

ARTICLE

Supporting Information

for

Origins of Peroxidase Mimicking Activities of Graphene Oxide from First Principles

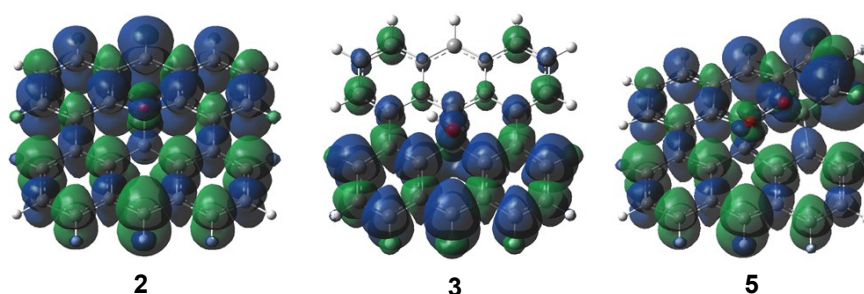


Fig. S1. The spin density distribution of 2, 3 and 5.

The coordinates for all the structures mentioned in the main text.

Fig. 3 (1, ts11, 2, ts12, int11, ts13, 3, ts14.)

1			
C	-2.45880400	3.58120100	0.03868300
C	-1.22211400	2.87368100	0.01550500
C	0.00000000	3.55617000	-0.00000700
C	-1.23025600	1.43201800	0.00790200
C	0.00000000	0.72609200	-0.00000200
C	1.23025600	1.43201800	-0.00790800
C	1.22211400	2.87368100	-0.01551600
C	-3.64733800	2.89432300	0.05661900
C	-3.66143600	1.48264600	0.04471300
C	-2.48856500	0.73632100	0.01308300
C	-2.48856500	-0.73632100	-0.01308400
C	-1.23025600	-1.43201800	-0.00790300
C	0.00000000	-0.72609200	0.00000200
C	1.23025600	-1.43201800	0.00790800
C	2.48856500	-0.73632100	0.01308500
C	2.48856500	0.73632100	-0.01308400
C	2.45880400	3.58120100	-0.03869400
C	3.66143600	1.48264600	-0.04471200
C	3.64733800	2.89432300	-0.05662300
C	1.22211400	-2.87368100	0.01551600

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C	2.45880400	-3.58120100	0.03869500
C	3.64733800	-2.89432300	0.05662400
C	3.66143600	-1.48264600	0.04471300
C	-1.22211400	-2.87368100	-0.01550500
C	0.00000000	-3.55617000	0.00000700
C	-3.66143600	-1.48264600	-0.04471400
C	-3.64733800	-2.89432300	-0.05662000
C	-2.45880400	-3.58120100	-0.03868400
H	-2.43854500	4.66705400	0.04480700
H	0.00000000	4.64279400	-0.00000900
H	-4.59058300	3.43146500	0.07965000
H	-4.62436400	0.98617700	0.06298800
H	2.43854500	4.66705400	-0.04482200
H	4.62436500	0.98617800	-0.06298000
H	4.59058300	3.43146500	-0.07965300
H	2.43854500	-4.66705400	0.04482300
H	4.59058300	-3.43146500	0.07965400
H	4.62436500	-0.98617800	0.06298100
H	0.00000000	-4.64279400	0.00000900
H	-4.62436400	-0.98617700	-0.06298900
H	-4.59058300	-3.43146500	-0.07965100
H	-2.43854500	-4.66705400	-0.04480700

2

C	-3.57115900	-0.18976300	2.46944600
C	-2.87147500	-0.06576900	1.24577200
C	-3.55701600	-0.08348200	0.00000000
C	-1.45353200	0.06035600	1.27481600
C	-0.74707400	0.32578500	0.00000000
C	-1.45353200	0.06035600	-1.27481600
C	-2.87147500	-0.06576900	-1.24577200
C	-2.87564900	-0.20592600	3.66830900
C	-1.48078200	-0.12258000	3.68390400
C	-0.74223400	0.00591200	2.49006000
C	0.74222700	0.00593900	2.49006700
C	1.45352500	0.06027700	1.27481600
C	0.74708700	0.32568900	0.00000000
C	1.45352500	0.06027700	-1.27481600
C	0.74222700	0.00593900	-2.49006700
C	-0.74223400	0.00591200	-2.49006000
C	-3.57115900	-0.18976300	-2.46944600
C	-1.48078200	-0.12258000	-3.68390400
C	-2.87564900	-0.20592600	-3.66830900
C	2.87146600	-0.06588200	-1.24577400
C	3.57115100	-0.18979800	-2.46945600
C	2.87565000	-0.20576600	-3.66832600
C	1.48078400	-0.12236800	-3.68392300
C	2.87146600	-0.06588200	1.24577400
C	3.55700200	-0.08366200	0.00000000
C	1.48078400	-0.12236800	3.68392300
C	2.87565000	-0.20576600	3.66832600
C	3.57115100	-0.18979800	2.46945600
H	-4.65383100	-0.27207000	2.45342900
H	-4.63965100	-0.16687000	0.00000000
H	-3.41357900	-0.29637400	4.60695600
H	-0.97515700	-0.16310200	4.64035000
H	-4.65383100	-0.27207000	-2.45342900

H	-0.97515700	-0.16310200	-4.64035000
H	-3.41357900	-0.29637400	-4.60695600
H	4.65381900	-0.27215800	-2.45344200
H	3.41358500	-0.29608700	-4.60698200
H	0.97517200	-0.16264600	-4.64038600
H	4.63963200	-0.16710300	0.00000000
H	0.97517200	-0.16264600	4.64038600
H	3.41358500	-0.29608700	4.60698200
H	4.65381900	-0.27215800	2.45344200
O	0.00004200	1.59716100	0.00000000

3

C	2.38497200	-3.57642100	-0.26530200
C	1.18698400	-2.85216600	-0.06097900
C	-0.06677600	-3.52057500	-0.02110000
C	1.24272900	-1.43440700	0.05228000
C	-0.00882700	-0.68669000	0.46720900
C	-1.29411800	-1.38632400	0.06779200
C	-1.29532700	-2.80774000	-0.03457000
C	3.59366700	-2.90569800	-0.38242200
C	3.63734900	-1.51363500	-0.30454500
C	2.46663200	-0.75859700	-0.07160000
C	2.49999200	0.71750200	-0.00959500
C	1.25259100	1.44002100	-0.01867300
C	0.01588700	0.77167100	0.06137600
C	-1.19436400	1.48530800	-0.03409800
C	-2.46983900	0.81135800	-0.03140800
C	-2.49343700	-0.66627100	-0.06278200
C	-2.52265700	-3.48808200	-0.21236100
C	-3.69522300	-1.37986000	-0.26780900
C	-3.70684300	-2.77346300	-0.32197600
C	-1.16323900	2.92480800	-0.13621500
C	-2.38960500	3.65355200	-0.17602100
C	-3.58708000	2.99047800	-0.11932100
C	-3.62331000	1.57428400	-0.05523100
C	1.27712500	2.87892800	-0.11560900
C	0.06974800	3.58370500	-0.16319500
C	3.68266200	1.43519600	-0.00723300
C	3.70103900	2.85214100	-0.05624800
C	2.53054900	3.56067800	-0.12934000
H	2.33974700	-4.65847200	-0.34653300
H	-0.08667500	-4.60442100	-0.08603200
H	4.51109900	-3.46136700	-0.55113500
H	4.59105700	-1.01694500	-0.43517000
H	-2.51943000	-4.57188400	-0.28253200
H	-4.63076100	-0.84888700	-0.39489500
H	-4.64704500	-3.29599500	-0.46988000
H	-2.34979300	4.73678200	-0.24334700
H	-4.52238900	3.54106600	-0.13641500
H	-4.59535900	1.09597400	-0.03176400
H	0.09080100	4.66896300	-0.21552200
H	4.63522300	0.91944600	0.02446700
H	4.65635400	3.36745000	-0.05156900
H	2.53378700	4.64505700	-0.18966300
O	0.06639900	-0.72777200	1.94813800
H	-0.72550000	-0.27279000	2.27875100

int11

C	2.08874800	-3.77061500	-0.04882400
C	0.96294500	-2.93552300	0.06799700
C	-0.36660700	-3.49714200	0.01232500
C	1.14902300	-1.52910300	0.10745600
C	-0.02367500	-0.66171800	0.33427600
C	-1.40478400	-1.28000100	0.27703100
C	-1.50204100	-2.73915600	-0.00891100
C	3.35957100	-3.21716800	-0.15195500
C	3.53089300	-1.83386700	-0.15786900
C	2.43251200	-0.96253800	-0.03160100
C	2.58662400	0.50899100	-0.04386300
C	1.40601200	1.34089700	-0.02924400
C	0.11554900	0.78922600	0.06768900
C	-1.03927500	1.59978500	0.02673000
C	-2.37458200	1.04222900	0.03137900
C	-2.55848500	-0.41262300	-0.06588200
C	-2.79979900	-3.27831100	-0.31609000
C	-3.71527000	-1.01658400	-0.46758000
C	-3.85613800	-2.44870900	-0.53720600
C	-0.88111600	3.03183600	-0.03715100
C	-2.03647100	3.86856800	-0.02302100
C	-3.28955700	3.31576000	0.04973700
C	-3.45516800	1.91047300	0.07186400
C	1.55005900	2.77401600	-0.11375000
C	0.40688500	3.57846700	-0.10011800
C	3.82443100	1.12380400	-0.10076500
C	3.96217000	2.53379600	-0.16551900
C	2.85708700	3.34303300	-0.18090400
H	1.94940400	-4.84715800	-0.07719100
H	-0.44775000	-4.57257800	-0.12488100
H	4.22709400	-3.86347100	-0.24286000
H	4.53437500	-1.43749500	-0.25721200
H	-2.90055000	-4.35560200	-0.41230600
H	-4.56877300	-0.41427100	-0.76095500
H	-4.82382600	-2.85712900	-0.81089600
H	-1.89897200	4.94513200	-0.06115900
H	-4.16918300	3.95133100	0.07978800
H	-4.46276300	1.51193400	0.11912100
H	0.52039600	4.65863200	-0.13581200
H	4.73048600	0.52923700	-0.10084900
H	4.95840100	2.96255800	-0.21072300
H	2.95262800	4.42322200	-0.24003400
O	-0.77227600	-0.96265800	1.55482300

ts11

C	3.84559100	-2.60238000	0.04430800
C	2.46205300	-2.34783700	-0.18873600
C	1.55212300	-3.39690800	-0.35729500
C	1.98969600	-0.98557800	-0.22967400
C	0.61581500	-0.73383400	-0.44380200
C	-0.29532700	-1.80234100	-0.61350600
C	0.18756100	-3.15937000	-0.56227800
C	4.71592600	-1.56033600	0.23927700
C	4.25883300	-0.22267300	0.19520100
C	2.92865500	0.09024900	-0.04540600
C	2.44618700	1.48086900	-0.13493200

C	1.05615100	1.72296500	-0.34690200
C	0.11839700	0.63812600	-0.40678800
C	-1.24822800	0.90081300	-0.73206600
C	-2.17746700	-0.17403400	-0.94480500
C	-1.69934400	-1.56290500	-0.82417700
C	-0.73593200	-4.23670400	-0.69793500
C	-2.55352200	-2.65439000	-0.91791400
C	-2.07491500	-3.98327200	-0.85822600
C	-1.69296000	2.26429200	-0.89419000
C	-3.06081700	2.52503600	-1.21083400
C	-3.93186300	1.48305600	-1.40136500
C	-3.48460900	0.14326400	-1.28563400
C	0.58538300	3.07043800	-0.48411800
C	-0.77571200	3.30412800	-0.75771000
C	3.30425700	2.57903300	-0.04913400
C	2.83615200	3.90091400	-0.15638400
C	1.49996300	4.15069000	-0.37580200
H	4.18823900	-3.63249000	0.07272500
H	1.91076700	-4.42165800	-0.31440300
H	5.76805800	-1.75158200	0.42657300
H	4.98582600	0.56470100	0.35563200
H	-0.35929300	-5.25449600	-0.65786500
H	-3.61891800	-2.50440300	-1.04883500
H	-2.78194000	-4.80249800	-0.94537200
H	-3.38516000	3.55635800	-1.30975200
H	-4.96958000	1.67217800	-1.65663200
H	-4.20164900	-0.64521200	-1.48208200
H	-1.11796700	4.32872600	-0.87481400
H	4.36729700	2.42823300	0.09716800
H	3.54205700	4.72147200	-0.07602600
H	1.12709000	5.16554100	-0.47465700
O	-0.56096200	0.64046300	1.57260500
H	-2.17699900	1.18057800	1.80636900
O	-0.63436000	0.25795400	3.41445800
O	-3.13106800	1.31262900	2.07742400
H	0.18989900	-0.25288500	3.39538200
H	-1.36897900	-0.42078100	3.32575400
H	-3.13139300	-0.37220300	2.60066900
H	-3.61050100	1.35300200	1.23735800
O	-2.78328900	-1.23632700	2.94001200
H	-2.51170200	-1.69818800	2.13178500

ts12

C	-3.56164900	-0.16547400	2.46438800
C	-2.85787500	-0.01853200	1.24449800
C	-3.54699700	0.00250400	0.00000000
C	-1.43884100	0.06467900	1.27205100
C	-0.70317600	0.40465600	0.00000000
C	-1.43884100	0.06467900	-1.27205100
C	-2.85787500	-0.01853200	-1.24449800
C	-2.86885700	-0.26535500	3.66069400
C	-1.47215400	-0.22452400	3.67504400
C	-0.73771500	-0.04651700	2.48530800
C	0.74359700	-0.03198200	2.48597500
C	1.44991400	-0.00441600	1.24772500
C	0.75338800	0.10096100	0.00000000
C	1.44991400	-0.00441600	-1.24772500

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C	0.74359700	-0.03198200	-2.48597500
C	-0.73771500	-0.04651700	-2.48530800
C	-3.56164900	-0.16547400	-2.46438800
C	-1.47215400	-0.22452400	-3.67504400
C	-2.86885700	-0.26535500	-3.66069400
C	2.88057800	-0.08465600	-1.23282100
C	3.58740900	-0.14083000	-2.46330700
C	2.89502300	-0.12579500	-3.65420200
C	1.48751200	-0.07804500	-3.66505200
C	2.88057800	-0.08465600	1.23282100
C	3.56244800	-0.10487600	0.00000000
C	1.48751200	-0.07804500	3.66505200
C	2.89502300	-0.12579500	3.65420200
C	3.58740900	-0.14083000	2.46330700
H	-4.64659500	-0.21227200	2.44569300
H	-4.63178700	-0.04817800	0.00000000
H	-3.40907600	-0.38878800	4.59422600
H	-0.96214000	-0.33736600	4.62391700
H	-4.64659500	-0.21227200	-2.44569300
H	-0.96214000	-0.33736600	-4.62391700
H	-3.40907600	-0.38878800	-4.59422600
H	4.67177000	-0.19116200	-2.44562500
H	3.43009400	-0.15916600	-4.59783700
H	0.98734100	-0.07805100	-4.62576100
H	4.64771100	-0.15098400	0.00000000
H	0.98734100	-0.07805100	4.62576100
H	3.43009400	-0.15916600	4.59783700
H	4.67177000	-0.19116200	2.44562500
O	-0.22950000	1.74633200	0.00000000

ts13

C	-0.75006500	-2.44583500	2.56346600
C	-1.16205100	-1.19424300	2.04203300
C	-0.59409100	-0.00430600	2.54276800
C	-2.21255600	-1.12898300	1.08079600
C	-2.52682000	0.19962100	0.42160500
C	-2.17646200	1.38717900	1.29575600
C	-1.10295500	1.27075800	2.22687700
C	-1.40223000	-3.60250600	2.16649100
C	-2.46262700	-3.52598300	1.26189300
C	-2.88242100	-2.30007500	0.69947000
C	-4.04545700	-2.22014700	-0.20647900
C	-4.59438000	-0.92064400	-0.50371500
C	-3.96134900	0.25964200	-0.07158500
C	-4.55471100	1.51686000	-0.30033300
C	-3.96129400	2.73342500	0.19804800
C	-2.78328200	2.63471000	1.08393800
C	-0.60287500	2.42063200	2.89037300
C	-2.28095400	3.74799100	1.78710600
C	-1.19033600	3.64980500	2.65979500
C	-5.78285900	1.59596200	-1.05303800
C	-6.35299700	2.87383600	-1.33297800
C	-5.73964800	4.01644000	-0.88993300
C	-4.55142800	3.94295700	-0.11993900
C	-5.82047100	-0.83596700	-1.25904500
C	-6.37869100	0.41950000	-1.52103900
C	-4.66753300	-3.34289400	-0.72126900

