

Supporting Information (SI)

for

**Mechanisms of Formation of Dibenzofuran, Dibenzo-*p*-Dioxin and
Their Hydroxylated Derivatives from Catechol**

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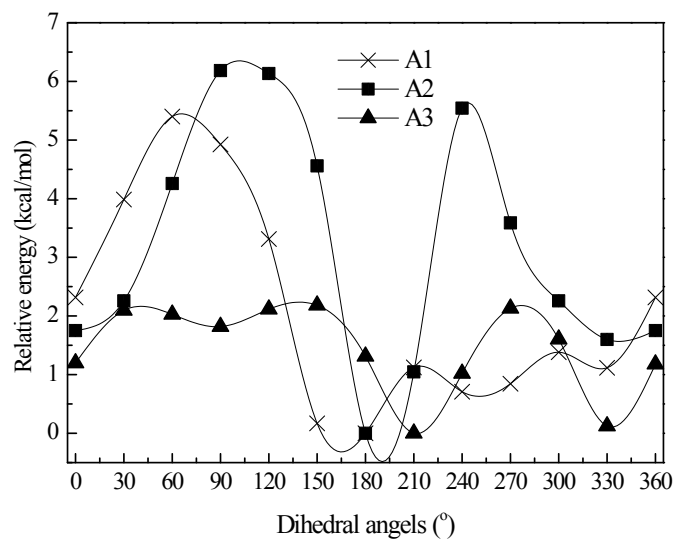
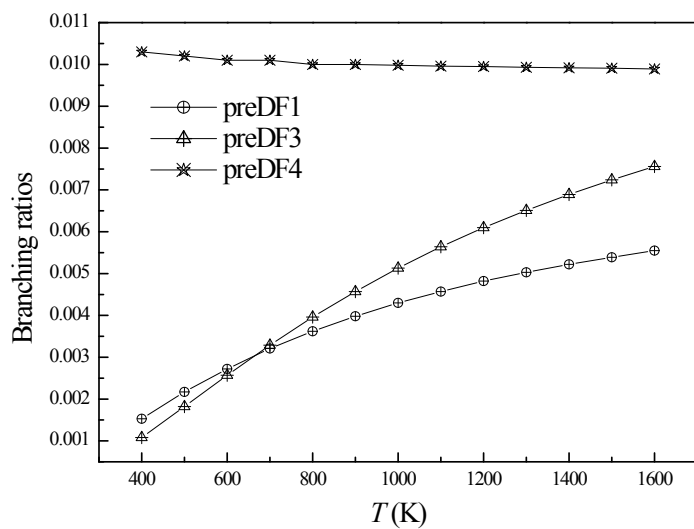
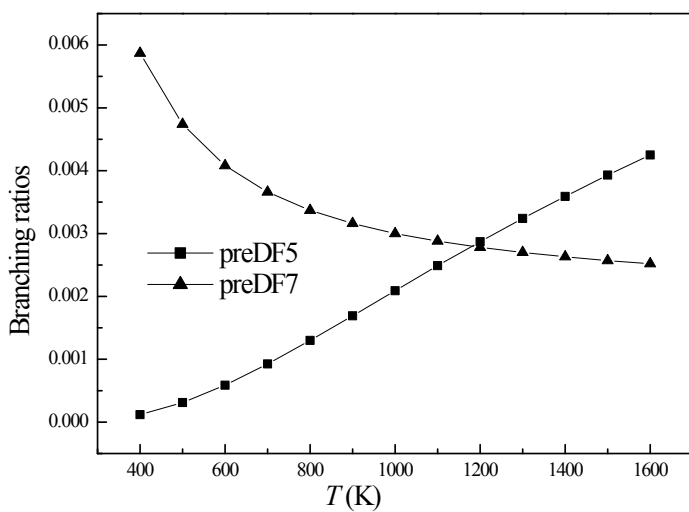


Figure S1: Energy potentials (in kcal/mol) for rotations about the O-C bonds in A1, A2 and A3 intermediates. Values are calculated by performing partial scanning of the corresponding dihedral angle at an interval of 30° at the M06-2X/6-311+G(d,p) level of theory.



(a)



(b)

Figure S2: Branching ratios at 1.0 atm for the minimal channels for A1 (a) and A2 (b) calculated at 1.0 atm.

Cartesian coordinates for transition structures

TS3

| | | | |
|---|-------------|-------------|-------------|
| C | -1.41534900 | -0.63003500 | 0.20552900 |
| C | -1.01180800 | 0.65963400 | 0.55107200 |
| C | -2.48707300 | -0.84380300 | -0.64759800 |
| C | -1.69320100 | 1.74546200 | 0.04607600 |
| C | -3.16988100 | 0.26963600 | -1.14238200 |
| C | -2.79816400 | 1.55821300 | -0.78926600 |
| H | -4.00619900 | 0.10769200 | -1.81176500 |
| H | -3.34109300 | 2.41184500 | -1.17175300 |
| C | 1.21707100 | -0.74899200 | -0.20020500 |
| C | 1.24775200 | 0.43307500 | 0.55943200 |
| C | 2.33113600 | -1.06671300 | -0.97728700 |
| C | 2.36638400 | 1.24901100 | 0.57261200 |
| C | 3.46153700 | -0.25864300 | -0.95161300 |
| H | 2.29227700 | -1.96838100 | -1.57646300 |
| C | 3.48602600 | 0.89524200 | -0.17339300 |
| H | 4.36759400 | 1.52355100 | -0.15310100 |
| O | 0.13788700 | -1.55381200 | -0.17141400 |
| O | 0.13800300 | 0.79209300 | 1.31246500 |
| H | 2.34278600 | 2.14805000 | 1.17652000 |
| H | 4.32619900 | -0.53112300 | -1.54463800 |
| H | -2.75870900 | -1.85016100 | -0.94382300 |
| H | -1.33684900 | 2.73486800 | 0.30858000 |
| O | -1.34059600 | -1.70740400 | 1.47497900 |
| H | -2.09661900 | -2.30769500 | 1.41801200 |
| H | -0.47831300 | -2.08818900 | 1.05231500 |

TS7

| | | | |
|---|-------------|-------------|-------------|
| C | -1.09713300 | 0.82861200 | 0.17918600 |
| C | -1.27121700 | -0.49774700 | 0.68550800 |
| C | -2.11952800 | 1.45914300 | -0.52571300 |
| C | -2.49442900 | -1.16852900 | 0.40986000 |
| C | -3.29412000 | 0.78046000 | -0.77493900 |
| C | -3.46714800 | -0.54950800 | -0.32456100 |
| H | -4.39187500 | -1.06990200 | -0.54022000 |
| C | 1.23053800 | 0.69827400 | 0.10415400 |
| C | 1.12368100 | -0.55826400 | -0.52442500 |
| C | 2.44702000 | 1.25161600 | 0.44905600 |
| C | 2.32101100 | -1.22453100 | -0.81879500 |
| C | 3.62189600 | 0.56994200 | 0.14603500 |
| H | 2.45656100 | 2.21580700 | 0.94240600 |

