

Coordinates of the computed structures

11A

C	-3.16535100	-1.12457600	0.39051400
C	-2.24634000	-1.48400500	-0.59161200
C	-2.01312500	-2.82238500	-0.89991600
C	-2.72603800	-3.79893100	-0.20225000
C	-3.65168900	-3.43853200	0.78217500
C	-3.87887300	-2.09616800	1.08790900
C	-3.24000600	0.37109200	0.53413400
C	-1.61299900	-0.25314800	-1.18547300
H	-1.30426100	-3.10355200	-1.67377600
H	-2.56491800	-4.84710300	-0.43018200
H	-4.19923700	-4.21122700	1.31114300
H	-4.59929100	-1.81661900	1.85061000
H	-2.86752200	0.69326400	1.51215600
N	-2.36686900	0.83584500	-0.55286900
C	-2.21606400	2.08778900	-1.06913100
O	-1.44847800	2.24209200	-2.02371000
C	-3.02181000	3.27972300	-0.51932800
C	-3.08509900	3.33291700	1.01657700
C	-2.34161300	4.56321600	-1.01231200
C	-4.43753300	3.21162700	-1.11846900
H	-3.83762900	2.66428600	1.43520500
H	-2.11562500	3.09821500	1.46698700
H	-3.35661200	4.34918500	1.31641000
H	-2.25939900	4.58022700	-2.09971800
H	-2.93375500	5.42456300	-0.69008300
H	-1.33581700	4.66014300	-0.59330200
H	-5.01851900	4.07147500	-0.77002400
H	-4.39698500	3.24806300	-2.21125500
H	-4.97268200	2.30443900	-0.82494400
C	0.70756300	-0.95136200	-1.97293100
C	1.55701200	-1.84362800	-1.30585200
C	2.42335800	-2.70445700	-1.98538800
C	2.40421900	-2.65677400	-3.37241100
C	1.54804200	-1.76999200	-4.04593400
C	0.68960900	-0.90888400	-3.36084600
C	-0.07671800	-0.16298800	-0.97041100
C	1.34048700	-1.65931700	0.09967600
H	3.08253100	-3.37601600	-1.44635200
H	3.05658500	-3.30474600	-3.94631700
H	1.55945900	-1.75085000	-5.13054100
H	0.04469500	-0.22233500	-3.89869800
H	1.83352200	-2.18328100	0.90251200
N	0.39650200	-0.76957900	0.30238800
C	-0.00082600	-0.20786900	1.57521000
O	-0.39313800	0.93001400	1.54935100
C	0.05486400	-1.07095100	2.83493300
C	-0.93415000	-0.44863300	3.83080300
C	-0.37374800	-2.52230500	2.56796500
C	1.47381000	-0.99875200	3.43218200
H	-0.68520800	0.59168300	4.04618700
H	-1.95729000	-0.48981700	3.44277500
H	-0.89640500	-1.01834200	4.76250600
H	0.36204200	-3.10287900	2.00995100

H	-0.51205700	-3.01864000	3.53225700
H	-1.32551700	-2.56071000	2.02933900
H	1.47828300	-1.56693100	4.36678500
H	2.24052200	-1.40849900	2.77284100
H	1.74469400	0.03711100	3.65479100
H	-1.75372600	-0.19244600	-2.26950700
H	0.24288500	0.88292000	-0.96869700
H	-4.26138600	0.73825300	0.41049600
C	3.37435800	0.71562100	0.22140000
O	2.52707600	1.20153300	-0.53930700
O	3.41512300	-0.39258200	0.79971400
C	4.61144800	1.61058100	0.54139700
F	5.76670100	0.99388700	0.21407100
F	4.60565500	2.78829300	-0.10024000
F	4.68540100	1.88719900	1.86170000

TS1A

C	3.20648000	0.28590300	-0.68928000
C	2.72450200	-0.56017600	0.30415300
C	3.21558100	-1.85419400	0.45044500
C	4.21706500	-2.28680600	-0.41936000
C	4.70370200	-1.43845600	-1.42015000
C	4.19923300	-0.14520000	-1.56610000
C	2.51173300	1.62002100	-0.63649300
C	1.65026800	0.13043000	1.10717400
H	2.83262800	-2.51242300	1.22521600
H	4.62200600	-3.28799900	-0.31886400
H	5.48217600	-1.78680900	-2.09057000
H	4.58069000	0.51203000	-2.34125700
H	1.91295700	1.78548700	-1.53743400
N	1.66545000	1.49301100	0.56098600
C	1.04552200	2.46585700	1.28529300
O	0.52749300	2.16297100	2.36427800
C	1.00678600	3.92595400	0.79503300
C	0.80367300	4.07137900	-0.72220900
C	-0.17038000	4.61207300	1.50049100
C	2.31392000	4.60739500	1.23542200
H	1.72784700	3.95742700	-1.28994800
H	0.06831200	3.35401900	-1.09977500
H	0.42645100	5.07760100	-0.92721500
H	-0.07849200	4.54637300	2.58512600
H	-0.19305900	5.66638700	1.21049500
H	-1.11988200	4.15234600	1.21032200
H	2.30012400	5.65419500	0.91575500
H	2.41678400	4.58166100	2.32423800
H	3.19626000	4.13347000	0.79654000
C	-0.04622700	-1.57065700	2.07229500
C	-0.74062600	-2.63678300	1.46837000
C	-1.27266000	-3.69959500	2.21629400
C	-1.06143100	-3.68054400	3.58264600
C	-0.34544100	-2.62536300	4.18811600
C	0.16376200	-1.56223900	3.45367600
C	0.30428300	-0.58583900	1.03963800
C	-0.73847400	-2.38379700	0.06717700
H	-1.82125000	-4.50151100	1.73472100
H	-1.44771600	-4.48214200	4.20170700
H	-0.19707100	-2.64409700	5.26267000