C	-5.84987600	-3.25070800	-1.49875200
C	-6.42561200	-2.03233600	-1.74800400
H	0.04745000	-2.47513500	3.29915000
H	0.22218200	-0.07824900	3.25665300
H	-1.10981200	-4.56498100	2.57211600
H	-2.98055400	-4.44233400	1.00445900
H	0.22222400	2.31209300	3.58730700
H	-2.75144500	4.71734300	1.67092400
H	-0.83090900	4.53746800	3.16912700
H	-7.27261700	2.91898300	-1.90910700
H	-6.16420400	4.99048400	-1.11162400
H	-4.11513100	4.87347900	0.22431500
H	-7.29214300	0.48324400	-2.10619500
H	-4.26269800	-4.33059500	-0.53305600
H	-6.30118300	-4.16082600	-1.88092900
H	-7.34231500	-1.95389700	-2.32517300
O	-1.68428600	0.38420500	-0.72812300
H	-0.82449400	-0.75573200	-0.98070900
N	0.26589500	-1.85915600	-1.28055400
C	1.55310000	-1.44556000	-1.08164400
H	0.04251100	-2.65999400	-0.69414800
C	2.49990800	-2.20865600	-0.31837500
C	2.01697100	-0.23859500	-1.70416800
C	3.80595400	-1.75315800	-0.17359900
C	2.08541500	-3.51553400	0.30360600
C	3.33228400	0.17161500	-1.52703200
C	1.07736700	0.58183000	-2.54780600
C	4.26389500	-0.55562000	-0.75662100
H	4.50107300	-2.36722200	0.39282800
H	2.92883300	-3.99089400	0.81141900
H	1.28355600	-3.38213100	1.04288100
H	1.70177600	-4.22313900	-0.44297400
H	3.64109100	1.10593700	-1.98866300
H	1.60608000	1.41273000	-3.02322900
H	0.61468700	-0.02503200	-3.33525900
H	0.25410200	0.99452900	-1.95361400
C	5.65424500	-0.08969600	-0.57600400
C	6.38754800	-0.40073000	0.58485200
C	6.30858700	0.68518300	-1.55246900
C	7.69847800	0.02921600	0.78309000
H	5.91443500	-0.97336300	1.37769700
C	7.61950600	1.13420800	-1.39911400
H	5.79205100	0.92866400	-2.47676000
C	8.32793100	0.80716800	-0.21800300
C	8.43695800	-0.31610800	2.05234700
C	8.28922200	1.94264600	-2.48248800
N	9.65926400	1.19590100	-0.07088000
H	9.35981500	-0.87399200	1.84909700
H	8.72909700	0.58209600	2.61317400
H	7.81481700	-0.92790200	2.71035600
H	7.61435500	2.09504900	-3.32837700
H	8.59873700	2.93330400	-2.12289700
H	9.19403200	1.44764300	-2.85695600
H	9.92608600	2.01847400	-0.59690500
H	9.98866300	1.24562500	0.88481900

ts14

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C	-3.47336300	3.77811800	-2.87667300
C	-3.13642900	2.43747900	-2.53481900
C	-2.39930600	1.63010000	-3.40776700
C	-3.55850600	1.90409400	-1.26424100
C	-3.23040400	0.56688600	-0.92449100
C	-2.48405800	-0.23900400	-1.82229500
C	-2.05746300	0.31283300	-3.08338100
C	-4.19124200	4.55634700	-2.00402900
C	-4.60254500	4.03985000	-0.75747600
C	-4.30512900	2.74006600	-0.36461200
C	-4.72642500	2.19030200	0.93475100
C	-4.38984200	0.83048100	1.25653500
C	-3.65531100	0.02134800	0.35251200
C	-3.33827500	-1.32093400	0.68660200
C	-2.59619200	-2.15876100	-0.21616000
C	-2.13209700	-1.59303800	-1.49387700
C	-1.29016100	-0.49240400	-3.97219000
C	-1.35876200	-2.32680400	-2.38894500
C	-0.94769600	-1.77412600	-3.62149900
C	-3.77617100	-1.86063300	1.94984500
C	-3.47299500	-3.21439900	2.27218500
C	-2.77980100	-3.99852000	1.38389400
C	-2.34443100	-3.48117300	0.14312000
C	-4.80824600	0.28130200	2.52175700
C	-4.49244200	-1.04563300	2.83321100
C	-5.43943900	2.93642400	1.86588900
C	-5.84282900	2.39630700	3.10497300
C	-5.53872000	1.09864900	3.43071600
H	-3.15184500	4.16814700	-3.83841300
H	-2.07976300	2.03932100	-4.36308800
H	-4.44989600	5.57831300	-2.26543200
H	-5.16787600	4.69102600	-0.10107500
H	-0.97822500	-0.06815100	-4.92277100
H	-1.03450300	-3.33670700	-2.14345900
H	-0.35200200	-2.38239200	-4.29667500
H	-3.80941000	-3.61114700	3.22628500
H	-2.55886400	-5.03483700	1.62260900
H	-1.79882700	-4.14415300	-0.52319000
H	-4.81735500	-1.45655100	3.78595000
H	-5.70372400	3.96532400	1.65159900
H	-6.39953900	3.01984300	3.79848000
H	-5.84840100	0.67383500	4.38151800
O	-0.10319800	-5.22841800	-1.39520400
H	0.65637000	-4.34973300	-0.52718000
N	1.06702400	-3.21618500	0.49401200
C	2.06290000	-2.34493900	0.51013700
H	0.24890300	-2.94113000	1.03302200
C	2.00942700	-1.11912000	1.28772000
C	3.25684700	-2.62294100	-0.26533800
C	3.08446900	-0.25943100	1.26286000
C	0.78632400	-0.81087800	2.10977400
C	4.29990500	-1.72422300	-0.24061500
C	3.32199700	-3.87502400	-1.09413600
C	4.25910500	-0.52081500	0.51016300
H	3.04021300	0.63713300	1.87299500
H	0.90228600	0.13850000	2.63701100
H	-0.11268100	-0.73776900	1.48600600

H	0.59483000	-1.58777900	2.86023700
H	5.17078900	-1.93109800	-0.85438000
H	2.52761800	-3.88924500	-1.84825000
H	4.28473200	-3.95604500	-1.60450700
H	3.17448800	-4.76849900	-0.47851600
C	5.38405700	0.41697000	0.50864600
C	5.19683000	1.79287000	0.75231500
C	6.70324300	-0.01310700	0.25924800
C	6.24634700	2.70224000	0.75093800
H	4.19294200	2.17477100	0.90952100
C	7.78599800	0.85661100	0.25860100
H	6.89825000	-1.06867700	0.09703700
C	7.56105900	2.23281300	0.50909100
C	5.99951600	4.17246400	0.98384200
C	9.18471500	0.35407800	-0.00179400
N	8.61797600	3.12766000	0.46297500
H	6.34967500	4.78060400	0.14037900
H	4.93453700	4.37381100	1.11871800
H	6.51384500	4.53884200	1.88363800
H	9.18486700	-0.72155000	-0.19149200
H	9.63544900	0.84567300	-0.87323800
H	9.85287300	0.53176000	0.85266600
H	9.54611800	2.74948900	0.57488200
H	8.48853800	4.01611500	0.92229500
H	0.44943900	-5.20639400	-2.19035600

Fig. 4 (4, ts41, int42, ts42, int43, TMB, ts43, int44, OXTMB)

4

C	-2.36538100	3.57152700	0.00002300
C	-1.20340700	2.82009200	0.00000600
C	-1.23852800	1.41083800	0.00000200
C	0.00000000	0.68903100	-0.00000100
C	1.23852800	1.41083700	-0.00001000
C	1.20340800	2.82009100	-0.00002200
C	-3.59717800	2.89939200	0.00003800
C	-3.66563100	1.51286900	0.00003000
C	-2.48908700	0.73302100	0.00000800
C	-2.48908700	-0.73302000	-0.00000800
C	-1.23852800	-1.41083700	-0.00000200
C	0.00000000	-0.68903100	0.00000200
C	1.23852800	-1.41083800	0.00001000
C	2.48908700	-0.73302100	0.00001400
C	2.48908700	0.73302000	-0.00001300
C	2.36538100	3.57152600	-0.00004600
C	3.66563100	1.51286800	-0.00004400
C	3.59717900	2.89939100	-0.00006000
C	1.20340700	-2.82009200	0.00002200
C	2.36538100	-3.57152700	0.00004600
C	3.59717800	-2.89939200	0.00006100
C	3.66563100	-1.51286900	0.00004500
C	-1.20340800	-2.82009100	-0.00000600
C	-3.66563100	-1.51286800	-0.00003100
C	-3.59717900	-2.89939100	-0.00003900
C	-2.36538200	-3.57152600	-0.00002300
H	-2.30945500	4.65464800	0.00002700
H	-4.51394600	3.48040500	0.00005600

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H	-4.63841600	1.03576100	0.00004700
H	2.30945600	4.65464800	-0.00005600
H	4.63841600	1.03576000	-0.00006200
H	4.51394700	3.48040400	-0.00008500
H	2.30945500	-4.65464800	0.00005600
H	4.51394600	-3.48040500	0.00008500
H	4.63841600	-1.03576100	0.00006300
H	-4.63841600	-1.03576000	-0.00004800
H	-4.51394700	-3.48040400	-0.00005700
H	-2.30945600	-4.65464800	-0.00002700
O	0.00000000	-3.50660600	0.00000900
O	0.00000000	3.50660600	-0.00000900

int41

C	2.83665400	-2.81496200	1.08603300
C	2.27766700	-1.55100300	0.95249500
C	1.00855700	-1.36149000	0.33012700
C	0.43241600	-0.03941800	0.07729200
C	1.18289800	1.20243100	-0.12129600
C	2.50403700	1.24680000	-0.65021500
C	2.12144000	-3.94559800	0.67871800
C	0.82835500	-3.81185100	0.20646200
C	0.23804400	-2.53687700	0.06321400
C	-1.18515900	-2.40973900	-0.25140000
C	-1.77238300	-1.12495800	-0.13186600
C	-0.95498600	0.04984500	0.02128800
C	-1.62916500	1.31818500	0.11255900
C	-0.89957900	2.52033800	0.29353800
C	0.54937200	2.46534800	0.10472300
C	3.24302300	2.41499300	-0.71494100
C	1.31715300	3.64908700	0.04874300
C	2.65184300	3.61876600	-0.31265800
C	-3.03893900	1.36298800	0.11628500
C	-3.73167200	2.54105400	0.33852200
C	-3.00116700	3.71483000	0.56355500
C	-1.61372800	3.71236800	0.53865400
C	-3.17076800	-0.99313900	-0.25813400
C	-2.01882100	-3.50393300	-0.56573100
C	-3.38825600	-3.33325400	-0.71293800
C	-3.98356700	-2.07656700	-0.54561500
H	3.81788300	-2.91241000	1.54276600
H	2.56534800	-4.93054000	0.78484300
H	0.25581500	-4.70329900	-0.01643700
H	4.25629500	2.38893300	-1.09500900
H	0.85329300	4.60431900	0.26065000
H	3.22868800	4.53751900	-0.34684800
H	-4.81608800	2.53451300	0.34079600
H	-3.53283000	4.64247200	0.75052000
H	-1.08824200	4.64472200	0.70326000
H	-1.60108400	-4.49480600	-0.69269000
H	-4.01297800	-4.18785200	-0.95295500
H	-5.05414200	-1.93430300	-0.64357500
O	-3.79431200	0.22869100	-0.10284300
O	2.95945100	0.06741400	-1.22128900
O	2.91262800	-0.45930500	1.48081300
H	3.78249100	-0.73295400	1.81002700
O	4.40657000	-0.03067500	-1.15452300

H 4.65124800 0.20920400 -2.06710400

int42

C -2.91424000 3.28787100 0.06316600
 C -2.52422900 1.95665900 0.02022000
 C -1.15987800 1.58783500 0.03556800
 C -0.82975500 0.21191700 0.01227800
 C -1.85328800 -0.76481700 -0.02482500
 C -3.19939000 -0.32695800 -0.06096200
 C -1.91738900 4.26159900 0.12080400
 C -0.55830600 3.93212500 0.13844400
 C -0.14870600 2.59668700 0.09685000
 C 1.25099400 2.15493000 0.08982300
 C 1.52418800 0.76048300 -0.04425200
 C 0.53268900 -0.19560900 -0.00732600
 C 0.85997900 -1.59637200 0.05604700
 C -0.14977600 -2.59079500 0.05471500
 C -1.55509800 -2.16583200 -0.03752600
 C -4.25421300 -1.22805000 -0.12334300
 C -2.63018300 -3.05443200 -0.10440600
 C -3.94949100 -2.58702800 -0.14849900
 C 2.20717100 -1.95403800 0.23465000
 C 2.57885300 -3.28300900 0.39532800
 C 1.58472200 -4.26469500 0.36044000
 C 0.24127400 -3.93275200 0.19368200
 C 2.93245700 0.27360600 -0.31169200
 C 2.32978200 2.99961500 0.30190800
 C 3.68388000 2.52472400 0.38085300
 C 3.99335000 1.22911500 0.15317300
 H -3.96669100 3.54562900 0.04899600
 H -2.20581000 5.30704300 0.14912900
 H 0.17195000 4.73184200 0.17226600
 H -5.27540200 -0.86713900 -0.15391300
 H -2.45849200 -4.12351700 -0.12421700
 H -4.76041700 -3.30608700 -0.20135700
 H 3.62309900 -3.53643900 0.54059400
 H 1.86597700 -5.30677500 0.47119700
 H -0.49829500 -4.72434100 0.19517700
 H 2.16289300 4.05825800 0.46785200
 H 4.46066500 3.23754500 0.63458600
 H 5.01074900 0.85300900 0.19408200
 O -3.50562900 1.00470600 -0.03767400
 O 3.18766100 -0.98588000 0.31846800
 O 3.00365400 0.12769800 -1.71904700
 H 3.93190500 -0.03790300 -1.95907200

int43

C 2.36059700 -3.58314500 -0.02901900
 C 1.19580100 -2.82491600 -0.01159600
 C 1.23134300 -1.41175500 -0.00463000
 C 0.00057700 -0.70492300 0.00031200
 C -1.22902100 -1.41371800 0.00497900
 C -1.19120000 -2.82681500 0.01146000
 C 3.57933500 -2.90868800 -0.04029100
 C 3.64844600 -1.51043100 -0.02995000
 C 2.48589200 -0.73229100 -0.00836600
 C 2.48467400 0.73632000 0.00874200

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C	1.22902300	1.41371800	0.00498700
C	-0.00057600	0.70492400	0.00031600
C	-1.23134200	1.41175400	-0.00462200
C	-2.48589000	0.73229000	-0.00836100
C	-2.48467400	-0.73632200	0.00873700
C	-2.35471400	-3.58696700	0.02861400
C	-3.64593500	-1.51639900	0.03010100
C	-3.57456800	-2.91453200	0.04009300
C	-1.19579800	2.82491600	-0.01157800
C	-2.36059600	3.58314700	-0.02899400
C	-3.57933200	2.90868900	-0.04027000
C	-3.64844400	1.51043000	-0.02993800
C	1.19119900	2.82681700	0.01147900
C	3.64593300	1.51640000	0.03011400
C	3.57456300	2.91453300	0.04011600
C	2.35471100	3.58696900	0.02864000
H	2.30215000	-4.66529000	-0.03490100
H	4.50005200	-3.48204400	-0.05688800
H	4.62432500	-1.04045800	-0.04183000
H	-2.29441800	-4.66900400	0.03417300
H	-4.62256900	-1.04801100	0.04204100
H	-4.49436700	-3.48937700	0.05652900
H	-2.30214800	4.66529100	-0.03486900
H	-4.50005100	3.48204300	-0.05686100
H	-4.62432300	1.04045900	-0.04182000
H	4.62256700	1.04801300	0.04205200
H	4.49436000	3.48938100	0.05655800
H	2.29441600	4.66900600	0.03420700
O	-0.00282100	3.49704400	-0.00029200
O	0.00281800	-3.49705100	-0.00031300

TMB

C	0.74140700	-0.00015700	0.00184600
C	1.47326700	-1.13676600	0.37624500
C	2.86764900	-1.16084700	0.38258600
C	3.57549400	0.00036400	0.00449500
C	2.86775600	1.15860000	-0.38300100
C	1.47351700	1.13499400	-0.37697100
C	-0.74140700	0.00012000	0.00185700
C	-1.47351500	-1.13500300	-0.37697800
C	-2.86777400	-1.15862400	-0.38293600
C	-3.57549400	-0.00038200	0.00453500
C	-2.86763200	1.16083100	0.38262400
C	-1.47326800	1.13673300	0.37631100
H	0.94037300	-2.02756500	0.69846700
H	0.94088200	2.02372600	-0.70511000
H	-0.94088800	-2.02373100	-0.70514300
H	-0.94036600	2.02752900	0.69852100
C	3.61765200	2.39363100	-0.81996300
H	2.92693800	3.18127200	-1.13053200
H	4.23809600	2.80924700	-0.01242500
H	4.28812900	2.18378700	-1.66292500
C	3.61629800	-2.40649000	0.79068200
H	2.92451200	-3.21716900	1.03187700
H	4.28072500	-2.76042600	-0.00793600
H	4.24232300	-2.24195700	1.67981000
C	-3.61758600	-2.39369300	-0.81994100

H	-2.92679700	-3.18137600	-1.13024000
H	-4.23822300	-2.80919600	-0.01250200
H	-4.28784600	-2.18400700	-1.66312300
C	-3.61635800	2.40645300	0.79063400
H	-2.92464100	3.21730100	1.03145200
H	-4.28108400	2.76002200	-0.00789000
H	-4.24211500	2.24204100	1.67998000
N	4.97635900	-0.01586800	-0.04911400
H	5.41589700	0.88896400	0.04773400
H	5.41658500	-0.70094100	0.54913300
N	-4.97635600	0.01612300	-0.04914800
H	-5.41601900	-0.88872000	0.04697300
H	-5.41654000	0.70082000	0.54957300