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|---|-------------|-------------|-------------|
| C | 3.55033300 | -0.66227000 | -0.49435800 |
| H | 4.57914100 | 1.00159400 | 0.40787100 |
| O | 0.08352000 | 1.45009400 | 0.33093900 |
| O | -0.05388200 | -1.09506600 | -0.81216100 |
| H | 2.25298600 | -2.18788500 | -1.30886500 |
| H | 4.45825500 | -1.20217000 | -0.73551700 |
| H | -2.63056200 | -2.17014900 | 0.80133900 |
| H | -4.08289000 | 1.26025600 | -1.34033200 |
| H | -1.94127500 | 2.45978200 | -0.89766300 |
| O | -0.47776600 | -0.86105500 | 1.71250800 |
| H | -0.42074400 | -1.82229900 | 1.75463400 |

TS6

| | | | |
|---|-------------|-------------|-------------|
| C | -1.02323800 | 0.40212200 | 0.32992600 |
| C | -0.96743200 | -0.94572000 | 0.76180000 |
| C | -2.21123800 | 0.94257600 | -0.20378300 |
| C | -2.13765600 | -1.74317100 | 0.67057100 |
| C | -3.31985100 | 0.13246900 | -0.30361800 |
| C | -3.27594300 | -1.21439200 | 0.12774100 |
| H | -4.17030600 | -1.81856500 | 0.03908700 |
| C | 1.29720500 | 0.55650000 | 0.21352800 |
| C | 1.37711900 | -0.71322900 | -0.39466300 |
| C | 2.42459900 | 1.26975400 | 0.58061400 |
| C | 2.65879300 | -1.21733500 | -0.65480500 |
| C | 3.68464700 | 0.74229800 | 0.32433000 |
| H | 2.29320600 | 2.23847700 | 1.04693500 |
| C | 3.79235100 | -0.49570500 | -0.30283300 |
| H | 4.57017600 | 1.29615700 | 0.60733000 |
| O | 0.06622900 | 1.17822400 | 0.34362000 |
| O | 0.28980000 | -1.40684500 | -0.70381500 |
| H | 2.73118800 | -2.18654100 | -1.13204200 |
| H | 4.76973800 | -0.91578500 | -0.50815100 |
| H | -2.10800600 | -2.76289200 | 1.02935400 |
| H | -4.23243100 | 0.53162500 | -0.73403200 |
| H | -0.17964700 | -1.22229400 | 1.45212200 |
| O | -2.16330800 | 2.23528500 | -0.60430700 |
| H | -3.01182500 | 2.48950100 | -0.97743500 |

TS18

| | | | |
|---|-------------|-------------|-------------|
| C | -2.72649400 | 1.55036700 | -0.18301000 |
| C | -1.87293700 | 1.70393100 | -1.29200300 |
| C | -0.98806700 | 0.67866900 | -1.65705300 |
| C | -0.99055800 | -0.48788000 | -0.93766000 |

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|---|-------------|-------------|-------------|
| C | -1.80867600 | -0.65564700 | 0.23658900 |
| C | -2.74271700 | 0.38641600 | 0.54533000 |
| H | -3.41122800 | 2.35042800 | 0.07229700 |
| H | -1.88776400 | 2.62611400 | -1.85870700 |
| H | -3.44400900 | 0.22361200 | 1.35476200 |
| C | 0.74017200 | -1.30218700 | 0.28418900 |
| C | 1.99611000 | -0.57541200 | -0.04508200 |
| C | 2.17966500 | 0.71090700 | 0.28866900 |
| C | 1.23996300 | 1.42090800 | 1.13378900 |
| C | 0.17986000 | 0.78165900 | 1.66803100 |
| C | -0.15436800 | -0.57966600 | 1.29944900 |
| O | -0.01740900 | -1.44007900 | -0.99916900 |
| H | -1.68748300 | -2.55671400 | 0.05389500 |
| O | -2.22431900 | -1.93666700 | 0.56269600 |
| H | 1.44117800 | 2.46236700 | 1.36323100 |
| H | -0.27468200 | 0.80012100 | -2.46312700 |
| H | 0.97269500 | -2.32699100 | 0.57580900 |
| H | -0.55502500 | -1.19996800 | 2.09415200 |
| H | -0.47807000 | 1.29617900 | 2.35860000 |
| O | 2.89042000 | -1.29499600 | -0.76704900 |
| H | 3.63895700 | -0.72036600 | -0.96943100 |
| O | 3.31878000 | 1.33205200 | -0.18289600 |
| H | 3.63394100 | 1.97034000 | 0.46242800 |

TS19

| | | | |
|---|-------------|-------------|-------------|
| C | 2.55728200 | -0.40719200 | 1.07017500 |
| C | 2.17853100 | -1.69975300 | 0.67386600 |
| C | 1.26651200 | -1.87866700 | -0.37713000 |
| C | 0.76880100 | -0.78326700 | -1.03649900 |
| C | 1.11118100 | 0.56884200 | -0.65278500 |
| C | 2.07739600 | 0.70163900 | 0.40563900 |
| H | 3.28300600 | -0.28479500 | 1.86589000 |
| H | 2.58223000 | -2.56229600 | 1.18851400 |
| H | 2.47138500 | 1.69404200 | 0.60120100 |
| C | -1.39950000 | -0.13154600 | -1.18848900 |
| C | -2.27487300 | -1.18058800 | -0.57182900 |
| C | -2.28597500 | -1.40984300 | 0.74658200 |
| C | -1.56045200 | -0.56394100 | 1.68862600 |
| C | -0.93248800 | 0.53538500 | 1.25044300 |
| C | -0.80953800 | 0.84606600 | -0.17105500 |
| O | -0.30287300 | -0.84414100 | -1.86478600 |
| H | -2.84902100 | -1.79443600 | -1.25532700 |
| H | -2.87913500 | -2.22295100 | 1.14913900 |
| H | 0.44099300 | 2.11281300 | -1.62480200 |
| O | 1.20595100 | 1.52098900 | -1.65557800 |
| H | -1.57972500 | -0.77740400 | 2.74982000 |
| H | 0.90735400 | -2.86221800 | -0.65471200 |

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|---|-------------|------------|-------------|
| H | -1.91395600 | 0.43050900 | -1.96845500 |
| O | -1.04699800 | 2.16899100 | -0.50066300 |
| H | -0.95883600 | 2.69783900 | 0.30480400 |
| O | -0.38872700 | 1.47445700 | 2.09698600 |
| H | 0.57563600 | 1.42372700 | 2.01099900 |

TS20

| | | | |
|---|-------------|-------------|-------------|
| C | -2.96237100 | -0.14042800 | 1.01987900 |
| C | -2.26755000 | 1.08191600 | 1.08780400 |
| C | -1.30272800 | 1.40811900 | 0.12921400 |
| C | -1.07217500 | 0.52508200 | -0.91392200 |
| C | -1.72780200 | -0.74242700 | -0.97777200 |
| C | -2.73718600 | -1.03014900 | -0.00037400 |
| H | -3.71022300 | -0.35705100 | 1.77358800 |
| H | -2.45995300 | 1.77117900 | 1.90363400 |
| H | -3.31366200 | -1.94393900 | -0.07489500 |
| C | 0.87457600 | -0.53288600 | -1.39643800 |
| C | 1.91520700 | -0.02189800 | -0.45500700 |
| C | 1.91708500 | -0.34126200 | 0.84809200 |
| C | 1.02103400 | -1.34375000 | 1.38693100 |
| C | 0.18520200 | -2.02621500 | 0.57733200 |
| C | 0.01484600 | -1.66165400 | -0.81409800 |
| O | 0.00891500 | 0.61610900 | -1.72694100 |
| H | 1.08144400 | -1.56904800 | 2.44677200 |
| H | 1.33988300 | -0.80925900 | -2.34335600 |
| H | -1.87815200 | -1.14052600 | -1.97801900 |
| O | -0.55503700 | 2.53966800 | 0.18393200 |
| H | -0.76063000 | 3.01890500 | 0.99072100 |
| H | -0.17739900 | -2.48688500 | -1.49158400 |
| H | -0.43138800 | -2.82392700 | 0.97454800 |
| O | 2.79485200 | 0.84104600 | -1.01308000 |
| H | 3.35156700 | 1.19324100 | -0.30782700 |
| O | 2.82767900 | 0.30554700 | 1.66391300 |
| H | 3.19841400 | -0.31834200 | 2.29398000 |

