

Supplementary material

Mechanism and kinetic properties for the gas-phase ozonolysis of β -ionone

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Keywords: β -Ionone; O₃; Degradation mechanisms; Oxidation products; Rate constants

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Scheme S The structure of β -ionone.

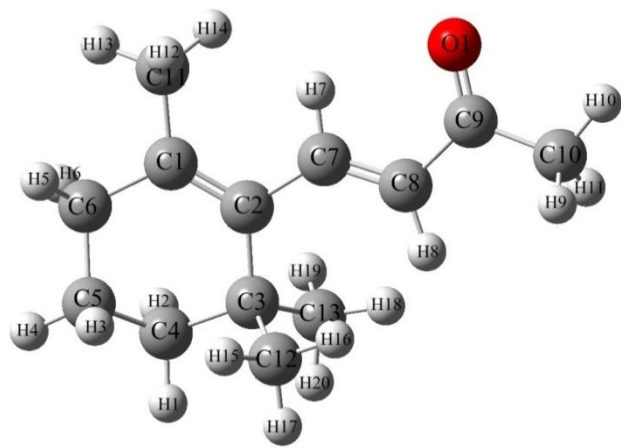
Fig. S1 (a) Profile of the potential energy surface for the reaction of β -ionone with O_3 at the MPWB1K/6-311++G(3df,2p)//MPWB1K/6-31+G(d,p) level. (b) Profile of the potential energy surface for the secondary reaction pathways of IM5. (c) Profile of the potential energy surface for the secondary reaction pathways of IM6. (d) Profile of the potential energy surface for the secondary reaction pathways of IM7. (e) Profile of the potential energy surface for the secondary reaction pathways of IM8. (Pages 4-6)

Fig. S2 The IRC trajectories of TS1 calculated at the MPWB1K/6-31+G(d,p) level.

Fig. S3 MPWB1K/6-31+G(d,p) optimized geometries with the bond lengths (\AA) for the intermediate states and products involved in the reaction of β -ionone with O_3 .

Fig. S4 MPWB1K/6-31+G(d,p) optimized geometries with the bond lengths (\AA) for the transition states involved in the secondary reactions of β -ionone with O_3 .

Table S Cartesian coordinates (bohr) for the optimized stationary points.



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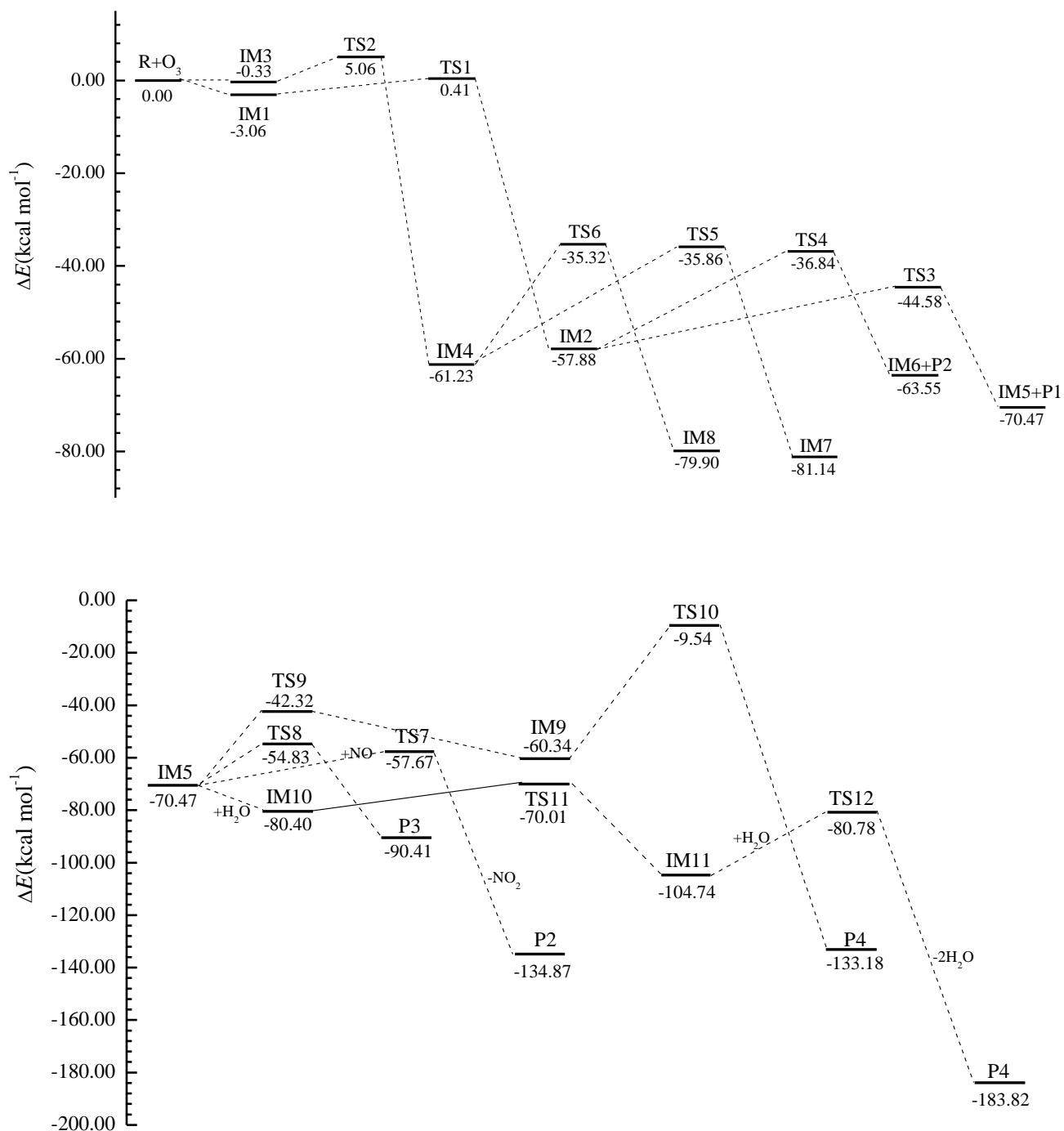


Fig. S1 (a) Profile of the potential energy surface for the reaction of β -ionone with O₃ at the MPWB1K/6-311++G(3df,2p)//MPWB1K/6-31+G(d,p) level. **(b)** Profile of the potential energy surface for the secondary reaction pathways of IM5.

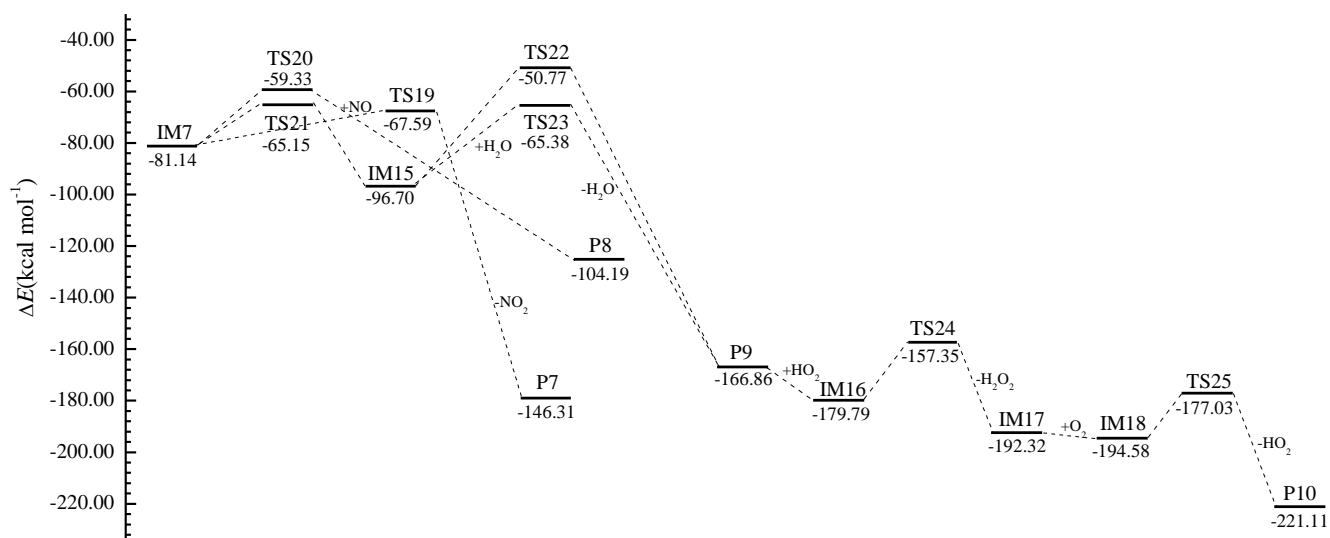
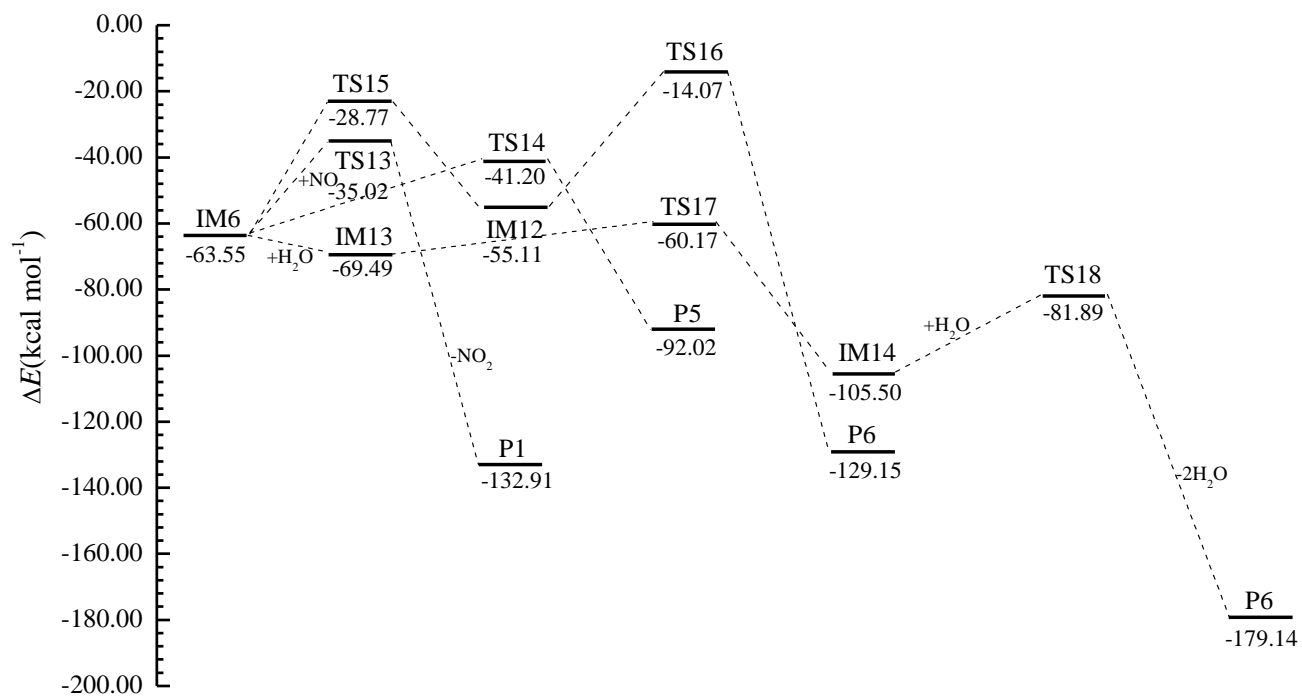


Fig. S1 (c) Profile of the potential energy surface for the secondary reaction pathways of IM6.

(d) Profile of the potential energy surface for the secondary reaction pathways of IM7.

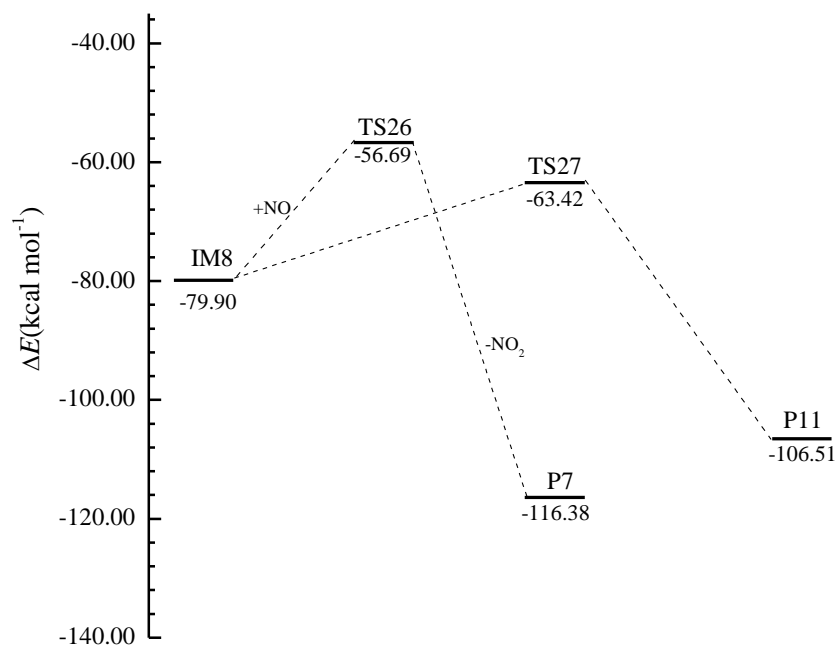


Fig. S1(e) Profile of the potential energy surface for the secondary reaction pathways of IM8.

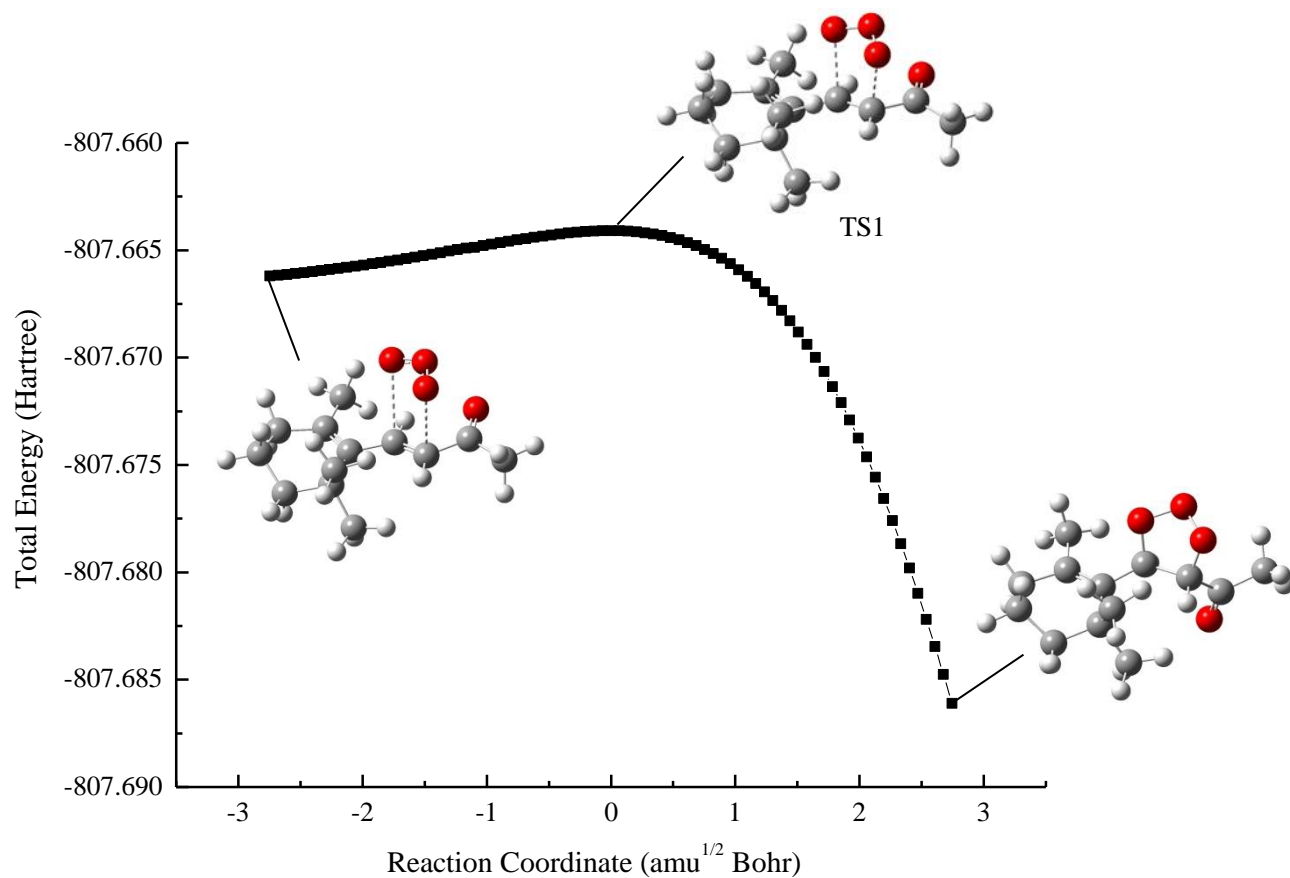
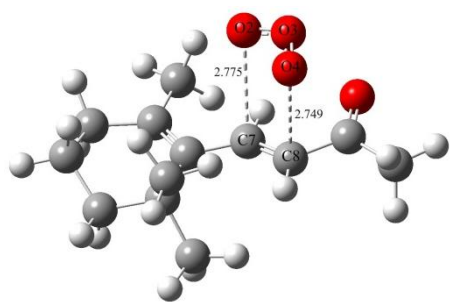
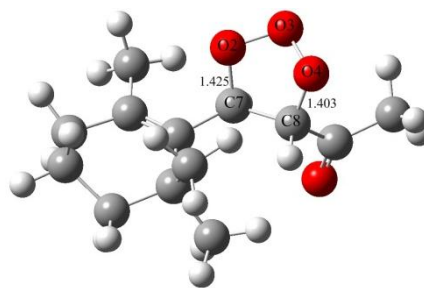


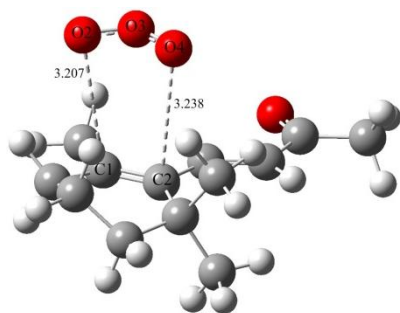
Fig. S2 The IRC trajectories of TS1 calculated at the MPWB1K/6-31+G(d,p) level.