H	0.68684700	-0.74519100	3.93898400	H	0.40436700	5.15197900	0.97157000
H	-1.21231300	-2.96676000	-0.70983700	H	1.93125800	4.71913400	0.17840800
N	-0.06540200	-1.27463500	-0.19224400	C	-0.84242400	-0.66538400	1.94523500
C	-0.06111400	-0.59428300	-1.47944800	C	-1.59708700	-1.79401100	1.46203000
O	-0.19214900	0.60018000	-1.45724400	C	-2.77550500	-2.22131200	2.15270200
C	0.16276200	-1.40920600	-2.75432400	C	-3.15160400	-1.54177600	3.27466000
C	0.81105900	-0.44929600	-3.76315400	C	-2.39368800	-0.41885400	3.76332100
C	1.10318700	-2.59775100	-2.52278000	C	-1.26862400	0.01945600	3.12670100
C	-1.19097200	-1.87436200	-3.32252700	C	0.21550500	-0.44771900	1.07468800
H	0.14950200	0.38684600	-3.99733100	C	-0.95606500	-2.24818000	0.32560000
H	1.75392700	-0.04858700	-3.37741700	H	-3.35295900	-3.06321500	1.78405300
H	1.02075800	-0.99933600	-4.68386300	H	-4.04182700	-1.84232200	3.81711300
H	0.66774900	-3.37453800	-1.89039500	H	-2.74079300	0.09153400	4.65573500
H	1.33128900	-3.05071500	-3.49136500	H	-0.72198900	0.88255700	3.49138900
H	2.04393500	-2.27083300	-2.06998900	H	-1.94619600	1.72296000	0.64618900
H	-1.01438200	-2.26724500	-4.32839600	N	0.14434500	-1.44515200	0.10463100
H	-1.65425000	-2.66312700	-2.72871300	C	0.99120000	-1.51846800	-1.04611400
H	-1.89792500	-1.04388100	-3.39006300	O	1.51400300	-0.50077100	-1.42872600
H	1.90726100	0.17024500	2.17021800	C	1.24963600	-2.87249600	-1.72146200
H	-0.82176400	0.36374800	1.14318200	C	2.55464600	-2.71309100	-2.51635300
H	3.22463200	2.44180700	-0.53391300	C	1.44486600	-4.00213900	-0.69925600
C	-3.10999500	0.01962800	-0.19644300	C	0.11680000	-3.19071300	-2.71705500
O	-2.49524500	0.55918700	0.74588000	H	2.46593300	-1.93841800	-3.27997700
O	-2.91417300	-1.05779600	-0.77955100	H	3.38683300	-2.45004900	-1.85588400
C	-4.33662100	0.81586500	-0.73215600	H	2.78687400	-3.66224200	-3.00642000
F	-5.45540100	0.06271000	-0.68919200	H	0.52956100	-4.27902800	-0.17616600
F	-4.59295500	1.93518500	-0.04016100	H	1.80716200	-4.88904200	-1.22682000
F	-4.16489500	1.18175200	-2.01861800	H	2.19612700	-3.72432100	0.04717800
16+TFA				H	0.40992300	-4.06366000	-3.30794300
C	3.45715300	0.83909300	0.27761200	H	-0.83293800	-3.42363500	-2.23359600
C	2.71327900	0.07651400	1.16931700	H	-0.04403000	-2.35345000	-3.40257700
C	3.27914100	-1.00007400	1.84252400	H	1.10900800	0.99755300	2.25423300
C	4.62508900	-1.29436900	1.61311600	H	2.99186500	2.89386100	-0.23583900
C	5.37838100	-0.52210200	0.72381000	H	-1.21559800	-3.05035200	-0.34181400
C	4.79796100	0.55143700	0.04511100	C	-2.43686100	0.55608500	-0.78011800
C	2.60135100	1.88351700	-0.38172800	O	-1.40057100	0.61882600	-1.40058300
C	1.29454400	0.58110200	1.25794800	O	-2.76934500	1.19517200	0.30410200
H	2.68629900	-1.60088700	2.52649100	C	-3.60240800	-0.31089300	-1.30538400
H	5.09036000	-2.12828500	2.12772100	F	-4.27784900	-0.91462700	-0.32365200
H	6.42237000	-0.76330000	0.55396800	F	-3.16088900	-1.24892600	-2.14606900
H	5.38022600	1.14074800	-0.65649900	F	-4.47214800	0.46495700	-1.97787800
H	2.51028400	1.67981800	-1.44870000	TS2A			
N	1.30385100	1.72353900	0.30107600	C	3.45992300	0.66332900	-0.78373900
C	0.24764300	2.54064900	0.27172200	C	3.05720900	-0.09144700	0.31177400
O	-0.68380700	2.34175000	1.09363000	C	3.73219400	-1.25048900	0.67817200
C	0.15509400	3.74594200	-0.67817900	C	4.83915400	-1.64014900	-0.07980500
C	0.73719100	3.49416000	-2.07779600	C	5.25115000	-0.87922800	-1.17747100
C	-1.33002800	4.10148300	-0.84345100	C	4.56242400	0.28029500	-1.53971800
C	0.87062100	4.92354400	0.00881000	C	2.52301900	1.81221400	-1.02248400
H	1.82147300	3.60082300	-2.11328300	C	1.84466400	0.53489500	0.95801800
H	0.46321700	2.50184500	-2.44928700	H	3.40672600	-1.84221800	1.52928800
H	0.32029200	4.23625400	-2.76427400	H	5.38313700	-2.54049800	0.18496000
H	-1.81472800	4.27736600	0.11778700	H	6.11091600	-1.19635700	-1.75791100
H	-1.40730300	5.01159000	-1.44451600	H	4.87339100	0.86145600	-2.40214800
H	-1.86762500	3.30438200	-1.36702000	H	2.02373700	1.69753600	-1.98613200
H	0.79607400	5.81022000	-0.62821500	N	1.56957200	1.69485400	0.09323000

C	0.61573300	2.57077900	0.51152700	C	3.08225100	0.00678400	0.21225000
O	0.00823500	2.31869200	1.55562600	C	3.81331000	-1.15409300	0.43239300
C	0.32698000	3.87312100	-0.25915300	C	4.90829800	-1.40972600	-0.39430300
C	0.34286400	3.72165800	-1.78939500	C	5.24946500	-0.51514600	-1.41257100
C	-1.06902200	4.35183700	0.15933100	C	4.50664500	0.64879100	-1.62379300
C	1.36273900	4.91913400	0.18826800	C	2.44970600	2.05462800	-0.83880700
H	1.35031700	3.72912700	-2.20641300	C	1.88298900	0.50945000	0.97469800
H	-0.16518100	2.80694400	-2.11037900	H	3.54118500	-1.84673500	1.22376800
H	-0.19089500	4.56998300	-2.22753200	H	5.49633000	-2.30904100	-0.24569700
H	-1.13966900	4.48317500	1.23972500	H	6.10279000	-0.72911500	-2.04730600
H	-1.27600800	5.30961500	-0.32655400	H	4.77423600	1.33638300	-2.41980100
H	-1.83701400	3.63588900	-0.14913400	H	1.91334700	2.06858900	-1.78831500
H	1.15513100	5.86939900	-0.31396700	N	1.54314700	1.75461400	0.28219600
H	1.30587100	5.08462100	1.26838300	C	0.44946500	2.41774500	0.74251900
H	2.38603800	4.62536300	-0.06175400	O	-0.19316400	1.89309300	1.65806100
C	0.08910400	-0.60299300	2.48477600	C	0.06408300	3.80328000	0.20138800
C	-0.86149600	-1.64008400	2.36508900	C	0.03173900	3.86992900	-1.33478500
C	-1.62478100	-2.03898000	3.47946500	C	-1.33653300	4.13387500	0.72946200
C	-1.39796600	-1.39667200	4.67904000	C	1.06542600	4.82646000	0.76521900
C	-0.44727000	-0.34850600	4.79789600	H	1.02234600	3.99768200	-1.77272400
C	0.29210400	0.06373600	3.71368700	H	-0.43720400	2.98039900	-1.76725400
C	0.69713500	-0.42610000	1.21082400	H	-0.56288300	4.73887300	-1.63093200
C	-0.90573200	-2.05508000	0.98809900	H	-1.37226500	4.09540300	1.81927600
H	-2.36563100	-2.82655700	3.39455100	H	-1.60884400	5.14189900	0.40417700
H	-1.96479100	-1.68930300	5.55693800	H	-2.07888500	3.43199700	0.33936700
H	-0.31660000	0.13885900	5.75751600	H	0.79006200	5.82765500	0.41925600
H	0.99383300	0.88605900	3.79512700	H	1.04709800	4.82704700	1.85934600
H	-2.07744400	-1.58052800	0.51696300	H	2.08943600	4.62828000	0.43758600
N	0.16323200	-1.32159500	0.36392100	C	0.30535800	-0.95727400	2.42807800
C	0.51733800	-1.42972900	-1.04465300	C	-0.59888500	-2.00441100	2.22834100
O	0.92446300	-0.44208900	-1.59101200	C	-1.23883900	-2.61214500	3.30324200
C	0.43616100	-2.79496500	-1.72954600	C	-0.94167700	-2.14263900	4.57935100
C	1.19402200	-2.65712500	-3.05635700	C	-0.03096800	-1.09109200	4.78314800
C	1.14084000	-3.86843000	-0.88457600	C	0.60156200	-0.48048000	3.71140100
C	-1.02279600	-3.17370900	-2.05133100	C	0.77551800	-0.52451200	1.12695900
H	0.73050500	-1.90947800	-3.70306000	C	-0.68943400	-2.28614700	0.77222200
H	2.23573200	-2.36853400	-2.88791400	H	-1.94836700	-3.41800700	3.15374100
H	1.17814100	-3.62119100	-3.57104300	H	-1.42583900	-2.59492000	5.43828600
H	0.64395000	-4.08047400	0.06227900	H	0.16907900	-0.74869500	5.79201300
H	1.16902800	-4.79764600	-1.46082600	H	1.28687700	0.34377600	3.86987100
H	2.17328400	-3.57352800	-0.67040500	H	-1.69364900	-2.15166500	0.34939700
H	-1.00949500	-4.08239500	-2.66025600	N	0.22645400	-1.28229300	0.19287500
H	-1.62836200	-3.37642100	-1.16827600	C	0.43490200	-1.12512600	-1.25231700
H	-1.50680200	-2.38058600	-2.62734400	O	0.75123100	-0.03657400	-1.63851200
H	2.10013300	0.90523800	1.95748600	C	0.41773900	-2.37028400	-2.14117800
H	3.04312000	2.77367600	-0.99841000	C	0.75432300	-1.88840300	-3.55785800
H	-0.96655400	-3.10918900	0.74216000	C	1.54519600	-3.29943800	-1.65207500
C	-3.08500500	-0.37077700	-0.86105700	C	-0.93037300	-3.11188300	-2.19716400
O	-2.06998000	-0.01131000	-1.43424900	H	-0.02278500	-1.22105600	-3.93927800
O	-3.21750500	-1.18701000	0.11395500	H	1.70841700	-1.35717000	-3.58483100
C	-4.44350400	0.22977300	-1.30643000	H	0.81898700	-2.75842500	-4.21590200
F	-4.86859200	1.13845000	-0.40931500	H	1.39221200	-3.65657900	-0.63022600
F	-5.39893200	-0.70905000	-1.39882900	H	1.58434200	-4.17377800	-2.30807800
F	-4.36280800	0.83960300	-2.49319400	H	2.51401200	-2.79212700	-1.69887400
17A				H	-0.88717000	-3.80535600	-3.04174400
C	3.41617100	0.90262100	-0.79760600	H	-1.13975200	-3.70390900	-1.30740900

