

Supporting information

Computational Study on Gold-catalyzed (4+3) Intramolecular Cycloaddition of Trienyne: Mechanism, Reactivity and Selectivity

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Contents:

Table S1 Cartesian coordinates of some key stationary points.

Table S1 Cartesian coordinates of some key stationary points optimized at the basis level 6-31g(d) for main group elements and lanl2dz for Au at 298 K using the B3LYP method

S1-1 Cartesian coordinates in Figure 1

1a

C	-4.33333400	0.70851600	0.79135200
C	-4.33731400	-0.72336400	1.33531800
C	-4.97206100	-1.73278600	0.70129100
C	-2.22626800	0.13112600	-0.54437200
C	-2.85843500	1.07865300	0.41339100
C	-5.44068800	1.06717900	-0.25225300
C	-5.92940200	2.51889600	-0.08305600
C	-5.10792600	0.79215900	-1.72898500
C	-2.07135100	-0.73907600	-1.40828900
C	-3.56195500	-0.91582200	2.62218400
C	-5.01744900	-3.13584400	1.09364700
C	-5.65046300	-4.07807100	0.37426700
C	-2.02265500	-1.73706000	-2.42980400
C	-2.59388000	-2.94402100	-2.28302000
O	-2.83092000	2.42304000	-0.11172000
C	-1.67778500	3.12471200	0.03280300
C	-1.82744000	4.52877100	-0.48810200
O	-0.67135200	2.64831800	0.52131400
H	-4.52117600	1.35870500	1.65859700
H	-5.51492100	-1.51260600	-0.21467400
H	-2.26294900	1.07495700	1.32873500
H	-6.29252900	0.43094000	0.01686000
H	-6.79755200	2.69908300	-0.72680300
H	-6.23911500	2.71735800	0.94982200
H	-5.15559800	3.24318200	-0.35196100
H	-5.98822300	1.00359500	-2.34611700
H	-4.82109500	-0.24734300	-1.91636500
H	-4.29844400	1.43836800	-2.08522200
H	-3.72245400	-0.07193100	3.30494100
H	-3.85471500	-1.82325900	3.15385800
H	-2.47808500	-0.98259300	2.44649500
H	-4.50709700	-3.43519800	2.00625400
H	-5.66951100	-5.11746500	0.68678500
H	-6.18474600	-3.83467200	-0.54182300
H	-1.52552200	-1.46227100	-3.35736100

H	-2.57110300	-3.66132700	-3.09752700
H	-3.10317000	-3.23736600	-1.36953300
H	-2.07742000	4.50661200	-1.55416000
H	-0.89709600	5.07638300	-0.33635600
H	-2.64756500	5.03697900	0.02900000
H	6.11761600	2.10176800	-2.30619100
C	5.14974200	2.22912900	-1.83039500
C	4.56173000	3.49301900	-1.76149300
C	4.49549700	1.12077200	-1.28925600
C	3.31463300	3.65226800	-1.15071600
H	5.07255400	4.35291900	-2.18497300
C	3.24262500	1.27866400	-0.67752200
H	4.95906900	0.14128300	-1.34695100
C	2.64914500	2.55160100	-0.61246300
H	2.85655600	4.63566400	-1.09744600
P	2.37060500	-0.14171100	0.07054300
H	1.67677300	2.68349300	-0.14486400
C	3.18257700	-1.66724200	-0.52406100
C	2.62971700	-0.05778200	1.87751400
Au	0.08029800	-0.12903800	-0.42622400
C	4.20977100	-2.27560800	0.21394200
C	2.79258500	-2.21820600	-1.75553500
C	3.64198000	0.73961100	2.43159000
C	1.81376900	-0.83149000	2.71974400
C	4.83881600	-3.41975900	-0.28028500
H	4.51507500	-1.86407500	1.17083000
C	3.42845700	-3.35770800	-2.24564600
H	1.99174400	-1.75745300	-2.32837400
C	3.83506100	0.75755800	3.81451300
H	4.27319500	1.34698800	1.79096600
C	2.01489200	-0.81179300	4.09859500
H	1.02588600	-1.45030000	2.29692000
C	4.45085300	-3.96019500	-1.50760600
H	5.63024500	-3.88865000	0.29688500
H	3.12251700	-3.77874300	-3.19883500
C	3.02446300	-0.01549700	4.64709600
H	4.61802200	1.37905600	4.23882700
H	1.38219600	-1.41287200	4.74502400
H	4.94091900	-4.85196200	-1.88718800
H	3.17587900	0.00372400	5.72237900
Ts _{1a}			
C	4.09217800	-0.33686400	1.23932600
C	4.58071600	0.97729600	0.65003700

C	2.57627400	1.57164200	0.00071700
C	4.70481500	1.10816200	-0.72652300
C	1.97268000	0.43380000	0.20688300
C	2.79711600	-0.80390000	0.53035700
C	5.21546600	-1.40327700	1.46040400
C	4.64206400	-2.65811400	2.14086300
C	6.05110900	-1.77622500	0.22580500
C	5.12631000	1.98655800	1.62601300
C	5.30616900	2.21308000	-1.45090600
C	5.44025400	2.18974800	-2.78913600
C	2.45344300	2.98866600	-0.20825000
C	1.79684900	3.78597100	0.65156900
O	3.08095200	-1.51935000	-0.69863900
C	2.19726400	-2.49362100	-1.06829600
C	2.61671100	-3.13533700	-2.36591000
O	1.21650300	-2.77964200	-0.41856000
H	3.73893700	-0.09293300	2.25066800
H	4.40104600	0.26316700	-1.33722700
H	2.24008100	-1.48208700	1.17631500
H	5.90324300	-0.93755100	2.18093600
H	5.45532400	-3.32439100	2.44689200
H	4.06428200	-2.40726900	3.03848400
H	3.99116600	-3.22592700	1.46637700
H	6.84619700	-2.46909100	0.52197100
H	6.53462100	-0.90364400	-0.22704800
H	5.44765100	-2.26759900	-0.54195500
H	4.43946000	2.12374400	2.46764400
H	6.07308200	1.61516300	2.04177200
H	5.32032000	2.96421400	1.18208700
H	5.68654700	3.06430000	-0.89327400
H	5.92406900	2.99941600	-3.32646100
H	5.08221700	1.35330000	-3.38477300
H	2.90751400	3.40583200	-1.10440200
H	1.67569700	4.84575200	0.44708300
H	1.34280500	3.39706300	1.55816000
H	2.59673200	-2.39380000	-3.17199100
H	1.93421800	-3.95160100	-2.60348200
H	3.64069300	-3.51538600	-2.29318700
H	-5.41080100	-2.07691500	-3.40997800
C	-4.49373500	-2.16629800	-2.83484900
C	-3.67506100	-3.28713700	-2.98811000
C	-4.13611000	-1.15393500	-1.94296800
C	-2.49331900	-3.39496800	-2.25111800
H	-3.95588900	-4.07291500	-3.68363200

C	-2.95058800	-1.26049100	-1.19857900
H	-4.77582800	-0.28395300	-1.83147600
C	-2.12456600	-2.38545200	-1.36176000
H	-1.85230900	-4.26370700	-2.37039000
P	-2.46822200	0.01923300	0.01742000
H	-1.19586400	-2.47530900	-0.80468700
C	-3.34888700	1.55416400	-0.45706500
C	-3.15467200	-0.49863600	1.63482800
Au	-0.11230100	0.30634600	0.11405700
C	-4.55678500	1.93236800	0.14781300
C	-2.80107100	2.35948300	-1.46950900
C	-4.18946000	-1.44107900	1.73090000
C	-2.63426200	0.07756400	2.80555900
C	-5.20856800	3.09801200	-0.26073500
H	-4.98677200	1.32427400	0.93748600
C	-3.45922400	3.51874900	-1.87724800
H	-1.86106500	2.07800700	-1.93794900
C	-4.69872700	-1.79478700	2.98204300
H	-4.59336000	-1.90347400	0.83580000
C	-3.15059900	-0.27502400	4.05156800
H	-1.82361300	0.79915500	2.74110500
C	-4.66297900	3.89027000	-1.27202500
H	-6.14207300	3.38565500	0.21420100
H	-3.03078300	4.13441600	-2.66293700
C	-4.18258600	-1.21297200	4.14109600
H	-5.49714100	-2.52811500	3.04862700
H	-2.74310800	0.17571300	4.95188600
H	-5.17179800	4.79697400	-1.58633200
H	-4.57937200	-1.49283200	5.11268900
2a			
C	-4.21315800	0.24149800	1.16996800
C	-4.32449200	-1.15680000	0.54424500
C	-2.79987300	-1.55754400	0.22634400
C	-4.13166300	-1.18977400	-0.89721000
C	-1.99814800	-0.42296600	0.33484500
C	-2.85747500	0.79964000	0.66105800
C	-5.48130600	1.13324300	1.12022000
C	-5.22280500	2.47725400	1.82334800
C	-6.10831800	1.34194200	-0.26864800
C	-5.18547300	-2.17486800	1.26529400
C	-4.50630600	-2.28443300	-1.78877700
C	-4.48233200	-2.13803800	-3.12319300
C	-2.32050100	-2.95808100	0.20905300
C	-1.46367400	-3.44211600	1.11472800

O	-2.98306500	1.61085700	-0.53525000
C	-2.11506400	2.66170800	-0.67125100
C	-2.36736100	3.39864600	-1.96128000
O	-1.26711600	2.92978500	0.14849400
H	-4.02615800	0.05649500	2.23805100
H	-3.92018100	-0.25112500	-1.39574200
H	-2.36458800	1.41323200	1.41775700
H	-6.22747400	0.59809200	1.72546300
H	-6.15692000	3.03991600	1.92229600
H	-4.81407500	2.33505600	2.83079900
H	-4.52171300	3.10231100	1.25900100
H	-7.02699400	1.93032600	-0.16986500
H	-6.38581200	0.39451500	-0.74540000
H	-5.43798700	1.88193000	-0.94330700
H	-4.92067900	-2.20599700	2.32672300
H	-6.24157400	-1.89357700	1.18587300
H	-5.07369100	-3.18618800	0.86830000
H	-4.87088000	-3.21127900	-1.35589700
H	-4.82899900	-2.92546700	-3.78526600
H	-4.13013500	-1.22310600	-3.59354100
H	-2.69280800	-3.61613600	-0.57192100
H	-1.12253400	-4.47201400	1.06821000
H	-1.07818600	-2.83315300	1.92791000
H	-2.07026700	2.76940000	-2.80797800
H	-1.78097400	4.31774900	-1.97275400
H	-3.43052900	3.62915600	-2.07623700
H	5.17415600	2.51079600	-3.29138400
C	4.30725000	2.53615800	-2.63744700
C	3.52605500	3.69014300	-2.55185000
C	3.97785400	1.40839800	-1.88332200
C	2.40871600	3.71570600	-1.71353300
H	3.78553400	4.56619700	-3.13940300
C	2.85794000	1.43105100	-1.03792800
H	4.58934900	0.51454600	-1.95781800
C	2.06785800	2.59095400	-0.96211100
H	1.79721900	4.61088900	-1.64501000
P	2.40985000	-0.00768700	0.00393400
H	1.18841000	2.62075300	-0.32415700
C	3.24051100	-1.46745300	-0.72737000
C	3.18384700	0.26934300	1.64104600
Au	0.03140000	-0.27927200	0.18225600
C	4.50563000	-1.89434700	-0.29617800
C	2.59349900	-2.16114000	-1.76329100
C	4.24382800	1.17149300	1.81561200

C	2.70578100	-0.45703900	2.74431600
C	5.11573800	-2.99539800	-0.90042900
H	5.01177100	-1.37438200	0.51130700
C	3.20998500	-3.25620100	-2.36731000
H	1.60749200	-1.84476900	-2.09469100
C	4.82046500	1.33655500	3.07656700
H	4.61503100	1.74801300	0.97415600
C	3.28852000	-0.29200700	3.99995600
H	1.87749700	-1.15031800	2.61981500
C	4.47125700	-3.67496400	-1.93570700
H	6.09395400	-3.32174000	-0.55942600
H	2.70415900	-3.78610800	-3.16932600
C	4.34589700	0.60608100	4.16734800
H	5.63878400	2.03907600	3.20492700
H	2.91364300	-0.85774300	4.84798200
H	4.94813100	-4.53198800	-2.40251000
H	4.79502200	0.73943300	5.14725900
Ts _{2a}			
C	3.82511300	0.44158200	-1.45425300
C	4.00641500	-0.99051100	-0.91005700
C	2.78006800	-1.25620100	0.11715800
C	4.31216400	-1.11753200	0.54546600
C	1.98654900	-0.04096600	0.10271100
C	2.81395900	1.12214100	-0.50551200
C	5.11697900	1.21105600	-1.86094200
C	4.76906400	2.61527000	-2.39939800
C	6.21986800	1.28590900	-0.78608500
C	4.42112400	-2.04439200	-1.91131300
C	4.98387400	-2.30368900	1.12827000
C	5.73573800	-2.24256000	2.23657500
C	2.13891400	-2.59185200	0.30688700
C	1.45866600	-3.25361500	-0.63889100
O	3.46913900	1.93982500	0.58648900
C	2.98997100	1.69522400	1.82493400
C	3.51164600	2.58183700	2.90349100
O	2.15614900	0.76766200	1.99012900
H	3.25182200	0.32841800	-2.38895100
H	4.55050600	-0.20244200	1.07339100
H	2.19204800	1.85512400	-1.01610100
H	5.53029800	0.63466200	-2.70299000
H	5.65751300	3.08443700	-2.83451500
H	4.00186900	2.57039200	-3.18261800
H	4.40846900	3.26961800	-1.59755200
H	7.11088800	1.75877900	-1.21412500

H	6.51579000	0.29388100	-0.42911600
H	5.90506900	1.88691100	0.07188500
H	3.86126600	-1.93468600	-2.84660200
H	5.48832700	-1.93890800	-2.14282200
H	4.25807600	-3.05912300	-1.54374800
H	4.86253400	-3.25486500	0.61730500
H	6.23598200	-3.11920700	2.63329000
H	5.88515600	-1.31494600	2.78340500
H	2.24389900	-3.02816500	1.29914700
H	1.00169700	-4.21721400	-0.43583900
H	1.33509800	-2.86112500	-1.64480000
H	3.27717800	2.15840800	3.87971500
H	3.04161700	3.56909900	2.82008000
H	4.59005100	2.72300900	2.79600800
H	-5.98765000	-1.97107500	2.96562700
C	-5.03706400	-1.45076400	2.91643400
C	-4.35458000	-1.12074900	4.09316200
C	-4.49453800	-1.11489600	1.67016500
C	-3.12443200	-0.45486400	4.02669100
H	-4.77655200	-1.38530400	5.05684500
C	-3.26310500	-0.44467500	1.60408500
H	-5.02330600	-1.38127800	0.76137400
C	-2.57564200	-0.11794000	2.78475600
H	-2.59088300	-0.20351200	4.93711700
P	-2.51162400	0.04647800	-0.04152600
H	-1.61686200	0.38975300	2.73580500
C	-3.25425900	-1.11092300	-1.31775900
C	-3.16976600	1.75668700	-0.44263400
Au	-0.06695100	-0.02580600	0.01517900
C	-4.35258400	-0.73067600	-2.10294400
C	-2.69288600	-2.39042200	-1.46469600
C	-4.27929100	2.29359000	0.22693200
C	-2.53042800	2.49885900	-1.45015400
C	-4.88894600	-1.63293800	-3.03061200
H	-4.78519100	0.25834600	-1.99951400
C	-3.23627100	-3.28770800	-2.38941400
H	-1.83771000	-2.68265900	-0.86247000
C	-4.74680600	3.56940700	-0.11394700
H	-4.77453700	1.72916600	1.00928800
C	-3.00540300	3.76958000	-1.78947900
H	-1.66811900	2.08711200	-1.96639400
C	-4.33389800	-2.90940900	-3.17339300
H	-5.73727500	-1.33655700	-3.63830100
H	-2.80347900	-4.27637100	-2.50001000

C	-4.11311100	4.30625400	-1.12057300
H	-5.60327200	3.98344000	0.40739400
H	-2.51180600	4.33922100	-2.56977000
H	-4.75190400	-3.60527300	-3.89294900
H	-4.47807900	5.29385100	-1.38165000
3a			
C	-3.57833700	0.64435400	1.35906600
C	-3.75072100	-0.84208700	0.99391100
C	-2.76040000	-1.17111300	-0.13493000
C	-4.28245600	-1.13496500	-0.39972100
C	-1.99451200	0.10439600	-0.46471800
C	-2.74801300	1.25965100	0.22709700
C	-4.82171200	1.41687000	1.87930500
C	-4.46167100	2.86726600	2.24449800
C	-6.06348200	1.36563800	0.97397000
C	-4.06535600	-1.76330100	2.15563500
C	-5.01516600	-2.38518100	-0.71670000
C	-6.07764200	-2.43428400	-1.52537600
C	-2.04149700	-2.47415400	-0.29764300
C	-1.44075700	-3.16505600	0.67502900
O	-3.54546300	1.88817600	-0.89461900
C	-3.13941700	1.38693300	-2.01411400
C	-3.65881800	1.91173000	-3.30307000
O	-2.27134500	0.45994900	-1.96138200
H	-2.86390200	0.65477300	2.19848300
H	-4.67469000	-0.28662100	-0.95394300
H	-2.12864900	2.09086900	0.55923700
H	-5.09158500	0.90812700	2.81502100
H	-5.29779200	3.34803000	2.76282000
H	-3.59002300	2.91613500	2.90888300
H	-4.24524400	3.46792500	1.35236100
H	-6.90272800	1.85627000	1.47922300
H	-6.36879900	0.33846500	0.75189600
H	-5.90284800	1.89100800	0.02653500
H	-3.37695500	-1.58835300	2.99155500
H	-5.08343100	-1.58243100	2.51971200
H	-3.99667000	-2.81724600	1.88186900
H	-4.65129900	-3.30409400	-0.26308300
H	-6.59111700	-3.36825300	-1.73139100
H	-6.47837900	-1.54473300	-2.00765500
H	-2.01225000	-2.86308500	-1.31628700
H	-0.92703800	-4.09932800	0.46579200
H	-1.44057000	-2.82915800	1.70853900
H	-3.46040400	1.20207700	-4.10693200

H	-3.15402700	2.85961000	-3.52715100
H	-4.72907800	2.11635400	-3.21842600
H	5.92614900	-3.26262100	-1.37679300
C	5.03580100	-2.71082600	-1.66397100
C	4.49448300	-2.86883900	-2.94130600
C	4.43414700	-1.84602700	-0.74798900
C	3.34538100	-2.16245600	-3.30516800
H	4.96377800	-3.54480800	-3.65023000
C	3.28111500	-1.13167500	-1.10848300
H	4.85891500	-1.73409700	0.24483400
C	2.73733800	-1.30094800	-2.39263900
H	2.91852200	-2.28761200	-4.29606000
P	2.47208600	0.03782100	0.04511700
H	1.83744900	-0.76111100	-2.67704000
C	2.98273200	-0.45641800	1.73311200
C	3.21657900	1.68376500	-0.26248100
Au	0.09908300	0.05889600	-0.21680700
C	4.05817200	0.15586700	2.39352700
C	2.28165900	-1.49508000	2.36856700
C	4.39768900	1.84048000	-1.00223400
C	2.58359300	2.81704400	0.27565800
C	4.42808400	-0.27006800	3.67103400
H	4.60376200	0.96433600	1.91711800
C	2.65977200	-1.92024000	3.64131500
H	1.44310100	-1.97105500	1.86584800
C	4.93718800	3.11407300	-1.19735000
H	4.89518800	0.97486600	-1.42785700
C	3.13095700	4.08471700	0.08518300
H	1.66524000	2.70526300	0.84713700
C	3.73201800	-1.30670700	4.29484000
H	5.26021800	0.21052700	4.17727700
H	2.11520700	-2.72588400	4.12535000
C	4.30752700	4.23487500	-0.65432000
H	5.85034700	3.22727200	-1.77441600
H	2.63797300	4.95509900	0.50867800
H	4.02163300	-1.63462600	5.28897500
H	4.72996700	5.22363500	-0.80805800
Ts _{3a}			
C	3.19104700	-0.74726400	1.36080800
C	3.47211100	0.75202400	1.11676800
C	2.78409300	1.15171400	-0.19309600
C	4.31915100	1.07252100	-0.11618300
C	2.08030900	-0.10551800	-0.69791200
C	2.56959200	-1.22469100	0.07974700

C	4.30032500	-1.61999700	2.02854000
C	3.83072500	-3.07474900	2.19289200
C	5.68027700	-1.55564300	1.35796400
C	3.53741500	1.61648800	2.35915700
C	5.13791900	2.30703300	-0.19123400
C	6.36140300	2.34820700	-0.72730800
C	2.13832700	2.47254800	-0.47104600
C	1.30884100	3.12322500	0.34964600
O	3.82113600	-1.79707700	-1.35414700
C	3.30416100	-1.20496700	-2.31542100
C	3.76384100	-1.35499600	-3.73011800
O	2.28990600	-0.37128400	-2.12594400
H	2.34516200	-0.80879800	2.07121100
H	4.79541500	0.22782900	-0.60155100
H	2.14741200	-2.21892400	0.00534700
H	4.40948800	-1.19585800	3.03582500
H	4.53180200	-3.62905500	2.82514700
H	2.84182200	-3.13733200	2.66427300
H	3.78545900	-3.59478400	1.22827300
H	6.39040200	-2.15518900	1.93827900
H	6.06971200	-0.53417000	1.31737800
H	5.65894900	-1.96014600	0.34108000
H	2.66986700	1.43649700	3.00686300
H	4.43880400	1.38809200	2.94000800
H	3.55890200	2.68180000	2.12314000
H	4.70381200	3.22150600	0.20728200
H	6.93379100	3.26991100	-0.76521300
H	6.83832100	1.46296700	-1.14320800
H	2.37420400	2.90997100	-1.44182600
H	0.86502400	4.07392800	0.06775100
H	1.04434000	2.73603600	1.33012900
H	4.42490400	-0.51443900	-3.97351100
H	2.90913200	-1.31604000	-4.40955600
H	4.31634200	-2.28726500	-3.85065900
H	-5.44583600	3.70772400	1.30525000
C	-4.63098700	3.38859400	0.66204600
C	-4.09130700	4.27049300	-0.27624900
C	-4.12490900	2.09288300	0.78038700
C	-3.03897700	3.85876100	-1.09825400
H	-4.48670700	5.27824400	-0.36439100
C	-3.06980000	1.67353800	-0.04463800
H	-4.54811100	1.41517500	1.51531700
C	-2.52511900	2.56781000	-0.98112300
H	-2.61477800	4.54400200	-1.82639300

P	-2.40156000	-0.02728600	0.04364000
H	-1.69924200	2.25609000	-1.61543600
C	-2.84988400	-0.68606600	1.69209400
C	-3.31023500	-1.02568900	-1.19197900
Au	-0.05206400	-0.07622400	-0.31944000
C	-3.97053100	-1.50844100	1.88017200
C	-2.05714900	-0.33363400	2.79736000
C	-4.52635100	-0.59090400	-1.73995500
C	-2.78026000	-2.26769400	-1.58034100
C	-4.29368900	-1.96672700	3.15941100
H	-4.58795600	-1.79357400	1.03425100
C	-2.38839300	-0.78856300	4.07246700
H	-1.18389400	0.29958200	2.65947000
C	-5.20346300	-1.39312400	-2.66079300
H	-4.94294700	0.36964400	-1.45403000
C	-3.46445500	-3.06689600	-2.49471900
H	-1.83447300	-2.60851700	-1.16611000
C	-3.50624300	-1.60774700	4.25439200
H	-5.16141300	-2.60514200	3.29725700
H	-1.77318500	-0.50875700	4.92277700
C	-4.67592200	-2.62930100	-3.03723300
H	-6.14263500	-1.04897200	-3.08390000
H	-3.05004100	-4.02689200	-2.78854200
H	-3.76018400	-1.96692600	5.24740300
H	-5.20470200	-3.24968800	-3.75495100
4a			
C	1.15209100	-1.10135600	0.64989900
C	1.18892200	0.44479200	0.72995400
C	-0.18580200	0.95764700	0.26685800
C	1.08635500	1.24320300	-0.56497300
C	-0.87277200	-0.28222400	-0.21548900
C	-0.14438800	-1.39262000	-0.07855500
C	2.43121700	-1.81706500	0.13150000
C	2.32848100	-3.33360200	0.36909900
C	2.79334500	-1.52765900	-1.33274100
C	1.89247000	1.01970600	1.94244200
C	1.65353800	2.60292100	-0.69738600
C	2.14414000	3.09285900	-1.84076300
C	-0.94734900	2.03289200	0.95071700
C	-2.03861700	1.83560900	1.69754700
O	-2.09538300	-0.15727600	-0.86064800
C	-3.20060500	-0.80764700	-0.37356100
C	-4.39101700	-0.50128300	-1.24857600
O	-3.20247500	-1.50056200	0.61317700

H	1.03462100	-1.45452100	1.68915500
H	1.12507200	0.67616500	-1.49037700
H	-0.44510700	-2.37750400	-0.41563700
H	3.25844600	-1.44766400	0.75586400
H	3.27513500	-3.82947500	0.12487500
H	2.08866500	-3.56282000	1.41429400
H	1.55117100	-3.78672500	-0.25869100
H	3.66934500	-2.11758000	-1.62819600
H	3.03729500	-0.47408900	-1.49452300
H	1.97158300	-1.79486400	-2.00871000
H	1.49868900	0.56653600	2.85995400
H	2.96988900	0.81513400	1.90185200
H	1.76561800	2.10079800	2.03735900
H	1.67561400	3.23588300	0.18757700
H	2.55706400	4.09575700	-1.89936100
H	2.15173700	2.50838400	-2.75835200
H	-0.58058900	3.04899300	0.81534700
H	-2.55484400	2.66935600	2.16546300
H	-2.45084000	0.84477300	1.87237700
H	-4.59526200	0.57441900	-1.22990800
H	-5.26014100	-1.05056200	-0.88559900
H	-4.17867500	-0.77501800	-2.28693800
Ts _{4a}			
C	-0.81298600	-1.31809700	-0.72933300
C	0.67451200	-1.36434700	-0.45078800
C	-1.59656500	-2.49182900	-0.06436600
C	-1.43535000	-2.64962500	1.45724300
C	-3.08419200	-2.52630100	-0.44546200
C	-1.20990500	0.18650400	-0.47767800
C	0.12611500	0.92074200	-0.43093000
C	1.15749200	-0.12076900	-0.30001700
O	2.44543500	0.33320900	-0.07071100
C	3.51903000	-0.50423500	0.05454600
C	4.77008300	0.31096400	0.27693200
O	3.46297400	-1.70821500	-0.00451600
C	-1.25353400	0.57090900	0.98705700
C	-1.66224500	1.75979400	1.60028500
C	-2.17149200	2.90377600	1.00746200
C	-0.46802000	3.33325300	-0.66258500
C	0.42235100	2.29335800	-0.47480800
C	-2.31304700	0.63148700	-1.43842900
H	1.24735500	-2.27804200	-0.40867200
H	-1.13508900	-3.38458800	-0.51462500
H	-1.80421400	-3.63478500	1.76729100

H	-0.38705400	-2.57401200	1.76737000
H	-2.01048800	-1.89994900	2.01038100
H	-3.53898300	-3.46798700	-0.11565600
H	-3.22990100	-2.44725500	-1.52923800
H	-3.64088500	-1.71256800	0.03375000
H	4.93900000	0.98077500	-0.57278700
H	5.62125800	-0.36026300	0.39455000
H	4.66106900	0.93608400	1.16918400
H	-0.77089000	-0.14395100	1.64155700
H	-1.32961500	1.85982600	2.63452000
H	-2.81107400	2.86727700	0.13879300
H	-2.28091100	3.80150200	1.61011200
H	-1.33049100	3.23587400	-1.30370000
H	-0.11710400	4.35287900	-0.52786100
H	1.42798000	2.54695000	-0.14259300
H	-2.56143500	1.68835400	-1.37333000
H	-3.23234000	0.07062400	-1.24907900
H	-2.00435800	0.43136200	-2.47088400
H	-0.95259000	-1.48155900	-1.81205100
5a			
C	-0.56658700	1.49205200	0.65676400
C	0.92762900	1.26852800	0.58180500
C	-1.00108600	2.47407900	-0.48716000
C	-0.99699000	1.85438200	-1.89242000
C	-2.30911200	3.23470300	-0.20171800
C	-1.13386600	0.00910400	0.72387100
C	-0.01350800	-0.81441900	0.07136200
C	1.19888300	0.00414600	0.22236600
O	2.40232100	-0.62717500	-0.04538400
C	3.60824000	0.01414000	0.00448500
C	4.70822100	-0.95301300	-0.36284200
O	3.76060400	1.17422500	0.30020500
C	-2.52231300	-0.19947500	0.15207100
C	-3.09413600	-1.36724800	-0.16215500
C	-2.46015100	-2.73560600	-0.06401000
C	-1.17236300	-2.91329400	-0.88287400
C	-0.02048200	-2.00393600	-0.55119900
C	-1.19826800	-0.35914400	2.23914100
H	1.65140900	2.05629700	0.72761800
H	-0.21317900	3.24269700	-0.48222700
H	-1.17690300	2.62874900	-2.64802200
H	-0.03369100	1.38521500	-2.11676500
H	-1.77486800	1.09191300	-2.00358800
H	-2.41773000	4.07017100	-0.90396800

H	-2.31402800	3.65199000	0.81269600
H	-3.20221900	2.61098200	-0.31055100
H	4.70131100	-1.81004800	0.31853200
H	5.67005900	-0.44234300	-0.30841700
H	4.54875300	-1.33899200	-1.37517200
H	-3.14262600	0.68844600	0.08134300
H	-4.12924700	-1.34028400	-0.50139400
H	-2.24131700	-2.97089500	0.98725000
H	-3.18292300	-3.49065200	-0.39459900
H	-0.83249900	-3.95383200	-0.77727000
H	-1.41047000	-2.79609800	-1.95250300
H	0.94411400	-2.35196200	-0.91925300
H	-1.46183800	-1.41101700	2.37862500
H	-1.95601000	0.25203200	2.74261900
H	-0.23233200	-0.17920300	2.72341400
H	-0.82181300	2.00044100	1.59814000
Ts _{1b}			
C	-5.22889300	-0.65437600	-0.13809700
C	-5.80326700	0.78149900	-0.07112900
C	-5.09878200	1.79118000	0.49884000
C	-2.61035300	-0.33448200	-0.62588200
C	-4.00152800	-0.42973700	-0.98107700
C	-5.26567500	-1.38742100	1.24162900
C	-5.20138100	-2.92370400	1.13335500
C	-4.30413400	-0.88300600	2.32926300
C	-1.69245900	0.63381600	-0.90909400
C	-7.15924200	0.93179600	-0.71130500
C	-5.52248500	3.17257300	0.66900400
C	-4.75528400	4.09544300	1.27243800
C	-2.14416800	1.87153400	-1.53371200
C	-1.32258000	2.87877600	-1.88336700
O	-3.60882300	-2.36895400	-1.59275100
C	-2.64996900	-2.58398700	-0.84608900
C	-1.95883200	-3.90027000	-0.69650600
O	-2.13665400	-1.58391800	-0.11521800
H	-5.91432900	-1.20992700	-0.79090200
H	-4.11003500	1.57159900	0.89515400
H	-4.25617800	0.04730600	-1.92549900
H	-6.28125800	-1.15726600	1.59325900
H	-5.61277100	-3.36864500	2.04551800
H	-5.77803000	-3.30716800	0.28480100
H	-4.17507100	-3.29447600	1.04475300
H	-4.48944800	-1.43854600	3.25530800
H	-4.45307100	0.17560400	2.55520200

H	-3.25446800	-1.03890000	2.06092400
H	-7.11459500	0.69402000	-1.78343900
H	-7.87335400	0.22644000	-0.26547500
H	-7.57253400	1.93679100	-0.61289000
H	-6.50077700	3.46524100	0.29690600
H	-5.08878300	5.12099300	1.39517300
H	-3.77046400	3.85171900	1.66517800
H	-3.20697600	1.99681400	-1.74144500
H	-1.70240200	3.76589800	-2.38198200
H	-0.25528900	2.84275700	-1.68180700
H	-1.02529300	-3.87247100	-1.27163500
H	-2.59191500	-4.70253200	-1.07589900
H	-1.69863100	-4.07284400	0.35116300
H	5.09876300	-0.36637900	4.43065100
C	4.21618600	-0.65877500	3.86918000
C	3.27210400	-1.51355200	4.44184000
C	4.02837100	-0.17191900	2.57447600
C	2.13389400	-1.88092600	3.71997900
H	3.41974900	-1.88760500	5.45082400
C	2.88911400	-0.54098400	1.84267600
H	4.76307500	0.49843900	2.13914100
C	1.93915800	-1.39389800	2.42779700
H	1.39422600	-2.53921200	4.16661200
P	2.61286200	0.04274700	0.12849200
H	1.04625600	-1.67089000	1.87265600
C	3.56970700	1.59569900	-0.04875000
C	3.40485000	-1.18469500	-0.97959100
Au	0.30076400	0.34971500	-0.39753900
C	4.84922800	1.62184300	-0.62284600
C	2.99705300	2.79098500	0.41803900
C	4.36572800	-2.09649700	-0.51776400
C	3.03989100	-1.19463800	-2.33661400
C	5.54598200	2.82807300	-0.72342600
H	5.30018100	0.70766900	-0.99598700
C	3.69999900	3.99100900	0.32090200
H	2.00297900	2.78124200	0.85882500
C	4.95551900	-3.00029400	-1.40409000
H	4.65112500	-2.10630200	0.52947100
C	3.63685200	-2.09471000	-3.21845100
H	2.28949600	-0.49786800	-2.70227800
C	4.97460000	4.01102000	-0.25198600
H	6.53497700	2.84100000	-1.17225300
H	3.25152900	4.91024000	0.68659300
C	4.59431200	-2.99978800	-2.75255200

H	5.69709100	-3.70464900	-1.03833400
H	3.35170000	-2.09256800	-4.26657300
H	5.51871500	4.94751900	-0.33344900
H	5.05527800	-3.70429900	-3.43886400
2b			
C	-5.15993500	-0.63389300	-0.00961700
C	-5.62535600	0.78608400	-0.36877300
C	-5.58401300	1.81068400	0.51074500
C	-2.53597600	-0.72419500	-0.69236100
C	-3.99922100	-1.03547000	-0.96708800
C	-5.01163700	-0.94612500	1.51317000
C	-5.31978400	-2.41875800	1.84646900
C	-3.70032300	-0.51704600	2.19906000
C	-1.71905300	0.33128300	-0.79006600
C	-6.19212300	0.93386500	-1.76847000
C	-6.03282100	3.17890000	0.28832300
C	-5.94565900	4.13553700	1.22602200
C	-2.28657000	1.61660800	-1.20525500
C	-1.57168200	2.73625400	-1.40271700
O	-3.95697800	-2.54371900	-1.04177900
C	-2.79755900	-2.94730100	-0.64892600
C	-2.47858200	-4.38709500	-0.51689400
O	-1.94862600	-2.02846800	-0.38203200
H	-5.97762100	-1.28277400	-0.36249900
H	-5.17805800	1.63575500	1.50331300
H	-4.27621500	-0.73795700	-1.98028800
H	-5.82142700	-0.36805900	1.97364800
H	-5.40490700	-2.54532500	2.93107700
H	-6.26273800	-2.75020500	1.39776500
H	-4.53102900	-3.10261300	1.51026600
H	-3.83277300	-0.55316400	3.28622100
H	-3.38455200	0.49446500	1.93215400
H	-2.86976000	-1.19028500	1.95958300
H	-6.70932000	0.01945600	-2.08494800
H	-6.91671000	1.74829700	-1.83117000
H	-5.41904700	1.14249000	-2.52286700
H	-6.45056600	3.43587700	-0.68203300
H	-6.28674600	5.14898000	1.03953900
H	-5.53176900	3.93448200	2.21176700
H	-3.36248400	1.67269200	-1.36300800
H	-2.04970800	3.65590500	-1.72737700
H	-0.49618600	2.76681900	-1.24878000
H	-1.40773100	-4.52457900	-0.36455100
H	-2.81055000	-4.91702100	-1.41502100

H	-3.02971300	-4.80376000	0.33485400
H	5.28326200	-0.36161900	4.30542400
C	4.43628900	-0.72142600	3.72845200
C	3.63425800	-1.74981800	4.22723800
C	4.15085800	-0.14674300	2.48867100
C	2.54097800	-2.20427900	3.48581400
H	3.85693400	-2.19202900	5.19402400
C	3.05631900	-0.60171700	1.73707300
H	4.77401200	0.65863700	2.11209000
C	2.24943000	-1.63064000	2.24862700
H	1.91147700	-2.99934800	3.87527700
P	2.65785100	0.09818400	0.09072700
H	1.39108800	-1.97683800	1.67837100
C	3.39739100	1.77553700	0.06167900
C	3.58206700	-0.89969900	-1.13873800
Au	0.31588900	0.17406100	-0.36842300
C	4.64615200	2.03272100	-0.52268100
C	2.68375700	2.82839400	0.65903400
C	4.68430800	-1.69061300	-0.78114000
C	3.17464200	-0.85095500	-2.48255100
C	5.17405000	3.32562500	-0.50331800
H	5.20390800	1.23059400	-0.99568200
C	3.21836500	4.11572200	0.68064700
H	1.71183900	2.63910100	1.10850800
C	5.37098800	-2.41620400	-1.75677300
H	5.00492800	-1.74527100	0.25451600
C	3.86830300	-1.57212700	-3.45376100
H	2.31553300	-0.24856400	-2.76761400
C	4.46359500	4.36598900	0.09761700
H	6.14044200	3.51786000	-0.96041100
H	2.66138600	4.92349100	1.14659700
C	4.96625700	-2.35681700	-3.09156100
H	6.22209600	-3.02786200	-1.47151600
H	3.54883500	-1.52535500	-4.49088800
H	4.87654700	5.37053600	0.10875900
H	5.50290000	-2.92256900	-3.84776200
Ts _{2b}			
C	-4.87223400	-0.67216600	0.20546400
C	-5.41184600	0.74836500	-0.01222600
C	-4.91486300	1.82101900	0.64227700
C	-2.59238400	-0.25639200	-1.00473600
C	-3.88482700	-0.97228000	-0.96853600
C	-4.45514700	-1.03565800	1.67006300
C	-4.77960000	-2.50643500	1.99573000

C	-3.01592200	-0.71373600	2.11520800
C	-1.80781400	0.72712000	-1.18792500
C	-6.56414500	0.82005300	-0.98875400
C	-5.35704500	3.20621100	0.54343300
C	-4.79692900	4.20259700	1.24729900
C	-2.09552300	2.05104600	-1.76094700
C	-1.19512400	3.02341800	-1.95320200
O	-3.72192400	-2.40184800	-1.17463100
C	-2.50744500	-2.86801500	-0.89338100
C	-2.36768400	-4.35305300	-1.03249700
O	-1.61786500	-2.09753100	-0.53983200
H	-5.71365700	-1.33909100	-0.03052600
H	-4.10239400	1.66577500	1.34736400
H	-4.39409100	-0.64441800	-1.88424000
H	-5.12466700	-0.42681400	2.29004700
H	-4.60514400	-2.70700800	3.05838500
H	-5.82688600	-2.74580400	1.78014700
H	-4.15566500	-3.20527100	1.42613400
H	-2.94089700	-0.84976800	3.19998700
H	-2.70745600	0.31075800	1.89176100
H	-2.28378600	-1.38230600	1.65312500
H	-7.45455300	0.33385800	-0.56657000
H	-6.83993400	1.84109300	-1.25726200
H	-6.34332400	0.28799900	-1.92540000
H	-6.18186700	3.44050700	-0.12496100
H	-5.14548200	5.22701700	1.16194800
H	-3.97585800	4.02285900	1.93810100
H	-3.13363700	2.22732000	-2.03351500
H	-1.49616000	3.97298400	-2.38542900
H	-0.14792600	2.90844200	-1.68885500
H	-1.31237400	-4.62419500	-1.07133100
H	-2.88906000	-4.69893200	-1.92877700
H	-2.83391100	-4.83912300	-0.16737400
H	4.45837100	-1.19153400	4.51031000
C	3.69720800	-1.42013300	3.77011100
C	2.82807000	-2.49490600	3.96636100
C	3.58981000	-0.63079800	2.62355000
C	1.84522400	-2.78225100	3.01546400
H	2.91274000	-3.10474400	4.86113700
C	2.60609200	-0.91793400	1.66481700
H	4.26499700	0.20728700	2.48124400
C	1.72890200	-1.99591100	1.87002500
H	1.16489700	-3.61471900	3.17025500
P	2.45157300	0.06164100	0.12779300

H	0.95548400	-2.21417500	1.13763500
C	3.25501300	1.67596700	0.43620800
C	3.43244800	-0.79537600	-1.15685700
Au	0.20430600	0.32446900	-0.52130300
C	4.56597800	1.94094400	0.01328900
C	2.53677800	2.66430100	1.13043400
C	4.46247100	-1.68701100	-0.81972000
C	3.15743200	-0.53369700	-2.50940900
C	5.15004800	3.17976200	0.28654800
H	5.12842800	1.18921100	-0.53131500
C	3.12782900	3.89638000	1.40498400
H	1.51756000	2.46899800	1.45521400
C	5.21010600	-2.30176700	-1.82577200
H	4.67833000	-1.90607100	0.22131000
C	3.91081800	-1.14743400	-3.50921300
H	2.35364400	0.14663500	-2.77947600
C	4.43430000	4.15602800	0.98125100
H	6.16393700	3.38021000	-0.04715900
H	2.56747900	4.65532200	1.94314600
C	4.93676900	-2.03270300	-3.16827300
H	6.00429200	-2.99268200	-1.55840500
H	3.69268300	-0.93984300	-4.55268800
H	4.89087400	5.11924800	1.18946500
H	5.51896600	-2.51494700	-3.94812600
3b			
C	-5.12823500	-0.75463800	-0.12141600
C	-5.11423900	0.56180100	-0.89111100
C	-5.91854800	1.60106200	-0.56697500
C	-2.49007800	-1.07788600	0.26014800
C	-3.81982000	-1.44160800	0.14513900
C	-6.08243400	-0.88652800	1.12978200
C	-6.39906500	-2.35667500	1.45735900
C	-5.58445500	-0.15544200	2.38564800
C	-1.83474300	0.16709500	0.44370800
C	-4.23221400	0.56086500	-2.12300000
C	-6.05534600	2.85537100	-1.29315800
C	-6.87479000	3.84283600	-0.89603300
C	-2.59208400	1.33186900	0.80798500
C	-2.01069800	2.53124400	1.04910600
O	-2.41658800	-2.83916300	-1.77896400
C	-1.60781600	-2.97296600	-0.89286200
C	-0.49045700	-3.97599500	-0.83768100
O	-1.59419900	-2.16977100	0.23322000
H	-5.57541200	-1.46088700	-0.84703700

H	-6.54225300	1.53094700	0.32080800
H	-3.95294000	-2.51777500	0.20654300
H	-7.02176500	-0.42558000	0.80264900
H	-7.20527700	-2.40431800	2.19659400
H	-6.73158200	-2.91059900	0.57167600
H	-5.53875100	-2.88169900	1.88864000
H	-6.31478100	-0.26894200	3.19411400
H	-5.44358900	0.91742000	2.22374200
H	-4.63543500	-0.57413400	2.74222800
H	-4.08115200	-0.45603200	-2.50130200
H	-4.66273000	1.15778200	-2.93057600
H	-3.23267000	0.96747300	-1.91616500
H	-5.46302300	2.99621300	-2.19394800
H	-6.96422900	4.76908200	-1.45479600
H	-7.48697400	3.75278700	-0.00120800
H	-3.67043700	1.26665100	0.89769300
H	-2.60723900	3.40240200	1.30609400
H	-0.93310700	2.66095300	1.00050800
H	-0.40976400	-4.41042400	0.16242600
H	0.45673700	-3.46969100	-1.05877800
H	-0.66359500	-4.75436100	-1.58165700
H	5.59053200	-3.51723000	-1.43236400
C	4.70915200	-2.92554200	-1.66192500
C	3.97914800	-3.17762900	-2.82454000
C	4.31144300	-1.91192000	-0.78701200
C	2.84434800	-2.41483700	-3.11581600
H	4.29184500	-3.96631300	-3.50266300
C	3.17346700	-1.14392600	-1.07261000
H	4.88462900	-1.72449700	0.11535100
C	2.43873300	-1.40565800	-2.24246600
H	2.27490100	-2.60590700	-4.02084800
P	2.61269200	0.20974300	0.02932000
H	1.55499500	-0.81547100	-2.47411400
C	3.47732200	-0.00753100	1.62782400
C	3.24636500	1.76843600	-0.69511600
Au	0.22742100	0.20178800	0.26868600
C	4.72870500	0.58051700	1.87025800
C	2.87841400	-0.79620100	2.62401500
C	4.24154200	1.77937500	-1.68336500
C	2.72622500	2.98577700	-0.22466400
C	5.37262700	0.37325800	3.09105400
H	5.19590400	1.20277100	1.11312800
C	3.52840400	-1.00243800	3.84061100
H	1.90391800	-1.24565600	2.44939100

C	4.70966400	2.99388000	-2.18999900
H	4.64878400	0.84683800	-2.06095500
C	3.20173000	4.19488100	-0.72899200
H	1.95367400	2.98669900	0.54052700
C	4.77516700	-0.41747900	4.07503300
H	6.33944700	0.83315400	3.27364400
H	3.05868300	-1.61251800	4.60657600
C	4.19275600	4.19989400	-1.71461700
H	5.47834300	2.99453600	-2.95727300
H	2.79674100	5.13182400	-0.35772700
H	5.27775400	-0.57315400	5.02521600
H	4.55835200	5.14219800	-2.11208500
T _{S3b}			
C	3.07222600	-0.85515100	-1.27956700
C	3.01287800	-1.30628600	0.18867300
C	4.05402100	-0.96129900	1.06000400
C	2.87130100	1.27348300	-0.21524900
C	3.30769400	0.63615500	-1.30421500
C	4.04486700	-1.71215700	-2.15233300
C	3.80674200	-1.41839600	-3.64370300
C	5.52715900	-1.54825800	-1.79118200
C	2.23000800	0.49810100	0.88633300
C	2.17397000	-2.53078900	0.48559200
C	4.31973600	-1.55111100	2.34447900
C	5.35946800	-1.14631000	3.10316200
C	2.48387400	0.97610400	2.25807800
C	1.73213100	0.66833400	3.32841800
O	1.13597100	3.07840900	-1.24724600
C	2.06550000	3.48265000	-0.59507500
C	2.39457300	4.91804300	-0.28618500
O	2.99862600	2.64590800	-0.01442300
H	2.06585200	-1.03610000	-1.69366500
H	4.73773800	-0.17876400	0.74476600
H	3.73157700	1.14841600	-2.15956300
H	3.76928100	-2.76271500	-1.98262100
H	4.40230400	-2.09667500	-4.26368900
H	2.75372700	-1.55101900	-3.91759300
H	4.09766900	-0.39512700	-3.90932400
H	6.14500800	-2.15934300	-2.45768800
H	5.74573000	-1.86798300	-0.76618300
H	5.85487400	-0.50713000	-1.89954100
H	2.78194100	-3.43234400	0.33017400
H	1.80996500	-2.54999400	1.51570100
H	1.31048300	-2.59047200	-0.18104900