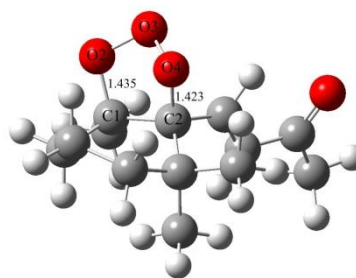
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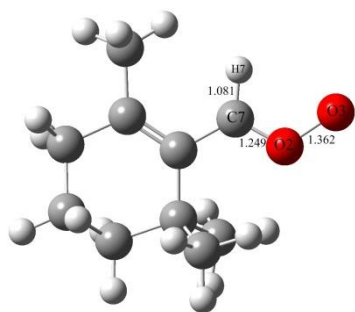
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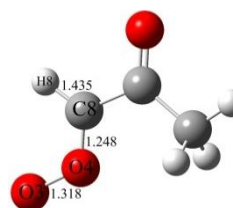
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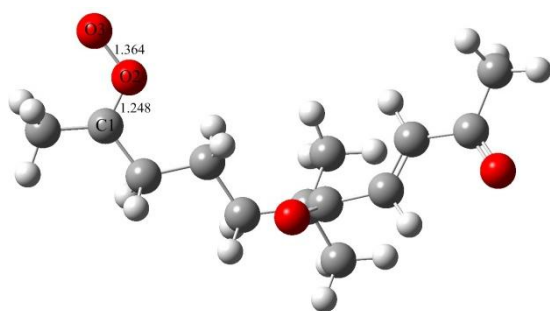
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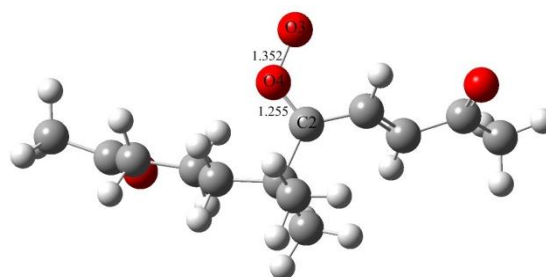
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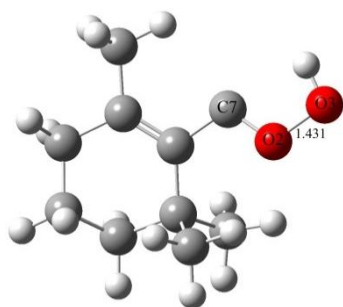
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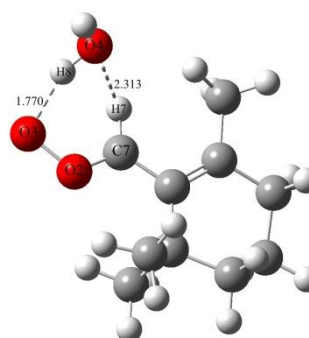
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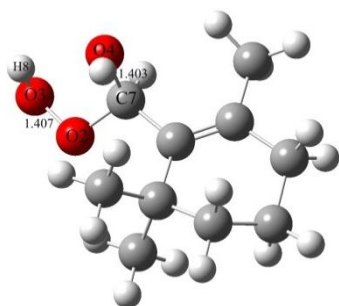
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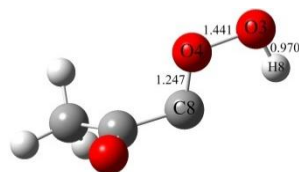
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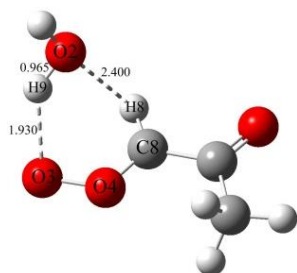
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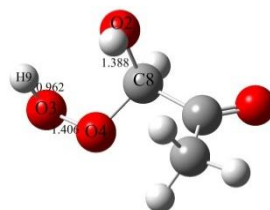
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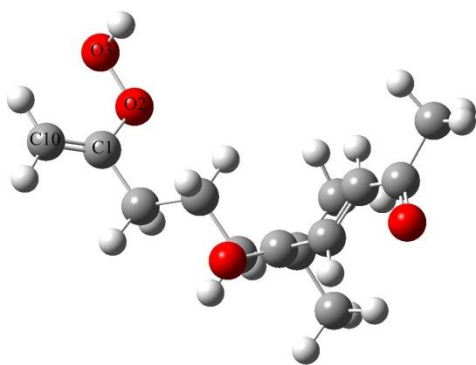
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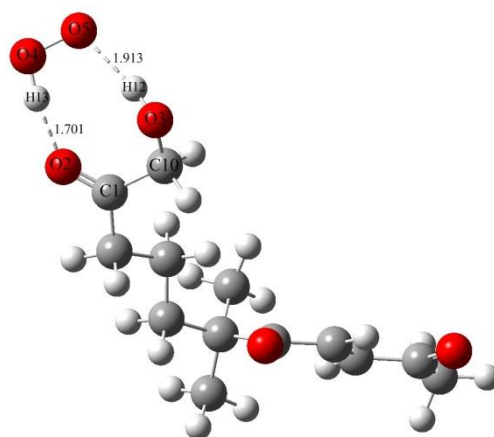
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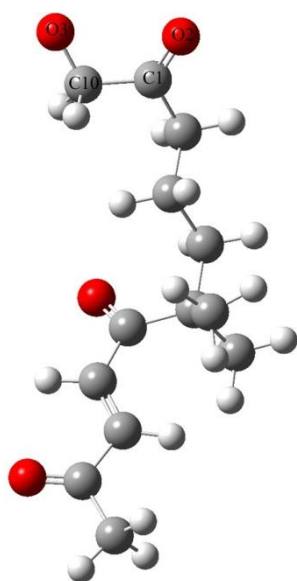
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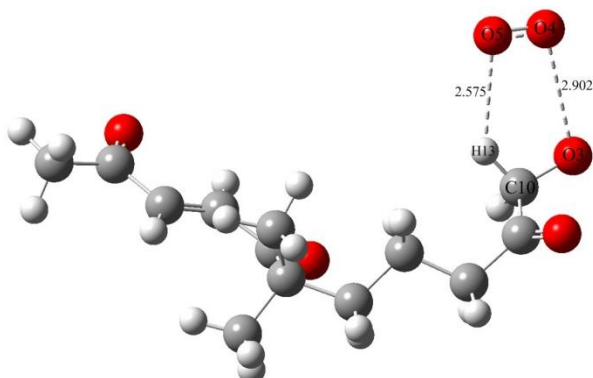
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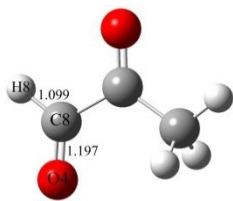
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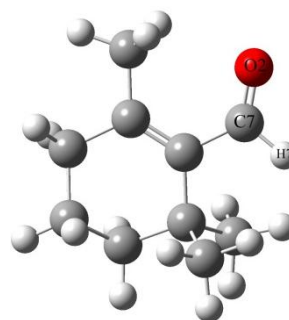
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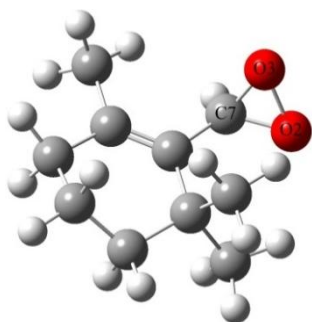
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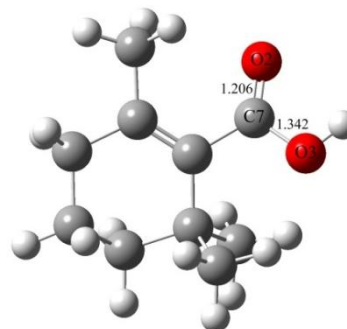
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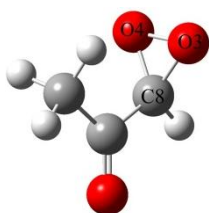
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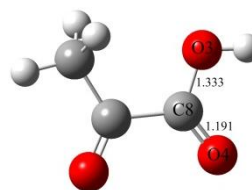
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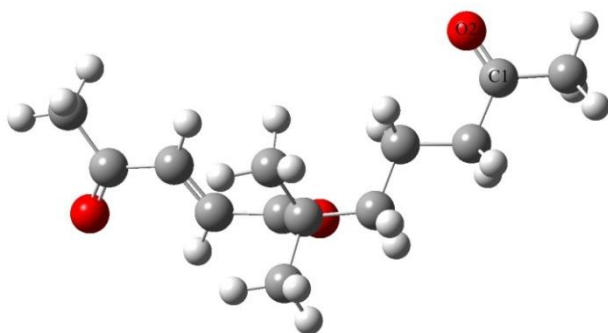
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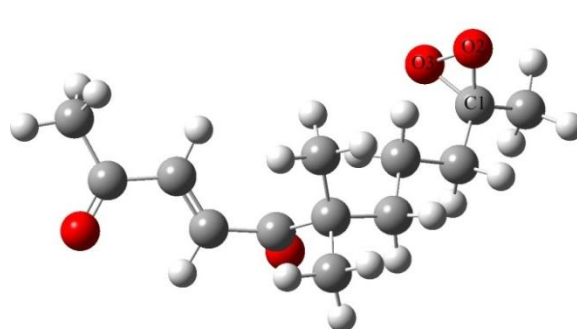
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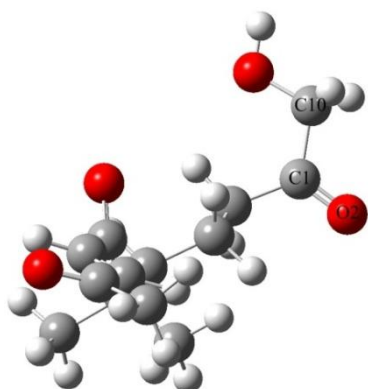
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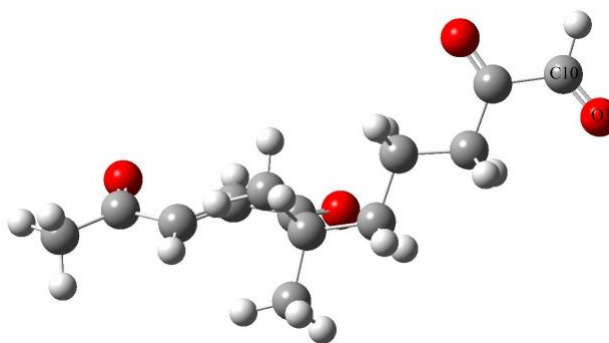
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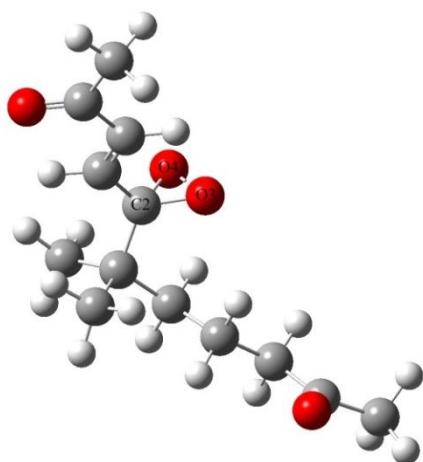
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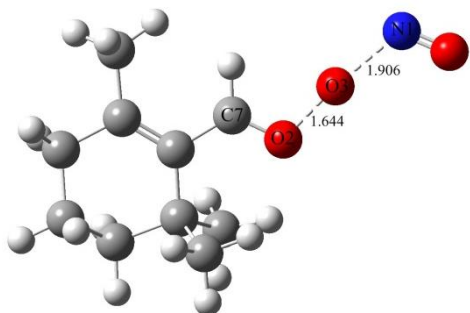


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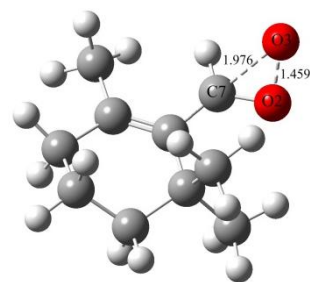


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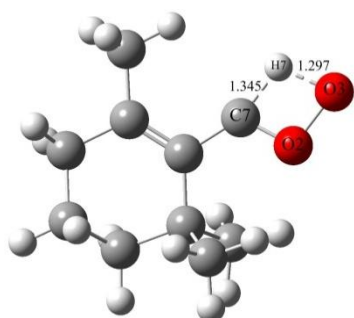
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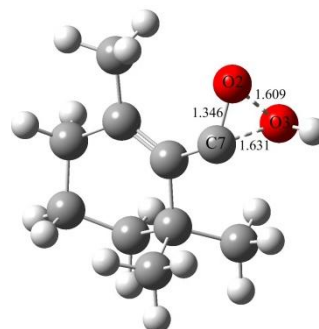
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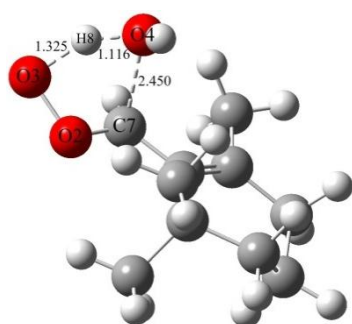
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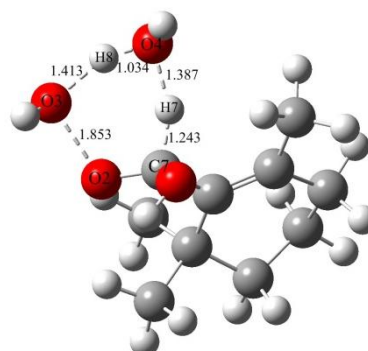
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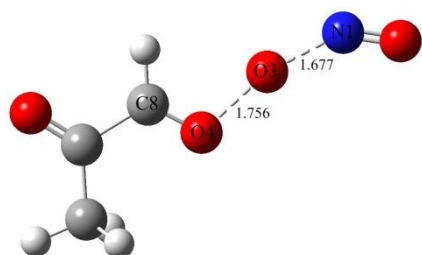
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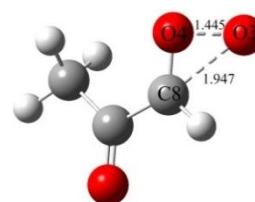
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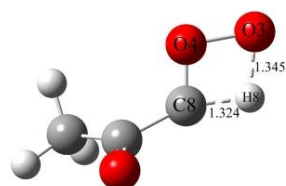
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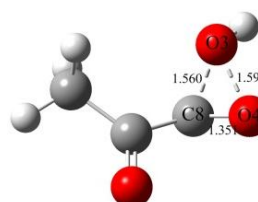
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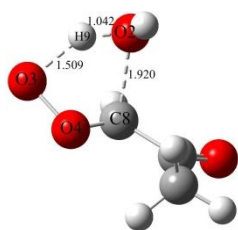
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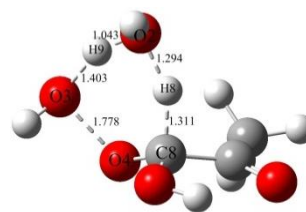
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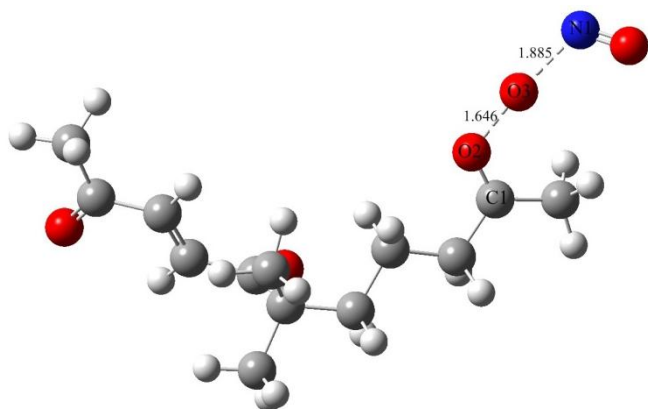
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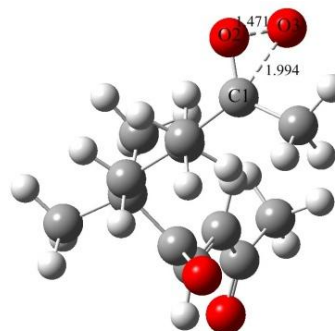
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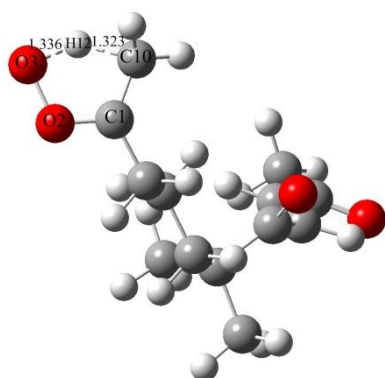
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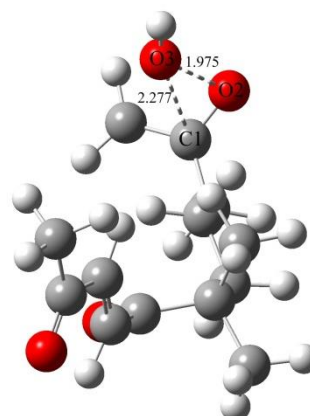
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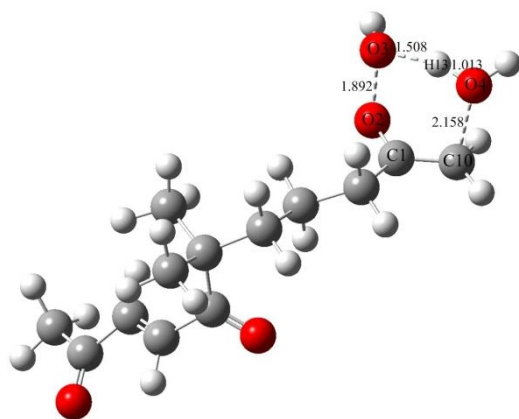
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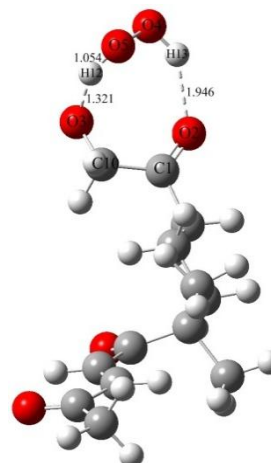
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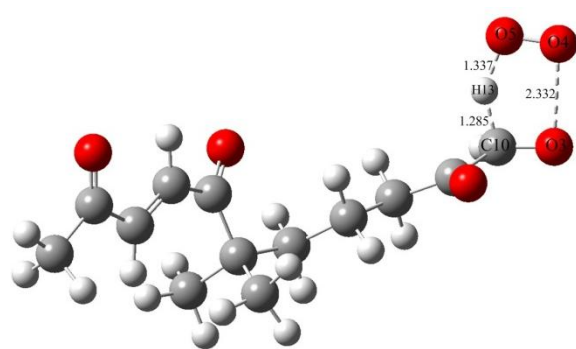
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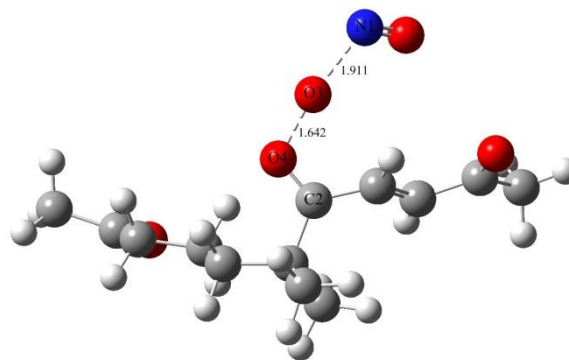
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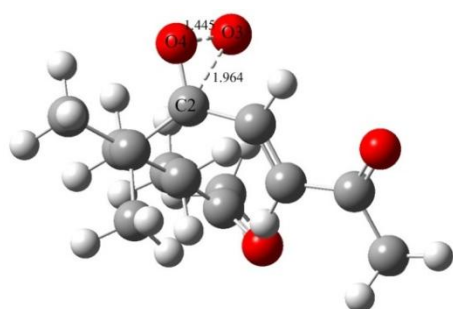
TS24



TS25



TS26



TS27

Fig. S4 MPWB1K/6-31+G(d,p) optimized geometries with the bond lengths (\AA) for the transition states involved in the secondary reactions of β -ionone with O_3 .

