 0.1983820000 2.2839920000

O -3.5831900000 -0.2622240000 0.9706500000

H -3.5036160000 1.4697300000 -0.1652920000

H -5.1395200000 0.9041990000 0.2528090000

H -4.7233320000 0.4177760000 -2.0834670000

H -4.8552770000 -1.0983110000 -1.1515270000

H -3.5911730000 -2.3382250000 -2.6653640000

H -3.4868130000 -0.9146720000 -3.7349180000

H -0.9988270000 -0.9523750000 -3.5225380000

H -1.6700860000 -2.4448530000 -4.2223240000

H 0.9156160000 -2.4490480000 -2.9831220000

H 0.0278940000 -3.9139540000 -3.4599580000

H 0.0393650000 -4.7123010000 -1.1114640000

H 1.6871190000 -4.4427840000 -1.7386920000

H 1.1500690000 -4.4846470000 1.0544190000

H 2.6959360000 -3.8965600000 0.3841880000

H 2.3913880000 -3.0053620000 2.6198630000

H 2.2871070000 -1.6690150000 1.4491520000

H 0.8738280000 -0.5271950000 3.2904210000

H 1.0630280000 -2.0190740000 4.2356980000

H -1.3920260000 -2.4516950000 4.0162130000

H -1.0112910000 -0.9588320000 4.9180420000

H -3.3265900000 -0.3908880000 4.2795180000

H -3.4888340000 -1.7479280000 3.1319700000

H -3.4932600000 1.2308060000 2.4010930000

H -4.9163300000 0.1648810000 2.4958480000

O -1.2181470000 1.6323630000 1.6485620000

O -1.0275890000 2.2434240000 -0.4602810000

N 3.3621820000 2.7272160000 -0.9754050000

N -0.9752400000 -1.0311220000 0.1591980000

C 1.9108940000 1.0273090000 -1.1404290000

C 0.6623420000 0.2085500000 -1.2391610000

C 3.2243570000 0.4894840000 -0.9045350000

C -0.0403140000 0.1310210000 0.1146720000

C 4.1098940000 1.5852950000 -0.8045710000

C 2.0449560000 2.3887550000 -1.1756270000

C 3.7325610000 -0.8152300000 -0.7980280000

C 5.4784450000 1.4156250000 -0.5798500000

C -0.8116980000 1.4353470000 0.3939500000

C 5.0862520000 -0.9870150000 -0.5750380000

C 5.9490250000 0.1208540000 -0.4620770000

H -0.0379950000 0.6207170000 -1.9685540000

H 0.9258170000 -0.8069990000 -1.5398180000

H 0.6925780000 -0.0291520000 0.9106510000

H 1.2911250000 3.1466070000 -1.3272300000

H 3.7225950000 3.6671660000 -0.9722430000

H 3.0711290000 -1.6696340000 -0.9073570000

H 6.1482590000 2.2640800000 -0.5064900000

H 5.5003680000 -1.9854170000 -0.4987130000

H -1.4149950000 -1.1277960000 1.0817600000

H -0.4291620000 -1.8857670000 -0.0361490000

H 7.0052610000 -0.0459540000 -0.2908580000

H -1.1423370000 0.8362420000 2.2070870000

H -1.7220260000 -0.9409180000 -0.5555780000

O 1.1305300000 3.4036670000 2.1413960000

H 0.8652550000 3.9287710000 1.3546660000

H 0.3064260000 2.9578650000 2.3865870000

O -2.0934180000 1.7904390000 -3.0991210000

H -1.3729370000 2.1651390000 -2.5695320000

H -2.3309070000 0.9931840000 -2.5860500000

O 2.6842850000 1.1087000000 2.2515400000

H 2.8432020000 0.7150510000 1.3819760000

H 2.1543290000 1.9114900000 2.0559300000

O -0.0351170000 4.8678400000 0.0683180000

H -0.6155180000 5.3834860000 0.6456490000

H -0.5714090000 4.0898630000 -0.1634320000

O -3.5003090000 3.6537560000 -1.4601920000

H -2.8188590000 3.5563740000 -0.7801960000

H -3.1881800000 3.0257300000 -2.1405530000