OXTMB

C	0.72332200	0.00001500	0.00004100
C	1.46816900	-1.19470600	0.20639500
C	2.84489400	-1.22388200	0.22025800
C	3.55661100	0.00000300	0.00001400
C	2.84490000	1.22389200	-0.22023500
C	1.46817500	1.19472700	-0.20634800
C	-0.72332200	0.00000900	0.00003600
C	-1.46816100	-1.19471100	-0.20634900
C	-2.84488700	-1.22389000	-0.22023800
C	-3.55661100	-0.00000900	0.00000800
C	-2.84490800	1.22388300	0.22025500
C	-1.46818200	1.19472200	0.20639500
H	0.94359200	-2.12194900	0.40609400
H	0.94360500	2.12196600	-0.40607900
H	-0.94358000	-2.12194600	-0.40607100
H	-0.94361800	2.12196900	0.40610300
C	3.60312100	2.50175700	-0.47097600
H	2.91836600	3.33621200	-0.63132700
H	4.24537600	2.76602400	0.37880500
H	4.24136300	2.42771800	-1.36049200
C	3.60311300	-2.50175900	0.47094000
H	2.91835800	-3.33622100	0.63125300
H	4.24537400	-2.76599500	-0.37884600
H	4.24135000	-2.42775000	1.36046100
C	-3.60309400	-2.50176500	-0.47097500
H	-2.91832900	-3.33621100	-0.63132800
H	-4.24534300	-2.76603800	0.37880800
H	-4.24133900	-2.42773500	-1.36048900
C	-3.60314000	2.50175200	0.47094100
H	-2.91839400	3.33622000	0.63126300
H	-4.24539900	2.76598600	-0.37884800
H	-4.24138100	2.42773100	1.36045800
N	4.90818700	0.00000100	0.00001700
H	5.43297500	0.84692100	-0.14922400
H	5.43298100	-0.84700500	0.14874800
N	-4.90818700	-0.00002300	0.00001300
H	-5.43296500	-0.84695000	-0.14922700
H	-5.43299200	0.84697600	0.14874400

int44

C	2.41109900	3.55541600	0.02070000
C	1.27679700	2.78643300	0.00616800

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C	1.24631100	1.38975000	0.00481300
C	-0.00027700	0.67736800	0.00070300
C	-1.24741800	1.38882200	0.00030300
C	-1.27893500	2.78547400	-0.00434200
C	3.63682400	2.86725100	0.02361400
C	3.67716100	1.48180000	0.01923100
C	2.49597200	0.70868500	0.00843800
C	2.49162700	-0.75550300	-0.00194700
C	1.23769300	-1.42756000	-0.00327000
C	0.00025800	-0.70143700	-0.00095500
C	-1.23660900	-1.42851000	0.00138600
C	-2.49105900	-0.75741000	0.00654400
C	-2.49656800	0.70680300	0.00004800
C	-2.41388000	3.55371300	-0.00483300
C	-3.67833100	1.47904000	-0.01096900
C	-3.63903600	2.86453900	-0.01482800
C	-1.19845800	-2.83730300	0.00163300
C	-2.35926300	-3.59198100	0.00989500
C	-3.59116600	-2.92480000	0.01973900
C	-3.66432400	-1.53784600	0.01838100
C	1.20064200	-2.83637100	-0.00900100
C	3.66554400	-1.53499600	-0.01150500
C	3.59347400	-2.92197700	-0.01925500
C	2.36205600	-3.59012400	-0.01694000
H	2.35789900	4.63865300	0.02630100
H	4.55923500	3.43694000	0.03265500
H	4.64359800	0.99301000	0.02581600
H	-2.36161100	4.63701300	-0.00345700
H	-4.64438600	0.98949700	-0.01892100
H	-4.56191100	3.43349900	-0.02243000
H	-2.29874800	-4.67458800	0.00993500
H	-4.50645600	-3.50773800	0.02835300
H	-4.63888100	-1.06541500	0.02838500
H	4.63977300	-1.06180900	-0.01542900
H	4.50924400	-3.50416700	-0.02733600
H	2.30239100	-4.67276600	-0.02200300
O	0.00134900	-3.52222700	-0.00658500
O	-0.00146000	3.47424600	0.02267400
H	-0.00006800	4.34607700	-0.43308600

ts42

C	2.41109900	3.55541600	0.02070000
C	1.27679700	2.78643300	0.00616800
C	1.24631100	1.38975000	0.00481300
C	-0.00027700	0.67736800	0.00070300
C	-1.24741800	1.38882200	0.00030300
C	-1.27893500	2.78547400	-0.00434200
C	3.63682400	2.86725100	0.02361400
C	3.67716100	1.48180000	0.01923100
C	2.49597200	0.70868500	0.00843800
C	2.49162700	-0.75550300	-0.00194700
C	1.23769300	-1.42756000	-0.00327000
C	0.00025800	-0.70143700	-0.00095500
C	-1.23660900	-1.42851000	0.00138600
C	-2.49105900	-0.75741000	0.00654400
C	-2.49656800	0.70680300	0.00004800
C	-2.41388000	3.55371300	-0.00483300

C	-3.67833100	1.47904000	-0.01096900
C	-3.63903600	2.86453900	-0.01482800
C	-1.19845800	-2.83730300	0.00163300
C	-2.35926300	-3.59198100	0.00989500
C	-3.59116600	-2.92480000	0.01973900
C	-3.66432400	-1.53784600	0.01838100
C	1.20064200	-2.83637100	-0.00900100
C	3.66554400	-1.53499600	-0.01150500
C	3.59347400	-2.92197700	-0.01925500
C	2.36205600	-3.59012400	-0.01694000
H	2.35789900	4.63865300	0.02630100
H	4.55923500	3.43694000	0.03265500
H	4.64359800	0.99301000	0.02581600
H	-2.36161100	4.63701300	-0.00345700
H	-4.64438600	0.98949700	-0.01892100
H	-4.56191100	3.43349900	-0.02243000
H	-2.29874800	-4.67458800	0.00993500
H	-4.50645600	-3.50773800	0.02835300
H	-4.63888100	-1.06541500	0.02838500
H	4.63977300	-1.06180900	-0.01542900
H	4.50924400	-3.50416700	-0.02733600
H	2.30239100	-4.67276600	-0.02200300
O	0.00134900	-3.52222700	-0.00658500
O	-0.00146000	3.47424600	0.02267400
H	-0.00006800	4.34607700	-0.43308600

ts43

C	2.41109900	3.55541600	0.02070000
C	1.27679700	2.78643300	0.00616800
C	1.24631100	1.38975000	0.00481300
C	-0.00027700	0.67736800	0.00070300
C	-1.24741800	1.38882200	0.00030300
C	-1.27893500	2.78547400	-0.00434200
C	3.63682400	2.86725100	0.02361400
C	3.67716100	1.48180000	0.01923100
C	2.49597200	0.70868500	0.00843800
C	2.49162700	-0.75550300	-0.00194700
C	1.23769300	-1.42756000	-0.00327000
C	0.00025800	-0.70143700	-0.00095500
C	-1.23660900	-1.42851000	0.00138600
C	-2.49105900	-0.75741000	0.00654400
C	-2.49656800	0.70680300	0.00004800
C	-2.41388000	3.55371300	-0.00483300
C	-3.67833100	1.47904000	-0.01096900
C	-3.63903600	2.86453900	-0.01482800
C	-1.19845800	-2.83730300	0.00163300
C	-2.35926300	-3.59198100	0.00989500
C	-3.59116600	-2.92480000	0.01973900
C	-3.66432400	-1.53784600	0.01838100
C	1.20064200	-2.83637100	-0.00900100
C	3.66554400	-1.53499600	-0.01150500
C	3.59347400	-2.92197700	-0.01925500
C	2.36205600	-3.59012400	-0.01694000
H	2.35789900	4.63865300	0.02630100
H	4.55923500	3.43694000	0.03265500
H	4.64359800	0.99301000	0.02581600
H	-2.36161100	4.63701300	-0.00345700

H	-4.64438600	0.98949700	-0.01892100
H	-4.56191100	3.43349900	-0.02243000
H	-2.29874800	-4.67458800	0.00993500
H	-4.50645600	-3.50773800	0.02835300
H	-4.63888100	-1.06541500	0.02838500
H	4.63977300	-1.06180900	-0.01542900
H	4.50924400	-3.50416700	-0.02733600
H	2.30239100	-4.67276600	-0.02200300
O	0.00134900	-3.52222700	-0.00658500
O	-0.00146000	3.47424600	0.02267400
H	-0.00006800	4.34607700	-0.43308600

Fig. 5 (5, int51, ts51, int52, int53, int54, ts52, int55, ts53.)

5			
C	-2.41169900	3.62508700	-0.62446500
C	-1.20170100	2.88883000	-0.51434300
C	0.06792900	3.51832800	-0.56083500
C	-1.28525800	1.47838200	-0.26318100
C	-0.07555800	0.75555100	-0.14760500
C	1.13543800	1.39730600	-0.11323600
C	1.24327200	2.80810700	-0.29350400
C	-3.62254200	2.99526800	-0.42882900
C	-3.68981900	1.61769300	-0.12748900
C	-2.54046000	0.83679500	-0.05044100
C	-2.55975200	-0.62839100	0.18261300
C	-1.35423200	-1.36513000	0.21741900
C	-0.03111300	-0.67225600	0.28420700
C	1.11395200	-1.45778000	-0.27028200
C	2.34127200	-0.79881000	-0.25788400
C	2.24668300	0.54999000	0.41701300
C	2.52673200	3.40986200	-0.10674500
C	3.51059600	1.29336800	0.64709500
C	3.60647600	2.64047600	0.36897400
C	1.02881100	-2.84581600	-0.51574400
C	2.20976600	-3.50762700	-0.94014200
C	3.41114700	-2.81650600	-1.03474600
C	3.50098800	-1.46518400	-0.65886200
C	-1.37858300	-2.78994200	0.09412900
C	-0.20183400	-3.51016500	-0.25817800
C	-3.77576100	-1.33748500	0.25161000
C	-3.79834600	-2.73351500	0.30003600
C	-2.62285400	-3.45939600	0.18637600
H	-2.36604500	4.68999500	-0.83245400
H	0.11474300	4.59080700	-0.72929400
H	-4.54534700	3.56343400	-0.49159100
H	-4.66738100	1.18144000	0.04111000
H	2.64969500	4.47381700	-0.28079400
H	4.36379100	0.74291100	1.02727400
H	4.56053100	3.13477200	0.52963400
H	2.16767900	-4.56779800	-1.17233700
H	4.30433700	-3.33710000	-1.36640400
H	4.45927700	-0.95697200	-0.66661200
H	-0.26460100	-4.58719100	-0.38094500
H	-4.71837900	-0.80399800	0.24644600
H	-4.75067300	-3.24981200	0.37116000
H	-2.64378300	-4.54346200	0.12829000

O	1.71987900	0.15772000	1.83477300
O	0.40197700	-0.51935600	1.77507200

int51

C	-2.61799000	3.52115700	-0.18817200
C	-1.35758000	2.85682800	-0.19607600
C	-0.15923400	3.57646800	-0.28002000
C	-1.31252600	1.42184800	-0.09102400
C	-0.06127600	0.77312700	-0.03495600
C	1.13936600	1.50091500	-0.15870900
C	1.08436400	2.93653500	-0.27526700
C	-3.78101300	2.79885300	-0.09158900
C	-3.74376800	1.38567500	-0.03909300
C	-2.54741800	0.68598100	-0.05569800
C	-2.48679900	-0.78293400	-0.11730900
C	-1.25387100	-1.43528000	-0.03140300
C	-0.01194300	-0.67281300	0.34874800
C	1.27303200	-1.35083500	-0.03546800
C	2.45736700	-0.62289200	-0.17679500
C	2.42236400	0.84900200	-0.17261700
C	2.29738800	3.68199800	-0.35379500
C	3.56640400	1.62529800	-0.24372800
C	3.50764600	3.03792300	-0.32515200
C	1.29077800	-2.77007000	-0.16101100
C	2.51173700	-3.45801400	-0.36058200
C	3.69004700	-2.73705600	-0.46404600
C	3.65645100	-1.34417400	-0.39392300
C	-1.17835600	-2.84853500	-0.17446100
C	0.07939700	-3.48646700	-0.18262500
C	-3.63850900	-1.57596500	-0.34268500
C	-3.57760200	-2.96466300	-0.45422700
C	-2.35277300	-3.60989900	-0.37730200
H	-2.63650200	4.60482300	-0.25268300
H	-0.19716900	4.66021000	-0.34710500
H	-4.74142900	3.30289000	-0.07238300
H	-4.68817500	0.85654700	0.00896200
H	2.23945500	4.76355600	-0.42938100
H	4.54542300	1.16097900	-0.24029100
H	4.43311300	3.60179900	-0.37549600
H	2.50192200	-4.53899500	-0.45396200
H	4.63470400	-3.24423000	-0.62420000
H	4.58926300	-0.80797800	-0.52178500
H	0.11413300	-4.56887800	-0.27245200
H	-4.60624500	-1.09996900	-0.44631700
H	-4.48805600	-3.52969600	-0.61881200
H	-2.27445400	-4.68644800	-0.48803300
O	0.96416400	-0.11887700	2.52091400
O	-0.14034000	-0.78195800	1.86192600
H	0.60933500	0.77998900	2.64512200

int52

C	-2.47303500	3.58394300	0.00941700
C	-1.23417800	2.89392600	0.00611000
C	-0.02170400	3.59332700	-0.08452700
C	-1.21935100	1.45638700	0.08206200
C	0.02329700	0.79332700	0.10719300
C	1.24247000	1.49290600	-0.03450500

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C	1.21306100	2.92894100	-0.12352200
C	-3.66639300	2.88414700	0.05836400
C	-3.66577000	1.48510300	0.06834400
C	-2.47250900	0.74207800	0.06116800
C	-2.48696200	-0.70065400	-0.04793900
C	-1.26403200	-1.43887000	0.30489700
C	0.06804800	-0.64824300	0.38662800
C	1.32032700	-1.37776800	0.14600200
C	2.52205600	-0.66778800	-0.02817500
C	2.50111700	0.80428200	-0.06629900
C	2.43284000	3.64873300	-0.22255600
C	3.66435500	1.56606600	-0.15830000
C	3.63264800	2.97197200	-0.23431400
C	1.29770500	-2.79804700	0.12100100
C	2.51611600	-3.50017500	-0.00462000
C	3.71059800	-2.80430700	-0.13404200
C	3.71476500	-1.41041300	-0.16453100
C	-1.17232000	-2.88171900	-0.00423100
C	0.05667900	-3.50965900	0.05415700
C	-3.57079400	-1.43573300	-0.50219000
C	-3.51938700	-2.84315200	-0.63972000
C	-2.35512700	-3.55017400	-0.41100500
H	-2.46809700	4.66868900	-0.02978700
H	-0.04139400	4.67792700	-0.13756800
H	-4.61071300	3.41711600	0.07353600
H	-4.61667100	0.96556800	0.09241500
H	2.39988500	4.73196500	-0.28243300
H	4.63314100	1.08221800	-0.17161200
H	4.56767900	3.51732100	-0.30466700
H	2.50182800	-4.58532000	-0.02405100
H	4.64632700	-3.34375700	-0.23370800
H	4.66213900	-0.90243100	-0.29702000
H	0.09901200	-4.58722800	-0.07784900
H	-4.48540700	-0.92865500	-0.78750700
H	-4.40688800	-3.36475400	-0.98087600
H	-2.31559000	-4.62079500	-0.58613900
O	-0.66654800	-1.04981200	1.55975800

int53

C	-2.55724800	3.53604600	-0.14719400
C	-1.29971800	2.86477200	-0.12640400
C	-0.09625700	3.57691400	-0.18516500
C	-1.26560400	1.42908500	-0.01290100
C	-0.02197400	0.77281200	0.07177300
C	1.18552600	1.49245100	-0.02961800
C	1.14298800	2.92852000	-0.14894800
C	-3.72503100	2.82109600	-0.06662900
C	-3.69751700	1.40680900	-0.00109100
C	-2.50667900	0.70062800	0.00858200
C	-2.45385300	-0.77092600	-0.04027500
C	-1.22818900	-1.42940700	0.07755600
C	0.01313600	-0.67364300	0.49690600
C	1.29912800	-1.36273200	0.09414400
C	2.49077000	-0.64222800	-0.03139800
C	2.46480700	0.83126000	-0.01521600
C	2.36303500	3.66473800	-0.19805200
C	3.61558200	1.59956500	-0.05295500

C	3.56785300	3.01267400	-0.13503400
C	1.31006600	-2.78062800	-0.03977400
C	2.52846500	-3.47621000	-0.23211700
C	3.71184200	-2.76282100	-0.32175600
C	3.68611100	-1.36940500	-0.24382700
C	-1.16049400	-2.84197900	-0.07069000
C	0.09305400	-3.48743700	-0.07307800
C	-3.60653100	-1.55621600	-0.28421400
C	-3.55520200	-2.94646800	-0.39001700
C	-2.33642200	-3.59801000	-0.29245900
H	-2.56860400	4.61940000	-0.21945600
H	-0.12550800	4.66076700	-0.25510500
H	-4.68289700	3.33057300	-0.06912100
H	-4.64604600	0.88398400	0.03566200
H	2.31516400	4.74655000	-0.27818800
H	4.59094000	1.12818600	-0.02516400
H	4.49788700	3.57081000	-0.16087000
H	2.51202700	-4.55669700	-0.33098500
H	4.65461900	-3.27465900	-0.47818900
H	4.62245600	-0.83786600	-0.36599900
H	0.12112100	-4.56958200	-0.16933200
H	-4.56842200	-1.07288000	-0.40810400
H	-4.46680300	-3.50515500	-0.56942000
H	-2.26113500	-4.67475900	-0.40410000
O	-0.05902300	-0.73041200	1.96619100
H	0.70751800	-0.24093000	2.30795400

int54

C	-2.85772700	3.34245600	-0.18063100
C	-1.55060100	2.77367200	-0.11359400
C	-0.40759800	3.57835300	-0.10013500
C	-1.40629700	1.34057100	-0.02908400
C	-0.11572800	0.78913400	0.06785100
C	1.03897900	1.59993900	0.02673300
C	0.88049200	3.03197500	-0.03724500
C	-3.96269500	2.53305300	-0.16509700
C	-3.82468500	1.12309100	-0.10038300
C	-2.58675000	0.50848900	-0.04365400
C	-2.43234100	-0.96305000	-0.03166200
C	-1.14869900	-1.52928300	0.10739900
C	0.02375900	-0.66170500	0.33418100
C	1.40482900	-1.27960000	0.27749600
C	2.55844000	-0.41216000	-0.06560700
C	2.37437800	1.04265100	0.03126500
C	2.03569100	3.86892300	-0.02338000
C	3.45481800	1.91113000	0.07125700
C	3.28890500	3.31635900	0.04901600
C	1.50263700	-2.73869900	-0.00872500
C	2.80047200	-3.27766200	-0.31570900
C	3.85676400	-2.44790200	-0.53667300
C	3.71538900	-1.01587900	-0.46719300
C	-0.96227800	-2.93571400	0.06767100
C	0.36735300	-3.49696400	0.01200200
C	-3.53045700	-1.83466000	-0.15828000
C	-3.35882300	-3.21792500	-0.15249100
C	-2.08789700	-3.77104700	-0.04928700
H	-2.95349300	4.42263200	-0.23978200