Table S Cartesian coordinates (bohr) for the optimized stationary points

| Optimized stationary points | Cartesian coordinates (bohr) | | | |
|-----------------------------|------------------------------|-------------|-------------|-------------|
| IM1 | C | -3.84760800 | 1.57468900 | -0.66670500 |
| | H | -4.80995300 | 1.22477800 | -1.02023100 |
| | H | -3.92585900 | 1.85686500 | 0.38227100 |
| | H | -3.54763800 | 2.46287300 | -1.21944700 |
| | C | -2.82455200 | 0.49041800 | -0.81428300 |
| | C | -1.44282200 | 0.82875900 | -0.44312000 |
| | H | -1.28458900 | 1.77635100 | 0.04291000 |
| | C | -0.45338900 | -0.04067800 | -0.73504900 |
| | H | -0.81289300 | -0.92148100 | -1.24783100 |
| | C | 0.96763900 | -0.00250700 | -0.46003000 |
| | C | 1.66144000 | -1.13458100 | -0.72473300 |
| | C | 3.09664100 | -1.31528700 | -0.34966200 |
| | H | 3.21390200 | -2.31708700 | 0.06653000 |
| | H | 3.69016400 | -1.31502400 | -1.26970300 |
| | C | 3.60819900 | -0.26740700 | 0.60756900 |
| | H | 4.69412200 | -0.30583600 | 0.66816500 |
| | H | 3.23178700 | -0.47098200 | 1.60936500 |
| | C | 3.14337900 | 1.08782500 | 0.13609200 |
| | H | 3.56465300 | 1.88576800 | 0.74780300 |
| | H | 3.50811600 | 1.24738500 | -0.88139300 |
| | C | 1.62072800 | 1.23343500 | 0.14144900 |
| | C | 1.31961600 | 2.47569000 | -0.69836500 |
| | H | 1.56786500 | 2.30136500 | -1.74354500 |
| | H | 0.28428200 | 2.79282100 | -0.65215700 |
| | H | 1.93082100 | 3.30401400 | -0.34199300 |
| | C | 1.14448200 | 1.44693300 | 1.57862300 |
| | H | 1.52750100 | 2.39253700 | 1.96115900 |
| | H | 0.06229700 | 1.45888700 | 1.65935500 |
| | H | 1.49570500 | 0.65044100 | 2.22985800 |
| | O | -3.12969300 | -0.62283100 | -1.19221100 |
| | C | 1.06116900 | -2.34505100 | -1.37742600 |
| | H | 0.36896800 | -2.85193400 | -0.70548500 |
| H | 0.51739200 | -2.10932300 | -2.28785900 | |
| H | 1.84293000 | -3.05338100 | -1.63716800 | |
| O | -2.28111500 | -0.29261800 | 1.92274100 | |
| O | -2.30460000 | -1.42709900 | 1.43256800 | |
| O | -1.21573100 | -1.93276000 | 1.14605600 | |
| IM2 | C | 4.16774400 | -0.37062600 | -0.47227500 |
| | H | 4.76689600 | -0.59319600 | -1.34669100 |
| | H | 4.31308400 | 0.66241900 | -0.16170300 |
| | H | 4.47419500 | -0.98823200 | 0.36934400 |
| | C | 2.72806900 | -0.59553400 | -0.78287000 |
| | C | 1.72295700 | -0.37880200 | 0.33305800 |
| | H | 1.37804000 | -1.34608100 | 0.67539800 |
| | C | 0.58659200 | 0.57729000 | -0.11773300 |
| | H | 0.90020700 | 0.99746500 | -1.07197000 |

| | | | | |
|-----|---|-------------|-------------|-------------|
| | C | -0.86796900 | 0.18341900 | -0.19540000 |
| | C | -1.70510500 | 1.15562100 | -0.58785600 |
| | C | -3.19572700 | 1.00551200 | -0.55973400 |
| | H | -3.62802500 | 1.94921500 | -0.22514600 |
| | H | -3.55547100 | 0.86173100 | -1.58260700 |
| | C | -3.64319300 | -0.13719800 | 0.31647900 |
| | H | -4.70804100 | -0.32474700 | 0.19196000 |
| | H | -3.48766400 | 0.12235200 | 1.36370800 |
| | C | -2.83855500 | -1.35718800 | -0.05299800 |
| | H | -3.18519400 | -2.24186000 | 0.48166700 |
| | H | -2.98622500 | -1.55785400 | -1.11625100 |
| | C | -1.33768600 | -1.20149400 | 0.21527700 |
| | C | -0.67551800 | -2.29857300 | -0.62565400 |
| | H | -0.76960700 | -2.07390300 | -1.68535900 |
| | H | 0.37726100 | -2.46424500 | -0.42892400 |
| | H | -1.18523100 | -3.24204800 | -0.43298700 |
| | C | -1.08934400 | -1.42906600 | 1.70830700 |
| | H | -1.26133600 | -2.47450300 | 1.96213100 |
| | H | -0.08451800 | -1.16473800 | 2.02608800 |
| | H | -1.76456200 | -0.82031900 | 2.30474900 |
| | O | 2.31985900 | -0.94847400 | -1.85971600 |
| | C | -1.27667700 | 2.51811000 | -1.03683800 |
| | H | -1.40678700 | 3.23543700 | -0.22732100 |
| | H | -0.24308400 | 2.58313400 | -1.35623600 |
| | H | -1.91023000 | 2.84424000 | -1.86042000 |
| | O | 2.27670000 | 0.25045700 | 1.45834900 |
| | O | 2.03907800 | 1.61120100 | 1.17683400 |
| | O | 0.67845700 | 1.58767900 | 0.88328400 |
| IM3 | C | 4.65057200 | 0.32753700 | -0.52343600 |
| | H | 4.47406700 | 0.26617100 | -1.59613700 |
| | H | 4.79672300 | 1.37957200 | -0.28358400 |
| | H | 5.54039200 | -0.23392500 | -0.26555000 |
| | C | 3.46876300 | -0.21311300 | 0.22602400 |
| | C | 2.17667900 | 0.44971100 | -0.02757200 |
| | H | 2.17633400 | 1.26147500 | -0.73623300 |
| | C | 1.08070100 | 0.01452900 | 0.60939700 |
| | H | 1.28694900 | -0.81905700 | 1.26683800 |
| | C | -0.30868200 | 0.43311200 | 0.53232600 |
| | C | -1.20781000 | -0.31546400 | 1.21607800 |
| | C | -2.68356500 | -0.09742400 | 1.11651600 |
| | H | -3.16872200 | -1.07207100 | 1.05100900 |
| | H | -3.03440400 | 0.34160100 | 2.05629100 |
| | C | -3.06265100 | 0.78041800 | -0.04881800 |
| | H | -4.11528000 | 1.05188300 | 0.00091100 |
| | H | -2.91927700 | 0.22642000 | -0.97742100 |
| | C | -2.18344000 | 2.00593000 | -0.02237500 |
| | H | -2.49128600 | 2.73610400 | -0.77103700 |
| | H | -2.29155000 | 2.49101900 | 0.95061900 |
| | C | -0.70821000 | 1.67602400 | -0.25471800 |
| | C | 0.08289400 | 2.88694200 | 0.24413100 |
| | H | 0.00019400 | 2.98021500 | 1.32528000 |

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|-----|---|-------------|-------------|-------------|
| | H | 1.13706200 | 2.84697200 | -0.00545900 |
| | H | -0.32852700 | 3.79075700 | -0.20386100 |
| | C | -0.48453800 | 1.49750600 | -1.75710200 |
| | H | -0.58884200 | 2.45832400 | -2.25984700 |
| | H | 0.49859200 | 1.10012400 | -1.98808300 |
| | H | -1.21213600 | 0.81283000 | -2.18499100 |
| | O | 3.58371100 | -1.14431900 | 0.99367800 |
| | C | -0.82638100 | -1.44087000 | 2.13739800 |
| | H | -0.45118600 | -2.31093100 | 1.60018900 |
| | H | -0.06226000 | -1.15055200 | 2.85306400 |
| | H | -1.69763300 | -1.76759800 | 2.69823600 |
| | O | -0.55667800 | -1.63460200 | -1.94706700 |
| | O | -0.77958900 | -2.55599300 | -1.16868300 |
| | O | -1.93684300 | -2.71738200 | -0.78009300 |
| IM4 | C | 4.49029500 | -0.00359400 | 1.00362600 |
| | H | 4.39228200 | 0.89388000 | 1.61256000 |
| | H | 4.34383100 | -0.85565200 | 1.66577900 |
| | H | 5.48074100 | -0.04444300 | 0.56720200 |
| | C | 3.45320300 | -0.00882900 | -0.07819400 |
| | C | 2.04016600 | 0.04371900 | 0.36860700 |
| | H | 1.86000800 | 0.13144300 | 1.42924400 |
| | C | 1.06118600 | -0.04090100 | -0.52548200 |
| | H | 1.36374500 | -0.14774800 | -1.56056100 |
| | C | -0.42732400 | 0.02912500 | -0.33441200 |
| | C | -1.04892500 | -1.14184100 | 0.51066700 |
| | C | -2.34691200 | -0.73889200 | 1.19006500 |
| | H | -2.88466000 | -1.66079800 | 1.40795600 |
| | H | -2.13661400 | -0.27098600 | 2.15006000 |
| | C | -3.17402600 | 0.15761600 | 0.30167200 |
| | H | -4.14039600 | 0.35251800 | 0.76125400 |
| | H | -3.36668300 | -0.38126600 | -0.62279800 |
| | C | -2.46884600 | 1.47239300 | -0.00935700 |
| | H | -2.76738900 | 1.79922100 | -1.00306800 |
| | H | -2.79776200 | 2.24989600 | 0.67966300 |
| | C | -0.92867200 | 1.43775400 | 0.04865000 |
| | C | -0.41702600 | 1.84005400 | 1.42891000 |
| | H | -0.62763000 | 1.10591300 | 2.20224500 |
| | H | 0.65362700 | 2.02189000 | 1.41286800 |
| | H | -0.89695100 | 2.77069100 | 1.72323800 |
| | C | -0.39405000 | 2.45373600 | -0.95629300 |
| | H | -0.80877900 | 3.43465100 | -0.73034400 |
| | H | 0.69025400 | 2.52923700 | -0.91296000 |
| | H | -0.68182400 | 2.19055700 | -1.97108700 |
| | O | 3.75278800 | -0.05576000 | -1.24750200 |
| | C | -0.12728000 | -1.85858800 | 1.46586700 |
| | H | 0.71548000 | -2.30012400 | 0.94650500 |
| | H | 0.24390300 | -1.18485500 | 2.23491600 |
| | H | -0.68631100 | -2.65090900 | 1.95692900 |
| | O | -1.00700200 | -0.24291400 | -1.60471200 |
| | O | -0.82128300 | -1.61857200 | -1.68782100 |
| | O | -1.45195400 | -2.06195700 | -0.51440900 |

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| IM5 | C | -1.45324000 | 0.79689600 | 0.01371400 | |
| | H | -1.74764400 | 1.83669100 | 0.01601100 | |
| | C | -0.09167500 | 0.35683400 | 0.08345200 | |
| | C | 0.86346300 | 1.31905000 | 0.08688000 | |
| | C | 2.31629500 | 0.98575100 | -0.00512800 | |
| | H | 2.78983900 | 1.71018900 | -0.66960600 | |
| | H | 2.76377100 | 1.16028600 | 0.97838400 | |
| | C | 2.57765000 | -0.43127400 | -0.45292800 | |
| | H | 3.62920800 | -0.67896400 | -0.32536100 | |
| | H | 2.35679900 | -0.53005400 | -1.51549800 | |
| | C | 1.70182700 | -1.35906200 | 0.35297700 | |
| | H | 1.92808700 | -2.40297400 | 0.13986700 | |
| | H | 1.90845200 | -1.20402800 | 1.41443500 | |
| | C | 0.21099600 | -1.13540500 | 0.10030500 | |
| | C | -0.54227900 | -1.82930400 | 1.23549100 | |
| | H | -0.37045500 | -1.32262900 | 2.18349200 | |
| | H | -1.61050300 | -1.87883100 | 1.05947200 | |
| | H | -0.17219300 | -2.84898000 | 1.33174700 | |
| | C | -0.18687300 | -1.77215400 | -1.23107000 | |
| | H | 0.01645000 | -2.84129100 | -1.19716900 | |
| | H | -1.24481900 | -1.64107300 | -1.43577200 | |
| | H | 0.37439500 | -1.34695600 | -2.06028100 | |
| | C | 0.61407800 | 2.79285200 | 0.14631300 | |
| | H | -0.33134300 | 3.08200700 | 0.58704700 | |
| | H | 1.40330900 | 3.26106600 | 0.73107400 | |
| | H | 0.67191600 | 3.22413400 | -0.85325500 | |
| | O | -3.65262100 | 0.51824600 | -0.19467800 | |
| | O | -2.40071900 | -0.00870700 | -0.10089900 | |
| | IM6 | C | -1.34220500 | 1.27609300 | 0.00017100 |
| | | H | -2.41706900 | 1.40447600 | -0.02129200 |
| | | H | -0.92726200 | 1.74980500 | 0.88702800 |
| | | H | -0.88819300 | 1.76155800 | -0.86051200 |
| C | | -1.03034000 | -0.18189100 | -0.00035800 | |
| C | | 0.38773900 | -0.59718300 | 0.00128700 | |
| H | | 0.69678600 | -1.63350500 | 0.00426700 | |
| O | | -1.85843200 | -1.05846500 | -0.00078100 | |
| O | | 1.25572700 | 0.29906800 | -0.00129700 | |
| O | | 2.53327700 | -0.02365900 | 0.00006700 | |
| IM7 | C | -4.87186500 | 2.41774000 | 0.55962000 | |
| | H | -4.71367200 | 2.29129400 | 1.62958600 | |
| | H | -4.25155400 | 3.25491200 | 0.24315800 | |
| | H | -5.91425100 | 2.63837900 | 0.36570400 | |
| | C | -4.46609300 | 1.17637500 | -0.17025400 | |
| | C | -3.05483500 | 0.73876600 | 0.00030900 | |
| | H | -2.42550400 | 1.31255500 | 0.66503100 | |
| | C | -2.59773800 | -0.30314400 | -0.68330800 | |
| | H | -3.28037100 | -0.79455900 | -1.36706400 | |
| | C | -1.18766200 | -0.78305500 | -0.71979800 | |
| | C | 4.09282100 | 0.41096100 | -0.18531800 | |
| | C | 3.16216700 | -0.73974200 | -0.25050400 | |
| | H | 3.14218500 | -1.08854800 | -1.28549500 | |

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| | H | 3.62050300 | -1.55526500 | 0.31654200 |
| | C | 1.75943000 | -0.45561300 | 0.24315600 |
| | H | 1.30829500 | 0.30038800 | -0.39634000 |
| | H | 1.81187000 | -0.03046500 | 1.24353900 |
| | C | 0.90655900 | -1.71045400 | 0.24369100 |
| | H | 1.00936200 | -2.22201800 | -0.71223100 |
| | H | 1.26620200 | -2.39607800 | 1.01349000 |
| | C | -0.57636800 | -1.46127100 | 0.49695100 |
| | C | -0.78964500 | -0.66452900 | 1.77880300 |
| | H | -0.41326200 | 0.35306400 | 1.70218900 |
| | H | -1.84024600 | -0.62506900 | 2.05189400 |
| | H | -0.25491500 | -1.15334200 | 2.59159600 |
| | C | -1.30509700 | -2.80151700 | 0.62367200 |
| | H | -0.93258400 | -3.33537200 | 1.49575500 |
| | H | -2.37682500 | -2.66110600 | 0.75194900 |
| | H | -1.14086500 | -3.42441100 | -0.25297500 |
| | O | -5.23544600 | 0.55279400 | -0.86014100 |
| | C | 5.47852700 | 0.37130200 | -0.65791000 |
| | H | 6.13274600 | 0.64560100 | 0.16922800 |
| | H | 5.73676600 | -0.59736200 | -1.06849200 |
| | H | 5.61395000 | 1.16719000 | -1.38981700 |
| | O | -0.59864300 | -0.70449400 | -1.77050400 |
| | O | 4.50730000 | 2.52766500 | 0.38737900 |
| | O | 3.65190800 | 1.46719700 | 0.31302700 |
| IMS | C | -4.75944100 | -2.11158400 | -0.89271900 |
| | H | -5.80077000 | -2.28292000 | -0.64970300 |
| | H | -4.66055800 | -1.87853300 | -1.95178100 |
| | H | -4.18408100 | -3.01786600 | -0.70995400 |
| | C | -4.21962800 | -0.98949000 | -0.06370600 |
| | C | -2.79507300 | -0.62441300 | -0.28847000 |
| | H | -2.27640000 | -1.09520300 | -1.10912900 |
| | C | -2.18874500 | 0.20421000 | 0.55833300 |
| | H | -2.73190600 | 0.54603900 | 1.43293200 |
| | C | -0.81497300 | 0.66397900 | 0.50075600 |
| | C | 4.34401800 | -1.04620500 | -0.09040400 |
| | C | 3.54619200 | 0.22438400 | 0.04405300 |
| | H | 3.61701000 | 0.57741800 | 1.07405200 |
| | H | 4.05656600 | 0.98250000 | -0.55716200 |
| | C | 2.10580900 | 0.07503800 | -0.38855400 |
| | H | 1.60692000 | -0.61548800 | 0.29064300 |
| | H | 2.08815000 | -0.39486200 | -1.36936300 |
| | C | 1.38207500 | 1.40813900 | -0.41331400 |
| | H | 1.55218700 | 1.93995400 | 0.52175000 |
| | H | 1.79827200 | 2.03326900 | -1.20533200 |
| | C | -0.12475900 | 1.31937500 | -0.66539600 |
| | C | -0.40482000 | 0.59306300 | -1.97580200 |
| | H | -0.15232200 | -0.46315500 | -1.92909900 |
| | H | -1.44425200 | 0.69383300 | -2.27443700 |
| | H | 0.20608700 | 1.04378600 | -2.75533100 |
| | C | -0.70338800 | 2.73610900 | -0.75725100 |
| | H | -0.26591100 | 3.24660300 | -1.61288100 |