H	-1.75653600	-2.41646200	-2.35356600	O	0.49939600	-1.39209900	1.07554500
H	2.15863500	0.75148100	2.00642200	C	2.41078800	-1.42834800	2.55321900
H	2.95210800	3.01527700	-0.69319500	C	2.48240600	-2.93216700	2.25401600
H	-0.32362300	-3.28906900	0.53998200	C	3.81982000	-0.83075600	2.49464500
C	-3.27971300	-0.66955400	-0.86367700	C	1.78358400	-1.21428000	3.94780400
O	-2.14418600	-0.28965100	-1.19888500	H	1.49867600	-3.39999500	2.32304100
O	-3.66434300	-1.74897800	-0.37570600	H	2.88575600	-3.10932400	1.25165500
C	-4.43196200	0.36261600	-1.06456000	H	3.14680200	-3.40274200	2.98310800
F	-5.42574100	-0.14614100	-1.82370400	H	3.85042100	0.23225600	2.73939100
F	-4.04488000	1.50469000	-1.65456300	H	4.43926800	-1.35154100	3.22977100
F	-4.98957600	0.70534300	0.11689100	H	4.27229200	-0.97682000	1.51150200
17A--H₂O				H	2.39858900	-1.74460700	4.68029300
C	1.86970200	-2.18739300	-1.57878500	H	1.75271500	-0.16046500	4.23465900
C	2.63419100	-1.05836500	-1.30056300	H	0.76947100	-1.62008400	3.98702700
C	4.00473500	-1.14688600	-1.08071000	H	2.11833300	0.85319200	-2.16088500
C	4.60388500	-2.40645200	-1.13665000	H	0.07917800	-2.15562800	-2.77726600
C	3.83870800	-3.54352300	-1.41248400	H	2.33745400	1.55615100	2.88878300
C	2.46428800	-3.44400100	-1.63526900	O	-1.08738300	1.07031600	0.66875400
C	0.42895700	-1.82196100	-1.79722200	H	-2.05424300	1.22052200	0.73176400
C	1.77374600	0.17991400	-1.36960000	C	-3.98028100	-0.16576500	1.19479700
H	4.59635100	-0.25931500	-0.87598300	O	-3.84757200	1.02712900	0.84102300
H	5.67137800	-2.50257800	-0.97036600	O	-3.13968400	-1.00512100	1.54663800
H	4.31987200	-4.51474900	-1.45755300	H	-1.02959800	0.11184400	0.79537700
H	1.87414700	-4.32806200	-1.85436400	C	-5.46270800	-0.64715400	1.15525300
H	-0.20999600	-2.25677100	-1.02564000	F	-5.63159100	-1.90564700	1.59046400
N	0.45005700	-0.34971500	-1.72094600	F	-5.95521100	-0.60254300	-0.10203100
C	-0.45415200	0.54636000	-2.23201900	F	-6.26308600	0.13508200	1.90904800
O	-0.11204200	1.72174800	-2.34129200	TS3A			
C	-1.84776800	0.09238700	-2.69996400	C	-1.67342500	0.05305500	2.60557300
C	-2.45905600	-1.04928100	-1.87362500	C	-1.82590500	-0.97957500	1.68553700
C	-2.77818900	1.30824700	-2.59286900	C	-1.95379100	-2.30298100	2.09002100
C	-1.72742900	-0.31613900	-4.17935200	C	-1.92059400	-2.58295000	3.45717100
H	-2.09630000	-2.03352100	-2.17298500	C	-1.75057000	-1.55216800	4.38585100
H	-2.28161500	-0.91576300	-0.80225200	C	-1.62324100	-0.22486700	3.96838400
H	-3.54225100	-1.04686500	-2.02966900	C	-1.59439500	1.38246900	1.90350500
H	-2.38941800	2.15911500	-3.15401800	C	-1.88382600	-0.41594800	0.28696600
H	-3.75966200	1.03794100	-2.99390500	H	-2.07860400	-3.10002700	1.36230900
H	-2.90594500	1.60453900	-1.54758900	H	-2.02319600	-3.60657000	3.80123600
H	-2.71331200	-0.61203700	-4.55160700	H	-1.72312000	-1.78494700	5.44514800
H	-1.36896800	0.52089800	-4.78583400	H	-1.49813600	0.57147500	4.69531600
H	-1.04823900	-1.16208600	-4.32201200	H	-0.60504700	1.83038900	2.01231900
C	1.84639900	2.47092000	-0.06984900	N	-1.87951500	1.02648400	0.49726000
C	1.74281300	2.87056700	1.26828200	C	-2.60358200	1.77731200	-0.39707600
C	1.80478600	4.21200600	1.62135300	O	-3.22326300	1.22222600	-1.30214300
C	1.98620300	5.13890600	0.59695000	C	-2.60961200	3.31456900	-0.29038000
C	2.09833900	4.74103100	-0.74530300	C	-1.32416200	3.89959200	0.31482000
C	2.02405900	3.40214200	-1.10017600	C	-2.75421000	3.85732400	-1.72079700
C	1.74367900	1.02695300	-0.10497700	C	-3.84395900	3.74459800	0.52142100
C	1.57257200	1.66054600	2.11870400	H	-1.30969400	3.85914400	1.40468300
H	1.71745700	4.52927300	2.65430300	H	-0.43197300	3.39103700	-0.06586900
H	2.04059700	6.19468700	0.84028400	H	-1.25402200	4.95460400	0.03404500
H	2.23278300	5.49363000	-1.51349400	H	-3.65108500	3.46773800	-2.20390800
H	2.07588300	3.09267900	-2.13633400	H	-2.81931600	4.94853600	-1.68279400
H	0.57641000	1.60611000	2.57178000	H	-1.88806900	3.58635300	-2.33229300
N	1.66785600	0.57006200	1.12577300	H	-3.88893700	4.83767500	0.55685800
C	1.45385600	-0.82752700	1.53315500	H	-4.76254000	3.37933100	0.05317000