H	3.68038500	-2.35274100	2.70136900
H	5.58248400	-1.61159000	4.05826300
H	6.02905000	-0.35332200	2.77825100
H	3.34575400	1.62799900	2.40487600
H	1.97477100	1.05599300	4.31387400
H	0.85987400	0.02385900	3.25086400
H	3.40641600	5.15551900	-0.62964900
H	2.37001500	5.08185700	0.79635000
H	1.67075600	5.56991000	-0.77546500
H	-5.87922500	2.68057300	-1.66587500
C	-4.80462100	2.52278300	-1.66677600
C	-3.96733600	3.39117600	-2.37337300
C	-4.26255600	1.45462900	-0.95354000
C	-2.58590500	3.19297200	-2.36358000
H	-4.39324100	4.22536000	-2.92365100
C	-2.87231800	1.24692100	-0.94855200
H	-4.91799400	0.79193000	-0.39616100
C	-2.03442600	2.12559900	-1.65239500
H	-1.92939800	3.87214200	-2.89922100
P	-2.14000600	-0.16659200	-0.05167400
H	-0.95704300	1.99625400	-1.63451800
C	-3.14486600	-0.40506600	1.46178800
C	-2.39371600	-1.66295100	-1.08140400
Au	0.17225600	0.10867000	0.44200300
C	-4.21982000	-1.30581600	1.50871300
C	-2.84589400	0.37263800	2.59279900
C	-3.01480800	-1.60698000	-2.33629900
C	-1.91211700	-2.89492000	-0.60327200
C	-4.98430400	-1.42226500	2.67154400
H	-4.45877300	-1.91887800	0.64531300
C	-3.61590800	0.25594900	3.74916700
H	-2.01357300	1.07177200	2.56601400
C	-3.15544200	-2.76922600	-3.09966900
H	-3.38931800	-0.66331000	-2.71905700
C	-2.06311400	-4.05193300	-1.36509700
H	-1.43082500	-2.95032700	0.37038800
C	-4.68483300	-0.64320000	3.79039500
H	-5.81354700	-2.12313900	2.70091600
H	-3.37986900	0.86314100	4.61832900
C	-2.68310300	-3.98972800	-2.61716700
H	-3.63828800	-2.71669700	-4.07114900
H	-1.69783900	-5.00126800	-0.98371600
H	-5.28096300	-0.73743300	4.69340900
H	-2.79698900	-4.89113400	-3.21229300

4b

C	-3.52136100	-0.41111800	1.45304900
C	-3.31869400	-1.20692100	0.13553900
C	-4.28383700	-0.96401300	-0.99517300
C	-3.09578800	1.15686900	-0.24503300
C	-3.46998800	1.04311800	1.03262100
C	-4.71798600	-0.83622100	2.35229000
C	-4.60743500	-0.15821400	3.72963700
C	-6.11013100	-0.59827600	1.74773700
C	-2.91030400	-0.16493800	-0.92695700
C	-2.63464400	-2.54939400	0.32088300
C	-4.57109400	-1.94937500	-2.05609200
C	-5.73962200	-1.98964200	-2.70601400
C	-1.93287200	-0.24659100	-2.00558100
C	-1.25382100	-1.33469800	-2.52541200
O	-2.03981000	3.56185000	0.63381600
C	-2.41982200	3.45374500	-0.50521100
C	-2.43412400	4.53263400	-1.55490400
O	-2.92198900	2.28010500	-1.03301900
H	-2.62386200	-0.61078000	2.06330600
H	-5.11294700	-0.29165300	-0.79741400
H	-3.67609400	1.86674600	1.70144900
H	-4.60743500	-1.91825700	2.51594900
H	-5.36895100	-0.55110700	4.41170100
H	-3.62654000	-0.32947800	4.18882600
H	-4.76123700	0.92550000	3.65978900
H	-6.88332500	-0.85938900	2.47865600
H	-6.28780400	-1.21059600	0.85874800
H	-6.25713600	0.45463300	1.47696500
H	-3.15813900	-3.11301800	1.10177700
H	-2.63620300	-3.17730900	-0.57235700
H	-1.59680500	-2.42100500	0.65198900
H	-3.80758700	-2.68025700	-2.30948600
H	-5.93771700	-2.73602500	-3.46904400
H	-6.54162600	-1.28702400	-2.49202400
H	-1.77416900	0.70652100	-2.51126800
H	-0.75724100	-1.23294600	-3.48799500
H	-1.43749100	-2.34884300	-2.18718700
H	-3.46944900	4.77149300	-1.82227500
H	-1.93258400	4.19369100	-2.46663800
H	-1.94362400	5.42466300	-1.16492000
H	4.57754900	4.23391200	1.11240400
C	3.62636100	3.71151600	1.06979300
C	2.44160500	4.38222400	1.38141900

C	3.59456100	2.36719400	0.69581300
C	1.21739800	3.71101500	1.32059800
H	2.47176500	5.42986900	1.66674100
C	2.36718000	1.68774900	0.63659900
H	4.51861200	1.85452300	0.44769600
C	1.17772300	2.36779900	0.94800800
H	0.28782100	4.22406300	1.54462900
P	2.29449400	-0.08052000	0.19030500
H	0.21794500	1.85960500	0.90231100
C	3.82667500	-0.49092700	-0.71572300
C	2.29621600	-1.05227400	1.73775200
Au	0.39202800	-0.56334200	-1.11709500
C	4.92352000	-1.07725100	-0.06598800
C	3.91235400	-0.18230700	-2.08386600
C	2.65782800	-0.47392700	2.96336200
C	1.94693200	-2.41255400	1.68603600
C	6.09284200	-1.34647000	-0.78003400
H	4.86676000	-1.32688900	0.98875900
C	5.08412600	-0.45030100	-2.78919700
H	3.06596900	0.26929500	-2.59576300
C	2.67286000	-1.25286400	4.12249700
H	2.92327700	0.57706200	3.01642900
C	1.96937700	-3.18497900	2.84581600
H	1.66434000	-2.86776500	0.73961500
C	6.17446600	-1.03405900	-2.13806500
H	6.93784000	-1.80306200	-0.27327600
H	5.14427100	-0.20961500	-3.84643500
C	2.33076800	-2.60474700	4.06549900
H	2.95139500	-0.79984400	5.06934300
H	1.70217200	-4.23659600	2.79929200
H	7.08457000	-1.24838900	-2.69052000
H	2.34284300	-3.20637900	4.96960700
T _{S_{4b}}			
C	-3.11677000	-0.59012700	1.38804600
C	-3.05945100	-1.13566500	-0.07302300
C	-4.23653600	-0.84814000	-0.89619600
C	-2.76482200	1.25770300	-0.00834800
C	-3.17654500	0.91367900	1.21996900
C	-4.16394400	-1.24100900	2.33190500
C	-3.89830100	-0.80042100	3.78296600
C	-5.63003200	-0.98512900	1.95334300
C	-2.42273200	0.08818300	-0.87354800
C	-2.45867000	-2.53279400	-0.18573500
C	-4.64222800	-1.57144100	-2.06095500

C	-5.65915000	-1.14365400	-2.84311800
C	-2.12555700	0.29686600	-2.31379500
C	-1.82296900	-0.59420500	-3.27600800
O	-1.21225700	3.24463800	1.06519800
C	-1.87874500	3.47944800	0.08965400
C	-1.99828600	4.79717200	-0.62661900
O	-2.66054000	2.52791400	-0.54345000
H	-2.13009900	-0.82954900	1.82726400
H	-4.82555400	0.02319800	-0.63362400
H	-3.41505500	1.60533400	2.01666400
H	-3.99064600	-2.32603900	2.28890800
H	-4.55422300	-1.34209500	4.47255800
H	-2.86205300	-0.99675300	4.08189600
H	-4.09144700	0.26999100	3.92222900
H	-6.29320600	-1.43768000	2.69857200
H	-5.89374200	-1.41875700	0.98240000
H	-5.85452800	0.08798200	1.91769400
H	-3.16557000	-3.27443500	0.20354600
H	-2.21187200	-2.81262500	-1.21222700
H	-1.53993000	-2.59625100	0.40554300
H	-4.13740500	-2.49893500	-2.31325300
H	-5.99570900	-1.71551600	-3.70230000
H	-6.19491900	-0.22221000	-2.62811700
H	-2.16281500	1.34936100	-2.58998800
H	-1.64009900	-0.25674400	-4.29074600
H	-1.74228700	-1.66220300	-3.10062700
H	-3.03719400	5.14256300	-0.60025200
H	-1.71915700	4.68401700	-1.67920000
H	-1.35197500	5.53175100	-0.14614000
H	5.65135000	3.33071700	0.36547900
C	4.62365700	3.06498000	0.59523300
C	3.79588100	3.97189800	1.26193900
C	4.13280300	1.81563900	0.21507700
C	2.47201100	3.63145200	1.54855300
H	4.18163600	4.94533000	1.55100500
C	2.80303200	1.46878300	0.50705700
H	4.78025900	1.11997500	-0.30979900
C	1.97214700	2.38486700	1.17193100
H	1.81836400	4.33537600	2.05463300
P	2.14130000	-0.17413000	0.06613300
H	0.93606700	2.14007300	1.38459400
C	3.09960500	-0.78934300	-1.36391900
C	2.48665800	-1.30803000	1.46004900
Au	-0.14941100	-0.08392600	-0.39147700

C	4.24197000	-1.58494400	-1.18173200
C	2.70894300	-0.42272100	-2.66217800
C	3.27668200	-0.91683600	2.55003800
C	1.94197500	-2.60342700	1.42624800
C	4.98604400	-2.00005200	-2.28763600
H	4.54843900	-1.88354900	-0.18405900
C	3.45878400	-0.83819400	-3.76163600
H	1.81814700	0.18168900	-2.81244400
C	3.52029100	-1.81513900	3.59215700
H	3.69994700	0.08150600	2.58945500
C	2.19466500	-3.49629400	2.46528400
H	1.32741800	-2.91409400	0.58470500
C	4.59687300	-1.62739200	-3.57554900
H	5.86759200	-2.61712500	-2.14074700
H	3.15120900	-0.55178500	-4.76306900
C	2.98244600	-3.10167400	3.55133900
H	4.13147100	-1.50529100	4.43468900
H	1.77537600	-4.49765100	2.43086100
H	5.17623200	-1.95529600	-4.43370600
H	3.17392100	-3.79682300	4.36353500
T _{S1c}			
C	-4.70722500	0.36539000	0.63356300
C	-4.87050900	-0.88563600	-0.23144800
C	-4.41346200	-2.08159100	0.32022900
C	-2.80435700	-0.85878900	-0.06438200
C	-3.17524000	0.52910500	0.41868600
C	-5.66692600	1.58154500	0.53954100
C	-5.29882100	2.58152400	1.65361000
C	-5.82442600	2.31948100	-0.80239000
C	-1.76860400	-1.52523800	-0.51245900
C	-5.36448600	-0.83502300	-1.64640300
C	-4.29428700	-2.47449000	1.72552200
C	-4.10570900	-3.75596500	2.07282900
C	-1.69182100	-2.85198400	-1.13472100
C	-2.24008300	-3.18379700	-2.31236300
O	-2.88295800	1.46207600	-0.64039500
C	-1.95803900	2.43547400	-0.38339600
C	-1.76111600	3.32032800	-1.58638600
O	-1.40563100	2.56171400	0.68719900
H	-4.80451600	0.03954600	1.67415400
H	-4.31718000	-2.91022100	-0.37733000
H	-2.62501200	0.84704900	1.30769000
H	-6.65548500	1.17034900	0.79298500
H	-6.03122300	3.39405200	1.69241100

H	-5.28212100	2.10374100	2.64040800
H	-4.31353900	3.03194600	1.48443300
H	-6.56092000	3.12026100	-0.67465500
H	-6.19147000	1.67587800	-1.60468100
H	-4.89027000	2.77576700	-1.13564000
H	-4.88982100	-0.03397900	-2.21915300
H	-5.21079500	-1.78840900	-2.15806300
H	-6.44356500	-0.62995600	-1.63472700
H	-4.39477700	-1.72196900	2.50182400
H	-4.06193500	-4.05798100	3.11435500
H	-4.00134400	-4.54339000	1.33034900
H	-1.06573700	-3.57665900	-0.61478100
H	-2.08676600	-4.16962600	-2.74078400
H	-2.81327700	-2.47327400	-2.90174700
H	-0.77843700	3.79121100	-1.53034900
H	-2.52501800	4.10738100	-1.58191800
H	-1.86368400	2.75493400	-2.51531200
H	4.86427800	3.79767000	-2.11624600
C	4.02169600	3.52198700	-1.48874200
C	3.17034500	4.50625200	-0.98457100
C	3.79699600	2.17675900	-1.18721900
C	2.08627400	4.14558800	-0.17873300
H	3.34996200	5.55168200	-1.21875300
C	2.70991400	1.81188400	-0.37940200
H	4.46645200	1.41855600	-1.58023200
C	1.84928000	2.80399100	0.12016500
H	1.42200700	4.90746700	0.21943600
P	2.38923000	0.06739000	0.07618200
H	0.99389800	2.53679600	0.73337600
C	3.50448000	-0.96244000	-0.94842000
C	2.94317100	-0.12282200	1.81134600
Au	0.13210300	-0.63975000	-0.21307600
C	4.78138000	-1.33472900	-0.50078100
C	3.07305500	-1.36997500	-2.22164200
C	3.82647000	0.79080100	2.40635600
C	2.48994100	-1.22748000	2.55132800
C	5.61328200	-2.10071600	-1.31938300
H	5.12511800	-1.03463400	0.48421500
C	3.91070400	-2.13003000	-3.03732800
H	2.08189000	-1.09479100	-2.57388000
C	4.25175900	0.59638800	3.72200500
H	4.17804800	1.65362700	1.84967500
C	2.92183100	-1.41896400	3.86293700
H	1.79992500	-1.93711200	2.10159600

C	5.18077900	-2.49779800	-2.58616100
H	6.59853500	-2.38843100	-0.96420900
H	3.56921100	-2.44025800	-4.02059100
C	3.80192700	-0.50622800	4.45021400
H	4.93300500	1.30965900	4.17675200
H	2.56696600	-2.27602900	4.42793400
H	5.82994900	-3.09594300	-3.21903400
H	4.13272700	-0.65262900	5.47435500
2c			
C	-4.37211200	0.57878100	0.84159400
C	-5.14882900	-0.52320900	0.23117900
C	-4.23753600	-1.60112800	-0.18453700
C	-2.83870700	-0.99209400	-0.18866000
C	-2.99531600	0.48788200	0.10375400
C	-5.04924900	1.93092300	1.18167700
C	-4.14279000	2.75558100	2.11255100
C	-5.48973600	2.77374700	-0.02956800
C	-1.67727900	-1.64810200	-0.38717400
C	-6.60774500	-0.56135900	0.06185200
C	-4.46161800	-2.59972100	0.97692400
C	-5.11692800	-3.75661500	0.85214800
C	-1.67234200	-3.07500500	-0.76397300
C	-2.19431200	-3.57706300	-1.89358600
O	-3.08783000	1.18972700	-1.16213700
C	-2.24145300	2.23996300	-1.37353600
C	-2.30872300	2.70319600	-2.80526100
O	-1.53607700	2.71202100	-0.50866000
H	-4.12129200	0.11453400	1.82494400
H	-4.56522300	-2.09026900	-1.10803200
H	-2.18573900	0.92353000	0.68612300
H	-5.95386600	1.67324800	1.75157300
H	-4.65888400	3.66920500	2.42406700
H	-3.87830500	2.19818700	3.01931700
H	-3.21617600	3.04942000	1.60794100
H	-6.14683200	3.57916300	0.31414900
H	-6.04086500	2.19902900	-0.78140700
H	-4.63507000	3.23803800	-0.52626100
H	-6.83763500	0.10259900	-0.79003800
H	-6.98251700	-1.55991000	-0.16799900
H	-7.14009100	-0.13160700	0.91784700
H	-3.99645600	-2.31207200	1.91696400
H	-5.17851600	-4.45019200	1.68609500
H	-5.57342800	-4.07361700	-0.08188900
H	-1.12146500	-3.74275700	-0.09968000

H	-2.09490300	-4.62917500	-2.14461400
H	-2.68325600	-2.94187500	-2.62929700
H	-1.76954000	1.98846400	-3.43792700
H	-1.83915900	3.68336300	-2.89465800
H	-3.34305500	2.74085700	-3.15795000
H	5.19310000	3.05206100	-2.76557400
C	4.24220100	2.91083700	-2.25973900
C	3.25487900	3.89512300	-2.33444000
C	4.01320400	1.73938800	-1.53489900
C	2.03154900	3.70580500	-1.68641400
H	3.43735500	4.80530200	-2.89884100
C	2.78659600	1.54645700	-0.88180300
H	4.78660300	0.97957000	-1.48302200
C	1.79210400	2.53477100	-0.96812300
H	1.25721900	4.46572600	-1.74155500
P	2.43292500	0.04727500	0.11082100
H	0.83147200	2.39497700	-0.48080000
C	3.70296800	-1.19245800	-0.34986100
C	2.77570900	0.50135000	1.85521900
Au	0.20341000	-0.80432700	-0.17773100
C	4.91652400	-1.30767300	0.34543600
C	3.45255700	-2.03737000	-1.44386300
C	3.54439300	1.62414500	2.19594100
C	2.26059500	-0.31629400	2.87487100
C	5.86550900	-2.25069300	-0.05373100
H	5.11920800	-0.66844900	1.19916000
C	4.40612700	-2.97408900	-1.84161400
H	2.51136800	-1.96334500	-1.98300200
C	3.79856500	1.91844700	3.53727800
H	3.94014400	2.27063800	1.41895200
C	2.52292200	-0.02196800	4.21229500
H	1.65501100	-1.18267600	2.62014300
C	5.61284900	-3.08263600	-1.14615100
H	6.80090600	-2.33582600	0.49191000
H	4.20384500	-3.62282100	-2.68901700
C	3.29116500	1.09684000	4.54512800
H	4.39286400	2.79121700	3.79231800
H	2.12386400	-0.66202700	4.99410500
H	6.35231700	-3.81713000	-1.45218800
H	3.49049800	1.32879400	5.58748300
Ts _{2c}			
C	4.23553500	-0.77664100	1.09157600
C	4.97339900	0.53697800	0.99019000
C	4.24472800	1.51338200	0.33537600

C	2.79303000	0.87318600	-0.00263200
C	2.97217100	-0.62026200	0.21386000
C	5.08582500	-2.07608100	1.01118300
C	4.22951900	-3.31671200	1.31180500
C	5.90245100	-2.24015500	-0.28212200
C	1.68438200	1.54479400	-0.41924500
C	6.23405100	0.76342700	1.75010000
C	4.50273900	2.97396600	0.36283000
C	5.63552200	3.54853300	-0.04943600
C	1.72527600	2.85655100	-1.06312600
C	2.45173400	3.14018000	-2.15882400
O	3.17045500	-1.20527200	-1.10137500
C	2.19924800	-2.03889900	-1.57782200
C	2.49633900	-2.45315700	-2.99563600
O	1.23538100	-2.37820500	-0.92743700
H	3.85438100	-0.74566900	2.13053100
H	3.91132500	1.13149000	-0.77416400
H	2.09082600	-1.08095700	0.65653400
H	5.80946200	-1.98482500	1.83320000
H	4.86135800	-4.21019200	1.35032100
H	3.72166100	-3.22848500	2.27961500
H	3.46353900	-3.48530200	0.54768600
H	6.60562300	-3.07210600	-0.16795100
H	6.49032200	-1.34439500	-0.51611300
H	5.26627500	-2.45249600	-1.14338500
H	7.07387500	0.25924400	1.25144200
H	6.47735200	1.82306400	1.84033000
H	6.16288800	0.31934300	2.75100400
H	3.70153600	3.58276700	0.77515400
H	5.78371900	4.62018500	0.04251000
H	6.44616900	2.98105600	-0.49956800
H	1.02139300	3.60110700	-0.69200100
H	2.38184000	4.10723300	-2.64717700
H	3.09256400	2.40120800	-2.63507600
H	2.34183900	-1.59830500	-3.66408300
H	1.82518400	-3.26200400	-3.28586400
H	3.53787400	-2.76995300	-3.10198200
H	-5.73402600	-2.01748600	-3.04456400
C	-4.72413700	-2.06339400	-2.64731700
C	-3.83082700	-3.03146800	-3.10979900
C	-4.32318900	-1.14773900	-1.67281700
C	-2.53163000	-3.08302700	-2.59855900
H	-4.14541500	-3.74206600	-3.86884200
C	-3.01893700	-1.19750500	-1.15712000

H	-5.02313500	-0.39663200	-1.32057800
C	-2.11948500	-2.16807100	-1.62968500
H	-1.83371900	-3.83431800	-2.95711900
P	-2.45819200	-0.03848300	0.14512000
H	-1.10360000	-2.21381300	-1.24692900
C	-3.64699500	1.35612300	0.14950500
C	-2.66640800	-0.90548500	1.74590200
Au	-0.22009300	0.74439500	-0.16719800
C	-4.75179000	1.38808700	1.01353400
C	-3.44905900	2.41012000	-0.75789400
C	-3.47256200	-2.04633300	1.87057800
C	-2.01126700	-0.39503700	2.87913200
C	-5.64670600	2.45894800	0.96477900
H	-4.91257200	0.58429500	1.72516100
C	-4.34941200	3.47349600	-0.80692300
H	-2.59109600	2.39715100	-1.42575400
C	-3.62349400	-2.66340900	3.11423200
H	-3.97749800	-2.45523900	1.00119400
C	-2.17066900	-1.01132900	4.11942700
H	-1.37897800	0.48518200	2.79013000
C	-5.44820200	3.49979800	0.05595900
H	-6.49795100	2.47851300	1.63913000
H	-4.19034200	4.28336900	-1.51305700
C	-2.97576200	-2.14752800	4.23783000
H	-4.24711900	-3.54832200	3.20228900
H	-1.66399200	-0.60820500	4.99164400
H	-6.14549300	4.33193100	0.02222200
H	-3.09503600	-2.63053400	5.20341300
3c			
C	-3.83133900	-0.59108800	1.40019200
C	-3.39123100	-1.85559300	0.67962100
C	-2.91139000	-1.61262400	-0.56223300
C	-2.94725400	-0.10376400	-0.86955900
C	-3.10415400	0.48536000	0.56114300
C	-5.38072900	-0.50429000	1.58365300
C	-5.78914500	0.56866700	2.60701800
C	-6.17086300	-0.36701700	0.27303900
C	-1.72752300	0.42809800	-1.54828400
C	-3.52577100	-3.19058900	1.35074800
C	-2.45619000	-2.56576800	-1.58152200
C	-3.00232200	-3.76196200	-1.84401600
C	-1.80668500	0.87737100	-2.91818900
C	-2.70034200	0.38744500	-3.80680100
O	-3.77194400	1.76111300	0.56756500

C	-3.16658400	2.75702800	-0.09723200
C	-3.88556000	4.06910400	0.04568100
O	-2.13810900	2.59601400	-0.74454300
H	-3.40964900	-0.58115500	2.41515000
H	-3.85092800	0.13994100	-1.44635300
H	-2.10336700	0.64128200	0.97465000
H	-5.65498600	-1.47363200	2.02403800
H	-6.86247700	0.50044400	2.81643100
H	-5.25810900	0.43498400	3.55715600
H	-5.58165900	1.57813600	2.24174600
H	-7.24322000	-0.47612000	0.46796100
H	-5.88929000	-1.13647300	-0.45490200
H	-6.02207500	0.61635900	-0.18643000
H	-4.55620300	-3.56766800	1.30633400
H	-2.88320200	-3.94186500	0.88296500
H	-3.26580000	-3.11454600	2.41379800
H	-1.60639600	-2.24673900	-2.18640300
H	-2.58790700	-4.40938200	-2.61127600
H	-3.88233000	-4.12715600	-1.32313400
H	-1.01166600	1.52916800	-3.27163800
H	-2.62209600	0.62834800	-4.86334500
H	-3.47841200	-0.31664200	-3.52824800
H	-4.92178800	3.96627200	-0.29279600
H	-3.37603000	4.83495800	-0.53917600
H	-3.91377100	4.36227400	1.10050400
H	6.43187400	2.80023900	-0.25301900
C	5.35662100	2.79219300	-0.10026300
C	4.66187300	3.99289300	0.05892300
C	4.67261300	1.57573200	-0.06898600
C	3.27755200	3.98005600	0.24707000
H	5.19710600	4.93756100	0.03051000
C	3.28245700	1.55661700	0.12410700
H	5.21910200	0.64699100	-0.20118600
C	2.58791200	2.76843400	0.27542100
H	2.73377000	4.91292900	0.36379100
P	2.34546700	-0.01340900	0.20945500
H	1.50913600	2.76487500	0.41138500
C	3.34444000	-1.27647200	-0.66114600
C	2.28858800	-0.50952800	1.97158200
Au	0.14515000	0.21242100	-0.72352700
C	4.24263600	-2.10906400	0.02345100
C	3.21829900	-1.39199100	-2.05553800
C	3.17592200	0.01871000	2.92089700
C	1.33505700	-1.46163000	2.37054800

C	5.00937400	-3.03828900	-0.68236300
H	4.34110600	-2.03758600	1.10220100
C	3.98984500	-2.31871900	-2.75526500
H	2.51743000	-0.75723900	-2.59237800
C	3.11276600	-0.40642800	4.24967200
H	3.91117300	0.76165000	2.62821700
C	1.28180700	-1.88735100	3.69705100
H	0.63661900	-1.86999000	1.64385200
C	4.88538800	-3.14308000	-2.06898400
H	5.70148200	-3.68133700	-0.14656200
H	3.88801600	-2.40139500	-3.83341300
C	2.16956700	-1.35910000	4.63835700
H	3.80146800	0.00893600	4.97957600
H	0.54556900	-2.62745200	3.99722800
H	5.48194100	-3.86883100	-2.61401800
H	2.12334800	-1.68746100	5.67264300
Ts _{3c}			
C	-5.03231200	1.16406300	-0.48224100
C	-3.91236400	2.15204500	-0.71822700
C	-2.67421100	1.58329700	-0.67143500
C	-2.80782700	0.11652100	-0.53328100
C	-4.31103300	-0.20525500	-0.64497000
C	-5.80651300	1.47010000	0.84398800
C	-7.12910700	0.69490900	0.95373400
C	-4.95855500	1.34051200	2.11889800
C	-1.75209300	-0.85052400	-0.52910800
C	-4.22516900	3.58414800	-1.01298600
C	-1.38993900	2.26786700	-0.87424700
C	-1.01823700	3.40321100	-0.26777900
C	-2.11419800	-2.25937700	-0.75046100
C	-1.28709800	-3.28954400	-0.50635900
O	-4.68688700	-1.19209400	0.32451400
C	-5.35989900	-2.30322700	-0.12729400
C	-5.73775700	-3.19947000	1.02123600
O	-5.58249300	-2.50487700	-1.29719400
H	-5.77148200	1.26937200	-1.28826400
H	-2.38348800	-0.30167300	0.58421600
H	-4.52088900	-0.61056500	-1.63964800
H	-6.08416000	2.52909600	0.74693900
H	-7.73075000	1.09865100	1.77545300
H	-7.72229900	0.78007400	0.03591200
H	-6.96820900	-0.36667300	1.15852000
H	-5.52782000	1.69910500	2.98340300
H	-4.04011100	1.93686900	2.06308300

H	-4.68213000	0.29993300	2.31406900
H	-4.51742900	4.11906100	-0.09915800
H	-3.36865800	4.10865100	-1.44264400
H	-5.07639400	3.65543000	-1.70082900
H	-0.71503300	1.81446700	-1.60017800
H	-0.06927500	3.87659900	-0.49889400
H	-1.63646000	3.88479300	0.48529300
H	-3.07551000	-2.47476300	-1.21050900
H	-1.58137700	-4.30876900	-0.74040000
H	-0.30199800	-3.14813800	-0.07070200
H	-4.85250800	-3.44711400	1.61568000
H	-6.19713700	-4.10876500	0.63309100
H	-6.44275100	-2.68650400	1.68407800
H	6.54347800	-2.44624300	-1.79740300
C	5.56819100	-2.01448300	-2.00226200
C	5.03645800	-2.06383400	-3.29253300
C	4.84856600	-1.41407000	-0.96794200
C	3.77877700	-1.51350000	-3.55129100
H	5.59851800	-2.53450400	-4.09389300
C	3.58516900	-0.85780100	-1.22180300
H	5.26815100	-1.38650700	0.03281400
C	3.05280300	-0.91717300	-2.52059100
H	3.35973700	-1.55458900	-4.55240900
P	2.61607300	-0.03042200	0.09356200
H	2.06998700	-0.49976700	-2.72570400
C	3.21606200	-0.68890300	1.69411000
C	3.09631400	1.73906900	0.07258200
Au	0.27388000	-0.38379100	-0.21943800
C	4.26992900	-0.07544300	2.38964300
C	2.62695600	-1.85019100	2.21980500
C	4.13386300	2.21826900	-0.73941900
C	2.40726900	2.62980900	0.91322200
C	4.72842200	-0.62218800	3.58938700
H	4.72785700	0.82898200	2.00140400
C	3.09097300	-2.39423700	3.41691700
H	1.80482500	-2.32786100	1.69328600
C	4.47920800	3.57171800	-0.70692700
H	4.67242300	1.54155700	-1.39471000
C	2.76379300	3.97710300	0.94915200
H	1.59686700	2.26970500	1.54176800
C	4.14147700	-1.78020700	4.10323300
H	5.54255000	-0.14030400	4.12282500
H	2.62910300	-3.29233600	3.81656700
C	3.79889400	4.45033700	0.13674800

H	5.28312700	3.93549800	-1.34012000
H	2.23449700	4.65765300	1.61011600
H	4.49848800	-2.20121300	5.03860000
H	4.07281400	5.50104300	0.16295200
4c			
C	-4.06769200	-0.39862400	1.14588800
C	-3.73825300	-1.82556200	0.74517800
C	-2.99963200	-1.87090700	-0.39694300
C	-2.64637800	-0.51478200	-0.84229300
C	-3.04058000	0.41142100	0.29574800
C	-5.59203600	-0.09116200	0.97502900
C	-6.02939400	1.20071900	1.68460500
C	-6.08192000	-0.12669500	-0.48041100
C	-2.02988800	-0.22002000	-2.01114900
C	-4.20505500	-2.97812000	1.57901900
C	-2.50861100	-3.06637100	-1.09627800
C	-3.19611100	-4.19363300	-1.31901100
C	-1.57220200	1.07404400	-2.48140200
C	-0.96008900	1.25850800	-3.66365900
O	-3.51650200	1.69089300	-0.17537300
C	-3.12576500	2.79359300	0.51803900
C	-3.67142400	4.04481700	-0.12967900
O	-2.43829700	2.76402900	1.51384300
H	-3.84694700	-0.25135800	2.21275500
H	-1.84248400	-1.04983900	-2.69251000
H	-2.16743200	0.61089800	0.92465600
H	-6.09397700	-0.91321400	1.50689400
H	-7.12364300	1.25177500	1.73544000
H	-5.64454900	1.24716100	2.71023800
H	-5.68668100	2.09327500	1.15430800
H	-7.17248300	-0.01555400	-0.51383600
H	-5.82730000	-1.07272200	-0.96955000
H	-5.64175900	0.68424100	-1.06838300
H	-5.27088300	-3.19612000	1.42025400
H	-3.64796800	-3.89122600	1.35062600
H	-4.09058400	-2.75132400	2.64729500
H	-1.48771200	-2.99926100	-1.47407700
H	-2.74279200	-5.03532000	-1.83537300
H	-4.23296100	-4.30988400	-1.01621000
H	-1.72610200	1.93066000	-1.83223100
H	-0.61690200	2.23802200	-3.98251100
H	-0.78331800	0.43238000	-4.34927200
H	-3.41215100	4.07009600	-1.19268300
H	-3.26727000	4.92095300	0.37849800

H -4.76485500 4.05523700 -0.06215600

S1-2 Cartesian coordinates of some key stationary points in Figure 3

1-2			
C	-4.65003300	-0.82815200	0.98430600
C	-4.46103000	-2.14511600	0.22525500
C	-4.94893000	-2.33343300	-1.02001100
C	-2.51240200	0.06193900	-0.10798900
C	-3.24156400	-0.16400300	1.16546700
C	-5.81325400	0.09742600	0.50051400
C	-6.48655100	0.82314200	1.68146000
C	-5.47205800	1.10790000	-0.60827700
C	-2.23371200	0.26868600	-1.29263300
C	-3.68208400	-3.20353300	0.97740000
C	-4.80851900	-3.51534500	-1.86125100
C	-5.31090100	-3.59416600	-3.10512300
C	-2.08637500	0.52840400	-2.69146900
C	-2.58146500	-0.29035400	-3.63371300
O	-3.38943400	1.08070700	1.88079000
C	-2.38271300	1.42048900	2.73401200
C	-2.71002300	2.69064700	3.47342300
O	-1.37055900	0.76432200	2.85493700
H	-4.90707800	-1.11117300	2.01567200
H	-5.51068100	-1.52640300	-1.48442500
H	-2.63576900	-0.82411900	1.78866800
H	-6.56783100	-0.59001400	0.09897000
H	-7.38268900	1.35054800	1.33577800
H	-6.79993400	0.11576800	2.45840500
H	-5.81902600	1.55879800	2.13872600
H	-6.38374600	1.63190500	-0.91662400
H	-5.04802200	0.63825900	-1.50113100
H	-4.76465900	1.86564100	-0.25538400
H	-4.00701000	-3.25386200	2.02456400
H	-3.80907600	-4.19981000	0.54968000
H	-2.60237400	-2.99384300	0.99029800
H	-4.26387400	-4.37005500	-1.46654000
H	-5.19162000	-4.48531100	-3.71339800
H	-5.87326700	-2.77425900	-3.54731400
H	-1.56716200	1.44469900	-2.95933600
H	-2.48043400	-0.03814400	-4.68477000
H	-3.09879600	-1.21285500	-3.38625800
H	-2.78234400	3.52373200	2.76598300
H	-1.92977200	2.89653300	4.20657800

H	-3.67974600	2.60060500	3.97258900
H	0.33033300	-5.78902500	-0.58708300
C	1.17250900	-5.14815700	-0.87477900
C	0.98674700	-3.75603400	-0.24417500
C	1.29522600	-5.07359900	-2.40204100
H	2.07552100	-5.61500800	-0.45567600
C	2.13775500	-2.80525800	-0.64882200
H	0.92351300	-3.85860900	0.84245900
H	0.03301400	-3.32456400	-0.58010400
C	2.40764900	-4.10235000	-2.81780200
H	0.33948900	-4.73413200	-2.82757100
H	1.48539600	-6.07057300	-2.81623400
P	1.99226200	-1.12767200	0.19219500
C	2.21583100	-2.71130000	-2.18826900
H	3.07474500	-3.24334000	-0.27824300
H	2.44270100	-4.00262400	-3.90917400
H	3.38293900	-4.50722800	-2.51100500
Au	-0.17774800	-0.30416100	-0.16199900
C	3.38176500	-0.07713400	-0.43491200
C	2.34405600	-1.35230900	2.02903000
H	1.28234000	-2.27029000	-2.56372700
H	3.02769400	-2.04824100	-2.50052400
C	3.32996000	1.32844000	-0.64166500
C	4.59283600	-0.75685500	-0.68152500
C	3.57767200	-2.24636400	2.37948000
C	1.08808900	-1.74680100	2.84787000
H	2.59471000	-0.32741800	2.31687400
C	2.12857700	2.23046800	-0.47585700
C	4.50699200	1.96761700	-1.07254800
C	5.73946900	-0.09584900	-1.11254700
H	4.64849600	-1.83111900	-0.54753800
C	3.17517400	-3.57758300	3.03144200
H	4.21479500	-2.42998300	1.50948800
H	4.20677100	-1.68524000	3.08159700
C	1.49927900	-2.09484700	4.28729900
H	0.57381300	-2.60600100	2.40162500
H	0.37285500	-0.91905300	2.84359800
C	1.34758000	2.55464500	-1.63174000
C	1.86314200	2.90714100	0.74643300
C	5.69577600	1.28250200	-1.30690000
H	4.47683500	3.04326000	-1.21470600
H	6.65192400	-0.65594400	-1.29335800
C	2.39013900	-3.35953800	4.34379600
H	2.56948700	-4.16080700	2.32608200

H	4.07294900	-4.17653400	3.22191800
H	0.60489000	-2.22887700	4.90567600
H	2.03521100	-1.23581600	4.71274600
C	0.27624400	3.44658800	-1.49705200
C	1.62569800	2.14653800	-3.09444400
C	0.78116800	3.80587600	0.79209400
C	2.64598100	2.87456400	2.08235400
H	6.57789700	1.82268500	-1.63815200
H	1.77596100	-4.24517300	4.54490400
H	3.08899000	-3.27477900	5.18423400
C	-0.03656600	4.08522500	-0.29506500
H	-0.29991900	3.69217800	-2.38686000
H	0.67336700	2.33202200	-3.60887800
C	2.64305100	3.09832600	-3.76292800
C	1.97060900	0.68373600	-3.40554400
H	0.59793900	4.33758300	1.72353200
C	4.07851300	2.32223700	2.12856400
C	1.79167300	2.25503200	3.21118100
H	2.75008300	3.93767000	2.34173600
C	-1.17008000	5.09648800	-0.19019800
H	2.66542200	2.92079200	-4.84466000
H	2.37591300	4.14715600	-3.59691700
H	3.65556700	2.93853000	-3.38167000
H	1.88950400	0.52003300	-4.48685200
H	1.27437500	-0.00276300	-2.91343100
H	2.98716800	0.41547900	-3.11198400
H	4.48388200	2.50500300	3.13040100
H	4.73610300	2.82106500	1.41302700
H	4.14123700	1.24641200	1.94329900
H	0.83802300	2.77553100	3.33198700
H	1.54815900	1.20796100	3.01547300
H	2.32939300	2.30995900	4.16479200
C	-0.87854900	6.36116700	-1.02194700
C	-2.53278900	4.48915400	-0.57339900
H	-1.22909500	5.40360600	0.86321700
H	0.07032700	6.82041100	-0.72546400
H	-0.81917700	6.12877000	-2.09185800
H	-1.67378000	7.10287300	-0.88599900
H	-3.33547000	5.21987100	-0.42226600
H	-2.76081800	3.60136800	0.02804100
H	-2.55586500	4.19208800	-1.62884100
Ts _{1a}			
C	-3.95391500	-2.39593000	0.04603300
C	-4.52083400	-1.69540500	-1.17786700

C	-2.71325200	-0.57983400	-1.56183900
C	-4.92358200	-0.36893100	-1.08407300
C	-2.06718200	-0.87113700	-0.46330100
C	-2.81862500	-1.54958700	0.67301300
C	-5.03050200	-2.99063300	1.01230000
C	-4.35608400	-3.76180600	2.16012500
C	-6.08121800	-2.00571500	1.54851000
C	-4.84987900	-2.56418200	-2.36457100
C	-5.65823300	0.38346000	-2.08574800
C	-6.12145500	1.62263800	-1.84335100
C	-2.61990600	-0.09057200	-2.91402300
C	-1.83267200	-0.66598500	-3.83753000
O	-3.31891600	-0.53444400	1.57835700
C	-2.56524500	-0.27613500	2.69102200
C	-3.18282300	0.81869000	3.52228400
O	-1.53419000	-0.85582100	2.94480500
H	-3.41494000	-3.27171000	-0.34058500
H	-4.77089100	0.13702200	-0.13561800
H	-2.15448600	-2.19184800	1.25002200
H	-5.57082400	-3.73213700	0.40599500
H	-5.10762400	-4.31137900	2.73645000
H	-3.62761900	-4.49139900	1.78638000
H	-3.83688600	-3.09152600	2.85453500
H	-6.81389700	-2.55051800	2.15384600
H	-6.63317700	-1.50926600	0.74278900
H	-5.63315700	-1.23390600	2.17992800
H	-4.06507000	-3.30827800	-2.53232800
H	-5.78138300	-3.11349900	-2.16959100
H	-4.98493700	-2.00054100	-3.28955900
H	-5.87511000	-0.08805700	-3.04018300
H	-6.71017100	2.16179700	-2.57911600
H	-5.93795500	2.12642200	-0.89799100
H	-3.21442300	0.78297200	-3.17300000
H	-1.74772800	-0.24803100	-4.83645300
H	-1.23685500	-1.54533000	-3.61141500
H	-2.92438300	1.78797300	3.08034700
H	-2.77661700	0.77494900	4.53384400
H	-4.27270400	0.73895100	3.54525200
Au	0.00192000	-0.59667400	-0.29721800
H	-1.75550300	6.40868300	0.93662100
C	-2.56442900	5.82389300	0.48654100
C	-2.51852400	4.35726400	0.95918200
H	-2.46022000	5.89185500	-0.60292600
H	-3.51706700	6.29077400	0.76267600

C	-1.16956100	3.71890400	0.65732000
C	-3.69331300	3.55514900	0.37088200
H	-2.63600700	4.36207800	2.05195600
C	-0.74844900	3.45704400	-0.64699300
C	-0.26614200	3.44092500	1.67465000
H	-4.64895400	4.00602300	0.66507700
H	-3.67860000	2.51550600	0.71924600
H	-3.65544800	3.54191600	-0.72485300
C	0.52138300	2.95131800	-0.95194200
H	-1.40981300	3.70318300	-1.47472400
C	1.01480400	2.90247500	1.45437500
H	-0.54855800	3.68477000	2.69715200
C	0.83017100	2.95738000	-2.46413800
C	1.41294000	2.62181100	0.11783700
C	1.80962800	2.75126900	2.77339900
H	-0.16050200	2.95869400	-2.93678400
C	1.50027100	4.28079600	-2.89700000
C	1.56341000	1.75759600	-3.07745500
C	2.82901900	2.20351300	-0.21382700
C	3.34213600	2.64466900	2.75015900
C	1.19276700	1.63377000	3.64656000
H	1.60690400	3.68981300	3.30819300
H	1.52395200	4.34816500	-3.99132500
H	0.95170900	5.14858200	-2.51557400
H	2.53219400	4.34536400	-2.54001500
H	1.48102900	1.81020100	-4.17017400
H	1.11532500	0.81267700	-2.75435200
H	2.62729000	1.74007900	-2.83339600
C	3.71846700	3.27229200	-0.43201500
C	3.33781900	0.88200100	-0.34483400
H	3.70299900	2.66831700	3.78506300
H	3.80285700	3.48282600	2.22189300
H	3.71370700	1.72322900	2.29518400
H	0.14545000	1.84160900	3.88509600
H	1.20969900	0.66372900	3.14340300
H	1.73926500	1.54166700	4.59243800
C	5.05420600	3.08566500	-0.77630300
H	3.33629900	4.28173400	-0.31584100
C	4.69252800	0.71326800	-0.69746900
P	2.36833200	-0.67236900	-0.04908000
C	5.54682300	1.79085700	-0.91414600
H	5.70012600	3.94444000	-0.93487100
H	5.09795100	-0.28406100	-0.82107500
C	3.05906600	-1.96584900	-1.23295400

C	2.84862400	-1.18610000	1.70241200
H	6.58294900	1.61440000	-1.18734200
C	3.01523800	-1.51133600	-2.70801100
C	2.33225800	-3.32318000	-1.08343800
H	4.10859400	-2.12225000	-0.95008100
C	4.32149300	-1.66918000	1.90587500
C	1.82357100	-2.14719500	2.35584200
H	2.74898100	-0.23240700	2.22775400
C	3.62700800	-2.57287600	-3.63847900
H	1.96828500	-1.34037700	-2.99434700
H	3.53674000	-0.55875400	-2.83887300
C	2.93648300	-4.38616000	-2.01875800
H	2.38179500	-3.68310600	-0.05226700
H	1.26726100	-3.18641300	-1.31862100
C	4.40875300	-3.15389300	2.28994600
H	4.94519000	-1.47356900	1.02868800
H	4.76498100	-1.07121300	2.71205100
C	2.34899700	-2.61078100	3.72391300
H	1.63726700	-3.02209300	1.72316000
H	0.86031100	-1.63920700	2.46909900
C	2.93152300	-3.93147500	-3.48362600
H	3.56523900	-2.22495500	-4.67677600
H	4.69728800	-2.68153000	-3.41026500
H	2.38117400	-5.32522500	-1.90518600
H	3.96937000	-4.59646000	-1.70548600
C	3.64118300	-3.45663000	3.59390500
H	4.00964500	-3.76650600	1.47157800
H	5.46089300	-3.44311500	2.39487700
H	1.57051200	-3.17808900	4.24592400
H	2.54073700	-1.72233700	4.34048700
H	1.89223000	-3.84941400	-3.83552700
H	3.41680500	-4.68364700	-4.11678700
H	3.39865700	-4.52545700	3.62596000
H	4.28959000	-3.26474000	4.45712300
2a-2			
C	-4.01791900	-2.40270900	0.42461800
C	-4.21273800	-2.02603400	-1.04831400
C	-2.80296600	-1.35494500	-1.48251000
C	-4.35564700	-0.60229400	-1.30317800
C	-2.03013000	-1.15676200	-0.33450600
C	-2.83453200	-1.52429300	0.91283700
C	-5.30238900	-2.51367900	1.28874300
C	-4.95259500	-2.96462100	2.71776800
C	-6.21890100	-1.27885200	1.30039300

C	-4.80618500	-3.07734100	-1.96269600
C	-4.91329500	-0.02094900	-2.52835200
C	-5.32786200	1.25315300	-2.57915200
C	-2.27336600	-1.40947700	-2.86829700
C	-1.33247100	-2.27920900	-3.24968900
O	-3.23591000	-0.29929200	1.57256900
C	-2.53031900	0.05343700	2.69590300
C	-3.04276300	1.34691000	3.27157900
O	-1.61338500	-0.60113700	3.13406700
H	-3.59174300	-3.41670000	0.40468300
H	-4.34328300	0.06727700	-0.45079200
H	-2.20195300	-2.07119400	1.61469400
H	-5.88035100	-3.33083800	0.83285500
H	-5.86605000	-3.17942800	3.28222700
H	-4.34274700	-3.87591700	2.71580900
H	-4.40168200	-2.19268800	3.26633400
H	-7.11383900	-1.49435200	1.89436000
H	-6.55944200	-1.00622300	0.29502200
H	-5.72644800	-0.40863900	1.74328100
H	-4.29611300	-4.03494100	-1.81754200
H	-5.86713300	-3.21865400	-1.72565200
H	-4.72696700	-2.81882700	-3.02053000
H	-5.05259900	-0.66517800	-3.39138800
H	-5.80896900	1.65443800	-3.46589600
H	-5.21568300	1.92685000	-1.73411700
H	-2.67304200	-0.70601000	-3.59501200
H	-0.95394200	-2.28548800	-4.26774200
H	-0.91083900	-3.00919400	-2.56363700
H	-2.58507400	2.17800000	2.72260500
H	-2.74821600	1.41440100	4.31997300
H	-4.12784700	1.42906000	3.17295100
Au	-0.04722200	-0.70614500	-0.19717400
H	-1.71600200	6.58568200	0.36841500
C	-2.55723300	6.01218400	-0.03448800
C	-2.59327300	4.58847800	0.55743400
H	-2.44991700	5.98173900	-1.12531600
H	-3.48173300	6.55328100	0.19830900
C	-1.27766700	3.86200600	0.30854200
C	-3.81560400	3.81265400	0.03674100
H	-2.70584000	4.68953800	1.64594400
C	-0.90257600	3.40990500	-0.95688200
C	-0.34935700	3.70243100	1.33066400
H	-4.74229600	4.33366200	0.30331300
H	-3.85642600	2.80174200	0.46023000