TS21

| | | | |
|---|-------------|-------------|-------------|
| C | 1.90975900 | 1.96674700 | 0.47720500 |
| C | 2.52167500 | 0.72061000 | 0.69084700 |
| C | 2.08277200 | -0.41928500 | 0.00321200 |
| C | 1.05322300 | -0.29038900 | -0.91189700 |
| C | 0.37723800 | 0.95385500 | -1.11747000 |
| C | 0.88556100 | 2.11103300 | -0.43277700 |
| H | 2.29138300 | 2.83237500 | 1.00611600 |
| H | 3.33419900 | 0.63056700 | 1.40430000 |
| H | 0.50408500 | 3.09545500 | -0.68262500 |
| C | -1.00216500 | -1.27044700 | -0.94103300 |
| C | -1.09698600 | -2.21371800 | 0.21942600 |
| C | -1.19245500 | -1.78133200 | 1.48156700 |

| | | | |
|---|-------------|-------------|-------------|
| C | -1.35157000 | -0.36793500 | 1.80466300 |
| C | -1.49047500 | 0.53212600 | 0.82167700 |
| C | -1.33274000 | 0.18388500 | -0.59014000 |
| O | 0.38533700 | -1.34940200 | -1.43127500 |
| H | -1.00559200 | -3.26834700 | -0.01011500 |
| H | -1.18592000 | -2.49217300 | 2.29980200 |
| H | -1.42468200 | -0.04226300 | 2.83472200 |
| H | -1.62668400 | -1.58120300 | -1.77870600 |
| O | -2.26429200 | 0.73903600 | -1.43874600 |
| H | -2.66372700 | 1.49420000 | -0.98824600 |
| O | -1.80710000 | 1.85110100 | 1.06046900 |
| H | -1.01551900 | 2.37869300 | 0.87589400 |
| H | -0.02871000 | 1.11166700 | -2.11570200 |
| O | 2.60624000 | -1.65397600 | 0.21256000 |
| H | 3.27666600 | -1.60393900 | 0.89882200 |

TS22

| | | | |
|---|-------------|-------------|-------------|
| C | -0.83348800 | 2.14110600 | -0.07513700 |
| C | -1.50900900 | 1.98315900 | -1.24309600 |
| C | -2.18571900 | 0.77463600 | -1.55890400 |
| C | -2.10603000 | -0.27645400 | -0.65632100 |
| C | -1.30817800 | -0.21406900 | 0.47940500 |
| C | -0.75835600 | 1.08615100 | 0.98909400 |
| H | -1.54460100 | 2.80268800 | -1.95074600 |
| H | -2.75374600 | 0.65442100 | -2.47107300 |
| C | 1.47257100 | 0.37169600 | 0.65489000 |
| C | 1.13965700 | -0.88789400 | 0.14310000 |
| C | 2.67617100 | 0.97631700 | 0.33512100 |
| C | 2.02392400 | -1.53164100 | -0.71850400 |
| C | 3.57111800 | 0.31308600 | -0.50177300 |
| H | 2.89976500 | 1.95049000 | 0.75287900 |
| C | 3.24278200 | -0.93405900 | -1.02592200 |
| H | 4.51895400 | 0.77461500 | -0.74931900 |
| H | 3.93747100 | -1.44436200 | -1.68223600 |
| O | 0.58282000 | 0.95540700 | 1.52047000 |
| O | -0.03818100 | -1.41899100 | 0.51293200 |
| H | -1.20774400 | -1.64797600 | 1.85162900 |
| H | 1.75339900 | -2.50306800 | -1.11496400 |
| H | -0.34710600 | 3.07617100 | 0.17474300 |
| O | -1.96626300 | -1.06348300 | 1.61272900 |
| H | -2.60935300 | -1.60405700 | 1.09686400 |
| H | -1.32239900 | 1.37935100 | 1.88549200 |
| O | -2.78431000 | -1.49294700 | -0.81986000 |
| H | -2.22983400 | -2.09036300 | -1.33514500 |

TS23

| | | | |
|---|-------------|-------------|-------------|
| C | -3.55415200 | -0.76687800 | -0.44365200 |
| C | -2.23520000 | -0.49480800 | -0.79242700 |
| C | -1.55139000 | 0.52911700 | -0.12938500 |
| C | -2.18044000 | 1.26926400 | 0.85815200 |
| C | -3.50080200 | 0.99448700 | 1.20403500 |
| C | -4.18312500 | -0.02438500 | 0.55093900 |
| H | -4.08760100 | -1.56065100 | -0.95771500 |
| H | -3.99072000 | 1.57586800 | 1.97452000 |
| H | -5.21159900 | -0.24579800 | 0.80922800 |
| O | -0.26973000 | 0.84355600 | -0.51555700 |
| C | 0.76341600 | 0.14713500 | 0.06387500 |
| C | 0.63701400 | -1.16982300 | 0.56371200 |
| C | 2.04975600 | 0.64237400 | -0.24933000 |
| C | 1.76558100 | -1.86686600 | 0.94333900 |
| C | 3.16621400 | -0.08675600 | 0.14155200 |
| C | 3.03933500 | -1.32830700 | 0.74954000 |
| H | -0.35152000 | -1.58222400 | 0.71393200 |
| H | 1.66398800 | -2.85023400 | 1.38450900 |
| H | 3.92601100 | -1.87854600 | 1.04495600 |
| O | 2.16133600 | 1.85240500 | -0.83064500 |
| H | 3.09922100 | 2.06808500 | -0.89785200 |
| O | -1.55428200 | -1.18034100 | -1.74588700 |
| H | -2.12293100 | -1.85252500 | -2.13085100 |
| H | -1.61786000 | 2.06124400 | 1.33819100 |
| H | 0.68659000 | 0.94056000 | 1.58934600 |
| O | 4.36466000 | 0.52000300 | -0.13269000 |
| H | 5.09330500 | -0.02809700 | 0.16788800 |

TS16

| | | | |
|---|------------|-------------|-------------|
| C | 2.73625100 | -0.82117000 | 1.03955400 |
| C | 1.56142700 | -0.08139300 | 0.96579500 |
| C | 1.11623800 | 0.40369600 | -0.29606000 |
| C | 1.79408400 | -0.00502800 | -1.46283400 |
| C | 2.96357800 | -0.73535700 | -1.37378200 |
| C | 3.43412000 | -1.14025300 | -0.11966500 |
| H | 3.09303500 | -1.15756200 | 2.00746900 |
| H | 3.50333000 | -1.00954100 | -2.27110100 |
| H | 4.34556700 | -1.72106800 | -0.04713100 |