H	-3.81470300	3.37826300	1.55144400	H	-0.61353300	-2.60860700	-0.12127500
C	-1.24266400	-1.81654600	-1.80640800	N	-0.38773400	-0.89639700	-1.36185100
C	-0.21153300	-2.68963700	-2.15109200	C	-1.47925200	-0.30642900	-1.90190100
C	-0.33934200	-3.54652500	-3.23797600	O	-1.43657800	0.90971100	-2.16939100
C	-1.52670300	-3.49641900	-3.96701300	C	-2.75483100	-1.10524600	-2.23156500
C	-2.55785200	-2.60798100	-3.62655000	C	-3.15272800	-2.12909700	-1.15126900
C	-2.42908900	-1.74867600	-2.54128300	C	-3.90517000	-0.10081000	-2.38568300
C	-0.81648100	-1.03162500	-0.64476600	C	-2.53445500	-1.79895900	-3.58874600
C	0.91709600	-2.51586300	-1.19012400	H	-2.63197800	-3.08087700	-1.25595800
H	0.45578500	-4.23126300	-3.51180400	H	-2.97479300	-1.74440700	-0.14315200
H	-1.65560500	-4.15609500	-4.81854300	H	-4.22255100	-2.33558900	-1.24557400
H	-3.46258300	-2.58842600	-4.22334500	H	-3.68544000	0.64931500	-3.14610600
H	-3.20411600	-1.03329100	-2.28532700	H	-4.81044500	-0.64243200	-2.67336100
H	1.82047900	-2.12104700	-1.66376500	H	-4.10680000	0.42483500	-1.44754900
N	0.38061600	-1.50781400	-0.25210900	H	-3.44384000	-2.34141400	-3.86567200
C	1.16512600	-0.86709000	0.76479500	H	-2.32475000	-1.06310200	-4.37066700
O	0.84153600	0.25373600	1.07313900	H	-1.71084700	-2.51720600	-3.56359900
C	2.25517400	-1.65324900	1.50145500	C	1.89745400	2.09785700	-0.76762400
C	2.89881800	-0.68402900	2.49893900	C	2.97716400	2.33565500	0.06798300
C	1.54963800	-2.78004100	2.27800800	C	3.90980700	3.32368900	-0.23825200
C	3.37011200	-2.23223000	0.61148600	C	3.72704000	4.06883300	-1.40301300
H	3.41324700	0.13012100	1.98063700	C	2.62971700	3.83459700	-2.23979300
H	2.15793600	-0.24725400	3.17179800	C	1.70195200	2.84231900	-1.92793000
H	3.63366100	-1.23156800	3.09492100	C	1.01738800	0.99013100	-0.22824700
H	1.01905800	-3.47342100	1.61868100	C	2.92986200	1.42152500	1.25586100
H	2.30421300	-3.34848600	2.82982600	H	4.75785500	3.51347200	0.41231800
H	0.83198700	-2.37021400	2.99500100	H	4.44180300	4.84265100	-1.66281200
H	4.19750300	-2.51847000	1.26688100	H	2.50157900	4.42826100	-3.13849300
H	3.06706200	-3.12990000	0.07320100	H	0.84656000	2.65941000	-2.57303700
H	3.73475700	-1.49208200	-0.10370700	H	2.80743600	1.99514600	2.17744500
H	-2.82821700	-0.68611700	-0.19168600	N	1.74510000	0.59099700	0.98366800
H	-2.34555200	2.07632700	2.28458400	C	1.25337700	-0.43191900	1.74437700
H	1.14846100	-3.43964100	-0.65630200	O	0.18883000	-0.95335600	1.41196800
O	-0.34864500	0.68936400	-1.73754800	C	2.04109900	-0.99323600	2.94520500
H	0.03641500	0.31246300	-2.54365900	C	1.11016700	-1.95502700	3.69424300
C	2.66321200	1.31370100	-1.08291100	C	3.22971200	-1.79845900	2.39235400
O	2.67451900	0.12707400	-1.44007900	C	2.52373100	0.07648500	3.94071700
O	1.71738500	2.13315500	-1.03932800	H	0.25122100	-1.42596300	4.11694700
H	0.40044200	1.24761700	-1.35753600	H	0.73334400	-2.74006200	3.03679600
C	4.01682500	1.91673100	-0.60984000	H	1.66638400	-2.41937500	4.51336400
F	3.91583700	2.45302600	0.62135400	H	3.94834200	-1.17328200	1.85736700
F	4.42103000	2.90538800	-1.43348800	H	3.75584100	-2.27813500	3.22398500
F	5.00948300	1.01568600	-0.56411000	H	2.88294000	-2.58086500	1.70949100
18+TFA				H	2.73185300	-0.41068900	4.89760200
C	1.31518100	-2.45635800	-1.08041200	H	3.44542200	0.56620400	3.62604000
C	1.91793000	-1.21135100	-1.22670900	H	1.76008200	0.84033100	4.11728100
C	3.30417500	-1.08908400	-1.27504300	H	0.94662500	0.39352800	-2.28539900
C	4.07990100	-2.24499200	-1.17431800	H	-0.62239300	-2.94490700	-1.87167300
C	3.47469600	-3.49649000	-1.02531800	H	3.83487000	0.81264900	1.33680100
C	2.08458100	-3.61180000	-0.97646100	O	-0.24877000	1.49816600	0.15734000
C	-0.18226900	-2.33026700	-1.08545700	H	-0.76475600	1.65643300	-0.66421700
C	0.87332900	-0.13238000	-1.32825400	C	-3.18641800	1.17278900	1.03462800
H	3.77570000	-0.11741100	-1.39593100	O	-3.03004400	2.22692000	0.47416300
H	5.16153800	-2.17164100	-1.21481800	O	-2.30574800	0.23854300	1.29141400
H	4.09092400	-4.38639600	-0.95148600	H	-1.39548500	0.49424800	0.95732100
H	1.61467700	-4.58399700	-0.86438400	C	-4.57151800	0.75232400	1.57795000