H	-3.79014700	3.72313300	-1.05581000
C	0.35243300	2.84658400	-1.22564500
H	-1.58415300	3.55178500	-1.79254600
C	0.91761900	3.11935300	1.14934900
H	-0.59779100	4.08523000	2.31913600
C	0.61006300	2.63469200	-2.73203300
C	1.27788600	2.66424800	-0.15038600
C	1.74007600	3.10889200	2.45932900
H	-0.39505700	2.53578800	-3.16240400
C	1.22161500	3.89881800	-3.37734700
C	1.36759300	1.38145400	-3.18780600
C	2.69758000	2.24290300	-0.46628100
C	3.27267000	3.00796600	2.41742300
C	1.13957100	2.08078900	3.44763600
H	1.54261400	4.09488200	2.90216700
H	1.21931600	3.80072300	-4.46951600
H	0.65126000	4.79649400	-3.11611900
H	2.25806900	4.04928500	-3.06100000
H	1.24874500	1.26860300	-4.27241500
H	0.96541000	0.48028300	-2.71398700
H	2.43830300	1.43583500	-2.98206900
C	3.54272500	3.30725900	-0.83415600
C	3.25296600	0.93451200	-0.44449500
H	3.65283600	3.14709500	3.43614900
H	3.71630600	3.78616000	1.79159900
H	3.64298100	2.04491200	2.05878700
H	0.11009600	2.33945000	3.71398300
H	1.10807700	1.07313600	3.02386500
H	1.72454400	2.04859800	4.37417300
C	4.87993200	3.12801100	-1.17611800
H	3.12369200	4.30877700	-0.83838200
C	4.60990200	0.77339700	-0.79307300
P	2.34583100	-0.61008500	0.04549600
C	5.42078600	1.84538800	-1.15546900
H	5.48984500	3.98308600	-1.45298500
H	5.05257600	-0.21580800	-0.79632000
C	3.09148000	-2.00503200	-0.98273200
C	2.85182400	-0.89401500	1.84125900
H	6.46013500	1.67359500	-1.41910600
C	3.05391200	-1.72130400	-2.50037300
C	2.40511300	-3.36140000	-0.69304300
H	4.14095100	-2.09589600	-0.67140800
C	4.34255100	-1.28662200	2.08995800
C	1.87044500	-1.82044100	2.60581800

H	2.71147100	0.10844800	2.25391300
C	3.72128200	-2.85718000	-3.29530700
H	2.00695200	-1.62504300	-2.81875200
H	3.54135400	-0.77044900	-2.73346700
C	3.06445100	-4.50113700	-1.49071400
H	2.44065500	-3.59996500	0.37314500
H	1.34175300	-3.28949100	-0.96266300
C	4.50108000	-2.73620800	2.57261300
H	4.96504200	-1.11165400	1.20764900
H	4.74347200	-0.61559600	2.86024700
C	2.44310100	-2.15120000	3.99311300
H	1.68985300	-2.75282400	2.05829900
H	0.89625600	-1.32908500	2.70069200
C	3.07296300	-4.21553800	-2.99781200
H	3.66586800	-2.63124000	-4.36711700
H	4.79056200	-2.89843900	-3.04144900
H	2.54034000	-5.44132300	-1.27958200
H	4.09729900	-4.63576500	-1.13810300
C	3.74471100	-2.98433400	3.89617800
H	4.13441600	-3.42191300	1.79819100
H	5.56555400	-2.96647000	2.69628700
H	1.69193300	-2.68293500	4.58750200
H	2.63750500	-1.20902700	4.52307700
H	2.03859500	-4.21300700	-3.37291600
H	3.59734200	-5.01543100	-3.53375000
H	3.51525600	-4.05303600	3.98320900
H	4.39429100	-2.74120000	4.74536300
Ts _{2a} -2			
C	-3.83777600	-2.39685000	-0.31692500
C	-4.13830800	-1.29769200	-1.35561800
C	-3.03664000	-0.12809300	-1.12359900
C	-4.60174800	0.01630200	-0.82373900
C	-2.19712800	-0.58713300	-0.03333000
C	-2.91432100	-1.73620900	0.72988800
C	-5.04195000	-3.25652600	0.16938500
C	-4.57929400	-4.31120400	1.19721900
C	-6.26082600	-2.46967100	0.69213600
C	-5.37817800	0.98448900	-1.63382500
C	-6.24355200	1.85589400	-1.09559600
C	-2.47903900	0.70082100	-2.23275200
C	-1.78239800	0.21783800	-3.26961000
O	-3.65966600	-1.21663800	1.93663700
C	-3.33676200	0.04664800	2.29794300
C	-3.96014900	0.52046100	3.56776700

O	-2.56377000	0.71896600	1.57320400
H	-3.16665600	-3.10611700	-0.82897900
H	-4.85426200	0.05286200	0.22835000
H	-2.21063300	-2.44358700	1.16489000
H	-5.37535300	-3.80214800	-0.72695900
H	-5.39198000	-5.01274100	1.41249200
H	-3.72863300	-4.89489500	0.82332900
H	-4.28819500	-3.84058300	2.14316300
H	-7.07540300	-3.16853000	0.91343300
H	-6.63721300	-1.75348800	-0.04594800
H	-6.02618400	-1.93017500	1.61419300
H	-5.23725500	0.96777100	-2.71104000
H	-6.81701400	2.54091200	-1.71047300
H	-6.41615800	1.91154400	-0.02382400
H	-2.66156700	1.77109200	-2.15694900
H	-1.38700800	0.87196900	-4.03996600
H	-1.57644100	-0.84293200	-3.38520200
H	-3.79639000	1.59102200	3.68558400
H	-3.51034500	-0.00970100	4.41510900
H	-5.03046100	0.29654700	3.57502600
Au	-0.14194300	-0.52454600	-0.03267100
H	-0.87346400	6.77467700	0.99736300
C	-1.74872000	6.31870200	0.52231200
C	-1.92067900	4.84551000	0.96387700
H	-1.61773300	6.39011400	-0.56427500
H	-2.63230800	6.90791700	0.79420700
C	-0.66850600	4.02773500	0.66167400
C	-3.19354200	4.23062400	0.34214800
H	-2.05101600	4.84167600	2.05587100
C	-0.27637800	3.72868100	-0.64613200
C	0.17384800	3.60148600	1.68508200
H	-4.07934100	4.80376400	0.64090500
H	-3.32336400	3.19183600	0.66284000
H	-3.14837100	4.24595300	-0.75372200
C	0.91143500	3.04327600	-0.95029800
H	-0.88860700	4.07631200	-1.47382700
C	1.37066300	2.89258800	1.46092800
H	-0.08994700	3.84953800	2.71042000
C	1.21734700	2.99559300	-2.46481000
C	1.74526500	2.58016200	0.12026200
C	2.11493000	2.57600800	2.78153800
H	0.23310300	3.12190400	-2.93789800
C	2.06134200	4.21479100	-2.91888600
C	1.78732000	1.69358600	-3.05147000

C	3.10281400	1.99279600	-0.20801000
C	3.63728000	2.34128500	2.77159100
C	1.37799600	1.44254200	3.54251200
H	1.97582200	3.48228700	3.38924900
H	2.08643300	4.26505100	-4.01423500
H	1.63609200	5.15198100	-2.54431800
H	3.09384100	4.13965000	-2.56556000
H	1.69648800	1.72041200	-4.14471700
H	1.23021900	0.82468600	-2.68888700
H	2.84429800	1.55555400	-2.81617200
C	4.12046100	2.94739700	-0.43433500
C	3.45350900	0.62117200	-0.33162700
H	3.98552100	2.28109900	3.80976800
H	4.17081900	3.16557200	2.29104200
H	3.93441500	1.41757600	2.26941200
H	0.34354700	1.72715500	3.76073200
H	1.34097300	0.52557500	2.94736000
H	1.88110500	1.22301600	4.49188400
C	5.42405100	2.59348300	-0.78141700
H	3.86433700	3.99522400	-0.32365800
C	4.77337500	0.27717500	-0.69238400
P	2.28663600	-0.84222700	-0.00550100
C	5.75425800	1.24393800	-0.91847700
H	6.17066500	3.36340200	-0.94456700
H	5.04652400	-0.76356200	-0.81302900
C	2.76722300	-2.21438200	-1.28655600
C	2.87190900	-1.50746700	1.73404300
H	6.75836400	0.94282300	-1.19689500
C	2.76747200	-1.70079500	-2.74205100
C	1.83236200	-3.44042000	-1.15545700
H	3.78542800	-2.52820600	-1.02106400
C	4.25728900	-2.22799200	1.76176900
C	1.76967000	-2.34716800	2.42758700
H	2.97116300	-0.57310400	2.29378600
C	3.19610500	-2.81845700	-3.71851400
H	1.75530500	-1.36329400	-3.00398100
H	3.43039900	-0.83732800	-2.85135400
C	2.24958300	-4.56130500	-2.13416700
H	1.83699300	-3.83054700	-0.13288000
H	0.80070500	-3.12670300	-1.37262400
C	4.13789700	-3.73867100	2.04320500
H	4.82471100	-2.06567500	0.84079900
H	4.86010100	-1.76963100	2.55731500
C	2.33096200	-2.98604600	3.71508700

H	1.39203800	-3.13575500	1.76530600
H	0.91317300	-1.70256300	2.65885600
C	2.29553300	-4.06090200	-3.58958700
H	3.17202500	-2.43309600	-4.74529700
H	4.23995400	-3.09976900	-3.51385200
H	1.55337100	-5.40429000	-2.04003400
H	3.24127100	-4.94106900	-1.84652300
C	3.45226600	-4.01660100	3.40308400
H	3.57172800	-4.21943300	1.23452900
H	5.13509700	-4.19421100	2.02654600
H	1.52134400	-3.46424000	4.27898400
H	2.72275700	-2.18636500	4.35892700
H	1.27673800	-3.80579900	-3.91899200
H	2.65012600	-4.85869100	-4.25325400
H	3.03905100	-5.03277100	3.39654600
H	4.19985700	-3.99275500	4.20550400
C	-4.49404800	-1.76575000	-2.74837600
H	-5.52918300	-2.12879400	-2.76580800
H	-4.40613800	-0.97204100	-3.49235300
H	-3.84315000	-2.58983600	-3.06073900

3a-2

C	3.63769800	-2.37363300	-0.08257000
C	3.92386600	-1.52332400	1.16892500
C	3.03929300	-0.26948500	1.10254700
C	4.57220400	-0.16899700	0.92896800
C	2.22543200	-0.34232500	-0.18593500
C	2.86234300	-1.46119800	-1.03809800
C	4.79030000	-3.24625700	-0.65142000
C	4.32703900	-4.04947800	-1.87894200
C	6.10501300	-2.50263700	-0.93942000
C	4.21677200	-2.31040300	2.43099100
C	5.40095100	0.50063400	1.96075400
C	6.53216500	1.15783400	1.68841500
C	2.41218300	0.40289800	2.28274000
C	1.82585100	-0.20828500	3.31522200
O	3.70721400	-0.71064400	-2.04539800
C	3.41129400	0.54500300	-1.96470000
C	3.99154900	1.51410500	-2.93011700
O	2.59481600	0.89912300	-1.05856300
H	2.86041800	-3.09153200	0.22736900
H	4.95421400	0.00989700	-0.07247700
H	2.17527200	-2.00718400	-1.68211200
H	5.00714600	-3.97346500	0.14324300
H	5.08962400	-4.78114100	-2.16554400

H	3.39994500	-4.60095500	-1.67847300
H	4.15752100	-3.40045600	-2.74685600
H	6.87322600	-3.22360600	-1.24022300
H	6.47845900	-1.97252200	-0.05781500
H	5.99913800	-1.78076600	-1.75632000
H	3.45642400	-3.08358000	2.59696500
H	5.18771500	-2.81247400	2.34742500
H	4.25004700	-1.67810000	3.31940300
H	5.05091000	0.45115400	2.98915100
H	7.11433900	1.63404400	2.47123400
H	6.92253300	1.24061500	0.67588900
H	2.43971800	1.49277200	2.26077700
H	1.38308200	0.36143600	4.12742100
H	1.76276500	-1.29026400	3.39034800
H	3.99474700	2.51686000	-2.50059300
H	3.37262700	1.51998700	-3.83602800
H	5.00023000	1.20450300	-3.21221900
Au	0.11936500	-0.45101500	-0.03421200
H	0.59463400	6.72595100	-1.28291900
C	1.45718500	6.43448100	-0.67443300
C	1.81269900	4.94763800	-0.88456300
H	1.20814100	6.63038800	0.37520400
H	2.30135200	7.07860000	-0.94699800
C	0.61097500	4.06167000	-0.58075200
C	3.07081200	4.57410100	-0.08166000
H	2.04575200	4.81677800	-1.95146300
C	0.24116700	3.72148900	0.71964800
C	-0.23029800	3.63243100	-1.60082100
H	3.92686100	5.17273000	-0.41363900
H	3.32403100	3.51365000	-0.19506300
H	2.93975900	4.76881200	0.98891700
C	-0.91967500	2.99590700	1.02118900
H	0.84981300	4.07112100	1.54988500
C	-1.40140300	2.88686000	-1.38191700
H	0.00937800	3.91815200	-2.62404800
C	-1.20269200	2.91460800	2.53540600
C	-1.74675400	2.53094200	-0.04812400
C	-2.15718000	2.59442300	-2.69722400
H	-0.21622000	3.05396900	2.99600500
C	-2.05934000	4.10611800	3.01867200
C	-1.73149300	1.59719800	3.11412500
C	-3.07831300	1.89061700	0.28595200
C	-3.66919500	2.32297800	-2.67382900
C	-1.40771600	1.51524200	-3.51108200

H	-2.05345800	3.52347900	-3.27388600
H	-2.07122300	4.13767000	4.11468300
H	-1.65824600	5.05880000	2.65667000
H	-3.09583300	4.02083300	2.67960200
H	-1.62759500	1.61882600	4.20597600
H	-1.15496400	0.74574300	2.74132700
H	-2.78755200	1.43009200	2.89347800
C	-4.11081300	2.81103600	0.55093000
C	-3.38754000	0.50587900	0.38936200
H	-4.03048300	2.28918200	-3.70841500
H	-4.21595800	3.11784600	-2.15990900
H	-3.94104500	1.37684500	-2.20005400
H	-0.38530200	1.83519000	-3.73938400
H	-1.33369400	0.57474700	-2.95739500
H	-1.91927600	1.31842100	-4.46084500
C	-5.39455400	2.42249900	0.92254500
H	-3.88407000	3.86814600	0.45396200
C	-4.69027200	0.13257200	0.78042600
P	-2.22767800	-0.89185800	0.00647300
C	-5.68663900	1.06685100	1.04784900
H	-6.15491500	3.17354200	1.11658900
H	-4.93750100	-0.91616900	0.89598500
C	-2.61703600	-2.27189200	1.23267700
C	-2.80292900	-1.50109200	-1.69464300
H	-6.67552200	0.73444900	1.34934900
C	-2.59388600	-1.80919000	2.70453000
C	-1.66044100	-3.47481300	1.05341300
H	-3.63248800	-2.61815300	0.99598400
C	-4.18598100	-2.22603100	-1.75529200
C	-1.70903700	-2.30166700	-2.44790200
H	-2.91608900	-0.55314600	-2.22861100
C	-2.97218500	-2.95912100	3.65442900
H	-1.58395500	-1.45605400	2.95153000
H	-3.27042800	-0.96382200	2.85783100
C	-2.02751800	-4.62691900	2.00654200
H	-1.67778100	-3.84128400	0.02307500
H	-0.63135900	-3.14330200	1.25286900
C	-4.05865400	-3.72516400	-2.06424100
H	-4.76598800	-2.08081000	-0.84049000
H	-4.77948200	-1.75385100	-2.54836500
C	-2.29053700	-2.90939300	-3.73427700
H	-1.29704300	-3.10188600	-1.82255600
H	-0.86989300	-1.63583000	-2.68025100
C	-2.05170000	-4.17276600	3.47146000

H	-2.93383500	-2.60097300	4.69023100
H	-4.01401300	-3.25748900	3.46693200
H	-1.31552300	-5.45029500	1.87036900
H	-3.01555100	-5.02215100	1.72930300
C	-3.37427100	-3.97205300	-3.42586700
H	-3.48933200	-4.21620500	-1.26484200
H	-5.05218200	-4.18760300	-2.05211800
H	-1.48735200	-3.34772200	-4.33765400
H	-2.71855600	-2.09907800	-4.33975700
H	-1.03217000	-3.90452800	3.78567800
H	-2.37192500	-4.99706800	4.11951000
H	-2.93087400	-4.97479800	-3.42963000
H	-4.12449700	-3.96605300	-4.22520000
T _{S3a} -2			
C	3.28732200	-2.43096800	-0.04977800
C	3.69899500	-1.59681300	1.18271300
C	3.07915600	-0.20432100	1.03585900
C	4.60195700	-0.39249300	0.90187400
C	2.30282400	-0.21890100	-0.28007800
C	2.66831400	-1.43204000	-0.98596500
C	4.30332800	-3.46785600	-0.62553000
C	3.71633900	-4.19523300	-1.84623400
C	5.70556400	-2.91995700	-0.92798600
C	3.81806800	-2.37028300	2.48013400
C	5.52105200	0.14356100	1.93507300
C	6.76058900	0.56798400	1.67133200
C	2.54133400	0.63268400	2.15098900
C	1.83646600	0.19074200	3.19589500
O	3.92396900	-0.49381600	-2.19081100
C	3.51632400	0.66981600	-2.03503600
C	4.03683800	1.83834300	-2.80942800
O	2.57802400	0.94068100	-1.14138400
H	2.42243500	-3.05080000	0.25179600
H	5.01902200	-0.32936400	-0.09717300
H	2.16305600	-1.75945200	-1.88557900
H	4.41396400	-4.21289800	0.17411700
H	4.35638000	-5.03719300	-2.12945700
H	2.71534500	-4.59671500	-1.64274000
H	3.64994700	-3.53223600	-2.71745000
H	6.34900700	-3.74228600	-1.26036900
H	6.17154600	-2.47557400	-0.04360700
H	5.68808200	-2.17020800	-1.72495000
H	2.91937000	-2.97336300	2.66254200
H	4.67391300	-3.05443000	2.43880100

H	3.96220000	-1.71789100	3.34254100
H	5.14878100	0.19962100	2.95573100
H	7.40575500	0.95655300	2.45332100
H	7.17880900	0.53910900	0.66708800
H	2.74913900	1.69971500	2.06745200
H	1.47594800	0.87342900	3.96015200
H	1.59611900	-0.86008000	3.33130000
H	4.77415400	2.36677800	-2.19352000
H	3.22391600	2.53490100	-3.02730900
H	4.51718400	1.49873000	-3.72748400
Au	0.15271000	-0.41824100	-0.05780700
H	0.62342300	6.74716200	-1.25944800
C	1.47866100	6.45855500	-0.63932700
C	1.83833500	4.97130200	-0.83888800
H	1.21696100	6.65862000	0.40647300
H	2.32569600	7.10196900	-0.90428700
C	0.63521500	4.08430000	-0.54492200
C	3.08655200	4.60028700	-0.01989500
H	2.08452000	4.83603900	-1.90226600
C	0.25805200	3.74267300	0.75260600
C	-0.19717700	3.65149500	-1.57111700
H	3.94800300	5.19298700	-0.34817000
H	3.33522900	3.53844100	-0.12648900
H	2.94474900	4.80487800	1.04757600
C	-0.90030000	3.01011700	1.04622700
H	0.85921000	4.09464500	1.58712800
C	-1.36524600	2.89921900	-1.36075700
H	0.04812700	3.93849500	-2.59259400
C	-1.19364700	2.93181000	2.55869600
C	-1.71595700	2.53894200	-0.02909300
C	-2.11395900	2.60605800	-2.67965200
H	-0.20644700	3.04525700	3.02474400
C	-2.02362600	4.14498300	3.03493200
C	-1.76099300	1.62997100	3.13595600
C	-3.04341500	1.88927100	0.30069400
C	-3.62558300	2.33218000	-2.66117200
C	-1.35933100	1.52996800	-3.49231100
H	-2.00995100	3.53607000	-3.25458500
H	-2.05007600	4.17390800	4.13073800
H	-1.59248500	5.08745900	2.68120700
H	-3.05740500	4.08855200	2.68104300
H	-1.64966500	1.64431000	4.22709600
H	-1.21415500	0.76222700	2.75710700
H	-2.82324800	1.49618600	2.92133400

C	-4.08322300	2.80074500	0.56752200
C	-3.34079100	0.50242700	0.40882500
H	-3.98398000	2.29869400	-3.69670400
H	-4.17537000	3.12563500	-2.14810400
H	-3.89752200	1.38504800	-2.18913200
H	-0.33446700	1.84829000	-3.71044200
H	-1.29139800	0.58658600	-2.94254900
H	-1.86365100	1.33794600	-4.44687000
C	-5.36100500	2.40167400	0.94812000
H	-3.86621600	3.85949500	0.46679100
C	-4.63679300	0.11757300	0.81170800
P	-2.18023400	-0.88766000	0.01168200
C	-5.63944500	1.04390100	1.08269400
H	-6.12719500	3.14633300	1.14364900
H	-4.87357900	-0.93285500	0.93399700
C	-2.53847800	-2.27418800	1.23921300
C	-2.75958100	-1.49320800	-1.68838300
H	-6.62273900	0.70380000	1.39355200
C	-2.50426200	-1.81487100	2.71189700
C	-1.57550300	-3.46938900	1.04609400
H	-3.55359400	-2.62692400	1.01065300
C	-4.14292400	-2.21876800	-1.73833700
C	-1.67146300	-2.29196000	-2.45180600
H	-2.87736700	-0.54349300	-2.21811100
C	-2.86473700	-2.97021700	3.66223400
H	-1.49413100	-1.45569200	2.95044500
H	-3.18449200	-0.97429200	2.87415300
C	-1.92436700	-4.62651500	2.00017900
H	-1.60091100	-3.83319200	0.01507600
H	-0.54677800	-3.13060300	1.23657000
C	-4.01652300	-3.71880100	-2.04256400
H	-4.71895100	-2.06889900	-0.82180800
H	-4.73934200	-1.74904200	-2.53055300
C	-2.26557100	-2.90347200	-3.73066600
H	-1.25084800	-3.09020100	-1.82995000
H	-0.83736300	-1.62418300	-2.69628500
C	-1.93739000	-4.17654500	3.46646900
H	-2.81827800	-2.61425800	4.69834300
H	-3.90627300	-3.27526800	3.48457600
H	-1.20782200	-5.44419000	1.85441000
H	-2.91200200	-5.02813800	1.73122100
C	-3.34211800	-3.96919300	-3.40862500
H	-3.44110000	-4.20675100	-1.24552600
H	-5.00963000	-4.18166000	-2.02139000

H	-1.46734600	-3.33979100	-4.34176300
H	-2.70241100	-2.09543300	-4.33270400
H	-0.91677500	-3.90230200	3.77192900
H	-2.24540400	-5.00502100	4.11493000
H	-2.89462600	-4.97005400	-3.41164500
H	-4.09875400	-3.96968000	-4.20179100
1d-2			
C	-4.70282000	0.79479300	0.21409200
C	-4.75691600	-0.46239900	-0.66429100
C	-4.89861200	-1.65759700	-0.04517900
C	-2.24606900	1.29863300	-0.44697200
C	-3.22724300	1.07164400	0.64608400
C	-5.54462700	2.00555500	-0.31320100
C	-6.23570500	2.75573700	0.84103600
C	-4.80906100	3.00249200	-1.22298100
C	-1.59671000	1.73481500	-1.40212000
C	-4.67228300	-0.31284500	-2.16460000
C	-4.97623900	-2.98285400	-0.64543100
C	-5.11121200	-4.10944400	0.07384600
C	-0.99931300	2.34658200	-2.54984100
C	-1.54210900	2.28550900	-3.77576800
O	-3.21331900	2.21547400	1.53237500
C	-2.23289500	2.24396600	2.47820300
C	-2.37455000	3.45316500	3.36445900
O	-1.37482100	1.39181800	2.56549000
H	-5.16259600	0.51091500	1.16825400
H	-4.97970700	-1.65537300	1.04365300
H	-2.89869600	0.20300800	1.21963200
H	-6.34940800	1.55195600	-0.90702500
H	-6.91839500	3.51522800	0.44376900
H	-6.82778300	2.07306100	1.46186100
H	-5.50961000	3.25921800	1.48580300
H	-5.51985800	3.74401900	-1.60434500
H	-4.34204000	2.52433700	-2.08911300
H	-4.03376100	3.54808100	-0.67385600
H	-3.70778000	0.10744200	-2.47288500
H	-4.79451200	-1.26638000	-2.68098100
H	-5.44953900	0.36170600	-2.54206600
H	-4.93336400	-3.06218300	-1.72926300
H	-5.18362300	-5.08352100	-0.39999200
H	-5.17047300	-4.09041300	1.16002100
H	-0.07514500	2.88885400	-2.37170400
H	-1.07172000	2.79407100	-4.61134100
H	-2.45922400	1.74108300	-3.97798800

H	-2.28249300	4.36652700	2.76715200
H	-1.60167900	3.43353200	4.13311500
H	-3.36500400	3.46675000	3.83043400
H	-2.30245300	-4.93629500	-1.55279700
C	-1.22294400	-4.77207800	-1.65035100
C	-0.83278500	-3.54440700	-0.80775200
C	-0.82762400	-4.60675900	-3.12297900
H	-0.73145200	-5.66493300	-1.23738000
C	0.67761800	-3.23450800	-0.93498100
H	-1.11200400	-3.72209700	0.23389300
H	-1.41127000	-2.67203000	-1.14273300
C	0.66497600	-4.27880700	-3.25495000
H	-1.41860800	-3.79392700	-3.57027000
H	-1.06946900	-5.51590700	-3.68587500
P	1.18221700	-1.77069200	0.13450600
C	1.05239600	-3.04520600	-2.42111800
H	1.22866100	-4.10003400	-0.54261300
H	0.92964900	-4.10183100	-4.30421800
H	1.26080500	-5.14209000	-2.92483400
Au	-0.25308700	0.01783700	-0.34770100
C	2.98964700	-1.47882100	-0.13844800
C	1.04127000	-2.26853100	1.94501600
H	0.52230500	-2.16587400	-2.81197400
H	2.12182500	-2.84402600	-2.53207100
C	3.64277300	-0.21583300	-0.12733200
C	3.76255600	-2.64291200	-0.33269700
C	1.63933500	-3.66683700	2.31028100
C	-0.38085900	-2.07219900	2.52812100
H	1.67656100	-1.51224500	2.41389300
C	3.01635700	1.15341700	0.02304200
C	5.04019400	-0.20625600	-0.29587700
C	5.14294900	-2.59824700	-0.50415100
H	3.28111600	-3.61351600	-0.36218400
C	0.56103000	-4.67983400	2.72281000
H	2.25155700	-4.07854500	1.50281700
H	2.33057200	-3.52403600	3.15018300
C	-0.44227100	-2.65942200	3.94739100
H	-1.13973600	-2.55516900	1.90249100
H	-0.62530200	-1.00538000	2.54703700
C	2.74473400	1.92027500	-1.15554400
C	2.90063100	1.78260400	1.29359200
C	5.78888000	-1.36497200	-0.48109800
H	5.54628200	0.75361900	-0.27045800
H	5.70039800	-3.51800400	-0.65326100

C	-0.24211600	-4.19519100	3.94876500
H	-0.11624500	-4.85624500	1.87749300
H	1.03153100	-5.64626500	2.93669300
H	-1.39811700	-2.39756300	4.41457900
H	0.33384100	-2.17708600	4.55642200
C	2.28835500	3.23797000	-1.01624400
C	3.02260500	1.52139000	-2.62048700
C	2.44710000	3.11334700	1.34539100
C	3.25966400	1.24262200	2.69877200
H	6.86584600	-1.30146200	-0.60664300
H	-1.21351500	-4.70326400	3.96337900
H	0.27253300	-4.49326300	4.86970800
C	2.12448800	3.86289500	0.22207100
H	2.11163100	3.81445300	-1.92245400
H	2.40570100	2.21488500	-3.20688000
C	4.48220600	1.82516200	-3.02688200
C	2.61134500	0.12142000	-3.09476400
H	2.37764800	3.59133600	2.32022600
C	4.19908800	0.03650200	2.85158000
C	1.98387100	1.05768500	3.55116100
H	3.80564600	2.07615900	3.16208400
C	1.67857100	5.31355700	0.34524300
H	4.59313900	1.73475700	-4.11388400
H	4.77263700	2.84130900	-2.74010400
H	5.18412000	1.12554900	-2.56428600
H	2.65021900	0.08910700	-4.19021500
H	1.58557600	-0.11655600	-2.79318800
H	3.27294000	-0.66312800	-2.72270600
H	4.42137500	-0.09169900	3.91721300
H	5.14958100	0.18782300	2.33429400
H	3.77339300	-0.90417100	2.49256100
H	1.41244400	1.98631800	3.63259900
H	1.30439200	0.31974500	3.11802100
H	2.24740700	0.73201200	4.56431700
C	2.71954100	6.27967700	-0.25385000
C	0.28787700	5.55099600	-0.27225200
H	1.60333000	5.53479800	1.41839900
H	3.70000800	6.14675700	0.21551500
H	2.83919800	6.11873400	-1.33191400
H	2.40904300	7.32006700	-0.10500300
H	-0.03668900	6.58389800	-0.10292900
H	-0.46301100	4.88230400	0.16540700
H	0.29653200	5.38534200	-1.35649600

C	-4.34360900	-1.58098100	0.66826000
C	-4.70958800	-0.85723800	-0.64296500
C	-2.87019500	-0.76599300	-1.28985800
C	-5.13323300	-1.69822600	-1.68108100
C	-2.18893700	-0.81901900	-0.16485600
C	-2.95507000	-1.07313600	1.11169800
C	-5.45877700	-1.74872800	1.74665100
C	-4.94942400	-2.68321400	2.86163700
C	-6.06765000	-0.47910800	2.36707400
C	-5.17743100	0.59236200	-0.61575800
C	-5.83135300	-1.32053200	-2.87514900
C	-6.14148600	-2.23102000	-3.82466400
C	-2.68976700	-0.55832800	-2.71115300
C	-1.74282300	-1.15870400	-3.44616700
O	-3.05860200	0.16901300	1.85151800
C	-2.20015000	0.34543300	2.89688700
C	-2.39611900	1.69639100	3.53526400
O	-1.38761700	-0.48460600	3.23996500
H	-4.12019900	-2.61288000	0.36331500
H	-4.88228300	-2.75534300	-1.59676500
H	-2.45151000	-1.79520000	1.75568000
H	-6.27482200	-2.27761700	1.23307500
H	-5.76938400	-2.94420800	3.53875300
H	-4.54146100	-3.61813600	2.45863100
H	-4.16733900	-2.20562900	3.46321000
H	-6.83041600	-0.77184200	3.09721600
H	-6.55858400	0.16101300	1.63021200
H	-5.31764600	0.11921600	2.88955300
H	-4.69160100	1.13587100	0.19377100
H	-4.94468200	1.10911800	-1.55208400
H	-6.26204100	0.64943500	-0.47010500
H	-6.14191200	-0.28668600	-2.99867900
H	-6.70051300	-1.95947900	-4.71484900
H	-5.85156900	-3.27458800	-3.72808600
H	-3.37565900	0.13806000	-3.19178900
H	-1.62555500	-0.92671700	-4.50046000
H	-1.05466500	-1.87741200	-3.01204000
H	-1.90781700	2.45450900	2.91185400
H	-1.93577900	1.69883500	4.52423700
H	-3.45628500	1.95349200	3.60695700
Au	-0.10191100	-0.60787600	-0.11959700
H	-1.02764900	6.72763000	-0.10184300
C	-1.93138900	6.15886000	-0.34489500
C	-1.97143600	4.82166300	0.42121400

H	-1.94171700	5.99449200	-1.42902100
H	-2.80116700	6.77588400	-0.09119900
C	-0.73040500	3.98498800	0.13962900
C	-3.27479100	4.05758300	0.12699700
H	-1.96359800	5.05878900	1.49416400
C	-0.47995000	3.43134600	-1.11649500
C	0.24713200	3.80184100	1.11008200
H	-4.14558900	4.66003600	0.41050400
H	-3.31312100	3.11315300	0.68130900
H	-3.36782900	3.82455400	-0.94053200
C	0.69355600	2.73072900	-1.42167000
H	-1.19900400	3.59243300	-1.91655000
C	1.43862300	3.08590100	0.89200200
H	0.10345100	4.27126800	2.08167800
C	0.83636600	2.41645500	-2.92579300
C	1.65934800	2.51073800	-0.39018900
C	2.35696300	3.09942700	2.13767800
H	-0.19880100	2.38246100	-3.28945200
C	1.51018800	3.58936500	-3.67322100
C	1.45583800	1.08168100	-3.35911100
C	2.98387400	1.87851100	-0.75554600
C	3.85895000	2.80611500	2.00126500
C	1.73561800	2.25615800	3.27587000
H	2.31001300	4.14131800	2.48429600
H	1.44125100	3.43465600	-4.75675000
H	1.02879900	4.54362700	-3.43493700
H	2.57127500	3.67028900	-3.41800400
H	1.24332800	0.92141300	-4.42345600
H	1.02239000	0.24539900	-2.80293700
H	2.54052700	1.05578700	-3.23815700
C	3.94196900	2.77904900	-1.25798700
C	3.34768700	0.50732300	-0.66402400
H	4.33336000	2.98825300	2.97264400
H	4.34020500	3.46239400	1.27242700
H	4.08324000	1.77500300	1.71679100
H	0.74906900	2.63370100	3.56082400
H	1.60258000	1.21010200	2.98616600
H	2.37345800	2.28667600	4.16692600
C	5.21221900	2.38159600	-1.66485100
H	3.66938100	3.82834300	-1.31570500
C	4.63995900	0.12432200	-1.07874700
P	2.26976700	-0.85035500	0.00468100
C	5.56622000	1.03807900	-1.57387800
H	5.91613500	3.11590800	-2.04588700

H	4.93804700	-0.91619600	-1.02617500
C	2.73104100	-2.40920600	-0.95106200
C	2.86583800	-1.07348800	1.78087600
H	6.54995200	0.69816500	-1.88383800
C	2.60490900	-2.23527800	-2.47946000
C	1.89734700	-3.62915300	-0.49413300
H	3.78162200	-2.62274400	-0.71356100
C	4.29571500	-1.68114900	1.96111100
C	1.82055600	-1.76711300	2.68877500
H	2.91479600	-0.03222900	2.11150900
C	3.03883000	-3.51005400	-3.22349700
H	1.55724300	-2.01232500	-2.72383300
H	3.19628000	-1.38284500	-2.82601300
C	2.32603100	-4.90629000	-1.23937700
H	1.99434400	-3.78927000	0.58319600
H	0.83414400	-3.42827700	-0.68764400
C	4.27043700	-3.05866800	2.64179700
H	4.84060300	-1.74509700	1.01476000
H	4.88051600	-0.99168300	2.58296800
C	2.42488100	-2.00614700	4.08131600
H	1.49484600	-2.72439500	2.26621100
H	0.92233900	-1.14711600	2.76385500
C	2.24193700	-4.73714900	-2.76174900
H	2.92158000	-3.35885600	-4.30350700
H	4.11065600	-3.68336200	-3.04876300
H	1.69993500	-5.74461400	-0.91027300
H	3.35797400	-5.15986400	-0.95650800
C	3.61094300	-3.00175800	4.03601300
H	3.73093600	-3.77010400	2.00339100
H	5.29342800	-3.44435300	2.72238400
H	1.64693800	-2.36590200	4.76351100
H	2.75899700	-1.04076800	4.48506300
H	1.18845700	-4.61808400	-3.05646500
H	2.60619100	-5.64041800	-3.26536500
H	3.27217000	-4.00746900	4.31161000
H	4.35758900	-2.71473100	4.78611500

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C	-4.36305800	-1.42558900	0.74079000
C	-4.56100800	-0.84651600	-0.70531700
C	-2.98568700	-0.87444100	-1.21337700
C	-5.09946900	-1.85110000	-1.58578100
C	-2.18149900	-0.85043600	-0.12757700
C	-2.95160700	-0.96520500	1.16530500
C	-5.55321500	-1.36653500	1.74194700

C	-5.28198900	-2.34530400	2.90214600
C	-5.96769800	0.00017300	2.31730900
C	-5.12976800	0.56814700	-0.85307400
C	-5.89748900	-1.65312900	-2.74551200
C	-6.27739300	-2.70687200	-3.51331100
C	-2.69431200	-0.78996100	-2.64520300
C	-1.65024700	-1.35528600	-3.26493000
O	-2.98614500	0.33561600	1.80510600
C	-2.16967100	0.52197500	2.88103000
C	-2.29860400	1.92366600	3.41948100
O	-1.43833600	-0.33753600	3.32151400
H	-4.20826300	-2.50204600	0.58115300
H	-4.81033300	-2.88125600	-1.37828300
H	-2.49484500	-1.66268800	1.87078200
H	-6.41880900	-1.75880100	1.18691900
H	-6.15239700	-2.39951300	3.56433400
H	-5.07295500	-3.36014600	2.54306400
H	-4.42857400	-2.02003200	3.50917100
H	-6.87832800	-0.13052600	2.91278300
H	-6.18468300	0.74701800	1.55127100
H	-5.19895100	0.41038800	2.97580500
H	-4.63493000	1.24150200	-0.15237200
H	-4.95924600	0.96051700	-1.86121900
H	-6.20778400	0.58967400	-0.66133400
H	-6.23295900	-0.65121900	-2.99685300
H	-6.92048100	-2.57998200	-4.37914100
H	-5.95802900	-3.72070100	-3.28393000
H	-3.40961100	-0.22336200	-3.24266900
H	-1.48838000	-1.21576200	-4.32952100
H	-0.92942300	-1.96376500	-2.72769900
H	-1.77023000	2.60977100	2.74781100
H	-1.84720500	1.97326600	4.41123100
H	-3.34540800	2.23716900	3.46060600
Au	-0.12448700	-0.61922900	-0.10196800
H	-0.97981800	6.72266700	-0.44323800
C	-1.88642600	6.14214000	-0.64409900
C	-1.92085500	4.85258500	0.19972600
H	-1.90719800	5.91403000	-1.71640800
H	-2.75316300	6.77434600	-0.41898300
C	-0.68346200	3.99801400	-0.04166600
C	-3.22701100	4.07341000	-0.03960300
H	-1.90466900	5.15219200	1.25682900
C	-0.44181200	3.37611500	-1.26709500
C	0.29692700	3.86133200	0.93387700

H	-4.09543100	4.69344600	0.21181200
H	-3.26302800	3.16424600	0.57104000
H	-3.32596500	3.77640300	-1.09058700
C	0.72705500	2.65458100	-1.53922500
H	-1.16371700	3.49733200	-2.07156200
C	1.48148200	3.12424800	0.75130100
H	0.16010800	4.38345900	1.87924000
C	0.86538500	2.26509300	-3.02597800
C	1.69428500	2.48204800	-0.50044700
C	2.40236100	3.19036500	1.99382600
H	-0.17072500	2.20817000	-3.38399000
C	1.53351400	3.40326600	-3.83008000
C	1.49037900	0.91393800	-3.39610500
C	3.01270200	1.82081200	-0.83490900
C	3.89966000	2.86927300	1.87048600
C	1.77378500	2.41467100	3.17568700
H	2.36939600	4.24919700	2.28674100
H	1.46705800	3.19523900	-4.90482300
H	1.04737300	4.36577700	-3.63924200
H	2.59386900	3.50157800	-3.57727200
H	1.27164900	0.69999200	-4.44969600
H	1.06419200	0.10443000	-2.79695900
H	2.57601600	0.89960000	-3.28139100
C	3.97887600	2.68715700	-1.38021400
C	3.36237400	0.45205800	-0.67684400
H	4.37882500	3.09233000	2.83091700
H	4.38920900	3.48071000	1.10893600
H	4.10661300	1.82179700	1.63753900
H	0.79250900	2.81804900	3.44240500
H	1.62896600	1.35581000	2.94260600
H	2.41396300	2.48510800	4.06279800
C	5.24633400	2.25904900	-1.76400100
H	3.71512800	3.73449200	-1.49131900
C	4.65242300	0.03861000	-1.06790400
P	2.26165900	-0.86127300	0.04420500
C	5.58829500	0.91887400	-1.60425900
H	5.95719000	2.96713000	-2.18019700
H	4.94135200	-1.00070100	-0.96514100
C	2.72668900	-2.46877500	-0.82533300
C	2.84398600	-1.00380000	1.83454100
H	6.56992900	0.55534500	-1.89349900
C	2.64194400	-2.37169600	-2.36367900
C	1.86373700	-3.65366900	-0.33054100
H	3.76773300	-2.68413900	-0.55010600

C	4.26615400	-1.61420100	2.05622500
C	1.78521100	-1.64469400	2.76584600
H	2.90070900	0.05182300	2.11404600
C	3.07654100	-3.68828500	-3.03063400
H	1.60494700	-2.14826900	-2.64888900
H	3.25417000	-1.54622400	-2.73795400
C	2.29177800	-4.97251900	-0.99908400
H	1.93063500	-3.76045600	0.75562800
H	0.80864900	-3.44757700	-0.56010900
C	4.22087600	-2.96967500	2.77837100
H	4.82595200	-1.70881200	1.12110200
H	4.84503200	-0.90984500	2.66696100
C	2.38177000	-1.84116600	4.16829700
H	1.44407400	-2.61233200	2.37991600
H	0.89661400	-1.00806500	2.81362600
C	2.24933300	-4.87951100	-2.52967800
H	2.98968700	-3.59030200	-4.11964500
H	4.14082200	-3.86741000	-2.81886400
H	1.64501900	-5.78462200	-0.64487500
H	3.31226400	-5.22546700	-0.67667100
C	3.54644500	-2.86246700	4.16277400
H	3.68154100	-3.69546600	2.15626600
H	5.23909200	-3.36233500	2.88253100
H	1.59602900	-2.15803400	4.86269500
H	2.73623000	-0.86822600	4.53474800
H	1.20573700	-4.76008600	-2.85753800
H	2.61241100	-5.81207600	-2.97783700
H	3.18218400	-3.85299400	4.46027600
H	4.28992300	-2.57185200	4.91465100

Ts_{2d}-2

C	-4.45183900	-1.57855500	0.38978700
C	-4.64086200	-0.50227400	-0.74416900
C	-3.11973400	-0.21092800	-1.21546600
C	-4.81956200	-1.16951300	-2.02046200
C	-2.24908300	-0.73524000	-0.29699400
C	-2.94595200	-1.53468700	0.78124200
C	-5.57469900	-1.74028600	1.45689400
C	-5.45264600	-3.12876900	2.11627400
C	-5.73802100	-0.67413900	2.55526800
C	-5.46218800	0.75384600	-0.46626700
C	-5.36432600	-0.63243000	-3.23051500
C	-5.42936700	-1.38909500	-4.34929200
C	-2.81260000	0.70913900	-2.32288700
C	-1.81344100	0.55950900	-3.19844700

O	-2.60412000	-1.09508400	2.12457200
C	-2.69874400	0.21595200	2.45298600
C	-2.19168800	0.45875200	3.85263500
O	-3.13220200	1.06791900	1.70792600
H	-4.51143900	-2.53628100	-0.14095300
H	-4.46931800	-2.19732900	-2.08879900
H	-2.54960400	-2.55368200	0.80495600
H	-6.50788300	-1.74585400	0.87413900
H	-6.29016000	-3.30032900	2.80062000
H	-5.45880000	-3.93760000	1.37559600
H	-4.52824400	-3.20769200	2.70035900
H	-6.69781300	-0.83474200	3.05889100
H	-5.72713300	0.34991900	2.18108200
H	-4.96076200	-0.76721100	3.31909000
H	-5.00943800	1.31481200	0.35007800
H	-5.51091600	1.41254000	-1.33788700
H	-6.48938200	0.48698400	-0.19667600
H	-5.77510200	0.37198400	-3.23312600
H	-5.89646100	-1.02285000	-5.25849300
H	-5.02663300	-2.39875200	-4.37852400
H	-3.47005500	1.57317900	-2.41782500
H	-1.62730300	1.30059300	-3.96964600
H	-1.14642700	-0.29710800	-3.16582500
H	-2.54259600	-0.31668100	4.53895300
H	-2.51868000	1.44321400	4.18983200
H	-1.09645400	0.42843100	3.84905200
H	6.33237500	2.80452400	-1.34319000
C	5.53423400	2.10672100	-1.10661600
C	4.28714900	2.58166500	-0.71129300
C	5.74263200	0.73272200	-1.19503000
C	3.21238100	1.73053600	-0.39205000
H	4.12488000	3.65246000	-0.63583700
C	4.69892000	-0.13406600	-0.88282500
H	6.70397200	0.33338700	-1.50450100
C	1.92842800	2.43890200	-0.02506500
C	3.42959300	0.32868000	-0.47898600
H	4.88563100	-1.19819800	-0.96905800
C	1.06433800	2.87400400	-1.07720900
C	1.66321000	2.87149200	1.30417000
P	2.17314700	-0.97194500	-0.05616300
C	-0.06693500	3.63461700	-0.75764400
C	1.29984000	2.74827800	-2.59681600
C	0.52473300	3.66361300	1.53740300
C	2.49259500	2.65826500	2.59387900

Au	-0.19492300	-0.55440700	-0.20835800
C	2.55180500	-2.44796500	-1.16855600
C	2.63713500	-1.46440900	1.70784600
C	-0.36080400	4.05344500	0.54026600
H	-0.71210100	3.95458900	-1.57246500
H	0.29747800	2.86024400	-3.02927300
C	2.12466700	3.94236800	-3.12800400
C	1.84241000	1.43228100	-3.16996200
H	0.34635700	4.01929600	2.55033500
C	3.96835200	2.23860700	2.51137900
C	1.72757500	1.75891600	3.59244200
H	2.51317900	3.65445500	3.05723500
C	2.52300300	-2.08405400	-2.66931200
C	1.59185700	-3.63205700	-0.90343200
H	3.56532100	-2.78558200	-0.91346600
C	3.99655300	-2.21368300	1.88927900
C	1.48498300	-2.16624800	2.46907200
H	2.75095900	-0.47816200	2.16573500
C	-1.53811700	4.96978300	0.84588800
H	2.13074800	3.93861000	-4.22480500
H	1.70520900	4.89688700	-2.79349300
H	3.16486200	3.89075000	-2.79170100
H	1.68029600	1.42273800	-4.25509600
H	1.32120300	0.56869800	-2.74738700
H	2.91417400	1.30542600	-3.00320000
H	4.38851800	2.25519400	3.52395400
H	4.55589200	2.92786700	1.90055400
H	4.11935000	1.23267800	2.11096400
H	0.74245900	2.17373800	3.82636700
H	1.56977300	0.75192700	3.19325500
H	2.28535200	1.66782600	4.53189300
C	2.88400900	-3.29579000	-3.54576700
H	1.51259700	-1.73885100	-2.92980300
H	3.20353100	-1.25508000	-2.88418100
C	1.94821900	-4.84548600	-1.78101800
H	1.61668000	-3.92996600	0.14827700
H	0.56182900	-3.31301400	-1.11618500
C	3.81537100	-3.66459600	2.36101900
H	4.60056100	-2.19034100	0.97791200
H	4.58623800	-1.67080700	2.63875800
C	1.98257900	-2.64563200	3.84166800
H	1.09266200	-3.01982100	1.90533100
H	0.64571300	-1.47057200	2.58270000
C	-1.32546800	6.36925000	0.23502700