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|---|-------------|-------------|-------------|
| O | -0.13324300 | 0.94956000 | -0.39777800 |
| C | -1.20291900 | 0.10456300 | -0.24624500 |
| C | -1.12398900 | -1.28007700 | -0.23738500 |
| C | -2.45113100 | 0.73398800 | -0.12443300 |
| C | -2.27899800 | -2.04998800 | -0.09532600 |
| C | -3.59289500 | -0.04115500 | 0.01490000 |
| C | -3.51202700 | -1.43243400 | 0.03146700 |
| H | -0.16107700 | -1.76527200 | -0.34351000 |
| H | -2.20163900 | -3.12980700 | -0.08827500 |
| H | -4.41462600 | -2.02022100 | 0.14175900 |
| H | -4.55476500 | 0.45306400 | 0.11295700 |
| O | -2.46693100 | 2.08999000 | -0.15219300 |
| H | -3.36923700 | 2.39976000 | -0.04021400 |
| O | 0.79735600 | 0.22878700 | 2.02181400 |
| H | 1.22858600 | -0.04233900 | 2.83731900 |
| H | 1.38168000 | 0.31440900 | -2.41219300 |
| O | 2.00183500 | 2.19622800 | 0.01015900 |
| H | 2.89456800 | 2.02969500 | -0.32900400 |

TS15

| | | | |
|---|-------------|-------------|-------------|
| C | 2.90236800 | 1.09122100 | 0.54578600 |
| C | 2.98057200 | -0.30101500 | 0.36150500 |
| C | 1.95958900 | -0.99198200 | -0.28927700 |
| C | 0.88224000 | -0.27246700 | -0.78915400 |
| C | 0.78693200 | 1.13432800 | -0.63187100 |
| C | 1.84577600 | 1.81318700 | 0.04205600 |
| H | 3.70986000 | 1.59627600 | 1.06230900 |
| H | 3.82790900 | -0.85410600 | 0.75423200 |
| H | 1.81495800 | 2.89205000 | 0.12881200 |
| C | -1.44403400 | -0.13120500 | -0.73001200 |
| C | -2.34807000 | -1.14936100 | -0.10079700 |
| C | -2.21622900 | -1.44662800 | 1.19796500 |
| C | -1.32563000 | -0.67618700 | 2.05666900 |
| C | -0.80369800 | 0.49609400 | 1.63734800 |
| C | -0.97777500 | 0.94626800 | 0.26688800 |
| O | -0.26554900 | -0.89192100 | -1.15027900 |
| H | -1.15915700 | -1.01254300 | 3.07311000 |
| H | -0.24018700 | 1.14196700 | 2.30435900 |
| O | -1.98769900 | 0.49941700 | -1.84049100 |
| H | -2.10010200 | -0.16910400 | -2.52465300 |
| H | -2.80846500 | -2.23703700 | 1.64381000 |
| H | 0.23249500 | 1.68585400 | -1.39002100 |
| O | 1.93581100 | -2.34544800 | -0.41953700 |
| H | 2.70929000 | -2.71893100 | 0.01060800 |
| O | -1.49257600 | 2.20737500 | 0.08248400 |
| H | -1.89917200 | 2.50126100 | 0.90237900 |
| H | -3.05956300 | -1.65459100 | -0.74500000 |

TS14

| | | | |
|---|-------------|-------------|-------------|
| C | -2.98813600 | 0.42893900 | 0.49162600 |
| C | -2.65604300 | 1.32577300 | -0.53829200 |
| C | -1.51986300 | 1.10724700 | -1.33243800 |
| C | -0.76960900 | -0.01763500 | -1.11636900 |
| C | -1.06701500 | -0.93897500 | -0.06002600 |
| C | -2.24668700 | -0.70922800 | 0.71233600 |
| H | -3.86667200 | 0.61815700 | 1.09672800 |
| H | -3.26593200 | 2.20419200 | -0.70519800 |
| H | -2.52972300 | -1.44461600 | 1.45569700 |
| C | 1.42931800 | -0.27232500 | -0.50321200 |
| C | 2.24876700 | 0.97473200 | -0.61638000 |
| C | 1.97507100 | 2.05031700 | 0.13036400 |
| C | 0.99510600 | 2.00667800 | 1.21308000 |
| C | 0.42670200 | 0.84762700 | 1.58735200 |
| C | 0.62335500 | -0.37812500 | 0.83053800 |
| O | 0.48061000 | -0.21757900 | -1.62116300 |
| H | 3.01451100 | 0.96725600 | -1.38349800 |
| H | 2.52834800 | 2.96998300 | -0.02270800 |
| H | -0.07899100 | -2.33316800 | -0.96036300 |
| O | -0.70827000 | -2.27655600 | -0.22526500 |
| H | 0.80108400 | 2.91362700 | 1.77289800 |
| H | -1.19352500 | 1.82537500 | -2.07474200 |
| O | 0.93347900 | -1.45818700 | 1.62186700 |
| H | 0.53881400 | -2.24565900 | 1.20928100 |
| O | 2.16239300 | -1.43733700 | -0.74236300 |
| H | 2.59681700 | -1.68105100 | 0.08418200 |
| H | -0.19621800 | 0.77302200 | 2.47163700 |

TS13

| | | | |
|---|-------------|-------------|-------------|
| C | -3.22380100 | -0.45820000 | 0.31769300 |
| C | -2.80737700 | 0.88428600 | 0.34172900 |
| C | -1.60215600 | 1.26962800 | -0.25116500 |
| C | -0.83740300 | 0.30832900 | -0.89297000 |
| C | -1.22579000 | -1.06132900 | -0.91017000 |
| C | -2.47814000 | -1.41926000 | -0.32221200 |
| H | -4.16577100 | -0.72154400 | 0.78377400 |
| H | -3.41212100 | 1.63083100 | 0.84673100 |
| H | -2.83121100 | -2.44076800 | -0.38886400 |
| C | 1.31189600 | -0.48117500 | -0.59800800 |
| C | 2.13362000 | 0.34742200 | 0.35598500 |
| C | 1.84134600 | 0.42882900 | 1.66090800 |
| C | 0.82988600 | -0.44061200 | 2.23911900 |
| C | 0.22525800 | -1.40540600 | 1.51166600 |

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|---|-------------|-------------|-------------|
| C | 0.44350700 | -1.52689800 | 0.08974900 |
| O | 0.44939800 | 0.52962800 | -1.24995800 |
| H | 0.62640800 | -0.35151300 | 3.29942200 |
| H | 0.57785800 | -2.52700100 | -0.30842800 |
| H | -0.44817700 | -2.11055400 | 1.98479800 |
| O | 3.10272700 | 1.03028300 | -0.30369100 |
| H | 3.54759900 | 1.63948600 | 0.29247500 |
| O | 2.07035800 | -1.09123600 | -1.57917500 |
| H | 2.65577100 | -0.42416700 | -1.95856100 |
| H | 2.38764100 | 1.11243700 | 2.30229000 |
| H | -0.87155000 | -1.64413500 | -1.75637900 |
| O | -1.12240200 | 2.54070400 | -0.19886200 |
| H | -1.73218000 | 3.08820700 | 0.30228300 |