F	-4.54905300	0.68354900	2.91724300	H	-1.70000100	2.52962900	2.10114200
F	-4.92834800	-0.45319600	1.11456100	H	-0.63466500	2.81443800	3.46609600
F	-5.50928800	1.62764600	1.22284000	H	0.05395600	2.64288100	1.84682600
11B				H	-1.99654400	0.77913000	4.40945400
C	2.33617400	1.91430100	0.27686600	H	-2.69835900	0.23843000	2.87569400
C	1.33599100	1.90067000	-0.69142400	H	-1.64255500	-0.84640900	3.78938800
C	0.64046700	3.06193400	-1.02107300	H	1.30136100	0.47131500	-2.32940900
C	0.96733500	4.24374800	-0.35433500	H	-0.16017300	-1.19507900	-0.95618700
C	1.97075600	4.25814100	0.61980300	H	4.02534600	0.56953300	0.28397800
C	2.66478500	3.09179300	0.94391900	F	-3.02580500	-2.63431800	2.06829100
C	2.94414000	0.54791800	0.44150400	F	-3.92687000	-0.85598200	0.91623700
C	1.16813700	0.50997600	-1.24356300	F	-4.48932200	-3.01508600	0.35223300
H	-0.13025600	3.05650600	-1.78681800	B	-3.42246800	-2.17986100	0.78023000
H	0.44176000	5.16066400	-0.59830100	O	-2.33258300	-2.14852800	-0.14818800
H	2.21297100	5.18607900	1.12670100	H	-1.92834200	-3.02061100	-0.22458800
H	3.44743200	3.10505900	1.69650600	TS1B			
H	2.74384700	0.14094600	1.43785100	C	0.62582000	2.82157800	-0.65239800
N	2.26318800	-0.22890000	-0.60511100	C	-0.34729300	2.04411600	-1.26949700
C	2.53160100	-1.48009500	-1.07396700	C	-1.59748200	2.57014300	-1.58236300
O	1.83681700	-1.92347800	-1.99371200	C	-1.85239600	3.90666000	-1.27263000
C	3.70350700	-2.30900500	-0.51772500	C	-0.87322300	4.69270400	-0.65555400
C	3.82300900	-2.26756600	1.01520800	C	0.37426400	4.15592400	-0.33738200
C	3.48035900	-3.76647800	-0.94073100	C	1.87495300	2.01826200	-0.41169300
C	4.99731000	-1.79931500	-1.17641100	C	0.13765700	0.62674700	-1.45242100
H	4.32630200	-1.37067700	1.37742200	H	-2.35758500	1.95648600	-2.05785300
H	2.84408000	-2.34270300	1.49883900	H	-2.81600900	4.34066400	-1.51714100
H	4.42209800	-3.12354000	1.33892700	H	-1.08510200	5.73065300	-0.42195600
H	3.38577000	-3.85875700	-2.02341800	H	1.13270800	4.76794000	0.14132600
H	4.33331400	-4.36591400	-0.61032700	H	2.06707600	1.90292000	0.65996800
H	2.57447500	-4.17553900	-0.48377600	N	1.55201300	0.72642900	-1.03885400
H	5.84267900	-2.39820400	-0.82313100	C	2.37264100	-0.32260800	-1.28229500
H	4.94203200	-1.89594500	-2.26478100	O	1.90872000	-1.32069600	-1.85703700
H	5.20553400	-0.75353100	-0.93577900	C	3.86542100	-0.29303900	-0.89893000
C	-1.26152100	0.33866000	-1.98417000	C	4.13534400	0.28446800	0.50001200
C	-2.34565700	0.91945500	-1.31067800	C	4.37765500	-1.73896600	-0.91632000
C	-3.46290700	1.42437500	-1.98330900	C	4.61977200	0.50826700	-1.97321600
C	-3.45618200	1.34150000	-3.36850400	H	4.11099700	1.37353300	0.52368500
C	-2.36799100	0.76721000	-4.04691800	H	3.42271600	-0.10054200	1.23543600
C	-1.25769700	0.26055600	-3.36986500	H	5.13940000	-0.01929200	0.81051200
C	-0.23873200	-0.10555500	-0.98726700	H	4.21109600	-2.21416700	-1.88363600
C	-2.04727400	0.86143800	0.08783800	H	5.45072000	-1.73572400	-0.70545300
H	-4.29604100	1.85805500	-1.44162300	H	3.88033700	-2.33964800	-0.14774300
H	-4.29903000	1.71709600	-3.93715300	H	5.68500800	0.53318300	-1.72232100
H	-2.39626400	0.71052600	-5.12986500	H	4.50959200	0.03658500	-2.95427800
H	-0.43230000	-0.19058800	-3.90990900	H	4.26754100	1.54020300	-2.04892600
H	-2.68706500	1.17747200	0.89850400	C	-1.95166100	-0.84373600	-1.34097600
N	-0.86825200	0.32846100	0.28668400	C	-3.00761200	-0.86708200	-0.39726600
C	-0.26776100	-0.04713300	1.55711400	C	-4.28505000	-1.37594800	-0.71867500
O	0.47021800	-0.99576400	1.52010600	C	-4.48525700	-1.82747800	-2.00308800
C	-0.55635500	0.77470100	2.81230500	C	-3.43581800	-1.78751900	-2.95839800
C	0.65726500	0.59036300	3.73532800	C	-2.17808400	-1.30719500	-2.65057000
C	-0.72541600	2.27371400	2.52031100	C	-0.74788700	-0.37007800	-0.68919000
C	-1.80589400	0.19556200	3.50411500	C	-2.49075600	-0.33333100	0.80365900
H	0.84309200	-0.46333900	3.94908900	H	-5.07286900	-1.40350500	0.02602000
H	1.55907700	1.02113200	3.28712100	H	-5.45135500	-2.22140800	-2.29748700
H	0.46193500	1.10975000	4.67665100	H	-3.63120200	-2.15606000	-3.96003700