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H	-0.52136800	4.65849300	-0.13580000
H	-4.95898400	2.96170500	-0.21015900
H	-4.73061000	0.52833400	-0.10036700
H	1.89799000	4.94547200	-0.06141600
H	4.46251900	1.51280600	0.11815800
H	4.16836900	3.95218000	0.07875000
H	2.90139700	-4.35494200	-0.41186400
H	4.82455900	-2.85619100	-0.81016700
H	4.56864600	-0.41318700	-0.76053300
H	0.44887100	-4.57233600	-0.12551800
H	-4.53402000	-1.43854800	-0.25789700
H	-4.22618600	-3.86443200	-0.24352100
H	-1.94825700	-4.84756100	-0.07765500
O	0.77232200	-0.96246400	1.55519100

int55

C	-1.43584600	4.17748700	-0.29030300
C	-0.47246200	3.13912000	-0.20210000
C	0.91283800	3.41825800	-0.24803100
C	-0.90770600	1.78184600	-0.06008400
C	0.07791300	0.76113100	0.06804100
C	1.43344200	1.06032500	0.01831600
C	1.86247700	2.41639800	-0.15140800
C	-2.77748000	3.87740500	-0.23956200
C	-3.20958700	2.54039100	-0.11880300
C	-2.31109400	1.48366600	-0.03691700
C	-2.75388100	0.07239800	0.02967600
C	-1.79507900	-0.95670800	0.13830300
C	-0.37022700	-0.63144000	0.33143500
C	0.64657800	-1.75461300	0.21320800
C	2.03519300	-1.40627100	-0.15119500
C	2.46456100	-0.01412300	0.17392600
C	3.28212200	2.73289500	-0.26342400
C	3.89371900	0.38833400	0.12622900
C	4.23967700	1.79420700	-0.17257800
C	0.14663300	-3.11272600	-0.12541000
C	1.10340600	-4.08848000	-0.57861900
C	2.38281000	-3.72651900	-0.86233900
C	2.83541400	-2.36446500	-0.68174900
C	-2.18405200	-2.32218300	0.10001100
C	-1.19361000	-3.36243900	-0.04420700
C	-4.11097200	-0.29153100	-0.02460600
C	-4.50361400	-1.63017100	0.00140800
C	-3.55355800	-2.64179300	0.04482200
H	-1.09436200	5.20285900	-0.39601900
H	1.23408400	4.44961200	-0.36585000
H	-3.51838700	4.66832400	-0.30127800
H	-4.27672000	2.35490900	-0.09711200
H	3.54144600	3.76960700	-0.46038400
H	4.63803300	-0.35611600	-0.14237900
H	5.28650200	2.04148500	-0.31766100
H	0.76095300	-5.10742400	-0.73525900
H	3.08741100	-4.45648300	-1.24703300
H	3.85479300	-2.12995800	-0.97019400
H	-1.55503800	-4.37270300	-0.21904700
H	-4.88049100	0.46881900	-0.08184000
H	-5.56000500	-1.87733200	-0.03385400

H	-3.85355200	-3.68504000	0.01882500
O	0.22834500	-1.24420900	1.51415800
O	3.26035900	0.11758800	1.40894600

ts51

C	0.37006000	-0.21440600	-1.87140400
C	1.56393500	-0.71685400	-1.30599100
C	1.72146900	-2.11001200	-1.06966100
C	2.63756900	0.17507500	-0.97783500
C	3.84467700	-0.33913400	-0.39339500
C	3.97305800	-1.74652300	-0.13424100
C	2.90115500	-2.63573500	-0.46221800
C	0.23823200	1.14708300	-2.11067900
C	1.27654300	2.01926400	-1.79969400
C	2.48576200	1.56309300	-1.23206700
C	3.57642000	2.46919300	-0.90411000
C	4.77290700	1.94626500	-0.33400300
C	4.90379900	0.53727600	-0.07527400
C	6.11588900	0.02084200	0.50879700
C	6.25323300	-1.37028400	0.77756400
C	5.15657100	-2.27416400	0.45065300
C	3.01811200	-4.01548800	-0.20312100
C	5.22842700	-3.65807400	0.69389200
C	4.17436200	-4.51400300	0.37507000
C	7.19339200	0.89445800	0.82711800
C	8.36378300	0.39718600	1.39387900
C	8.49368700	-0.96677800	1.65872900
C	7.45420900	-1.83258500	1.35483500
C	5.83700800	2.84056100	-0.02332300
C	7.09587400	2.34361100	0.56554800
C	3.48794400	3.85905400	-1.13523900
C	4.53391500	4.71332300	-0.82642400
C	5.70959400	4.20382200	-0.27057800
H	-0.41475000	-0.90599500	-2.14650300
H	-0.67422500	1.53491600	-2.55069500
H	1.13989200	3.07258900	-2.00942300
H	2.19585600	-4.67255900	-0.45789200
H	6.11764600	-4.08665200	1.13860900
H	4.26726300	-5.57556000	0.57848600
H	9.16668000	1.08803400	1.62476000
H	9.40563900	-1.35235000	2.10211400
H	7.58164500	-2.88604300	1.57066200
H	2.58815800	4.28140300	-1.56447800
H	4.43722000	5.77693100	-1.01711200
H	6.53730400	4.85914100	-0.02385800
O	8.03366300	3.11272100	0.83034900
O	0.74300900	-2.93918000	-1.43580100
O	-0.19803000	-3.21314800	-0.12213000
H	-1.33841400	-1.75747800	0.09690100
N	-1.74203700	-0.88252500	0.43576900
C	-3.07060900	-0.62835600	0.43452900
H	-1.12088400	-0.28412100	0.96174000
C	-3.57718400	0.54098800	1.08787700
C	-3.97397400	-1.51487600	-0.23457900
C	-4.93579600	0.79020100	1.05305500
C	-2.63441600	1.47333500	1.80182500
C	-5.32519900	-1.22110600	-0.22849400

ARTICLE

Journal Name

C	-3.45128600	-2.73919700	-0.93321400
C	-5.85785000	-0.06940400	0.40140800
H	-5.30053700	1.66778400	1.57630600
H	-3.18381500	2.29640400	2.26347800
H	-2.07288700	0.95876200	2.59195600
H	-1.89634000	1.90539300	1.11439200
H	-5.98730600	-1.89165500	-0.76523300
H	-4.26496700	-3.28600200	-1.41453900
H	-2.70940100	-2.48527100	-1.69969000
H	-2.95627600	-3.42091500	-0.22805000
C	-7.28828900	0.22297100	0.37249200
C	-7.78362700	1.53094300	0.59349100
C	-8.24630900	-0.78741200	0.11423500
C	-9.13413100	1.83657100	0.55742600
H	-7.08842200	2.34567400	0.76598500
C	-9.60734100	-0.53607800	0.07549700
H	-7.92017900	-1.81231600	-0.02802700
C	-10.07041200	0.79405300	0.29550800
C	-9.61969300	3.24655500	0.77532300
C	-10.59627800	-1.64244600	-0.18372500
N	-11.40290400	1.07414200	0.22107500
H	-8.78034700	3.92237400	0.95397200
H	-10.17693300	3.62167600	-0.09229800
H	-10.29314500	3.31552700	1.63965700
H	-10.08301500	-2.59533000	-0.33117500
H	-11.29628000	-1.76582500	0.65306100
H	-11.20130300	-1.44382800	-1.07738700
H	-11.74538700	1.96293100	0.55406500
H	-12.07191900	0.31867300	0.20526600
H	-0.73026900	-3.92761400	-0.51920500

ts52

C	-2.81081200	2.09180100	-1.62991800
C	-1.45102400	2.02977600	-1.17413100
C	-0.68475000	3.18717200	-1.03777400
C	-0.86825400	0.75315300	-0.84891600
C	0.45697000	0.70743800	-0.37829700
C	1.24020200	1.87574400	-0.26727700
C	0.64755500	3.14530100	-0.60053400
C	-3.55719400	0.95572900	-1.74506200
C	-2.99280800	-0.32064200	-1.44150400
C	-1.65214100	-0.45092900	-1.05764100
C	-0.99077800	-1.75837700	-0.99963600
C	0.26303500	-1.85584100	-0.21796600
C	1.01766800	-0.57777300	0.10049100
C	2.46952300	-0.66080700	0.34483600
C	3.24210200	0.51513600	0.43787900
C	2.61162600	1.82790500	0.17544800
C	1.41815500	4.33519900	-0.46075400
C	3.30320800	3.02087500	0.30417400
C	2.71167000	4.26835000	-0.00902700
C	3.06250600	-1.93963000	0.51350200
C	4.42562800	-2.02124700	0.85290000
C	5.18015300	-0.86267800	0.98999600
C	4.60345500	0.38783600	0.77030200
C	1.03898900	-3.12481300	-0.27152800
C	2.32249700	-3.13769500	0.19637200

C	-1.45394400	-2.88368100	-1.61794900
C	-0.78723300	-4.15494800	-1.50212600
C	0.40289200	-4.27662100	-0.85132500
H	-3.22656800	3.06331200	-1.88077500
H	-1.13231400	4.14932900	-1.27173200
H	-4.58684900	1.00273400	-2.08494300
H	-3.56832400	-1.20241400	-1.68729500
H	0.96035800	5.28686000	-0.71368600
H	4.33077700	3.02233300	0.64786400
H	3.30029600	5.17310100	0.10587400
H	4.88127200	-2.99810400	0.98454400
H	6.23154400	-0.92692600	1.25238900
H	5.22806700	1.26810400	0.86426500
H	2.86384800	-4.07999400	0.22661100
H	-2.35203400	-2.83926100	-2.22512100
H	-1.24058700	-5.01855100	-1.97802900
H	0.91978500	-5.23057100	-0.79986400
O	0.19494300	-1.24606100	1.10460300
O	-3.19505000	-0.77604300	0.65290700
O	-3.88607400	-1.39606900	2.16992500
H	-3.14797800	0.78837000	1.25506300
H	-4.37112500	-2.14128800	1.78070600
H	-4.58699900	-0.68845100	2.38021200
O	-3.26358800	1.69048400	1.68476300
O	-5.48792400	0.58697600	2.68954600
H	-3.52519300	2.25656300	0.94436200
H	-4.75645600	1.18364900	2.37171800
H	-6.13335700	0.60252800	1.96669000

ts53

C	-2.16365400	3.77197100	-0.63376300
C	-1.00703800	2.95342500	-0.52397000
C	0.29753900	3.49852300	-0.57837900
C	-1.17838400	1.55148800	-0.25798100
C	-0.02005700	0.74826900	-0.13604500
C	1.22896900	1.30717800	-0.13915500
C	1.42113700	2.70460600	-0.32168200
C	-3.41232200	3.22731800	-0.43007200
C	-3.56771300	1.85746300	-0.12251700
C	-2.47619300	0.99877400	-0.04299000
C	-2.60326700	-0.46226700	0.18807900
C	-1.45173400	-1.28022500	0.22548500
C	-0.07583100	-0.67698200	0.35320300
C	1.01888500	-1.54133400	-0.22814500
C	2.28885400	-0.96782100	-0.25841300
C	2.30451700	0.39875100	0.40047600
C	2.72870000	3.24029800	-0.10210100
C	3.60358000	1.07793900	0.61814200
C	3.76150400	2.43980700	0.39252100
C	0.83257900	-2.91487000	-0.48903700
C	1.95586800	-3.66148100	-0.93032400
C	3.20166800	-3.05955400	-1.04667100
C	3.38853900	-1.71378800	-0.68385300
C	-1.57232100	-2.70029800	0.10332600
C	-0.44540400	-3.49433700	-0.23917700
C	-3.86413100	-1.08508600	0.24282800
C	-3.98437900	-2.47886200	0.29231000

C	-2.86245900	-3.28329700	0.18897000
H	-2.04426600	4.82955100	-0.84903500
H	0.41754100	4.56540100	-0.74533900
H	-4.29596700	3.85439100	-0.49234800
H	-4.57220800	1.48794200	0.04807500
H	2.89748600	4.30055100	-0.26418200
H	4.42348000	0.48119600	1.00116200
H	4.72566800	2.89456300	0.59767500
H	1.83135400	-4.71542500	-1.16204700
H	4.05076600	-3.64275900	-1.38985400
H	4.37935900	-1.27226500	-0.71812700
H	-0.57791100	-4.56531900	-0.36121100
H	-4.76873200	-0.48933000	0.22363400
H	-4.97130500	-2.92647100	0.35685000
H	-2.95626100	-4.36388700	0.13629000
O	1.94155900	0.18709300	1.79215900
O	0.23047900	-0.58356800	1.77935000

Fig. 6 (6, int61, ts61_0H₂O, ts61_1H₂O, ts61_2H₂O, ts61_3H₂O, int62, ts62, int63,, .)**6**

C	-3.58786900	2.45050800	-0.11425100
C	-2.89111400	1.20821700	-0.03409700
C	-3.57374100	-0.02785400	-0.00434800
C	-1.44771600	1.21772400	-0.02609000
C	-0.72837800	-0.00564400	-0.01342300
C	-1.42848500	-1.24033600	-0.00315300
C	-2.87135900	-1.25353400	0.00886500
C	-2.89812200	3.63551600	-0.15859700
C	-1.49195400	3.65062700	-0.11840200
C	-0.75385700	2.47601700	-0.04489100
C	0.71514500	2.48768800	0.00490200
C	1.42848600	1.24036300	-0.00318000
C	0.72837500	0.00567200	-0.01343400
C	1.44771300	-1.21769500	-0.02609900
C	0.75385900	-2.47598900	-0.04486900
C	-0.71514300	-2.48766100	0.00493900
C	-3.54951400	-2.50690700	0.07016800
C	-1.43500500	-3.67429800	0.06631400
C	-2.84132900	-3.68145400	0.10270700
C	2.89110900	-1.20818700	-0.03413300
C	3.58787100	-2.45047100	-0.11424800
C	2.89812900	-3.63548300	-0.15855600
C	1.49196000	-3.65060000	-0.11835600
C	2.87136100	1.25355900	0.00882200
C	3.57374000	0.02787500	-0.00440900
C	1.43500800	3.67432600	0.06625000
C	2.84133200	3.68147900	0.10263600
C	3.54951600	2.50693300	0.07010800
H	-4.66981800	2.45899200	-0.14429700
H	-3.43730200	4.57498700	-0.22730500
H	-0.99332100	4.61087400	-0.15779700
H	-4.63138500	-2.53048900	0.09418100
H	-0.92154800	-4.62703500	0.09662000
H	-3.36596000	-4.63004600	0.15764200
H	4.66982300	-2.45894400	-0.14429300
H	3.43731700	-4.57495200	-0.22724000

H	0.99333200	-4.61085000	-0.15771800
H	0.92155000	4.62706300	0.09653900
H	3.36596700	4.63007000	0.15755800
H	4.63138700	2.53051700	0.09411500
C	5.07012700	0.05876300	-0.02871500
C	-5.07013600	-0.05876700	-0.02862200
O	5.73622000	0.61283500	-0.88937200
O	-5.73624100	-0.61278900	-0.88929800
O	-5.63063100	0.57886900	1.01823900
H	-6.59966600	0.53545600	0.90956800
O	5.63063800	-0.57918100	1.01795500
H	6.59966800	-0.53584100	0.90921400

int61

C	3.55159400	2.46212900	0.00061000
C	2.84675300	1.26275400	0.00026700
C	3.62345700	0.00000000	0.00001200
C	1.42651300	1.25207700	0.00012100
C	0.69821900	0.00000000	0.00000300
C	1.42651300	-1.25207700	-0.00011600
C	2.84675300	-1.26275400	-0.00025800
C	2.86602200	3.67692500	0.00086900
C	1.47982400	3.68572100	0.00065600
C	0.72923600	2.49145900	0.00018700
C	-0.72923600	2.49145900	-0.00018600
C	-1.42651300	1.25207700	-0.00012200
C	-0.69821900	0.00000000	-0.00000300
C	-1.42651300	-1.25207700	0.00011700
C	-0.72923600	-2.49145900	0.00019500
C	0.72923600	-2.49145900	-0.00019200
C	3.55159400	-2.46212900	-0.00061500
C	1.47982400	-3.68572100	-0.00069000
C	2.86602200	-3.67692500	-0.00090200
C	-2.84675300	-1.26275400	0.00025800
C	-3.55159300	-2.46212900	0.00061500
C	-2.86602200	-3.67692500	0.00090400
C	-1.47982400	-3.68572100	0.00069300
C	-2.84675300	1.26275400	-0.00026800
C	-3.62345700	0.00000000	-0.00001500
C	-1.47982400	3.68572100	-0.00065400
C	-2.86602200	3.67692500	-0.00086800
C	-3.55159400	2.46212900	-0.00061100
H	4.63510600	2.41566200	0.00069600
H	3.41282500	4.61466900	0.00125700
H	0.97218400	4.64266600	0.00096600
H	4.63510500	-2.41566300	-0.00069600
H	0.97218400	-4.64266600	-0.00103400
H	3.41282500	-4.61466900	-0.00131300
H	-4.63510500	-2.41566300	0.00069500
H	-3.41282500	-4.61466900	0.00131600
H	-0.97218400	-4.64266600	0.00104000
H	-0.97218400	4.64266600	-0.00096300
H	-3.41282500	4.61466900	-0.00125500
H	-4.63510600	2.41566200	-0.00069800
O	-4.85363600	0.00000000	-0.00003500
O	4.85363600	0.00000000	0.00002800
H	4.91974432	-0.16784043	1.04456583

ts61_OH₂O

C	-2.98923300	2.68482500	-0.39830400
C	-2.35984000	1.44629400	-0.28206500
C	-0.94585300	1.34955700	-0.18288300
C	-0.29760100	0.05985900	-0.14054200
C	-1.09413500	-1.14272200	-0.21933300
C	-2.51597500	-1.07731900	-0.29219800
C	-2.22594200	3.85236100	-0.40492300
C	-0.84771100	3.78167000	-0.28493900
C	-0.17850700	2.54520700	-0.17186400
C	1.27104400	2.45976700	-0.04704000
C	1.89172900	1.18251600	0.00938200
C	1.09543700	-0.02248500	-0.05776700
C	1.74771900	-1.31217800	-0.04364000
C	0.98317400	-2.50536800	-0.14642800
C	-0.46791800	-2.41807300	-0.25154000
C	-3.27976200	-2.24121000	-0.39062800
C	-1.27409000	-3.56873500	-0.38003600
C	-2.65393600	-3.48562400	-0.45213800
C	3.16179900	-1.40673300	0.06930600
C	3.78993700	-2.64961300	0.08003300
C	3.03697100	-3.81945500	-0.02295600
C	1.65745100	-3.74539500	-0.13354500
C	3.30656300	1.10923700	0.12955900
C	3.99728900	-0.19453200	0.17700300
C	2.08280300	3.61196100	0.02593700
C	3.46047600	3.52206700	0.14916200
C	4.07301600	2.26988700	0.20046300
H	-4.06736500	2.74303300	-0.48625200
H	-2.71310600	4.81647000	-0.50095900
H	-0.28433900	4.70597400	-0.28926800
H	-4.36278500	-2.19547500	-0.40750400
H	-0.81787400	-4.54928800	-0.42399600
H	-3.24970400	-4.38693400	-0.54220100
H	4.86965700	-2.68834600	0.16884800
H	3.52716800	-4.78714200	-0.01451500
H	1.09905200	-4.67008800	-0.20550800
H	1.63369800	4.59649800	-0.00847700
H	4.05815300	4.42568600	0.20531300
H	5.14933600	2.17982600	0.29358000
O	5.23022600	-0.26862500	0.29472300
C	-3.16136200	0.22566700	-0.18748600
O	-4.02773500	0.38527800	1.28998300
O	-4.15254800	-0.81338700	2.04369100
H	-3.45680800	-0.68589200	2.71632700
O	-4.47149900	0.37856200	-0.81886400
H	-4.86245400	0.36369000	0.27903400
H	-4.73144100	-0.39122400	-1.36421800

ts61_1H₂O

C	2.70588500	-2.76841400	-0.70143500
C	2.12571700	-1.51980000	-0.51953200
C	0.72101900	-1.38202000	-0.36980100
C	0.11463500	-0.07177600	-0.26939100
C	0.93401300	1.11062400	-0.43524800
C	2.34055200	1.00089400	-0.61219800