C	-2.88395800	4.36868600	0.40220600
H	-1.57665300	5.08984100	1.93722200
C	1.95955100	-4.48940400	-3.27300600
H	2.83691600	-3.00666700	-4.60268800
H	3.92603100	-3.58740300	-3.34950600
H	1.23598000	-5.65636300	-1.58440200
H	2.93807100	-5.22414600	-1.48773700
C	3.06607100	-3.74437500	3.70890500
H	3.26765200	-4.23021800	1.59653800
H	4.79607900	-4.14679600	2.44509900
H	1.13896100	-3.01207600	4.43759300
H	2.38782000	-1.78188500	4.38585400
H	-0.38753800	6.81677300	0.58135300
H	-1.28961100	6.32236500	-0.86005900
H	-2.14659200	7.03984200	0.51379900
H	-3.70764400	5.03818900	0.67764900
H	-3.05373900	3.39569900	0.87250700
H	-2.91912300	4.23550700	-0.68653700
H	0.93780400	-4.23695000	-3.59385900
H	2.26901100	-5.35647400	-3.86854100
H	2.61084500	-4.73694000	3.80734000
H	3.77995300	-3.65220800	4.53595200

3d-2

C	-4.32007500	-1.91934300	0.71401100
C	-4.23590700	-1.76640000	-0.82404600
C	-3.02987200	-0.89887600	-1.20255700
C	-2.97035100	-2.41681500	-1.39370600
C	-2.29520400	-0.49852900	0.06055100
C	-3.00650100	-1.24285700	1.22929600
C	-5.67776400	-1.51870100	1.36527800
C	-5.77180900	-1.99274100	2.82627300
C	-6.10689200	-0.04221000	1.23830700
C	-5.50587700	-1.80867600	-1.65293000
C	-2.93337600	-3.07831600	-2.72019300
C	-2.28507500	-4.22515800	-2.94925700
C	-3.03655900	0.06813800	-2.34100200
C	-2.27617800	-0.01141500	-3.43528900
O	-3.23896500	-0.15478500	2.22102800
C	-3.11728600	0.98675300	1.62237800
C	-3.36647500	2.25255400	2.35501100
O	-2.73833600	0.96230900	0.41335300
H	-4.21443300	-2.98721100	0.94828700
H	-2.35551800	-2.94587800	-0.66263400
H	-2.36114300	-1.93448400	1.76420300

H	-6.41220200	-2.10807500	0.80248100
H	-6.77761100	-1.81027100	3.22046400
H	-5.57446000	-3.06757800	2.91146100
H	-5.06346200	-1.46494300	3.47435700
H	-7.19814100	0.03416700	1.28992400
H	-5.79497800	0.41086700	0.29087600
H	-5.71830400	0.56698000	2.06082600
H	-6.24326100	-1.07264100	-1.32030100
H	-5.29534500	-1.59700700	-2.70418200
H	-5.97346100	-2.79943300	-1.60335800
H	-3.47501300	-2.60685700	-3.53509200
H	-2.29316500	-4.69549200	-3.92780700
H	-1.73354900	-4.74138700	-2.16586200
H	-3.71290900	0.91571300	-2.22741700
H	-2.33161400	0.74485100	-4.21353100
H	-1.58327100	-0.83197300	-3.59756200
H	-4.12711100	2.83685500	1.82807100
H	-2.44103000	2.83908500	2.35486400
H	-3.68933700	2.04676600	3.37566100
Au	-0.18476600	-0.51900600	0.07407500
H	-0.64300500	6.93178600	0.28096000
C	-1.49035600	6.58582900	-0.32015000
C	-1.91133200	5.15529000	0.07800600
H	-1.19136700	6.62332000	-1.37425400
H	-2.31985700	7.28829800	-0.17838100
C	-0.73319400	4.19674100	-0.04910800
C	-3.15229300	4.71753000	-0.71912200
H	-2.18989500	5.18631900	1.14181400
C	-0.36169600	3.62569300	-1.26480800
C	0.08729500	3.92781100	1.04237700
H	-4.00184600	5.37048800	-0.48934300
H	-3.43790600	3.68350400	-0.49308900
H	-2.98096700	4.78121900	-1.79952700
C	0.78842600	2.84051900	-1.42390400
H	-0.96003600	3.82976100	-2.14855400
C	1.24618500	3.13456000	0.96808900
H	-0.15055300	4.39491300	1.99793900
C	1.07463600	2.48560100	-2.89717100
C	1.60285500	2.55760100	-0.28374800
C	1.97516500	3.03895200	2.32634700
H	0.09015500	2.54296500	-3.37830400
C	1.94236000	3.56346500	-3.58434800
C	1.59650400	1.08159600	-3.22151100
C	2.95105400	1.89481900	-0.49301400

C	3.49006100	2.78466900	2.37244400
C	1.21464900	2.07319100	3.26354100
H	1.85169100	4.03718000	2.76724000
H	1.96422500	3.39105400	-4.66694800
H	1.54318100	4.56833000	-3.40953900
H	2.97521300	3.53915600	-3.22475700
H	1.50240000	0.90440100	-4.29980000
H	1.00884100	0.31559100	-2.70574800
H	2.64833900	0.95062400	-2.96094200
C	3.96374400	2.79312500	-0.88205300
C	3.30236900	0.52109500	-0.37022700
H	3.82854800	2.90210100	3.40856100
H	4.04018700	3.50553000	1.76191400
H	3.78012100	1.78481000	2.04259600
H	0.19486300	2.42842200	3.44946700
H	1.13302300	1.07274000	2.82861600
H	1.72001800	1.98949600	4.23299500
C	5.26734100	2.39346600	-1.16117800
H	3.70488700	3.84446500	-0.95893900
C	4.62575100	0.13490500	-0.66759400
P	2.18183300	-0.84311000	0.20330200
C	5.60205100	1.04617600	-1.05928300
H	6.00952900	3.12890800	-1.45796700
H	4.90731900	-0.90970400	-0.60448900
C	2.64929400	-2.38418400	-0.77854200
C	2.72153800	-1.14505800	1.99363500
H	6.60796800	0.70209800	-1.28060300
C	2.60369700	-2.16698100	-2.30597500
C	1.75627800	-3.58782600	-0.39456800
H	3.68091700	-2.63597400	-0.49922400
C	4.11270500	-1.82863800	2.20933200
C	1.61663600	-1.81570100	2.84767500
H	2.80933400	-0.11879300	2.36243200
C	3.02904200	-3.43789100	-3.06177900
H	1.57952600	-1.89945900	-2.59780400
H	3.24522800	-1.33064000	-2.59814100
C	2.17635000	-4.85911100	-1.15447600
H	1.79694900	-3.78028900	0.68161600
H	0.71138500	-3.34649000	-0.63456800
C	3.99941600	-3.21086900	2.87125500
H	4.67989800	-1.91448200	1.27866200
H	4.71534700	-1.17731500	2.85459500
C	2.14834800	-2.10307200	4.26058600
H	1.26730100	-2.74771800	2.38970800

H	0.74334700	-1.15467100	2.89342400
C	2.16589600	-4.64511700	-2.67345900
H	2.96956500	-3.25409400	-4.14123500
H	4.08417300	-3.65563800	-2.84041100
H	1.50829200	-5.68378500	-0.87678700
H	3.18530500	-5.15562500	-0.83290800
C	3.30160600	-3.13873000	4.24469700
H	3.44744500	-3.88885400	2.20777200
H	4.99970200	-3.64575200	2.97905300
H	1.33103900	-2.45086500	4.90258500
H	2.49709400	-1.15765500	4.69773400
H	1.13247300	-4.47541600	-3.00973400
H	2.51899400	-5.54761000	-3.18625800
H	2.92133400	-4.13320500	4.50573900
H	4.03397600	-2.87879400	5.01805100

Ts_{3d}-2

C	-4.38917000	-1.86166600	0.68201800
C	-4.28890500	-1.70929300	-0.85757500
C	-3.01556800	-0.92801400	-1.20478200
C	-3.10002100	-2.48315800	-1.40114900
C	-2.24552000	-0.67505900	0.02308600
C	-3.01004400	-1.31637400	1.19792800
C	-5.71223100	-1.36283700	1.33049100
C	-5.84815100	-1.85035600	2.78415400
C	-6.02896000	0.14170200	1.22562100
C	-3.05779000	-3.09866100	-2.74615400
C	-2.44467300	-4.26204800	-2.99216400
C	-2.89168900	0.01904500	-2.35284700
C	-2.11433300	-0.13750400	-3.42596900
O	-3.09294900	-0.31592900	2.26719800
C	-3.00781700	0.91544500	1.80163100
C	-3.13427900	2.01093700	2.81189000
O	-2.81149700	1.09950400	0.59159600
H	-4.37804100	-2.93798500	0.89957800
H	-2.55150000	-3.07490000	-0.66725600
H	-2.41610600	-2.10820200	1.65474100
H	-6.48780600	-1.88691500	0.75735700
H	-6.83574200	-1.58927600	3.18009100
H	-5.74259800	-2.93930800	2.85341100
H	-5.09697000	-1.39447400	3.43785800
H	-7.11074900	0.29744600	1.29615600
H	-5.69180200	0.58917000	0.28551800
H	-5.58508300	0.70692900	2.05039400
H	-3.56949400	-2.58635300	-3.55480600

H	-2.45679600	-4.70993900	-3.98106100
H	-1.92275000	-4.81488700	-2.21375900
H	-3.48297600	0.92858100	-2.24928900
H	-2.07443100	0.62175200	-4.20195500
H	-1.49924100	-1.02041900	-3.57297100
H	-2.83508100	2.95870700	2.36562200
H	-2.50716100	1.78144300	3.67839800
H	-4.17030700	2.07738600	3.15987200
Au	-0.17879200	-0.52676400	0.07228100
H	-0.79460800	6.88307000	0.06569200
C	-1.65348300	6.47113800	-0.47471800
C	-1.99694800	5.04980100	0.01835400
H	-1.40522500	6.46261800	-1.54266800
H	-2.50407100	7.14762500	-0.33143400
C	-0.78602600	4.13329600	-0.10657700
C	-3.25007200	4.51444600	-0.69601100
H	-2.23223400	5.12773700	1.09034200
C	-0.40477500	3.55976300	-1.31826700
C	0.05124700	3.90682200	0.98047900
H	-4.11059200	5.15961100	-0.48554600
H	-3.49173300	3.49608000	-0.37395500
H	-3.11726500	4.49931100	-1.78401400
C	0.76652300	2.80671100	-1.47541700
H	-1.01429500	3.73748100	-2.20034900
C	1.23060800	3.14508900	0.90997900
H	-0.19653600	4.37646700	1.93164000
C	1.06017800	2.44898800	-2.94656800
C	1.59247400	2.55765400	-0.33525200
C	1.97318700	3.09489300	2.26369200
H	0.07377000	2.47618600	-3.42654600
C	1.89651400	3.54547800	-3.64306600
C	1.62006000	1.05769800	-3.26266900
C	2.94744500	1.91045700	-0.54010000
C	3.49119600	2.85931200	2.30428900
C	1.23296600	2.14721900	3.23481100
H	1.84093900	4.10352500	2.67769000
H	1.92086700	3.36703900	-4.72471800
H	1.47031800	4.53995000	-3.47327500
H	2.93058500	3.55191200	-3.28607500
H	1.52912500	0.87008000	-4.33956200
H	1.05389200	0.28025100	-2.74038300
H	2.67562900	0.95604500	-3.00330700
C	3.95218200	2.80881600	-0.94838800
C	3.30895200	0.54189400	-0.39527300

H	3.83601300	3.00366600	3.33493600
H	4.02868800	3.57257500	1.67395100
H	3.79078100	1.85561400	1.99445000
H	0.20830000	2.49132000	3.41248900
H	1.16662300	1.13215700	2.83222400
H	1.74425600	2.10245100	4.20377800
C	5.25696800	2.41237700	-1.22651900
H	3.68584800	3.85696900	-1.04115600
C	4.63316600	0.15784600	-0.69152200
P	2.19666500	-0.81466900	0.20780700
C	5.60119100	1.06902400	-1.10332300
H	5.99332700	3.14716800	-1.53903700
H	4.92221800	-0.88363500	-0.61185300
C	2.66522100	-2.37182700	-0.74850100
C	2.73858400	-1.08468000	2.00181600
H	6.60843700	0.72809700	-1.32342800
C	2.61126700	-2.18181200	-2.27902000
C	1.78434600	-3.57595200	-0.33932300
H	3.69992700	-2.61060000	-0.46935600
C	4.13357300	-1.75779000	2.22532500
C	1.63788000	-1.74647200	2.86808100
H	2.82226000	-0.05196900	2.35305600
C	3.04420300	-3.46202900	-3.01454900
H	1.58335100	-1.92840100	-2.57091900
H	3.24369600	-1.34484800	-2.58838800
C	2.21256800	-4.85675100	-1.07861700
H	1.83099200	-3.74872100	0.73988000
H	0.73613200	-3.34805700	-0.57897300
C	4.02878100	-3.12825100	2.91259600
H	4.69857000	-1.85778900	1.29466300
H	4.73481900	-1.09194000	2.85679200
C	2.17308600	-2.00629000	4.28511000
H	1.29330300	-2.68840700	2.42686900
H	0.76048700	-1.09013000	2.90365200
C	2.19374300	-4.66994800	-2.60106400
H	2.97851800	-3.29775200	-4.09677200
H	4.10209600	-3.66682900	-2.79428300
H	1.55365600	-5.68256500	-0.78307700
H	3.22563600	-5.13810800	-0.75659600
C	3.33254900	-3.03519600	4.28552600
H	3.47978500	-3.82146000	2.26247200
H	5.03166400	-3.55542900	3.02674200
H	1.35854300	-2.34777000	4.93388500
H	2.51667200	-1.05136200	4.70521000

H	1.15719400	-4.51575500	-2.93593200
H	2.55250300	-5.57820500	-3.09947800
H	2.95865200	-4.02703000	4.56511200
H	4.06453100	-2.75707500	5.05286100
C	-5.54756700	-1.61978400	-1.69880500
H	-5.30832300	-1.42374500	-2.74710800
H	-6.11083500	-2.55941000	-1.65745700
H	-6.20791000	-0.81554900	-1.36444100
4d-2			
C	-4.31993500	-1.91980400	0.71355300
C	-4.23590900	-1.76608500	-0.82443800
C	-3.02990700	-0.89832000	-1.20261000
C	-2.97041300	-2.41617500	-1.39455500
C	-2.29513000	-0.49864900	0.06066100
C	-3.00631100	-1.24360500	1.22907500
C	-5.67756600	-1.51945700	1.36513900
C	-5.77154300	-1.99430800	2.82587600
C	-6.10665100	-0.04287500	1.23902100
C	-2.93346600	-3.07699700	-2.72138900
C	-2.28487000	-4.22353500	-2.95114800
C	-3.03666600	0.06934300	-2.34049300
C	-2.27671800	-0.00983300	-3.43511200
O	-3.23871100	-0.15605400	2.22142600
C	-3.11703400	0.98580400	1.62339300
C	-3.36618500	2.25126700	2.35668200
O	-2.73817800	0.96200300	0.41431300
H	-4.21431500	-2.98780200	0.94727100
H	-2.35549700	-2.94561300	-0.66382100
H	-2.36090800	-1.93551700	1.76354800
H	-6.41207300	-2.10848000	0.80206600
H	-6.77731800	-1.81202600	3.22022600
H	-5.57422700	-3.06920000	2.91046500
H	-5.06315200	-1.46689000	3.47422200
H	-7.19790100	0.03351600	1.29060200
H	-5.79466800	0.41077300	0.29188200
H	-5.71809700	0.56581200	2.06193300
H	-3.47537100	-2.60528200	-3.53596100
H	-2.29298500	-4.69337100	-3.92993500
H	-1.73306800	-4.74000600	-2.16810700
H	-3.71261800	0.91713000	-2.22613400
H	-2.33218100	0.74691800	-4.21287900
H	-1.58416100	-0.83053600	-3.59813900
H	-4.12773400	2.83526300	1.83070800
H	-2.44109000	2.83833100	2.35574600

H	-3.68793300	2.04497600	3.37758200
Au	-0.18471600	-0.51900900	0.07395000
H	-0.64386900	6.93171100	0.27944200
C	-1.49149300	6.58513600	-0.32092900
C	-1.91184900	5.15475700	0.07841600
H	-1.19315100	6.62204200	-1.37524000
H	-2.32108400	7.28749300	-0.17911800
C	-0.73356300	4.19640600	-0.04875700
C	-3.15315400	4.71611800	-0.71771500
H	-2.18981200	5.18639700	1.14236300
C	-0.36196000	3.62558000	-1.26454700
C	0.08694600	3.92742500	1.04269400
H	-4.00270300	5.36912800	-0.48806000
H	-3.43847400	3.68224000	-0.49065800
H	-2.98237200	4.77890700	-1.79825900
C	0.78823500	2.84055000	-1.42372700
H	-0.96030800	3.82972000	-2.14827700
C	1.24597600	3.13436300	0.96830400
H	-0.15096100	4.39438600	1.99831300
C	1.07446700	2.48577700	-2.89702900
C	1.60271200	2.55760200	-0.28358900
C	1.97508300	3.03887800	2.32651400
H	0.08993900	2.54287900	-3.37810300
C	1.94184400	3.56396600	-3.58415000
C	1.59672200	1.08196100	-3.22152100
C	2.95096100	1.89496800	-0.49297400
C	3.49000000	2.78471700	2.37246700
C	1.21477300	2.07311200	3.26386300
H	1.85157000	4.03713100	2.76734200
H	1.96379600	3.39162900	-4.66676100
H	1.54234900	4.56869500	-3.40928800
H	2.97470100	3.53996500	-3.22454000
H	1.50261500	0.90485700	-4.29982600
H	1.00927500	0.31574800	-2.70582100
H	2.64860200	0.95120700	-2.96100600
C	3.96356000	2.79338500	-0.88200800
C	3.30239100	0.52125100	-0.37027300
H	3.82859200	2.90224500	3.40854100
H	4.04002600	3.50556300	1.76182900
H	3.78010600	1.78485100	2.04266900
H	0.19494300	2.42819200	3.44984600
H	1.13326900	1.07259400	2.82906400
H	1.72022500	1.98959300	4.23329000
C	5.26717800	2.39385200	-1.16121800

H	3.70461700	3.84470800	-0.95880600
C	4.62581200	0.13521200	-0.66769500
P	2.18195200	-0.84301800	0.20317600
C	5.60201600	1.04658000	-1.05939300
H	6.00928500	3.12936900	-1.45802000
H	4.90748900	-0.90937400	-0.60461400
C	2.64950500	-2.38406300	-0.77873200
C	2.72163200	-1.14499100	1.99352500
H	6.60795600	0.70260600	-1.28075700
C	2.60371800	-2.16680700	-2.30612400
C	1.75675100	-3.58782100	-0.39465500
H	3.68120600	-2.63567800	-0.49950600
C	4.11286700	-1.82833700	2.20921800
C	1.61679800	-1.81576900	2.84753100
H	2.80922700	-0.11869800	2.36231500
C	3.02914900	-3.43763300	-3.06205800
H	1.57947600	-1.89942900	-2.59785600
H	3.24510400	-1.33036900	-2.59833600
C	2.17685900	-4.85903200	-1.15470900
H	1.79768200	-3.78036800	0.68150600
H	0.71176200	-3.34665300	-0.63442000
C	3.99980700	-3.21055200	2.87125600
H	4.68004000	-1.91426800	1.27853000
H	4.71550600	-1.17688800	2.85435900
C	2.14852500	-2.10300800	4.26048100
H	1.26759500	-2.74785400	2.38959500
H	0.74341600	-1.15485900	2.89325000
C	2.16618300	-4.64497200	-2.67368000
H	2.96951800	-3.25377300	-4.14149300
H	4.08433400	-3.65525700	-2.84082200
H	1.50892900	-5.68378400	-0.87694700
H	3.18589300	-5.15544500	-0.83329200
C	3.30189000	-3.13853600	4.24464800
H	3.44800600	-3.88866900	2.20775900
H	5.00017400	-3.64523400	2.97910600
H	1.33124500	-2.45084500	4.90249100
H	2.49716900	-1.15751800	4.69756000
H	1.13270000	-4.47536000	-3.00983000
H	2.51929400	-5.54741200	-3.18656800
H	2.92168700	-4.13306600	4.50559800
H	4.03414900	-2.87858400	5.01810400
C	-5.50606000	-1.80792500	-1.65303600
H	-6.24287000	-1.07121000	-1.32061000
H	-5.29572600	-1.59708100	-2.70448800

H	-5.97431400	-2.79833500	-1.60276000
Ts _{4d} -2			
C	3.60332800	-2.08886500	-0.33803600
C	4.04523100	-1.31572200	0.93943000
C	3.27387200	0.01512500	0.95960200
C	2.90426800	-1.10068900	1.93623300
C	2.40663400	0.04129300	-0.32710900
C	2.88457200	-1.05175600	-1.15622000
C	4.61243900	-3.02933800	-1.07157100
C	3.85308800	-4.06715000	-1.91783100
C	5.69922400	-2.35806200	-1.92730300
C	5.46699200	-1.44365400	1.44962900
C	3.12707100	-1.02521600	3.40087700
C	2.30829700	-1.58505200	4.29691300
C	3.89417000	1.29721400	1.40804200
C	3.49738800	2.02293100	2.45598000
O	4.14091400	0.12897300	-2.11528300
C	3.58585800	1.21825500	-1.90776100
C	4.00404300	2.50207100	-2.54910200
O	2.56138600	1.29401800	-1.06951300
H	2.79203600	-2.77601800	-0.04067000
H	1.97730700	-1.62033900	1.68668900
H	2.42355600	-1.30448900	-2.10566100
H	5.11238800	-3.57680400	-0.26223800
H	4.55463600	-4.77015900	-2.37880000
H	3.14675200	-4.64915200	-1.31390500
H	3.29191300	-3.59156900	-2.73287300
H	6.44666900	-3.10819100	-2.20789200
H	6.21907700	-1.54913100	-1.40823900
H	5.28549400	-1.94163300	-2.85040100
H	6.20284800	-1.23775600	0.66751600
H	5.65512200	-0.73770900	2.26240500
H	5.66058700	-2.44999500	1.83898700
H	4.00655100	-0.49266700	3.75170100
H	2.50467900	-1.52315300	5.36295200
H	1.41485300	-2.13002300	3.99839500
H	4.73928000	1.65276500	0.81519400
H	3.99827700	2.94953900	2.72255200
H	2.67078300	1.71101800	3.08811400
H	4.65203000	3.04930700	-1.85441000
H	3.12774000	3.12364600	-2.74665400
H	4.55777700	2.30144500	-3.46682300
Au	0.27845600	-0.36374000	-0.14301800
H	-0.21321300	6.74460700	-1.49220200

C	0.65765700	6.67257400	-0.83229000
C	1.26457100	5.25312000	-0.85075600
H	0.33336100	6.94001400	0.18031800
H	1.39530800	7.41459700	-1.15935700
C	0.21021300	4.21842300	-0.47198500
C	2.53328800	5.20125000	0.01363800
H	1.55887200	5.04239500	-1.89037300
C	0.08049900	3.69375900	0.81152200
C	-0.73552400	3.81621200	-1.40962600
H	3.30290000	5.85910700	-0.40567100
H	2.93847700	4.18558700	0.08031900
H	2.33772400	5.54844900	1.03497000
C	-0.95267300	2.81873000	1.18017700
H	0.78273700	3.99892000	1.58140600
C	-1.78260800	2.92465700	-1.12836300
H	-0.67987800	4.23824600	-2.41187900
C	-0.99808900	2.54317000	2.69746300
C	-1.88767100	2.39037400	0.18860300
C	-2.69452000	2.69887100	-2.35699300
H	0.02201200	2.76352000	3.03694400
C	-1.90848400	3.55214700	3.43245000
C	-1.27893400	1.11381900	3.17646700
C	-3.09270900	1.58021900	0.61638400
C	-4.13714700	2.20231700	-2.17392200
C	-1.95056900	1.86182800	-3.42375500
H	-2.80222200	3.70155800	-2.79272600
H	-1.76245000	3.46720200	4.51587300
H	-1.67888900	4.58221200	3.13970700
H	-2.96646600	3.36589600	3.22609600
H	-1.04103300	1.03932700	4.24442400
H	-0.64998200	0.38981400	2.64757400
H	-2.32415300	0.82362600	3.05398400
C	-4.16698500	2.34924700	1.10282600
C	-3.25047700	0.16686300	0.59677300
H	-4.64051200	2.23906300	-3.14709800
H	-4.70248000	2.83677900	-1.48681200
H	-4.20716200	1.17541300	-1.80716700
H	-1.03151500	2.35954400	-3.74888200
H	-1.66130000	0.88035500	-3.03639500
H	-2.58164000	1.71111200	-4.30749900
C	-5.35304200	1.78594800	1.56468800
H	-4.05624400	3.42909900	1.10518200
C	-4.45796800	-0.38604700	1.07146400
P	-2.00280800	-1.04498200	-0.04565100

C	-5.50014700	0.40149800	1.55194200
H	-6.15171600	2.42470200	1.93058900
H	-4.59294200	-1.46142200	1.08163300
C	-2.15762400	-2.59294800	1.01916400
C	-2.63506700	-1.48769400	-1.77124200
H	-6.41202200	-0.06618100	1.91100500
C	-2.02651400	-2.31011100	2.53121700
C	-1.13719400	-3.67831100	0.60274700
H	-3.16161300	-2.99587300	0.82891600
C	-3.94700300	-2.33381200	-1.84003800
C	-1.53035100	-2.06485300	-2.69303400
H	-2.87555000	-0.49552300	-2.16190800
C	-2.21755600	-3.59532300	3.35564700
H	-1.02890200	-1.89726500	2.73316700
H	-2.74923800	-1.55468900	2.85165300
C	-1.32029400	-4.96411200	1.42959900
H	-1.22967800	-3.91651100	-0.46044800
H	-0.12002600	-3.28793100	0.75074900
C	-3.71025300	-3.75876600	-2.36273800
H	-4.46334700	-2.36816800	-0.87688300
H	-4.64111100	-1.82186100	-2.51827500
C	-2.15054400	-2.55739300	-4.01005600
H	-0.99433200	-2.89081200	-2.21089800
H	-0.78126200	-1.28788000	-2.88758400
C	-1.23088800	-4.69286300	2.93668900
H	-2.10291000	-3.36189900	4.42093800
H	-3.24721900	-3.95943200	3.22672200
H	-0.56684400	-5.70078700	1.12504500
H	-2.29937200	-5.40607000	1.19474300
C	-3.10316700	-3.75668700	-3.78301200
H	-3.04636100	-4.29559700	-1.67342800
H	-4.65671700	-4.31117400	-2.35736800
H	-1.35916700	-2.82789000	-4.71823700
H	-2.69765300	-1.72331600	-4.46949400
H	-0.20733400	-4.37800100	3.18932300
H	-1.42147600	-5.61360900	3.50028500
H	-2.56747000	-4.69929100	-3.94585900
H	-3.90481000	-3.72752800	-4.53010000
5d-2			
C	-1.11172300	1.06972700	-0.54291400
C	-1.36216500	-0.35980700	0.04019000
C	-0.84630800	-1.49125800	-0.85287700
C	0.98198600	0.05960300	-0.12543700
C	0.40120300	1.14945700	-0.64107300

C	0.00598000	-0.97742400	0.32680600
C	-1.44160600	-2.84416200	-0.83673900
C	-1.60385400	-3.60132400	-1.92684200
C	0.35942400	-1.86688700	1.47367200
C	0.15416900	-1.57068600	2.75864600
O	3.20721700	1.67820600	-0.69905500
C	3.34141900	0.55118900	-0.28855700
C	4.65629300	-0.13537000	-0.00689100
O	2.31195600	-0.30422000	-0.00750500
H	-0.48716600	-1.18520300	-1.83485300
H	0.92304300	1.97094900	-1.10495600
H	-1.74982600	-3.24416300	0.12764600
H	-2.04074500	-4.59421900	-1.87073300
H	-1.30715700	-3.25455100	-2.91453200
H	0.84431500	-2.80913800	1.21691700
H	0.45834400	-2.24775900	3.55278700
H	-0.31932000	-0.64107000	3.06549500
H	4.70686500	-0.43560800	1.04490400
H	5.47582400	0.54524900	-0.23936000
H	4.74402900	-1.04482900	-0.61036000
C	-2.56093500	-0.63952900	0.92658000
H	-2.44712100	-1.58694900	1.45787600
H	-2.69241700	0.13609400	1.68733100
C	-1.74397400	2.25735500	0.24941900
H	-1.63384300	2.04346800	1.32232700
C	-1.02352900	3.58991400	-0.02131000
H	-1.53515100	4.40832100	0.49868500
H	0.01530200	3.57364200	0.32059800
H	-1.02315200	3.83107900	-1.09261000
C	-3.23867400	2.42401600	-0.07533200
H	-3.68353300	3.21651100	0.53820700
H	-3.36862700	2.70971400	-1.12755400
H	-3.81577900	1.51106700	0.09074500
H	-1.53932300	1.11445100	-1.55862200
H	-3.48419900	-0.69782700	0.33850500

T_{Sd}-2

C	0.75715000	1.38779100	0.48992600
C	-0.73659000	1.13717400	0.53583100
C	1.12742200	2.60540000	-0.42178700
C	0.07329500	3.72620700	-0.35557600
C	2.49787000	3.20327500	-0.05699400
C	1.35436800	-0.03290500	0.09494600
C	0.14843200	-0.84848800	-0.35796100
C	-1.03465600	-0.07377100	0.04235700

O	-2.25413900	-0.70986900	-0.11836500
C	-3.45362800	-0.08685200	0.08981700
C	-4.57814200	-1.04605100	-0.21802600
O	-3.58182600	1.05417400	0.46090000
C	1.30183500	-0.96796800	1.28591500
C	1.81369500	-2.25830600	1.45868700
C	2.53441500	-3.03092400	0.56309600
C	1.09109500	-2.91697100	-1.40473300
C	0.05775400	-2.11210900	-0.96769600
C	2.63712100	0.01046400	-0.73286000
H	1.11806700	1.63982300	1.49853800
H	-1.44964800	1.84766800	0.91972700
H	1.15328000	2.25642400	-1.46338700
H	0.40057100	4.58375400	-0.95486700
H	-0.89935400	3.40309000	-0.73728400
H	-0.06855600	4.08042600	0.67405800
H	2.75758600	4.02083500	-0.73995800
H	3.30970000	2.47348100	-0.09125900
H	2.47043400	3.61953600	0.95869500
H	-4.52898500	-1.35928800	-1.26626900
H	-5.53277100	-0.55688700	-0.02246700
H	-4.48644200	-1.94718700	0.39693700
H	0.67826800	-0.60054400	2.09704900
H	1.40610900	-2.77989800	2.32599400
H	3.24144700	-2.60257000	-0.13039600
H	2.70831700	-4.07778300	0.79724600
H	2.00035700	-2.51221400	-1.82169900
H	0.86539100	-3.93360900	-1.71509300
H	-0.92991400	-2.56608400	-0.90197300
H	2.91585100	-0.96070600	-1.13319300
H	3.47250800	0.35456400	-0.11496500
H	2.53689400	0.68693200	-1.58536600

6d-2

C	-0.68614500	1.29919300	-0.36520200
C	0.81885100	1.21228000	-0.21583900
C	-1.32237700	2.57898300	0.24085500
C	-0.64484900	3.84848500	-0.30768600
C	-2.83526200	2.67024600	-0.02429500
C	-1.18679000	-0.10995500	0.16698300
C	0.06069900	-0.99350400	-0.01148000
C	1.19616600	-0.06451900	-0.04512400
O	2.45621700	-0.63304900	0.04653900
C	3.61116800	0.09454500	-0.01303100
C	4.79730000	-0.83362100	0.09726300

O	3.66599700	1.29444800	-0.13183600
C	-2.39757800	-0.61181100	-0.60490200
C	-2.88365200	-1.85722700	-0.59675600
C	-2.30008400	-3.02697300	0.16274700
C	-0.86731600	-3.39352000	-0.25948500
C	0.18709400	-2.32300700	-0.15458300
C	-1.49379000	-0.03375300	1.68991000
H	-0.91249000	1.33103400	-1.44623100
H	1.48989900	2.04991500	-0.31261500
H	-1.16357500	2.56558900	1.32728800
H	-1.14274200	4.74409300	0.08209400
H	0.41106300	3.91407000	-0.02921900
H	-0.70725300	3.88687900	-1.40332300
H	-3.24484700	3.58722700	0.41562600
H	-3.39276900	1.82624200	0.39188600
H	-3.04032800	2.70444100	-1.10269800
H	4.74915700	-1.39892500	1.03370900
H	5.71687800	-0.24873100	0.06278500
H	4.78652200	-1.55868700	-0.72329900
H	-2.91549000	0.12856800	-1.21152400
H	-3.76883900	-2.05928300	-1.19896900
H	-2.31198400	-2.82553600	1.24186200
H	-2.93500500	-3.90862500	0.01717100
H	-0.54001600	-4.26149000	0.33208500
H	-0.88442600	-3.75001000	-1.30247800
H	1.20541900	-2.69372600	-0.26845800
H	-1.70614200	-1.02784900	2.08945400
H	-2.35913700	0.60216000	1.89574200
H	-0.63221100	0.36639400	2.23524400
Ts _{1c} -2			
C	-4.57221400	0.06011500	-1.06267900
C	-4.74814000	0.72059700	0.31826200
C	-5.02572400	-0.11660300	1.40189100
C	-2.98489100	-0.09796900	0.52502800
C	-3.39240900	-0.87551000	-0.69304000
C	-5.82769600	-0.44233400	-1.82396600
C	-5.40258900	-1.07525500	-3.16063000
C	-6.77839900	-1.36312200	-1.04510600
C	-1.94768900	0.40333300	1.14733800
C	-4.87803400	2.21829800	0.39694500
C	-5.39013700	0.28551300	2.74547600
C	-5.82371300	-0.61408400	3.64790100
C	-1.85908300	1.37221500	2.24248900
C	-2.28980400	1.18312800	3.49811500

O	-3.80865400	-2.22217400	-0.37962000
C	-2.98820400	-3.24157300	-0.77677200
C	-3.55179100	-4.57417300	-0.35631000
O	-1.95687100	-3.06487000	-1.38496200
H	-4.11651700	0.82341100	-1.70468300
H	-5.08531800	-1.18425800	1.21266400
H	-2.59555500	-0.93345600	-1.43548700
H	-6.39339500	0.47046000	-2.06281600
H	-6.28226300	-1.30544200	-3.77061700
H	-4.76283500	-0.40092100	-3.74211200
H	-4.85386600	-2.01129600	-3.00579200
H	-7.65061200	-1.59451400	-1.66626800
H	-7.15234400	-0.89016200	-0.13032100
H	-6.30129200	-2.30927300	-0.77381300
H	-5.90826200	2.50804500	0.14822300
H	-4.65020200	2.61158100	1.38987600
H	-4.21443700	2.70591000	-0.32176500
H	-5.37238400	1.33998300	3.00170200
H	-6.16565400	-0.31155200	4.63265500
H	-5.86086400	-1.67739300	3.42322300
H	-1.30069100	2.27549900	1.99677200
H	-2.11849500	1.93724100	4.26087000
H	-2.78387200	0.26863600	3.80807200
H	-4.56799200	-4.69853500	-0.74395000
H	-3.60824400	-4.62804500	0.73627200
H	-2.91210800	-5.37361500	-0.73072300
H	2.54401000	-1.99787400	4.94518300
C	3.16462300	-1.85897000	4.05280900
C	2.27162200	-1.59469900	2.83046700
C	4.08409500	-3.08677600	3.83889500
H	3.77125900	-0.96271300	4.24053900
C	3.14703800	-1.19511600	1.61517600
H	1.67079400	-2.48609200	2.61791700
H	1.55648600	-0.79125000	3.04214200
C	4.37339400	-3.34564000	2.34416700
H	3.62497300	-3.98166500	4.27537300
H	5.02601800	-2.93220000	4.37829400
P	2.15628200	-1.03656100	0.01443500
C	4.46173900	-2.03777100	1.54341800
H	3.44335600	-0.15568400	1.77758700
H	3.58849700	-3.98192800	1.91668600
H	5.30844600	-3.90628400	2.23198000
Au	-0.03870300	-0.25255500	0.48378500
C	3.21822400	0.03963600	-1.06480600

C	2.12550500	-2.73498800	-0.79440400
H	4.75837800	-2.25087700	0.51263900
H	5.27503700	-1.42726600	1.95570600
C	3.04400400	1.43532600	-1.27778600
C	4.30370600	-0.60669400	-1.69159400
C	1.66439100	-2.70649400	-2.26799600
C	1.25531500	-3.73609500	0.00123000
H	3.16054000	-3.10198900	-0.76273600
C	1.95947300	2.34483200	-0.73761200
C	3.97927200	2.09164800	-2.10078300
C	5.21025700	0.06955200	-2.50298000
H	4.44571800	-1.67244500	-1.55839700
C	1.75134000	-4.11073800	-2.89224000
H	0.62584000	-2.35586500	-2.31002700
H	2.26749600	-2.00519500	-2.85218400
C	1.33651000	-5.14272100	-0.62024700
H	1.57046500	-3.78639900	1.04723100
H	0.21378100	-3.39227400	-0.00873000
C	0.83095600	2.64852000	-1.56366500
C	2.15357300	3.09356000	0.45708800
C	5.04627500	1.43638100	-2.70855100
H	3.85761100	3.15963300	-2.25284400
H	6.03002500	-0.47087000	-2.96683800
C	0.93041900	-5.13747800	-2.10032000
H	1.40609200	-4.06575200	-3.93226800
H	2.80451200	-4.42742100	-2.92712400
H	0.69679000	-5.82709400	-0.04887600
H	2.36393300	-5.52298700	-0.52050000
C	-0.07531400	3.63203000	-1.14467800
C	0.53359700	2.11259300	-2.97984400
C	1.21008400	4.08015200	0.79631500
C	3.30838300	3.02765100	1.48395600
H	5.73971000	1.99093500	-3.33419600
H	-0.13425800	-4.88220500	-2.18011800
H	1.05664000	-6.13820800	-2.53121300
C	0.09553900	4.37906500	0.02222100
H	-0.91596400	3.85878500	-1.79654600
H	-0.53370300	2.32513700	-3.12490400
C	1.26954800	2.93004200	-4.06529100
C	0.68468700	0.60905800	-3.24470400
H	1.38815200	4.67051700	1.69326900
C	4.67471400	2.45127300	1.08219600
C	2.80654900	2.40395700	2.80721300
H	3.51318800	4.08171000	1.71613000

C	-0.81889000	5.54150800	0.38780300
H	0.88356100	2.66650300	-5.05728400
H	1.12473600	4.00592900	-3.92016500
H	2.34422200	2.72645000	-4.06444000
H	0.20987900	0.36422100	-4.20262500
H	0.19308700	0.01325100	-2.46773600
H	1.72804600	0.29606700	-3.31053000
H	5.37597200	2.62095500	1.90762400
H	5.08182700	2.94670000	0.19726000
H	4.65973200	1.37772800	0.88061300
H	1.97594900	2.97980900	3.22769100
H	2.44483700	1.38175200	2.66314700
H	3.61054800	2.38245600	3.55221500
C	-0.57889500	6.74188500	-0.55080100
C	-2.30821300	5.15793900	0.41139300
H	-0.54497900	5.85886400	1.40316800
H	0.47181900	7.05008300	-0.53787100
H	-0.84167700	6.49204700	-1.58571700
H	-1.18989200	7.59938600	-0.24599000
H	-2.91802600	6.01205500	0.72703500
H	-2.49691100	4.33152500	1.10593200
H	-2.65982000	4.85433900	-0.58231700

2c-2

C	-4.23234700	-0.62270900	-0.84314500
C	-5.05674200	-0.48053600	0.37438800
C	-4.27950400	-0.83292200	1.57480400
C	-2.80444600	-0.85853100	1.07568800
C	-2.92529500	-1.29648500	-0.36464600
C	-4.91144200	-0.99425400	-2.19121600
C	-3.89580800	-0.93553600	-3.34256800
C	-5.65293200	-2.34217500	-2.15723900
C	-1.67732000	-0.52397200	1.72396600
C	-6.42253700	0.06096300	0.41467100
C	-4.71591400	-0.18722600	2.86130900
C	-5.52362100	-0.76035300	3.75525800
C	-1.59800900	-0.20857600	3.15950100
C	-1.85637700	-1.06510400	4.15941600
O	-3.11044000	-2.74422300	-0.38659500
C	-2.15125800	-3.49966200	-0.99540800
C	-2.38932300	-4.96854700	-0.75143100
O	-1.23331100	-3.03229500	-1.63265700
H	-3.92736900	0.45096300	-0.93143500
H	-4.54956500	-1.92131800	1.60372300
H	-2.06263400	-1.04514500	-0.97644400

H	-5.65953700	-0.21089000	-2.37636400
H	-4.40285300	-1.11862500	-4.29548500
H	-3.41291900	0.04680000	-3.40573900
H	-3.11001500	-1.68965300	-3.23026900
H	-6.20014000	-2.48200800	-3.09521700
H	-6.38318400	-2.39393300	-1.34039900
H	-4.96263400	-3.17988000	-2.04061400
H	-6.98146000	-0.09554500	-0.50960900
H	-6.97034200	-0.30036000	1.29109000
H	-6.32602300	1.15176700	0.56663100
H	-4.35855200	0.82808000	3.01680300
H	-5.83233900	-0.23552000	4.65411600
H	-5.88320800	-1.78157400	3.64399000
H	-1.19490000	0.77555800	3.40388800
H	-1.70349500	-0.78510400	5.19776700
H	-2.19955000	-2.07889500	3.96962300
H	-2.00018600	-5.23153300	0.23954200
H	-1.85776900	-5.55363500	-1.50314500
H	-3.45555300	-5.20914900	-0.76305700
H	3.83848300	-1.08447600	4.72758400
C	4.24309900	-0.76980900	3.75898400
C	3.14208100	-0.82631500	2.68884700
C	5.46070700	-1.64470100	3.37335100
H	4.55520500	0.27603000	3.88441700
C	3.64820500	-0.18286600	1.37101300
H	2.83835400	-1.86761800	2.53517200
H	2.24372000	-0.30046100	3.03067600
C	5.59893300	-1.80467900	1.84331800
H	5.37221300	-2.63652300	3.83247300
H	6.37368700	-1.19744100	3.78417300
P	2.42823100	-0.40976400	-0.06153900
C	5.14347700	-0.54154800	1.09685400
H	3.60209900	0.90048300	1.51666700
H	5.00709000	-2.66328900	1.50189800
H	6.63813900	-2.03219900	1.57916700
Au	0.18727600	-0.41098700	0.78442200
C	2.91598200	0.92883500	-1.25768800
C	2.85388800	-2.05133400	-0.88703100
H	5.35314700	-0.64245200	0.02907900
H	5.75953800	0.30307700	1.43091600
C	2.23404800	2.16343600	-1.44587200
C	4.09047200	0.69203600	-2.00151200
C	2.24787700	-2.19760000	-2.29889100
C	2.41361300	-3.24667300	-0.00739700

H	3.94897700	-2.08369300	-0.97267900
C	0.92773500	2.61199800	-0.82448200
C	2.79914300	3.09524600	-2.33737400
C	4.61802500	1.62704900	-2.88771600
H	4.60696500	-0.25552000	-1.90177400
C	2.65254600	-3.53612800	-2.94181800
H	1.15507100	-2.15817600	-2.22361000
H	2.55997500	-1.37048600	-2.94330500
C	2.80364900	-4.58925400	-0.65254300
H	2.85592800	-3.18582700	0.99130700
H	1.32430100	-3.20619100	0.12430700
C	-0.27920900	2.46246900	-1.57753900
C	0.89186900	3.36762300	0.37937200
C	3.96952500	2.84831700	-3.04906100
H	2.29329900	4.04753700	-2.46331000
H	5.52443300	1.39897200	-3.44074700
C	2.23405300	-4.72682000	-2.06987000
H	2.19644300	-3.61063300	-3.93652100
H	3.74183800	-3.55637800	-3.09506500
H	2.45412700	-5.41060100	-0.01434100
H	3.90008600	-4.66943900	-0.68836500
C	-1.47006900	2.99392100	-1.06638800
C	-0.43426200	1.87124000	-2.99393900
C	-0.34206200	3.87826800	0.82121100
C	2.05301300	3.77122000	1.31595300
H	4.36428900	3.60135900	-3.72510800
H	1.13686900	-4.76073200	-2.01854000
H	2.56471800	-5.66943100	-2.52281700
C	-1.53474200	3.70631200	0.13146000
H	-2.37168900	2.88832400	-1.66724800
H	-1.50856600	1.65334200	-3.07261300
C	-0.14804900	2.91972300	-4.09168900
C	0.26818100	0.54565500	-3.31075600
H	-0.35315900	4.46814000	1.73592200
C	3.49260500	3.81633100	0.78129000
C	1.97489200	2.97854500	2.64038900
H	1.82469000	4.81260300	1.58167100
C	-2.82516100	4.34575300	0.62598700
H	-0.46756900	2.53474600	-5.06758000
H	-0.68744600	3.85400000	-3.90177300
H	0.91873100	3.14894300	-4.16127400
H	-0.13961900	0.13604600	-4.24305300
H	0.10041300	-0.19295400	-2.52130100
H	1.34409500	0.66289500	-3.45104100

H	4.13315200	4.25956600	1.55271700
H	3.57489100	4.43936500	-0.11315000
H	3.90328000	2.83384500	0.53775000
H	1.01656800	3.14044100	3.14484000
H	2.07160400	1.90249500	2.47237600
H	2.77173400	3.29312100	3.32469300
C	-3.22045800	5.55773500	-0.24047000
C	-3.98581100	3.33771500	0.71759300
H	-2.63469600	4.71357600	1.64302000
H	-2.41668800	6.30052200	-0.26630200
H	-3.42738300	5.25423400	-1.27378100
H	-4.12013900	6.04331700	0.15547500
H	-4.86914200	3.80733700	1.16667000
H	-3.70136600	2.47259000	1.32852600
H	-4.27426600	2.97733200	-0.27941400