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| | H | -1.78258700 | 2.71467100 | -0.89143100 |
| | H | -0.47717100 | 3.31037900 | 0.13785600 |
| | O | -4.89087700 | -0.40158400 | 0.74755200 |
| | C | 5.69472700 | -1.06553900 | 0.55983000 |
| | H | 6.26419500 | -1.91758800 | 0.20790100 |
| | H | 6.23756700 | -0.14262000 | 0.36895400 |
| | H | 5.56719300 | -1.14487900 | 1.63866500 |
| | O | -0.18815400 | 0.69018200 | 1.58790400 |
| | O | -0.78427600 | 0.15408900 | 2.67676200 |
| | O | 3.91453800 | -1.99990500 | -0.68987800 |
| IM9 | C | 1.46953200 | 0.84303700 | -0.08009000 |
| | H | 3.46069400 | 1.34558900 | -0.00317900 |
| | C | 0.10550100 | 0.35433600 | -0.09846800 |
| | C | -0.82453600 | 1.34435300 | -0.08076600 |
| | C | -2.28878100 | 1.06483000 | 0.02146000 |
| | H | -2.73258500 | 1.79322600 | 0.70114400 |
| | H | -2.72711900 | 1.28075400 | -0.95784600 |
| | C | -2.61079200 | -0.35171600 | 0.43285800 |
| | H | -3.66888800 | -0.55644100 | 0.28255300 |
| | H | -2.41419800 | -0.48255200 | 1.49657600 |
| | C | -1.75612800 | -1.29470600 | -0.37816700 |
| | H | -2.02487600 | -2.33412800 | -0.18997500 |
| | H | -1.94075400 | -1.11072600 | -1.43932100 |
| | C | -0.26289600 | -1.12659700 | -0.10120500 |
| | C | 0.47770800 | -1.87009700 | -1.21289500 |
| | H | 0.33387500 | -1.37746600 | -2.17294300 |
| | H | 1.54246200 | -1.94894300 | -1.02383400 |
| | H | 0.07794500 | -2.88047500 | -1.29306600 |
| | C | 0.08477400 | -1.76836800 | 1.24211200 |
| | H | -0.17723300 | -2.82571200 | 1.22166300 |
| | H | 1.14610500 | -1.69102300 | 1.45565800 |
| | H | -0.45594600 | -1.30103400 | 2.06187800 |
| | C | -0.51113400 | 2.80065500 | -0.14457900 |
| | H | 0.51864400 | 2.99192900 | -0.41075300 |
| | H | -1.17942800 | 3.28054100 | -0.85919000 |
| | H | -0.71121300 | 3.26048000 | 0.82336200 |
| | O | 3.64905000 | 0.40979300 | 0.17919300 |
| | O | 2.30757800 | -0.08709100 | 0.15902200 |
| IM10 | C | -1.21089200 | 0.03721100 | -0.39567100 |
| | H | -1.82304400 | 0.87977300 | -0.67789800 |
| | C | 0.17797400 | 0.17066400 | -0.08898500 |
| | C | 0.66545000 | 1.43703500 | -0.11609900 |
| | C | 2.12714900 | 1.71036700 | -0.00117400 |
| | H | 2.37730000 | 2.50374700 | -0.70755100 |
| | H | 2.31071100 | 2.13856300 | 0.98901200 |
| | C | 2.98105000 | 0.48344700 | -0.21159700 |
| | H | 4.01425500 | 0.69348300 | 0.05604500 |
| | H | 2.97781100 | 0.20902200 | -1.26635300 |
| | C | 2.42356500 | -0.64308600 | 0.62475300 |
| | H | 3.06823000 | -1.52035000 | 0.58777100 |
| | H | 2.39123100 | -0.32218400 | 1.66839200 |

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| | C | 1.01981400 | -1.06399500 | 0.19272600 |
| | C | 0.42124200 | -1.87910700 | 1.33975000 |
| | H | 0.23708200 | -1.25060000 | 2.20893100 |
| | H | -0.50708300 | -2.36615200 | 1.06377300 |
| | H | 1.13257800 | -2.65111400 | 1.63002700 |
| | C | 1.09955500 | -1.93920800 | -1.05731600 |
| | H | 1.67094100 | -2.83941300 | -0.83720300 |
| | H | 0.11194800 | -2.24535100 | -1.39056800 |
| | H | 1.58886700 | -1.41955300 | -1.87840000 |
| | C | -0.16403900 | 2.67319100 | -0.26884900 |
| | H | -1.18041400 | 2.58139000 | 0.09649300 |
| | H | 0.31117300 | 3.48402700 | 0.27899100 |
| | H | -0.19251300 | 2.98258300 | -1.31407200 |
| | O | -3.12991600 | -1.05203300 | -0.73163600 |
| | O | -1.78753900 | -1.07116500 | -0.39897400 |
| | O | -3.56411700 | 1.10617600 | 0.82812500 |
| | H | -3.65112000 | 0.28832200 | 0.30009900 |
| | H | -4.23059600 | 1.07086600 | 1.50715600 |
| IM11 | C | -1.39734400 | 0.58769500 | -0.02290200 |
| | H | -1.62580000 | 1.47987500 | -0.59644800 |
| | C | 0.08055700 | 0.28750100 | -0.02385900 |
| | C | 0.90645200 | 1.33960600 | -0.08881700 |
| | C | 2.39651800 | 1.20628200 | -0.12695900 |
| | H | 2.78068700 | 1.87779600 | -0.89707000 |
| | H | 2.79556300 | 1.58964500 | 0.81671700 |
| | C | 2.86833600 | -0.21021500 | -0.35530100 |
| | H | 3.92703100 | -0.29972000 | -0.11914000 |
| | H | 2.75955300 | -0.47314500 | -1.40673500 |
| | C | 2.04600400 | -1.14338700 | 0.50177400 |
| | H | 2.42129200 | -2.16526300 | 0.44437100 |
| | H | 2.13666000 | -0.83135400 | 1.54517100 |
| | C | 0.56796500 | -1.14782700 | 0.11385400 |
| | C | -0.18691400 | -1.87521300 | 1.22663900 |
| | H | -0.05587900 | -1.36998000 | 2.18565700 |
| | H | -1.24691100 | -1.96755300 | 1.00639900 |
| | H | 0.21650200 | -2.88025100 | 1.34264400 |
| | C | 0.38705800 | -1.93045800 | -1.18881700 |
| | H | 0.78817600 | -2.93659300 | -1.06779900 |
| | H | -0.65871300 | -2.00997700 | -1.46350400 |
| | H | 0.91108400 | -1.45283400 | -2.01282600 |
| | C | 0.43359500 | 2.76419200 | -0.11952900 |
| | H | -0.47457000 | 2.92366200 | 0.45233300 |
| | H | 1.20138500 | 3.41317800 | 0.29630300 |
| | H | 0.26090700 | 3.09831600 | -1.14323800 |
| | O | -3.42827800 | -0.05018700 | -0.75621400 |
| | O | -2.09337200 | -0.47189600 | -0.61411300 |
| | O | -1.92095100 | 0.83015000 | 1.25549300 |
| | H | -3.70830600 | 0.03404500 | 0.16221200 |
| | H | -1.50120700 | 0.23656000 | 1.87710500 |
| IM12 | C | -1.79138500 | -1.07595400 | -0.03545600 |
| | H | -2.82453300 | -0.84201100 | -0.26492800 |

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| | H | -1.36596600 | -1.69285000 | -0.82531800 |
| | H | -1.73367000 | -1.64338200 | 0.89064100 |
| | C | -1.01645400 | 0.19322800 | 0.08476800 |
| | C | 0.39123800 | 0.07144800 | 0.56175400 |
| | H | 2.47459600 | -0.01817600 | 0.91566200 |
| | O | -1.46379800 | 1.29687400 | -0.08635500 |
| | O | 1.15810700 | -0.04313800 | -0.41506800 |
| | O | 2.54933800 | -0.12072500 | -0.04638300 |
| IM13 | C | -0.01072300 | 0.04233600 | -0.50285000 |
| | H | -0.56819800 | 0.75097200 | -1.09995600 |
| | C | 1.40741200 | 0.26564500 | -0.11759600 |
| | O | -1.83293700 | -1.23517800 | -0.42355000 |
| | O | -0.55043700 | -1.00383600 | -0.10834800 |
| | O | -2.23170600 | 1.30819300 | 0.53843800 |
| | H | -2.52166900 | 0.42578400 | 0.27776300 |
| | H | -2.86450800 | 1.64038400 | 1.16791300 |
| | O | 1.95132400 | 1.23133100 | -0.58700400 |
| | C | 2.04845600 | -0.70455800 | 0.81340900 |
| | H | 3.08271100 | -0.42003100 | 0.96046700 |
| | H | 1.52300900 | -0.70769200 | 1.76597900 |
| | H | 1.98783900 | -1.71403400 | 0.41376200 |
| IM14 | C | 0.29607700 | -0.46988400 | -0.14450200 |
| | H | 0.53382200 | -1.15172000 | -0.95341400 |
| | C | -1.17735800 | -0.07102600 | -0.21421700 |
| | O | 2.36212000 | 0.37621900 | -0.49940400 |
| | O | 1.01701900 | 0.71579300 | -0.26814700 |
| | O | 0.61266800 | -1.12351800 | 1.03799200 |
| | H | 2.65449500 | 0.08296800 | 0.36930400 |
| | H | 0.30606800 | -0.60966700 | 1.78546100 |
| | O | -1.92539500 | -0.71415600 | -0.89713400 |
| | C | -1.60612700 | 1.11017500 | 0.59574000 |
| | H | -1.09036000 | 1.99631800 | 0.23169300 |
| | H | -2.67883200 | 1.23589900 | 0.51461700 |
| | H | -1.33203700 | 0.99589700 | 1.64375100 |
| IM15 | C | -4.87674600 | -2.45068400 | -0.52475000 |
| | H | -4.73176200 | -2.32896000 | -1.59713400 |
| | H | -4.24065100 | -3.27612500 | -0.20881800 |
| | H | -5.91357700 | -2.68594100 | -0.31854200 |
| | C | -4.48290400 | -1.19766400 | 0.19289900 |
| | C | -3.08133500 | -0.73914700 | 0.00249100 |
| | H | -2.44765800 | -1.31572200 | -0.65488300 |
| | C | -2.63705600 | 0.32816500 | 0.65617400 |
| | H | -3.32273400 | 0.82181300 | 1.33490200 |
| | C | -1.23741900 | 0.84002600 | 0.68518900 |
| | C | 4.09534900 | -0.35871400 | 0.43990600 |
| | C | 3.18976300 | 0.81396100 | 0.28111000 |
| | H | 3.19514900 | 1.37126200 | 1.21449200 |
| | H | 3.60316600 | 1.46844000 | -0.48829900 |
| | C | 1.76375700 | 0.43286800 | -0.09008600 |
| | H | 1.34461700 | -0.18420400 | 0.70366800 |
| | H | 1.78471800 | -0.16865100 | -0.99749700 |

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| | C | 0.89801000 | 1.66077500 | -0.29613700 |
| | H | 0.96469100 | 2.29941500 | 0.58355000 |
| | H | 1.28549900 | 2.23812400 | -1.13827100 |
| | C | -0.57435100 | 1.37419400 | -0.57431900 |
| | C | -0.73474400 | 0.44436700 | -1.77118800 |
| | H | -0.37721800 | -0.56203600 | -1.56589500 |
| | H | -1.76941500 | 0.38702100 | -2.09740300 |
| | H | -0.14891300 | 0.83719200 | -2.60048500 |
| | C | -1.29728300 | 2.68960500 | -0.87895100 |
| | H | -0.88955400 | 3.12318300 | -1.79007200 |
| | H | -2.36368400 | 2.53253600 | -1.03154600 |
| | H | -1.16471500 | 3.40687300 | -0.07203000 |
| | O | -5.25636300 | -0.58323200 | 0.88628700 |
| | C | 4.70618900 | -0.73979100 | 1.55119200 |
| | H | 5.36404600 | -1.58912000 | 1.57832000 |
| | H | 4.55015500 | -0.16831500 | 2.44943900 |
| | H | 4.44990000 | -2.82061100 | -0.75550000 |
| | O | -0.70281400 | 0.90918900 | 1.76542700 |
| | O | 5.06595500 | -2.08592200 | -0.70701800 |
| | O | 4.19829000 | -0.98677800 | -0.76834300 |
| IM16 | C | -3.43698500 | 0.32470800 | -0.42874500 |
| | C | -2.28350400 | 1.25990200 | -0.61722400 |
| | H | -2.17336500 | 1.40711900 | -1.69444900 |
| | H | -2.56647700 | 2.21812100 | -0.18836900 |
| | C | -0.96140600 | 0.76361400 | -0.04845900 |
| | H | -0.66488300 | -0.15674600 | -0.54783000 |
| | H | -1.09065400 | 0.53416900 | 1.00946900 |
| | C | 0.12684600 | 1.80583300 | -0.22955700 |
| | H | 0.14674700 | 2.11719200 | -1.27244900 |
| | H | -0.12191500 | 2.68822600 | 0.36271700 |
| | C | 1.53656800 | 1.36756700 | 0.17063000 |
| | C | 1.53688300 | 0.85787000 | 1.61020000 |
| | H | 1.05115400 | -0.11109000 | 1.69973400 |
| | H | 2.53672300 | 0.76087900 | 2.01923500 |
| | H | 0.99296900 | 1.56218800 | 2.23756900 |
| | C | 2.45357900 | 2.58515200 | 0.03587000 |
| | H | 2.12648800 | 3.35996900 | 0.72664700 |
| | H | 3.49125000 | 2.35800500 | 0.26035800 |
| | H | 2.40970000 | 2.99101500 | -0.97220100 |
| | C | -3.20863500 | -1.13962200 | -0.69390700 |
| | H | -2.56221100 | -1.50478000 | 0.11524700 |
| | H | -2.62527200 | -1.23784900 | -1.60898100 |
| | O | -4.51967300 | 0.73785700 | -0.07128300 |
| | O | -4.36007200 | -1.87962800 | -0.83796900 |
| | H | -4.90643300 | -1.82310600 | -0.04564800 |
| | O | -6.27958800 | -1.51037600 | 1.24942400 |
| | O | -6.69784300 | -0.29558900 | 1.06925900 |
| | H | -5.98946000 | 0.14384800 | 0.54422800 |
| | C | 6.50730500 | -0.99842300 | 1.17624400 |
| | H | 6.93757500 | -0.03142800 | 0.91986600 |
| | H | 6.14593800 | -0.92563400 | 2.20096200 |

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| | H | 7.26692100 | -1.76731000 | 1.10898800 |
| | C | 5.37426000 | -1.31668000 | 0.25257400 |
| | C | 4.24181600 | -0.34754300 | 0.23540900 |
| | H | 4.31929600 | 0.50892500 | 0.88661200 |
| | C | 3.20585000 | -0.55263800 | -0.57237600 |
| | H | 3.23835100 | -1.42517100 | -1.21237500 |
| | C | 2.01244200 | 0.29935000 | -0.80923000 |
| | O | 5.36464800 | -2.30195700 | -0.44234600 |
| | O | 1.41845900 | 0.10955800 | -1.84682000 |
| IM17 | C | -4.31937500 | -0.11579700 | 0.25731300 |
| | C | -3.30431100 | 0.83654600 | -0.30805400 |
| | H | -3.35201800 | 0.78257900 | -1.39748000 |
| | H | -3.60231600 | 1.83864600 | -0.01038000 |
| | C | -1.88086800 | 0.53374200 | 0.14313000 |
| | H | -1.58112400 | -0.45439700 | -0.20257200 |
| | H | -1.84703600 | 0.52496400 | 1.23294000 |
| | C | -0.90781300 | 1.56291900 | -0.40110200 |
| | H | -1.01413400 | 1.61108900 | -1.48343600 |
| | H | -1.17345300 | 2.54613900 | -0.00861400 |
| | C | 0.56578000 | 1.32220700 | -0.06843600 |
| | C | 0.74571300 | 1.19184800 | 1.44223900 |
| | H | 0.37626500 | 0.24039700 | 1.81753400 |
| | H | 1.78189200 | 1.28460600 | 1.74873000 |
| | H | 0.18708200 | 1.98423500 | 1.93759200 |
| | C | -4.08465600 | -1.59510500 | -0.05101500 |
| | H | -3.30613100 | -1.93338300 | 0.65334400 |
| | H | -3.65092100 | -1.73403800 | -1.04859700 |
| | O | -5.25618000 | 0.23795100 | 0.91558500 |
| | O | -5.14213600 | -2.39470900 | 0.18202400 |
| | C | 1.03763300 | 0.07416800 | -0.80698900 |
| | O | 0.37000600 | -0.40069500 | -1.69847100 |
| | C | 2.31398400 | -0.62300800 | -0.50467900 |
| | H | 2.36331300 | -1.61779000 | -0.92881200 |
| | C | 3.39576700 | -0.17356100 | 0.12437000 |
| | H | 3.46001700 | 0.81378900 | 0.55404000 |
| | C | 4.60077800 | -1.04306500 | 0.24108800 |
| | C | 5.78685800 | -0.44621100 | 0.93055000 |
| | H | 5.52091800 | -0.15036800 | 1.94427400 |
| | H | 6.59827700 | -1.16283500 | 0.95853400 |
| | H | 6.10762000 | 0.45424700 | 0.40882900 |
| | O | 4.60703600 | -2.16589200 | -0.19849000 |
| | C | 1.35934300 | 2.51921700 | -0.59732200 |
| | H | 2.42949300 | 2.41659500 | -0.44403500 |
| | H | 1.18467300 | 2.65774900 | -1.66188300 |
| | H | 1.03477500 | 3.42113500 | -0.08174800 |
| IM18 | C | 3.76642800 | -0.98996900 | -0.07002200 |
| | C | 2.56581500 | -1.88334500 | -0.19940800 |
| | H | 2.48690500 | -2.20496600 | -1.23969100 |
| | H | 2.75097600 | -2.76401800 | 0.41030400 |
| | C | 1.26663700 | -1.19928700 | 0.20785000 |
| | H | 1.08079200 | -0.34174000 | -0.43695800 |