C	1.90121000	-3.91254000	-0.73565800
C	0.53445100	-3.80497200	-0.55195600
C	-0.08587500	-2.55118200	-0.35883300
C	-1.52130800	-2.42420200	-0.13911000
C	-2.09304400	-1.13094400	0.00515100
C	-1.26578700	0.05001900	-0.09782800
C	-1.87846200	1.35786600	-0.03476200
C	-1.09596000	2.52806100	-0.22828200
C	0.33301200	2.39732600	-0.48548100
C	3.10473500	2.12095400	-0.91862600
C	1.14239200	3.51342400	-0.78554400
C	2.49874300	3.37744700	-1.02051000
C	-3.27219600	1.49352300	0.20979700
C	-3.85936300	2.75526800	0.28112700
C	-3.08616200	3.90233100	0.10442400
C	-1.72783200	3.78705200	-0.15037200
C	-3.49128500	-1.01712400	0.23767300
C	-4.13013200	0.30517600	0.38503900
C	-2.36515400	-3.55145200	-0.04874600
C	-3.72641100	-3.42317300	0.18221600
C	-4.28957900	-2.15564300	0.32741600
H	3.77898900	-2.85318700	-0.81620800
H	2.35264700	-4.88683500	-0.89016500
H	-0.06034400	-4.70965700	-0.56389900
H	4.17377400	2.04656900	-1.08624100
H	0.70393900	4.50077600	-0.85359300
H	3.09680100	4.24652500	-1.27232200
H	-4.92368700	2.82558200	0.47496600
H	-3.54318400	4.88437400	0.16562800
H	-1.15061300	4.69424900	-0.27952900
H	-1.95327300	-4.54732800	-0.15387000
H	-4.34908000	-4.30908500	0.24962900
H	-5.35159200	-2.03557500	0.50902200
O	-5.34228700	0.41433800	0.63075400
C	2.98762800	-0.32127800	-0.36922600
O	4.24104700	-0.53289300	-0.83645500
H	4.80206600	0.24585500	-0.69383900
O	3.15196800	-0.19585500	1.32413100
H	3.90112400	0.68196700	1.61502400
O	3.85515200	-1.33888800	1.84844200
O	4.70531900	1.55645800	1.94004600
H	3.11228200	-1.86979300	2.18981100
H	4.26252700	2.41990100	1.86671600
H	4.92536600	1.44769800	2.88169800

ts61_2H₂O

C	-2.94106600	1.92851600	-0.86889700
C	-2.09928900	0.84432300	-0.63005600
C	-0.70243000	1.03140900	-0.44907000
C	0.17996600	-0.10343400	-0.29323400
C	-0.35388200	-1.44403400	-0.39394400
C	-1.74880100	-1.65975300	-0.58162700
C	-2.41417000	3.22033800	-0.92215200
C	-1.06136600	3.42726400	-0.70951200
C	-0.18047900	2.35309700	-0.46484900
C	1.24229200	2.56169800	-0.22729800
C	2.08983300	1.43617700	-0.04267900

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C	1.55083500	0.09590300	-0.10600500
C	2.43995300	-1.03655100	0.01773900
C	1.93816800	-2.36012100	-0.10683400
C	0.51574300	-2.56645100	-0.34764800
C	-2.24541300	-2.94735400	-0.76271400
C	-0.02706900	-3.85612800	-0.53319600
C	-1.37948800	-4.04422800	-0.75055800
C	3.82862900	-0.84552800	0.25701100
C	4.68384600	-1.93859700	0.37685100
C	4.18756900	-3.23668200	0.25814600
C	2.83752200	-3.44037800	0.01837500
C	3.47545900	1.64890100	0.19487700
C	4.39699900	0.51091700	0.37950400
C	1.80660000	3.85341500	-0.16327000
C	3.15916800	4.04328000	0.07515100
C	3.99398700	2.94060100	0.25495000
H	-4.00224300	1.77146700	-1.01179100
H	-3.06714600	4.06360200	-1.11966400
H	-0.68519100	4.44185100	-0.74215700
H	-3.30206800	-3.13293400	-0.92263100
H	0.61687000	-4.72621400	-0.51737700
H	-1.77253500	-5.04354700	-0.90212900
H	5.73702900	-1.76049800	0.56202300
H	4.85415200	-4.08740000	0.35282100
H	2.47923600	-4.45858400	-0.06464800
H	1.18076000	4.72715300	-0.29484800
H	3.56350100	5.04892700	0.12245200
H	5.05414400	3.07015100	0.44086000
O	5.60257400	0.68790500	0.61659200
C	-2.66281900	-0.50624000	-0.48356300
O	-2.89211100	-0.49847800	1.36218300
O	-3.66552300	-1.65941200	1.71270000
H	-2.96705900	-2.26569700	2.01808000
O	-3.92121000	-0.62378500	-0.93574400
H	-3.63869700	0.36172600	1.66932500
O	-4.45824100	1.22213500	2.03799900
H	-4.04832400	2.09070400	1.89232100
H	-5.22009700	1.16080900	1.37682000
O	-6.28149200	0.89520400	0.18347700
H	-6.94998600	0.29119600	0.54183100
H	-5.71127900	0.32591000	-0.36154200
H	-4.25483900	-1.52932000	-0.83039800

ts61_3H₂O

C	1.84222300	3.13698800	0.55106500
C	1.41358400	1.81689500	0.42482100
C	2.39580800	0.72204200	0.34887100
C	0.02853900	1.51737900	0.29721500
C	-0.43118500	0.14727100	0.23152400
C	0.52688700	-0.93189900	0.32311000
C	1.91685600	-0.66199700	0.43874800
C	0.91731800	4.18037900	0.55848300
C	-0.43271400	3.90858100	0.41624400
C	-0.90717200	2.58857800	0.27892600
C	-2.32691300	2.29723200	0.12076100
C	-2.75646100	0.94555300	0.04169700
C	-1.79551300	-0.13246600	0.11845100

C	-2.25740900	-1.50245200	0.08007300
C	-1.33385900	-2.57587300	0.19521100
C	0.08723400	-2.28412100	0.34082400
C	2.83493600	-1.70049500	0.59339600
C	1.04375200	-3.30716200	0.49991900
C	2.39316800	-3.02266100	0.63224600
C	-3.64088000	-1.79688500	-0.06549400
C	-4.08545500	-3.11680300	-0.09811300
C	-3.17617000	-4.16810900	0.01354800
C	-1.82392100	-3.89853200	0.15788300
C	-4.14352100	0.67190500	-0.10885200
C	-4.63867800	-0.71609700	-0.18461300
C	-3.29329300	3.32199300	0.03806400
C	-4.64168700	3.03772000	-0.11356500
C	-5.06747200	1.71179300	-0.18589200
H	2.89540900	3.38524200	0.63832300
H	1.25786100	5.20426000	0.66627700
H	-1.12648600	4.73944500	0.41836300
H	3.89136600	-1.48165500	0.67940200
H	0.73223000	-4.34352600	0.52736500
H	3.10684100	-3.82933300	0.76039300
H	-5.14647500	-3.30785700	-0.21177200
H	-3.52253000	-5.19585000	-0.01300600
H	-1.13988700	-4.73394900	0.23754600
H	-2.99032800	4.36027400	0.08640400
H	-5.36074500	3.84769300	-0.17633800
H	-6.11762500	1.46939000	-0.30279100
O	-5.84533500	-0.96424300	-0.33632300
O	3.63062400	0.90075400	0.84748700
H	3.89579000	1.83458600	0.83803100
O	2.87838300	0.89543300	-1.45937300
O	1.79746000	0.58471800	-2.35089100
H	1.42734200	1.47122700	-2.51082800
H	5.18918900	-0.05048300	1.80196200
O	6.07922100	-0.43790300	1.84053500
H	6.51218200	-0.39335400	0.15601400
O	6.73416800	-0.37408400	-0.80977000
H	5.39329400	-0.61022100	-1.59053300
O	4.53201300	-0.74629400	-2.11965500
H	4.20924300	-1.63125800	-1.88722300
H	3.66984100	0.08644500	-1.74275000
H	6.96715300	0.54977900	-0.98500000
H	5.91606000	-1.37044900	2.04679100

int62

C	3.12808100	-2.71464800	0.03531300
C	2.50412600	-1.44866700	-0.01540200
C	3.28884400	-0.25510000	-0.01142600
C	1.07977400	-1.34766500	-0.04750200
C	0.45030600	-0.06071600	-0.03014700
C	1.25923300	1.12411200	-0.04976300
C	2.69636500	1.03930200	-0.07736300
C	2.35986400	-3.86547500	0.01790100
C	0.97041300	-3.77707000	-0.03099100
C	0.30528900	-2.53793900	-0.05641300
C	-1.14739800	-2.44460700	-0.06718300
C	-1.76149600	-1.16326400	-0.02187100

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C	-0.95608900	0.03339000	-0.00977400
C	-1.59287200	1.32571400	0.02531900
C	-0.80830900	2.50973300	0.00152700
C	0.64206100	2.40424000	-0.08206000
C	3.45983400	2.21978500	-0.23778500
C	1.45228700	3.54507200	-0.22053400
C	2.83636700	3.45163200	-0.32233200
C	-3.00993400	1.43465000	0.08462900
C	-3.61978400	2.68236000	0.14057700
C	-2.84495400	3.84503500	0.13710400
C	-1.46498700	3.75862200	0.06504400
C	-3.18130700	-1.07965400	0.00714200
C	-3.86305700	0.22916900	0.08028500
C	-1.97033700	-3.59081400	-0.11243500
C	-3.35108800	-3.48870100	-0.09519200
C	-3.95780200	-2.23210300	-0.02625900
H	4.20648000	-2.78292000	0.08893800
H	2.83674100	-4.83827700	0.05403300
H	0.40232800	-4.69857600	-0.02943900
H	4.53372800	2.16411700	-0.30591400
H	1.00330000	4.52845600	-0.27391300
H	3.42936100	4.34851200	-0.46020300
H	-4.70141300	2.73513600	0.18803000
H	-3.32227600	4.81759700	0.19041000
H	-0.89279200	4.67734300	0.06949400
H	-1.52828700	-4.57727800	-0.16725400
H	-3.95931800	-4.38612000	-0.13185600
H	-5.03726400	-2.13626800	-0.00222900
O	-5.09772100	0.31164000	0.13132000
O	4.60717400	-0.52452100	-0.00463900
O	5.42704500	0.45984600	0.66259700
H	6.11685700	0.59420700	-0.01677600

ts62

C	0.37006000	-0.21440600	-1.87140400
C	1.56393500	-0.71685400	-1.30599100
C	1.72146900	-2.11001200	-1.06966100
C	2.63756900	0.17507500	-0.97783500
C	3.84467700	-0.33913400	-0.39339500
C	3.97305800	-1.74652300	-0.13424100
C	2.90115500	-2.63573500	-0.46221800
C	0.23823200	1.14708300	-2.11067900
C	1.27654300	2.01926400	-1.79969400
C	2.48576200	1.56309300	-1.23206700
C	3.57642000	2.46919300	-0.90411000
C	4.77290700	1.94626500	-0.33400300
C	4.90379900	0.53727600	-0.07527400
C	6.11588900	0.02084200	0.50879700
C	6.25323300	-1.37028400	0.77756400
C	5.15657100	-2.27416400	0.45065300
C	3.01811200	-4.01548800	-0.20312100
C	5.22842700	-3.65807400	0.69389200
C	4.17436200	-4.51400300	0.37507000
C	7.19339200	0.89445800	0.82711800
C	8.36378300	0.39718600	1.39387900
C	8.49368700	-0.96677800	1.65872900
C	7.45420900	-1.83258500	1.35483500

C	5.83700800	2.84056100	-0.02332300
C	7.09587400	2.34361100	0.56554800
C	3.48794400	3.85905400	-1.13523900
C	4.53391500	4.71332300	-0.82642400
C	5.70959400	4.20382200	-0.27057800
H	-0.41475000	-0.90599500	-2.14650300
H	-0.67422500	1.53491600	-2.55069500
H	1.13989200	3.07258900	-2.00942300
H	2.19585600	-4.67255900	-0.45789200
H	6.11764600	-4.08665200	1.13860900
H	4.26726300	-5.57556000	0.57848600
H	9.16668000	1.08803400	1.62476000
H	9.40563900	-1.35235000	2.10211400
H	7.58164500	-2.88604300	1.57066200
H	2.58815800	4.28140300	-1.56447800
H	4.43722000	5.77693100	-1.01711200
H	6.53730400	4.85914100	-0.02385800
O	8.03366300	3.11272100	0.83034900
O	0.74300900	-2.93918000	-1.43580100
O	-0.19803000	-3.21314800	-0.12213000
H	-1.33841400	-1.75747800	0.09690100
N	-1.74203700	-0.88252500	0.43576900
C	-3.07060900	-0.62835600	0.43452900
H	-1.12088400	-0.28412100	0.96174000
C	-3.57718400	0.54098800	1.08787700
C	-3.97397400	-1.51487600	-0.23457900
C	-4.93579600	0.79020100	1.05305500
C	-2.63441600	1.47333500	1.80182500
C	-5.32519900	-1.22110600	-0.22849400
C	-3.45128600	-2.73919700	-0.93321400
C	-5.85785000	-0.06940400	0.40140800
H	-5.30053700	1.66778400	1.57630600
H	-3.18381500	2.29640400	2.26347800
H	-2.07288700	0.95876200	2.59195600
H	-1.89634000	1.90539300	1.11439200
H	-5.98730600	-1.89165500	-0.76523300
H	-4.26496700	-3.28600200	-1.41453900
H	-2.70940100	-2.48527100	-1.69969000
H	-2.95627600	-3.42091500	-0.22805000
C	-7.28828900	0.22297100	0.37249200
C	-7.78362700	1.53094300	0.59349100
C	-8.24630900	-0.78741200	0.11423500
C	-9.13413100	1.83657100	0.55742600
H	-7.08842200	2.34567400	0.76598500
C	-9.60734100	-0.53607800	0.07549700
H	-7.92017900	-1.81231600	-0.02802700
C	-10.07041200	0.79405300	0.29550800
C	-9.61969300	3.24655500	0.77532300
C	-10.59627800	-1.64244600	-0.18372500
N	-11.40290400	1.07414200	0.22107500
H	-8.78034700	3.92237400	0.95397200
H	-10.17693300	3.62167600	-0.09229800
H	-10.29314500	3.31552700	1.63965700
H	-10.08301500	-2.59533000	-0.33117500
H	-11.29628000	-1.76582500	0.65306100
H	-11.20130300	-1.44382800	-1.07738700
H	-11.74538700	1.96293100	0.55406500

H	-12.07191900	0.31867300	0.20526600
H	-0.73026900	-3.92761400	-0.51920500

int63

C	3.55775200	-2.46329000	-0.00040700
C	2.85894600	-1.26282300	-0.00002100
C	3.62631400	-0.00001600	0.00039500
C	1.43358900	-1.24688700	0.00000800
C	0.72174600	-0.00005400	0.00007300
C	1.43361000	1.24674000	0.00011500
C	2.85898900	1.26276900	0.00024000
C	2.86108500	-3.67250600	-0.00082400
C	1.46976000	-3.67893600	-0.00069900
C	0.73097100	-2.48471100	-0.00014400
C	-0.73106000	-2.48470800	0.00020500
C	-1.43363700	-1.24683900	0.00000400
C	-0.72176700	-0.00004400	-0.00008500
C	-1.43358000	1.24684500	-0.00014500
C	-0.73094900	2.48465600	-0.00004900
C	0.73104100	2.48460600	0.00002500
C	3.55782700	2.46318100	0.00023400
C	1.46979900	3.67882300	-0.00000700
C	2.86109900	3.67238500	0.00010500
C	-2.85893300	1.26285500	-0.00028400
C	-3.55770000	2.46333800	-0.00028400
C	-2.86098600	3.67252600	-0.00014000
C	-1.46965500	3.67891500	-0.00001700
C	-2.85903400	-1.26274300	0.00002000
C	-3.62627900	0.00008800	-0.00044500
C	-1.46990200	-3.67891400	0.00080300
C	-2.86121200	-3.67239800	0.00091800
C	-3.55785700	-2.46314400	0.00044300
H	4.64116300	-2.44286500	-0.00041800
H	3.40182400	-4.61254300	-0.00122900
H	0.96588800	-4.63608700	-0.00112700
H	4.64126800	2.44285500	0.00034300
H	0.96587200	4.63596200	-0.00014200
H	3.40182300	4.61243700	0.00009100
H	-4.64112000	2.44295400	-0.00040400
H	-3.40168200	4.61259200	-0.00012500
H	-0.96572000	4.63604300	0.00012500
H	-0.96610600	-4.63610300	0.00127300
H	-3.40201600	-4.61240300	0.00135600
H	-4.64127800	-2.44272900	0.00044100
O	-4.86180700	0.00013500	-0.00014200
O	4.86183400	0.00006500	0.00009200

Fig. 7 (7, ts71_0H₂O, ts71_1H₂O, ts71_2H₂O, ts71_3H₂O, int71, ts72, int72, ts73, int73, .)**7**

C	3.58786900	-2.45050800	-0.11425100
C	2.89111400	-1.20821700	-0.03409700
C	3.57374100	0.02785400	-0.00434800
C	1.44771600	-1.21772400	-0.02609000
C	0.72837800	0.00564400	-0.01342300
C	1.42848500	1.24033600	-0.00315300