H	-1.38668600	-1.30686900	-3.39247400	H	0.29482700	4.78875500	-0.87314000
H	-2.98009400	-0.28015700	1.76625100	C	0.82395100	-1.54156400	-1.33552200
N	-1.22157800	0.01593800	0.62390600	C	0.90510000	-2.75292800	-0.55765200
C	-0.28126600	0.39402700	1.66122800	C	1.85338900	-3.76657200	-0.89368900
O	0.83134400	-0.05151900	1.56168900	C	2.67157700	-3.56410200	-1.96861300
C	-0.72444900	1.33708900	2.77719600	C	2.58693400	-2.36196400	-2.75491400
C	0.51286600	2.15683500	3.17235400	C	1.68712800	-1.37126100	-2.46389500
C	-1.83691300	2.30634500	2.35476500	C	-0.14519300	-0.72860600	-0.75872200
C	-1.15228300	0.46965200	3.97672100	C	-0.03706700	-2.65233100	0.45013800
H	1.34118700	1.51385300	3.47470200	H	1.92040200	-4.67108700	-0.29775000
H	0.84167300	2.78666500	2.33847900	H	3.40446900	-4.31530600	-2.24274500
H	0.25027700	2.80765400	4.01022200	H	3.25804300	-2.24556700	-3.59969800
H	-2.81240100	1.82958200	2.25158200	H	1.64444700	-0.46688100	-3.06195400
H	-1.93199300	3.07583400	3.12560600	H	-0.26428100	-3.31668000	1.26825500
H	-1.59318200	2.80386000	1.40970300	N	-0.66623600	-1.43853800	0.31381800
H	-1.42543300	1.13228100	4.80317500	C	-1.61321600	-0.91267200	1.26105700
H	-2.01306800	-0.16537200	3.75494100	O	-1.48118100	0.23238000	1.61541100
H	-0.32867700	-0.17250500	4.30004400	C	-2.75432400	-1.80326500	1.75807100
H	0.10326600	0.30766100	-2.49845800	C	-3.96959000	-0.87750800	1.93063000
H	-0.13407500	-1.55710500	-0.40643700	C	-3.12415400	-2.92289800	0.77857200
H	2.74915000	2.48078600	-0.87622200	C	-2.36155200	-2.37708200	3.13173600
F	1.50130300	-3.20280500	1.84194200	H	-3.75939000	-0.06866100	2.63234400
F	-0.74113000	-2.63168200	1.88123500	H	-4.26293300	-0.43786700	0.97101800
F	-0.07654200	-4.64926300	1.03529300	H	-4.80935800	-1.46414000	2.31239200
B	0.27341600	-3.29695100	1.17479300	H	-2.38516500	-3.72433700	0.74748700
O	0.36891000	-2.67340500	-0.16541700	H	-4.07465000	-3.35964000	1.09733600
H	1.25861300	-2.59611600	-0.54911100	H	-3.25415400	-2.53271700	-0.23550300
16+BF₃·H₂O				H	-3.20556600	-2.95175100	3.52469400
C	-2.61988600	1.83105600	-0.69846700	H	-1.49680400	-3.04239800	3.07257500
C	-2.17475300	0.69116300	-1.35647800	H	-2.13203700	-1.57361500	3.83678700
C	-3.06707400	-0.17277200	-1.98249800	H	-0.23681900	0.67859400	-2.28578300
C	-4.42775800	0.13893100	-1.95073100	H	3.47725500	-0.81442200	-0.86724600
C	-4.87655200	1.29064700	-1.29763200	H	-1.41115700	3.60224200	-0.39375900
C	-3.97495000	2.14478300	-0.65983400	F	2.15900000	-0.09024100	1.60625500
C	-1.47561800	2.56502000	-0.05739800	F	3.69435100	-1.77987500	1.26784000
C	-0.67157000	0.57448400	-1.28607300	F	4.39430600	0.31812700	1.88352800
H	-2.71294500	-1.06738300	-2.48704500	B	3.44504600	-0.41709800	1.18877100
H	-5.14189200	-0.51837000	-2.43524800	O	3.55994900	-0.03405700	-0.28783100
H	-5.93693100	1.51890400	-1.27977400	H	2.81280100	0.66968900	-0.60892100
H	-4.32565900	3.03185700	-0.14150500	TS2B			
H	-1.56284300	2.53778700	1.02897600	C	-1.19736200	-0.45052100	1.59261400
N	-0.29961700	1.79677900	-0.51131600	C	0.11702700	-0.72478100	1.15649200
C	0.98564200	2.13835600	-0.44632000	C	0.98747500	-1.52087400	1.93837700
O	1.80602600	1.43519300	-1.10040500	C	0.52357900	-1.99523400	3.13898800
C	1.49202900	3.37204800	0.31322600	C	-0.79813300	-1.70871200	3.57865800
C	0.77168200	3.61908300	1.64793300	C	-1.66501000	-0.95862800	2.82215000
C	2.98429200	3.16526600	0.60936000	C	-1.88771500	0.28936800	0.57552200
C	1.33929500	4.58454300	-0.62418200	C	0.26998000	-0.09493700	-0.10988500
H	-0.19398400	4.10962900	1.52595500	H	1.98635100	-1.75334500	1.59929900
H	0.63155200	2.68729800	2.20481700	H	1.16249300	-2.60449200	3.76286000
H	1.39398300	4.28093800	2.25603500	H	-1.12532100	-2.10314700	4.53163500
H	3.55981300	2.98642000	-0.30085400	H	-2.68083200	-0.76005000	3.13199800
H	3.37237000	4.06817400	1.08796600	H	-2.52202100	1.13017900	0.82391900
H	3.13909300	2.32827100	1.29622100	N	-0.86570800	0.53062900	-0.41182600
H	1.74430800	5.46959000	-0.12421700	C	-1.10424100	1.21301000	-1.66968200
H	1.89510700	4.43111600	-1.55371600	O	-0.75560400	0.64859800	-2.67693600

C	-1.73343800	2.59867100	-1.63497300	C	-1.24856400	-1.88063600	3.70738900
C	-1.22687700	3.41185500	-0.43273000	C	-1.81572400	-0.74552700	3.20159000
C	-1.33053700	3.30860700	-2.93780900	C	-1.66268100	0.87851300	1.19962400
C	-3.26961400	2.44552400	-1.61057200	C	-0.00137700	-0.20353700	0.08762500
H	-1.60839800	3.03623600	0.51577900	H	1.14009000	-2.60353600	1.34383300
H	-0.13676300	3.41098900	-0.38976800	H	0.25021100	-3.44174800	3.47334000
H	-1.57086800	4.44114700	-0.54334000	H	-1.61054900	-2.29280600	4.64329600
H	-1.66847500	2.75477900	-3.81219700	H	-2.62655200	-0.23975900	3.71567600
H	-1.78916700	4.29775500	-2.95150700	H	-2.43383900	1.61726900	1.34571600
H	-0.24736100	3.42893000	-2.99803400	N	-0.86353800	0.87677300	0.08350500
H	-3.71186000	3.44189800	-1.66147400	C	-0.95844000	1.84060900	-0.99517700
H	-3.61213700	1.87109600	-2.47309300	O	-0.92029200	1.42214600	-2.12419500
H	-3.63826200	1.96142900	-0.70833300	C	-1.12749500	3.32493400	-0.65943800
C	1.71734800	-1.50805300	-1.58013700	C	-0.55874300	3.72641100	0.70730500
C	2.97406100	-1.97372600	-1.22614800	C	-0.38345700	4.10320700	-1.75654600
C	3.40575400	-3.22710900	-1.64161300	C	-2.63107600	3.65820400	-0.74377900
C	2.54697600	-4.00371900	-2.41747200	H	-1.17888400	3.39259000	1.54012000
C	1.28263700	-3.53021400	-2.77277000	H	0.45284400	3.33479400	0.83866900
C	0.85452100	-2.27261500	-2.35430400	H	-0.51425100	4.81847100	0.75063800
C	1.48598000	-0.12904700	-1.00782200	H	-0.76518200	3.85549300	-2.74855700
C	3.72550100	-0.94869700	-0.41905100	H	-0.52614500	5.17342600	-1.58504600
H	4.38686900	-3.59404100	-1.36967600	H	0.68652900	3.88063800	-1.72508200
H	2.86369900	-4.98346600	-2.74851200	H	-2.75539100	4.73552700	-0.59903500
H	0.62938800	-4.14491800	-3.37685700	H	-3.03671700	3.39115100	-1.72320600
H	-0.12199800	-1.89539200	-2.62598300	H	-3.21509300	3.14632800	0.02539700
H	4.57794700	-0.58016900	-0.98650900	C	1.15327900	-1.92978100	-1.31525800
N	2.71278900	0.11274700	-0.22688700	C	2.41408600	-2.42876400	-1.01333800
C	2.80971800	1.34384300	0.36262900	C	2.72012100	-3.76926000	-1.23190800
O	1.89566100	2.14324500	0.15222200	C	1.73269600	-4.60057100	-1.76158200
C	3.95521700	1.71565300	1.32107800	C	0.46439300	-4.09591500	-2.06746900
C	3.81572500	3.21093200	1.63288100	C	0.16291600	-2.75217300	-1.84326400
C	3.78740000	0.93302700	2.63630000	C	1.05355000	-0.46696300	-0.95694000
C	5.35602500	1.48723100	0.72231300	C	3.29855400	-1.35337500	-0.44457100
H	3.92792300	3.81420200	0.73141700	H	3.70323500	-4.16229800	-0.99171100
H	2.84400700	3.43380100	2.07133300	H	1.95034700	-5.64840600	-1.93893900
H	4.59437200	3.49736300	2.34166400	H	-0.29025000	-4.75630300	-2.48110800
H	3.92071500	-0.13960700	2.50776500	H	-0.82272900	-2.35652800	-2.07149200
H	4.53845400	1.27715500	3.35009200	H	4.16864900	-1.19245100	-1.08474000
H	2.80032500	1.11115100	3.06786300	N	2.41618500	-0.17639600	-0.44773400
H	6.07978300	2.04255600	1.32168800	C	2.70532400	1.12220000	-0.17081300
H	5.66360000	0.44580400	0.73691200	O	1.85982700	1.98472500	-0.43633300
H	5.41457800	1.85946000	-0.30267000	C	3.99841500	1.50674400	0.57230900
H	-2.88403500	-0.57772000	0.08544800	C	4.09790900	3.03631900	0.58280700
H	4.07757800	-1.35244800	0.52964500	C	3.85295500	1.00503800	2.02002000
F	-5.75386200	0.29326500	-0.05517800	C	5.28307600	0.94686200	-0.06192000
F	-4.66592200	-0.29552900	1.86769100	H	4.20861800	3.43168400	-0.43093900
F	-5.95518000	-1.84849600	0.74249100	H	3.21207700	3.49251900	1.02805600
B	-5.11545100	-0.74767900	0.62051700	H	4.97575100	3.33180800	1.16452100
O	-3.89293400	-1.16446600	-0.14089900	H	3.79035300	-0.08521200	2.07398200
H	-3.90185500	-1.98372400	-0.65469000	H	4.72308900	1.32017900	2.60446400
H	1.38465200	0.62405600	-1.78660900	H	2.95571800	1.42278700	2.48794800
17B				H	6.13602500	1.50643000	0.33323000
C	-1.31210300	-0.22607300	1.96685700	H	5.45354300	-0.10313900	0.17663800
C	-0.24586800	-0.90575900	1.26758800	H	5.28279900	1.06665700	-1.14983200
C	0.32894400	-2.08349300	1.84252500	H	-2.62571100	-1.02433600	0.57438200
C	-0.17077500	-2.54644400	3.02816900	H	3.64637100	-1.60288900	0.56391400