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| | H | 1.36575900 | -0.82716100 | 1.22774400 |
| | C | 0.09246800 | -2.15604500 | 0.10930500 |
| | H | 0.08901700 | -2.60843200 | -0.88082300 |
| | H | 0.22913500 | -2.96430800 | 0.82974600 |
| | C | -1.28475100 | -1.54090200 | 0.36483500 |
| | C | -1.30734400 | -0.84852600 | 1.72535100 |
| | H | -0.73640800 | 0.07703900 | 1.72322600 |
| | H | -2.31338300 | -0.61013900 | 2.05348700 |
| | H | -0.86710700 | -1.50971800 | 2.46983300 |
| | C | -2.31137300 | -2.67549300 | 0.32996600 |
| | H | -2.09017400 | -3.38427100 | 1.12568600 |
| | H | -3.32961900 | -2.32584800 | 0.47181000 |
| | H | -2.26759400 | -3.20718800 | -0.61780700 |
| | C | 3.71722400 | 0.30736200 | -0.87896100 |
| | H | 3.09642100 | 1.00475000 | -0.28991500 |
| | H | 3.18154400 | 0.17355300 | -1.82636000 |
| | O | 4.70908300 | -1.25117400 | 0.62219700 |
| | O | 4.90433400 | 0.92328000 | -1.02489800 |
| | O | 3.57518600 | 3.15774500 | 1.03958300 |
| | O | 4.66868600 | 3.31573500 | 0.59999100 |
| | C | -6.04075600 | 1.39905700 | 0.73955200 |
| | H | -6.55563600 | 0.45608100 | 0.56158200 |
| | H | -5.75285200 | 1.41213900 | 1.78974900 |
| | H | -6.70808900 | 2.22626300 | 0.53185800 |
| | C | -4.82540800 | 1.49113800 | -0.12832300 |
| | C | -3.80549200 | 0.41844400 | 0.04530300 |
| | H | -4.01247700 | -0.33862900 | 0.78516700 |
| | C | -2.71099100 | 0.41768600 | -0.70959400 |
| | H | -2.61719800 | 1.20420800 | -1.44758600 |
| | C | -1.60607600 | -0.57372600 | -0.76954900 |
| | O | -4.66720700 | 2.38152600 | -0.92594100 |
| | O | -0.95612000 | -0.58535700 | -1.79079200 |
| P1 | C | 0.85008800 | 1.27310000 | 0.00077800 |
| | H | 0.47097100 | 1.73323200 | 0.91114500 |
| | H | 1.92271500 | 1.40490700 | -0.06688600 |
| | H | 0.34697900 | 1.77001800 | -0.82521600 |
| | C | 0.51789900 | -0.17658000 | -0.00035900 |
| | C | -0.95473700 | -0.55647400 | 0.00619500 |
| | H | -1.14038500 | -1.64014000 | 0.02031600 |
| | O | 1.32004700 | -1.07318700 | -0.00408900 |
| | O | -1.83002000 | 0.25965000 | -0.00579200 |
| P2 | C | 1.24757000 | -1.53207500 | 0.13770100 |
| | H | 0.69171000 | -2.46705100 | 0.30932400 |
| | C | 0.41058700 | -0.33658900 | -0.01197300 |
| | C | 0.97064400 | 0.88882100 | -0.06715400 |
| | C | 0.13897500 | 2.13239000 | -0.07950700 |
| | H | 0.60980600 | 2.85908500 | 0.58376900 |
| | H | 0.20511500 | 2.57079700 | -1.08006600 |
| | C | -1.30427000 | 1.90243700 | 0.30238500 |
| | H | -1.90000900 | 2.78467200 | 0.07666000 |
| | H | -1.37634800 | 1.74294000 | 1.37828800 |

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| | C | -1.82672200 | 0.69500800 | -0.43814300 |
| | H | -2.89266500 | 0.55148800 | -0.26056900 |
| | H | -1.70704900 | 0.86292300 | -1.51089400 |
| | C | -1.08899700 | -0.58530400 | -0.05602000 |
| | C | -1.42582500 | -1.63313500 | -1.11757400 |
| | H | -1.01968900 | -1.34932300 | -2.08646800 |
| | H | -1.05052000 | -2.62292600 | -0.86946300 |
| | H | -2.50759600 | -1.71487300 | -1.21650900 |
| | C | -1.57909700 | -1.08526400 | 1.30194400 |
| | H | -2.64233400 | -1.31871800 | 1.25809100 |
| | H | -1.05549800 | -1.99015300 | 1.60497800 |
| | H | -1.42312800 | -0.34201500 | 2.08010900 |
| | C | 2.44472200 | 1.13247000 | -0.11026100 |
| | H | 2.91922200 | 0.58763800 | -0.92062100 |
| | H | 2.64468500 | 2.19492200 | -0.22305800 |
| | H | 2.92827600 | 0.77786100 | 0.79799300 |
| | O | 2.45631200 | -1.57497800 | 0.11375600 |
| P3 | C | 1.58017300 | 0.80967200 | -0.29369800 |
| | H | 1.77820100 | 1.60141300 | -1.00625400 |
| | C | 0.17578700 | 0.33688900 | -0.19899400 |
| | C | -0.78736300 | 1.26767800 | -0.16750800 |
| | C | -2.23339000 | 0.91891700 | 0.01288000 |
| | H | -2.68828500 | 1.65425300 | 0.67765300 |
| | H | -2.73976000 | 1.03942900 | -0.94931700 |
| | C | -2.43616800 | -0.48297600 | 0.53693400 |
| | H | -3.48580700 | -0.76386600 | 0.47458200 |
| | H | -2.16066300 | -0.52335000 | 1.59067200 |
| | C | -1.57684700 | -1.43273800 | -0.26219500 |
| | H | -1.76301900 | -2.46855500 | 0.02149400 |
| | H | -1.84521300 | -1.34313200 | -1.31756000 |
| | C | -0.08145600 | -1.15640400 | -0.10966100 |
| | C | 0.62226600 | -1.90426900 | -1.24259500 |
| | H | 0.37650800 | -1.46760500 | -2.20936300 |
| | H | 1.70095600 | -1.91648700 | -1.12761600 |
| | H | 0.28157200 | -2.93913600 | -1.25124800 |
| | C | 0.41398800 | -1.69525800 | 1.23248300 |
| | H | 0.26789000 | -2.77445300 | 1.27050700 |
| | H | 1.46987500 | -1.48795900 | 1.37490700 |
| | H | -0.12868400 | -1.24826500 | 2.06214800 |
| | C | -0.54930400 | 2.74294200 | -0.25063700 |
| | H | 0.45344400 | 3.02891000 | -0.54507500 |
| | H | -1.24988100 | 3.19174000 | -0.95390400 |
| | H | -0.74377700 | 3.20123800 | 0.71887300 |
| | O | 2.33374500 | 0.91723600 | 0.86686000 |
| | O | 2.63007100 | -0.06859800 | -0.16342800 |
| P4 | C | 0.12456400 | 1.41419000 | -0.02897000 |
| | C | -0.32388700 | 0.14626300 | 0.01192800 |
| | C | -1.78642200 | -0.05870100 | -0.01228400 |
| | H | -3.12232200 | -1.23389600 | -0.53392200 |
| | O | -2.61938700 | 0.70556800 | 0.40746800 |
| | O | -2.16283300 | -1.21399700 | -0.58166400 |

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| | C | 1.58638000 | 1.73880400 | -0.05266600 |
| | H | 1.75337500 | 2.49183500 | -0.82357100 |
| | H | 1.81924600 | 2.24021700 | 0.89187800 |
| | C | -0.75119500 | 2.63032000 | -0.03955500 |
| | H | -1.56402200 | 2.55134600 | -0.75493800 |
| | H | -1.22017700 | 2.77496900 | 0.93017100 |
| | H | -0.15999800 | 3.51121600 | -0.27498100 |
| | C | 2.49281100 | 0.54776800 | -0.25396000 |
| | H | 3.51201500 | 0.79909000 | 0.03332100 |
| | H | 2.52526500 | 0.28100200 | -1.30952300 |
| | C | 1.97502300 | -0.61318000 | 0.55866400 |
| | H | 2.65296700 | -1.46489000 | 0.50468700 |
| | H | 1.92369900 | -0.31602600 | 1.60875300 |
| | C | 0.58823700 | -1.07103700 | 0.11035100 |
| | C | 0.69571900 | -1.80834200 | -1.22416500 |
| | H | -0.26857200 | -2.19212300 | -1.53895800 |
| | H | 1.06860800 | -1.15862500 | -2.01195600 |
| | H | 1.38117100 | -2.64947600 | -1.12309100 |
| | C | 0.07709500 | -2.04164600 | 1.17402200 |
| | H | -0.85541700 | -2.51300900 | 0.88101500 |
| | H | 0.81486100 | -2.82772500 | 1.32940400 |
| | H | -0.07287900 | -1.53312400 | 2.12507700 |
| P5 | C | -1.06393700 | 1.29951700 | 0.04103100 |
| | H | -2.06110700 | 1.49416400 | 0.41647100 |
| | H | -0.31007500 | 1.78737800 | 0.65178600 |
| | H | -0.97506200 | 1.70588100 | -0.96519600 |
| | C | -0.83035000 | -0.17009500 | -0.01301900 |
| | C | 0.60428100 | -0.63184100 | -0.09421500 |
| | H | 0.74873100 | -1.69232400 | -0.26263000 |
| | O | -1.69271600 | -1.00732700 | -0.00300700 |
| | O | 1.48784600 | -0.00770100 | 0.75392200 |
| | O | 1.49706400 | 0.22995500 | -0.68131700 |
| P6 | C | -1.59151500 | 0.95483200 | 0.00237000 |
| | H | -2.63265800 | 0.65677900 | -0.00064900 |
| | H | -1.37449500 | 1.56398500 | 0.87701000 |
| | H | -1.37078600 | 1.57106500 | -0.86628000 |
| | C | -0.73117900 | -0.26249100 | -0.00033300 |
| | C | 0.79309800 | -0.06202000 | 0.00039700 |
| | H | 2.07862100 | 1.29520900 | -0.00290100 |
| | O | -1.14227900 | -1.38532400 | -0.00298700 |
| | O | 1.58263900 | -0.95373200 | 0.00321100 |
| | O | 1.11925200 | 1.23043600 | -0.00294800 |
| P7 | C | -3.50908000 | 0.24192000 | -0.17190400 |
| | H | -3.57141500 | 0.54796800 | -1.21779300 |
| | H | -4.01826800 | 1.03114200 | 0.38911600 |
| | C | -2.07131600 | 0.10614100 | 0.27287500 |
| | H | -1.57783100 | -0.63189000 | -0.35746400 |
| | H | -2.05964500 | -0.29384500 | 1.28458500 |
| | C | -1.32902700 | 1.42718900 | 0.20320400 |
| | H | -1.49042800 | 1.88405600 | -0.77233100 |
| | H | -1.73699500 | 2.11420200 | 0.94785900 |

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| | C | 0.17462400 | 1.32918300 | 0.43936300 |
| | C | 0.48102900 | 0.62957300 | 1.75870000 |
| | H | 0.21750700 | -0.42536900 | 1.74252300 |
| | H | 1.53039200 | 0.72146400 | 2.02514200 |
| | H | -0.10205100 | 1.10063900 | 2.54828400 |
| | C | 0.77567900 | 2.73690400 | 0.48359200 |
| | H | 0.36920200 | 3.27573200 | 1.33732300 |
| | H | 1.85824800 | 2.70518600 | 0.59358900 |
| | H | 0.53557400 | 3.29634700 | -0.41793600 |
| | C | -4.31674300 | -1.01502300 | 0.01143700 |
| | O | -3.89098400 | -1.95713300 | 0.63192800 |
| | C | -5.67667400 | -1.04054900 | -0.62153200 |
| | H | -6.21046700 | -0.10910200 | -0.44732400 |
| | H | -5.56425300 | -1.14830000 | -1.69957400 |
| | H | -6.24793400 | -1.87890400 | -0.24053500 |
| | C | 4.82092500 | -2.07836800 | 0.70397500 |
| | H | 4.69298700 | -1.83939500 | 1.75864700 |
| | H | 4.26400900 | -2.99498900 | 0.51565500 |
| | H | 5.87039600 | -2.23446600 | 0.48688500 |
| | C | 4.28110800 | -0.96955100 | -0.14392800 |
| | C | 2.84623000 | -0.62992300 | 0.04588400 |
| | H | 2.29419300 | -1.17338400 | 0.79841400 |
| | C | 2.27588200 | 0.29020100 | -0.72301700 |
| | H | 2.88747200 | 0.75304800 | -1.48878300 |
| | C | 0.83062700 | 0.65261400 | -0.75387600 |
| | O | 4.96752500 | -0.37429700 | -0.93863100 |
| | O | 0.24342400 | 0.48368100 | -1.79516100 |
| P8 | C | -1.80680200 | 0.27575300 | 0.17312600 |
| | H | -1.83157100 | -0.18360800 | 1.15941400 |
| | H | -1.32419400 | -0.43220100 | -0.49716400 |
| | C | -4.11876600 | -0.69516900 | -0.13070200 |
| | O | -4.03472500 | -1.35659200 | 1.08045100 |
| | O | -3.50769500 | -1.93388700 | -0.15325400 |
| | C | -5.47936300 | -0.63279200 | -0.73959800 |
| | H | -6.02667000 | 0.22234300 | -0.35097300 |
| | H | -5.40136000 | -0.52374000 | -1.81820400 |
| | H | -6.01935300 | -1.54358100 | -0.50710700 |
| | C | -3.22920800 | 0.50208900 | -0.29302100 |
| | H | -3.69116600 | 1.32030600 | 0.26330900 |
| | H | -3.24228400 | 0.80092100 | -1.34126800 |
| | C | -1.01887600 | 1.57187300 | 0.20799800 |
| | H | -1.42265000 | 2.22342500 | 0.98593500 |
| | H | -1.13870000 | 2.09639700 | -0.73915300 |
| | C | 0.47287300 | 1.40124300 | 0.47488400 |
| | C | 0.71578600 | 0.60841400 | 1.75344300 |
| | H | 0.39309800 | -0.42643000 | 1.66631200 |
| | H | 1.76423600 | 0.62265000 | 2.03791100 |
| | H | 0.14600800 | 1.06235900 | 2.56253200 |
| | C | 1.12593100 | 2.77857600 | 0.62100500 |
| | H | 2.20284400 | 2.69746100 | 0.75847600 |
| | H | 0.93455600 | 3.39966500 | -0.25142000 |

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| | H | 0.71540300 | 3.28176200 | 1.49427000 |
| | C | 1.13709200 | 0.77340000 | -0.74032100 |
| | C | 2.56439700 | 0.34700100 | -0.68579000 |
| | H | 3.23313500 | 0.85917900 | -1.36788600 |
| | C | 3.05599200 | -0.67270400 | 0.00786100 |
| | H | 2.44378900 | -1.26480100 | 0.67222400 |
| | C | 4.48370900 | -1.05696500 | -0.14715500 |
| | C | 4.93250300 | -2.26945000 | 0.60662800 |
| | H | 4.34648800 | -3.13511800 | 0.30172100 |
| | H | 5.98375500 | -2.45326400 | 0.42222600 |
| | H | 4.76326400 | -2.13029600 | 1.67331700 |
| | O | 0.57775300 | 0.69650200 | -1.80720100 |
| | O | 5.23463600 | -0.41615600 | -0.84182500 |
| P9 | C | 5.22379600 | -2.07553300 | 0.59506900 |
| | H | 5.11706100 | -1.86310900 | 1.65773600 |
| | H | 4.66706800 | -2.98990500 | 0.39584200 |
| | H | 6.26921700 | -2.22076700 | 0.35231900 |
| | C | 4.66114300 | -0.94874800 | -0.21334500 |
| | C | 3.22783800 | -0.62476200 | 0.01072000 |
| | H | 2.69425100 | -1.18811900 | 0.76217500 |
| | C | 2.63644900 | 0.30530000 | -0.72949400 |
| | H | 3.23176700 | 0.78832400 | -1.49578200 |
| | C | 1.18707300 | 0.65334900 | -0.72550700 |
| | C | -3.89008100 | -1.07568600 | 0.14647900 |
| | C | -3.12432700 | 0.19809500 | -0.02048700 |
| | H | -3.22130100 | 0.51098600 | -1.06159700 |
| | H | -3.65314200 | 0.97147200 | 0.54126400 |
| | C | -1.67697000 | 0.07791800 | 0.39398700 |
| | H | -1.19011200 | -0.66274100 | -0.23781900 |
| | H | -1.63418900 | -0.30863100 | 1.41071400 |
| | C | -0.95356600 | 1.40752100 | 0.29099700 |
| | H | -1.15243300 | 1.85220300 | -0.68315400 |
| | H | -1.34826200 | 2.09686400 | 1.04042200 |
| | C | 0.55796900 | 1.33271200 | 0.48073400 |
| | C | 0.91650200 | 0.65194400 | 1.79629900 |
| | H | 0.65434600 | -0.40355100 | 1.80229100 |
| | H | 1.97536500 | 0.74784700 | 2.02054100 |
| | H | 0.36276800 | 1.13189400 | 2.60152700 |
| | C | 1.14066600 | 2.74884600 | 0.48880200 |
| | H | 0.75337400 | 3.29388500 | 1.34749800 |
| | H | 2.22649300 | 2.73269200 | 0.56577200 |
| | H | 0.86537100 | 3.29304700 | -0.41197300 |
| | O | 5.32915100 | -0.32807700 | -1.00448000 |
| | C | -5.33914100 | -1.09244500 | -0.27917100 |
| | H | -5.91721700 | -1.48715900 | 0.55770000 |
| | H | -5.41678000 | -1.80501900 | -1.10322800 |
| | O | 0.57485000 | 0.47131800 | -1.74973200 |
| | O | -3.40526500 | -2.08471500 | 0.59379600 |
| | O | -5.75313100 | 0.19107800 | -0.65277300 |
| | H | -6.65257800 | 0.16188200 | -0.96722800 |