C	2.87135900	1.25353400	0.00886500
C	2.89812200	-3.63551600	-0.15859700
C	1.49195400	-3.65062700	-0.11840200
C	0.75385700	-2.47601700	-0.04489100
C	-0.71514500	-2.48768800	0.00490200
C	-1.42848600	-1.24036300	-0.00318000
C	-0.72837500	-0.00567200	-0.01343400
C	-1.44771300	1.21769500	-0.02609900
C	-0.75385900	2.47598900	-0.04486900
C	0.71514300	2.48766100	0.00493900
C	3.54951400	2.50690700	0.07016800
C	1.43500500	3.67429800	0.06631400
C	2.84132900	3.68145400	0.10270700
C	-2.89110900	1.20818700	-0.03413300
C	-3.58787100	2.45047100	-0.11424800
C	-2.89812900	3.63548300	-0.15855600
C	-1.49196000	3.65060000	-0.11835600
C	-2.87136100	-1.25355900	0.00882200
C	-3.57374000	-0.02787500	-0.00440900
C	-1.43500800	-3.67432600	0.06625000
C	-2.84133200	-3.68147900	0.10263600
C	-3.54951600	-2.50693300	0.07010800
H	4.66981800	-2.45899200	-0.14429700
H	3.43730200	-4.57498700	-0.22730500
H	0.99332100	-4.61087400	-0.15779700
H	4.63138500	2.53048900	0.09418100
H	0.92154800	4.62703500	0.09662000
H	3.36596000	4.63004600	0.15764200
H	-4.66982300	2.45894400	-0.14429300
H	-3.43731700	4.57495200	-0.22724000
H	-0.99333200	4.61085000	-0.15771800
H	-0.92155000	-4.62706300	0.09653900
H	-3.36596700	-4.63007000	0.15755800
H	-4.63138700	-2.53051700	0.09411500
C	-5.07012700	-0.05876300	-0.02871500
C	5.07013600	0.05876700	-0.02862200
O	-5.73622000	-0.61283500	-0.88937200
O	5.73624100	0.61278900	-0.88929800
O	5.63063100	-0.57886900	1.01823900
H	6.59966600	-0.53545600	0.90956800
O	-5.63063800	0.57918100	1.01795500
H	-6.59966800	0.53584100	0.90921400

ts71_OH₂O

C	3.86282600	-2.64022100	-0.02821100
C	3.25362300	-1.35101000	-0.00238700
C	4.02033700	-0.17234000	0.10580300
C	1.81456100	-1.25380500	-0.04989300
C	1.18417900	0.01782600	-0.03695000
C	1.97381200	1.19366900	0.05100200
C	3.40950200	1.09854700	0.15561900
C	3.09249600	-3.77140800	-0.12179500
C	1.68957800	-3.68056600	-0.16948200
C	1.03495600	-2.45534900	-0.11482900
C	-0.43026100	-2.36002000	-0.12258100
C	-1.05704900	-1.06570300	-0.15736500
C	-0.26733500	0.11576700	-0.11526700

C	-0.89471900	1.39034400	-0.14898400
C	-0.09901000	2.58916000	-0.11083800
C	1.35810200	2.48830300	0.04420200
C	4.17817700	2.29374800	0.27094100
C	2.16032400	3.61532700	0.18281900
C	3.55912800	3.51783300	0.29372800
C	-2.33394400	1.49432000	-0.25248800
C	-2.90210300	2.79389700	-0.40319200
C	-2.11392000	3.91772900	-0.39619900
C	-0.72350900	3.82270000	-0.23788700
C	-2.49565000	-0.97535800	-0.21083100
C	-3.12011100	0.30508100	-0.25967900
C	-1.22740000	-3.49686600	-0.08215600
C	-2.62670700	-3.40263200	-0.08870400
C	-3.25206700	-2.18107800	-0.15141500
H	4.94119000	-2.72685400	0.01680500
H	3.56285500	-4.74882300	-0.15510900
H	1.12609900	-4.60143500	-0.24925800
H	5.25608900	2.23236800	0.35037700
H	1.71916500	4.60347300	0.20975500
H	4.14805200	4.42388500	0.39368000
H	-3.96752900	2.89935300	-0.53062900
H	-2.57013800	4.89507600	-0.51954600
H	-0.14459500	4.73742600	-0.23795300
H	-0.78144300	-4.48162800	-0.02574900
H	-3.22076500	-4.30981900	-0.03780900
H	-4.33006000	-2.14304000	-0.14595400
C	-4.58954100	0.38640600	-0.35044500
C	5.51352200	-0.25880800	0.20962300
O	6.15822400	0.10997400	1.17762800
O	6.08577100	-0.77794100	-0.89285500
H	7.04881300	-0.82646100	-0.73981700
O	-5.22774400	-0.44077100	1.47628700
O	-6.29494500	-1.38975800	1.26655100
H	-6.98397600	-0.86061400	0.82759200
O	-5.15895600	-0.36521100	-1.27992500
H	-6.11927400	-0.19105200	-1.28084300
O	-5.30632800	1.40776000	0.11482600
H	-5.56343800	0.89276200	1.01143300

ts71_1H₂O

C	4.19673200	-2.57728500	-0.00936700
C	3.55723800	-1.30231900	-0.01474500
C	4.29393200	-0.09693200	-0.04305900
C	2.11654200	-1.24756500	0.05194600
C	1.45084600	0.00583100	0.05815700
C	2.20536700	1.20813300	0.05651600
C	3.64715100	1.15892700	0.01171400
C	3.45379600	-3.73055700	0.02906900
C	2.04898600	-3.68118600	0.08231000
C	1.36640000	-2.47080000	0.11288600
C	-0.10018600	-2.41134600	0.19882000
C	-0.76275700	-1.13840400	0.09779800
C	-0.00364200	0.05766900	0.05586900
C	-0.67393700	1.30711700	0.07146200
C	0.07656600	2.53110600	0.15106300
C	1.54480400	2.48333800	0.09488400

C	4.37639900	2.38419200	-0.02034400
C	2.31366300	3.64054000	0.05977200
C	3.71799900	3.58813800	0.00151800
C	-2.11596100	1.35683200	0.00504000
C	-2.75169600	2.62731700	0.16277000
C	-2.01115900	3.77215000	0.31938600
C	-0.60665300	3.73223200	0.28619800
C	-2.20866900	-1.08647500	0.05220300
C	-2.85978000	0.15645700	-0.15781200
C	-0.86259200	-3.55565200	0.38898700
C	-2.26477200	-3.49196400	0.46080700
C	-2.92347800	-2.30224100	0.28001200
H	5.27724300	-2.63638900	-0.04057400
H	3.95092400	-4.69551800	0.02206800
H	1.50728600	-4.61869200	0.09954500
H	5.45768400	2.36329100	-0.06307800
H	1.84112200	4.61467500	0.06489000
H	4.28246000	4.51491500	-0.02929400
H	-3.82851000	2.67815800	0.19174500
H	-2.51204800	4.72321200	0.47212400
H	-0.06640500	4.66507300	0.38893000
H	-0.38698200	-4.52019700	0.51533200
H	-2.82878900	-4.39610500	0.66777700
H	-3.99683800	-2.28353100	0.37486700
C	-4.32229700	0.28611500	-0.62321500
C	5.78764000	-0.13313200	-0.09705000
O	6.52578400	0.36374400	0.74025100
O	6.26436200	-0.76097300	-1.19200900
H	7.23868000	-0.76123900	-1.13320000
O	-4.76772400	-0.97908900	-1.29454000
H	-5.13831900	-0.63543400	-2.12705000
O	-4.65634200	1.28939900	-1.33964300
O	-5.14826900	0.29842100	0.74888200
H	-6.18745900	-0.99857500	0.77212400
O	-6.21346600	1.28056400	0.57060000
O	-6.57510500	-1.72998800	0.18821000
H	-5.90034900	1.63603800	-0.31696800
H	-5.85860400	-1.58042000	-0.59447500
H	-6.40391200	-2.58730500	0.61964700

ts71_2H₂O

C	4.30277800	-2.47508300	0.35495700
C	3.63294800	-1.23106900	0.15801000
C	4.31657300	0.00380400	0.22518900
C	2.20555900	-1.23709100	-0.05842700
C	1.49899700	-0.01407000	-0.19584500
C	2.20151100	1.21759700	-0.13257500
C	3.62609300	1.23077700	0.10051900
C	3.60395600	-3.65585600	0.33016400
C	2.21706800	-3.66704700	0.09551700
C	1.50822000	-2.49094100	-0.11801900
C	0.06287800	-2.49687200	-0.38351500
C	-0.65171200	-1.25023000	-0.45033000
C	0.05270300	-0.02173200	-0.37707800
C	-0.65300300	1.19695100	-0.53922300
C	0.06067700	2.44543500	-0.57042900
C	1.50366700	2.46200200	-0.29334000

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C	4.29910300	2.48611700	0.17282500
C	2.21086600	3.65227000	-0.17216900
C	3.59956200	3.66067900	0.05097500
C	-2.09176400	1.19243800	-0.69773100
C	-2.73175500	2.43368700	-1.00889600
C	-2.01191800	3.59642000	-1.11823200
C	-0.62747200	3.61066500	-0.87947000
C	-2.09030900	-1.25775500	-0.60503500
C	-2.80958900	-0.03088800	-0.60806700
C	-0.62860700	-3.68362500	-0.58277100
C	-2.01765900	-3.69058800	-0.79552600
C	-2.73588000	-2.52205000	-0.78309200
H	5.36974600	-2.48734600	0.53740400
H	4.12113000	-4.59552500	0.49768100
H	1.70703300	-4.62220200	0.10010500
H	5.36812300	2.51204500	0.33898000
H	1.70014800	4.60434400	-0.24472000
H	4.11913600	4.61086300	0.12636600
H	-3.79359600	2.43818000	-1.19520100
H	-2.51410900	4.51891800	-1.39317100
H	-0.10123500	4.55325400	-0.96565000
H	-0.10281000	-4.63036500	-0.59390500
H	-2.52449700	-4.63494700	-0.96865700
H	-3.80025700	-2.54831900	-0.94971900
C	-4.34414800	-0.01247100	-0.50252400
C	5.79162400	0.03103800	0.46826400
O	6.33436100	0.59433500	1.40691500
O	6.49515800	-0.62217600	-0.47999200
H	7.43831700	-0.57748600	-0.23361000
O	-4.49239700	-1.11755300	0.84341400
O	-5.91060800	-1.28281900	1.08512700
H	-6.14037300	-1.94025100	0.40517200
O	-4.92561700	-0.73354800	-1.54985300
H	-5.86167000	-0.46968100	-1.54238600
O	-4.98876200	1.04359700	-0.17381300
H	-4.03180500	-0.48052000	2.10188600
O	-3.75113800	0.07361500	2.94418700
H	-2.78918800	-0.02527500	3.03545700
H	-3.97229000	1.14604100	2.58102000
O	-4.29895600	2.21772000	1.97533600
H	-5.11849500	2.54348200	2.38019700
H	-4.57542200	1.80434400	1.06743300

ts71_3H₂O

C	-1.45214700	-3.40514100	-0.13509300
C	-1.12214900	-2.02813700	-0.20875800
C	-2.06804700	-1.00182700	-0.35090300
C	0.27737500	-1.62592300	-0.13228600
C	0.63509100	-0.24942400	-0.19003400
C	-0.34705600	0.74596800	-0.32952000
C	-1.66978600	0.32327800	-0.41562600
C	-0.46160500	-4.35215200	0.00241300
C	0.89684100	-3.97746800	0.07572900
C	1.29352500	-2.64503800	0.01358400
C	2.70902800	-2.22691000	0.09591000
C	2.97748000	-0.82546500	0.03595600
C	1.99342700	0.16996900	-0.09928400

C	2.35257200	1.54575600	-0.14535100
C	1.33617600	2.56770400	-0.27779500
C	-0.07936100	2.15019500	-0.36255800
C	-2.77029300	1.18596800	-0.53914100
C	-1.18987000	3.01046100	-0.45871500
C	-2.53235500	2.55234700	-0.53536000
C	3.75167300	1.94666500	-0.05693000
C	4.08586800	3.32432600	-0.10607900
C	3.09601900	4.27227700	-0.23606100
C	1.73656800	3.89952800	-0.32132900
C	4.30028600	-0.40249000	0.11730500
C	4.70300000	0.92433400	0.07470800
C	3.81665100	-3.08831300	0.23194600
C	5.15468200	-2.62406800	0.31138700
C	5.39726100	-1.26138700	0.25350600
H	-2.49426200	-3.69462600	-0.18991200
H	-0.72132600	-5.40236400	0.05695100
H	1.64070000	-4.75644900	0.18557800
H	-1.02895900	4.08121700	-0.47077900
H	-3.34547700	3.26028300	-0.58474400
H	5.12972600	3.60516300	-0.03988100
H	3.35559100	5.32330700	-0.27523600
H	0.99411900	4.68073500	-0.42621300
H	3.65503100	-4.15759600	0.27945700
H	5.96262800	-3.33820000	0.41586700
C	-3.95893500	0.34036800	-0.51764800
O	-3.46342800	-1.06284700	-0.43689800
O	-5.18273800	0.49473200	-0.77954800
C	6.60173700	-0.40286500	0.30132500
O	7.79110100	-0.59719100	0.40767400
O	6.08552300	1.00217800	0.18068800
O	-4.62097000	0.89005400	1.41378600
O	-4.40277600	2.36765400	1.55729700
H	-3.71428100	2.35622900	2.28407400
H	-5.66977000	0.89404600	0.47817200
O	-6.94923700	1.09815900	0.72676000
H	-7.44533200	0.13374500	0.73224600
H	-6.93953600	1.47014400	1.64505100
O	-7.92476300	-1.19959800	0.62302200
H	-7.22794700	-1.65625700	-0.03459500
H	-8.81274800	-1.22876900	0.18400600
O	-6.18975900	-1.91107000	-1.05505800
H	-5.36585400	-2.33356300	-0.69341900
H	-5.89788000	-0.94882500	-1.22018600

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C	-3.97308200	2.52613400	-0.13889500
C	-3.31498700	1.26335000	-0.05246700
C	-4.03176000	0.04663300	-0.07281700
C	-1.87308000	1.23214100	0.00771600
C	-1.18676400	-0.00988700	0.03030900
C	-1.92210100	-1.22331400	0.02170100
C	-3.36362900	-1.19797100	-0.04415000
C	-3.24880200	3.69130400	-0.14118300
C	-1.84518700	3.66590900	-0.05015800
C	-1.14428000	2.46900200	0.03479900
C	0.32151000	2.43659100	0.13388100

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C	1.00612700	1.17291800	0.07656100
C	0.27022000	-0.03929000	0.04690000
C	0.96032900	-1.27773000	0.08661500
C	0.22452800	-2.51197700	0.16207500
C	-1.24308700	-2.48691600	0.08007200
C	-4.07558800	-2.43354600	-0.04680000
C	-1.99430900	-3.65583700	0.05161100
C	-3.39935500	-3.62674400	-0.00588400
C	2.40871600	-1.30883100	0.06429200
C	3.05113600	-2.57216200	0.25515000
C	2.32035800	-3.72473500	0.39451600
C	0.91786300	-3.70363500	0.32256600
C	2.45055900	1.14514200	0.05701100
C	3.12791200	-0.09498600	-0.09088700
C	1.06307000	3.59948100	0.29065900
C	2.46586000	3.56430800	0.36401000
C	3.14703500	2.38088600	0.23212500
H	-5.05270000	2.56539600	-0.20784400
H	-3.75850000	4.64660300	-0.21734700
H	-1.31839800	4.61185600	-0.06129900
H	-5.15710400	-2.42949200	-0.08699300
H	-1.50796400	-4.62279700	0.07348300
H	-3.94940000	-4.56247400	-0.01658000
H	4.12579200	-2.61312600	0.32340300
H	2.82966000	-4.66794200	0.56665300
H	0.38719800	-4.64238100	0.41844100
H	0.57015100	4.55920500	0.38094000
H	3.01308700	4.48747900	0.52760300
H	4.22385700	2.37896700	0.29531200
C	4.63093100	-0.07995200	-0.43525600
C	-5.52562200	0.05670900	-0.16039000
O	-6.17155400	-0.46715700	-1.05486300
O	-6.11141200	0.69293400	0.87410300
H	-7.07620600	0.67568700	0.72788600
O	5.27805700	0.13997100	0.81594900
O	6.70779500	0.33744100	0.58160200
H	6.75704000	1.31069500	0.58034900
O	4.87705900	0.94586200	-1.35675500
H	5.81400100	0.85939700	-1.60180700
O	5.16980000	-1.26733500	-0.95136100
H	4.75437300	-1.42877600	-1.81368800

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C	-4.22548600	-2.56775400	0.15928000
C	-3.58346300	-1.29631100	0.09367200
C	-4.31153500	-0.09418100	0.21120100
C	-2.14880300	-1.24092000	-0.05023000
C	-1.48502700	0.01228600	-0.08589300
C	-2.23688800	1.21163800	0.00942000
C	-3.66699600	1.16027900	0.18812400
C	-3.49013400	-3.72235500	0.06907100
C	-2.09307500	-3.67178500	-0.08862000
C	-1.40756500	-2.46393600	-0.15249800
C	0.05279600	-2.40876700	-0.30249500
C	0.71959300	-1.13370900	-0.28441900
C	-0.03460100	0.06780500	-0.20148800
C	0.62504900	1.32361800	-0.27746000

C	-0.13857600	2.54228700	-0.28874700
C	-1.58771900	2.48711300	-0.06213100
C	-4.39508900	2.37998700	0.31286200
C	-2.34711600	3.64025000	0.09864300
C	-3.74137900	3.58591000	0.28005200
C	2.06587700	1.38695400	-0.37337600
C	2.66244600	2.65728200	-0.63211500
C	1.89692200	3.79423200	-0.72382200
C	0.50865400	3.74717500	-0.52853900
C	2.16154400	-1.08299200	-0.34971500
C	2.81735700	0.18018600	-0.26820900
C	0.80778500	-3.56361800	-0.46020500
C	2.20447900	-3.50663600	-0.57644800
C	2.87156200	-2.30821400	-0.50818500
H	-5.29995800	-2.62208200	0.28267400
H	-3.98354600	-4.68728300	0.12407100
H	-1.55807000	-4.61103300	-0.14900400
H	-5.46881400	2.35213800	0.44794300
H	-1.87260500	4.61357100	0.09413100
H	-4.29846800	4.51028800	0.39306700
H	3.72523800	2.72853000	-0.80874200
H	2.37070600	4.74273300	-0.95639700
H	-0.05301100	4.67006200	-0.59839500
H	0.33044600	-4.53392900	-0.50672700
H	2.76356700	-4.42549400	-0.72274000
H	3.94519400	-2.29773500	-0.60518000
C	4.29987000	0.24310100	-0.06372100
C	-5.79851700	-0.13689800	0.40188700
O	-6.37567300	0.27566400	1.39423100
O	-6.44444500	-0.66763600	-0.65270400
H	-7.39899800	-0.68039600	-0.44818000
O	4.96671400	-0.28423000	-1.12348900
O	6.40314300	-0.33748800	-0.87775600
H	6.68751400	0.52780100	-1.22935400
O	4.63080600	-0.96310500	1.26197800
H	3.98706800	-0.72747300	1.95282500
O	4.90168200	1.33378500	0.42144600
H	4.39987200	1.70453100	1.16807400
O	6.92041200	-0.37072800	2.24001600
H	7.09356300	0.56090500	2.01918200
H	5.75504400	-0.64909300	1.74830500
H	6.84235800	-0.39831700	3.20930600

int72,

C	-3.86835600	2.40636700	-0.04907900
C	-3.14902800	1.17555800	0.00450600
C	-3.81016100	-0.07134000	0.04667000
C	-1.70665000	1.20813200	-0.02754500
C	-0.96874700	-0.00400100	-0.03729800
C	-1.64775200	-1.25013600	-0.01323600
C	-3.08921400	-1.28579700	0.03660900
C	-3.19972500	3.60261900	-0.11129000
C	-1.79316600	3.64006900	-0.11341700
C	-1.03426900	2.47775400	-0.06197200
C	0.43491100	2.51351100	-0.05007400
C	1.16567500	1.27741500	-0.07926700
C	0.48640100	0.03054200	-0.07626200