TS12

| | | | |
|---|-------------|-------------|-------------|
| C | 2.90236800 | 1.09122100 | 0.54578600 |
| C | 2.98057200 | -0.30101500 | 0.36150500 |
| C | 1.95958900 | -0.99198200 | -0.28927700 |
| C | 0.88224000 | -0.27246700 | -0.78915400 |
| C | 0.78693200 | 1.13432800 | -0.63187100 |
| C | 1.84577600 | 1.81318700 | 0.04205600 |
| H | 3.70986000 | 1.59627600 | 1.06230900 |
| H | 3.82790900 | -0.85410600 | 0.75423200 |
| H | 1.81495800 | 2.89205000 | 0.12881200 |
| C | -1.44403400 | -0.13120500 | -0.73001200 |
| C | -2.34807000 | -1.14936100 | -0.10079700 |
| C | -2.21622900 | -1.44662800 | 1.19796500 |
| C | -1.32563000 | -0.67618700 | 2.05666900 |
| C | -0.80369800 | 0.49609400 | 1.63734800 |
| C | -0.97777500 | 0.94626800 | 0.26688800 |
| O | -0.26554900 | -0.89192100 | -1.15027900 |
| H | -1.15915700 | -1.01254300 | 3.07311000 |
| H | -0.24018700 | 1.14196700 | 2.30435900 |
| O | -1.98769900 | 0.49941700 | -1.84049100 |
| H | -2.10010200 | -0.16910400 | -2.52465300 |
| H | -2.80846500 | -2.23703700 | 1.64381000 |
| H | 0.23249500 | 1.68585400 | -1.39002100 |
| O | 1.93581100 | -2.34544800 | -0.41953700 |
| H | 2.70929000 | -2.71893100 | 0.01060800 |
| O | -1.49257600 | 2.20737500 | 0.08248400 |
| H | -1.89917200 | 2.50126100 | 0.90237900 |
| H | -3.05956300 | -1.65459100 | -0.74500000 |

TS17

| | | | |
|---|-------------|-------------|-------------|
| C | -1.08121300 | -1.62148500 | 0.61204300 |
| C | -1.71107500 | -1.30007000 | 1.77412100 |
| C | -2.27205500 | -0.01486100 | 1.97696900 |
| C | -2.11986500 | 0.98046100 | 1.00628000 |
| C | -1.36428300 | 0.71737900 | -0.12649700 |
| C | -1.08093700 | -0.70306900 | -0.57148600 |
| H | -1.76349000 | -2.03032900 | 2.57298100 |
| H | -2.77980500 | 0.21778800 | 2.90308900 |
| C | 1.26466300 | -0.41204300 | -0.61258000 |
| C | 1.25979900 | 0.87250200 | -0.05555300 |
| C | 2.37051400 | -1.23659900 | -0.50216600 |
| C | 2.37927900 | 1.31243100 | 0.64745700 |
| C | 3.50023100 | -0.77660100 | 0.17107000 |
| H | 2.33595700 | -2.22156500 | -0.95227700 |
| C | 3.49862300 | 0.49165200 | 0.74524700 |
| H | 4.37381900 | -1.41113300 | 0.25311300 |
| H | 4.37383200 | 0.84453100 | 1.27754300 |
| O | 0.14588900 | -0.80883600 | -1.30636200 |
| O | 0.16555900 | 1.62894600 | -0.22078200 |
| H | -0.91718900 | 2.12057700 | -1.40866200 |
| H | 2.35984800 | 2.30158900 | 1.08845500 |
| H | -0.60836400 | -2.58409800 | 0.44973100 |
| O | -1.73983900 | 1.55884300 | -1.34686400 |
| H | -2.56683300 | 2.04016500 | -1.19214000 |
| O | -2.08250400 | -1.02311700 | -1.50660700 |
| H | -2.15003100 | -1.98332000 | -1.53785300 |
| H | -2.43265300 | 2.00091300 | 1.20151800 |

TS27

| | | | |
|---|-------------|-------------|-------------|
| C | 3.02312800 | -1.45412100 | -0.39067300 |
| C | 3.35700400 | -0.06768200 | -0.43167600 |
| C | 2.37524200 | 0.90711500 | -0.17292700 |
| C | 1.16494100 | 0.47926300 | 0.29327800 |
| C | 0.89049900 | -0.92727500 | 0.72282100 |
| C | 1.82884600 | -1.89812000 | 0.07459000 |
| H | 3.75087000 | -2.16470700 | -0.76624100 |
| H | 4.33689100 | 0.24494100 | -0.77417100 |
| H | 1.59001800 | -2.95451000 | 0.09529000 |
| C | -1.04245700 | 0.40148300 | 0.36283600 |
| C | -2.21227600 | 0.70757400 | -0.44463300 |
| C | -2.91218100 | -0.31671900 | -0.99082300 |
| C | -2.50664600 | -1.69264700 | -0.86897800 |
| C | -1.36666100 | -2.01329400 | -0.20356100 |
| C | -0.62643400 | -1.00436300 | 0.49963800 |
| O | 0.02930800 | 1.24758900 | 0.28733600 |
| H | -3.10770100 | -2.45596100 | -1.34411900 |
| H | -3.79178300 | -0.08098800 | -1.58389500 |

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|---|-------------|-------------|-------------|
| H | -1.02492300 | -3.04134400 | -0.15622200 |
| O | -2.47871100 | 2.03525500 | -0.59134500 |
| H | -3.08990100 | 2.16348800 | -1.32198300 |
| O | -1.51256300 | 0.50839000 | 2.04693700 |
| H | -2.45441600 | 0.70080400 | 2.16027800 |
| H | -1.22513900 | -0.67793000 | 1.72217300 |
| H | 1.09174400 | -0.98454400 | 1.81173300 |
| O | 2.55467200 | 2.23152500 | -0.43894500 |
| H | 3.34466900 | 2.34141300 | -0.97405100 |

TS28

| | | | |
|---|-------------|-------------|-------------|
| C | -2.56906300 | 1.76536800 | -0.33883800 |
| C | -3.14790700 | 0.48415400 | -0.41015100 |
| C | -2.37498800 | -0.66067000 | -0.17080300 |
| C | -1.06391600 | -0.48812300 | 0.21839400 |
| C | -0.50119500 | 0.80187100 | 0.44089600 |
| C | -1.25651700 | 1.94723700 | 0.02963400 |
| H | -3.17690400 | 2.62591700 | -0.59206100 |
| H | -4.18494700 | 0.37092000 | -0.70634000 |
| C | 1.17960800 | -0.94334700 | 0.25750700 |
| C | 1.73185000 | -1.23512900 | -1.10224900 |
| C | 2.32672500 | -0.29367100 | -1.84937100 |
| C | 2.46541200 | 1.07761700 | -1.39275600 |
| C | 1.89434500 | 1.48620900 | -0.24053800 |
| C | 1.00784400 | 0.58178000 | 0.49939400 |
| O | -0.16347000 | -1.48926600 | 0.37700600 |
| H | -0.00387100 | 1.00945000 | 1.91915600 |
| H | 3.01439200 | 1.78254600 | -2.00422600 |
| O | 1.16088900 | 0.79587100 | 2.03664900 |
| H | 1.82935900 | 1.47065700 | 2.27471600 |
| H | 1.91561700 | 2.52990300 | 0.05839200 |
| O | 1.97775100 | -1.58935900 | 1.18367200 |
| H | 1.59261900 | -1.45870800 | 2.05951200 |
| H | 1.65324400 | -2.26930700 | -1.41364100 |
| H | 2.73389300 | -0.55671900 | -2.81854400 |
| H | -0.82188600 | 2.93924900 | 0.06611200 |
| O | -2.84629800 | -1.92853000 | -0.32303200 |
| H | -3.73568600 | -1.89341500 | -0.68415900 |