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| P10 | C | -0.98704100 | 1.30821500 | -0.15882500 |
| | H | -1.31675800 | 2.23290600 | 0.31928600 |
| | H | -1.14357200 | 1.43079500 | -1.22903500 |
| | C | -4.14952500 | -0.79714900 | 0.42512800 |
| | C | -5.60907900 | -0.79122500 | -0.00205500 |
| | H | -6.20008500 | -1.62204300 | 0.41052500 |
| | O | -6.07042000 | 0.04874000 | -0.71905200 |
| | O | -3.79765200 | -1.66919800 | 1.17676100 |
| | C | -3.26833400 | 0.27844100 | -0.11167200 |
| | H | -3.71003300 | 1.23507900 | 0.17758800 |
| | H | -3.34875900 | 0.25994800 | -1.20017300 |
| | C | -1.83314600 | 0.15422500 | 0.34529800 |
| | H | -1.43240500 | -0.79177500 | -0.01310300 |
| | H | -1.81257500 | 0.10726300 | 1.43269600 |
| | C | 5.90544900 | -0.20700200 | 0.71107100 |
| | H | 6.13104800 | 0.74554900 | 0.23396400 |
| | H | 5.66452200 | 0.00625200 | 1.75150600 |
| | H | 6.77036100 | -0.85680400 | 0.66082900 |
| | C | 4.73804500 | -0.85524600 | 0.03504400 |
| | C | 3.46769300 | -0.07788700 | 0.02116500 |
| | H | 3.47995300 | 0.89069300 | 0.49608500 |
| | C | 2.38914300 | -0.57728400 | -0.57472800 |
| | H | 2.48622900 | -1.54321500 | -1.05369500 |
| | C | 1.05751400 | 0.04933500 | -0.78342000 |
| | C | 0.51583100 | 1.17550400 | 0.09228200 |
| | C | 0.77875700 | 0.92354900 | 1.57433300 |
| | H | 0.46937800 | -0.07385900 | 1.87731600 |
| | H | 1.82423000 | 1.03962100 | 1.83936300 |
| | H | 0.20947200 | 1.64090400 | 2.16338100 |
| | C | 1.17891800 | 2.48099300 | -0.35287100 |
| | H | 0.79935200 | 3.30126900 | 0.25352900 |
| | H | 2.25956100 | 2.46337800 | -0.24611200 |
| | H | 0.94757600 | 2.69499200 | -1.39393100 |
| O | 4.81105700 | -1.94758500 | -0.47084400 | |
| O | 0.40916000 | -0.37542700 | -1.71243000 | |
| P11 | C | -4.94687100 | -2.34824300 | 0.01868000 |
| | H | -5.96221000 | -2.35624800 | -0.35810400 |
| | H | -4.36649800 | -3.13343500 | -0.46339900 |
| | H | -4.94506900 | -2.56256200 | 1.08622200 |
| | C | -4.31468900 | -1.01680000 | -0.23675000 |
| | C | -2.91757400 | -0.84549200 | 0.23678400 |
| | H | -2.41055900 | -1.68195700 | 0.69579100 |
| | C | -2.30919500 | 0.32507500 | 0.11303200 |
| | H | -2.84378900 | 1.14357600 | -0.34934800 |
| | C | -0.92236500 | 0.57110000 | 0.57466300 |
| | C | 4.39202000 | -1.04718600 | -0.26568900 |
| | C | 3.54764300 | 0.06693700 | 0.29206500 |
| | H | 3.46145600 | -0.07211600 | 1.37165800 |
| | H | 4.11410800 | 0.99422100 | 0.16797000 |
| | C | 2.18654000 | 0.17403700 | -0.35567500 |
| | H | 1.63924400 | -0.74852600 | -0.17528600 |

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| | H | 2.32114400 | 0.24272500 | -1.43303900 |
| | C | 1.41071000 | 1.36781900 | 0.16984600 |
| | H | 1.42343900 | 1.36951800 | 1.26005000 |
| | H | 1.91633700 | 2.28221700 | -0.14651800 |
| | C | -0.04856800 | 1.47278700 | -0.28046100 |
| | C | -0.21362900 | 1.10867900 | -1.75007100 |
| | H | 0.01910100 | 0.06362800 | -1.93923500 |
| | H | -1.22860400 | 1.29555500 | -2.09426300 |
| | H | 0.45802800 | 1.71477900 | -2.35476300 |
| | C | -0.53652800 | 2.90007600 | -0.04580000 |
| | H | 0.01883000 | 3.58412200 | -0.68328100 |
| | H | -1.59241500 | 3.01833700 | -0.28194800 |
| | H | -0.38143500 | 3.19783000 | 0.98910400 |
| | O | -4.90154100 | -0.12155100 | -0.79652600 |
| | C | 5.68281000 | -1.33588200 | 0.44285700 |
| | H | 6.29258000 | -2.00232500 | -0.15579700 |
| | H | 6.22694700 | -0.41921800 | 0.65863800 |
| | H | 5.46744000 | -1.81271300 | 1.39810600 |
| | O | -0.77876500 | 0.71979700 | 1.94729000 |
| | O | -0.32665900 | -0.47508700 | 1.24515000 |
| | O | 4.04572700 | -1.68251500 | -1.23009500 |
| TS1 | C | 3.95207600 | -1.24432400 | -0.85091100 |
| | H | 4.89169600 | -0.80697800 | -1.16575800 |
| | H | 4.07434500 | -1.71487500 | 0.12280200 |
| | H | 3.65046500 | -2.01864000 | -1.55381200 |
| | C | 2.90329400 | -0.18215700 | -0.76199700 |
| | C | 1.55026700 | -0.60010500 | -0.34945800 |
| | H | 1.40051200 | -1.62899300 | -0.07717000 |
| | C | 0.51216700 | 0.28551800 | -0.55305700 |
| | H | 0.84084000 | 1.20503100 | -1.01297100 |
| | C | -0.91669900 | 0.10400400 | -0.40906800 |
| | C | -1.67359800 | 1.21350800 | -0.58465800 |
| | C | -3.14117500 | 1.24773800 | -0.30564700 |
| | H | -3.36546100 | 2.18443900 | 0.20602600 |
| | H | -3.67015200 | 1.30697300 | -1.26236300 |
| | C | -3.62516700 | 0.06306100 | 0.49298900 |
| | H | -4.71259400 | 0.02172700 | 0.49258700 |
| | H | -3.31465500 | 0.17149800 | 1.53165500 |
| | C | -3.03897500 | -1.19145200 | -0.10296500 |
| | H | -3.43402100 | -2.08357800 | 0.38307300 |
| | H | -3.33537500 | -1.24990700 | -1.15297700 |
| | C | -1.51196600 | -1.24103500 | -0.01830700 |
| | C | -1.08825400 | -2.34303800 | -0.99205000 |
| | H | -1.26769900 | -2.03743700 | -2.02101500 |
| | H | -0.04729000 | -2.63214600 | -0.90604100 |
| | H | -1.68357900 | -3.23465700 | -0.79916700 |
| | C | -1.09817700 | -1.61207200 | 1.40530100 |
| | H | -1.42998600 | -2.62369300 | 1.63695500 |
| | H | -0.02384000 | -1.55943000 | 1.55268700 |
| | H | -1.54143600 | -0.93348000 | 2.12978200 |
| | O | 3.14040400 | 0.98689200 | -0.97412700 |

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| | C | -1.10994100 | 2.53515900 | -1.01223100 |
| | H | -0.47521700 | 2.95723100 | -0.23327200 |
| | H | -0.51016700 | 2.46359000 | -1.91603600 |
| | H | -1.91300900 | 3.24012400 | -1.20652300 |
| | O | 2.14446000 | -0.17569200 | 1.68598000 |
| | O | 2.04704800 | 1.08130600 | 1.61368600 |
| | O | 0.86602700 | 1.45304000 | 1.36244900 |
| TS2 | C | -4.62213500 | 0.71172800 | 0.12859500 |
| | H | -4.51372000 | 1.16363900 | 1.11335000 |
| | H | -4.68475400 | 1.52605300 | -0.59158900 |
| | H | -5.52968200 | 0.12147000 | 0.09428700 |
| | C | -3.43682800 | -0.15490700 | -0.17315400 |
| | C | -2.11966800 | 0.51381900 | -0.16576100 |
| | H | -2.11237300 | 1.57622500 | 0.01066300 |
| | C | -1.01343000 | -0.21750500 | -0.35414200 |
| | H | -1.22442000 | -1.27035500 | -0.48904500 |
| | C | 0.39354500 | 0.13489100 | -0.33494800 |
| | C | 1.27871200 | -0.81259100 | -0.86136200 |
| | C | 2.75340700 | -0.59389600 | -0.78375800 |
| | H | 3.21772700 | -1.55624300 | -0.57175400 |
| | H | 3.11904100 | -0.28937900 | -1.76916900 |
| | C | 3.10888300 | 0.44231000 | 0.25133200 |
| | H | 4.18367900 | 0.60858200 | 0.27462400 |
| | H | 2.80289200 | 0.08673900 | 1.23507000 |
| | C | 2.37198100 | 1.70670000 | -0.11072700 |
| | H | 2.67002800 | 2.54528000 | 0.51769900 |
| | H | 2.64049100 | 1.97784800 | -1.13415200 |
| | C | 0.84881100 | 1.55558700 | -0.00347000 |
| | C | 0.25978700 | 2.51477900 | -1.04646800 |
| | H | 0.46782100 | 2.16554300 | -2.05611200 |
| | H | -0.81002800 | 2.65870900 | -0.95635300 |
| | H | 0.73237400 | 3.48866400 | -0.92671200 |
| | C | 0.42409300 | 1.98936000 | 1.39850600 |
| | H | 0.50444600 | 3.07203700 | 1.48319200 |
| | H | -0.59395300 | 1.69543600 | 1.63439800 |
| | H | 1.07216300 | 1.54332600 | 2.14809800 |
| | O | -3.55931400 | -1.33607200 | -0.40959200 |
| | C | 0.87037200 | -1.86093500 | -1.85284600 |
| | H | -0.11871900 | -2.27099900 | -1.69301000 |
| | H | 0.88357400 | -1.41673700 | -2.84882500 |
| | H | 1.58163300 | -2.68102900 | -1.84600400 |
| | O | 0.48643500 | -0.75347100 | 1.91379700 |
| | O | 0.37370400 | -1.93576900 | 1.49304600 |
| | O | 1.32500000 | -2.26479400 | 0.73031800 |
| TS3 | C | -3.41043500 | 1.40467700 | -0.09656700 |
| | H | -4.32336600 | 1.12037300 | 0.42357500 |
| | H | -3.40723200 | 2.47551600 | -0.26311300 |
| | H | -3.41705100 | 0.85196700 | -1.03308300 |
| | C | -2.24516900 | 1.01740300 | 0.75201000 |
| | C | -1.88894000 | -0.44926500 | 0.77362300 |
| | H | -1.23588600 | -0.72028500 | 1.60273000 |

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| | C | -0.64177200 | -0.47080000 | -0.64556400 |
| | H | -1.24435600 | 0.09228100 | -1.34380400 |
| | C | 0.68554600 | 0.03426800 | -0.30004200 |
| | C | 0.95573500 | 1.32713200 | -0.57346500 |
| | C | 2.27864300 | 1.95070500 | -0.24933600 |
| | H | 2.54096500 | 2.64479400 | -1.04762500 |
| | H | 2.13763000 | 2.56876100 | 0.64200000 |
| | C | 3.38221400 | 0.94937300 | -0.01510100 |
| | H | 4.25394300 | 1.44247600 | 0.41026100 |
| | H | 3.69855000 | 0.51598400 | -0.96336000 |
| | C | 2.87059700 | -0.12590300 | 0.91000100 |
| | H | 3.66058300 | -0.82884700 | 1.17300300 |
| | H | 2.53900900 | 0.33929200 | 1.84049100 |
| | C | 1.70712100 | -0.91935400 | 0.31591100 |
| | C | 1.13118200 | -1.75757100 | 1.45474700 |
| | H | 0.77100100 | -1.12576400 | 2.26388700 |
| | H | 0.32960800 | -2.41626000 | 1.13534500 |
| | H | 1.92583800 | -2.38289000 | 1.85895200 |
| | C | 2.23795700 | -1.86517200 | -0.76531900 |
| | H | 3.00719600 | -2.50833700 | -0.33977000 |
| | H | 1.45523700 | -2.50463000 | -1.16113400 |
| | H | 2.67492900 | -1.31674000 | -1.59629200 |
| | O | -1.60596500 | 1.78959500 | 1.41906500 |
| | C | 0.02599600 | 2.31756100 | -1.19863100 |
| | H | -0.95476700 | 1.94857000 | -1.46881500 |
| | H | -0.12281900 | 3.14769700 | -0.50981200 |
| | H | 0.48595600 | 2.72359400 | -2.09869200 |
| | O | -2.78141000 | -1.27111200 | 0.39378500 |
| | O | -2.00473100 | -2.05801100 | -1.16989200 |
| | O | -0.77127200 | -1.77870600 | -0.85524900 |
| TS4 | C | -4.13275400 | -0.27607500 | -0.35169000 |
| | H | -4.85796500 | -1.04245600 | -0.60111200 |
| | H | -4.31520200 | 0.08327000 | 0.65763200 |
| | H | -4.21927400 | 0.57792600 | -1.01629800 |
| | C | -2.77545900 | -0.89106400 | -0.39375300 |
| | C | -1.57430400 | -0.04208400 | -0.74078300 |
| | H | -0.97381700 | -0.41650100 | -1.55925000 |
| | C | -0.51643300 | -0.09709800 | 0.79530900 |
| | H | -0.76678300 | -1.15552700 | 0.92726900 |
| | C | 0.89613900 | 0.12870200 | 0.35149200 |
| | C | 1.41421100 | 1.34180600 | 0.11090000 |
| | C | 2.79488700 | 1.51443300 | -0.45039600 |
| | H | 2.76176100 | 2.31964000 | -1.18584600 |
| | H | 3.45296100 | 1.87391200 | 0.34593700 |
| | C | 3.35423600 | 0.24889400 | -1.05250300 |
| | H | 4.40712500 | 0.37371500 | -1.29844500 |
| | H | 2.83643300 | 0.02334200 | -1.98583500 |
| | C | 3.16009200 | -0.87227800 | -0.06236200 |
| | H | 3.64410800 | -1.79107700 | -0.39409600 |
| | H | 3.63652200 | -0.58887500 | 0.87872500 |
| | C | 1.68613900 | -1.16877800 | 0.20454200 |

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| | C | 1. 62742500 | -1. 97746400 | 1. 50296600 |
| | H | 1. 92098400 | -1. 36591700 | 2. 35356900 |
| | H | 0. 64252700 | -2. 39128700 | 1. 70536600 |
| | H | 2. 31837200 | -2. 81684300 | 1. 43507000 |
| | C | 1. 12230900 | -2. 03193200 | -0. 92500000 |
| | H | 1. 69409500 | -2. 95531900 | -1. 00639600 |
| | H | 0. 08560800 | -2. 31510900 | -0. 74521800 |
| | H | 1. 17954200 | -1. 51917800 | -1. 88458100 |
| | O | -2. 57944600 | -2. 06599700 | -0. 22011900 |
| | C | 0. 72323000 | 2. 64948300 | 0. 33466600 |
| | H | -0. 15018200 | 2. 58221100 | 0. 96518000 |
| | H | 1. 43035700 | 3. 34287500 | 0. 79057800 |
| | H | 0. 43209600 | 3. 08887800 | -0. 62004300 |
| | O | -1. 68425600 | 1. 26983700 | -0. 79740200 |
| | O | -2. 30072500 | 1. 71285700 | 0. 25748300 |
| | O | -1. 16526700 | 0. 69993400 | 1. 54722000 |
| TS5 | C | 4. 43777900 | 0. 60958000 | 0. 88961400 |
| | H | 4. 39282100 | 1. 69408200 | 0. 80231900 |
| | H | 4. 19570900 | 0. 36278500 | 1. 92228700 |
| | H | 5. 43714600 | 0. 26419600 | 0. 65470900 |
| | C | 3. 44615100 | -0. 02154300 | -0. 04095700 |
| | C | 2. 02595500 | 0. 34906700 | 0. 16688300 |
| | H | 1. 80633500 | 0. 98666500 | 1. 00738500 |
| | C | 1. 10096800 | -0. 11697000 | -0. 67120400 |
| | H | 1. 46307600 | -0. 75950400 | -1. 46501300 |
| | C | -0. 38353500 | 0. 05233200 | -0. 72456500 |
| | C | -0. 94197300 | -1. 24728100 | 0. 63657000 |
| | C | -1. 18068900 | -0. 48190100 | 1. 88945800 |
| | H | -1. 39638600 | -1. 17730000 | 2. 70218700 |
| | H | -0. 22770000 | -0. 02037800 | 2. 14586900 |
| | C | -2. 29465400 | 0. 55265400 | 1. 74280100 |
| | H | -2. 12714800 | 1. 33580100 | 2. 48032900 |
| | H | -3. 24810300 | 0. 09497800 | 1. 99670100 |
| | C | -2. 40114800 | 1. 15869400 | 0. 34535100 |
| | H | -3. 00620000 | 0. 52629800 | -0. 29937600 |
| | H | -2. 92429900 | 2. 11248100 | 0. 41656600 |
| | C | -1. 06718800 | 1. 40906600 | -0. 34508500 |
| | C | -0. 23824500 | 2. 36010400 | 0. 50908700 |
| | H | 0. 00722300 | 1. 97296600 | 1. 49445700 |
| | H | 0. 68174600 | 2. 65215300 | 0. 01156700 |
| | H | -0. 82482700 | 3. 26435300 | 0. 66454000 |
| | C | -1. 33813400 | 2. 12201600 | -1. 66876400 |
| | H | -1. 81444300 | 3. 08275800 | -1. 47931000 |
| | H | -0. 41105100 | 2. 30452200 | -2. 20937200 |
| | H | -1. 98542100 | 1. 52376000 | -2. 30170600 |
| | O | 3. 79066800 | -0. 78893400 | -0. 90901200 |
| | C | 0. 08072700 | -2. 33771400 | 0. 61864300 |
| | H | 0. 35123100 | -2. 62055400 | -0. 39045100 |
| | H | 0. 96636700 | -2. 04235300 | 1. 16629300 |
| | H | -0. 36778000 | -3. 20197100 | 1. 10956900 |
| | O | -0. 88248500 | -0. 50630900 | -1. 76793400 |