Ts_{2c}-2

C	-4.47492400	-0.80613400	-0.96032800
C	-5.22580500	-0.26216100	0.23201100
C	-4.42619900	-0.12041800	1.35081200
C	-2.91182400	-0.51907700	0.89682500
C	-3.09800900	-1.25041900	-0.41968100
C	-5.26399400	-1.71703200	-1.94165200
C	-4.43219600	-2.03359300	-3.19500600
C	-5.86350200	-2.98787400	-1.31515900
C	-1.76289500	-0.27030500	1.57961800
C	-6.60445900	0.28231700	0.08307700
C	-4.74064300	0.67516000	2.56331100
C	-5.80749000	0.47180000	3.34073400
C	-1.71784500	0.01158200	3.01515500
C	-2.22606600	-0.79188700	3.96612500
O	-3.09621300	-2.66982600	-0.09833700
C	-2.10217900	-3.44373700	-0.62170600
C	-2.16878700	-4.84531800	-0.07090500
O	-1.28098800	-3.03310800	-1.41212000
H	-4.25603600	0.11685100	-1.53177300
H	-3.87929900	-1.16775300	1.64386000
H	-2.28307200	-1.05962100	-1.11490100
H	-6.11058300	-1.09934000	-2.27266200
H	-5.03705200	-2.59244100	-3.91681700
H	-4.08978200	-1.11693800	-3.69003700
H	-3.54837900	-2.63748200	-2.96442400
H	-6.55897900	-3.45126500	-2.02311700
H	-6.42429900	-2.77224800	-0.39786300
H	-5.09679500	-3.72452300	-1.06764000

H	-7.33397700	-0.53689700	0.01501000
H	-6.88751500	0.92080700	0.92105400
H	-6.69349000	0.84916500	-0.85214900
H	-4.04702500	1.47985600	2.79170400
H	-6.01101200	1.11723100	4.18979300
H	-6.50570300	-0.34366600	3.16977500
H	-1.12146500	0.87248300	3.31682800
H	-2.08837000	-0.57422400	5.02088500
H	-2.74757600	-1.71563300	3.72504000
H	-3.20052500	-5.20348100	-0.02003800
H	-1.76723000	-4.84896400	0.94947100
H	-1.56625700	-5.50957400	-0.69146500
H	3.41216100	-1.28012000	4.84842400
C	3.90828800	-1.01399200	3.90820900
C	2.88001000	-0.97356100	2.76702200
C	5.05919400	-2.00453400	3.60698000
H	4.31009700	-0.00184900	4.05188700
C	3.53105200	-0.39723000	1.48236000
H	2.48390800	-1.98129700	2.59770800
H	2.01889100	-0.35630900	3.04697600
C	5.28511500	-2.18883900	2.09027100
H	4.84455800	-2.97975000	4.05983600
H	5.98060900	-1.64388300	4.07923900
P	2.39682000	-0.53303900	-0.02998200
C	5.00222400	-0.89503700	1.31268100
H	3.57447300	0.68779500	1.61550400
H	4.63982200	-2.99099600	1.71094300
H	6.31381600	-2.51451600	1.89800700
Au	0.12079700	-0.32522100	0.68647100
C	3.05857800	0.75552200	-1.19112800
C	2.73968800	-2.20812000	-0.82370500
H	5.27524100	-1.02051700	0.26162900
H	5.66837300	-0.10803800	1.68862200
C	2.48641300	2.03753100	-1.41882300
C	4.25280600	0.42149400	-1.86239400
C	2.21949900	-2.31904900	-2.27234900
C	2.16133500	-3.36515300	0.02560600
H	3.83273000	-2.31955200	-0.83809600
C	1.19247600	2.59756500	-0.86472000
C	3.16960500	2.91324800	-2.28441500
C	4.89940900	1.30491300	-2.72183900
H	4.68862400	-0.56113100	-1.72509500
C	2.58223300	-3.68323600	-2.88565300
H	1.12906900	-2.20814900	-2.26839800

H	2.62588100	-1.51644800	-2.89438700
C	2.51465600	-4.73260600	-0.58830400
H	2.53237100	-3.32394100	1.05387900
H	1.07036900	-3.25799400	0.07237500
C	0.01209500	2.53480200	-1.67010500
C	1.16755000	3.38078500	0.32304700
C	4.35442500	2.56936000	-2.92860400
H	2.74593500	3.89979500	-2.44465000
H	5.81617800	1.00391500	-3.22006000
C	2.03858900	-4.84373700	-2.04230700
H	2.18769300	-3.73537800	-3.90759200
H	3.67594200	-3.76844200	-2.96856400
H	2.07261900	-5.52847900	0.02433100
H	3.60409400	-4.87792600	-0.54549900
C	-1.14832900	3.18406300	-1.22907600
C	-0.13298500	1.92797000	-3.08129700
C	-0.03264600	4.01580800	0.68913600
C	2.31030000	3.68773500	1.31714500
H	4.84169300	3.28230200	-3.58752400
H	0.94046700	-4.81741500	-2.06718500
H	2.34737200	-5.80511200	-2.47031000
C	-1.20275100	3.93717100	-0.05618100
H	-2.02946800	3.13360500	-1.86473100
H	-1.21697200	1.80491100	-3.20602200
C	0.29817700	2.92285400	-4.18192500
C	0.46208800	0.53948800	-3.34344900
H	-0.03286900	4.63022400	1.58791800
C	3.77547600	3.58857400	0.86569600
C	2.08325500	2.92081000	2.63950300
H	2.16807100	4.74899000	1.56263400
C	-2.44223300	4.72386300	0.34885900
H	-0.00878400	2.54681300	-5.16523300
H	-0.16358700	3.90524500	-4.03557500
H	1.38361800	3.05473200	-4.20343700
H	0.06552900	0.15031000	-4.28915600
H	0.18826500	-0.16732400	-2.55392300
H	1.54982600	0.55714600	-3.43051000
H	4.41069900	3.98400100	1.66705000
H	3.96652400	4.18387700	-0.03083100
H	4.10465600	2.56723400	0.66014500
H	1.12006200	3.18414100	3.08878500
H	2.07918300	1.83900000	2.47878500
H	2.86957100	3.15850600	3.36563800
C	-2.58494500	5.99955500	-0.50669900

C	-3.73201400	3.88733600	0.29600900
H	-2.29710900	5.04081200	1.39073700
H	-1.68861000	6.62464100	-0.43668400
H	-2.73577900	5.74811100	-1.56341000
H	-3.44332400	6.59596800	-0.17591800
H	-4.58026400	4.46636800	0.67848800
H	-3.63985200	2.97664300	0.89890900
H	-3.97651100	3.58912900	-0.73075000
3c-2			
C	4.50612900	-0.36037300	1.10517800
C	3.80354100	0.71886200	1.90919200
C	3.05732700	1.54666100	1.14490300
C	3.10776200	1.11000600	-0.34084800
C	3.71139600	-0.31803900	-0.22511000
C	6.05743200	-0.16439800	1.07619400
C	6.80119800	-1.41741800	0.58415000
C	6.52350400	1.10062800	0.33877200
C	1.74934200	1.14967000	-0.95114500
C	3.99487200	0.79894300	3.39586000
C	2.30568700	2.74446200	1.53679200
C	2.70310600	3.66165800	2.43012200
C	1.41639300	2.18894800	-1.89782600
C	2.30340500	2.80689600	-2.71299800
O	4.52753600	-0.67438200	-1.35567600
C	3.90252200	-0.81669200	-2.54460000
C	4.84231100	-1.30096900	-3.61698400
O	2.71834700	-0.57698600	-2.70128700
H	4.34052200	-1.33935000	1.57761400
H	3.81281000	1.76610600	-0.87022600
H	2.88357300	-1.03124000	-0.17474500
H	6.33283700	-0.03888600	2.13316300
H	7.88101500	-1.29365700	0.72391000
H	6.49549000	-2.30712200	1.14802300
H	6.61867300	-1.60859600	-0.47648200
H	7.59784700	1.25071800	0.49188000
H	6.01079100	1.99741000	0.70518200
H	6.35409700	1.02158700	-0.74027700
H	4.95468700	1.26220800	3.66026000
H	3.20525100	1.38823100	3.87023700
H	3.99945400	-0.20575200	3.83651700
H	1.35114500	2.89791400	1.03215600
H	2.07769200	4.51669500	2.67036800
H	3.66413400	3.60725700	2.93285500
H	0.35948500	2.41491000	-2.02199100

H	1.96659500	3.51506700	-3.46534700
H	3.36621200	2.58715400	-2.70303700
H	5.73443900	-0.66840900	-3.65896100
H	4.33222200	-1.29762100	-4.58062400
H	5.17519300	-2.31805100	-3.38234300
H	-0.65025500	-3.67042700	-4.35665400
C	-1.40213900	-3.66008300	-3.55980100
C	-0.92505400	-2.76714000	-2.40414800
C	-1.70360000	-5.10204600	-3.08223100
H	-2.30418600	-3.21200000	-3.99818600
C	-2.06824900	-2.58053700	-1.37290800
H	-0.03810000	-3.21574600	-1.94309900
H	-0.60446300	-1.78905500	-2.77985400
C	-2.09132400	-5.15099800	-1.58804900
H	-0.83083700	-5.74456900	-3.24818100
H	-2.51339700	-5.52323700	-3.68945600
P	-1.49182700	-1.67602200	0.18853800
C	-2.87642200	-3.90095900	-1.16290300
H	-2.75791000	-1.84671200	-1.80031300
H	-1.18933800	-5.24285200	-0.96986500
H	-2.68891600	-6.04619100	-1.38145000
Au	0.23561500	-0.09537700	-0.36239900
C	-3.04766100	-0.98199600	0.92138400
C	-0.86291000	-2.99224700	1.38373600
H	-3.22530300	-4.00995100	-0.13256900
H	-3.78868500	-3.83702100	-1.76928800
C	-3.46883100	0.37500100	0.84455000
C	-3.87970600	-1.91249900	1.57787100
C	-0.74544200	-2.50043700	2.84223000
C	0.49574000	-3.57095000	0.92194500
H	-1.59830800	-3.80783100	1.35568000
C	-2.74824300	1.55882500	0.22908000
C	-4.71359900	0.70230100	1.41658300
C	-5.10142500	-1.55568200	2.14066400
H	-3.56489800	-2.94599800	1.66697700
C	-0.28842600	-3.63611100	3.77406500
H	-0.01567600	-1.68135300	2.88739000
H	-1.69776300	-2.09436100	3.19436700
C	0.96445300	-4.70285600	1.85397100
H	0.43707400	-3.94642100	-0.10333400
H	1.24235400	-2.76389800	0.91901800
C	-2.01757800	2.44721100	1.07975300
C	-2.98469400	1.94843400	-1.12022400
C	-5.52486700	-0.23228700	2.05375300

H	-5.04898700	1.73223400	1.34484600
H	-5.70930100	-2.30501900	2.63878800
C	1.04326900	-4.24516100	3.31610300
H	-0.20354000	-3.25293400	4.79801800
H	-1.06023500	-4.41918200	3.79769000
H	1.93941400	-5.07243700	1.51307000
H	0.26658700	-5.54861000	1.77164100
C	-1.51566900	3.64477900	0.54754500
C	-1.78925900	2.32005900	2.59975100
C	-2.45577600	3.16937700	-1.57514500
C	-3.78652100	1.21983100	-2.22096800
H	-6.47646100	0.07449400	2.47812500
H	1.83958500	-3.49301000	3.41888900
H	1.32207200	-5.08566700	3.96246800
C	-1.72723300	4.04219800	-0.77258400
H	-0.98087800	4.31121100	1.21933800
H	-0.94234700	2.98929300	2.79726700
C	-2.97168300	2.89288400	3.41257300
C	-1.35726900	0.95799300	3.15421100
H	-2.66569700	3.46574800	-2.60167400
C	-4.90791500	0.24161500	-1.83846800
C	-2.81728200	0.59322000	-3.24927400
H	-4.30037900	2.03043600	-2.75459400
C	-1.29130400	5.40134700	-1.30770900
H	-2.68951900	2.98028100	4.46848500
H	-3.25610200	3.88846200	3.05537900
H	-3.85152100	2.24553600	3.35802300
H	-0.99886000	1.08562500	4.18270200
H	-0.53495000	0.53706700	2.56569500
H	-2.17382900	0.23441300	3.18107400
H	-5.44856300	-0.03647100	-2.75062300
H	-5.62829700	0.69789300	-1.15446400
H	-4.55148300	-0.68083900	-1.37463800
H	-2.18986900	1.35807300	-3.71897900
H	-2.14294400	-0.12810100	-2.77871500
H	-3.37162600	0.08010500	-4.04389000
C	-2.35900800	6.46913000	-0.98631100
C	0.09168400	5.85508400	-0.81178700
H	-1.23934400	5.31301100	-2.40224300
H	-3.33830000	6.18526700	-1.38585000
H	-2.46407600	6.60137200	0.09705600
H	-2.08075800	7.43654100	-1.41998100
H	0.38322100	6.78598800	-1.31030300
H	0.86482100	5.10507200	-1.01424400

H	0.09143900	6.05436800	0.26608000
Ts _{3c} -2			
C	4.46866100	-0.77891400	0.89346600
C	5.20648600	0.04321100	-0.15073700
C	4.42471400	0.37430900	-1.21384300
C	3.04539600	-0.15839800	-0.97622600
C	3.15872400	-1.17831300	0.17677500
C	5.30688100	-1.85815500	1.63401900
C	4.51057200	-2.50056400	2.78176900
C	5.97577700	-2.91779100	0.74079800
C	1.77258800	0.31694000	-1.41195900
C	6.59088400	0.54485000	0.12093600
C	4.83318500	1.19872100	-2.36459400
C	5.92854900	0.96585500	-3.09793400
C	1.63094700	1.27101000	-2.52271500
C	1.88735100	1.06848000	-3.82106400
O	3.24019900	-2.47774300	-0.45605200
C	2.36297700	-3.44542600	-0.06232600
C	2.59504500	-4.71875200	-0.83464400
O	1.53265900	-3.28476900	0.80529000
H	4.16215900	-0.07047200	1.68239900
H	2.57414500	-0.79601600	-1.91413100
H	2.28783700	-1.17057300	0.83005400
H	6.12033200	-1.28627900	2.10179600
H	5.15080800	-3.18160900	3.35283100
H	4.13131500	-1.74196200	3.47710200
H	3.65226800	-3.07712900	2.42096900
H	6.74159100	-3.45095600	1.31482000
H	6.46548500	-2.47440300	-0.13310500
H	5.26276000	-3.65868800	0.37314600
H	7.32802900	-0.26579700	0.06557700
H	6.88837100	1.32040100	-0.58708200
H	6.65290000	0.95019700	1.13936800
H	4.19636700	2.03852800	-2.62425800
H	6.20187800	1.61842800	-3.92189400
H	6.57819400	0.11452100	-2.91216100
H	1.14246100	2.19257000	-2.19899300
H	1.66187200	1.83156100	-4.55893900
H	2.30422800	0.13618300	-4.19447200
H	2.68651000	-4.51472100	-1.90524900
H	1.77568400	-5.41336400	-0.64736400
H	3.53499500	-5.17841700	-0.50818200
H	-3.62399100	-1.25516700	-4.83574500
C	-3.75626700	-0.59323200	-3.97167400

C	-2.89677300	-1.13744500	-2.80135700
C	-5.25702300	-0.49201600	-3.60912600
H	-3.38429200	0.39171200	-4.27737600
C	-3.49448600	-0.69637900	-1.44696400
H	-2.86240900	-2.23130700	-2.84810600
H	-1.86135300	-0.79303800	-2.90674800
C	-5.63767400	-1.55656800	-2.57450600
H	-5.87003400	-0.59501200	-4.51107400
H	-5.48156200	0.50274500	-3.20063000
P	-2.30615000	-0.83235200	0.02008400
C	-4.89121100	-1.34047000	-1.23257100
H	-3.63825500	0.38750900	-1.50702400
H	-5.39459800	-2.54866400	-2.97681400
H	-6.71780300	-1.55689800	-2.39093100
Au	-0.08187700	-0.26519600	-0.65429300
C	-3.04030300	0.29582100	1.29727400
C	-2.45340900	-2.58239700	0.69218400
H	-4.80588900	-2.30626100	-0.72363300
H	-5.48383700	-0.69222000	-0.57775300
C	-2.56626300	1.59349000	1.63811300
C	-4.19305300	-0.19529400	1.94456100
C	-1.74932400	-2.77471200	2.05109200
C	-1.94239700	-3.62047500	-0.33281000
H	-3.52591800	-2.76431400	0.83966400
C	-1.35529000	2.32809500	1.09788400
C	-3.29162800	2.31889300	2.60277400
C	-4.88259800	0.54323500	2.90187300
H	-4.56773600	-1.18296100	1.70061300
C	-1.95016200	-4.20863500	2.57339100
H	-0.67654500	-2.58470700	1.93215700
H	-2.13184700	-2.05876600	2.78479500
C	-2.12579200	-5.05485200	0.19846300
H	-2.46828400	-3.51953700	-1.28744200
H	-0.87842000	-3.43501000	-0.52770400
C	-0.14388300	2.33166800	1.85995100
C	-1.46178800	3.20907000	-0.01572600
C	-4.42698700	1.81672500	3.23221100
H	-2.94669700	3.31761900	2.85136000
H	-5.76427000	0.12509100	3.37831800
C	-1.45347000	-5.25149100	1.56371500
H	-1.42464900	-4.32051300	3.52934800
H	-3.01740500	-4.37533600	2.78215600
H	-1.72465900	-5.76496600	-0.53558500
H	-3.20056800	-5.27248500	0.28343600

C	0.91891200	3.14926800	1.44948600
C	0.12514600	1.61917900	3.20125800
C	-0.35755700	4.01393800	-0.35063300
C	-2.66291600	3.45725700	-0.95496400
H	-4.94947700	2.41832500	3.97035700
H	-0.36614100	-5.14870500	1.45181900
H	-1.64592200	-6.26478700	1.93635700
C	0.84030700	4.01253700	0.35611700
H	1.82373300	3.14440500	2.05263300
H	1.22041800	1.59599000	3.27311900
C	-0.35073000	2.46472000	4.40377800
C	-0.31996500	0.16058000	3.35418700
H	-0.46477500	4.70573500	-1.18462800
C	-4.09411000	3.17528100	-0.47176900
C	-2.39539500	2.80793700	-2.33197400
H	-2.64144300	4.54123400	-1.12991700
C	1.95654500	4.98806600	0.00439000
H	0.03789200	2.03820900	5.33610600
H	0.00408300	3.49827800	4.33017900
H	-1.44171400	2.48193400	4.47814200
H	0.15713700	-0.27020300	4.24268000
H	-0.01788800	-0.44127300	2.49092500
H	-1.39902900	0.06041200	3.48480000
H	-4.79311300	3.56314100	-1.22202000
H	-4.31104700	3.68090000	0.47276000
H	-4.31434100	2.11398400	-0.33633500
H	-1.49800700	3.22721900	-2.79892200
H	-2.23653300	1.72897200	-2.24431400
H	-3.23762100	2.97982400	-3.01253300
C	1.95822100	6.18417700	0.97902600
C	3.34607300	4.33089200	-0.05125200
H	1.73638300	5.38212500	-0.99740100
H	0.98625400	6.68849000	0.98887700
H	2.17655200	5.85663100	2.00246900
H	2.72006500	6.91703100	0.68962400
H	4.09794900	5.05807200	-0.37730200
H	3.36632400	3.48793700	-0.75155500
H	3.65783600	3.95887800	0.93175100
4c-2			
C	-4.06769200	-0.39862400	1.14588800
C	-3.73825300	-1.82556200	0.74517800
C	-2.99963200	-1.87090700	-0.39694300
C	-2.64637800	-0.51478200	-0.84229300
C	-3.04058000	0.41142100	0.29574800

C	-5.59203600	-0.09116200	0.97502900
C	-6.02939400	1.20071900	1.68460500
C	-6.08192000	-0.12669500	-0.48041100
C	-2.02988800	-0.22002000	-2.01114900
C	-4.20505500	-2.97812000	1.57901900
C	-2.50861100	-3.06637100	-1.09627800
C	-3.19611100	-4.19363300	-1.31901100
C	-1.57220200	1.07404400	-2.48140200
C	-0.96008900	1.25850800	-3.66365900
O	-3.51650200	1.69089300	-0.17537300
C	-3.12576500	2.79359300	0.51803900
C	-3.67142400	4.04481700	-0.12967900
O	-2.43829700	2.76402900	1.51384300
H	-3.84694700	-0.25135800	2.21275500
H	-1.84248400	-1.04983900	-2.69251000
H	-2.16743200	0.61089800	0.92465600
H	-6.09397700	-0.91321400	1.50689400
H	-7.12364300	1.25177500	1.73544000
H	-5.64454900	1.24716100	2.71023800
H	-5.68668100	2.09327500	1.15430800
H	-7.17248300	-0.01555400	-0.51383600
H	-5.82730000	-1.07272200	-0.96955000
H	-5.64175900	0.68424100	-1.06838300
H	-5.27088300	-3.19612000	1.42025400
H	-3.64796800	-3.89122600	1.35062600
H	-4.09058400	-2.75132400	2.64729500
H	-1.48771200	-2.99926100	-1.47407700
H	-2.74279200	-5.03532000	-1.83537300
H	-4.23296100	-4.30988400	-1.01621000
H	-1.72610200	1.93066000	-1.83223100
H	-0.61690200	2.23802200	-3.98251100
H	-0.78331800	0.43238000	-4.34927200
H	-3.41215100	4.07009600	-1.19268300
H	-3.26727000	4.92095300	0.37849800
H	-4.76485500	4.05523700	-0.06215600

S1-3 Cartesian coordinates of some key stationary points in Figure 5

1-3			
C	-2.06688100	2.47013400	2.12243300
C	-2.92458900	3.23072600	1.11614900
C	-0.67353100	1.29744500	-0.79115200
C	-2.43153400	4.19071500	0.30159100
C	-0.47351000	1.53336600	0.40584700

C	-0.59058600	2.19325500	1.73612800
C	-2.22582200	3.02639400	3.58505200
C	-1.55612500	2.12036000	4.63143400
C	-1.82039500	4.49471500	3.78240000
C	-3.17617400	4.96194000	-0.68621600
C	-2.60974200	5.88752200	-1.47672800
C	-0.93933300	1.10806100	-2.18064800
C	-2.08733600	0.58760400	-2.64254700
O	0.19527000	3.40757900	1.72432700
C	1.50930700	3.28899700	2.06507400
C	2.18761000	4.63345900	2.06753000
O	2.03139400	2.22590800	2.32500100
H	-2.48480300	1.45197600	2.17171700
H	-1.37411700	4.43529500	0.36546100
H	-0.15939300	1.53817600	2.49369900
H	-3.30726600	2.97204700	3.76831800
H	-1.86310000	2.41848900	5.63966500
H	-1.83611100	1.06719800	4.49995400
H	-0.46154600	2.18953100	4.59895000
H	-2.17481400	4.84530000	4.75823200
H	-2.25633700	5.13973300	3.01432100
H	-0.73455300	4.62657400	3.76017900
H	-4.24335900	4.77535800	-0.78624700
H	-3.18810600	6.45152200	-2.20187200
H	-1.54705000	6.11379100	-1.41796700
H	-0.15893800	1.43544800	-2.86261000
H	-2.26037200	0.49827700	-3.71032300
H	-2.87763300	0.25603900	-1.97709100
H	2.22844200	5.02811300	1.04632300
H	3.19931500	4.53019400	2.46085100
H	1.61953100	5.34804300	2.67084900
Au	1.04989200	-0.19491500	0.13934800
H	4.68081000	4.54456200	-3.83295800
C	3.60657500	4.74117200	-3.75237100
C	3.05149400	4.26011100	-2.39694500
H	3.10908700	4.23354400	-4.58735100
H	3.44677300	5.81860200	-3.87377000
C	3.33478500	2.78066700	-2.17409300
C	1.55506700	4.60028800	-2.26496400
H	3.58608700	4.81016500	-1.61001300
C	2.73591300	1.78573200	-2.94943000
C	4.26589900	2.36222900	-1.23235800
H	1.40047300	5.68219600	-2.34876300
H	1.14953700	4.27004000	-1.30120200

H	0.96319000	4.12592200	-3.05697400
C	3.02107000	0.42259900	-2.79757200
H	2.05938400	2.07940700	-3.74972800
C	4.59737900	1.01358800	-1.00610400
H	4.79548000	3.12083000	-0.65996300
C	2.39941200	-0.45771200	-3.90301400
C	3.92824100	0.01606600	-1.76729700
C	5.73488700	0.86281100	0.03317600
H	1.54175300	0.12838900	-4.25867100
C	3.34648000	-0.57982800	-5.11818200
C	1.82006900	-1.82938500	-3.53199200
C	4.29082600	-1.44737100	-1.66010800
C	6.54517400	-0.44035000	0.11146900
C	5.25957000	1.28932100	1.43981900
H	6.46443800	1.62478400	-0.27572300
H	2.81364300	-1.03037300	-5.96388600
H	3.71746300	0.40064900	-5.43433100
H	4.20884800	-1.21530500	-4.89584700
H	1.20286000	-2.19115200	-4.36315400
H	1.17970600	-1.76565100	-2.64735300
H	2.58973500	-2.58166400	-3.34849800
C	5.30597000	-1.87834900	-2.53360400
C	3.69686600	-2.41924100	-0.80902600
H	7.36694400	-0.29087600	0.82121100
H	6.98807100	-0.70936600	-0.85036500
H	5.96462500	-1.29853400	0.46085100
H	4.85580500	2.30507100	1.44361300
H	4.46391200	0.64252500	1.81686700
H	6.09551200	1.25502300	2.14808300
C	5.73326900	-3.20130400	-2.60069200
H	5.77281800	-1.13581600	-3.17302100
C	4.13804500	-3.75625200	-0.89363600
P	2.40008100	-2.08836500	0.47168400
C	5.14000500	-4.15278900	-1.77473200
H	6.52091400	-3.48355300	-3.29322700
H	3.68509200	-4.51710200	-0.26861800
C	1.28393400	-3.60243500	0.53904900
C	3.34614000	-1.96733400	2.09452900
H	5.44863500	-5.19317600	-1.81105600
C	0.70750000	-3.98626800	-0.84077300
C	0.12995500	-3.42713000	1.55419200
H	1.91725900	-4.42641200	0.89546700
C	3.96619000	-3.30170600	2.62112700
C	2.56930900	-1.20657600	3.19975500

H	4.17684000	-1.32133600	1.79671400
C	-0.14424500	-5.26445900	-0.75078800
H	0.08038600	-3.15993900	-1.20335700
H	1.50657900	-4.12246400	-1.57483200
C	-0.72852300	-4.70221500	1.64361200
H	0.51313200	-3.18029700	2.54788900
H	-0.49945800	-2.58285900	1.23782700
C	3.27259600	-3.81586800	3.89176500
H	3.97692100	-4.08245400	1.85511000
H	5.02181800	-3.10944400	2.84974600
C	3.31848000	-1.33054600	4.53578400
H	1.55312900	-1.60051800	3.31737100
H	2.46455200	-0.15491800	2.91452400
C	-1.27705500	-5.12145400	0.27381300
H	-0.54965300	-5.49834600	-1.74239000
H	0.49990700	-6.11055100	-0.47081300
H	-1.54884000	-4.53414300	2.35175000
H	-0.12012500	-5.51759600	2.06078900
C	3.35360900	-2.79152400	5.04552500
H	2.22308600	-4.04544600	3.66775300
H	3.72771600	-4.76536300	4.19559700
H	2.85484800	-0.67644000	5.28240800
H	4.34103300	-0.95443900	4.39733500
H	-1.99231500	-4.36392000	-0.07910500
H	-1.83458600	-6.06130700	0.36003300
H	2.52399000	-2.96824400	5.74014600
H	4.27305400	-2.95231000	5.62044300
H	-13.27712800	-2.96727800	-0.26596200
C	-12.27201500	-2.62821500	-0.50130600
C	-11.42075100	-2.19325600	0.51730300
C	-11.82702500	-2.61795000	-1.82435100
C	-10.12954600	-1.75831700	0.21716900
H	-11.76361200	-2.19220000	1.54869200
C	-10.53824700	-2.17326200	-2.12446300
H	-12.48532600	-2.94572100	-2.62439500
C	-9.67725100	-1.74543800	-1.10780300
H	-9.46927400	-1.41074700	1.00530900
H	-10.20132300	-2.15566400	-3.15900400
C	-8.26427800	-1.32434800	-1.43941400
O	-7.84127700	-0.29693300	-0.55774600
H	-7.57880900	-2.18768500	-1.35062500
H	-8.20553600	-0.98030000	-2.48570800
C	-6.49508300	0.08059900	-0.74636900
C	-6.16441700	1.19774400	0.23766200

H	-5.82649700	-0.78615800	-0.58555000
H	-6.33259600	0.42367300	-1.78432000
C	-4.70604100	1.66277100	0.14513300
H	-6.84167700	2.04019500	0.04877800
H	-6.38258000	0.84237100	1.25304600
C	-4.38776600	2.82038400	1.11568700
H	-4.47875000	1.99001900	-0.87879300
H	-4.03631000	0.81476700	0.35622300
H	-4.68161000	2.51137300	2.12776900
H	-5.02832200	3.67379400	0.86995800
Ts1a-3			
C	-1.98924900	2.58361900	1.85873200
C	-2.51014500	3.06794200	0.51797100
C	-1.06438900	1.84649400	-0.62386500
C	-1.75304300	3.98027300	-0.20696400
C	-0.34426000	1.44400100	0.38598100
C	-0.51898500	2.11060800	1.74328900
C	-2.35296600	3.51713400	3.06158500
C	-1.86985400	2.90304400	4.38695000
C	-1.91625100	4.98530000	2.93898800
C	-2.17096400	4.68996500	-1.40539900
C	-1.43053700	5.67620000	-1.94129600
C	-1.44431500	1.65606700	-1.99916800
C	-2.01627400	0.52537200	-2.44554200
O	0.42853200	3.20209800	1.85369800
C	1.60027200	2.93808100	2.50883600
C	2.50255600	4.14493900	2.51464300
O	1.86133300	1.86278700	2.99823300
H	-2.51574300	1.64672800	2.07106200
H	-0.80382000	4.29658800	0.21469300
H	-0.29484300	1.41401900	2.55007100
H	-3.45254100	3.51552400	3.09189000
H	-2.26652400	3.47434500	5.23278300
H	-2.20702700	1.86560900	4.50111800
H	-0.77713900	2.91370900	4.46827200
H	-2.29007700	5.54843300	3.80119100
H	-2.31973700	5.46356500	2.03985100
H	-0.82802900	5.08784200	2.91926400
H	-3.12943700	4.44411800	-1.85318000
H	-1.77049700	6.23269100	-2.80929000
H	-0.47196200	5.96536700	-1.51848200
H	-1.24638300	2.47438900	-2.68823500
H	-2.25009500	0.39712500	-3.49844000
H	-2.23847700	-0.30405700	-1.78062200

H	3.04128200	4.18575200	1.56079000
H	3.22950700	4.04703200	3.32234300
H	1.93437500	5.07222300	2.62213800
Au	0.93988800	-0.20427000	0.21048500
H	5.47115800	4.62148600	-2.98561900
C	4.43268200	4.96575300	-2.94100100
C	3.72407800	4.43192500	-1.68015100
H	3.92736500	4.62387300	-3.85203100
H	4.43622300	6.06197500	-2.94964300
C	3.78357300	2.91200300	-1.61409900
C	2.28428600	4.96930200	-1.59199700
H	4.27394400	4.81514100	-0.80910400
C	3.08030600	2.10345000	-2.50780900
C	4.60977100	2.26729500	-0.70291500
H	2.28667200	6.06578900	-1.56736800
H	1.77829900	4.60289000	-0.69087800
H	1.69005700	4.65845900	-2.45947400
C	3.19016300	0.70744300	-2.52302600
H	2.45586200	2.57332600	-3.26427700
C	4.75316100	0.86945600	-0.63421000
H	5.20784400	2.87576000	-0.02690000
C	2.48743000	0.05636300	-3.73291900
C	4.00940700	0.06485000	-1.54151300
C	5.78237900	0.44929200	0.44228500
H	1.73776500	0.79918400	-4.03473500
C	3.44623100	-0.08218500	-4.93655900
C	1.69925800	-1.24188200	-3.52019500
C	4.24320400	-1.42682300	-1.64459100
C	6.45776100	-0.92905300	0.37683600
C	5.22069900	0.71964900	1.85709700
H	6.60479100	1.16592400	0.30904800
H	2.88071700	-0.34999800	-5.83714600
H	3.97488800	0.85633600	-5.13450000
H	4.19136400	-0.86539600	-4.76973100
H	1.07749300	-1.43116400	-4.40402600
H	1.03371400	-1.16171500	-2.65487300
H	2.34358400	-2.11254000	-3.38487800
C	5.26760100	-1.79654100	-2.53654800
C	3.54996200	-2.46671000	-0.96630900
H	7.23475200	-0.96734900	1.14925200
H	6.94325300	-1.10232600	-0.58660000
H	5.77551400	-1.76317300	0.55855200
H	4.95582500	1.77262100	1.99040800
H	4.31299800	0.14391100	2.05501200

H	5.96516300	0.46214600	2.61963300
C	5.61642100	-3.12179600	-2.78004300
H	5.80900500	-1.00377600	-3.04343300
C	3.91792600	-3.80302700	-1.22624300
P	2.19738100	-2.22279000	0.28171000
C	4.93301500	-4.13804700	-2.11780200
H	6.41514400	-3.35443000	-3.47845600
H	3.39385500	-4.61252900	-0.73196300
C	1.01878700	-3.68016000	0.07570100
C	3.06404500	-2.42794700	1.94704600
H	5.18125000	-5.18125900	-2.28928000
C	0.51195600	-3.84596600	-1.37292300
C	-0.18793900	-3.58202200	1.03927600
H	1.58574200	-4.58041600	0.34909900
C	3.56387800	-3.86658600	2.29660600
C	2.27912400	-1.78529500	3.11963600
H	3.95199400	-1.80892800	1.79333400
C	-0.40204500	-5.07618100	-1.50691400
H	-0.04926800	-2.94558600	-1.65714700
H	1.34806400	-3.92886600	-2.07311700
C	-1.10756000	-4.80926600	0.90590800
H	0.14386800	-3.49044000	2.07692700
H	-0.75630600	-2.66973300	0.80886400
C	2.78712900	-4.49668000	3.46228400
H	3.54101900	-4.53235500	1.42917000
H	4.62268100	-3.79734600	2.57644900
C	2.96049600	-2.13483900	4.45222800
H	1.23997800	-2.13359900	3.14303500
H	2.23515100	-0.69983200	2.98529500
C	-1.58887700	-5.00989000	-0.53659500
H	-0.75545600	-5.15532800	-2.54213500
H	0.18264700	-5.98591100	-1.30734400
H	-1.96202300	-4.69601300	1.58439400
H	-0.56409200	-5.70551300	1.23837800
C	2.90124300	-3.65328400	4.75077900
H	1.73235800	-4.60605200	3.17985600
H	3.15662400	-5.51301000	3.64127700
H	2.49703500	-1.56627400	5.26610800
H	4.00562600	-1.80013800	4.40608800
H	-2.24262300	-4.17188100	-0.82110400
H	-2.19598900	-5.91974800	-0.61232600
H	2.04772700	-3.87706400	5.40177600
H	3.79722600	-3.94928900	5.30934200
H	-13.29290300	-1.79373900	-2.14803500

C	-12.32376600	-1.72594200	-1.66146100
C	-11.82235200	-0.48332300	-1.26517600
C	-11.57167500	-2.87904200	-1.43307200
C	-10.58001500	-0.39486600	-0.63749000
H	-12.40178700	0.41858900	-1.44407800
C	-10.32359800	-2.78766200	-0.81328600
H	-11.95082700	-3.84879800	-1.74390900
C	-9.81955900	-1.54801600	-0.40572400
H	-10.18536500	0.57032600	-0.33539800
H	-9.73697500	-3.68877700	-0.64673500
C	-8.49485100	-1.46299300	0.31490100
O	-7.78266300	-0.31165900	-0.11759500
H	-8.65411600	-1.40398800	1.40672500
H	-7.90021100	-2.37279300	0.12868000
C	-6.56455700	-0.11962500	0.56642800
C	-5.91488700	1.14966600	0.02356400
H	-6.73748200	-0.03125100	1.65404500
H	-5.89575100	-0.98720500	0.41752000
C	-4.54471800	1.43533700	0.65161600
H	-5.81715900	1.04755000	-1.06495200
H	-6.59578100	1.99246800	0.19927900
C	-3.93255500	2.73419000	0.10285000
H	-3.86614800	0.59452200	0.45069500
H	-4.65350900	1.49766400	1.74217200
H	-4.57032900	3.58138400	0.40093500
H	-3.98608200	2.70040400	-0.99124500
2a-3			
C	-2.44291300	0.77532600	2.01747200
C	-2.95548100	0.85081100	0.57108900
C	-1.59863200	0.55181400	-0.34798700
C	-2.49325600	1.99467900	-0.18869200
C	-0.51139200	0.47258400	0.51967400
C	-0.90315300	0.93058400	1.92269900
C	-3.20539400	1.59434000	3.09646700
C	-2.57511300	1.37068500	4.48308800
C	-3.39246500	3.09170300	2.80210800
C	-3.11478300	2.47197800	-1.43453300
C	-2.92859000	3.71883800	-1.88736600
C	-1.64456100	-0.07498500	-1.69495500
C	-1.54628300	-1.39335100	-1.89251500
O	-0.42901200	2.28874200	2.09470400
C	0.71964200	2.45112700	2.82820200
C	1.09991500	3.90555400	2.92251500
O	1.33200100	1.52887000	3.31321100

H	-2.57244600	-0.27715700	2.30919600
H	-1.90532200	2.74135300	0.33328600
H	-0.40334400	0.31994000	2.67583300
H	-4.20933200	1.15120700	3.13830200
H	-3.20084300	1.82374400	5.25919000
H	-2.48061900	0.30332800	4.71627400
H	-1.57988000	1.82150200	4.56020300
H	-3.98400900	3.55011000	3.60231700
H	-3.93132700	3.26416100	1.86384400
H	-2.43629300	3.61985400	2.75091200
H	-3.78324200	1.79974500	-1.96467900
H	-3.44348800	4.08002500	-2.77237900
H	-2.27166300	4.42162500	-1.38180700
H	-1.75107300	0.58669300	-2.55181100
H	-1.55823500	-1.81302100	-2.89431600
H	-1.44970300	-2.09419100	-1.06727700
H	1.66509100	4.17945000	2.02422800
H	1.73877900	4.05282900	3.79476800
H	0.21923000	4.54952900	2.97995600
Au	1.31121500	-0.38100800	0.18802700
H	3.72348200	6.18307500	-2.17289500
C	2.63071700	6.11501000	-2.15921500
C	2.14536000	5.19677300	-1.01938500
H	2.30673500	5.73589700	-3.13575000
H	2.22735100	7.12732900	-2.04045300
C	2.76773000	3.81092000	-1.12770700
C	0.60755000	5.15444200	-0.96926500
H	2.49584800	5.63547200	-0.07454100
C	2.41363600	2.91558600	-2.13784400
C	3.78192200	3.41312500	-0.26575300
H	0.20096100	6.16167600	-0.82046100
H	0.25338900	4.51625900	-0.15068900
H	0.19123600	4.76403000	-1.90547900
C	3.04148100	1.67572900	-2.31422400
H	1.65449500	3.20805200	-2.85947100
C	4.44324400	2.17451500	-0.35823200
H	4.11215400	4.11157800	0.50122300
C	2.62624100	0.96556900	-3.61966200
C	4.05393400	1.27116300	-1.38660000
C	5.56441200	2.04192900	0.70095400
H	1.65402400	1.41183500	-3.86512700
C	3.56158000	1.33702600	-4.79226700
C	2.37667600	-0.54722200	-3.58845200
C	4.84695700	0.01293200	-1.66787100

C	6.71722600	1.04718500	0.49488700
C	4.95810500	1.89200600	2.11529800
H	6.04729200	3.02899600	0.69126900
H	3.12490400	0.99809300	-5.73935900
H	3.71043800	2.42020700	-4.85637100
H	4.54174200	0.86207500	-4.69247400
H	1.86889800	-0.84444000	-4.51435700
H	1.72876700	-0.82374400	-2.75034500
H	3.29942500	-1.12670100	-3.52448900
C	5.92912700	0.19091400	-2.55041000
C	4.61835400	-1.29392300	-1.15754900
H	7.45354500	1.20652500	1.29137800
H	7.22676400	1.20165500	-0.45919500
H	6.40931600	-0.00039600	0.53959200
H	4.29756600	2.72863900	2.36152600
H	4.36042200	0.98180700	2.21189400
H	5.75310900	1.86060600	2.86947600
C	6.76729900	-0.85090700	-2.93717800
H	6.11494400	1.19060200	-2.93071600
C	5.47795300	-2.33646700	-1.56050500
P	3.28441100	-1.74968000	0.04781000
C	6.53969700	-2.13011500	-2.43678900
H	7.58999000	-0.66160300	-3.62069700
H	5.31433200	-3.34283900	-1.19264800
C	2.75597600	-3.50961200	-0.38402700
C	4.17103700	-1.82579000	1.71391000
H	7.17639000	-2.96214500	-2.72256100
C	2.36682300	-3.68308800	-1.86855300
C	1.59266500	-3.99248400	0.51486500
H	3.62235400	-4.15216500	-0.17628000
C	5.17785300	-3.00296500	1.91375500
C	3.19856900	-1.68467600	2.91364200
H	4.75696800	-0.90321200	1.67942500
C	2.00155700	-5.14501800	-2.17973200
H	1.50408400	-3.04014200	-2.08895800
H	3.17753800	-3.35673200	-2.52609900
C	1.21666400	-5.45239600	0.20400700
H	1.84885200	-3.90457300	1.57413200
H	0.72132700	-3.34310000	0.34825600
C	4.69172400	-4.02719100	2.95018600
H	5.41354700	-3.50444900	0.97071100
H	6.12922000	-2.57905200	2.25927200
C	3.95560400	-1.92580900	4.22885100
H	2.36898800	-2.39710400	2.83872800

H	2.74506800	-0.68776400	2.90714200
C	0.87000900	-5.65268700	-1.27673600
H	1.71896300	-5.23198100	-3.23587000
H	2.89059700	-5.77776400	-2.04266500
H	0.37536800	-5.75325500	0.84041100
H	2.05889500	-6.10575700	0.47403100
C	4.47601500	-3.38067800	4.33598400
H	3.75654000	-4.48338800	2.60122400
H	5.41609100	-4.84653800	3.02385600
H	3.30720000	-1.68742000	5.07919000
H	4.79578700	-1.22026800	4.28154800
H	-0.05486900	-5.10474100	-1.51148300
H	0.66484600	-6.71055100	-1.47905500
H	3.77073100	-3.99255300	4.91085000
H	5.41720500	-3.38940900	4.89844300
H	-8.18761600	0.90835600	1.32854100
C	-8.07551000	0.63360100	0.26445300
O	-9.09563600	-0.25846000	-0.12667600
C	-6.73570800	-0.05899800	0.03255800
H	-8.13258000	1.57101000	-0.31771700
C	-10.40194400	0.27810900	0.02459000
C	-5.53525800	0.79953600	0.45123600
H	-6.73583100	-1.00425500	0.59014000
H	-6.66027900	-0.32251700	-1.03058000
C	-11.42758700	-0.71609400	-0.46825800
H	-10.47708100	1.22191600	-0.54544200
H	-10.59274500	0.52911500	1.08109300
C	-4.20317500	0.06605700	0.18883600
H	-5.62324700	1.05764800	1.51319300
H	-5.54457200	1.74959400	-0.09978600
C	-12.67766000	-0.80215800	0.15441900
C	-11.16151100	-1.53142400	-1.57511300
H	-4.15803300	-0.21199900	-0.86948500
H	-4.19161100	-0.88041700	0.74420900
H	-12.89151700	-0.18072300	1.02156000
C	-13.65162300	-1.68033100	-0.32455800
C	-12.13035600	-2.41654800	-2.04854600
H	-10.18762700	-1.47721300	-2.05128900
C	-13.37946300	-2.49130000	-1.42749700
H	-14.61770200	-1.73693200	0.16969000
H	-11.91057700	-3.04892800	-2.90481900
H	-14.13373900	-3.17995200	-1.79824100
Ts _{2a} -3			
C	-1.80750000	2.49902500	2.17920400

C	-2.13059500	2.85612300	0.71350500
C	-0.82177900	2.44904600	-0.16455000
C	-1.29760600	3.94250000	0.11075000
C	0.11351200	1.86500500	0.78223400
C	-0.27961200	2.28144400	2.22609300
C	-2.48002200	3.37358600	3.27943200
C	-2.05631700	2.90125700	4.68693700
C	-2.30324400	4.89802400	3.13097600
C	-1.74801100	4.75895600	-1.04299200
C	-1.36793300	6.03158100	-1.22641700
C	-0.88620500	1.97372800	-1.57873300
C	-1.47782900	0.84551100	-1.99097500
O	0.48709800	3.51084700	2.66314700
C	1.54617300	3.80913700	1.87899900
C	2.40453000	4.92902000	2.36131700
O	1.74111300	3.14732200	0.82857800
H	-2.20233300	1.48479000	2.33815100
H	-0.66953800	4.50249800	0.79211600
H	0.01253900	1.53881500	2.96608100
H	-3.55726900	3.16809100	3.17846800
H	-2.65493800	3.40568400	5.45260600
H	-2.20099700	1.82069300	4.81300700
H	-1.00364600	3.13512700	4.88186500
H	-2.89284500	5.40762200	3.90144400
H	-2.65230900	5.26118300	2.15885400
H	-1.25889300	5.19618000	3.26072600
H	-2.42214900	4.29609600	-1.75829000
H	-1.72503200	6.61596500	-2.06737600
H	-0.69338100	6.53802900	-0.54064500
H	-0.39232700	2.61546800	-2.30624800
H	-1.47122900	0.55381700	-3.03622600
H	-1.98142500	0.16987300	-1.30565700
H	3.05390000	5.27313200	1.55679300
H	3.02474600	4.57822600	3.19481100
H	1.78887100	5.75103600	2.73480100
Au	1.08954800	0.07390200	0.50588200
H	5.41988300	3.76108800	-4.22172900
C	4.43004300	4.21762200	-4.11457200
C	3.83814000	3.94682700	-2.71023500
H	3.78229500	3.80601800	-4.89812400
H	4.52873600	5.29518500	-4.29043400
C	3.76813600	2.44990200	-2.42206100
C	2.47264200	4.64899300	-2.54636400
H	4.52630600	4.38416900	-1.97222500