TS20

| | | | |
|---|-------------|-------------|-------------|
| C | -3.43872100 | 0.39016000 | -1.01997200 |
| C | -3.47382700 | -1.00926600 | -0.89559600 |
| C | -2.40806500 | -1.69502600 | -0.28253000 |

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|---|-------------|-------------|-------------|
| C | -1.39428100 | -0.95285300 | 0.26316600 |
| C | -1.40356600 | 0.47750300 | 0.30053400 |
| C | -2.40852100 | 1.13675700 | -0.48970500 |
| H | -4.23763500 | 0.89439100 | -1.55140900 |
| H | -4.29690900 | -1.56821500 | -1.32093500 |
| H | -2.40145000 | 2.21603900 | -0.59921700 |
| C | 0.71736700 | -0.42407700 | 0.98172100 |
| C | 1.96221900 | -0.68446600 | 0.20438700 |
| C | 2.44922700 | 0.18566100 | -0.69589700 |
| C | 1.79922600 | 1.44484100 | -0.97650200 |
| C | 0.69686000 | 1.83022800 | -0.29807900 |
| C | 0.02409000 | 0.90144200 | 0.61366400 |
| O | -0.25177400 | -1.47740000 | 0.77861700 |
| H | -1.35155100 | 1.14877500 | 1.70718000 |
| H | 2.19698100 | 2.06100700 | -1.77544200 |
| O | -0.28313800 | 1.60515700 | 2.00257200 |
| H | -0.18902900 | 2.57348700 | 1.93834400 |
| H | 0.96358700 | -0.44376300 | 2.04818000 |
| O | 2.58667600 | -1.83630700 | 0.53874400 |
| H | 3.38358500 | -1.90840600 | -0.00149000 |
| O | 3.60213700 | -0.18189900 | -1.36321000 |
| H | 4.16361000 | 0.58685200 | -1.49240300 |
| H | -2.35970900 | -2.77627300 | -0.26323300 |
| H | 0.16526400 | 2.73428500 | -0.57450700 |

TS31

| | | | |
|---|-------------|-------------|-------------|
| C | 3.07160700 | -0.30928600 | -1.12388200 |
| C | 3.17142700 | 1.08130000 | -0.81392400 |
| C | 2.12224800 | 1.74774100 | -0.17155000 |
| C | 1.04738100 | 1.00066800 | 0.24375000 |
| C | 1.08896700 | -0.50227400 | 0.31118800 |
| C | 2.03446400 | -1.07356600 | -0.68997900 |
| H | 3.83593100 | -0.75450500 | -1.75051700 |
| H | 4.02664400 | 1.64253100 | -1.16674900 |
| H | 1.95457900 | -2.12424400 | -0.94039900 |
| C | -1.10565500 | 0.44698900 | 0.55599700 |
| C | -2.32502000 | 0.76511100 | -0.12252400 |
| C | -2.91273600 | -0.14720600 | -0.95497900 |
| C | -2.17194900 | -1.29695300 | -1.37758800 |
| C | -0.95188100 | -1.62730300 | -0.88517500 |
| C | -0.42226800 | -0.84969000 | 0.23004200 |
| O | -0.12810100 | 1.49456400 | 0.63134700 |
| H | -2.59916200 | -1.90530500 | -2.16797200 |
| H | -1.27847100 | -0.48819900 | 1.73890900 |
| H | -3.89940700 | 0.03952000 | -1.36297300 |
| O | -0.85556400 | -1.57097000 | 1.60220700 |
| H | -0.04866200 | -1.70215900 | 2.13831000 |

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|---|-------------|-------------|-------------|
| O | 1.52188500 | -0.89227800 | 1.65036600 |
| H | 2.46997100 | -0.73351900 | 1.70871800 |
| H | 2.10236200 | 2.82616500 | -0.07987200 |
| H | -0.37071800 | -2.43832100 | -1.30264800 |
| O | -2.84348300 | 1.98174800 | 0.16005400 |
| H | -3.63047900 | 2.12033900 | -0.37486600 |

TS32

| | | | |
|---|-------------|-------------|-------------|
| C | 3.49269100 | -1.21323700 | 0.02103800 |
| C | 3.62064200 | 0.12107400 | -0.36306300 |
| C | 2.52500600 | 0.98153000 | -0.36785000 |
| C | 1.29515200 | 0.45565800 | 0.01756700 |
| C | 1.16313100 | -0.87353700 | 0.38625500 |
| C | 2.25583800 | -1.72783400 | 0.39883200 |
| H | 4.36975700 | -1.84834200 | 0.02338000 |
| H | 4.59132100 | 0.50680100 | -0.65944100 |
| H | 2.15109400 | -2.76555100 | 0.69268600 |
| C | -0.78279600 | 0.35697800 | 0.85095500 |
| C | -2.17998500 | 0.60876700 | 0.40089400 |
| C | -2.79874100 | -0.23968200 | -0.42743500 |
| C | -2.15023900 | -1.45647900 | -0.90718100 |
| C | -0.99219500 | -1.87357600 | -0.39271800 |
| C | -0.29870800 | -1.10494100 | 0.70624800 |
| O | 0.13707500 | 1.16171700 | 0.06875300 |
| H | -2.63992100 | -2.00051700 | -1.70876300 |
| H | -0.67565700 | 0.68733400 | 1.88949700 |
| H | -0.52178600 | -0.64843300 | 3.74163500 |
| O | 2.58417500 | 2.29097200 | -0.72196800 |
| H | 3.49676500 | 2.53655400 | -0.89564800 |
| H | -0.42372600 | -1.64967300 | 1.64680000 |
| H | -0.50647500 | -2.77221700 | -0.75614000 |
| O | -2.73096000 | 1.75883100 | 0.85445800 |
| H | -3.59293300 | 1.86141800 | 0.43191100 |
| O | -4.05364800 | 0.10575700 | -0.89018800 |
| H | -4.64035300 | -0.65392500 | -0.83561100 |

TS33

| | | | |
|---|-------------|-------------|-------------|
| C | -2.03333300 | 1.98884700 | -0.78329100 |
| C | -2.94639400 | 0.92579800 | -0.65427000 |
| C | -2.53384000 | -0.29786400 | -0.09905800 |
| C | -1.25263500 | -0.38934200 | 0.39034300 |
| C | -0.35435200 | 0.72262000 | 0.40539900 |
| C | -0.74254900 | 1.90468800 | -0.31397600 |
| H | -2.36411100 | 2.90130500 | -1.26569900 |
| H | -3.96162600 | 1.02770000 | -1.02143000 |