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| | O | -1.87847300 | -2.02414700 | -1.16134300 |
| | O | -2.08525700 | -1.53115500 | 0.02372200 |
| TS6 | C | 4.46310700 | 0.28269600 | 0.97166600 |
| | H | 5.45272700 | 0.07560000 | 0.58338900 |
| | H | 4.40114400 | 1.32291000 | 1.28766500 |
| | H | 4.27763500 | -0.33040800 | 1.85235800 |
| | C | 3.43287900 | -0.00128800 | -0.07824000 |
| | C | 2.02155000 | 0.24580400 | 0.30332800 |
| | H | 1.83609600 | 0.63368500 | 1.29162200 |
| | C | 1.05095700 | -0.05235000 | -0.55881000 |
| | H | 1.35415800 | -0.50486700 | -1.49655700 |
| | C | -0.39495300 | 0.15617400 | -0.45131300 |
| | C | -1.06145000 | -1.41478900 | 0.59665100 |
| | C | -2.32575300 | -0.83757200 | 1.22912200 |
| | H | -2.90460400 | -1.70035800 | 1.55799700 |
| | H | -2.07633900 | -0.27339900 | 2.12547000 |
| | C | -3.14114800 | -0.00874500 | 0.26697000 |
| | H | -4.14874000 | 0.12444600 | 0.65542300 |
| | H | -3.23972700 | -0.58117000 | -0.65346900 |
| | C | -2.53877500 | 1.36147600 | -0.02327100 |
| | H | -2.87304700 | 1.68030000 | -1.00874900 |
| | H | -2.92872200 | 2.09571700 | 0.68098200 |
| | C | -0.99919800 | 1.46708500 | 0.02702800 |
| | C | -0.50593700 | 1.85294500 | 1.42027400 |
| | H | -0.53422600 | 1.03702400 | 2.13548700 |
| | H | 0.50756300 | 2.24110800 | 1.38243500 |
| | H | -1.13686800 | 2.65029300 | 1.80539800 |
| | C | -0.56443900 | 2.57792200 | -0.93124600 |
| | H | -1.01952400 | 3.51803500 | -0.62371100 |
| | H | 0.51599800 | 2.70445100 | -0.92434300 |
| | H | -0.88261200 | 2.36368400 | -1.94842100 |
| | O | 3.73324800 | -0.40973300 | -1.17461200 |
| | C | 0.02532600 | -1.80086100 | 1.57265900 |
| | H | 0.85661200 | -2.26167800 | 1.05230200 |
| | H | 0.38615000 | -0.96321300 | 2.16319100 |
| | H | -0.39945700 | -2.53322800 | 2.25789000 |
| | O | -1.04402900 | -0.21823500 | -1.56662400 |
| | O | -0.69770200 | -1.40515800 | -1.94093100 |
| | O | -1.26866800 | -2.25061300 | -0.34849200 |
| TS7 | C | 0.70602800 | 0.43245100 | -0.11575900 |
| | H | 1.15743900 | 1.41803700 | -0.17849900 |
| | C | -0.72952300 | 0.27276800 | -0.11830400 |
| | C | -1.47277500 | 1.40411300 | -0.08627800 |
| | C | -2.95755600 | 1.36051000 | 0.07503200 |
| | H | -3.24931300 | 2.16287000 | 0.75436700 |
| | H | -3.40100400 | 1.62428200 | -0.89004500 |
| | C | -3.47528700 | 0.02093400 | 0.54033500 |
| | H | -4.55901600 | -0.01342700 | 0.45236400 |
| | H | -3.24067900 | -0.11911500 | 1.59514300 |
| | C | -2.82902700 | -1.06226700 | -0.28911500 |
| | H | -3.24747300 | -2.04110300 | -0.05793600 |

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|-----|---|-------------|-------------|-------------|
| | H | -3.04284100 | -0.87164600 | -1.34341700 |
| | C | -1.31619100 | -1.12989000 | -0.09550700 |
| | C | -0.74972100 | -1.96711600 | -1.24195100 |
| | H | -0.87602200 | -1.45784700 | -2.19584800 |
| | H | 0.30196600 | -2.19217800 | -1.10647800 |
| | H | -1.29330200 | -2.90948900 | -1.29312200 |
| | C | -0.98862700 | -1.81414900 | 1.23102700 |
| | H | -1.38939500 | -2.82672700 | 1.22793000 |
| | H | 0.08415400 | -1.87862000 | 1.38480700 |
| | H | -1.42164400 | -1.28125400 | 2.07480900 |
| | C | -0.95089700 | 2.80390700 | -0.17395200 |
| | H | 0.02135700 | 2.90756300 | -0.63679100 |
| | H | -1.65446200 | 3.40530500 | -0.74619800 |
| | H | -0.90457200 | 3.24515900 | 0.82146600 |
| | O | 3.02958900 | 0.08501400 | -0.00493400 |
| | O | 1.49372800 | -0.50159600 | -0.00821400 |
| | N | 4.86806900 | 0.58829600 | 0.03053800 |
| | O | 5.62915500 | -0.23560000 | 0.20946300 |
| TS8 | C | 1.48714100 | 0.76029400 | -0.27863300 |
| | H | 1.74961200 | 1.80661200 | -0.32022100 |
| | C | 0.12640400 | 0.33393100 | -0.21920300 |
| | C | -0.81765700 | 1.31004900 | -0.14842900 |
| | C | -2.25018400 | 0.99093000 | 0.11401600 |
| | H | -2.64725300 | 1.74594500 | 0.79440700 |
| | H | -2.79321200 | 1.13763400 | -0.82531400 |
| | C | -2.47318600 | -0.40820700 | 0.63632400 |
| | H | -3.53444400 | -0.64652400 | 0.62394000 |
| | H | -2.14949300 | -0.46826800 | 1.67478900 |
| | C | -1.68920800 | -1.37827800 | -0.21545200 |
| | H | -1.89609900 | -2.40895700 | 0.06982700 |
| | H | -2.00863300 | -1.27118500 | -1.25483700 |
| | C | -0.18084100 | -1.15174400 | -0.13030400 |
| | C | 0.45839800 | -1.89913000 | -1.29972900 |
| | H | 0.15043400 | -1.46947000 | -2.25168100 |
| | H | 1.54176000 | -1.89174200 | -1.24817800 |
| | H | 0.12796700 | -2.93680500 | -1.28057600 |
| | C | 0.35755600 | -1.71135400 | 1.18648600 |
| | H | 0.19790100 | -2.78825400 | 1.21605200 |
| | H | 1.42026500 | -1.51934700 | 1.29593100 |
| | H | -0.14909500 | -1.27058300 | 2.04192700 |
| | C | -0.56124600 | 2.77655300 | -0.28091700 |
| | H | 0.30802700 | 3.03617300 | -0.87043600 |
| | H | -1.42762200 | 3.24848000 | -0.73897200 |
| | H | -0.44918000 | 3.22112500 | 0.70816200 |
| | O | 3.13481900 | 0.64764900 | 0.80649800 |
| | O | 2.46718200 | -0.05553600 | -0.28397000 |
| TS9 | C | 1.53377400 | 0.60279400 | -0.03343400 |
| | H | 2.66585400 | 1.32916400 | -0.02802800 |
| | C | 0.13453100 | 0.29995600 | -0.08681900 |
| | C | -0.68851500 | 1.38041500 | -0.08470700 |
| | C | -2.17223000 | 1.23701500 | -0.01653200 |

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| | H | -2.56548000 | 2.01768200 | 0.63540900 |
| | H | -2.56671500 | 1.46599400 | -1.01142500 |
| | C | -2.62468700 | -0.13655700 | 0.41950400 |
| | H | -3.69673400 | -0.24366500 | 0.26888800 |
| | H | -2.44337900 | -0.26239700 | 1.48664600 |
| | C | -1.86143900 | -1.17459800 | -0.36834200 |
| | H | -2.22703300 | -2.17873900 | -0.15581900 |
| | H | -2.02858700 | -1.00000900 | -1.43380900 |
| | C | -0.35943900 | -1.14058600 | -0.09114000 |
| | C | 0.32425000 | -1.94251300 | -1.19770000 |
| | H | 0.21700500 | -1.44731400 | -2.16113900 |
| | H | 1.38066000 | -2.09742700 | -1.00669500 |
| | H | -0.14884100 | -2.92080800 | -1.27088100 |
| | C | -0.06329900 | -1.79761900 | 1.25631600 |
| | H | -0.39017300 | -2.83635200 | 1.23776300 |
| | H | 1.00033600 | -1.78556100 | 1.47484500 |
| | H | -0.58032800 | -1.29372200 | 2.06983300 |
| | C | -0.22940800 | 2.79731100 | -0.13491800 |
| | H | 0.82316200 | 2.90142300 | -0.35550000 |
| | H | -0.81008600 | 3.33486300 | -0.88359900 |
| | H | -0.43443500 | 3.28019300 | 0.82029500 |
| | O | 3.59781000 | 0.44506600 | 0.14876600 |
| | O | 2.38263400 | -0.32219600 | 0.14371600 |
| TS10 | C | -0.01504500 | 1.37521700 | 0.01099900 |
| | C | 0.29418200 | 0.07346600 | 0.14151500 |
| | C | 1.61184800 | -0.38744500 | 0.60300100 |
| | H | 3.05982700 | -1.53184000 | -0.37663600 |
| | O | 2.67025200 | 0.36082900 | 0.23922200 |
| | O | 2.41194100 | -0.90431400 | -0.72110000 |
| | C | -1.41375400 | 1.83543400 | -0.27648800 |
| | H | -1.63625300 | 2.69276500 | 0.36077500 |
| | H | -1.42484500 | 2.22810000 | -1.29828500 |
| | C | 0.96984900 | 2.50501700 | 0.12866900 |
| | H | 1.66524300 | 2.37553100 | 0.95421600 |
| | H | 1.57068500 | 2.61168000 | -0.77133100 |
| | H | 0.43934700 | 3.44155500 | 0.28494800 |
| | C | -2.47615300 | 0.77089900 | -0.11526500 |
| | H | -3.39234000 | 1.07832100 | -0.61644900 |
| | H | -2.72528500 | 0.65876400 | 0.93904600 |
| | C | -1.98088100 | -0.54464200 | -0.66717000 |
| | H | -2.75474900 | -1.31056300 | -0.60414300 |
| | H | -1.74245200 | -0.42147600 | -1.72609500 |
| | C | -0.73744300 | -1.04016300 | 0.06143800 |
| | C | -1.08703200 | -1.51221400 | 1.47238600 |
| | H | -0.19329800 | -1.86550300 | 1.98033300 |
| | H | -1.50898100 | -0.71114300 | 2.07345400 |
| | H | -1.80878800 | -2.32803200 | 1.42890000 |
| | C | -0.17817500 | -2.23347800 | -0.70672800 |
| | H | 0.67373100 | -2.66796200 | -0.18490700 |
| | H | -0.94049600 | -3.00657500 | -0.79463700 |
| | H | 0.13673600 | -1.94828400 | -1.70830800 |

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| TS11 | C | -1.31101400 | 0.39409900 | -0.39998000 |
| | H | -1.68754800 | 1.33441200 | -0.77045500 |
| | C | 0.10323300 | 0.23741900 | -0.13579800 |
| | C | 0.82844200 | 1.37535800 | -0.11786300 |
| | C | 2.31520700 | 1.36035700 | 0.00158500 |
| | H | 2.71675100 | 2.09039300 | -0.70346400 |
| | H | 2.57648500 | 1.74311800 | 0.99268900 |
| | C | 2.91591100 | -0.00848800 | -0.21223000 |
| | H | 3.96276500 | -0.01131100 | 0.08369800 |
| | H | 2.88760700 | -0.26194000 | -1.27167400 |
| | C | 2.12558900 | -1.01746300 | 0.58747700 |
| | H | 2.58946100 | -2.00249500 | 0.54993800 |
| | H | 2.12598900 | -0.70978300 | 1.63578900 |
| | C | 0.67998500 | -1.14707900 | 0.11002200 |
| | C | -0.10077900 | -1.85984500 | 1.21458500 |
| | H | -0.11398600 | -1.26098100 | 2.12495600 |
| | H | -1.12129700 | -2.08193500 | 0.91960500 |
| | H | 0.39313600 | -2.80123500 | 1.45093400 |
| | C | 0.62855400 | -1.98986100 | -1.16359100 |
| | H | 1.02777000 | -2.98281500 | -0.96156400 |
| | H | -0.38941700 | -2.10303200 | -1.52311000 |
| | H | 1.22017900 | -1.54275500 | -1.95947100 |
| | C | 0.23019800 | 2.74632500 | -0.19966000 |
| | H | -0.72479100 | 2.81587300 | 0.31111500 |
| | H | 0.90741900 | 3.46392100 | 0.25669600 |
| | H | 0.09855800 | 3.05504900 | -1.23679500 |
| | O | -3.38247700 | -0.22408700 | -0.58502800 |
| | O | -2.02471500 | -0.63531100 | -0.68740400 |
| | O | -2.31516800 | 0.86723200 | 1.21515600 |
| | H | -3.07374900 | 0.40307900 | 0.54024500 |
| | H | -2.10840600 | 0.24482800 | 1.91179900 |
| | TS12 | C | -1.16809700 | -0.03758300 |
| H | | -1.65315800 | 0.76399500 | -0.27781200 |
| C | | 0.31341300 | 0.14166000 | 0.20846400 |
| C | | 0.80773600 | 1.38179900 | 0.12538800 |
| C | | 2.25038300 | 1.65026500 | -0.17936500 |
| H | | 2.30222800 | 2.48870400 | -0.87583000 |
| H | | 2.73238000 | 2.00206000 | 0.73736700 |
| C | | 2.98143100 | 0.44699500 | -0.72449300 |
| H | | 4.05621200 | 0.61891700 | -0.71074600 |
| H | | 2.70334600 | 0.28613800 | -1.76541000 |
| C | | 2.62280200 | -0.76358300 | 0.10347900 |
| H | | 3.20145700 | -1.63545000 | -0.20207700 |
| H | | 2.87728700 | -0.56403300 | 1.14695200 |
| C | | 1.13706500 | -1.11907800 | 0.01855300 |
| C | | 0.84566400 | -2.11749400 | 1.13331500 |
| H | | 0.98690500 | -1.66242800 | 2.11280900 |
| H | | -0.16490300 | -2.51456700 | 1.06880400 |
| H | | 1.53045700 | -2.96082300 | 1.05517200 |
| C | | 0.83754500 | -1.77500900 | -1.32908600 |
| H | | 1.43670800 | -2.67887200 | -1.43744300 |

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| | H | -0.20997800 | -2.04655000 | -1.40649100 |
| | H | 1.07340100 | -1.10947300 | -2.15576500 |
| | C | 0.00444100 | 2.62708700 | 0.32593200 |
| | H | -0.91405300 | 2.46343600 | 0.87676200 |
| | H | 0.59312600 | 3.35541700 | 0.88185100 |
| | H | -0.23307100 | 3.07944500 | -0.63742600 |
| | O | -3.19168200 | -1.00189000 | -0.86029700 |
| | O | -1.68578700 | -1.16301000 | 0.20742800 |
| | O | -1.57710500 | 0.46361200 | 1.78067500 |
| | H | -3.79464000 | -1.31886400 | -0.18779700 |
| | H | -1.73656400 | -0.28271000 | 2.35851100 |
| | O | -2.59453400 | 1.30001000 | -1.14406500 |
| | H | -3.11994800 | 1.93461400 | -0.65717100 |
| | H | -3.06862100 | 0.38091600 | -1.12248200 |
| TS13 | C | -2.32619700 | -0.19093500 | 0.00002500 |
| | C | -2.78197700 | 1.22273900 | 0.00003100 |
| | H | -2.38460700 | 1.73832000 | -0.87167300 |
| | H | -2.38466900 | 1.73828800 | 0.87178300 |
| | C | -0.83090300 | -0.44435800 | -0.00001500 |
| | O | 1.58631300 | -0.15768400 | -0.00010600 |
| | O | -0.05158800 | 0.47669100 | -0.00009200 |
| | N | 3.25545600 | -0.31600100 | -0.00002000 |
| | O | 4.24683400 | 0.27029300 | 0.00011900 |
| | H | -3.86403200 | 1.25691300 | 0.00000000 |
| | H | -0.48838600 | -1.48080700 | 0.00002000 |
| | O | -3.03556300 | -1.15997300 | 0.00004900 |
| TS14 | C | 1.37315400 | 1.22752800 | 0.12057400 |
| | H | 2.45169900 | 1.29519400 | 0.18562900 |
| | H | 1.00366200 | 1.80208600 | -0.72637000 |
| | H | 0.91615500 | 1.65694200 | 1.01035900 |
| | C | 0.96945600 | -0.19716400 | -0.00460900 |
| | C | -0.48140000 | -0.48999500 | -0.25011800 |
| | H | -0.80700600 | -1.51803800 | -0.34265000 |
| | O | 1.70544000 | -1.14574800 | 0.07390100 |
| | O | -1.28615400 | 0.46157900 | -0.43985000 |
| | O | -2.26075800 | -0.12563100 | 0.45069300 |
| TS15 | C | 1.69869900 | 1.10680300 | 0.07335000 |
| | H | 2.76303200 | 0.96003800 | -0.06773700 |
| | H | 1.29752000 | 1.73562900 | -0.71963100 |
| | H | 1.51364100 | 1.61890500 | 1.01581200 |
| | C | 1.01091200 | -0.21298400 | 0.06069900 |
| | C | -0.46125600 | -0.23153100 | 0.34877000 |
| | H | -1.60173500 | -0.51556800 | 0.95848700 |
| | O | 1.53561900 | -1.27535400 | -0.13152300 |
| | O | -1.22031500 | 0.28640800 | -0.48810800 |
| | O | -2.49812800 | 0.01735400 | 0.10915100 |
| TS16 | C | 1.58644500 | 1.04703400 | -0.02849500 |
| | H | 2.64282400 | 0.80353100 | -0.04140500 |
| | H | 1.32899800 | 1.55315500 | -0.95761200 |
| | H | 1.36575600 | 1.72424500 | 0.79268200 |
| | C | 0.78008500 | -0.20585100 | 0.08359000 |