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C	1.22376800	-1.18187600	-0.10904900
C	0.55190800	-2.45185000	-0.11230800
C	-0.91531100	-2.48638600	-0.02908500
C	-3.74707300	-2.54935600	0.10828200
C	-1.61591200	-3.68402600	0.04137100
C	-3.02073200	-3.71315200	0.11393800
C	2.66522400	-1.14929400	-0.15263900
C	3.38554200	-2.37628800	-0.24084600
C	2.71544400	-3.57323900	-0.26885500
C	1.31028800	-3.61287200	-0.19971800
C	2.60671900	1.31404900	-0.10133000
C	3.32278300	0.09866300	-0.13364000
C	1.13980600	3.71030300	-0.00247200
C	2.54668600	3.73830400	-0.00657900
C	3.27100500	2.57384700	-0.06021400
H	-4.95079800	2.39715300	-0.04559000
H	-3.75575700	4.53338100	-0.16064800
H	-1.31101300	4.60805300	-0.16718800
H	-4.82765500	-2.58909600	0.16023500
H	-1.08785000	-4.62923700	0.05028000
H	-3.52915000	-4.67006200	0.17552500
H	4.46772700	-2.36494100	-0.29518700
H	3.26885100	-4.50373000	-0.34530100
H	0.82900000	-4.58237200	-0.22560400
H	0.61401300	4.65552200	0.04648000
H	3.05837800	4.69459500	0.03363200
H	4.35381100	2.61113800	-0.06944700
C	4.81627700	0.15386700	-0.19532000
C	-5.30661300	-0.12516600	0.05945600
O	5.49630800	0.57488400	-1.10646700
O	-5.98505600	-0.67173600	-0.79587200
O	-5.84823200	0.48326800	1.13276100
H	-6.81922300	0.42781600	1.04910900
O	5.32331400	-0.33479500	0.96982100
O	6.77864400	-0.35854500	0.90885900
H	6.95147600	-0.57014900	1.84485600

ts73

C	-7.78845400	0.66919000	0.66737500
C	-6.46424700	1.06118100	0.32076000
C	-6.17075200	2.38017600	-0.08179100
C	-5.39627600	0.09901900	0.40990900
C	-4.06700700	0.48247600	0.08180400
C	-3.79007800	1.81738400	-0.32321200
C	-4.85655000	2.78202200	-0.39794700
C	-8.04812900	-0.61847700	1.07085300
C	-7.01109100	-1.56176900	1.14859100
C	-5.69262500	-1.23525600	0.83115900
C	-4.60931200	-2.21673000	0.92022700
C	-3.27635400	-1.81663000	0.58476600
C	-2.99796200	-0.48083400	0.16724100
C	-1.66510500	-0.09392500	-0.16287800
C	-1.37220000	1.24428100	-0.57966000
C	-2.46021800	2.22105000	-0.66001300
C	-4.56797300	4.11328000	-0.81237800
C	-2.23901000	3.53971900	-1.05743800
C	-3.28228000	4.47608900	-1.13450600

C	-0.59745900	-1.05063900	-0.07526400
C	0.71952100	-0.65668500	-0.40155300
C	0.97948900	0.63766000	-0.80637800
C	-0.05235900	1.57807800	-0.89386500
C	-2.21179300	-2.77646000	0.67746900
C	-0.88606600	-2.37290800	0.36053900
C	-4.83457900	-3.53511800	1.32505400
C	-3.79003400	-4.46160900	1.41111100
C	-2.49631800	-4.09537100	1.09695400
H	-8.59706700	1.38758100	0.60932800
H	-9.05822600	-0.91444800	1.33278200
H	-7.26444700	-2.56417400	1.46917500
H	-5.36511500	4.84417000	-0.87140000
H	-1.24279800	3.87269500	-1.31932600
H	-3.06497100	5.49057600	-1.45093200
H	1.53157700	-1.37207600	-0.33321600
H	1.99437400	0.93187500	-1.05275700
H	0.20052900	2.58169000	-1.21031700
H	-5.83101700	-3.86804100	1.58541300
H	-4.00290900	-5.47590100	1.73241200
H	-1.69498800	-4.82246600	1.17338200
C	0.21541900	-3.37309300	0.43125400
C	-7.27048900	3.40498800	-0.13203800
O	0.93680100	-3.67404600	1.37502600
O	-7.33894600	4.35589700	0.62561100
O	-8.16021700	3.16280100	-1.10646700
H	-8.85020600	3.85374500	-1.07043600
O	0.22188500	-3.86617200	-0.77631200
O	1.60391800	-5.15557800	-0.89484000
H	1.81856200	-5.05004300	0.05105800
H	2.80779700	-3.82293300	-1.97881000
N	3.39407400	-3.17531100	-2.50651300
C	4.09523200	-2.18733100	-1.80955000
H	2.87555500	-2.81562900	-3.29762300
C	4.24716600	-0.89572000	-2.37500000
C	4.73564700	-2.48016900	-0.58091200
C	5.01203800	0.06219300	-1.70673500
C	3.57103700	-0.54898900	-3.67991000
C	5.49240300	-1.49013700	0.04990300
C	4.62024400	-3.85118500	0.03588100
C	5.65188700	-0.20059000	-0.48367900
H	5.08963500	1.05169900	-2.14956000
H	3.76919600	0.48978600	-3.95550700
H	3.91998700	-1.18251100	-4.50575300
H	2.48177900	-0.67536700	-3.62132300
H	5.99694200	-1.74978300	0.97695700
H	5.34201600	-3.97471300	0.84783500
H	3.62171000	-4.02245600	0.45282000
H	4.79451100	-4.64301500	-0.70200800
C	6.46135000	0.83395800	0.20730800
C	7.16475500	1.81671100	-0.50991300
C	6.55989500	0.87542200	1.60841700
C	7.92705800	2.80299600	0.11825100
H	7.13863600	1.80690900	-1.59621500
C	7.31425400	1.83953500	2.27945700
H	6.01382700	0.14889300	2.20427600
C	8.00521200	2.81969100	1.53010500

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C	8.67573100	3.82971800	-0.69513400
C	7.38861500	1.84394500	3.78641100
N	8.81481200	3.76010600	2.17707700
H	8.52480000	3.66475000	-1.76487800
H	8.34493700	4.85253300	-0.46892000
H	9.75485300	3.79889400	-0.49813200
H	6.79784200	1.02716000	4.20842000
H	8.42044500	1.73140700	4.14293200
H	7.00985700	2.78213300	4.21427600
H	8.55373100	3.94955000	3.13700700
H	8.94552400	4.62388000	1.66469100

int73,

C	3.53941200	-2.45674800	-0.12427800
C	2.84599000	-1.22065000	-0.04649700
C	3.53400700	0.01728700	-0.01307400
C	1.40687900	-1.22676400	-0.03468000
C	0.68955100	0.00654600	-0.00962100
C	1.39762700	1.24546100	0.00820800
C	2.83641500	1.25052300	0.01057200
C	2.84461600	-3.64946200	-0.16977800
C	1.44850300	-3.66112700	-0.13164800
C	0.70875500	-2.47158800	-0.05814400
C	-0.75006300	-2.47458000	-0.01189100
C	-1.45182200	-1.23424600	0.00204500
C	-0.74166900	0.00102600	-0.00369600
C	-1.46135900	1.23077000	-0.00394600
C	-0.76905000	2.47655600	-0.00023400
C	0.69016400	2.48503500	0.03154100
C	3.52156800	2.49211200	0.06760500
C	1.42147700	3.68057800	0.09035300
C	2.81804400	3.67981600	0.11117400
C	-2.89756400	1.22104000	-0.01759800
C	-3.60131900	2.44924200	-0.04849800
C	-2.91594200	3.64939500	-0.06002800
C	-1.51904900	3.66184600	-0.03508900
C	-2.88782000	-1.23567600	0.03056900
C	-3.59983100	-0.01007400	0.01010700
C	-1.49048200	-3.66579500	0.02683200
C	-2.88702400	-3.66418400	0.06779400
C	-3.58172000	-2.46933100	0.06718900
H	4.62163100	-2.46969900	-0.14934300
H	3.38503400	-4.58766700	-0.23547300
H	0.94413100	-4.61796700	-0.17004800
H	4.60389600	2.51147100	0.07768600
H	0.91033000	4.63379500	0.12930400
H	3.35193600	4.62270600	0.16169200
H	-4.68487000	2.44357800	-0.07527100
H	-3.45901400	4.58761500	-0.09011500
H	-1.01959500	4.62219400	-0.05185700
H	-0.98343100	-4.62230000	0.03432200
H	-3.42247700	-4.60664400	0.10159400
H	-4.66492000	-2.47207400	0.10659300
C	-5.12387400	-0.01619600	0.01542200
C	5.03522000	0.03975100	-0.04763800
O	-5.67219700	0.13621900	-1.10530100
O	5.68464200	0.54777400	-0.94518600

O	5.58940200	-0.54994100	1.02384600
H	6.56013300	-0.51690000	0.92163600
O	-5.66442400	-0.17298800	1.13924700

Fig. 8 (8, ts81_0H₂O, ts81_1H₂O, ts81_2H₂O, ts81_3H₂O,, int81, ts82, int82, TMB, OXTMB)**8**

C	2.76417300	3.37532500	-0.00005600
C	2.43788400	1.99353500	-0.00002500
C	3.37982600	0.95311000	0.00000100
C	1.03712300	1.58809600	0.00000000
C	0.67972500	0.21064300	0.00002100
C	1.66264400	-0.79331600	0.00002600
C	2.98926600	-0.37172200	0.00003500
C	1.76346100	4.32132800	-0.00006900
C	0.40385200	3.94433800	-0.00005000
C	0.01316000	2.60834800	-0.00001000
C	-1.40094300	2.19378400	0.00001700
C	-1.66264400	0.79331600	0.00003700
C	-0.67972500	-0.21064300	0.00003100
C	-1.03712300	-1.58809600	0.00002000
C	-0.01315900	-2.60834800	0.00000000
C	1.40094300	-2.19378400	0.00002300
C	4.09853800	-1.22352100	0.00005700
C	2.52091100	-3.05420000	-0.00000900
C	3.85887700	-2.59381200	0.00000700
C	-2.43788400	-1.99353500	-0.00000300
C	-2.76417300	-3.37532500	-0.00006000
C	-1.76346000	-4.32132800	-0.00008000
C	-0.40385100	-3.94433800	-0.00005100
C	-2.98926700	0.37172200	0.00007100
C	-3.37982700	-0.95311000	0.00003800
C	-2.52091000	3.05420100	-0.00002500
C	-3.85887600	2.59381300	0.00000100
C	-4.09853800	1.22352300	0.00010200
H	3.80812800	3.67031200	-0.00007300
H	2.01706300	5.37628300	-0.00009200
H	-0.34631300	4.72724900	-0.00006000
H	2.36787100	-4.12745400	-0.00006100
H	4.66905400	-3.31575700	-0.00001800
H	-3.80812700	-3.67031300	-0.00008400
H	-2.01706200	-5.37628300	-0.00011800
H	0.34631400	-4.72724900	-0.00007300
H	-2.36786900	4.12745500	-0.00007400
H	-4.66905300	3.31575800	-0.00000100
C	5.26398200	-0.33162800	0.00012100
O	4.76978900	1.00713200	0.00001100
O	6.46172200	-0.52658400	-0.00012400
C	-5.26398200	0.33163000	0.00025500
O	-6.46172500	0.52658300	-0.00011000
O	-4.76978900	-1.00713300	-0.00001300

int81

C	2.28377500	3.36526000	-0.12768700
C	1.95229800	1.98642000	-0.11289100
C	2.90544300	0.95141700	-0.13426500
C	0.55427800	1.58112600	-0.07350600

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C	0.19675000	0.20582300	-0.05926300
C	1.17911200	-0.79789900	-0.07997500
C	2.50916000	-0.38103800	-0.11282500
C	1.28721000	4.31694700	-0.10451100
C	-0.07048900	3.93997900	-0.06549700
C	-0.46637200	2.60402300	-0.05002100
C	-1.87993100	2.19556200	-0.01148700
C	-2.14467800	0.79693900	-0.00059500
C	-1.16414200	-0.21124000	-0.02341800
C	-1.52886300	-1.58957300	-0.01025000
C	-0.50834800	-2.61398500	-0.03356500
C	0.91014700	-2.19900100	-0.06968000
C	3.60404300	-1.24388400	-0.13857000
C	2.02010600	-3.05877300	-0.09461100
C	3.36848500	-2.60314000	-0.12758800
C	-2.93279100	-1.98836900	0.02716900
C	-3.26205200	-3.36947400	0.03868300
C	-2.26311300	-4.31704500	0.01574400
C	-0.90139100	-3.94791500	-0.02031000
C	-3.47412600	0.37835600	0.03542300
C	-3.86820100	-0.94144600	0.04946100
C	-2.99746400	3.06350000	0.01485400
C	-4.33354400	2.60780700	0.05238200
C	-4.58149300	1.23681100	0.06305500
H	3.32872700	3.65597000	-0.15737000
H	1.54292500	5.37116900	-0.11554000
H	-0.81973600	4.72385200	-0.04742100
H	1.86481300	-4.13207100	-0.08879300
H	4.17452400	-3.32880400	-0.14222900
H	-4.30627600	-3.66251900	0.06629800
H	-2.52099600	-5.37145200	0.02505200
H	-0.15469100	-4.73398900	-0.03761400
H	-2.83905500	4.13592400	0.00733400
H	-5.14085500	3.33314600	0.07191900
C	4.82674200	-0.35312500	-0.15528900
O	4.26798300	1.04367100	-0.18627400
O	5.64676800	-0.52810000	-1.23586000
C	-5.74762500	0.35391500	0.09856300
O	-6.94826600	0.55653300	0.13339400
O	-5.26351700	-0.98396400	0.08838200
H	6.46290900	-0.02334200	-1.05771600
O	5.49026300	-0.50320900	1.08054700
O	6.70544600	0.29875300	1.03984800
H	6.38075500	1.15478900	1.37861300

int82

C	2.25866500	3.57852900	0.03890900
C	2.01117500	2.20594800	0.03497800
C	3.15756800	1.27878700	0.05266400
C	0.67757000	1.71207200	0.02031800
C	0.44788200	0.28932800	0.01930200
C	1.53824800	-0.64436700	0.02293700
C	2.87834700	-0.16992000	0.02318300
C	1.20101900	4.48893500	0.02639100
C	-0.10856600	4.02882400	0.01235700
C	-0.40621600	2.65171500	0.00981800
C	-1.77246800	2.15366400	-0.00150100

C	-1.93076700	0.75186900	0.00010600
C	-0.86756600	-0.19514200	0.01024700
C	-1.17127200	-1.60484700	0.00981800
C	-0.10332900	-2.54143000	0.01718300
C	1.27587600	-2.04699900	0.02194800
C	3.94231800	-1.07870400	0.01554500
C	2.37818000	-2.92198600	0.02671800
C	3.68335600	-2.45347000	0.02571100
C	-2.54008300	-2.09201600	0.00138500
C	-2.79351000	-3.47783700	0.00254800
C	-1.73195700	-4.37191900	0.01115800
C	-0.41213300	-3.91819800	0.01814400
C	-3.22947200	0.24905400	-0.00933700
C	-3.54509200	-1.10247000	-0.00832100
C	-2.95460600	2.95571300	-0.01308100
C	-4.24571200	2.41847400	-0.02259400
C	-4.38818400	1.02332100	-0.02036100
H	3.28661300	3.92350200	0.05133300
H	1.39968500	5.55538800	0.02805500
H	-0.91694800	4.75086400	0.00412000
H	2.22458800	-3.99348800	0.02965800
H	4.50890100	-3.15748700	0.02709300
H	-3.81915700	-3.83027000	-0.00358200
H	-1.92599000	-5.43948000	0.01216000
H	0.38047900	-4.65615400	0.02395700
H	-2.86131600	4.03537600	-0.01501600
H	-5.10602900	3.07927200	-0.03122900
C	5.38475900	-0.65520500	0.02816000
O	4.32792900	1.69467900	0.09796100
O	5.86077400	-0.41985700	-1.20735400
C	-5.49480700	0.06762800	-0.02680700
O	-6.70246000	0.18580900	-0.03721300
O	-4.91681500	-1.24439700	-0.01870500
H	6.80824100	-0.20022800	-1.12802000
O	6.07876900	-0.65915700	1.02985300

ts1_OH₂O

C	2.07557700	3.62269000	-0.20671200
C	1.84109700	2.22543400	-0.23772100
C	2.84172200	1.24188600	-0.34590200
C	0.47582600	1.72515000	-0.15420300
C	0.20978500	0.32297000	-0.17973300
C	1.25175900	-0.61290000	-0.28810200
C	2.54312500	-0.10034800	-0.36955000
C	1.01522000	4.49750400	-0.10031500
C	-0.31155900	4.03038400	-0.01937200
C	-0.61041600	2.67053100	-0.04243900
C	-1.98992200	2.15881500	0.04392700
C	-2.15758900	0.74466100	0.01310800
C	-1.11351000	-0.18930900	-0.09525700
C	-1.37791900	-1.58718400	-0.11827000
C	-0.29191700	-2.53368600	-0.22680700
C	1.08501200	-2.02612300	-0.31260700
C	3.71166400	-0.87239900	-0.47509500
C	2.26153300	-2.80905100	-0.41518900
C	3.55971500	-2.26336600	-0.48874100
C	-2.74388900	-2.08820200	-0.03232200