C	2.87096600	1.60915700	-3.08642700
C	4.65225400	1.84897300	-1.52961600
H	2.58085200	5.73080800	-2.68833400
H	2.05411200	4.46619900	-1.55128100
H	1.75019700	4.29280400	-3.29098400
C	2.84388700	0.21777700	-2.89701000
H	2.19038400	2.03547900	-3.81791500
C	4.67057000	0.46433700	-1.26891400
H	5.38452500	2.47480100	-1.02492800
C	1.89742800	-0.51359300	-3.87586700
C	3.73467200	-0.37538400	-1.94297700
C	5.77385300	0.07661000	-0.25376600
H	1.17619700	0.26022200	-4.17425600
C	2.62651800	-0.93231700	-5.17922600
C	1.04891300	-1.67535400	-3.33301200
C	3.81906200	-1.88540700	-1.85913000
C	6.35102500	-1.35144300	-0.25177700
C	5.35176900	0.51132600	1.17440200
H	6.62279400	0.72198600	-0.52366700
H	1.89409000	-1.25277500	-5.93012200
H	3.20010600	-0.09829700	-5.59740100
H	3.31090200	-1.76761500	-5.00474900
H	0.25321800	-1.90813900	-4.05185800
H	0.57672900	-1.40401500	-2.38399400
H	1.63254600	-2.58611100	-3.18645900
C	4.64563900	-2.48609500	-2.83558900
C	3.15626000	-2.74701200	-0.94392900
H	7.21284600	-1.37715500	0.42601700
H	6.70142100	-1.64791700	-1.24390100
H	5.64087100	-2.10893100	0.08829200
H	5.16690800	1.58971000	1.21557500
H	4.42760200	0.01333900	1.48156300
H	6.13694900	0.26954600	1.90079000
C	4.81661200	-3.86662100	-2.93511700
H	5.16719700	-1.83341800	-3.52678900
C	3.33038800	-4.14221400	-1.06128600
P	2.05533000	-2.17868500	0.49677300
C	4.14746800	-4.70584200	-2.04238200
H	5.46263500	-4.28002700	-3.70228900
H	2.81108900	-4.81009500	-0.38517500
C	0.63466200	-3.49042800	0.63753600
C	3.18679600	-2.45016500	2.06328300
H	4.25597000	-5.78324800	-2.10438800
C	-0.09218500	-3.73571700	-0.70203900

C	-0.38940900	-3.08887300	1.72694000
H	1.12215200	-4.42335700	0.95014000
C	3.44958800	-3.93350900	2.47477400
C	2.71142300	-1.59563500	3.26603000
H	4.13497400	-2.02938600	1.71570900
C	-1.16947100	-4.83127700	-0.54734200
H	-0.57195200	-2.80263700	-1.02745200
H	0.61650500	-4.02022600	-1.48511200
C	-1.47498600	-4.17687600	1.88735600
H	0.10229000	-2.92132200	2.69024200
H	-0.86008300	-2.13714700	1.43958700
C	2.74353300	-4.32210900	3.78851700
H	3.17638200	-4.63557600	1.68195700
H	4.53256700	-4.05769600	2.60982800
C	3.50902400	-1.97986200	4.52910500
H	1.64065500	-1.73790100	3.45579500
H	2.84530700	-0.53233400	3.03374700
C	-2.18559800	-4.47679500	0.55459600
H	-1.68083500	-4.97766700	-1.50667300
H	-0.68277400	-5.78710900	-0.30201900
H	-2.20104000	-3.85838300	2.64610800
H	-1.00854300	-5.09780700	2.26776600
C	3.21021300	-3.43856200	4.97238000
H	1.65669000	-4.23181600	3.66125100
H	2.93616300	-5.37850900	4.00991000
H	3.28120600	-1.28155500	5.34313100
H	4.58045500	-1.86223800	4.31486400
H	-2.76447500	-3.59335900	0.24400500
H	-2.90556500	-5.29381600	0.68527600
H	2.43848000	-3.44442400	5.75205600
H	4.11027300	-3.87174700	5.42580700
H	-12.89452100	-1.63194500	-2.67588700
C	-11.94730100	-1.62562700	-2.14620300
C	-11.25694200	-2.82262500	-1.92695300
C	-11.40766700	-0.41858800	-1.68370900
C	-10.03280500	-2.81049000	-1.24874600
H	-11.66465000	-3.76117800	-2.28881600
C	-10.18936100	-0.40799200	-0.99786800
H	-11.93659400	0.51340600	-1.85703300
H	-9.49478000	-3.74163800	-1.09059400
C	-9.49263600	-1.60603300	-0.77343100
H	-9.76152200	0.52489000	-0.64900500
C	-8.20236800	-1.60996400	0.00756200
O	-7.42094100	-0.42999200	-0.34255500

H	-8.40038500	-1.59324600	1.09310600
H	-7.62347100	-2.52144000	-0.20677900
C	-6.19449100	-0.29229200	0.41283100
C	-5.52088700	0.99705400	-0.04759100
H	-6.41300300	-0.25792500	1.49365800
H	-5.53846100	-1.16170600	0.23451700
C	-4.17405300	1.24957900	0.65328600
H	-5.37736300	0.94312600	-1.13422600
H	-6.20705800	1.83322100	0.13883600
C	-3.53447200	2.57727400	0.19746300
H	-3.48863000	0.41580100	0.44109200
H	-4.33065200	1.25690700	1.74122000
H	-4.17844500	3.41245800	0.51288900
H	-3.52730300	2.59788200	-0.89727600
3a-3			
C	-1.54707600	2.64438400	2.08722000
C	-1.85705400	2.96800800	0.61225700
C	-0.61000600	2.61571400	-0.21819900
C	-1.02621900	4.08836800	0.00210000
C	0.44950000	2.07610300	0.73596900
C	-0.03201000	2.42524400	2.15978600
C	-2.22825400	3.51286500	3.18081600
C	-1.83544400	3.03791600	4.59056000
C	-2.04464300	5.03271400	3.03849400
C	-1.51354600	4.90963300	-1.13345600
C	-1.33541100	6.23153200	-1.21650200
C	-0.58773600	2.09276200	-1.61930600
C	-1.44059600	1.23025200	-2.17727100
O	0.78381600	3.64703400	2.52711800
C	1.70585100	3.80127200	1.63484300
C	2.74457600	4.85020200	1.80501100
O	1.69971300	3.01043000	0.64101400
H	-1.92862400	1.62586200	2.25391200
H	-0.43655700	4.67973600	0.69729600
H	0.25712300	1.71986200	2.93679200
H	-3.30292600	3.31479100	3.06338000
H	-2.44569600	3.54181000	5.34736200
H	-1.98425000	1.95769000	4.71274900
H	-0.78627800	3.26524200	4.81572800
H	-2.64040700	5.54453900	3.80243900
H	-2.37813400	5.39746300	2.06226900
H	-1.00212500	5.33588500	3.18247700
H	-2.03179300	4.39291800	-1.93746100
H	-1.70591800	6.80207500	-2.06251100

H	-0.81768700	6.79433600	-0.44203800
H	0.23987000	2.47084100	-2.22034900
H	-1.31843400	0.91481000	-3.20960800
H	-2.28140500	0.80530400	-1.63880000
H	3.14153800	5.14730800	0.83311500
H	3.56349200	4.43827500	2.40795300
H	2.32885800	5.70772000	2.33820300
Au	1.09738100	0.07968200	0.48618700
H	6.33353300	3.13429100	-3.66937300
C	5.41665400	3.72947800	-3.73588200
C	4.56275400	3.58325100	-2.45938400
H	4.86123000	3.39164600	-4.61880600
H	5.69982800	4.77632700	-3.89622200
C	4.23399900	2.11973800	-2.19449300
C	3.31668500	4.48269600	-2.53293500
H	5.17542100	3.93159800	-1.61548700
C	3.26254900	1.42901300	-2.91807900
C	4.96335300	1.38269700	-1.26887000
H	3.60978100	5.53511800	-2.62184300
H	2.68745100	4.37100700	-1.64243700
H	2.69754500	4.24653200	-3.40607400
C	3.01294900	0.06001500	-2.75193300
H	2.69887700	1.95693400	-3.68386200
C	4.76293500	0.01155500	-1.03259100
H	5.75886800	1.88457900	-0.72020700
C	2.02573400	-0.50383600	-3.79503400
C	3.74724400	-0.66596500	-1.76318300
C	5.75769300	-0.54836000	0.00918000
H	1.42546500	0.36723600	-4.08805500
C	2.75882700	-0.95769100	-5.07710400
C	1.00729500	-1.56142200	-3.35315100
C	3.58628800	-2.17010900	-1.69895300
C	6.09372000	-2.04749700	0.02813500
C	5.38891200	-0.04202700	1.42229300
H	6.70732000	-0.05637700	-0.24165100
H	2.03133700	-1.16894300	-5.86993700
H	3.44226300	-0.18356700	-5.44176300
H	3.33696200	-1.87097400	-4.90751000
H	0.22786500	-1.64830100	-4.12021400
H	0.52153300	-1.27299800	-2.41679200
H	1.45012900	-2.55159000	-3.22896600
C	4.36156500	-2.87478800	-2.63965800
C	2.73749800	-2.92687300	-0.84420900
H	6.91368100	-2.20903100	0.73775500

H	6.43056900	-2.40068100	-0.94980100
H	5.26094400	-2.68289000	0.33868500
H	5.40340400	1.05210500	1.46545600
H	4.38392900	-0.36157800	1.71264500
H	6.10011600	-0.41715400	2.16784900
C	4.31573100	-4.25931600	-2.77385700
H	5.02286300	-2.30176300	-3.28215100
C	2.69659600	-4.32766000	-1.00342000
P	1.69080600	-2.23638400	0.52519400
C	3.46688600	-4.99514700	-1.95127400
H	4.93394200	-4.75420500	-3.51731800
H	2.03570900	-4.92146700	-0.38288100
C	0.13190600	-3.29517500	0.59658400
C	2.69414800	-2.61946200	2.08546700
H	3.40060400	-6.07534900	-2.04096400
C	-0.60124100	-3.37230500	-0.75970800
C	-0.84957100	-2.80256800	1.68693300
H	0.45400400	-4.30771100	0.87532900
C	2.81140500	-4.12185000	2.49671500
C	2.29657600	-1.72718500	3.28942600
H	3.69159400	-2.29566400	1.77470900
C	-1.83537100	-4.28664900	-0.67652900
H	-0.91968100	-2.36136500	-1.04777800
H	0.07085000	-3.72710100	-1.54596900
C	-2.09006200	-3.71079400	1.77197500
H	-0.36492100	-2.76491200	2.66667600
H	-1.16072500	-1.77548900	1.44921500
C	2.02735600	-4.45331400	3.77503200
H	2.51117400	-4.79202400	1.68703900
H	3.87257100	-4.34094700	2.67041400
C	3.00136400	-2.21408900	4.56537200
H	1.21217200	-1.73043300	3.44804200
H	2.56750700	-0.68713800	3.07271300
C	-2.80613100	-3.83182100	0.42087400
H	-2.33871100	-4.30590600	-1.65061600
H	-1.51070700	-5.31769400	-0.47384800
H	-2.77329300	-3.31964700	2.53599700
H	-1.78244300	-4.70969600	2.11369600
C	2.52232300	-3.62590300	4.98215000
H	0.95909200	-4.26728200	3.60744900
H	2.11449500	-5.52431100	3.99054400
H	2.83587100	-1.49999600	5.38027400
H	4.08452400	-2.22209100	4.38374100
H	-3.23172600	-2.85484600	0.14632000

H	-3.64873800	-4.52899000	0.49910900
H	1.71490300	-3.54705500	5.71977300
H	3.34315200	-4.15264100	5.48284800
H	-12.70299400	-1.41866800	-2.64761600
C	-11.74253000	-1.40223600	-2.13982200
C	-11.04152900	-2.59012200	-1.92640900
C	-11.20021300	-0.19142500	-1.70199400
C	-9.80414100	-2.56437300	-1.28008200
H	-11.45200400	-3.53574500	-2.27019200
C	-9.96835800	-0.16832400	-1.04772700
H	-11.73887300	0.73751900	-1.86981800
H	-9.25712800	-3.49233600	-1.12601600
C	-9.25969900	-1.35646600	-0.83069200
H	-9.54117200	0.77192500	-0.71370500
C	-7.94853800	-1.34659200	-0.07994700
O	-7.20970300	-0.17994900	-0.40772000
H	-8.13095700	-1.36946600	1.00996600
H	-7.36439500	-2.25042900	-0.32236900
C	-6.00084900	-0.06589800	0.31049000
C	-5.31346100	1.22866100	-0.11119100
H	-6.19402800	-0.06494900	1.39853900
H	-5.34637700	-0.93306900	0.10245300
C	-3.95153000	1.43079000	0.56517600
H	-5.19395100	1.21741500	-1.20224700
H	-5.97866200	2.07017900	0.12107500
C	-3.29793700	2.76343500	0.15592200
H	-3.28575100	0.59371100	0.30883000
H	-4.08212400	1.39258200	1.65565200
H	-3.90245300	3.59098900	0.55346500
H	-3.34796700	2.86077200	-0.93228000
Ts _{3a} -3			
C	-1.33821900	2.43649600	2.07559800
C	-1.67426900	2.93251300	0.65110400
C	-0.40476600	2.78703400	-0.19984000
C	-0.91010100	4.18359200	0.20404700
C	0.66596700	2.20189400	0.71892900
C	0.15354800	2.27089500	2.07499600
C	-2.01274500	3.14383900	3.29236600
C	-1.56844600	2.50414200	4.61806400
C	-1.86081400	4.67154200	3.33810500
C	-1.46486200	5.11070000	-0.81226000
C	-1.39982300	6.44165500	-0.70760000
C	-0.34177400	2.43321300	-1.65019400
C	-1.10245200	1.54080100	-2.28926700

O	1.20759900	3.88788100	2.51790200
C	2.04796700	3.83296300	1.60402600
C	3.20643100	4.77201300	1.49066300
O	1.94931700	2.91940000	0.65178500
H	-1.68657200	1.39134000	2.15183300
H	-0.35941500	4.70536100	0.97866900
H	0.65613500	1.80807200	2.91441600
H	-3.08365700	2.93102100	3.17015600
H	-2.18217500	2.87814100	5.44400200
H	-1.66924200	1.41136700	4.60091800
H	-0.52561800	2.74904500	4.85386500
H	-2.42681100	5.06377300	4.19048000
H	-2.25234600	5.15056200	2.43599200
H	-0.81693700	4.97399700	3.46622100
H	-1.93443000	4.67216200	-1.68985200
H	-1.81358400	7.09193300	-1.47224000
H	-0.93570800	6.93100500	0.14646400
H	0.41942700	2.97252300	-2.21464300
H	-0.97302400	1.35392000	-3.35163900
H	-1.87702000	0.96756300	-1.78866300
H	2.91161100	5.61369400	0.85235300
H	4.05407800	4.27059900	1.01935200
H	3.47577500	5.15778600	2.47481300
Au	1.07963600	0.08602300	0.45924200
H	6.47201100	2.91067700	-3.63034100
C	5.57928500	3.53704400	-3.73033400
C	4.68973700	3.44618600	-2.47337700
H	5.03349900	3.20336200	-4.62081200
H	5.90387700	4.56990400	-3.90173700
C	4.29913800	2.00155400	-2.19001000
C	3.47955800	4.38899000	-2.59353400
H	5.29426300	3.78789000	-1.62071200
C	3.32737800	1.33237900	-2.93251200
C	4.96496100	1.25886700	-1.22158500
H	3.81336200	5.42786900	-2.69632500
H	2.82906800	4.32015300	-1.71446100
H	2.87331000	4.15703500	-3.47699700
C	3.01956700	-0.02239400	-2.74853900
H	2.80981400	1.86535600	-3.72648700
C	4.70155800	-0.09722000	-0.96297000
H	5.75733700	1.74234500	-0.65209200
C	2.04756500	-0.56923800	-3.81461900
C	3.69044500	-0.75366800	-1.71944700
C	5.61859000	-0.66793000	0.14093700

H	1.49466100	0.31887000	-4.14567400
C	2.80443400	-1.08069900	-5.06101000
C	0.97157000	-1.57467200	-3.38853500
C	3.48618600	-2.25209900	-1.64330500
C	5.92760900	-2.17240900	0.18460000
C	5.16752000	-0.14696600	1.52451700
H	6.59033300	-0.19301600	-0.04985600
H	2.09674300	-1.27234700	-5.87640300
H	3.53589900	-0.34591900	-5.41364100
H	3.33274800	-2.01662900	-4.85567500
H	0.22259300	-1.65520000	-4.18580200
H	0.45655900	-1.24216800	-2.48228100
H	1.37106200	-2.57615500	-3.21757100
C	4.27769500	-2.98711700	-2.54688000
C	2.58895400	-2.97967400	-0.81347500
H	6.70471900	-2.34436600	0.93859800
H	6.31155400	-2.53537700	-0.77244900
H	5.06883600	-2.79301000	0.45135100
H	5.19261800	0.94725400	1.55928800
H	4.14137700	-0.45047800	1.75253200
H	5.82453600	-0.52508400	2.31687800
C	4.20271800	-4.37151700	-2.66788200
H	4.97645900	-2.43830800	-3.17045300
C	2.51738400	-4.38102400	-0.95975300
P	1.51273900	-2.25563100	0.51104000
C	3.30578800	-5.07773300	-1.87063600
H	4.83593500	-4.88947100	-3.38240300
H	1.81827000	-4.95116400	-0.35911100
C	-0.09120300	-3.24681500	0.51861900
C	2.42621900	-2.67384900	2.11878200
H	3.21586400	-6.15681800	-1.95202800
C	-0.75499100	-3.35802200	-0.87027600
C	-1.11228500	-2.68270000	1.53492600
H	0.18165400	-4.25728600	0.85239500
C	2.45959400	-4.17934500	2.53418400
C	2.00822300	-1.76682400	3.30509500
H	3.45016200	-2.39234600	1.85613700
C	-2.01019700	-4.24583800	-0.81221300
H	-1.03849300	-2.35356300	-1.21150000
H	-0.05284500	-3.75485200	-1.60842900
C	-2.37556700	-3.56099100	1.59581600
H	-0.67581400	-2.61030400	2.53525700
H	-1.38694500	-1.66141700	1.23420400
C	1.58834200	-4.47701600	3.76344700

H	2.18409900	-4.83861600	1.70731800
H	3.49938700	-4.43792100	2.77084400
C	2.62243800	-2.28807700	4.61365300
H	0.91832400	-1.72129100	3.40950300
H	2.33749200	-0.73990800	3.10821000
C	-3.02448300	-3.72842500	0.21591700
H	-2.46537900	-4.29565800	-1.80853200
H	-1.71623600	-5.27323400	-0.55254900
H	-3.08806900	-3.12248400	2.30530000
H	-2.10683300	-4.54898000	1.99683100
C	2.05323800	-3.67505100	4.99947300
H	0.54087100	-4.24114500	3.53589000
H	1.61362900	-5.55120700	3.97877600
H	2.44912300	-1.56738600	5.42089800
H	3.71190600	-2.34799400	4.48891200
H	-3.41732000	-2.75739900	-0.12060600
H	-3.88310900	-4.40706900	0.28063100
H	1.21024900	-3.55700800	5.69045200
H	2.81825200	-4.24094600	5.54366800
H	-12.77336700	-0.80379400	-2.44898600
C	-11.77888900	-0.89163300	-2.02016700
C	-11.10925000	-2.11575800	-2.04678700
C	-11.16160500	0.22167000	-1.44404200
C	-9.82823100	-2.22340500	-1.50136300
H	-11.57851600	-2.98511600	-2.49939600
C	-9.88600100	0.11017100	-0.89113200
H	-11.67585700	1.17895000	-1.42470300
H	-9.30631900	-3.17761900	-1.53478000
C	-9.20803700	-1.11512800	-0.91486800
H	-9.40116800	0.97590900	-0.45086300
C	-7.84577600	-1.25256100	-0.27618000
O	-7.07602000	-0.08598800	-0.52557200
H	-7.94672900	-1.39652200	0.81503300
H	-7.32914400	-2.14467700	-0.66819700
C	-5.82389000	-0.08830800	0.12375400
C	-5.12310600	1.22726800	-0.19773300
H	-5.95287400	-0.20110500	1.21561600
H	-5.21325100	-0.94505900	-0.21732700
C	-3.73483000	1.35104800	0.44456200
H	-5.04313200	1.32195300	-1.28813600
H	-5.76477300	2.05117500	0.14004800
C	-3.10305300	2.72531600	0.16080500
H	-3.07999400	0.54922900	0.07252600
H	-3.82703900	1.19333200	1.52863600

H	-3.73478600	3.49972100	0.61868800
H	-3.14410200	2.91282600	-0.91623800
4a-3			
C	-2.47073700	1.20879000	-0.92894400
C	-1.94742400	0.77653600	0.46197100
C	-2.66092000	-0.54158100	0.81952700
C	-2.95072600	0.76243900	1.61075400
C	-3.66414700	-0.71209900	-0.28240300
C	-3.61981600	0.25948800	-1.20420700
C	-2.75010200	2.72454000	-1.14383000
C	-2.99699300	3.01196700	-2.63535800
C	-3.88565000	3.31329800	-0.29309900
C	-2.56720100	0.94923400	3.02723800
C	-3.34809000	1.55789900	3.92621300
C	-1.97286500	-1.68977200	1.45396300
C	-1.95194400	-2.95314100	1.01595300
O	-4.52641300	-1.78652700	-0.13887300
C	-5.55417000	-2.04190500	-1.00432600
C	-6.28985100	-3.28255300	-0.55788100
O	-5.82476500	-1.37153200	-1.97094200
H	-1.67372100	0.97402600	-1.65303200
H	-3.93296400	1.16864200	1.39076600
H	-4.29466100	0.35736700	-2.04009900
H	-1.82293500	3.24730000	-0.86402900
H	-3.07146600	4.09072700	-2.81499900
H	-2.18471100	2.62286900	-3.26126900
H	-3.93267500	2.55660600	-2.98193700
H	-4.05379000	4.36231300	-0.56512700
H	-3.65653500	3.28516000	0.77579100
H	-4.82744000	2.77483800	-0.45611200
H	-1.60046700	0.57494100	3.35673300
H	-3.03602000	1.68248700	4.95904700
H	-4.32657900	1.95312800	3.66162100
H	-1.42494600	-1.45708400	2.36527000
H	-1.40298800	-3.71838100	1.55732900
H	-2.48101000	-3.27138000	0.12376800
H	-5.60907700	-4.14005200	-0.53946300
H	-7.11484700	-3.47828400	-1.24341900
H	-6.67202900	-3.14926100	0.45941600
H	5.92606500	-0.13079500	1.49128000
C	6.79637700	-0.19621700	0.84699500
C	8.08057700	-0.03265700	1.36844800
C	6.61277100	-0.43038100	-0.52006500
C	9.19620900	-0.10842900	0.53270100

H	8.20948300	0.15487100	2.43150400
C	7.73496600	-0.49671900	-1.35398000
C	5.23247300	-0.65768200	-1.09498300
H	10.19550900	0.01875600	0.94070200
C	9.01966900	-0.34217400	-0.83237300
H	7.60314300	-0.66758100	-2.42078300
O	4.25683700	-0.01732500	-0.29633500
H	5.18962900	-0.28368300	-2.13256200
H	5.01954400	-1.74178900	-1.14436800
H	9.88096600	-0.39508600	-1.49336600
C	2.93142300	-0.26563500	-0.73272000
C	1.96718500	0.45916700	0.19775700
H	2.80154300	0.08584600	-1.77146400
H	2.72706300	-1.35085400	-0.73188700
C	0.49849700	0.24657300	-0.19147400
H	2.14164900	0.10649800	1.22293700
H	2.21204500	1.52949200	0.18883000
C	-0.46549700	0.99855100	0.74304700
H	0.25798500	-0.82430500	-0.16711600
H	0.35252000	0.57373700	-1.22935000
H	-0.25746000	2.07757700	0.68869400
H	-0.23018100	0.70919900	1.77235200

Ts_{4a}-3

C	-2.70794500	1.37315700	-0.71479000
C	-4.14176400	0.92248000	-0.89906900
C	-2.67377100	2.85384000	-0.20350300
C	-3.38693200	3.13997100	1.12909200
C	-1.28880400	3.51259800	-0.20507900
C	-2.00791400	0.15544200	0.02714500
C	-3.04334600	-0.97027300	-0.05219700
C	-4.29533700	-0.35196900	-0.51329000
O	-5.41135700	-1.17145200	-0.51378900
C	-6.64138800	-0.75612800	-0.94339200
C	-7.62455300	-1.89625500	-0.83157900
O	-6.89060200	0.35320600	-1.34751300
C	-2.33900800	0.07313800	1.50304800
C	-1.84060500	-0.77166600	2.50071300
C	-0.88920100	-1.76956200	2.37327600
C	-1.85290100	-3.09292100	0.60177100
C	-2.95674800	-2.34627400	0.23244200
C	-0.58382400	-0.14734100	-0.48341100
H	-4.91649700	1.56493700	-1.28881900
H	-3.25909300	3.37448900	-0.97731800
H	-3.53662600	4.22054600	1.24154400

H	-4.37102300	2.66094500	1.17886100
H	-2.79713700	2.80441000	1.98860000
H	-1.39040000	4.59859700	-0.09041500
H	-0.74786800	3.32856900	-1.14108400
H	-0.67134200	3.15663800	0.62565700
H	-8.60833500	-1.55680600	-1.15684100
H	-7.67514000	-2.25295800	0.20231700
H	-7.29726100	-2.73725800	-1.45189700
H	-3.17072300	0.69858300	1.79954100
H	-2.43389000	-0.77807500	3.41597600
H	-0.06829600	-1.68890800	1.67606700
H	-0.71200200	-2.44161000	3.20835100
H	-0.86494700	-2.91475400	0.20797100
H	-2.01576700	-4.11048500	0.94817100
H	-3.92817500	-2.82422000	0.35023500
H	-0.38164000	-1.21368800	-0.38175900
H	-0.57598700	0.03378600	-1.56679400
H	-2.23746400	1.42276900	-1.71117300
C	0.58348800	0.61515500	0.16539800
H	0.56563600	1.66544700	-0.13810300
H	0.46854300	0.60456800	1.25678800
C	1.94338900	0.01301000	-0.21556600
H	2.00709600	-1.03060400	0.12094800
H	2.05954400	-0.00388000	-1.30751500
C	3.11254400	0.78324000	0.38495800
H	3.03025000	0.80941500	1.48571900
H	3.10548300	1.83118600	0.03618900
O	4.32081500	0.14953600	0.00111100
C	5.47103900	0.80226200	0.50200000
H	5.46864100	0.79781000	1.60568600
H	5.45940300	1.86426300	0.19357700
C	6.72348700	0.13079100	-0.01531100
C	7.91754000	0.23022200	0.70821100
C	6.72441000	-0.55609800	-1.23422700
C	9.09512600	-0.33672900	0.22005500
H	7.92642600	0.75270800	1.66298000
C	7.89988400	-1.13129900	-1.71921800
H	5.79629500	-0.64597000	-1.78865600
C	9.08943000	-1.02089100	-0.99692400
H	10.01396100	-0.25176500	0.79459100
H	7.88564000	-1.66761500	-2.66474200
H	10.00407500	-1.46878700	-1.37644000
5a-3			
C	2.68285400	-0.62176700	-1.50283300

C	2.69075200	0.87856900	-1.32706400
C	3.96212900	-1.04831400	-2.30723900
C	5.27557600	-0.95520000	-1.51581000
C	3.82774700	-2.39148500	-3.04844000
C	2.41815400	-1.15270200	-0.02668100
C	2.85597200	0.03030600	0.85008000
C	2.81877700	1.20542200	-0.03202200
O	2.94511700	2.43922400	0.58474600
C	2.95109200	3.62081800	-0.10267200
C	3.12956500	4.76565100	0.86562200
O	2.82982800	3.72286400	-1.29901200
C	3.07960300	-2.47567300	0.31857700
C	3.24316200	-2.99833900	1.53958900
C	2.85168300	-2.36338900	2.85432100
C	3.49888900	-0.99902900	3.13153700
C	3.25981100	0.09663200	2.12959600
H	2.66637200	1.57017900	-2.15606100
H	4.02668200	-0.28950500	-3.10214500
H	6.13116500	-1.11148400	-2.18396800
H	5.38822300	0.03041700	-1.05258600
H	5.33156200	-1.70578900	-0.72094500
H	4.64436800	-2.50286500	-3.77206300
H	2.88347000	-2.44518000	-3.60400600
H	3.87183400	-3.26055300	-2.38426300
H	2.33411500	4.75315300	1.61776900
H	3.10912200	5.70787100	0.31729900
H	4.08246900	4.66511300	1.39589000
H	3.36505900	-3.09606700	-0.52372700
H	3.68245800	-3.99365200	1.59927900
H	1.75947200	-2.24966200	2.90511700
H	3.11831700	-3.04094100	3.67375500
H	3.16496200	-0.64689100	4.11861800
H	4.58820700	-1.13555000	3.23012800
H	3.51945700	1.09092800	2.49168100
H	-9.45561200	1.22986300	0.58008000
C	-8.61364600	0.60817600	0.28649600
C	-8.81742700	-0.72638000	-0.06930800
C	-7.32570400	1.14455800	0.27722000
H	-9.81890900	-1.14846900	-0.05708500
C	-7.72578500	-1.51627800	-0.43436900
C	-6.22811200	0.36054800	-0.09653700
H	-7.17184900	2.18260700	0.56604800
C	-6.43904100	-0.97618500	-0.45183100
H	-7.87555000	-2.55797600	-0.70699300

C	-4.84773600	0.97556500	-0.15859500
H	-5.58670600	-1.58788500	-0.72776800
O	-3.85901500	-0.01975000	0.01681200
H	-4.70353000	1.47544200	-1.13451600
H	-4.74856200	1.76037100	0.61128200
C	-2.53908400	0.47561100	-0.13401600
C	-1.55911300	-0.67438500	0.06115600
H	-2.41424900	0.92445700	-1.13527900
H	-2.34691000	1.27477100	0.60328900
C	-0.09616200	-0.23449000	-0.09465700
H	-1.72301100	-1.10759400	1.05660000
H	-1.79751500	-1.46186400	-0.66607600
C	0.86957800	-1.40840800	0.12024100
H	0.12470300	0.56033800	0.62954800
H	0.04480800	0.20674100	-1.08912900
H	0.61375500	-2.21341500	-0.58331900
H	0.69159900	-1.81430400	1.12202600
H	1.83157200	-0.92029900	-2.13300800

1d-3

C	2.28225200	-2.20025000	0.34848700
C	3.25054800	-1.63557500	1.38486000
C	0.21026700	0.14755100	1.74802600
C	3.04550900	-1.98333500	2.67819200
C	0.48901300	-0.48134200	0.71904100
C	1.34118300	-1.14464100	-0.30641700
C	2.90733700	-3.19137800	-0.69701100
C	1.86114500	-4.22258000	-1.15854600
C	3.59879200	-2.57099200	-1.92335100
C	3.82529800	-1.56948300	3.83769400
C	3.58401600	-2.00660600	5.08549600
C	-0.03611300	0.87444600	2.95135700
C	0.55894500	0.57135600	4.11688600
O	2.09366600	-0.12497100	-0.99927600
C	1.48471100	0.45695900	-2.07169700
C	2.39418700	1.46524000	-2.72293500
O	0.36085700	0.17409700	-2.42697800
H	1.57692700	-2.81729200	0.92026100
H	2.21474600	-2.65290200	2.90761500
H	0.70703300	-1.64411400	-1.04020800
H	3.66855400	-3.74284100	-0.13016200
H	2.32285400	-4.96746600	-1.81588300
H	1.41822800	-4.75694600	-0.30994100
H	1.04684100	-3.75475900	-1.72823200

H	4.11569700	-3.35772100	-2.48420800
H	4.33917500	-1.81278800	-1.65787200
H	2.87506800	-2.11349600	-2.60755400
H	4.64013600	-0.86604500	3.68029500
H	4.18039200	-1.67825700	5.93101300
H	2.79293700	-2.72364100	5.29641900
H	-0.70857700	1.72340000	2.87024800
H	0.37150300	1.18031000	4.99603500
H	1.25513200	-0.25468900	4.22062200
H	2.64062800	2.26062300	-2.01156800
H	1.90050100	1.88964200	-3.59746600
H	3.33457600	0.98955100	-3.01912700
Au	-1.77776300	-0.33875500	0.36607700
H	-0.73808200	6.76794900	0.21491700
C	0.02522300	6.18512000	0.74116700
C	0.20877400	4.79657900	0.09820500
H	-0.28004200	6.10291600	1.79114300
H	0.96453300	6.74880900	0.71196600
C	-1.10130600	4.02350600	0.03839700
C	1.31797500	4.00094300	0.81224600
H	0.53344000	4.95560300	-0.93910400
C	-1.79355300	3.64518300	1.19118400
C	-1.69632200	3.71125600	-1.17633500
H	2.26644000	4.54924200	0.77957100
H	1.47261000	3.02108800	0.34480800
H	1.07380000	3.83115400	1.86781200
C	-3.01635300	2.96223800	1.16035300
H	-1.39667300	3.93972300	2.16060500
C	-2.91468200	3.01713700	-1.29559200
H	-1.21094300	4.04990400	-2.08898600
C	-3.67892500	2.82815100	2.54855500
C	-3.56805200	2.58745400	-0.10783000
C	-3.37138400	2.90503800	-2.77080400
H	-2.84540800	2.94673200	3.25364500
C	-4.63109900	4.00923300	2.84227700
C	-4.33797400	1.49539300	2.92941100
C	-4.92881400	1.92894400	-0.14070800
C	-4.84034000	2.60585800	-3.10788100
C	-2.43104800	1.97850900	-3.57385800
H	-3.19736000	3.91549800	-3.16666700
H	-4.91064000	4.00777300	3.90243600
H	-4.15478300	4.96948700	2.61859600
H	-5.55332300	3.94032600	2.25853000
H	-4.52742100	1.48641200	4.00947400

H	-3.68439900	0.64688000	2.70188400
H	-5.29628500	1.33722200	2.43063100
C	-6.02204900	2.81266400	-0.07971400
C	-5.21086800	0.53651600	-0.19669600
H	-4.96794100	2.69692200	-4.19273000
H	-5.52453000	3.31583000	-2.63706500
H	-5.16163700	1.59907700	-2.82645300
H	-1.38597000	2.28998600	-3.50063600
H	-2.46836500	0.94721100	-3.21501200
H	-2.71231500	1.98212900	-4.63338500
C	-7.34428500	2.37877400	-0.05841300
H	-5.81202200	3.87718700	-0.05713300
C	-6.55632600	0.11315900	-0.16721500
P	-3.95619100	-0.81433200	-0.36436000
C	-7.61549500	1.01336700	-0.09734800
H	-8.15290200	3.10232100	-0.01064700
H	-6.79260500	-0.94444300	-0.18689900
C	-4.60295200	-2.29817400	0.59208000
C	-3.95193700	-1.23604300	-2.19883300
H	-8.63726100	0.64670800	-0.07412200
C	-4.95009300	-1.96333900	2.05855200
C	-3.61845000	-3.49101700	0.54929300
H	-5.52246600	-2.61046800	0.07804900
C	-5.23602100	-1.94714800	-2.73521200
C	-2.65390700	-1.94533000	-2.66215200
H	-3.93148200	-0.23378300	-2.63504700
C	-5.54086600	-3.18719100	2.78069300
H	-4.03380500	-1.64692200	2.57566800
H	-5.65077000	-1.12543200	2.11423400
C	-4.20492800	-4.71661900	1.27461600
H	-3.37438000	-3.76393700	-0.48109800
H	-2.67588100	-3.19612800	1.03225700
C	-4.97492800	-3.40183400	-3.15322900
H	-6.06061900	-1.90249600	-2.01798600
H	-5.58654900	-1.38622600	-3.61042900
C	-2.81057700	-2.41105500	-4.11858700
H	-2.42393000	-2.80956900	-2.02851300
H	-1.80674100	-1.25694800	-2.57053700
C	-4.59439400	-4.39321900	2.72263400
H	-5.76093100	-2.92079000	3.82126800
H	-6.50217100	-3.45164700	2.31683300
H	-3.47557800	-5.53501300	1.24541200
H	-5.09034300	-5.06896900	0.72611500
C	-3.90716300	-3.49463600	-4.26506300

H	-4.65503000	-3.98158700	-2.27812600
H	-5.91240000	-3.85904100	-3.48945800
H	-1.85108300	-2.78508100	-4.49242900
H	-3.05615300	-1.53787900	-4.73759400
H	-3.68687600	-4.17123000	3.30288600
H	-5.06056000	-5.26639200	3.19372000
H	-3.45566700	-4.49349800	-4.24489200
H	-4.38534800	-3.39552600	-5.24658400
O	9.25836600	-0.34508400	0.07495300
C	10.56930600	-0.88593700	0.03526700
C	8.28004400	-1.28418100	0.47181600
C	11.54115100	0.15136500	-0.47786600
H	10.57967800	-1.77574900	-0.62054500
H	10.87380300	-1.22896000	1.03810500
C	6.92765300	-0.57988200	0.49730400
H	8.25944100	-2.13962600	-0.22722100
H	8.51884900	-1.69106700	1.47036000
C	12.85090100	0.19187200	0.01270500
C	11.16206200	1.05488300	-1.47823800
C	5.77776000	-1.50349900	0.91628000
H	6.99619300	0.27408300	1.18405900
H	6.73448200	-0.16264600	-0.50009700
C	13.77206100	1.11126100	-0.49281100
H	13.15322700	-0.49838000	0.79758100
C	12.07872100	1.98028200	-1.97781200
H	10.14218300	1.03543200	-1.84917900
C	4.42387600	-0.75885100	0.97243700
H	5.98823200	-1.94179800	1.90040900
H	5.70781200	-2.34782100	0.21799900
C	13.38743300	2.00923500	-1.48976900
H	14.78561800	1.13115000	-0.10137200
H	11.77160600	2.68037300	-2.75058300
H	4.22654000	-0.29716600	0.00265100
H	4.52134800	0.07326100	1.68164800
H	14.10084400	2.72956000	-1.88086600
T _{S1d} -3			
C	-1.76033300	-3.26729000	0.86243200
C	-2.41988000	-2.78202400	-0.44917300
C	-0.80402800	-1.97466200	-1.16766900
C	-2.40577400	-3.72879000	-1.48605000
C	-0.09862300	-1.75021700	-0.07511600
C	-0.65097800	-2.26099200	1.23364100
C	-2.69966900	-3.80839900	1.98821800
C	-1.92566800	-4.81377600	2.86368300

C	-3.40409100	-2.78569600	2.90066600
C	-3.12548800	-3.69172600	-2.72897900
C	-2.98560800	-4.67456400	-3.64429800
C	-0.76420900	-1.67754000	-2.58632900
C	0.31910300	-1.83508700	-3.35944000
O	-1.18300400	-1.12766400	1.96192700
C	-0.43617500	-0.64872500	2.99776500
C	-1.10093000	0.54299500	3.63604500
O	0.62376900	-1.12887900	3.33435600
H	-1.17679100	-4.14751700	0.56135400
H	-1.74231300	-4.58446800	-1.36417300
H	0.11737100	-2.71904500	1.85826200
H	-3.48085900	-4.37796700	1.46582200
H	-2.58926700	-5.25254100	3.61648400
H	-1.50671300	-5.63496000	2.27026200
H	-1.10155800	-4.32715300	3.39967700
H	-4.20149400	-3.29364300	3.45495700
H	-3.85257200	-1.94982400	2.35978000
H	-2.71307700	-2.36840300	3.63813500
H	-3.80924600	-2.87063300	-2.92228800
H	-3.54736800	-4.67296400	-4.57328800
H	-2.31333100	-5.51342400	-3.48071700
H	-1.68162300	-1.29213500	-3.02865600
H	0.30398500	-1.54460300	-4.40559400
H	1.24805500	-2.23551200	-2.96498200
H	-0.95026300	1.41682000	2.99195900
H	-0.64592500	0.73315500	4.60908300
H	-2.17755000	0.38523800	3.74192500
Au	1.71223300	-0.69744900	-0.11559300
H	-2.14930100	5.61936700	0.04241000
C	-2.75972100	4.73043200	-0.14873100
C	-2.21902300	3.50724700	0.61867200
H	-2.75955700	4.55011600	-1.23035500
H	-3.78979700	4.95184700	0.15362200
C	-0.76065300	3.23960200	0.27009800
C	-3.11745500	2.27799300	0.39374300
H	-2.25451900	3.75094300	1.68951600
C	-0.36998100	2.79468900	-0.99333200
C	0.25485400	3.51203100	1.17925700
H	-4.14245400	2.48720100	0.72125500
H	-2.74781700	1.40917800	0.94967000
H	-3.16120700	2.00474200	-0.66734400
C	0.97112900	2.64261900	-1.36768800
H	-1.13208200	2.61283400	-1.74771000

C	1.62301900	3.34731300	0.89406900
H	-0.01988800	3.91283800	2.15332400
C	1.14938000	2.38358800	-2.87916100
C	1.99407700	2.87973100	-0.39729000
C	2.51726800	3.78573300	2.07972900
H	0.21353100	1.89288200	-3.17646100
C	1.19661500	3.71666200	-3.65974300
C	2.26370200	1.44604800	-3.36248300
C	3.43736700	2.85627500	-0.84667600
C	4.00067000	4.11809000	1.85640900
C	2.35183100	2.81642500	3.27399200
H	2.06768700	4.73365000	2.40748500
H	1.13959500	3.52481700	-4.73807400
H	0.36122500	4.36952800	-3.38602000
H	2.12836900	4.25831600	-3.46928500
H	2.07561100	1.18614700	-4.41171200
H	2.27829200	0.51626700	-2.78657700
H	3.25538900	1.90051100	-3.31494000
C	3.89396700	4.06431900	-1.40649900
C	4.34641000	1.76529700	-0.79098300
H	4.40859500	4.51162400	2.79470500
H	4.13939500	4.88461200	1.09070600
H	4.60741000	3.25429000	1.57355600
H	1.31094400	2.76282100	3.60649100
H	2.65794200	1.79687200	3.02233700
H	2.95545600	3.15332100	4.12477200
C	5.18490300	4.22705800	-1.90043200
H	3.20196800	4.90018300	-1.44080000
C	5.65081100	1.95037700	-1.29352700
P	3.96757700	0.09189500	-0.07694500
C	6.07465500	3.15767700	-1.84244600
H	5.48976900	5.17984500	-2.32367100
H	6.36000200	1.13135500	-1.27146400
C	5.02003200	-1.13960100	-1.04191400
C	4.65563600	0.18501100	1.67639400
H	7.08829700	3.25439100	-2.21999500
C	4.76645300	-1.07865100	-2.56405500
C	4.81322100	-2.58875000	-0.54058600
H	6.06833800	-0.87304200	-0.85132000
C	6.20904000	0.29909200	1.79862400
C	4.07385400	-0.89527800	2.62296800
H	4.23629000	1.13992800	2.00455900
C	5.67286800	-2.06301600	-3.32351600
H	3.71520200	-1.33536500	-2.75479600

H	4.91586000	-0.06492100	-2.94679200
C	5.71797000	-3.57597900	-1.29948700
H	5.01639000	-2.66712800	0.53031900
H	3.76020300	-2.87048200	-0.68204700
C	6.84841200	-0.95932600	2.40353200
H	6.68025000	0.53750100	0.84039100
H	6.43350900	1.15395100	2.44908500
C	4.81527300	-0.85603000	3.96863900
H	4.16620200	-1.89867100	2.19261300
H	3.00269200	-0.72560500	2.76883600
C	5.50181500	-3.50094600	-2.81581500
H	5.45343000	-2.00480700	-4.39663600
H	6.72184900	-1.75547500	-3.20416900
H	5.52990200	-4.59284200	-0.93380800
H	6.76955400	-3.35222000	-1.06850500
C	6.30362000	-1.25568900	3.81878300
H	6.66034800	-1.81619300	1.74420500
H	7.93741400	-0.83817900	2.43439600
H	4.31256900	-1.51290900	4.68688700
H	4.73801900	0.15941200	4.38055300
H	4.48699000	-3.85214000	-3.05581300
H	6.19562800	-4.17383900	-3.33355400
H	6.43056700	-2.32318500	4.03501400
H	6.90116700	-0.71941300	4.56563400
O	-8.19500400	-0.29778300	-0.18921300
C	-9.57800700	-0.58837500	-0.04125600
C	-7.37510700	-1.44334600	-0.11526200
C	-10.38013400	0.69137800	-0.07134100
H	-9.73866000	-1.12054700	0.91380000
H	-9.91385200	-1.26660100	-0.84304400
C	-5.92533400	-0.99573200	-0.27676000
H	-7.51491400	-1.96151500	0.85035400
H	-7.64506100	-2.16392600	-0.90830700
C	-11.64526100	0.71413600	-0.66833900
C	-9.89174900	1.85709300	0.53168900
C	-4.93376500	-2.16629400	-0.26481800
H	-5.84015000	-0.43730900	-1.21816000
H	-5.68560200	-0.28872000	0.52783000
C	-12.41682800	1.87775400	-0.65610800
H	-12.03046000	-0.18306500	-1.14838900
C	-10.65731100	3.02321400	0.53588200
H	-8.90474400	1.84617800	0.98346200
C	-3.47840700	-1.67684100	-0.43799600
H	-5.18853600	-2.87050300	-1.06767800

H	-5.03472700	-2.72617100	0.67094500
C	-11.92350900	3.03649500	-0.05453100
H	-13.39763300	1.88034600	-1.12383300
H	-10.26610000	3.92360400	1.00244900
H	-3.22633700	-0.96643600	0.35291700
H	-3.41994000	-1.10911600	-1.37543800
H	-12.51960600	3.94491600	-0.04854900
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C	-1.78552000	-3.17759100	0.95416200
C	-2.36128300	-2.65731800	-0.41138800
C	-0.95371900	-1.99496200	-1.05603200
C	-2.40303800	-3.71002900	-1.38895500
C	-0.10221400	-1.74494300	-0.03556400
C	-0.61531700	-2.23672500	1.29595400
C	-2.76886800	-3.63473800	2.07133600
C	-2.05700200	-4.64226400	2.99628000
C	-3.44215700	-2.54999700	2.93502900
C	-3.13476200	-3.75129400	-2.61446200
C	-3.00784900	-4.80620200	-3.45483100
C	-0.88031200	-1.63795000	-2.47530100
C	0.21939300	-1.70972600	-3.23527400
O	-1.05875700	-1.08019700	2.05017200
C	-0.28968200	-0.69532600	3.10807900
C	-0.86523700	0.52781000	3.77391500
O	0.72127900	-1.27199200	3.44449600
H	-1.25590500	-4.10045500	0.68096600
H	-1.73746100	-4.55580200	-1.22005100
H	0.15249900	-2.73653400	1.88951300
H	-3.56524600	-4.18782700	1.55373400
H	-2.75161400	-5.02212700	3.75318300
H	-1.66772500	-5.50322600	2.43995700
H	-1.21871300	-4.17461800	3.52690700
H	-4.28301100	-2.99613000	3.47826100
H	-3.82547200	-1.70475300	2.35978600
H	-2.75000300	-2.15141900	3.68138100
H	-3.81899100	-2.94490900	-2.85844100
H	-3.58471900	-4.87750700	-4.37202600
H	-2.33106600	-5.62890100	-3.23667200
H	-1.80646600	-1.28961500	-2.93230900
H	0.20565300	-1.38715200	-4.27190700
H	1.16146000	-2.08025900	-2.84235800
H	-0.70649400	1.39509200	3.12329100
H	-0.36129700	0.69248100	4.72711600
H	-1.94272900	0.41912400	3.92733500