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|---|-------------|-------------|-------------|
| H | -0.05596900 | 2.73566600 | -0.41462500 |
| C | 0.76037600 | -1.39084800 | 0.73392900 |
| C | 1.25072000 | -2.16414800 | -0.45531600 |
| C | 2.05880500 | -1.63030500 | -1.37962700 |
| C | 2.55099600 | -0.26289200 | -1.28865800 |
| C | 2.11385900 | 0.52991500 | -0.29671700 |
| C | 1.02936200 | 0.11327600 | 0.60638300 |
| O | -0.67644400 | -1.52858400 | 0.86311500 |
| O | -3.33828400 | -1.39783100 | -0.04022000 |
| H | -4.15600700 | -1.20890900 | -0.50713200 |
| H | 0.21491400 | 1.06001200 | 1.86791100 |
| H | 3.25607800 | 0.10990700 | -2.02252100 |
| H | 2.38602200 | -2.23024700 | -2.22051400 |
| O | 1.32228400 | 0.67755800 | 2.03138000 |
| H | 1.95016400 | 1.42009200 | 1.94663900 |
| H | 1.17841500 | -1.78661400 | 1.66329600 |
| H | 0.91350800 | -3.19118600 | -0.51889200 |
| O | 2.46586000 | 1.83912000 | -0.09177400 |
| H | 3.04519900 | 2.14170000 | -0.79787800 |

TS24

| | | | |
|---|-------------|-------------|-------------|
| C | -2.34011300 | 1.38846400 | -0.97704600 |
| C | -1.93295300 | 0.22925600 | -1.66320000 |
| C | -1.43505600 | -0.87463400 | -0.96065400 |
| C | -1.39208100 | -0.82599000 | 0.42301600 |
| C | -1.73810100 | 0.36305500 | 1.13715600 |
| C | -2.28732500 | 1.45956200 | 0.39302500 |
| H | -2.73361800 | 2.22066600 | -1.54913300 |
| H | -1.98119800 | 0.19339000 | -2.74669300 |
| H | -2.65191100 | 2.33585500 | 0.91505300 |
| C | 0.50399000 | -0.94619300 | 1.65530300 |
| C | 1.60937800 | -1.22631700 | 0.69143900 |
| C | 2.06756900 | -0.30556100 | -0.16572200 |
| C | 1.65236600 | 1.09759400 | -0.05932500 |
| C | 0.80430500 | 1.48568200 | 0.91556300 |
| C | 0.12178500 | 0.53465500 | 1.76306500 |
| H | 1.93932400 | -2.25730200 | 0.61670300 |
| H | 0.56361600 | 2.53904400 | 1.02566600 |
| O | -0.67368900 | -1.70390400 | 1.16872700 |
| O | -0.96366400 | -1.98993600 | -1.57976400 |
| H | -1.00507600 | -1.86268100 | -2.53119300 |
| O | 2.24038600 | 1.92642200 | -0.95320300 |
| H | 1.88166700 | 2.81169400 | -0.84168800 |
| O | 2.96214700 | -0.54316200 | -1.15637800 |
| H | 3.14072100 | -1.48745600 | -1.19237600 |
| H | 0.70975100 | -1.37748500 | 2.63484900 |
| H | -2.11306400 | 0.20879100 | 2.14591200 |

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|---|-------------|------------|------------|
| H | -0.07424000 | 0.88269100 | 2.77212200 |
|---|-------------|------------|------------|

TS34

| | | | |
|---|-------------|-------------|-------------|
| C | 3.43590000 | -0.40990800 | -0.01573600 |
| C | 3.65613200 | 0.84200900 | -0.50573300 |
| C | 2.56309700 | 1.71562700 | -0.71878400 |
| C | 1.25976900 | 1.32020400 | -0.44609100 |
| C | 0.98292400 | 0.04458500 | 0.03351000 |
| C | 2.09783500 | -0.87150600 | 0.30992800 |
| H | 4.66110000 | 1.17773100 | -0.73121300 |
| H | 2.74142900 | 2.70832300 | -1.11395000 |
| H | 0.44872300 | 2.01718400 | -0.61772800 |
| C | -0.40356000 | -0.43073100 | 0.30115500 |
| C | -1.44999500 | 0.55742500 | 0.44545500 |
| C | -0.81076200 | -1.73700100 | -0.17830400 |
| C | -2.71835700 | 0.41236000 | -0.18346400 |
| C | -2.06744700 | -1.89251100 | -0.67286800 |
| H | -0.08350200 | -2.53492000 | -0.21314100 |
| C | -3.01383300 | -0.81688700 | -0.69671000 |
| H | -2.37469500 | -2.85078700 | -1.07152500 |
| H | -4.01847500 | -0.98884400 | -1.06708700 |
| H | -0.35190400 | 0.27912100 | 1.50655600 |
| H | 4.24013600 | -1.10997900 | 0.17553900 |
| O | -1.19039800 | 1.41779000 | 1.36141600 |
| O | 1.91326800 | -1.98499100 | 0.82417900 |
| O | -3.62000100 | 1.41899000 | -0.11056200 |
| H | -3.27599300 | 2.08586400 | 0.49814600 |

TS35

| | | | |
|---|-------------|-------------|-------------|
| C | -3.50717300 | 0.82698400 | 0.21939400 |
| C | -3.66194300 | -0.46366200 | -0.33696100 |
| C | -2.58084300 | -1.26689600 | -0.62652900 |
| C | -1.27089400 | -0.77674200 | -0.38878100 |
| C | -1.12561800 | 0.51919800 | 0.22512000 |
| C | -2.24561800 | 1.31790900 | 0.49103000 |
| H | -4.38562500 | 1.42121200 | 0.44716200 |
| H | -4.66406000 | -0.83188300 | -0.53799900 |
| H | -2.11441900 | 2.29891300 | 0.93952100 |
| C | 1.04993900 | -0.40162500 | 0.41614700 |
| C | 2.39390900 | -0.38750700 | -0.10586100 |
| C | 2.96094800 | 0.78862000 | -0.50847200 |

| | | | |
|---|-------------|-------------|-------------|
| C | 2.22640100 | 2.00310000 | -0.44783800 |
| C | 0.90443900 | 2.01336800 | -0.05088200 |
| C | 0.27289300 | 0.81588800 | 0.31558900 |
| O | -0.19401700 | -1.40263600 | -0.72710600 |
| O | 0.81949800 | -1.20771700 | 1.48002300 |
| H | 1.31401700 | -2.03211200 | 1.33332500 |
| H | 3.99619700 | 0.79977700 | -0.84104900 |
| H | 2.70487700 | 2.91945900 | -0.77534200 |
| H | 0.31170100 | 2.91966400 | -0.12659700 |
| O | 3.01345000 | -1.59647900 | -0.03296200 |
| H | 3.92543400 | -1.51965400 | -0.34743600 |
| H | -2.69819600 | -2.25252200 | -1.06295900 |