F	-4.05798400	0.51437300	-1.14487000	C	-2.26327200	-2.50665000	3.10835600
F	-4.99870400	-0.21537800	0.81106700	H	-3.58808000	-0.13205300	3.24413700
F	-5.30263300	-1.42849900	-1.11942800	H	-4.34580000	-0.15109500	1.63890800
B	-4.49090400	-0.56746800	-0.42156400	H	-4.76741100	-1.39324200	2.83590600
O	-3.17966500	-1.41511400	-0.14256100	H	-2.71154100	-3.34524000	0.44697500
H	-3.35170800	-2.35100200	0.07460400	H	-4.22650500	-3.23799600	1.33838100
H	0.85818200	0.14422500	-1.83837200	H	-3.88840700	-2.08069500	0.04575200
17B--H₂O				H	-3.09217900	-3.00606300	3.61756300
C	-3.03223800	1.63895500	-0.76681900	H	-1.55461100	-3.27484600	2.79373300
C	-2.53777800	0.49848200	-1.39072400	H	-1.76929400	-1.84349600	3.82375700
C	-3.38361200	-0.41397900	-2.01293500	H	-0.59770700	0.55273700	-2.33457200
C	-4.75622600	-0.16516400	-1.98734900	H	-1.90400200	3.47632600	-0.61060700
C	-5.25885600	0.97422400	-1.35188800	H	-0.71624100	-3.46133600	0.72958500
C	-4.40124000	1.88711500	-0.73615000	O	1.29730200	-0.30311900	2.18133700
C	-1.92001900	2.46737600	-0.18924500	H	0.82076300	0.51775400	2.00430300
C	-1.02963000	0.48577700	-1.33115700	F	4.78682700	0.76527100	1.69946600
H	-2.98853800	-1.29703100	-2.50695500	F	5.28263700	0.48807500	-0.52356800
H	-5.43808400	-0.86085700	-2.46401400	F	5.30689100	-1.32115800	0.90974400
H	-6.32848500	1.15369300	-1.34154500	B	4.63690000	-0.11549500	0.59034500
H	-4.79459100	2.77394700	-0.24971100	H	2.06083700	-0.31183600	1.55691400
H	-2.00640500	2.53090700	0.89619500	H	2.85074800	0.27011300	-0.26890100
N	-0.71765900	1.71426500	-0.58719900	O	3.25719400	-0.39656400	0.30705800
C	0.59466200	2.04472000	-0.48190800	TS3B			
O	1.41670700	1.26953100	-0.98870200	C	2.25547400	-2.21217500	-0.72882100
C	1.05760400	3.33823200	0.20489800	C	2.02770300	-0.97817300	-1.32668700
C	0.28783700	3.65827100	1.49675000	C	3.02207100	-0.32510300	-2.04727100
C	2.54060200	3.16134900	0.55551300	C	4.27041100	-0.93891100	-2.15555100
C	0.90935900	4.48741100	-0.80728200	C	4.50989800	-2.17245700	-1.54214900
H	-0.66961000	4.14575800	1.30971300	C	3.50434100	-2.81983100	-0.82166000
H	0.11226300	2.76175000	2.10105600	C	1.01248600	-2.71570800	-0.05013200
H	0.88897900	4.34724400	2.09598800	C	0.59508300	-0.55244400	-1.10419300
H	3.13967300	2.93175400	-0.32740300	H	2.83418300	0.63629800	-2.51715800
H	2.91285200	4.08897200	0.99862300	H	5.06210600	-0.45337000	-2.71581000
H	2.68449300	2.35450500	1.28105000	H	5.48674300	-2.63514700	-1.63389000
H	1.27981800	5.41169100	-0.35358300	H	3.69030100	-3.78103800	-0.35311100
H	1.49525300	4.29088700	-1.70974600	H	1.14134100	-2.76760700	1.03240800
H	-0.13278300	4.65101800	-1.09585900	N	-0.00017900	-1.70547700	-0.42703300
C	0.58416600	-1.58096000	-1.37261400	C	-1.33168800	-1.92671800	-0.64524100
C	0.84379400	-2.67988200	-0.54501500	O	-1.96518500	-1.11576500	-1.32813900
C	1.81134000	-3.61548600	-0.88783600	C	-2.04697300	-3.13969200	-0.02298800
C	2.50111500	-3.41820900	-2.08146200	C	-1.50100500	-3.53151400	1.35948400
C	2.24067800	-2.31553200	-2.91390900	C	-3.52528400	-2.75630200	0.14084000
C	1.28171000	-1.37718400	-2.56942100	C	-1.95057600	-4.32074800	-1.00464000
C	-0.43320700	-0.78000700	-0.73367000	H	-0.58995500	-4.12764200	1.30817500
C	-0.04747100	-2.60323200	0.64605000	H	-1.30887800	-2.64978000	1.98122800
H	2.03121500	-4.46366100	-0.24955200	H	-2.25419000	-4.13714000	1.87081100
H	3.26741600	-4.12784900	-2.37471800	H	-3.97082400	-2.45529800	-0.80872600
H	2.80946600	-2.19332000	-3.82841000	H	-4.07334800	-3.62137800	0.52434500
H	1.09755300	-0.51027800	-3.19313100	H	-3.64376600	-1.93631800	0.85614800
H	0.49976700	-2.45741400	1.58262800	H	-2.50445100	-5.17047100	-0.59374800
N	-0.82066300	-1.37047600	0.37910400	H	-2.39258700	-4.05937900	-1.97035900
C	-1.75212500	-0.80793500	1.36696200	H	-0.92042100	-4.64523200	-1.17353200
O	-1.57487400	0.33110700	1.69910500	C	-0.10603700	1.95199400	-1.15601300
C	-2.84742500	-1.70786700	1.92317700	C	0.39443300	3.14130600	-0.62365800
C	-3.95234600	-0.77965700	2.44445400	C	-0.03792100	4.37094700	-1.10380500
C	-3.43823700	-2.64635500	0.86511000	C	-0.98453700	4.36956900	-2.12754600