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C	-2.97917300	-3.48762800	-0.05829200
C	-1.92072400	-4.36360500	-0.16256300
C	-0.59427000	-3.89415100	-0.24525700
C	-3.44875900	0.23382200	0.09480500
C	-3.75094300	-1.11583000	0.07332600
C	-3.16101100	2.93887000	0.15476600
C	-4.46302800	2.38825200	0.23512800
C	-4.60814600	1.00602700	0.20396700
H	3.09467700	3.98913200	-0.26859700
H	1.19885600	5.56669600	-0.07763500
H	-1.10942500	4.75954700	0.06336300
H	2.17898300	-3.88975700	-0.43716000
H	4.41221000	-2.92909900	-0.56283800
H	-3.99879500	-3.85225700	0.00593200
H	-2.10320600	-5.43282400	-0.18175900
H	0.20369500	-4.62365000	-0.32572300
H	-3.08072900	4.01965000	0.18233800
H	-5.31660000	3.05279700	0.31818900
C	4.76971400	0.09609800	-0.44822200
O	4.22820000	1.37273500	-0.44728800
O	6.04608100	0.00476200	-0.78247400
C	-5.70958300	0.03454900	0.25433300
O	-6.91202000	0.14479400	0.34774200
O	-5.12629300	-1.26814100	0.16971500
H	6.39413300	-0.13132500	0.18156500
O	5.60909000	-0.13016900	1.53263000
O	5.50786400	-1.50402800	1.94728800
H	4.84647100	-1.45169700	2.65731100

ts1_1H₂O

C	-2.14548200	-3.26442100	-0.35332700
C	-1.77728200	-1.90327800	-0.31520400
C	-2.75132900	-0.85841600	-0.37686400
C	-0.38185500	-1.53520200	-0.21365700
C	0.00341800	-0.16723400	-0.17780600
C	-0.96303900	0.85967000	-0.23568200
C	-2.31154500	0.48932200	-0.32317300
C	-1.17947900	-4.25329700	-0.29458300
C	0.17834100	-3.91325200	-0.19463800
C	0.60944300	-2.58415000	-0.15237300
C	2.02564900	-2.21832300	-0.05146800
C	2.32574900	-0.83060800	-0.02607500
C	1.37015500	0.20683600	-0.08601500
C	1.78198600	1.57536700	-0.05079900
C	0.79438300	2.62408700	-0.11138000
C	-0.63119700	2.24953600	-0.21047200
C	-3.34726800	1.42022900	-0.39441400
C	-1.69248500	3.16538900	-0.28562000
C	-3.04605000	2.77192800	-0.37981900
C	3.19422800	1.93196900	0.04749200
C	3.55951200	3.30216000	0.08019100
C	2.58729400	4.27850200	0.02304200
C	1.22079600	3.95059700	-0.07174200
C	3.66600300	-0.44856600	0.06794100
C	4.09693800	0.85636300	0.10463200
C	3.11921400	-3.12364400	0.02223300
C	4.45876100	-2.70723100	0.11895100

C	4.74841000	-1.33998900	0.14331100
H	-3.19685700	-3.52184000	-0.43153600
H	-1.46702600	-5.29886300	-0.32471800
H	0.90725200	-4.71538700	-0.15023700
H	-1.48630700	4.22964300	-0.27520200
H	-3.82475100	3.52484800	-0.43685800
H	4.60918900	3.56719600	0.15291200
H	2.87553700	5.32499500	0.05074800
H	0.49981900	4.75892300	-0.11332100
H	2.92754200	-4.19039800	0.00612100
H	5.24440800	-3.45471200	0.17366700
C	-4.67738100	0.76797500	-0.52469500
O	-4.04492400	-0.99269400	-0.48826900
O	-5.56878800	0.91577600	-1.31485800
C	5.93292400	-0.49821900	0.23651800
O	7.12960300	-0.73512800	0.32803100
O	5.49193100	0.85347900	0.20747600
O	-5.37322200	0.65878400	1.00023700
O	-4.45297200	0.34860000	2.06606000
H	-4.33708600	1.23260800	2.46106500
H	-6.01594700	-0.27332500	0.95484800
O	-6.67328600	-1.39379600	0.85460600
H	-7.37691200	-1.25602400	0.19749300
H	-6.03847100	-1.99242700	0.42170200

ts1_2H₂O

C	-1.87290900	3.24138700	-0.28263500
C	-1.48855300	1.87738900	-0.26795000
C	-2.40393500	0.80733000	-0.34208200
C	-0.07902200	1.52672300	-0.17661600
C	0.33123700	0.16614800	-0.16227000
C	-0.61060100	-0.87428600	-0.23287900
C	-1.95451200	-0.51119500	-0.31406600
C	-0.91618000	4.23199900	-0.21124300
C	0.45195200	3.90810300	-0.12181600
C	0.89920000	2.58787600	-0.10262300
C	2.32461400	2.23465900	-0.01254200
C	2.64376400	0.84805700	-0.00771900
C	1.70484900	-0.19769900	-0.07949900
C	2.12389000	-1.56127200	-0.06630900
C	1.14574900	-2.62371600	-0.13994800
C	-0.28492300	-2.26311200	-0.23009000
C	-3.01378000	-1.41403800	-0.39911100
C	-1.35761200	-3.16568800	-0.31706600
C	-2.71988300	-2.76393000	-0.40215700
C	3.54044100	-1.90515900	0.02250700
C	3.92300000	-3.27226200	0.03426100
C	2.96255300	-4.25726800	-0.03461800
C	1.59012800	-3.94196000	-0.12122300
C	3.98668600	0.48106500	0.07613600
C	4.43162700	-0.82189800	0.09251100
C	3.40538600	3.14625400	0.06896200
C	4.75492800	2.74315600	0.15537900
C	5.05725500	1.38226900	0.15999600
H	-2.92664600	3.49104400	-0.35197600
H	-1.21325200	5.27531000	-0.22279900
H	1.16830700	4.72068200	-0.06696500

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H	-1.15783200	-4.23179800	-0.32234400
H	-3.49470100	-3.52047000	-0.46723000
H	4.97595100	-3.52529800	0.10028900
H	3.26146000	-5.30086300	-0.02321900
H	0.87656100	-4.75686400	-0.17363900
H	3.20430800	4.21145500	0.06739100
H	5.53131100	3.49930900	0.21705900
O	-3.75778600	0.85364100	-0.46344300
C	6.25433300	0.54655000	0.23739600
O	7.44445900	0.79458100	0.32802600
O	5.82511200	-0.80909700	0.18998700
C	-4.26887800	-0.58326900	-0.45531400
O	-5.27550500	-0.81441800	-1.13443600
O	-4.67185400	-0.49539100	1.27182200
H	-6.59143100	0.33335600	-1.08741000
H	-5.57084700	0.42790400	1.41738300
O	-5.39103800	-1.70496900	1.59776200
O	-7.29395800	0.99396800	-0.85776800
O	-6.36817600	1.23397400	1.49515900
H	-4.67343800	-2.25518700	1.95804900
H	-6.82744300	1.22010700	0.56650300
H	-8.10879400	0.47222100	-0.79677100
H	-5.90837400	2.08748900	1.56459800

ts1_3H₂O

C	1.80868600	3.05143600	-0.17501700
C	1.35272500	1.70897300	-0.17462800
C	2.20957400	0.59123300	-0.22697400
C	-0.07648500	1.43396800	-0.12022500
C	-0.56015000	0.09805600	-0.12235300
C	0.32564200	-0.99186600	-0.17175300
C	1.68837800	-0.70107800	-0.21664800
C	0.90434100	4.09085800	-0.12265200
C	-0.48130000	3.84025500	-0.06951000
C	-0.99838600	2.54599400	-0.06792200
C	-2.44289800	2.26931700	-0.01682000
C	-2.83586000	0.90204300	-0.02720200
C	-1.95277600	-0.19216100	-0.07796200
C	-2.44427000	-1.53126800	-0.08345500
C	-1.52270700	-2.64425000	-0.13623800
C	-0.07307500	-2.36032900	-0.18433500
C	2.69990900	-1.65706600	-0.27831500
C	0.95254900	-3.31935200	-0.24400300
C	2.33459200	-2.99024300	-0.29066000
C	-3.87895900	-1.79964100	-0.03578500
C	-4.33381500	-3.14466700	-0.04269900
C	-3.42574800	-4.17914700	-0.09345200
C	-2.03656500	-3.93696700	-0.14002700
C	-4.19815000	0.60695600	0.01857700
C	-4.71264300	-0.67054200	0.01496900
C	-3.47522300	3.23703800	0.04034800
C	-4.84639900	2.90657800	0.08902800
C	-5.22074400	1.56383400	0.07851400
H	2.87540600	3.24606200	-0.21624100
H	1.25628600	5.11704300	-0.12169400
H	-1.15437200	4.68978600	-0.02959300
H	0.69676500	-4.37325200	-0.25688700

H	3.06906500	-3.78772500	-0.33535600
H	-5.40013400	-3.34169300	-0.00752900
H	-3.77962800	-5.20543900	-0.09847400
H	-1.36612700	-4.78834400	-0.17939500
H	-3.21786300	4.29002500	0.04875700
H	-5.58239900	3.70321800	0.13372000
O	3.56662900	0.55838600	-0.31527000
C	-6.46270700	0.79307000	0.11753300
O	-7.63952600	1.10456100	0.17696200
O	-6.10557900	-0.58348400	0.07334400
C	3.99524900	-0.89462900	-0.32484800
O	5.00146200	-1.16367800	-0.99185900
O	4.58130500	-1.00949400	1.36538600
O	3.61132900	-0.61713900	2.36707200
H	3.22948700	-1.48107200	2.60009900
H	5.87676400	0.13729800	-1.79826600
O	6.46312600	0.83398800	-2.17649200
H	7.53465600	0.82609200	-0.86500300
O	8.05101500	0.78000000	-0.01257400
H	6.95120800	0.75712500	1.01255500
O	6.18542900	0.77146500	1.71223000
H	5.70560400	1.60429400	1.57198500
H	5.43215900	-0.08975500	1.50988700
H	8.43362900	-0.11047400	-0.01033100
H	5.96127000	1.65157100	-2.04154100

ts82

C	-1.66687800	1.80644600	-2.43614000
C	-2.34595600	0.75895800	-1.77295700
C	-1.80616300	-0.54217900	-1.61076700
C	-3.66213100	0.99705300	-1.21041500
C	-4.36791600	-0.04818800	-0.54327000
C	-3.80573000	-1.33005000	-0.41148100
C	-2.53405400	-1.52513500	-0.95181300
C	-2.25605300	3.05082300	-2.55210400
C	-3.52980500	3.29756000	-2.01099200
C	-4.24971200	2.30747300	-1.34034900
C	-5.58250500	2.54778000	-0.76572200
C	-6.21638700	1.44560500	-0.12840400
C	-5.66090400	0.15832500	0.00000600
C	-6.37297400	-0.88412200	0.66023000
C	-5.78756000	-2.19637400	0.78120200
C	-4.45119100	-2.43116000	0.21768100
C	-1.84664300	-2.73895200	-0.92074300
C	-3.74483400	-3.65779700	0.24699800
C	-2.45242200	-3.82266700	-0.29032500
C	-7.69561800	-0.64436800	1.22212600
C	-8.37825600	-1.70270100	1.87343400
C	-7.79105000	-2.94726800	1.97311700
C	-6.51376800	-3.19339500	1.43584000
C	-7.47945700	1.64064500	0.42234500
C	-8.20319400	0.65682200	1.07064100
C	-6.29138300	3.77174200	-0.78694900
C	-7.57326100	3.93882900	-0.21694900
C	-8.18113200	2.84920400	0.40157200
H	-0.68222500	1.61800800	-2.85092400
H	-1.73391800	3.85175500	-3.06460600

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H	-3.95516400	4.28842600	-2.12611500
H	-4.20303700	-4.52473000	0.70926600
H	-1.95665200	-4.78388900	-0.20821600
H	-9.36287000	-1.51837900	2.28992600
H	-8.31715900	-3.75350200	2.47332900
H	-6.09370600	-4.18712400	1.54269400
H	-5.84221400	4.63862300	-1.25798400
H	-8.05701400	4.90852300	-0.27016300
C	-0.47627500	-2.47822700	-1.51534100
O	-0.60963700	-1.01335700	-2.02361400
O	-0.00456200	-3.23235600	-2.56299800
C	-9.44193700	2.57076300	1.09844500
O	-10.41297700	3.24540500	1.36848500
O	-9.40947100	1.19714200	1.49355000
O	0.30986900	-2.52226900	-0.43176400
O	2.07873500	-2.12219400	-0.97584000
H	2.30651700	-3.06765200	-0.98079300
H	3.35733800	-1.13375500	2.17538900
N	3.87469200	-1.61349600	1.44923500
C	5.13160900	-1.06410000	1.19595000
H	3.27532800	-1.78339200	0.64004500
C	5.84196100	-1.41262800	0.02072600
C	5.73978300	-0.20469400	2.14439800
C	7.11632600	-0.88198000	-0.18966500
C	5.23398800	-2.35469700	-0.98434700
C	7.02006300	0.29038700	1.89675400
C	5.01507200	0.15724500	3.41770100
C	7.74006100	-0.02417900	0.73088300
H	7.63060400	-1.14172900	-1.11124500
H	5.91570400	-2.52570700	-1.82165400
H	4.99927000	-3.32678800	-0.53236900
H	4.28638000	-1.97129600	-1.39312200
H	7.47541100	0.92844800	2.64952400
H	5.62486100	0.81920600	4.03770300
H	4.06588800	0.67284000	3.21788200
H	4.77148000	-0.72947900	4.01694400
C	9.10129000	0.51630500	0.49162700
C	10.07323500	-0.22321600	-0.20358700
C	9.47740900	1.78907500	0.95351300
C	11.35970900	0.26452400	-0.43797300
H	9.83215100	-1.22156100	-0.55890800
C	10.75299300	2.31648900	0.74533900
H	8.74844900	2.40456400	1.47403200
C	11.70910500	1.54839800	0.04120600
C	12.37645200	-0.56747900	-1.18020600
C	11.10887900	3.69168300	1.25439900
N	13.01322000	2.02618900	-0.12558100
H	11.95437600	-1.53299600	-1.46977000
H	12.72042500	-0.06863100	-2.09643900
H	13.26976100	-0.75851200	-0.57236300
H	10.26275800	4.14527900	1.77665700
H	11.95630600	3.66186600	1.95105100
H	11.39634400	4.36931300	0.43886800
H	13.09685700	3.03510400	-0.10990000
H	13.50215700	1.63673700	-0.92231300
H	-0.67216600	-3.23687300	-3.26836700

oxTMB

C	0.72402200	-0.00001000	0.00000000
C	1.47254600	1.20540400	-0.12574200
C	2.84944200	1.23450800	-0.13281600
C	3.56620900	0.00000300	-0.00000200
C	2.84945300	-1.23450900	0.13281400
C	1.47255800	-1.20541800	0.12574300
C	-0.72402200	-0.00001000	0.00000300
C	-1.47254700	1.20540400	0.12574500
C	-2.84944200	1.23450800	0.13281700
C	-3.56620900	0.00000300	0.00000200
C	-2.84945300	-1.23450900	-0.13281300
C	-1.47255700	-1.20541800	-0.12574100
H	0.95701700	2.15037800	-0.24803500
H	0.95703900	-2.15039600	0.24804000
H	-0.95701800	2.15037800	0.24803800
H	-0.95703900	-2.15039600	-0.24803800
C	3.60381700	-2.52828800	0.28298900
H	2.91247300	-3.37006800	0.35733000
H	4.26643300	-2.71068200	-0.57216800
H	4.23248100	-2.52758800	1.18237300
C	3.60379400	2.52829400	-0.28299300
H	2.91244200	3.37006800	-0.35733100
H	4.26641000	2.71069400	0.57216300
H	4.23245500	2.52760000	-1.18237800
C	-3.60379400	2.52829400	0.28299200
H	-2.91244200	3.37006800	0.35733100
H	-4.26640900	2.71069300	-0.57216600
H	-4.23245700	2.52760100	1.18237600
C	-3.60381700	-2.52828800	-0.28299100
H	-2.91247300	-3.37006800	-0.35733200
H	-4.26643500	-2.71068300	0.57216500
H	-4.23247900	-2.52758700	-1.18237600
N	4.91283100	0.00000900	-0.00000600
H	5.43664000	-0.85716400	0.09985900
H	5.43663200	0.85719100	-0.09984100
N	-4.91283100	0.00001000	-0.00000300
H	-5.43663200	0.85718800	0.09986100
H	-5.43664000	-0.85716700	-0.09983900

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C	0.74220100	-0.00017500	-0.00335700
C	1.47636900	1.14651300	-0.34966700
C	2.87204200	1.17008500	-0.35418500
C	3.58285900	0.00031000	0.00122400
C	2.87158700	-1.16953000	0.35522200
C	1.47578500	-1.14631300	0.34627400
C	-0.74220100	0.00017200	-0.00334700
C	-1.47578000	1.14631300	0.34628200
C	-2.87158200	1.16953300	0.35524400
C	-3.58285800	-0.00031000	0.00126400
C	-2.87204700	-1.17008900	-0.35414000
C	-1.47637400	-1.14651900	-0.34964000
H	0.94849000	2.04793800	-0.64977800
H	0.94726800	-2.04802900	0.64434700
H	-0.94725900	2.04803100	0.64434100
H	-0.94849900	-2.04794700	-0.64974900

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C	3.61673200	-2.41885700	0.75642600
H	2.92150500	-3.21948400	1.02090200
H	4.25732000	-2.79252100	-0.05407900
H	4.27266800	-2.24277800	1.61834900
C	3.61778600	2.42339000	-0.74112100
H	2.92290700	3.23191000	-0.98140200
H	4.27328300	2.77333600	0.06649000
H	4.25821600	2.26524400	-1.61947600
C	-3.61672000	2.41886600	0.75644300
H	-2.92148800	3.21949400	1.02090100
H	-4.25731700	2.79252100	-0.05405900
H	-4.27264600	2.24279900	1.61837600
C	-3.61779800	-2.42339600	-0.74105600
H	-2.92292500	-3.23193200	-0.98129800
H	-4.27331800	-2.77330800	0.06655000
H	-4.25820600	-2.26526600	-1.61943000
N	4.98032400	0.02016800	0.06692100
H	5.42065900	-0.88342200	-0.05546000
H	5.41827600	0.71575400	-0.52429100
N	-4.98032400	-0.02016800	0.06696900
H	-5.42065500	0.88342800	-0.05538600
H	-5.41827900	-0.71573000	-0.52427100