Au	1.68413000	-0.70123500	-0.12791100
H	-2.10331500	5.62297800	0.23310600
C	-2.71891300	4.73147100	0.07306800
C	-2.13958800	3.51298300	0.81918700
H	-2.76806500	4.54759500	-1.00683300
H	-3.73471100	4.95088100	0.42175100
C	-0.69682200	3.24887200	0.40867500
C	-3.04042200	2.27820900	0.63661200
H	-2.12950800	3.75911900	1.88994000
C	-0.35850600	2.81284400	-0.87263900
C	0.35477600	3.51272800	1.27855300
H	-4.05290400	2.48503800	1.00278600
H	-2.64481800	1.41447000	1.18265500
H	-3.12314400	1.99921700	-0.42067100
C	0.96627600	2.65837800	-1.30031100
H	-1.15056000	2.63817900	-1.59716800
C	1.70981900	3.34340600	0.93939200
H	0.11977900	3.90979400	2.26446000
C	1.08491300	2.41185300	-2.81965900
C	2.02712800	2.88150800	-0.36842200
C	2.65204800	3.77325000	2.09103200
H	0.14292700	1.91326100	-3.08241300
C	1.08800300	3.75288100	-3.58845200
C	2.18825100	1.49142900	-3.35783400
C	3.45186000	2.84503500	-0.87158700
C	4.13033600	4.08698300	1.81335600
C	2.52079800	2.80816500	3.29296700
H	2.22546700	4.72675300	2.43320600
H	0.99354100	3.57054800	-4.66582900
H	0.25654900	4.39427700	-3.27811000
H	2.02030400	4.30334200	-3.42717200
H	1.95852100	1.23871600	-4.40051600
H	2.23645400	0.55687300	-2.79215600
H	3.17618500	1.95650700	-3.34783800
C	3.90311600	4.05072200	-1.44039800
C	4.34659700	1.74099800	-0.85702500
H	4.57846900	4.47177400	2.73685700
H	4.25100500	4.85427500	1.04545100
H	4.71414000	3.21597400	1.50534600
H	1.49299800	2.76609900	3.66521400
H	2.80764100	1.78536600	3.03165300
H	3.15954300	3.14001100	4.11968700
C	5.17716400	4.19942900	-1.98048100
H	3.22129000	4.89567000	-1.44485700

C	5.63428000	1.91247900	-1.40480900
P	3.96174900	0.06676400	-0.14601800
C	6.05403400	3.11805100	-1.96092600
H	5.47913400	5.15058000	-2.40946500
H	6.33286400	1.08413800	-1.41378600
C	4.97340400	-1.16846200	-1.15042000
C	4.70152900	0.13854200	1.58745600
H	7.05472100	3.20412200	-2.37403400
C	4.67383700	-1.09339100	-2.66371300
C	4.76768000	-2.61915200	-0.65299100
H	6.03006000	-0.91449000	-0.99115900
C	6.25818500	0.24087700	1.66779500
C	4.13937200	-0.94565800	2.54178000
H	4.29920100	1.09398500	1.93485200
C	5.54461500	-2.08201300	-3.45851900
H	3.61433400	-1.33574600	-2.82463400
H	4.82386400	-0.07853100	-3.04309800
C	5.63800500	-3.60946200	-1.44732400
H	5.00435300	-2.70658200	0.41031500
H	3.70807100	-2.89025500	-0.76204000
C	6.90644600	-1.03112000	2.23354200
H	6.70401200	0.49350600	0.70104600
H	6.50622100	1.08312700	2.32622000
C	4.92439200	-0.93025300	3.86299100
H	4.20548400	-1.94525600	2.09811300
H	3.07567900	-0.76669800	2.72637100
C	5.37410200	-3.52160900	-2.95544700
H	5.29184000	-2.01371200	-4.52370100
H	6.60023600	-1.78674400	-3.37037700
H	5.45234100	-4.62722600	-1.08277100
H	6.69859400	-3.39702700	-1.24916400
C	6.40176400	-1.34607300	3.65971900
H	6.69245100	-1.87592600	1.56673800
H	7.99675700	-0.91802400	2.23362300
H	4.43717900	-1.58908500	4.59002500
H	4.87360000	0.08146400	4.28800500
H	4.34833800	-3.86017600	-3.16512000
H	6.04375100	-4.19817500	-3.49965800
H	6.52081400	-2.41887600	3.85320900
H	7.02909200	-0.83109700	4.39710100
O	-8.21904100	-0.30269800	-0.24985000
C	-9.59641500	-0.59665100	-0.06089400
C	-7.38371400	-1.43163400	-0.11826900
C	-10.41002300	0.67342900	-0.14613900

H	-9.73471900	-1.07632700	0.92495000
H	-9.94034000	-1.32081500	-0.81781600
C	-5.94247500	-0.97313500	-0.31972100
H	-7.50689400	-1.89429100	0.87737100
H	-7.65141600	-2.20094800	-0.86514400
C	-9.92533800	1.87111100	0.39416500
C	-11.68082700	0.65728100	-0.73103500
C	-4.92690200	-2.12065400	-0.23521600
H	-5.87217300	-0.47586100	-1.29604100
H	-5.71198800	-0.21013200	0.43493400
C	-10.70006000	3.03022700	0.34899600
H	-8.93384600	1.89019300	0.83578500
C	-12.46151900	1.81434700	-0.76808600
H	-12.06341200	-0.26522100	-1.16275400
C	-3.48641600	-1.60470500	-0.42856100
H	-5.16615500	-2.87492500	-0.99709800
H	-5.02582900	-2.62668000	0.73025900
C	-11.97189600	3.00484900	-0.22882800
H	-10.31158400	3.95531900	0.76697300
H	-13.44675900	1.78670800	-1.22556700
H	-3.24980900	-0.85819400	0.33486400
H	-3.44557200	-1.06362400	-1.38266700
H	-12.57528400	3.90787900	-0.26136400
T _{S_{2d-3}}			
C	-2.16176400	-2.25133100	2.31503400
C	-2.65562100	-2.14529500	0.82837200
C	-1.68243200	-1.16019000	0.13274200
C	-1.85524900	-3.14830700	0.03589800
C	-0.47113900	-1.09824900	0.84880800
C	-0.66303900	-1.78047500	2.20063200
C	-3.08949500	-1.69525900	3.43361700
C	-2.72869400	-2.33307800	4.78964300
C	-3.23830500	-0.16918500	3.59023900
C	-4.16123300	-2.11437100	0.51202500
C	-2.10788500	-3.64172700	-1.29307000
C	-1.39835400	-4.66999100	-1.80270000
C	-1.99959000	-0.47841800	-1.12496400
C	-1.44152900	0.67365100	-1.52021100
O	-0.15486200	-1.00727100	3.31493200
C	-0.18559200	0.34189500	3.23864800
C	0.37849900	0.97201500	4.48612500
O	-0.61658000	0.94428100	2.27638300
H	-2.12727600	-3.32580800	2.53580400
H	-1.02758100	-3.62878500	0.54941500

H	-0.00800500	-2.65649800	2.24378700
H	-4.07984800	-2.08814900	3.16874700
H	-3.43158800	-2.00260300	5.56230900
H	-2.77527500	-3.42770600	4.74668600
H	-1.72041800	-2.04977400	5.10933300
H	-4.20385800	0.05401900	4.05787800
H	-3.18609300	0.37605200	2.64595500
H	-2.47419700	0.24440400	4.25377100
H	-4.30110400	-2.43460400	-0.52627300
H	-4.64481800	-2.89605100	1.11321000
H	-2.92116100	-3.22085800	-1.87505400
H	-1.63298600	-5.09349700	-2.77416000
H	-0.58257100	-5.13116000	-1.25123700
H	-2.79934000	-0.90399600	-1.72600500
H	-1.76078300	1.15052000	-2.44223600
H	-0.68450000	1.18521400	-0.93451400
H	-0.19411400	0.65248400	5.36278100
H	0.34146400	2.05736300	4.39276300
H	1.41221900	0.64361900	4.63337800
H	6.49379700	3.55881500	-3.33719400
C	5.93180400	2.76749200	-2.84950400
C	4.84095800	3.08172400	-2.04508300
C	6.29171300	1.43271700	-3.01607300
C	4.06699100	2.10746100	-1.38462300
H	4.56781600	4.12283000	-1.90580100
C	5.55588200	0.44743500	-2.36461100
H	7.13658200	1.15553400	-3.63954800
C	2.90774100	2.67357500	-0.59316400
C	4.44632100	0.74650000	-1.54604300
H	5.86174100	-0.58289100	-2.50144400
C	1.71485700	3.04738900	-1.28707100
C	3.05983700	3.07326000	0.76356100
P	3.65795900	-0.71926100	-0.71754100
C	0.70257400	3.71906900	-0.58868500
C	1.42453500	2.91825600	-2.79702200
C	2.00468000	3.75973100	1.38896600
C	4.27416600	2.89695300	1.70183700
Au	1.40588100	-0.64271900	0.14006300
C	3.68692900	-2.11101000	-1.98856100
C	4.90066800	-1.18164700	0.63335400
C	0.81672000	4.09282400	0.75037700
H	-0.19331900	3.99993000	-1.13783800
H	0.32970800	2.96504300	-2.86076300
C	1.93403400	4.14623700	-3.58452100

C	1.81397200	1.61820900	-3.51115600
H	2.14270900	4.07829900	2.42094300
C	5.68656700	2.74716900	1.11526200
C	3.98118100	1.80248700	2.75226800
H	4.31105000	3.83974000	2.26383700
C	2.82056300	-1.78810400	-3.22337500
C	3.25551200	-3.45681300	-1.36143300
H	4.72429600	-2.22301400	-2.32620900
C	6.24082900	-1.79252200	0.13539100
C	4.31113500	-2.02958200	1.78222200
H	5.12997900	-0.19878200	1.05775500
C	-0.25845200	4.90288600	1.46137500
H	1.53121200	4.12977000	-4.60437000
H	1.61858300	5.08157600	-3.11039000
H	3.02514500	4.15276700	-3.66111500
H	1.31811200	1.58347900	-4.48888500
H	1.48932200	0.74218900	-2.94199400
H	2.88869300	1.53911200	-3.68894900
H	6.40972600	2.79406900	1.93808700
H	5.92424700	3.55809900	0.42167500
H	5.85021800	1.80476100	0.58748800
H	3.10321400	2.06306600	3.35192600
H	3.77434800	0.83654100	2.28214700
H	4.83128800	1.68062500	3.43438900
C	2.85504200	-2.93140800	-4.25209700
H	1.78290700	-1.62263000	-2.90060300
H	3.15909300	-0.86021300	-3.69293100
C	3.28301200	-4.59382200	-2.39914000
H	3.90448900	-3.72164600	-0.52105800
H	2.23926000	-3.35337000	-0.95409400
C	7.00023500	-2.52243400	1.27297700
H	6.07708000	-2.50226000	-0.68283800
H	6.86569200	-0.98881900	-0.26838500
C	5.24483800	-1.98886400	3.01936300
H	4.18588000	-3.06555700	1.44795500
H	3.31138400	-1.67480200	2.05747800
C	-0.28925700	6.35392800	0.93963800
C	-1.65052700	4.25276200	1.37447500
H	0.02148500	4.94264000	2.52335500
C	2.42922200	-4.26773000	-3.63048600
H	2.20745700	-2.67661600	-5.09970700
H	3.87324500	-3.02640100	-4.65633800
H	2.94318800	-5.52444200	-1.92733100
H	4.32159500	-4.76976200	-2.71412300

C	6.73825500	-1.86819300	2.63363700
H	6.68482300	-3.57340100	1.31511000
H	8.07132500	-2.53363100	1.04237600
H	5.08275000	-2.90061300	3.60671100
H	4.96381500	-1.15005000	3.66692700
H	0.68907600	6.83583200	1.04326900
H	-0.56789000	6.38643200	-0.12051700
H	-1.02303500	6.94807800	1.49656800
H	-2.37593100	4.83219300	1.95755900
H	-1.62967200	3.22887200	1.75924700
H	-2.01485600	4.22201300	0.34036400
H	1.37010400	-4.20848500	-3.33548800
H	2.50440300	-5.07451300	-4.36932600
H	7.36526100	-2.32373600	3.40781700
H	7.03285500	-0.81101600	2.58673100
C	-4.91762100	-0.78490100	0.68111900
H	-5.03202300	-0.53969600	1.74072700
H	-4.33531100	0.03220700	0.23557800
C	-6.30322100	-0.84197700	0.02224300
H	-6.20322200	-1.05910800	-1.04978800
H	-6.89518600	-1.66232300	0.45055500
C	-7.08927300	0.46291600	0.16699900
H	-7.28810600	0.67240900	1.22834500
H	-6.49817800	1.30478400	-0.22392100
O	-8.29802200	0.38221600	-0.57182400
C	-9.48586700	0.50051200	0.19989800
H	-9.55267500	-0.31308700	0.94069200
H	-9.46620300	1.44800100	0.76598800
C	-10.69187300	0.46902600	-0.71033600
C	-11.88591200	-0.11661700	-0.27535000
C	-10.64858600	1.06481900	-1.97688200
C	-13.02330500	-0.09875900	-1.08489300
H	-11.92811200	-0.59154000	0.70279400
C	-11.78167400	1.07476700	-2.79064900
H	-9.71955100	1.50659800	-2.32278100
C	-12.97342700	0.49691800	-2.34621500
H	-13.94371000	-0.55726200	-0.73344300
H	-11.73500300	1.53582900	-3.77382500
H	-13.85560800	0.50733000	-2.98050500
3d-3			
C	-2.08162200	-2.09829800	2.27411600
C	-2.57897100	-1.86139400	0.82017200
C	-1.59403400	-0.94312200	0.07730100
C	-1.56813700	-2.44845000	-0.18523300

C	-0.45967300	-0.57930300	1.01047300
C	-0.66888700	-1.42336400	2.29895600
C	-3.06811400	-1.80044200	3.44441700
C	-2.61641400	-2.50556200	4.73664000
C	-3.41747300	-0.32562600	3.74125600
C	-1.95290500	-3.06961500	-1.47612000
C	-1.43677500	-4.22317200	-1.91399000
C	-1.99265600	0.06805100	-0.94843200
C	-1.67819900	0.03433000	-2.24550500
O	-0.49601200	-0.41464900	3.38248100
C	-0.63708900	0.76727100	2.87246300
C	-0.58593400	1.97440600	3.73340700
O	-0.77145700	0.83531200	1.61407400
H	-1.89138800	-3.17597800	2.36540400
H	-0.72812100	-2.97753400	0.26913400
H	0.13220000	-2.13239800	2.48905500
H	-3.99684000	-2.29298800	3.13164200
H	-3.36483600	-2.37194100	5.52556800
H	-2.48723500	-3.58291900	4.58260000
H	-1.66908400	-2.09992100	5.11116700
H	-4.41454000	-0.26292600	4.18992300
H	-3.43087700	0.30151700	2.84380700
H	-2.72596500	0.11154000	4.46795100
H	-2.68997700	-2.55892200	-2.08831200
H	-1.74746600	-4.66060000	-2.85790500
H	-0.69642900	-4.77822700	-1.34119300
H	-2.55866600	0.91696000	-0.56632400
H	-1.99532200	0.82554000	-2.91934400
H	-1.10316800	-0.77735500	-2.68122400
H	-1.51180400	2.54626800	3.61674300
H	0.23953500	2.60731100	3.38967900
H	-0.44624000	1.69534700	4.77782700
Au	1.50714800	-0.50436800	0.24457400
H	0.98953600	6.85639500	0.91709900
C	-0.01575500	6.48858900	0.68656200
C	-0.19711400	5.02833000	1.15211800
H	-0.16286100	6.57150900	-0.39671300
H	-0.74185200	7.14638100	1.17826400
C	0.86706700	4.13348900	0.52735300
C	-1.63692100	4.55380800	0.89139600
H	-0.03237600	5.01417800	2.23988700
C	0.73904600	3.59646300	-0.75204300
C	2.07117900	3.89902200	1.18460900
H	-2.34670000	5.15978300	1.46577200

H	-1.77467700	3.50202800	1.16806300
H	-1.91000400	4.65443700	-0.16509800
C	1.75999100	2.87428100	-1.38553600
H	-0.17336600	3.77837800	-1.31355800
C	3.13393400	3.16710200	0.62568800
H	2.22090300	4.34582700	2.16712600
C	1.44458000	2.56079300	-2.86231700
C	2.97510600	2.61907600	-0.67852600
C	4.35779000	3.10872100	1.56734600
H	0.34811700	2.54097800	-2.89818000
C	1.87854400	3.72069100	-3.78636400
C	1.88781700	1.21373400	-3.44426600
C	4.13739900	2.00569400	-1.43198900
C	5.76501100	2.88975400	0.99070800
C	4.07662100	2.14239200	2.74092800
H	4.39744900	4.11133200	2.01424300
H	1.48351100	3.56246600	-4.79692200
H	1.50382100	4.68342100	-3.42273600
H	2.96808900	3.78629400	-3.86376400
H	1.35251700	1.03831000	-4.38544400
H	1.64353200	0.39239100	-2.76450300
H	2.95597300	1.17724700	-3.66746900
C	4.88648900	2.93552600	-2.17856400
C	4.52724800	0.63926100	-1.49851900
H	6.49411900	3.02311300	1.79850800
H	6.00046800	3.61810500	0.21049200
H	5.92014700	1.89423000	0.56888000
H	3.20731600	2.46997200	3.32178000
H	3.86434300	1.12943500	2.38651600
H	4.93434200	2.09723100	3.42237100
C	5.96518900	2.57126100	-2.97904800
H	4.60135600	3.98114700	-2.11701000
C	5.61746800	0.28911500	-2.32177800
P	3.75243300	-0.75445200	-0.54667900
C	6.33168400	1.23048100	-3.05749800
H	6.50860300	3.32850300	-3.53681100
H	5.91695000	-0.74887800	-2.40708300
C	3.83979400	-2.28054000	-1.65028400
C	4.95995800	-1.03371200	0.88364400
H	7.16248800	0.91440200	-3.68131200
C	3.17124900	-2.07052300	-3.02538400
C	3.22488600	-3.51809100	-0.95359700
H	4.90532900	-2.49127400	-1.81205100
C	6.35457700	-1.64100700	0.51741000

C	4.31660900	-1.76374000	2.08963600
H	5.13577500	-0.00464400	1.20935000
C	3.29973100	-3.32584100	-3.90594200
H	2.10716900	-1.84521400	-2.87285100
H	3.60622700	-1.20965600	-3.54139600
C	3.34799600	-4.77360500	-1.83586900
H	3.70814800	-3.70718500	0.00930600
H	2.16434600	-3.32078100	-0.74336500
C	6.56898900	-3.04047300	1.11415000
H	6.51960600	-1.67162000	-0.56281800
H	7.12980300	-0.96980800	0.90767100
C	5.38243600	-2.04554800	3.16054000
H	3.84611800	-2.70512400	1.78520400
H	3.51260500	-1.14298800	2.50213200
C	2.71441500	-4.56540700	-3.21694400
H	2.79953300	-3.14706000	-4.86533200
H	4.36085400	-3.50111700	-4.13595700
H	2.88158200	-5.62335700	-1.32211400
H	4.41110900	-5.02869600	-1.95430400
C	6.46350300	-3.03328400	2.65341100
H	5.83074500	-3.73456800	0.69273700
H	7.54891700	-3.42215700	0.80544900
H	4.90587900	-2.43376400	4.06789500
H	5.84748600	-1.09215400	3.44556400
H	1.62799800	-4.43721700	-3.10276100
H	2.86267100	-5.45476100	-3.84076400
H	6.24165700	-4.04858600	3.00241500
H	7.43304000	-2.76502000	3.08931100
H	-10.49917700	-1.63661200	-0.71147900
C	-11.16741800	-0.84954600	-1.04548400
C	-12.35442300	-1.16346000	-1.70863800
C	-10.81570500	0.48630000	-0.81880400
C	-13.20754400	-0.14739500	-2.14519900
H	-12.61421900	-2.20415200	-1.88424800
C	-11.67051700	1.49987700	-1.26654400
C	-9.55724300	0.84008100	-0.06004200
H	-14.13218800	-0.39346600	-2.66012000
C	-12.86287000	1.18678400	-1.92127500
H	-11.40186600	2.54199900	-1.10514900
O	-8.55171800	-0.13026500	-0.30247400
H	-9.20355100	1.84147100	-0.35853000
H	-9.76602700	0.88858400	1.02447500
H	-13.51644300	1.98447200	-2.26404700
C	-7.36257400	0.10672300	0.41971900

C	-6.37570700	-1.01000100	0.09601300
H	-6.93510400	1.08830200	0.14522200
H	-7.56883900	0.13889200	1.50498700
C	-5.01456300	-0.82230300	0.78107000
H	-6.82100100	-1.96779600	0.39536400
H	-6.24668100	-1.05159700	-0.99317400
C	-4.05977700	-1.98805800	0.46008500
H	-5.16983300	-0.72816900	1.86042600
H	-4.56765400	0.12295400	0.44499900
H	-4.12962600	-2.16509600	-0.61663600
H	-4.44533200	-2.90887800	0.92107800
Ts _{3d} -3			
C	-2.04091700	-2.49014300	2.03396900
C	-2.55729100	-2.13884700	0.60670400
C	-1.56047900	-1.17816900	-0.06140300
C	-1.58230600	-2.70222700	-0.42560000
C	-0.40465900	-0.97623600	0.82330900
C	-0.60800800	-1.84919300	2.07567600
C	-3.00570800	-2.28874800	3.23900700
C	-2.54376000	-3.12547300	4.44701000
C	-3.32174300	-0.84799700	3.68927900
C	-1.95034100	-3.17809600	-1.77812000
C	-1.38795200	-4.25364100	-2.34146100
C	-1.92119000	-0.10817600	-1.03984600
C	-1.59676600	-0.07354800	-2.33373000
O	-0.32206200	-1.00922600	3.24380600
C	-0.51087400	0.27155100	2.98800100
C	-0.27716600	1.21473500	4.12442500
O	-0.83586000	0.62455000	1.84515200
H	-1.86993400	-3.57454200	2.02862300
H	-0.76212700	-3.28988300	-0.01225700
H	0.16700800	-2.61301300	2.13829200
H	-3.94759600	-2.73391200	2.89451600
H	-3.27224800	-3.05227500	5.26202100
H	-2.44160400	-4.18582300	4.18897800
H	-1.57979100	-2.77440600	4.83344500
H	-4.30497500	-0.81703100	4.17081100
H	-3.33853400	-0.12944900	2.86540500
H	-2.60346600	-0.50399500	4.43924400
H	-2.71537500	-2.63530200	-2.32348500
H	-1.69236900	-4.60145800	-3.32381100
H	-0.61603500	-4.83220700	-1.83805500
H	-2.46727100	0.72852800	-0.60621400
H	-1.88882500	0.76553600	-2.95887900

H	-1.03741800	-0.86979100	-2.81558500
H	-0.33194400	2.24221400	3.76616100
H	0.70835100	1.01833000	4.55843800
H	-1.02329100	1.05103300	4.90792200
Au	1.51517200	-0.56119200	0.15439300
H	0.28720700	6.68025700	1.24140500
C	-0.66772000	6.18928300	1.02571100
C	-0.64910700	4.70961000	1.46321900
H	-0.85229400	6.27421400	-0.05186700
H	-1.45998600	6.73822600	1.54789400
C	0.50565400	3.97089900	0.79788100
C	-2.01942500	4.05339300	1.22165300
H	-0.45920300	4.69434200	2.54669500
C	0.44647400	3.52391400	-0.52116000
C	1.71619400	3.79998400	1.46037200
H	-2.79385400	4.56952800	1.80040600
H	-2.01428400	2.99744700	1.51173400
H	-2.31267900	4.11094100	0.16691400
C	1.53737100	2.94521700	-1.18344700
H	-0.47019100	3.66903800	-1.08674400
C	2.84946500	3.21023000	0.87367300
H	1.80667600	4.17950800	2.47725500
C	1.28003200	2.72306100	-2.68818600
C	2.76010400	2.74772200	-0.46965600
C	4.06116700	3.20219700	1.83405100
H	0.18856100	2.63640200	-2.75795300
C	1.65665500	3.97275300	-3.51523900
C	1.82456200	1.45333800	-3.35299000
C	3.98332900	2.29381900	-1.23837700
C	5.49099900	3.12967000	1.27598200
C	3.84652100	2.15849900	2.95430900
H	4.01038100	4.18015800	2.33164200
H	1.28683800	3.86785800	-4.54227000
H	1.21783900	4.88071000	-3.08810200
H	2.74099800	4.10966100	-3.56731700
H	1.32997500	1.31747300	-4.32259900
H	1.61339600	0.56819500	-2.74524000
H	2.89891700	1.49944600	-3.54136000
C	4.66964200	3.33441100	-1.89320800
C	4.48211700	0.97176800	-1.39924700
H	6.19328900	3.26923400	2.10621000
H	5.68195200	3.92100400	0.54668600
H	5.73264500	2.17740800	0.79793000
H	2.93715200	2.37559700	3.52480200

H	3.74016700	1.14732100	2.55033200
H	4.68968400	2.16175400	3.65514200
C	5.78962700	3.11847300	-2.69072600
H	4.30049100	4.34643800	-1.75946600
C	5.61255300	0.77162300	-2.21850900
P	3.80029200	-0.54302600	-0.57224600
C	6.26381000	1.82054400	-2.86123900
H	6.28182400	3.95674500	-3.17534600
H	5.99445700	-0.23035700	-2.37519500
C	4.05520900	-1.97470000	-1.77239900
C	4.97161800	-0.81444000	0.88737100
H	7.12918500	1.61996600	-3.48583300
C	3.42159700	-1.71503800	-3.15625900
C	3.51437700	-3.30543000	-1.19672600
H	5.14025500	-2.08728600	-1.90193800
C	6.43107000	-1.24882600	0.54013900
C	4.35890400	-1.69850500	2.00399400
H	5.02941200	0.19889600	1.29400300
C	3.68546000	-2.88446900	-4.12054400
H	2.33763500	-1.58929100	-3.03013500
H	3.79882700	-0.78445400	-3.58986600
C	3.77288800	-4.47706600	-2.16118900
H	3.97073600	-3.53027700	-0.22875400
H	2.43384500	-3.20507700	-1.02156000
C	6.73876300	-2.69289100	0.96271800
H	6.65592500	-1.11129900	-0.52085300
H	7.11787300	-0.57497600	1.06776600
C	5.42525700	-2.01881300	3.06331800
H	3.95513400	-2.63432500	1.60143700
H	3.51002200	-1.17254600	2.45690300
C	3.17873200	-4.21567200	-3.55096000
H	3.20822900	-2.67249000	-5.08485200
H	4.76507500	-2.95697500	-4.31719600
H	3.35839300	-5.39736400	-1.73134600
H	4.85714200	-4.63768400	-2.25023500
C	6.56239500	-2.89570000	2.48406800
H	6.08238600	-3.38100800	0.41536700
H	7.76061300	-2.95192800	0.66309800
H	4.96150200	-2.51500400	3.92346000
H	5.83515000	-1.07258000	3.44163600
H	2.08152900	-4.18391600	-3.47725100
H	3.42397400	-5.04040700	-4.23042100
H	6.36006100	-3.95443700	2.68453100
H	7.49952100	-2.65994900	3.00174500

H	-10.47776300	-1.50590800	-0.77333100
C	-11.10792500	-0.66914800	-1.05726800
C	-12.29647400	-0.88485000	-1.75519700
C	-10.70418600	0.63137700	-0.73130400
C	-13.10008400	0.19518400	-2.12837700
H	-12.59672400	-1.89847000	-2.00779300
C	-11.50943700	1.70924700	-1.11563600
C	-9.44175200	0.87232000	0.06376000
H	-14.02632000	0.02556600	-2.67057900
C	-12.70396800	1.49413100	-1.80552400
H	-11.20021500	2.72490700	-0.87709000
O	-8.45589600	-0.08452600	-0.29114000
H	-9.06772300	1.89404700	-0.11692300
H	-9.65104200	0.79782800	1.14656200
H	-13.31877000	2.34110100	-2.09807600
C	-7.26578900	0.03193800	0.45845200
C	-6.31010400	-1.06441800	-0.00044900
H	-6.81063400	1.02774700	0.30803400
H	-7.47662100	-0.06484300	1.53885800
C	-4.95041200	-1.01678000	0.71005400
H	-6.79092200	-2.03695800	0.16850700
H	-6.17154500	-0.96885800	-1.08513900
C	-4.04304600	-2.17329200	0.24963200
H	-5.11039800	-1.05425100	1.79204000
H	-4.46174100	-0.05605600	0.49958600
H	-4.12353400	-2.22567900	-0.83991700
H	-4.45719700	-3.12580800	0.60991100
4d-3			
C	-2.08162200	-2.09829800	2.27411600
C	-2.57897100	-1.86139400	0.82017200
C	-1.59403400	-0.94312200	0.07730100
C	-1.56813700	-2.44845000	-0.18523300
C	-0.45967300	-0.57930300	1.01047300
C	-0.66888700	-1.42336400	2.29895600
C	-3.06811400	-1.80044200	3.44441700
C	-2.61641400	-2.50556200	4.73664000
C	-3.41747300	-0.32562600	3.74125600
C	-1.95290500	-3.06961500	-1.47612000
C	-1.43677500	-4.22317200	-1.91399000
C	-1.99265600	0.06805100	-0.94843200
C	-1.67819900	0.03433000	-2.24550500
O	-0.49601200	-0.41464900	3.38248100
C	-0.63708900	0.76727100	2.87246300
C	-0.58593400	1.97440600	3.73340700

O	-0.77145700	0.83531200	1.61407400
H	-1.89138800	-3.17597800	2.36540400
H	-0.72812100	-2.97753400	0.26913400
H	0.13220000	-2.13239800	2.48905500
H	-3.99684000	-2.29298800	3.13164200
H	-3.36483600	-2.37194100	5.52556800
H	-2.48723500	-3.58291900	4.58260000
H	-1.66908400	-2.09992100	5.11116700
H	-4.41454000	-0.26292600	4.18992300
H	-3.43087700	0.30151700	2.84380700
H	-2.72596500	0.11154000	4.46795100
H	-2.68997700	-2.55892200	-2.08831200
H	-1.74746600	-4.66060000	-2.85790500
H	-0.69642900	-4.77822700	-1.34119300
H	-2.55866600	0.91696000	-0.56632400
H	-1.99532200	0.82554000	-2.91934400
H	-1.10316800	-0.77735500	-2.68122400
H	-1.51180400	2.54626800	3.61674300
H	0.23953500	2.60731100	3.38967900
H	-0.44624000	1.69534700	4.77782700
Au	1.50714800	-0.50436800	0.24457400
H	0.98953600	6.85639500	0.91709900
C	-0.01575500	6.48858900	0.68656200
C	-0.19711400	5.02833000	1.15211800
H	-0.16286100	6.57150900	-0.39671300
H	-0.74185200	7.14638100	1.17826400
C	0.86706700	4.13348900	0.52735300
C	-1.63692100	4.55380800	0.89139600
H	-0.03237600	5.01417800	2.23988700
C	0.73904600	3.59646300	-0.75204300
C	2.07117900	3.89902200	1.18460900
H	-2.34670000	5.15978300	1.46577200
H	-1.77467700	3.50202800	1.16806300
H	-1.91000400	4.65443700	-0.16509800
C	1.75999100	2.87428100	-1.38553600
H	-0.17336600	3.77837800	-1.31355800
C	3.13393400	3.16710200	0.62568800
H	2.22090300	4.34582700	2.16712600
C	1.44458000	2.56079300	-2.86231700
C	2.97510600	2.61907600	-0.67852600
C	4.35779000	3.10872100	1.56734600
H	0.34811700	2.54097800	-2.89818000
C	1.87854400	3.72069100	-3.78636400
C	1.88781700	1.21373400	-3.44426600

C	4.13739900	2.00569400	-1.43198900
C	5.76501100	2.88975400	0.99070800
C	4.07662100	2.14239200	2.74092800
H	4.39744900	4.11133200	2.01424300
H	1.48351100	3.56246600	-4.79692200
H	1.50382100	4.68342100	-3.42273600
H	2.96808900	3.78629400	-3.86376400
H	1.35251700	1.03831000	-4.38544400
H	1.64353200	0.39239100	-2.76450300
H	2.95597300	1.17724700	-3.66746900
C	4.88648900	2.93552600	-2.17856400
C	4.52724800	0.63926100	-1.49851900
H	6.49411900	3.02311300	1.79850800
H	6.00046800	3.61810500	0.21049200
H	5.92014700	1.89423000	0.56888000
H	3.20731600	2.46997200	3.32178000
H	3.86434300	1.12943500	2.38651600
H	4.93434200	2.09723100	3.42237100
C	5.96518900	2.57126100	-2.97904800
H	4.60135600	3.98114700	-2.11701000
C	5.61746800	0.28911500	-2.32177800
P	3.75243300	-0.75445200	-0.54667900
C	6.33168400	1.23048100	-3.05749800
H	6.50860300	3.32850300	-3.53681100
H	5.91695000	-0.74887800	-2.40708300
C	3.83979400	-2.28054000	-1.65028400
C	4.95995800	-1.03371200	0.88364400
H	7.16248800	0.91440200	-3.68131200
C	3.17124900	-2.07052300	-3.02538400
C	3.22488600	-3.51809100	-0.95359700
H	4.90532900	-2.49127400	-1.81205100
C	6.35457700	-1.64100700	0.51741000
C	4.31660900	-1.76374000	2.08963600
H	5.13577500	-0.00464400	1.20935000
C	3.29973100	-3.32584100	-3.90594200
H	2.10716900	-1.84521400	-2.87285100
H	3.60622700	-1.20965600	-3.54139600
C	3.34799600	-4.77360500	-1.83586900
H	3.70814800	-3.70718500	0.00930600
H	2.16434600	-3.32078100	-0.74336500
C	6.56898900	-3.04047300	1.11415000
H	6.51960600	-1.67162000	-0.56281800
H	7.12980300	-0.96980800	0.90767100
C	5.38243600	-2.04554800	3.16054000

H	3.84611800	-2.70512400	1.78520400
H	3.51260500	-1.14298800	2.50213200
C	2.71441500	-4.56540700	-3.21694400
H	2.79953300	-3.14706000	-4.86533200
H	4.36085400	-3.50111700	-4.13595700
H	2.88158200	-5.62335700	-1.32211400
H	4.41110900	-5.02869600	-1.95430400
C	6.46350300	-3.03328400	2.65341100
H	5.83074500	-3.73456800	0.69273700
H	7.54891700	-3.42215700	0.80544900
H	4.90587900	-2.43376400	4.06789500
H	5.84748600	-1.09215400	3.44556400
H	1.62799800	-4.43721700	-3.10276100
H	2.86267100	-5.45476100	-3.84076400
H	6.24165700	-4.04858600	3.00241500
H	7.43304000	-2.76502000	3.08931100
H	-10.49917700	-1.63661200	-0.71147900
C	-11.16741800	-0.84954600	-1.04548400
C	-12.35442300	-1.16346000	-1.70863800
C	-10.81570500	0.48630000	-0.81880400
C	-13.20754400	-0.14739500	-2.14519900
H	-12.61421900	-2.20415200	-1.88424800
C	-11.67051700	1.49987700	-1.26654400
C	-9.55724300	0.84008100	-0.06004200
H	-14.13218800	-0.39346600	-2.66012000
C	-12.86287000	1.18678400	-1.92127500
H	-11.40186600	2.54199900	-1.10514900
O	-8.55171800	-0.13026500	-0.30247400
H	-9.20355100	1.84147100	-0.35853000
H	-9.76602700	0.88858400	1.02447500
H	-13.51644300	1.98447200	-2.26404700
C	-7.36257400	0.10672300	0.41971900
C	-6.37570700	-1.01000100	0.09601300
H	-6.93510400	1.08830200	0.14522200
H	-7.56883900	0.13889200	1.50498700
C	-5.01456300	-0.82230300	0.78107000
H	-6.82100100	-1.96779600	0.39536400
H	-6.24668100	-1.05159700	-0.99317400
C	-4.05977700	-1.98805800	0.46008500
H	-5.16983300	-0.72816900	1.86042600
H	-4.56765400	0.12295400	0.44499900
H	-4.12962600	-2.16509600	-0.61663600
H	-4.44533200	-2.90887800	0.92107800

C	-2.10238000	-0.37947100	1.88614700
C	-2.63266800	0.36485800	0.62014700
C	-1.48127600	1.25393100	0.10692600
C	-1.87051500	-0.00763100	-0.65690300
C	-0.28826300	1.05058500	1.07491400
C	-0.81985100	0.33292600	2.22078700
C	-3.05880700	-0.70708800	3.08208100
C	-2.46085900	-1.83239700	3.94590000
C	-3.49151700	0.46293600	3.98149100
C	-2.49165400	0.01985400	-2.00434300
C	-2.23332700	-0.88482400	-2.95450400
C	-1.69862100	2.62462600	-0.44518800
C	-1.40067100	3.01300600	-1.68735400
O	-1.14643900	2.00054800	3.21384300
C	-0.35226700	2.74738500	2.62249600
C	-0.04125200	4.14354900	3.05608300
O	0.27274300	2.32266200	1.53467800
H	-1.75995000	-1.37762900	1.56202200
H	-1.16479400	-0.83268200	-0.54339900
H	-0.18993800	-0.00712200	3.03638100
H	-3.95888000	-1.11242800	2.60741300
H	-3.16059200	-2.11413900	4.73965000
H	-2.24625300	-2.73176900	3.35636900
H	-1.53065000	-1.51667100	4.43582900
H	-4.33274700	0.14045500	4.60496300
H	-3.81263600	1.34260300	3.41843700
H	-2.68592400	0.77808400	4.64991000
H	-3.18877700	0.82538400	-2.21908700
H	-2.70809600	-0.83560100	-3.92971000
H	-1.54315600	-1.71031800	-2.79147200
H	-2.12805700	3.35513700	0.24316500
H	-1.57974800	4.03250500	-2.01764400
H	-0.98185000	2.32577700	-2.41707900
H	-0.65183600	4.83951600	2.46898200
H	1.00824400	4.37137000	2.85621200
H	-0.27616400	4.27087400	4.11326400
Au	1.37033900	-0.17941200	0.39658500
H	4.74229000	6.31471800	-0.09884600
C	3.72087000	6.52433000	-0.43336400
C	2.72220200	5.48536700	0.12050400
H	3.71866700	6.51479800	-1.52977300
H	3.45389100	7.53479500	-0.10259300
C	3.14570000	4.07675900	-0.27854000
C	1.28686700	5.84840800	-0.29120500

H	2.77899800	5.53646500	1.21830900
C	2.68151500	3.43887000	-1.42641300
C	4.10472900	3.39939600	0.46774100
H	0.99496000	6.80369700	0.15943800
H	0.56921300	5.08050400	0.01784400
H	1.19736600	5.96680800	-1.37727800
C	3.15240700	2.18733100	-1.85053300
H	1.94784000	3.94028000	-2.05058300
C	4.61255800	2.13688000	0.12193400
H	4.50844400	3.88679900	1.35408200
C	2.62273900	1.78370300	-3.24182800
C	4.11593700	1.49880500	-1.05091600
C	5.68921000	1.65240700	1.11963200
H	1.70463000	2.37407700	-3.35551900
C	3.56251700	2.25482300	-4.37400400
C	2.19385100	0.32889300	-3.46634700
C	4.76878800	0.24875100	-1.60355900
C	6.75369400	0.63688900	0.67666500
C	5.02325700	1.22490900	2.44755100
H	6.25895700	2.56119800	1.35581300
H	3.06408700	2.14263000	-5.34426400
H	3.83414100	3.30886500	-4.25295400
H	4.48373500	1.66579500	-4.40568400
H	1.60816000	0.26467100	-4.39126200
H	1.55925300	-0.02722800	-2.64765500
H	3.04260900	-0.34949000	-3.57128300
C	5.84426300	0.50201500	-2.47680900
C	4.42512200	-1.11000400	-1.36283700
H	7.49299500	0.53804700	1.48017400
H	7.28377100	0.97014600	-0.21923900
H	6.35681300	-0.36017200	0.47186400
H	4.46156900	2.05352700	2.89117500
H	4.31607600	0.40384000	2.29708100
H	5.77757100	0.90227000	3.17508400
C	6.56237200	-0.50881900	-3.10888700
H	6.12037900	1.53717800	-2.65142500
C	5.15937600	-2.12088800	-2.01780000
P	3.10417200	-1.70141500	-0.20440900
C	6.21387700	-1.83730800	-2.88045200
H	7.38383400	-0.25762500	-3.77361800
H	4.89884100	-3.16170100	-1.86484200
C	2.35656500	-3.25068800	-0.97901700
C	4.05383800	-2.26258000	1.33303500
H	6.75099500	-2.64705600	-3.36519500

C	1.89475800	-3.05241200	-2.43825700
C	1.18311600	-3.80607400	-0.13720500
H	3.15325000	-4.00703000	-0.97083600
C	4.90503900	-3.56584600	1.19205300
C	3.17108100	-2.29034600	2.60698600
H	4.75628900	-1.43402200	1.45850100
C	1.36906400	-4.36994200	-3.03463500
H	1.09685200	-2.29826000	-2.46196500
H	2.70989600	-2.66738500	-3.05701500
C	0.65090300	-5.12353300	-0.72962700
H	1.48410100	-3.97230300	0.90109900
H	0.37593300	-3.06010800	-0.11650000
C	4.33660000	-4.73832300	2.00557900
H	5.03150900	-3.86181400	0.14727400
H	5.91771900	-3.34604100	1.55262200
C	3.94915100	-2.91865700	3.77359900
H	2.24512600	-2.85235900	2.43931300
H	2.86449700	-1.26747100	2.85571900
C	0.22903900	-4.96253500	-2.19562500
H	1.03645000	-4.19436800	-4.06466000
H	2.19475300	-5.09396800	-3.09387500
H	-0.19114900	-5.47957100	-0.12352000
H	1.43363900	-5.89224400	-0.65581700
C	4.26808400	-4.41145300	3.51322600
H	3.33593500	-4.99072400	1.63246500
H	4.95183700	-5.63001000	1.84023500
H	3.38208800	-2.80649200	4.70463300
H	4.88005000	-2.35311100	3.91464700
H	-0.64677400	-4.29889700	-2.25131200
H	-0.08623800	-5.92818600	-2.60789300
H	3.50896700	-5.04681300	3.98442500
H	5.22051400	-4.66645900	3.99232700
H	-9.77662800	-2.13377100	-0.12824400
C	-9.79074400	-1.29408500	-0.84727000
C	-11.14723100	-0.62736000	-0.84298800
O	-8.78559800	-0.35715000	-0.49632500
H	-9.58315600	-1.72592300	-1.84074500
C	-11.43901300	0.40283700	0.05885300
C	-12.14669400	-1.06840000	-1.71764100
C	-7.49731900	-0.92833900	-0.40898900
C	-12.70914900	0.98012500	0.08339500
H	-10.66100600	0.75580200	0.72801600
C	-13.42053500	-0.49833500	-1.68737700
H	-11.92763700	-1.86139400	-2.42986700

C	-6.51434300	0.16854300	-0.01325000
H	-7.48609200	-1.74402300	0.33656400
H	-7.20632800	-1.37400800	-1.37690700
C	-13.70481900	0.52937700	-0.78638300
H	-12.92239900	1.78356200	0.78374600
H	-14.18635100	-0.85056300	-2.37323800
C	-5.07163100	-0.33818500	0.10601500
H	-6.57186400	0.97147600	-0.75978100
H	-6.84474900	0.60329100	0.93934800
H	-14.69383800	0.97893300	-0.76512300
C	-4.09428000	0.78482800	0.50534900
H	-4.74915200	-0.77342300	-0.84790000
H	-5.03263300	-1.15454800	0.83988900
H	-4.42722000	1.23691000	1.44615900
H	-4.16589200	1.58612800	-0.24074300

5d-3

C	2.59374800	1.34464600	-0.63665200
C	1.94368000	-0.02681600	-0.24354300
C	2.38646400	-1.21584700	-1.10819500
C	4.32084900	-0.12672500	0.01615900
C	4.08327800	1.06951300	-0.53216400
C	3.08270600	-0.93143400	0.23699100
C	1.56405200	-2.43332000	-1.27592300
C	1.50596300	-3.14873400	-2.40472000
C	3.03659100	-1.91135000	1.36329300
C	2.67157600	-1.61687300	2.61272800
O	6.88700900	1.00788700	0.00756200
C	6.71525300	-0.14591800	0.31674600
C	7.78850600	-1.11190900	0.75702200
O	5.50251800	-0.77957800	0.31961300
H	2.98232800	-0.96901800	-1.98577000
H	4.83840000	1.76320300	-0.86459500
H	0.99915400	-2.77578900	-0.41014500
H	0.90307500	-4.04929000	-2.47759800
H	2.05848200	-2.85848000	-3.29589400
H	3.35859300	-2.92627300	1.12868500
H	2.68669700	-2.36582400	3.40035600
H	2.34868200	-0.61772800	2.89580600
H	7.57523700	-1.47674900	1.76719300
H	8.75575200	-0.60887900	0.73990800
H	7.80868300	-1.98250000	0.09321700
H	-10.05533700	0.81809000	-0.41332500
C	-9.13256900	0.41151300	-0.00743000
C	-9.12698600	-0.19671800	1.24916000

C	-7.94983900	0.50978100	-0.74117500
H	-10.04558900	-0.26888100	1.82554300
C	-7.93263100	-0.70523400	1.76296000
C	-6.75089600	-0.00592100	-0.23576500
H	-7.95846900	0.99510000	-1.71531900
C	-6.75211700	-0.61429600	1.02432700
H	-7.91888600	-1.17481700	2.74336200
C	-5.49066100	0.05599500	-1.06963800
H	-5.82019700	-1.00097600	1.42293500
O	-4.35036900	0.05937600	-0.23330900
H	-5.44881400	-0.81331300	-1.75198500
H	-5.50441800	0.95495000	-1.70983600
C	-3.13062400	0.01457700	-0.95447200
C	-1.97665700	0.01446800	0.03984800
H	-3.09620300	-0.88961000	-1.58760000
H	-3.05712500	0.88438100	-1.63077500
C	-0.60360100	-0.03690700	-0.64166800
H	-2.05792300	0.91218100	0.66728100
H	-2.09645900	-0.84634000	0.71138500
C	0.55193400	-0.08697100	0.37582400
H	-0.48795300	0.83095800	-1.30349700
H	-0.54541900	-0.91811800	-1.29215600
H	0.45754800	-1.00666600	0.96394000
H	0.43860200	0.72655700	1.10274500
C	2.17709400	2.58139800	0.23295600
H	2.07198400	2.23293500	1.27091600
C	3.25554500	3.68133900	0.23519700
H	2.90543900	4.54792600	0.80784900
H	4.19372700	3.34178800	0.68211800
H	3.47280900	4.02789900	-0.78394500
C	0.84669500	3.20950400	-0.21608700
H	0.60426600	4.07910700	0.40621100
H	0.91948200	3.55977500	-1.25430400
H	0.00124400	2.52164800	-0.15758600
H	2.33521400	1.58469300	-1.68072400
T _{Sd} -3			
C	2.49407100	1.25820300	-0.69077800
C	4.00238100	1.12283500	-0.63367800
C	2.02222400	2.49025900	0.16465500
C	3.03910200	3.64849600	0.12901900
C	0.65559300	3.04658300	-0.27093300
C	1.98575000	-0.17987700	-0.23558300
C	3.20568100	-0.81429400	0.43168200
C	4.35343900	0.01920900	0.04055600