TS37

| | | | |
|---|-------------|-------------|-------------|
| C | -1.86375700 | 1.77661200 | 0.30742300 |
| C | -3.03928800 | 1.25277000 | -0.14230000 |
| C | -3.19215200 | -0.15938800 | -0.31709800 |
| C | -2.22154500 | -1.06157500 | 0.03246900 |
| C | -1.08008000 | -0.51666700 | 0.69023300 |
| C | -0.77888200 | 0.89485000 | 0.63907900 |
| H | -3.87133100 | 1.89528700 | -0.40141400 |
| H | -4.13819200 | -0.53601500 | -0.69838400 |
| C | 0.59324800 | 1.29351700 | -0.10129500 |
| C | 1.78081800 | 0.60261200 | 0.45423000 |
| C | 0.43336000 | 1.04680500 | -1.56866800 |
| C | 2.48740000 | -0.34302900 | -0.24749400 |
| C | 1.15054000 | 0.10080500 | -2.22497500 |
| H | -0.35612100 | 1.59295900 | -2.07200500 |
| C | 2.18153700 | -0.63300300 | -1.57806800 |
| H | 0.94795100 | -0.09775100 | -3.27084400 |
| H | 2.74777600 | -1.38506700 | -2.11422900 |
| H | -0.15029400 | 0.24239000 | 1.73695500 |
| H | -1.71208700 | 2.85112300 | 0.34183900 |
| O | -0.29402500 | -1.08507700 | 1.52509600 |
| H | 0.67442000 | 2.36563000 | 0.12052300 |
| O | 3.51330700 | -0.94085900 | 0.44687000 |
| H | 3.72853800 | -1.78830800 | 0.05023300 |
| O | -2.31956600 | -2.41070000 | -0.06826200 |
| H | -3.14543600 | -2.64336200 | -0.50196300 |
| O | 2.07548100 | 0.89741800 | 1.73529500 |
| H | 2.76601000 | 0.29100000 | 2.03608100 |

TS38

| | | | |
|---|-------------|-------------|-------------|
| C | 1.68978000 | 1.01899000 | -1.55891600 |
| C | 2.94809600 | 1.17286600 | -1.06348300 |
| C | 3.37529100 | 0.44003400 | 0.09234500 |
| C | 2.59199200 | -0.49607900 | 0.70806200 |
| C | 1.35621100 | -0.80656600 | 0.05214900 |
| C | 0.78614400 | 0.08008100 | -0.94409900 |
| H | 3.64097300 | 1.87211000 | -1.51374100 |
| H | 4.38136400 | 0.60527500 | 0.46966400 |
| C | -0.61011500 | 0.66270600 | -0.62506300 |
| C | -1.77454300 | -0.33349900 | -0.70083600 |
| C | -0.58786500 | 1.53508900 | 0.59693200 |
| C | -2.94356700 | -0.05407600 | 0.17594900 |
| C | -1.64134900 | 1.61779900 | 1.41345900 |
| H | 0.31475200 | 2.11210000 | 0.76914000 |
| C | -2.85179900 | 0.84375600 | 1.17544100 |
| H | -1.61743900 | 2.26640500 | 2.28093300 |
| H | -3.69409000 | 0.98147100 | 1.84768600 |
| O | -1.77232300 | -1.25745300 | -1.47328600 |
| H | 0.33289200 | -1.27035100 | -1.07871800 |
| H | 1.33423300 | 1.64847500 | -2.36842500 |
| O | 0.72093100 | -1.90658200 | 0.08024400 |
| H | -0.84510600 | 1.32629400 | -1.47565200 |
| O | -4.00820300 | -0.83916300 | -0.08411200 |
| H | -4.69159400 | -0.69235900 | 0.57677300 |
| O | 2.93684000 | -1.24328700 | 1.78324900 |
| H | 3.79639700 | -0.96414000 | 2.11194000 |

TS39

| | | | |
|---|-------------|-------------|-------------|
| C | 1.81242700 | 1.68766400 | 0.70759900 |
| C | 3.14185100 | 1.40855200 | 0.43513300 |
| C | 3.48895900 | 0.18099900 | -0.13551200 |
| C | 2.52624000 | -0.76856700 | -0.43675000 |
| C | 1.16144900 | -0.50748100 | -0.16922000 |
| C | 0.84462600 | 0.73474400 | 0.40054700 |
| H | 3.91261100 | 2.13539700 | 0.65684700 |
| H | 4.53154900 | -0.04206200 | -0.34397300 |
| C | -0.64751800 | 0.96791900 | 0.55169700 |
| C | -1.39867700 | -0.31675800 | 0.61084600 |
| C | -1.19337300 | 1.96201500 | -0.41963000 |
| C | -2.67204700 | -0.44037500 | -0.04293000 |
| C | -2.35740300 | 1.76220800 | -1.05667100 |
| H | -0.60605800 | 2.85883700 | -0.57781400 |
| C | -3.11971700 | 0.55705500 | -0.84855200 |
| H | -2.74312300 | 2.50158400 | -1.74747500 |
| H | -4.07346700 | 0.42477900 | -1.34675300 |
| O | -1.12110900 | -1.24321200 | 1.51346300 |
| H | 1.52648800 | 2.63768800 | 1.14667700 |

| | | | |
|---|-------------|-------------|-------------|
| O | 0.20525800 | -1.37981300 | -0.38859000 |
| H | -0.32316100 | -1.66754400 | 0.98411200 |
| H | -0.80869500 | 1.38931500 | 1.56330600 |
| O | 2.81655000 | -1.98612700 | -0.96836500 |
| H | 3.76511000 | -2.05533500 | -1.10375200 |
| O | -3.37709400 | -1.56976700 | 0.14518700 |
| H | -2.89097800 | -2.11916300 | 0.77592500 |

TS40

| | | | |
|---|-------------|-------------|-------------|
| C | 1.85856300 | 1.91735900 | 0.02387400 |
| C | 3.16676200 | 1.47617000 | -0.14146600 |
| C | 3.46952800 | 0.11796600 | -0.24442600 |
| C | 2.46319000 | -0.84590900 | -0.19198900 |
| C | 1.16537600 | -0.38890600 | -0.02888400 |
| C | 0.84760600 | 0.96187900 | 0.07983400 |
| H | 3.97417100 | 2.19650000 | -0.19095800 |
| H | 4.49863000 | -0.20230300 | -0.37039600 |
| C | -0.61026800 | 1.02652500 | 0.27460700 |
| C | -1.01324500 | -0.40645000 | 0.26954200 |
| C | -1.56172600 | 2.00960400 | -0.18149700 |
| C | -2.30779200 | -0.76746700 | -0.30187900 |
| C | -2.80512700 | 1.62598000 | -0.55944500 |
| H | -1.27479500 | 3.05501000 | -0.18596600 |
| C | -3.15911700 | 0.22702700 | -0.64494800 |
| H | -3.54509500 | 2.36009900 | -0.84953500 |
| H | -4.13507900 | -0.03851200 | -1.04132800 |
| O | -1.15755900 | -0.45994400 | 1.97560600 |
| H | 1.63413400 | 2.97307000 | 0.10857000 |
| O | 0.05211500 | -1.20604000 | 0.00351300 |
| H | -2.07297800 | -0.59416700 | 2.26146200 |
| H | -0.85931200 | 0.72516000 | 1.61413700 |
| O | 2.67615700 | -2.18133000 | -0.29737400 |
| H | 3.61603800 | -2.34891000 | -0.40583100 |
| O | -2.52430600 | -2.10266700 | -0.43896800 |
| H | -3.28947200 | -2.24875600 | -1.00230900 |