C	-1.49277600	3.17348800	-2.65640900	C	-4.03656800	-2.28436700	-0.13929500
C	-1.06134800	1.94347700	-2.17594300	C	-2.65075800	-3.70337700	-1.65134300
C	0.50866800	0.83995100	-0.44290600	H	-1.25008800	-4.16234000	0.62416900
C	1.37607500	2.82070300	0.45450400	H	-1.84095600	-2.82020800	1.62473100
H	0.34432100	5.30117900	-0.69858400	H	-2.91225400	-4.15507200	1.18916900
H	-1.34268400	5.31492800	-2.52081600	H	-4.46214100	-1.75268200	-0.99149800
H	-2.23891700	3.21295400	-3.44184700	H	-4.66450300	-3.15330200	0.07499100
H	-1.47019700	1.01364300	-2.55612000	H	-4.06378800	-1.62524100	0.73359600
H	1.01586100	3.13924200	1.43720000	H	-3.29163200	-4.55973000	-1.42078500
N	1.43207400	1.34249300	0.39972900	H	-3.07293300	-3.18361700	-2.51614100
C	2.05332300	0.52708400	1.40298400	H	-1.66473800	-4.08555600	-1.92653800
O	1.50507000	-0.51427600	1.67806800	C	0.36367100	2.19283100	-0.76296800
C	3.37273000	0.97274800	2.02982300	C	1.49836500	2.93025500	-0.46012700
C	3.85470100	-0.17365500	2.92597400	C	1.71444500	4.17379600	-1.04808100
C	4.40686100	1.21314100	0.91887200	C	0.76024500	4.65992100	-1.94131900
C	3.20282600	2.23157600	2.90348100	C	-0.38568500	3.91535000	-2.24306200
H	3.16090600	-0.35040400	3.75139000	C	-0.59209000	2.66673700	-1.65835000
H	3.96171000	-1.10380900	2.36250400	C	0.35861400	0.87752900	-0.02677000
H	4.82871500	0.09513700	3.34245500	C	2.35521600	2.20670500	0.53615200
H	4.09330800	1.97900400	0.20523400	H	2.60194400	4.75326400	-0.81470200
H	5.34170600	1.54550100	1.37962600	H	0.90771700	5.62713700	-2.40994300
H	4.60478800	0.28925700	0.36773000	H	-1.11571700	4.31008100	-2.94091500
H	4.09037400	2.31818700	3.53618300	H	-1.47247400	2.07968600	-1.90420300
H	3.13049900	3.15012200	2.32165600	H	2.42439900	2.77682100	1.46441700
H	2.33011000	2.15428400	3.55837600	N	1.62069200	0.94720000	0.73878500
H	0.08268000	-0.42020100	-2.05984100	C	1.88730200	-0.04985500	1.62564900
H	0.72803200	-3.69863000	-0.42739900	O	1.03346800	-0.93329800	1.78383500
H	2.36303800	3.24999600	0.27111600	C	3.23823300	-0.14250600	2.35427700
O	-1.01615900	0.61956600	1.00056200	C	3.15100500	-1.30551500	3.34971900
H	-0.93113600	-0.24305600	1.43256600	C	4.31824600	-0.46894900	1.30983200
F	-4.14267900	0.07230100	2.12402400	C	3.60705200	1.13251200	3.13336500
F	-5.60818700	0.09567900	0.35495200	H	2.40055200	-1.11352300	4.12129600
F	-4.89508200	2.07312400	1.30546100	H	2.89247200	-2.24117000	2.85034200
B	-4.50805000	0.76831600	0.93798400	H	4.12288600	-1.42578900	3.83616400
H	-1.95731600	0.69732200	0.63899000	H	4.44324700	0.32876600	0.57418100
H	-3.35079900	0.07969700	-0.58333700	H	5.27748300	-0.60827200	1.81814500
O	-3.39677400	0.84212700	0.01392400	H	4.07550900	-1.39242900	0.77468500
18+BF₃·H₂O				H	4.38179300	0.87715500	3.86182900
C	1.75248400	-2.19985400	-1.08802500	H	4.01393700	1.91658400	2.49465400
C	1.66243800	-0.85740000	-1.44026900	H	2.75002900	1.53289000	3.68403400
C	2.72856600	-0.20347300	-2.05217700	H	-0.20689400	0.09480900	-1.95106200
C	3.89277000	-0.92750600	-2.31190100	H	0.07944800	-3.55431600	-0.97782400
C	3.98401400	-2.27775700	-1.95893100	H	3.36444600	2.02649500	0.15350100
C	2.91313700	-2.92551500	-1.34104700	O	-0.74970800	0.83084200	0.84730800
C	0.47142800	-2.67727000	-0.46257300	H	-0.63774400	0.01594000	1.37498300
C	0.30937600	-0.31004100	-1.07790600	F	-4.08799100	0.42079800	2.11227300
H	2.65317700	0.84504100	-2.32821200	F	-5.49566900	0.75127800	0.32107100
H	4.73271100	-0.43982400	-2.79500100	F	-4.65992300	2.54918300	1.49387300
H	4.89487300	-2.82752400	-2.17109700	B	-4.43430000	1.25572900	1.05209900
H	2.98284000	-3.97450600	-1.07051100	H	-2.37787700	1.43821500	0.53474500
H	0.60197400	-2.89840300	0.59832300	H	-3.06066900	0.49048900	-0.49488100
N	-0.42743200	-1.51634900	-0.65295900	O	-3.25055800	1.32129500	0.08895200
C	-1.76403400	-1.54182100	-0.79442600	H₂O			
O	-2.33870100	-0.52899300	-1.26515000	O	0.00000000	0.00000000	0.11791300
C	-2.60812400	-2.77160200	-0.42557000	H	0.00000000	0.76425200	-0.47165300
C	-2.10469900	-3.51625700	0.82174100	H	0.00000000	-0.76425200	-0.47165300