O	5.60375300	-0.47698800	0.36909300
C	6.74507300	0.27258200	0.27800100
C	7.92144800	-0.54281000	0.75763300
O	6.79157000	1.40845200	-0.12622600
C	2.29037400	-1.22134900	-1.29789600
C	1.93411200	-2.57308300	-1.36873100
C	1.20010400	-3.31658100	-0.45720600
C	2.37038400	-2.86391600	1.60380300
C	3.35567900	-1.98767000	1.19078600
H	2.16778300	1.43811700	-1.72555800
H	4.68365300	1.84541300	-1.05106600
H	1.95676400	2.15962700	1.21108400
H	2.65468300	4.49819500	0.70484000
H	4.00652700	3.36667000	0.55283300
H	3.20949900	3.99872300	-0.89775100
H	0.39090500	3.92251800	0.33305700
H	-0.15985900	2.32807300	-0.17485000
H	0.69151600	3.37131600	-1.31931500
H	7.76922900	-0.84992600	1.79756800
H	8.83062300	0.05344200	0.67568500
H	8.01780100	-1.45416000	0.15836200
H	2.96889100	-0.87285500	-2.07159200
H	2.49052100	-3.13757700	-2.11821900
H	0.38219700	-2.89049600	0.10398400
H	1.15299800	-4.39547900	-0.57763600
H	1.38458600	-2.53275200	1.89194800
H	2.67059300	-3.81166200	2.04314100
H	4.38595900	-2.33059400	1.27149300
H	-7.86822700	1.30485100	2.65169500
C	-7.88849600	0.80354700	1.68725100
C	-9.09642800	0.33095700	1.17152800
C	-6.70207200	0.63622100	0.97126700
H	-10.01924000	0.46255700	1.73039500
C	-9.11071000	-0.31780700	-0.06478500
C	-6.70962400	-0.01384300	-0.26748900
H	-5.76015800	0.99573300	1.37151000
C	-7.92307700	-0.49232100	-0.77552300
H	-10.04464000	-0.69634600	-0.47226100
C	-5.44234200	-0.16576700	-1.07909000
H	-7.93915100	-1.00874200	-1.73352200
O	-4.31022600	-0.13253400	-0.23278100
H	-5.47098900	-1.11032600	-1.64949800
H	-5.37361700	0.64773700	-1.82510900
C	-3.08485900	-0.20637900	-0.94106500

C	-1.93786700	-0.14445000	0.05974200
H	-3.03835800	-1.14365000	-1.52270800
H	-3.01225000	0.62550100	-1.66394600
C	-0.56174800	-0.23837700	-0.61104000
H	-2.02363300	0.78996700	0.63058900
H	-2.06294600	-0.96218200	0.78219900
C	0.59097400	-0.21473600	0.40886500
H	-0.44642100	0.58136700	-1.33194700
H	-0.50012900	-1.16104200	-1.19949900
H	0.48755200	-1.08292800	1.06075700
H	0.48158200	0.64568100	1.07668500
6d-3			
C	-3.04858800	-0.84514600	1.33424400
C	-3.08931500	0.66879400	1.31680900
C	-2.26335800	-1.47588300	2.51684900
C	-2.72133600	-0.88562900	3.86339000
C	-2.41153400	-3.00685600	2.57055700
C	-2.62194600	-1.22229000	-0.14984800
C	-3.02856200	0.03522900	-0.93753300
C	-3.10188100	1.11721200	0.05186100
O	-3.22934500	2.40129000	-0.45268400
C	-3.35610200	3.50751600	0.33951800
C	-3.49858300	4.73472600	-0.52890700
O	-3.35047200	3.49636800	1.54645300
C	-3.34684700	-2.47449200	-0.62740000
C	-3.45297100	-2.90266000	-1.89016400
C	-2.90031900	-2.20665300	-3.11356100
C	-3.47527900	-0.79996500	-3.34522000
C	-3.34184800	0.20570500	-2.23318000
H	-4.08988000	-1.19441600	1.45722200
H	-3.18754000	1.28602300	2.19486100
H	-1.19750800	-1.24037700	2.40361900
H	-2.21431600	-1.39208800	4.69296800
H	-2.50063300	0.18248500	3.94850800
H	-3.80188900	-1.01906000	4.00620100
H	-1.84910700	-3.41479500	3.41863000
H	-2.04926100	-3.50257700	1.66530600
H	-3.46343300	-3.29130800	2.70708200
H	-2.63275100	4.83172200	-1.19201500
H	-3.58214200	5.61760500	0.10546000
H	-4.38731400	4.64689600	-1.16271000
H	-3.81253000	-3.07854500	0.14849500
H	-3.99907100	-3.82937800	-2.06336200
H	-1.80616200	-2.13545100	-3.05385100

H	-3.11088200	-2.81251000	-4.00239000
H	-3.01787700	-0.37970400	-4.25338400
H	-4.54791500	-0.89048900	-3.58336700
H	-3.61333000	1.21996500	-2.52470500
H	9.15495900	1.45038400	-0.86545500
C	8.33858200	0.82546500	-0.51250400
C	8.59066300	-0.47448600	-0.07088600
C	7.03461900	1.32241400	-0.51295600
H	9.60446100	-0.86624000	-0.07506700
C	7.53123300	-1.27019500	0.36973300
C	5.96948200	0.53355300	-0.06392700
H	6.84282400	2.33286200	-0.86892000
C	6.22905100	-0.76900400	0.37700300
H	7.71880100	-2.28575500	0.70932700
C	4.57126700	1.10715700	-0.01316700
H	5.40148200	-1.38641000	0.71023300
O	3.61413500	0.07734400	-0.16764800
H	4.41106400	1.62127900	0.95279100
H	4.44753200	1.87261700	-0.79861200
C	2.27951800	0.53367500	-0.02257600
C	1.33535800	-0.64798300	-0.20439000
H	2.14096500	0.99106900	0.97310500
H	2.06262300	1.31721500	-0.76974500
C	-0.14027100	-0.25270800	-0.05101900
H	1.51135700	-1.08522400	-1.19610000
H	1.60004300	-1.42101100	0.52936200
C	-1.07361100	-1.45235100	-0.27976100
H	-0.38325900	0.53858700	-0.77189800
H	-0.29873600	0.18248800	0.94284800
H	-0.78749400	-2.26522100	0.39741300
H	-0.88215900	-1.83152800	-1.28860600
Ts _{ic} -3			
C	-0.79070600	4.53986600	-0.76820200
C	0.06888300	4.56005500	0.51082100
C	-0.57526000	4.89187500	1.70353300
C	-0.95387700	2.86006800	0.73426800
C	-1.81890300	3.46258700	-0.32822700
C	-1.21706200	5.88834100	-1.40765100
C	-2.01298500	5.61852400	-2.69732200
C	-1.94544200	6.88679000	-0.49555800
C	-0.49281000	1.74902100	1.23887500
C	0.03887300	5.14105400	2.99241800
C	-0.67173900	5.64864400	4.01694300
C	0.53775700	1.48718900	2.24376300

C	0.49058800	1.89353000	3.52118500
O	-3.03829800	3.99065500	0.23893900
C	-4.22212500	3.60202800	-0.32613200
C	-5.38764800	4.20243600	0.41641500
O	-4.29396900	2.87893500	-1.29366100
H	-0.19709000	4.02944100	-1.53216100
H	-1.64124000	5.09460800	1.66188000
H	-2.09620300	2.75129200	-1.10784900
H	-0.27154200	6.36547600	-1.70629100
H	-2.22856400	6.55833300	-3.21625500
H	-1.45099900	4.97935200	-3.38864400
H	-2.96953000	5.12491400	-2.49237300
H	-2.13793100	7.81132600	-1.05079400
H	-1.34786900	7.15804800	0.38154400
H	-2.90848200	6.50154400	-0.14793400
H	1.10486600	4.97426600	3.11007000
H	-0.20361900	5.90146100	4.96306100
H	-1.73966200	5.83663400	3.93450800
H	1.33943700	0.82438400	1.92137500
H	1.26558200	1.59721100	4.22234200
H	-0.32718800	2.49127300	3.90909100
H	-5.36962200	3.88603600	1.46451100
H	-6.31857300	3.88310600	-0.05256600
H	-5.32329600	5.29561200	0.40259200
H	-5.53010900	-2.02928000	3.45447800
C	-4.69523600	-2.60434100	3.03645700
C	-4.14381000	-1.84196100	1.80423200
C	-5.16404600	-4.03726900	2.68841700
H	-3.92793500	-2.64790600	3.81815800
C	-3.46596300	-2.82435800	0.82381300
H	-4.96143400	-1.31988600	1.29570500
H	-3.44101100	-1.06577000	2.12876200
C	-5.65225000	-4.11099800	1.23777700
H	-5.95409200	-4.35329700	3.37836100
H	-4.33815900	-4.74866400	2.82490100
P	-2.33500200	-1.99998600	-0.44680300
C	-4.50300600	-3.82319200	0.23753200
H	-2.74710100	-3.40617200	1.40991000
H	-6.45993300	-3.38123800	1.09363700
H	-6.08410000	-5.09371800	1.01778800
Au	-1.33132100	-0.02829900	0.41454700
C	-1.19257000	-3.35861900	-0.99356900
C	-3.39226200	-1.54866800	-1.93559100
H	-4.94017000	-3.44695900	-0.69367800

H	-3.98971800	-4.75820400	-0.01216800
C	0.16606200	-3.53662800	-0.60641300
C	-1.78397500	-4.31474500	-1.84628900
C	-2.55488200	-0.98504400	-3.10160200
C	-4.51297100	-0.55992900	-1.54294000
H	-3.86979800	-2.47403100	-2.28152700
C	1.04771700	-2.66980500	0.27516500
C	0.83199200	-4.67922800	-1.09367900
C	-1.09330700	-5.42631400	-2.31905300
H	-2.81581100	-4.19449500	-2.15517500
C	-3.44295200	-0.63177300	-4.30668400
H	-2.03202000	-0.08047100	-2.76073700
H	-1.78699600	-1.70338500	-3.40365700
C	-5.38944400	-0.19555800	-2.75487300
H	-5.14571300	-0.98695000	-0.75846900
H	-4.06855000	0.35584800	-1.13379700
C	2.00279300	-1.79943900	-0.33662900
C	1.15638800	-2.92042200	1.67313800
C	0.23109200	-5.61215200	-1.93332300
H	1.86061400	-4.83300600	-0.78340100
H	-1.58957400	-6.13492800	-2.97545400
C	-4.55637900	0.35068800	-3.92126300
H	-2.81811500	-0.21405400	-5.10569300
H	-3.88832200	-1.55295400	-4.71004600
H	-6.13601400	0.54353600	-2.44259600
H	-5.94291900	-1.08738300	-3.08411500
C	2.98947800	-1.19136900	0.45585700
C	2.18298100	-1.51397000	-1.84110700
C	2.18123200	-2.28879400	2.39656200
C	0.29191500	-3.83461800	2.56671000
H	0.79409800	-6.47475700	-2.27809300
H	-4.11507400	1.31166600	-3.62415200
H	-5.20124100	0.55152000	-4.78526000
C	3.12085200	-1.43707200	1.82364800
H	3.71415300	-0.54607000	-0.03618100
H	2.70186700	-0.54670300	-1.86591000
C	3.14971400	-2.52079700	-2.50366900
C	0.92942900	-1.32431200	-2.70176200
H	2.26757900	-2.51195000	3.45855000
C	-0.36813600	-5.08865500	1.97147800
C	-0.71468500	-2.98107200	3.37020900
H	0.99962100	-4.22815600	3.30802400
C	4.28981700	-0.91176500	2.64829600
H	3.40355400	-2.18542900	-3.51691400

H	4.07922900	-2.61352900	-1.93175500
H	2.70032100	-3.51461200	-2.58918700
H	1.21340500	-0.87294600	-3.66042900
H	0.21309900	-0.65444100	-2.21553000
H	0.42544600	-2.26713900	-2.92357400
H	-0.79190400	-5.67935300	2.79226700
H	0.35968700	-5.71908200	1.45284400
H	-1.17625000	-4.87458000	1.26914300
H	-0.19439000	-2.24585600	3.99299500
H	-1.38629400	-2.42174400	2.71236500
H	-1.32216500	-3.61349800	4.02894200
C	5.55830600	-1.74589500	2.36805000
C	4.57682500	0.58552500	2.44545700
H	4.02573400	-1.06032000	3.70463300
H	5.38098400	-2.81090900	2.55333300
H	5.88238400	-1.63141500	1.32725600
H	6.38238900	-1.41982900	3.01309300
H	5.36706900	0.91108700	3.13176000
H	3.68862600	1.19741700	2.64717600
H	4.92067300	0.80159300	1.42810800
H	8.55778300	-2.87386900	-1.47996800
C	8.42351000	-1.82191500	-1.24321900
C	9.30458300	-1.18150000	-0.37133600
C	7.36341600	-1.11087500	-1.81218500
H	10.12926200	-1.73209300	0.07273700
C	9.12284400	0.17214600	-0.07221700
C	7.17890500	0.24540600	-1.52343400
H	6.67815500	-1.61416600	-2.49089000
C	8.06918500	0.88126300	-0.64680300
H	9.80690500	0.67560200	0.60563700
C	6.05261100	1.02366000	-2.15745600
H	7.92529000	1.93211900	-0.41163000
O	5.30502200	1.68523700	-1.13938100
H	6.44497000	1.77639400	-2.86239300
H	5.39955300	0.34944000	-2.73453400
C	4.20693800	2.42647700	-1.63987700
C	3.60640100	3.22274100	-0.48250300
H	4.53002800	3.09696100	-2.45380300
H	3.45392300	1.74055800	-2.06795000
C	2.15335000	3.64110000	-0.73665500
H	3.64183200	2.58778300	0.41020100
H	4.23434500	4.09766200	-0.27145000
C	1.58068400	4.45162600	0.43915200
H	1.55368000	2.73273100	-0.88013400

H	2.08167400	4.21871800	-1.66789500
H	1.99275200	5.47202700	0.41477400
H	1.93892400	4.00745900	1.37442100
2c-3			
C	-2.19303100	2.43073600	0.39193400
C	-3.03179800	2.24953700	-0.81041500
C	-2.19192700	1.87596200	-1.97007200
C	-0.79653700	1.57979300	-1.37304500
C	-0.73676000	2.44142500	-0.13375700
C	-2.67865800	3.34564100	1.54646500
C	-1.80921500	3.15012600	2.79890800
C	-2.78903500	4.83284900	1.16410800
C	0.16647900	0.74275400	-1.80280100
C	-2.84838400	0.99960400	-3.00456300
C	-3.48122800	1.45176800	-4.08858700
C	0.12697200	0.02419500	-3.08657800
C	0.09484000	0.59887100	-4.29897200
O	-0.38573100	3.79478000	-0.55345800
C	0.65406100	4.40718600	0.07627600
C	1.01467400	5.69901300	-0.61224000
O	1.20666800	3.95135600	1.05466300
H	-2.28719600	1.37926100	0.76854800
H	-2.09478600	2.91393700	-2.38787800
H	-0.01272900	2.11035400	0.60636400
H	-3.69125600	2.99669900	1.79435300
H	-2.21309500	3.73909200	3.62879000
H	-1.78834700	2.10017700	3.11537900
H	-0.77779700	3.47289100	2.62593200
H	-3.29632700	5.37701100	1.96751300
H	-3.36531800	4.98856300	0.24429300
H	-1.80760800	5.29017900	1.02369700
H	-2.80888900	-0.06630500	-2.79518700
H	-3.96172500	0.77134900	-4.78499900
H	-3.51780400	2.50932800	-4.34297700
H	0.24648900	-1.05826500	-3.02211000
H	0.14925800	0.00644900	-5.20793400
H	0.04570000	1.67817300	-4.41986300
H	1.54966900	5.47361500	-1.54225000
H	1.66039000	6.29116700	0.03713400
H	0.11835200	6.26621100	-0.87856400
H	6.06937100	0.13762600	-4.23855600
C	6.28151900	-0.23657500	-3.23067300
C	5.10902200	0.09055000	-2.29308400
C	7.61483000	0.35189800	-2.70617200

H	6.36170100	-1.32833700	-3.32190000
C	5.31178600	-0.61611900	-0.92781800
H	5.03176200	1.17735400	-2.17699700
H	4.15867000	-0.23284600	-2.73272100
C	7.60698400	0.53512200	-1.17267600
H	7.81299000	1.31955600	-3.18234300
H	8.44172200	-0.30714700	-2.99655100
P	4.00412700	-0.12865900	0.34904400
C	6.80554100	-0.57217800	-0.47176500
H	5.05929000	-1.66799200	-1.08671900
H	7.17981500	1.51255300	-0.91504900
H	8.63343500	0.54496400	-0.78816300
Au	1.90350300	0.31650000	-0.72425200
C	4.06258300	-1.52452300	1.57967900
C	4.65878300	1.39180500	1.24975200
H	6.90303700	-0.47496100	0.61303200
H	7.26119300	-1.54060900	-0.71472200
C	3.14763500	-2.61205900	1.64461100
C	5.13082900	-1.49251700	2.49952500
C	3.91197800	1.69786500	2.56598000
C	4.63202000	2.64299200	0.34081600
H	5.70972500	1.18102500	1.49136800
C	1.91511800	-2.85273500	0.79799800
C	3.37418000	-3.60251000	2.61964300
C	5.32618900	-2.48347200	3.45755400
H	5.82927600	-0.66412300	2.48321800
C	4.54386500	2.90196800	3.28702800
H	2.86357500	1.92811500	2.33803700
H	3.91540400	0.82732900	3.22847800
C	5.25452000	3.85683000	1.05593400
H	5.16852400	2.46121700	-0.59481600
H	3.59058700	2.86516900	0.07591700
C	0.63827700	-2.46057500	1.30818000
C	1.96460800	-3.65872700	-0.37299900
C	4.43783900	-3.55353300	3.51606800
H	2.68644800	-4.44174000	2.65844700
H	6.16279200	-2.41404700	4.14657900
C	4.56288100	4.14981400	2.39424700
H	3.98940800	3.10252400	4.21208500
H	5.57088100	2.64686900	3.58833500
H	5.19996100	4.73188300	0.39596600
H	6.32412000	3.66456100	1.22710700
C	-0.51714100	-2.82181500	0.60409600
C	0.33932800	-1.76974500	2.65445100

C	0.75733200	-4.00221300	-1.00823300
C	3.18711900	-4.27944800	-1.08712600
H	4.56793400	-4.34403100	4.24968200
H	3.53044500	4.46971600	2.20295000
H	5.06801200	4.97718300	2.90787500
C	-0.49206600	-3.60257500	-0.55209300
H	-1.47812100	-2.52109900	1.01670300
H	-0.66874000	-1.35391000	2.52033200
C	0.21526000	-2.79399700	3.80459700
C	1.21193400	-0.58298900	3.08338400
H	0.80615900	-4.64376900	-1.88606000
C	4.50190400	-4.49793600	-0.32357700
C	3.43697500	-3.55878800	-2.43246500
H	2.85079900	-5.29111600	-1.35293900
C	-1.76658800	-4.06300900	-1.24730200
H	-0.18431200	-2.30483100	4.70132100
H	-0.45813500	-3.61516400	3.53649000
H	1.18691000	-3.22177300	4.06768500
H	0.71392000	-0.04758000	3.90145400
H	1.35929200	0.12247400	2.25931100
H	2.19259100	-0.89217400	3.44933900
H	5.18431000	-5.06469300	-0.96780700
H	4.35081000	-5.07959000	0.58930100
H	5.00793900	-3.57116400	-0.04407800
H	2.56067500	-3.62023400	-3.08577700
H	3.65333400	-2.49646400	-2.28838800
H	4.28276000	-4.01351900	-2.96160600
C	-2.61390400	-4.97268300	-0.33655200
C	-2.60257900	-2.88341400	-1.77755800
H	-1.46115200	-4.66070400	-2.11646200
H	-2.03400500	-5.83515800	0.00811900
H	-2.96733900	-4.43266100	0.55013200
H	-3.49345400	-5.34633900	-0.87371800
H	-3.49246500	-3.24724400	-2.30471900
H	-2.01797000	-2.27093800	-2.47348800
H	-2.94013000	-2.23834800	-0.95568100
H	-13.12217400	1.38910800	1.32121200
C	-12.72518400	0.42585300	1.01203700
C	-13.59418300	-0.58941500	0.60283300
C	-11.34840100	0.20641500	1.02843900
H	-14.66704000	-0.41822100	0.59353800
C	-13.07760700	-1.82223300	0.20255900
C	-10.82266700	-1.02861500	0.62692400
H	-10.67188900	0.99669700	1.34018800

C	-11.69759600	-2.03677900	0.20951100
H	-13.74581500	-2.61473500	-0.12296000
C	-9.33626800	-1.28386400	0.68517800
H	-11.29924900	-2.99628200	-0.11324500
O	-8.63363500	-0.15875200	0.16377100
H	-9.01401700	-1.45827800	1.72709600
H	-9.08007800	-2.18996100	0.11301000
C	-7.23534700	-0.28393900	0.26170600
C	-6.62105200	0.99029000	-0.31846300
H	-6.92524700	-0.41692100	1.31403400
H	-6.87924000	-1.16959800	-0.29426100
C	-5.08989400	0.97197000	-0.25676300
H	-6.95740200	1.09935800	-1.35615300
H	-7.01274100	1.85032200	0.23812900
C	-4.49805600	2.31212700	-0.83372900
H	-4.69549500	0.12726700	-0.83311900
H	-4.75062400	0.85022400	0.77906100
H	-4.86707900	3.13712800	-0.21654200
H	-4.85623900	2.41967500	-1.86187100
Ts _{2c} -3			
C	-2.35397500	2.52921600	0.30686800
C	-3.11260700	2.17730100	-0.95335800
C	-2.29391300	1.65347300	-1.93540100
C	-0.79623200	1.55755300	-1.30503600
C	-0.86016000	2.44296200	-0.07313300
C	-2.87849700	3.72386200	1.14929400
C	-2.11748800	3.84507700	2.47972900
C	-2.94763100	5.06772300	0.40339600
C	0.25864400	0.84337100	-1.79023000
C	-2.73988400	0.90085200	-3.13534700
C	-3.43538100	1.43459000	-4.14256600
C	0.34769300	0.37644400	-3.17384200
C	0.25348000	1.16686700	-4.25728800
O	-0.34977400	3.74242000	-0.48765200
C	0.76287400	4.22261800	0.13480200
C	1.23414600	5.49791900	-0.51581600
O	1.29032300	3.67393600	1.07798300
H	-2.51768300	1.63424100	0.93740300
H	-1.36109400	2.40648700	-2.20655400
H	-0.23377200	2.07453100	0.73615300
H	-3.91234300	3.45078200	1.40358600
H	-2.57237100	4.62146200	3.10387400
H	-2.14846300	2.90587900	3.04528800
H	-1.06554600	4.11050200	2.33311900

H	-3.50811700	5.79216600	1.00401700
H	-3.45711000	4.97682100	-0.56315100
H	-1.95608600	5.48458600	0.21624300
H	-2.49132800	-0.15734800	-3.14402200
H	-3.77788700	0.82279000	-4.97174700
H	-3.68133100	2.49298300	-4.18329200
H	0.63173700	-0.66733100	-3.30669900
H	0.41194700	0.77444800	-5.25717600
H	0.06842600	2.23575900	-4.17896400
H	1.94795100	5.99864200	0.13917000
H	0.39417200	6.16091000	-0.74061500
H	1.72702900	5.25692600	-1.46516800
H	6.17980000	0.36852800	-4.07799900
C	6.36689700	-0.05891700	-3.08641200
C	5.16597300	0.20863100	-2.16591900
C	7.68083100	0.50716900	-2.49462600
H	6.45723000	-1.14359500	-3.23463600
C	5.33641400	-0.56912200	-0.83527200
H	5.07276200	1.28664300	-1.99316500
H	4.23253800	-0.10090300	-2.65015700
C	7.63846200	0.58960100	-0.95272300
H	7.87762800	1.50588100	-2.90211300
H	8.52085000	-0.12291600	-2.81006200
P	4.01214400	-0.13982800	0.44231100
C	6.81879200	-0.55716200	-0.34204500
H	5.08146100	-1.60976000	-1.05203000
H	7.20848700	1.54974800	-0.64186400
H	8.65568900	0.57008100	-0.54511500
Au	1.93515100	0.35130700	-0.65037400
C	4.04045600	-1.58848200	1.60633300
C	4.63950500	1.33668000	1.42676000
H	6.88919100	-0.52875700	0.74907800
H	7.27795800	-1.51009800	-0.63424200
C	3.13422200	-2.68446700	1.58426300
C	5.07405900	-1.59081500	2.56589000
C	3.83746800	1.58494300	2.72310900
C	4.66419400	2.62848800	0.57656900
H	5.67755200	1.10293800	1.69999200
C	1.94778900	-2.89944600	0.66857400
C	3.32715500	-3.71387600	2.52529300
C	5.23845500	-2.62263500	3.48576600
H	5.76886700	-0.76056000	2.61343600
C	4.44175200	2.75019900	3.52661700
H	2.80144100	1.82991500	2.45942300

H	3.81009600	0.68430100	3.34335100
C	5.26246400	3.80035600	1.37777000
H	5.24450900	2.48612600	-0.33956300
H	3.63878000	2.87666600	0.27756900
C	0.64296500	-2.53098700	1.12487200
C	2.06486200	-3.66975000	-0.52199500
C	4.35393400	-3.69726600	3.46489100
H	2.64425300	-4.55744400	2.49972900
H	6.04790700	-2.58013400	4.20848300
C	4.50904200	4.03689500	2.69375600
H	3.84560800	2.91209900	4.43291800
H	5.45236000	2.47453800	3.86315500
H	5.24725200	4.70594500	0.75817900
H	6.32083500	3.58905600	1.59081900
C	-0.47219700	-2.88203600	0.35285300
C	0.26931600	-1.89222000	2.47926000
C	0.89368000	-4.00946300	-1.22300100
C	3.32632400	-4.25869400	-1.19590200
H	4.45969200	-4.51706300	4.16961100
H	3.48813000	4.37074000	2.46817300
H	4.99236200	4.83689300	3.26776300
C	-0.38107600	-3.63593400	-0.81811400
H	-1.45564400	-2.59981400	0.72247100
H	-0.73837100	-1.48864400	2.31263500
C	0.11108300	-2.96099100	3.58410900
C	1.09861900	-0.70833100	2.99260900
H	0.99171600	-4.62915800	-2.11231100
C	4.61719300	-4.46608000	-0.38935100
C	3.61373500	-3.51482700	-2.52167700
H	3.01883200	-5.27201700	-1.48863900
C	-1.61337500	-4.09033000	-1.58938800
H	-0.34739100	-2.51445800	4.47463600
H	-0.52735300	-3.78612600	3.25094200
H	1.07766100	-3.37632000	3.88372000
H	0.56233700	-0.22543200	3.81887500
H	1.25181400	0.04286000	2.21044800
H	2.07550600	-1.01084000	3.37377700
H	5.33229900	-5.00836000	-1.01893100
H	4.44582100	-5.06708300	0.50692600
H	5.09661200	-3.53573400	-0.07608900
H	2.76705400	-3.58923700	-3.21166100
H	3.79940600	-2.44927400	-2.35667600
H	4.49106400	-3.94244300	-3.02098300
C	-2.54671800	-4.95708900	-0.72263700

C	-2.37796800	-2.90444600	-2.20580300
H	-1.25965700	-4.71648300	-2.41932400
H	-2.01274300	-5.81758600	-0.30626200
H	-2.96297500	-4.38423100	0.11454300
H	-3.38616900	-5.33308500	-1.31873400
H	-3.24177700	-3.25618400	-2.78180200
H	-1.72928500	-2.33133200	-2.87899500
H	-2.74752900	-2.22497000	-1.42732500
H	-13.35733000	1.30804900	0.60635500
C	-12.89864800	0.32339800	0.64229600
C	-13.69032400	-0.82110300	0.51609900
C	-11.51966700	0.20809000	0.81630000
H	-14.76477600	-0.72977100	0.38272300
C	-13.09345800	-2.08187800	0.55735500
C	-10.91384700	-1.05413900	0.85728400
H	-10.90203200	1.09640700	0.90636600
C	-11.71137600	-2.19540300	0.72146500
H	-13.70033500	-2.97717300	0.45294500
C	-9.42719000	-1.18696700	1.08789500
H	-11.25009500	-3.18057700	0.74156600
O	-8.73500800	-0.17429100	0.36927300
H	-9.19376100	-1.09368800	2.16393100
H	-9.08010700	-2.18456800	0.77186300
C	-7.34105900	-0.19686000	0.57795000
C	-6.72795100	0.93792600	-0.23838800
H	-7.10449000	-0.07478400	1.65045600
H	-6.91714600	-1.16763400	0.26339400
C	-5.19937000	0.98614300	-0.13309200
H	-7.02819500	0.81014300	-1.28581800
H	-7.16146400	1.88739200	0.10070000
C	-4.60712800	2.14056100	-0.98736900
H	-4.77146900	0.03457700	-0.47607100
H	-4.89991700	1.10799100	0.91624600
H	-5.00212300	3.09160200	-0.60936000
H	-4.95488600	2.02634600	-2.01645000

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C	-2.14490300	2.93215800	-0.81528600
C	-2.52676900	1.45806400	-0.88069500
C	-1.66430000	0.73010800	-1.63030900
C	-0.52994300	1.62780100	-2.18591600
C	-0.66572200	2.88085200	-1.27893600
C	-3.13108200	3.87777700	-1.57628600
C	-2.93977500	5.35829300	-1.20345900
C	-3.16346800	3.67253900	-3.09879800

C	0.79828800	0.95687100	-2.08826200
C	-1.67110600	-0.70282700	-1.94512800
C	-2.74195800	-1.48624900	-2.14054900
C	1.46152900	0.49575800	-3.28789600
C	1.28149900	1.01182900	-4.52624500
O	-0.26144000	4.09788000	-1.93357600
C	1.04145500	4.22483500	-2.25916100
C	1.34713300	5.58468200	-2.82932400
O	1.85418300	3.33036800	-2.10013800
H	-2.16798600	3.26493700	0.23222300
H	-0.77540100	1.89752500	-3.22233700
H	-0.01649300	2.73935400	-0.40973900
H	-4.12123900	3.59878300	-1.19601400
H	-3.74957400	5.95975000	-1.63185400
H	-2.96512800	5.49895900	-0.11592500
H	-1.99253900	5.75661600	-1.57473800
H	-3.98588800	4.24759500	-3.53847800
H	-3.31906700	2.62041600	-3.36357000
H	-2.23641600	4.01559600	-3.57024800
H	-0.68807300	-1.16556300	-2.03856300
H	-2.62258200	-2.54542700	-2.34972100
H	-3.75888200	-1.10940200	-2.12579200
H	2.22017100	-0.27282000	-3.15846400
H	1.87407300	0.65841100	-5.36585600
H	0.59416700	1.82569300	-4.73457700
H	0.66038400	5.81856500	-3.64875100
H	2.37838700	5.61179400	-3.18227100
H	1.20384800	6.34808000	-2.05666200
H	5.72756000	3.97320900	0.41949100
C	5.72233000	3.11123600	1.09592700
C	4.39606400	2.34744600	0.95763400
C	5.97326700	3.56690900	2.55515200
H	6.53772700	2.45635700	0.76026300
C	4.46813700	1.02031700	1.75566800
H	3.57375500	2.98241800	1.30566500
H	4.18192500	2.13260800	-0.09525400
C	5.23880600	2.67467500	3.57907000
H	5.64862300	4.60577300	2.68733100
H	7.05044400	3.55494800	2.75897900
P	2.81853700	0.09394800	1.77865100
C	5.19210500	1.20690100	3.12753100
H	5.08014500	0.33652700	1.16068600
H	4.21599300	3.04308000	3.72985400
H	5.72829300	2.74064400	4.55744000

Au	1.66941400	0.47108800	-0.29945000
C	3.28392200	-1.65866800	2.17108600
C	1.83234000	0.74072900	3.24826100
H	4.75068200	0.58855700	3.91383100
H	6.22057000	0.84007300	3.01940200
C	3.37404000	-2.72110700	1.22949100
C	3.60383200	-1.92080400	3.51926700
C	0.63477500	-0.15998700	3.61813400
C	1.34100200	2.18784700	3.00722700
H	2.52475100	0.76283900	4.10058900
C	3.04074600	-2.70499500	-0.24883000
C	3.80763300	-3.97486200	1.70208000
C	4.01913000	-3.17472200	3.95780500
H	3.51609700	-1.13075500	4.25629200
C	-0.11416100	0.38310800	4.84767200
H	-0.05709900	-0.20127800	2.76634200
H	0.96341500	-1.18562400	3.80819900
C	0.58311600	2.73260500	4.23217800
H	2.17678300	2.85364600	2.77438900
H	0.67677400	2.19557600	2.13114300
C	1.76634800	-3.19499400	-0.67482700
C	4.04033700	-2.45817600	-1.23301500
C	4.12846700	-4.21208600	3.03558000
H	3.89682600	-4.78346600	0.98342600
H	4.25305700	-3.33296300	5.00633900
C	-0.58787500	1.82585800	4.63082900
H	-0.96515300	-0.27136500	5.07111600
H	0.54823100	0.34282200	5.72454800
H	0.22873800	3.74794800	4.01578700
H	1.28129600	2.82103800	5.07695300
C	1.52112700	-3.36102500	-2.04634900
C	0.61211500	-3.71202400	0.20837400
C	3.72079300	-2.66379800	-2.58705500
C	5.50721500	-2.00760700	-1.04707200
H	4.45713600	-5.19909900	3.34792900
H	-1.34804300	1.84236700	3.83571800
H	-1.07354700	2.20917200	5.53588700
C	2.48106900	-3.11788700	-3.02819200
H	0.55063900	-3.75063500	-2.34242600
H	-0.26765600	-3.65683900	-0.44548700
C	0.78623900	-5.20872900	0.55103300
C	0.22844200	-2.91304400	1.45869300
H	4.50314600	-2.49852600	-3.32626100
C	6.23459100	-2.27540200	0.27965200

C	5.67383200	-0.53606500	-1.48953600
H	6.06004900	-2.60136000	-1.78749900
C	2.25281900	-3.42989800	-4.50278500
H	-0.13373200	-5.59676900	1.00399500
H	0.99904400	-5.80161700	-0.34488400
H	1.59897300	-5.36648500	1.26598600
H	-0.74466800	-3.26416400	1.82243200
H	0.13143800	-1.84661000	1.23208800
H	0.94379000	-3.03356600	2.27422000
H	7.29087400	-2.01139400	0.15232300
H	6.19023400	-3.33059000	0.56174900
H	5.84955100	-1.69355100	1.12022300
H	5.37011000	-0.39851800	-2.53249600
H	5.06255900	0.14106800	-0.88591600
H	6.72076500	-0.22293100	-1.40102900
C	2.59824400	-4.90610200	-4.79459000
C	0.83577300	-3.10058100	-5.00090600
H	2.95943400	-2.81152500	-5.07463600
H	3.62539600	-5.14083000	-4.49624100
H	1.92745600	-5.57814100	-4.24621600
H	2.49472300	-5.12330200	-5.86394000
H	0.77362300	-3.24935800	-6.08451200
H	0.55594600	-2.06329200	-4.78414700
H	0.08308100	-3.75336000	-4.54386900
H	-13.55941000	-2.90712900	0.72007600
C	-12.70208300	-2.36335900	1.10764800
C	-12.47936000	-2.29373600	2.48379600
C	-11.81657000	-1.74309900	0.22422800
H	-13.16413600	-2.78018800	3.17311600
C	-11.36869900	-1.59936900	2.96953900
C	-10.70720100	-1.03852900	0.70437300
H	-11.98941300	-1.80975500	-0.84796800
C	-10.48995900	-0.97199500	2.08607500
H	-11.18719400	-1.54513000	4.03986000
C	-9.78942300	-0.32091500	-0.25790500
H	-9.62200900	-0.43822700	2.46005500
O	-8.45359400	-0.36416100	0.21973900
H	-9.85391700	-0.77925400	-1.25891000
H	-10.10358100	0.73280700	-0.37064800
C	-7.55174600	0.36291400	-0.58717900
C	-6.16183000	0.25261200	0.03153400
H	-7.54666200	-0.03675400	-1.61717000
H	-7.86075400	1.42155700	-0.65549500
C	-5.09280700	1.00084800	-0.77437900

H	-6.20446700	0.64451100	1.05612300
H	-5.90010900	-0.81036900	0.11359200
C	-3.69983700	0.90773000	-0.10607800
H	-5.38987800	2.05073500	-0.88183600
H	-5.04216400	0.59544100	-1.79359800
H	-3.49935100	-0.14884300	0.11176700
H	-3.75131700	1.42709800	0.86161700
Ts _{3c} -3			
C	2.92713800	-1.73571700	0.44417900
C	3.62576400	-0.41345700	0.16213800
C	2.79465100	0.52218500	-0.38183300
C	1.42837700	-0.05623000	-0.52543500
C	1.51955100	-1.55900100	-0.18017100
C	3.74363700	-3.02810100	0.15492500
C	3.07682900	-4.27109900	0.76799800
C	4.13804800	-3.25939200	-1.31528500
C	0.16695700	0.59410300	-0.68865000
C	3.10100600	1.94790900	-0.57882700
C	4.18686600	2.43995300	-1.18679700
C	0.05758300	1.94789100	-1.24637100
C	0.50729300	2.35692300	-2.44223100
O	1.35300900	-2.24661200	-1.44326800
C	0.44451100	-3.26274500	-1.52434700
C	0.36984300	-3.79437700	-2.93309200
O	-0.19261100	-3.66850100	-0.57940300
H	2.76874700	-1.74904300	1.53589300
H	0.97091300	-0.08442600	-1.67201500
H	0.71849600	-1.87976600	0.48550200
H	4.67768800	-2.87729600	0.71302900
H	3.71602300	-5.14973700	0.62811800
H	2.91854100	-4.14616100	1.84591400
H	2.10517400	-4.49181400	0.31488800
H	4.96211200	-3.97986800	-1.36611300
H	4.46990100	-2.33797900	-1.80498500
H	3.31199300	-3.66329800	-1.90400600
H	2.37240100	2.64711200	-0.17558200
H	4.35433500	3.51104800	-1.24904200
H	4.93039600	1.80316400	-1.65659200
H	-0.57877000	2.61207300	-0.66187800
H	0.29004300	3.35634700	-2.80437900
H	1.06731300	1.70829400	-3.11252100
H	0.10742600	-2.99165500	-3.62985500
H	-0.37479500	-4.58929000	-2.98074700
H	1.34501000	-4.18622900	-3.24116700

H	-3.60504500	-3.39320500	-4.08168400
C	-4.33888000	-3.08249000	-3.32910700
C	-3.63037300	-2.35661100	-2.17431300
C	-5.14817900	-4.30358900	-2.82927300
H	-5.00508400	-2.36897700	-3.83249300
C	-4.67860400	-1.73141500	-1.21738800
H	-2.97295000	-3.05670500	-1.64661300
H	-2.98118200	-1.56338200	-2.56397300
C	-5.60393900	-4.13611300	-1.36349300
H	-4.54693900	-5.21623700	-2.91682800
H	-6.02101200	-4.44815500	-3.47668200
P	-3.88709400	-1.02230900	0.35276100
C	-5.91378100	-2.66942800	-1.02820300
H	-5.03911200	-0.81859200	-1.70112100
H	-4.82604900	-4.50888600	-0.68587100
H	-6.49071600	-4.75052100	-1.17076400
Au	-1.70138500	-0.20232100	-0.20160500
C	-5.13372000	0.20992200	0.97545700
C	-3.83604200	-2.41272900	1.62709200
H	-6.33605200	-2.59757900	-0.02304000
H	-6.70802700	-2.31592200	-1.69784900
C	-5.07163900	1.62764500	0.86525900
C	-6.26811300	-0.36661700	1.58664600
C	-3.62023600	-1.91895000	3.07325000
C	-2.76596300	-3.46781100	1.27094200
H	-4.81806200	-2.90282400	1.57558700
C	-3.98109500	2.51911600	0.29886600
C	-6.17002000	2.36474000	1.35320900
C	-7.33343600	0.39009000	2.06385200
H	-6.32227900	-1.44111800	1.71068700
C	-3.65103400	-3.09273200	4.06808800
H	-2.64641300	-1.41617400	3.14038900
H	-4.37810600	-1.18178900	3.35189900
C	-2.78689900	-4.64052000	2.26733900
H	-2.90878300	-3.85433300	0.25907700
H	-1.77515300	-2.99949900	1.27824300
C	-3.07932300	3.16621900	1.19995100
C	-4.03295100	2.97044200	-1.05159100
C	-7.28578900	1.77513500	1.93887200
H	-6.13377000	3.44534300	1.25719300
H	-8.18368200	-0.10170400	2.52683500
C	-2.61168600	-4.16427500	3.71465200
H	-3.48203700	-2.71120400	5.08230400
H	-4.65521300	-3.54143500	4.06747700

H	-1.99733600	-5.35111200	1.99593200
H	-3.74043700	-5.18081200	2.17323500
C	-2.26390500	4.20490100	0.72520300
C	-2.94595200	2.94419200	2.72000500
C	-3.18914600	4.02147000	-1.44892500
C	-4.92002800	2.46420100	-2.20902000
H	-8.10342800	2.39454200	2.29599900
H	-1.60254500	-3.74477000	3.83937600
H	-2.68644700	-5.01128600	4.40690700
C	-2.30997300	4.67228000	-0.58856500
H	-1.60451100	4.69477600	1.43722300
H	-1.95466200	3.34935500	2.96026300
C	-3.94905000	3.79751800	3.52778600
C	-2.92812300	1.49987700	3.23100000
H	-3.25623300	4.36804500	-2.47876000
C	-6.32005100	1.90277600	-1.91413000
C	-4.10697500	1.51596800	-3.11745600
H	-5.10649900	3.36145800	-2.81321600
C	-1.52321700	5.89106000	-1.05654900
H	-3.68628600	3.77221300	4.59199100
H	-3.93578000	4.84307400	3.20172700
H	-4.97133700	3.42130600	3.42979700
H	-2.56433800	1.48455300	4.26536400
H	-2.25664700	0.87442700	2.63153000
H	-3.91936100	1.04412600	3.22777900
H	-6.84303400	1.75979200	-2.86711700
H	-6.91503300	2.59509600	-1.31199200
H	-6.31101600	0.94078200	-1.39703600
H	-3.20579900	2.01098500	-3.49453400
H	-3.77934400	0.62331800	-2.57609200
H	-4.70543400	1.19590700	-3.97885600
C	-2.26181300	7.18767600	-0.66176200
C	-0.06911800	5.92523900	-0.55543800
H	-1.49522100	5.85259900	-2.15464700
H	-3.28221300	7.20007500	-1.05899700
H	-2.32456100	7.28455300	0.42865200
H	-1.73363000	8.06641600	-1.04919400
H	0.46012600	6.77875600	-0.99317000
H	0.47775500	5.01496800	-0.82728100
H	-0.01646000	6.03671700	0.53372900
H	15.36807100	1.64863500	-0.45250600
C	14.52230900	1.24221600	0.09557700
C	14.57312100	1.13662500	1.48635900
C	13.37856400	0.83611000	-0.59470400

H	15.45986200	1.45728100	2.02630900
C	13.47568000	0.62149700	2.18080600
C	12.27964700	0.31082500	0.09366700
H	13.34053200	0.93091700	-1.67796600
C	12.33746600	0.20707200	1.48900900
H	13.50706500	0.54131600	3.26430000
C	11.07011000	-0.18034500	-0.66684000
H	11.48048600	-0.18630700	2.02669500
O	9.88825800	0.10006500	0.06865800
H	11.02519300	0.29621900	-1.66027000
H	11.14314100	-1.26949600	-0.83980000
C	8.72014500	-0.40442500	-0.54122000
C	7.53018300	-0.03719700	0.34022500
H	8.59583800	0.02390800	-1.55215000
H	8.78819900	-1.50053200	-0.66322600
C	6.19292600	-0.51590200	-0.23816500
H	7.68785600	-0.46976700	1.33671500
H	7.51760300	1.05248400	0.46969900
C	5.00960200	-0.13853900	0.68760500
H	6.22452900	-1.60062000	-0.38911800
H	6.03789200	-0.07238100	-1.23032800
H	5.08659600	0.93119500	0.91087700
H	5.13358500	-0.67674900	1.63769200

4c-3

C	2.45530800	-1.02496200	-0.40888300
C	1.62098000	0.23384700	-0.62865800
C	2.38404700	1.36318800	-0.53829200
C	3.79699300	1.00469500	-0.32157800
C	3.88369100	-0.46647400	-0.67728500
C	2.19772700	-1.72274400	0.96594000
C	2.79139300	-3.14070400	1.02790700
C	2.61496400	-0.88904900	2.18623300
C	4.85351900	1.74668100	0.07967100
C	1.95034600	2.74634300	-0.78569600
C	0.82331200	3.33009200	-0.35766300
C	4.86291700	3.13725900	0.49864200
C	5.97948400	3.80077100	0.84337600
O	4.95516900	-1.12964500	0.01915500
C	5.81394800	-1.88750500	-0.71645600
C	6.88122600	-2.48387900	0.17056300
O	5.71870200	-2.06455600	-1.90964400
H	2.20126000	-1.76682000	-1.17922400
H	5.81395300	1.23556900	0.13840700
H	4.08694900	-0.56901200	-1.74791000

H	1.10810400	-1.85060100	1.01630100
H	2.41891500	-3.66710900	1.91494400
H	2.51115200	-3.73233500	0.14777500
H	3.88252200	-3.12050000	1.09080300
H	2.30518200	-1.39328000	3.10964400
H	2.15240700	0.10320800	2.17532100
H	3.69990800	-0.75407200	2.22431200
H	2.63940900	3.33813200	-1.38897700
H	0.58609600	4.35499500	-0.62906000
H	0.11638400	2.82376400	0.29251100
H	3.90827800	3.65466900	0.55381000
H	5.95043700	4.83666800	1.16737600
H	6.95808900	3.32631500	0.81127900
H	7.30761700	-1.72229700	0.82970900
H	7.65952700	-2.93007600	-0.44957500
H	6.43984800	-3.25919800	0.80735300
H	-10.29424300	0.45929200	1.08323000
C	-9.41493900	0.17457800	0.51115800
C	-9.54111100	-0.20710700	-0.82590800
C	-8.15693700	0.20302400	1.11349500
H	-10.51919200	-0.22405100	-1.29945800
C	-8.40229300	-0.56045100	-1.55173800
C	-7.01217900	-0.15836500	0.39365800
H	-8.06387100	0.51241200	2.15285000
C	-7.14526100	-0.54045000	-0.94560300
H	-8.49154700	-0.85328700	-2.59485000
C	-5.66535200	-0.17549000	1.08140800
H	-6.25696500	-0.80764000	-1.50801200
O	-4.62826000	-0.00892400	0.13386000
H	-5.62147800	0.61946400	1.84574000
H	-5.52868000	-1.13306400	1.61740300
C	-3.33478400	-0.09391700	0.70481600
C	-2.30250600	0.08282600	-0.40194600
H	-3.20853000	0.68405100	1.47834300
H	-3.20196500	-1.06970300	1.20494500
C	-0.86061000	0.01454400	0.11651000
H	-2.46734400	-0.69413400	-1.16005200
H	-2.48076100	1.04625500	-0.89685600
C	0.17082000	0.16628100	-1.02636800
H	-0.70665700	-0.93780300	0.63864500
H	-0.69676500	0.80172700	0.86447700
H	-0.07916900	1.07610900	-1.58630600
H	0.03801900	-0.68083600	-1.71567900