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| | C | -0.59146900 | -0.11901900 | 0.63878000 |
| | H | -2.15026000 | 1.17215600 | 0.29526600 |
| | O | 1.21129700 | -1.31062700 | -0.14567400 |
| | O | -1.51583300 | -0.73650600 | -0.12922900 |
| | O | -1.42517500 | 0.84887300 | -0.25661800 |
| TS17 | C | -0.22801700 | 0.14233300 | -0.49984600 |
| | H | -0.56780600 | 0.85314700 | -1.24054800 |
| | C | 1.24464600 | 0.08172200 | -0.18435000 |
| | O | -2.27425600 | -0.53020500 | -0.32445600 |
| | O | -0.90494100 | -0.90164500 | -0.26927900 |
| | O | -1.08105900 | 1.27516100 | 0.79476300 |
| | H | -1.87758000 | 0.67674600 | 0.49077000 |
| | H | -0.88187600 | 1.05490700 | 1.70533000 |
| | O | 1.94502400 | 0.93668800 | -0.65154700 |
| | C | 1.71556000 | -1.03587000 | 0.67849300 |
| | H | 1.23201500 | -0.99142400 | 1.65227300 |
| | H | 1.43360600 | -1.98953100 | 0.23757400 |
| | H | 2.79036500 | -0.97294700 | 0.79297900 |
| TS18 | C | -0.05831800 | 0.40524800 | -0.28015200 |
| | H | 0.49997700 | 0.12943000 | 0.87403000 |
| | C | -1.41259000 | -0.14633500 | 0.05289300 |
| | O | 2.27230400 | -0.58111700 | -0.57446700 |
| | O | 0.60883100 | -0.28639100 | -1.12964500 |
| | O | 0.00397900 | 1.77417900 | -0.41120000 |
| | H | 2.67667000 | 0.06168200 | -1.15925700 |
| | H | -0.84632800 | 2.11573600 | -0.11637800 |
| | O | 1.51469300 | -0.12002900 | 1.63764300 |
| | H | 1.79563900 | 0.69274300 | 2.05990100 |
| | H | 2.09093800 | -0.30340300 | 0.78844200 |
| | O | -2.27387800 | 0.64431000 | 0.35165700 |
| | C | -1.58580300 | -1.62298400 | 0.00267800 |
| | H | -2.46690800 | -1.90117500 | 0.56830700 |
| | H | -1.71263300 | -1.92306500 | -1.03561900 |
| | H | -0.70451900 | -2.13513000 | 0.37615700 |
| TS19 | C | 2.16852400 | -1.59461200 | -0.25872300 |
| | H | 2.05803600 | -1.99572400 | -1.26876700 |
| | H | 2.49071800 | -2.44379800 | 0.35073100 |
| | C | 0.86606400 | -1.01309500 | 0.24159200 |
| | H | 0.56157700 | -0.21249400 | -0.42936700 |
| | H | 1.03395000 | -0.55656400 | 1.21509500 |
| | C | -0.22002000 | -2.06945700 | 0.32359100 |
| | H | -0.24178000 | -2.64059600 | -0.60352100 |
| | H | 0.01296600 | -2.77166900 | 1.12655000 |
| | C | -1.62057200 | -1.52148300 | 0.57520900 |
| | C | -1.65450500 | -0.63449500 | 1.81423300 |
| | H | -1.10555900 | 0.29466500 | 1.67914000 |
| | H | -2.67376300 | -0.39443300 | 2.10342200 |
| | H | -1.19475600 | -1.17002400 | 2.64321700 |
| | C | -2.59148800 | -2.68715100 | 0.78340700 |
| | H | -2.31451200 | -3.23241600 | 1.68370300 |
| | H | -3.61394900 | -2.33540300 | 0.90822500 |

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| | H | -2.56424400 | -3.37910100 | -0.05560900 |
| | C | 3.30902100 | -0.63507300 | -0.28941700 |
| | O | 4.45978800 | 1.46208700 | 0.05947800 |
| | O | 3.12397500 | 0.50316900 | 0.12243000 |
| | N | 6.10633400 | 2.37937900 | 0.09341500 |
| | O | 7.03521600 | 1.77795600 | 0.35658300 |
| | C | 4.62711700 | -1.06540500 | -0.80509400 |
| | H | 4.61726200 | -2.10302300 | -1.11927500 |
| | H | 4.90191600 | -0.41018600 | -1.62819600 |
| | H | 5.37286500 | -0.89343500 | -0.03284400 |
| | C | -5.09468600 | 3.09026100 | 0.50164000 |
| | H | -4.97517900 | 2.95852800 | 1.57591900 |
| | H | -4.31658400 | 3.77956800 | 0.17723500 |
| | H | -6.06988100 | 3.51023400 | 0.28844400 |
| | C | -4.93728800 | 1.77784600 | -0.19926900 |
| | C | -3.64700100 | 1.06703900 | 0.00633200 |
| | H | -2.92815700 | 1.50848100 | 0.68101200 |
| | C | -3.39543200 | -0.05210300 | -0.66221300 |
| | H | -4.14871800 | -0.40047000 | -1.35929700 |
| | C | -2.11208500 | -0.80805400 | -0.67500600 |
| | O | -5.80539700 | 1.31000600 | -0.89509100 |
| | O | -1.54263700 | -0.91485400 | -1.73432700 |
| TS20 | C | 1.85995100 | 0.42250600 | -0.13100400 |
| | H | 1.93815900 | -0.03202200 | -1.11625800 |
| | H | 1.40289800 | -0.31204800 | 0.52828900 |
| | C | 4.07873800 | -0.50181300 | 0.24822900 |
| | O | 4.52712700 | -0.75474900 | -0.91272400 |
| | O | 3.94172200 | -2.10430700 | -0.93079600 |
| | C | 4.38672700 | -1.32635200 | 1.43420600 |
| | H | 4.83032400 | -0.67610900 | 2.19043900 |
| | H | 3.46910400 | -1.72770100 | 1.85930300 |
| | H | 5.03790900 | -2.14638300 | 1.16582400 |
| | C | 3.27589300 | 0.73146200 | 0.37201200 |
| | H | 3.72316400 | 1.49203400 | -0.26809600 |
| | H | 3.24241400 | 1.08589600 | 1.39881500 |
| | C | 1.01164100 | 1.67882000 | -0.17292100 |
| | H | 1.39767500 | 2.34865900 | -0.94326500 |
| | H | 1.08968300 | 2.20304600 | 0.77823300 |
| | C | -0.46443800 | 1.42912500 | -0.46582700 |
| | C | -0.64124800 | 0.61548500 | -1.74282200 |
| | H | -0.28336200 | -0.40636100 | -1.63898800 |
| | H | -1.68089800 | 0.58993000 | -2.05611100 |
| | H | -0.06792500 | 1.08370600 | -2.54106200 |
| | C | -1.17890100 | 2.77250100 | -0.63647900 |
| | H | -2.24731700 | 2.63714000 | -0.79407800 |
| | H | -1.03596100 | 3.40941000 | 0.23378300 |
| | H | -0.77650700 | 3.28830600 | -1.50612400 |
| | C | -1.11452100 | 0.77503200 | 0.74365200 |
| | C | -2.52805600 | 0.30981300 | 0.68762700 |
| | H | -3.19483100 | 0.75935200 | 1.41424200 |
| | C | -3.00712400 | -0.68071400 | -0.05560600 |

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| | H | -2.39537400 | -1.21530700 | -0.76714600 |
| | C | -4.42084100 | -1.11350200 | 0.11073800 |
| | C | -4.85471300 | -2.29766900 | -0.69398900 |
| | H | -4.24121400 | -3.16192500 | -0.44407900 |
| | H | -5.89689600 | -2.51754900 | -0.49809000 |
| | H | -4.71124000 | -2.10208200 | -1.75554700 |
| | O | -0.55101500 | 0.70322100 | 1.80958000 |
| | O | -5.17014200 | -0.53018500 | 0.85556600 |
| TS21 | C | 5.82753500 | -0.45842700 | 1.09417800 |
| | H | 6.13760700 | 0.51856000 | 0.72634100 |
| | H | 5.48793800 | -0.32034400 | 2.11965900 |
| | H | 6.66776400 | -1.14136600 | 1.07513800 |
| | C | 4.71341800 | -0.99427800 | 0.25131200 |
| | C | 3.48029800 | -0.16043100 | 0.17643200 |
| | H | 3.47992900 | 0.76395000 | 0.73224000 |
| | C | 2.45239400 | -0.56372300 | -0.56446300 |
| | H | 2.56515800 | -1.49391800 | -1.10647500 |
| | C | 1.16255200 | 0.11778500 | -0.84531100 |
| | C | -4.15802200 | -0.40981900 | -0.18175700 |
| | C | -3.19268700 | 0.63983800 | -0.58086900 |
| | H | -3.12400300 | 0.66054900 | -1.66736800 |
| | H | -3.57693300 | 1.60074500 | -0.24423700 |
| | C | -1.80676200 | 0.38812100 | 0.00634600 |
| | H | -1.43161100 | -0.56652500 | -0.35585600 |
| | H | -1.89053500 | 0.31758100 | 1.08988800 |
| | C | -0.84723500 | 1.49752000 | -0.38248800 |
| | H | -0.89878000 | 1.65282000 | -1.45859600 |
| | H | -1.16471000 | 2.42803600 | 0.09151200 |
| | C | 0.61414200 | 1.26213100 | 0.00211000 |
| | C | 0.72051500 | 0.96671600 | 1.49639800 |
| | H | 0.34275900 | -0.02198800 | 1.74585800 |
| | H | 1.73982400 | 1.03048000 | 1.86093700 |
| | H | 0.12994900 | 1.69697300 | 2.04710000 |
| | C | 1.39644200 | 2.53057600 | -0.34543400 |
| | H | 1.01249900 | 3.36198800 | 0.24263200 |
| | H | 2.45824000 | 2.43940900 | -0.13690000 |
| | H | 1.28095700 | 2.77971800 | -1.39782800 |
| | O | 4.79623000 | -2.04333100 | -0.33740300 |
| | C | -4.09912000 | -1.79509500 | -0.38025600 |
| | H | -4.98424800 | -2.23204300 | -0.83516600 |
| | H | -3.17280000 | -2.18904700 | -0.76923600 |
| | H | -4.76226600 | -1.90499300 | 0.75942900 |
| | O | 0.55104000 | -0.27769100 | -1.81230500 |
| | O | -5.76063600 | -1.10293400 | 1.13825200 |
| | O | -5.07132800 | -0.01430300 | 0.63692200 |
| TS22 | C | -4.75241200 | -2.35770900 | -0.62468100 |
| | H | -4.57909400 | -2.21871100 | -1.69073200 |
| | H | -4.14000000 | -3.20128300 | -0.30983900 |
| | H | -5.79830400 | -2.57623800 | -0.44780100 |
| | C | -4.35167400 | -1.12644800 | 0.12594300 |
| | C | -2.93713500 | -0.69362400 | -0.02004200 |

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| | H | -2.29810900 | -1.27005000 | -0.67293800 |
| | C | -2.48853400 | 0.34970700 | 0.66742700 |
| | H | -3.18206900 | 0.84544500 | 1.33690900 |
| | C | -1.07786300 | 0.82804500 | 0.73048600 |
| | C | 4.18609000 | -0.40324000 | 0.29130400 |
| | C | 3.29787100 | 0.79782200 | 0.38181800 |
| | H | 3.24398400 | 1.14083000 | 1.41426900 |
| | H | 3.74897000 | 1.59680300 | -0.20513000 |
| | C | 1.90090000 | 0.49705700 | -0.14305200 |
| | H | 1.43835500 | -0.25197800 | 0.49767500 |
| | H | 1.99728900 | 0.05044500 | -1.13078100 |
| | C | 1.04035300 | 1.74498800 | -0.19385400 |
| | H | 1.11761400 | 2.27872800 | 0.75254500 |
| | H | 1.41793200 | 2.41526700 | -0.96857900 |
| | C | -0.43512900 | 1.48659200 | -0.47954900 |
| | C | -0.61287100 | 0.66637400 | -1.75206100 |
| | H | -0.22913700 | -0.34596700 | -1.64748000 |
| | H | -1.65624500 | 0.61532500 | -2.05093600 |
| | H | -0.05965900 | 1.14504800 | -2.55832000 |
| | C | -1.16565400 | 2.82126900 | -0.64991900 |
| | H | -0.77072400 | 3.33972800 | -1.52135200 |
| | H | -2.23345100 | 2.67553300 | -0.80415700 |
| | H | -1.02545100 | 3.46104300 | 0.21871700 |
| | O | -5.13007000 | -0.50902100 | 0.81156000 |
| | C | 4.35774000 | -1.29959200 | 1.33934800 |
| | H | 5.00140900 | -2.14902400 | 1.19232100 |
| | H | 3.86058000 | -1.16599800 | 2.28848200 |
| | H | 3.12704300 | -3.04644900 | -1.20982500 |
| | O | -0.52032400 | 0.76282400 | 1.79923100 |
| | O | 3.44011100 | -2.36210800 | -0.59948500 |
| | O | 4.61640500 | -0.79243800 | -0.82656300 |
| TS23 | C | 5.43011700 | -2.39423900 | 0.42634800 |
| | H | 5.24118600 | -2.37013700 | 1.49849200 |
| | H | 4.83283900 | -3.20708600 | 0.01608300 |
| | H | 6.48094200 | -2.58087700 | 0.24229400 |
| | C | 5.02298600 | -1.09587400 | -0.19717300 |
| | C | 3.60142400 | -0.69648000 | -0.02500500 |
| | H | 2.96374100 | -1.34234500 | 0.56011600 |
| | C | 3.14739600 | 0.40545800 | -0.61118100 |
| | H | 3.84256400 | 0.96951400 | -1.22201000 |
| | C | 1.73411500 | 0.87584400 | -0.65836000 |
| | C | -3.52597500 | -0.62317500 | -0.64609900 |
| | C | -2.68598300 | 0.59714900 | -0.44469800 |
| | H | -2.69702100 | 1.20875300 | -1.34573200 |
| | H | -3.16213700 | 1.18581700 | 0.34391000 |
| | C | -1.26210000 | 0.26730300 | -0.03919300 |
| | H | -0.77178100 | -0.26806600 | -0.85206200 |
| | H | -1.30406600 | -0.40532300 | 0.81511700 |
| | C | -0.47271900 | 1.51649600 | 0.29952400 |
| | H | -0.54236000 | 2.22313200 | -0.52650400 |
| | H | -0.91987500 | 2.00014000 | 1.17037600 |

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| | C | 1. 00232200 | 1. 28244100 | 0. 61025700 |
| | C | 1. 17079900 | 0. 28049700 | 1. 74620700 |
| | H | 0. 86484600 | -0. 72430300 | 1. 46437200 |
| | H | 2. 19787800 | 0. 24576900 | 2. 09910100 |
| | H | 0. 54386900 | 0. 58976300 | 2. 58066600 |
| | C | 1. 64782100 | 2. 60638000 | 1. 03083700 |
| | H | 1. 18686200 | 2. 95501500 | 1. 95296100 |
| | H | 2. 71478300 | 2. 48985500 | 1. 21361500 |
| | H | 1. 50827400 | 3. 37105300 | 0. 26986400 |
| | O | 5. 80180500 | -0. 40235000 | -0. 80512400 |
| | C | -4. 56501000 | -0. 68681500 | -1. 56189800 |
| | H | -5. 09593700 | -1. 61751600 | -1. 66329100 |
| | H | -4. 70980700 | 0. 07223300 | -2. 31376900 |
| | H | -4. 77316600 | -1. 92177300 | 1. 92087000 |
| | O | 1. 24354900 | 1. 02019300 | -1. 75240200 |
| | O | -4. 65224300 | -1. 04394700 | 1. 55778300 |
| | O | -3. 46394500 | -1. 57854900 | 0. 18573400 |
| | O | -6. 08799900 | -0. 00045600 | -0. 19545200 |
| | H | -5. 65584900 | -0. 44392800 | 0. 60629200 |
| | H | -6. 94628400 | -0. 39874000 | -0. 33245700 |
| TS24 | C | -3. 51062900 | 0. 49630800 | -0. 35592600 |
| | C | -2. 33462100 | 1. 40914700 | -0. 53706700 |
| | H | -2. 23463200 | 1. 60328000 | -1. 60764100 |
| | H | -2. 58205000 | 2. 35207000 | -0. 05592500 |
| | C | -1. 01849500 | 0. 85091700 | -0. 01083000 |
| | H | -0. 74829800 | -0. 04951700 | -0. 55905300 |
| | H | -1. 14099800 | 0. 57391500 | 1. 03637100 |
| | C | 0. 09545600 | 1. 87116700 | -0. 15712700 |
| | H | 0. 11916500 | 2. 22147200 | -1. 18772300 |
| | H | -0. 12828800 | 2. 73626900 | 0. 46962700 |
| | C | 1. 49492700 | 1. 38223100 | 0. 21918600 |
| | C | 1. 48862600 | 0. 82445900 | 1. 64076100 |
| | H | 0. 98252300 | -0. 13617700 | 1. 70069500 |
| | H | 2. 48737500 | 0. 69497400 | 2. 04275700 |
| | H | 0. 96214600 | 1. 51911500 | 2. 29318300 |
| | C | -3. 33844700 | -0. 94280100 | -0. 79997800 |
| | H | -2. 66067700 | -1. 44489700 | -0. 09951400 |
| | H | -2. 81389300 | -0. 95979500 | -1. 76406900 |
| | O | -4. 54531400 | 0. 88359000 | 0. 12915700 |
| | O | -4. 49820100 | -1. 63854900 | -0. 98278100 |
| | H | -5. 11034000 | -1. 92476300 | 0. 15218100 |
| | O | -5. 36424700 | -1. 72529100 | 1. 15531800 |
| | O | -6. 45709100 | -0. 90761600 | 1. 07215900 |
| | H | -6. 04829800 | -0. 03746700 | 0. 95470400 |
| | C | 1. 93827800 | 0. 33618900 | -0. 79852100 |
| | O | 1. 31618000 | 0. 17752500 | -1. 82535200 |
| | C | 3. 13225300 | -0. 52857100 | -0. 61822600 |
| | H | 3. 16651500 | -1. 35270000 | -1. 31923900 |
| | C | 4. 16277100 | -0. 39193400 | 0. 21093900 |
| | H | 4. 24130400 | 0. 40897700 | 0. 92910000 |
| | C | 5. 28893100 | -1. 36772000 | 0. 16091800 |

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| | C | 6.41935500 | -1.12612800 | 1.11057700 |
| | H | 6.05335300 | -1.12535300 | 2.13622100 |
| | H | 7.17422900 | -1.89336700 | 0.99105300 |
| | H | 6.85744300 | -0.14606300 | 0.92724100 |
| | O | 5.27674600 | -2.29787400 | -0.60611900 |
| | C | 2.44409300 | 2.57867400 | 0.12173200 |
| | H | 3.47503300 | 2.31675300 | 0.33936200 |
| | H | 2.41195200 | 3.01724600 | -0.87307500 |
| | H | 2.13687200 | 3.34013700 | 0.83606100 |
| TS25 | C | -0.04806300 | -1.71281500 | -0.48061400 |
| | H | 0.10610100 | -2.76123600 | -0.21691500 |
| | H | 0.10724100 | -1.62933200 | -1.55487900 |
| | C | 3.42625000 | -0.37211200 | 0.50443100 |
| | C | 4.82005200 | -0.36453400 | -0.13071600 |
| | H | 4.75930500 | 0.81174800 | -0.64399600 |
| | H | 4.92631400 | -0.96668300 | -1.04641500 |
| | O | 5.83062800 | -0.22446800 | 0.61289800 |
| | O | 6.23516800 | 1.99437900 | 0.02161400 |
| | O | 5.28891800 | 2.03702900 | -0.72733100 |
| | O | 3.23438400 | 0.15264800 | 1.56366300 |
| | C | 2.36797500 | -1.07760500 | -0.28960400 |
| | H | 2.62705600 | -2.14065500 | -0.29365700 |
| | H | 2.44370100 | -0.76091500 | -1.33245500 |
| | C | 0.97235700 | -0.85868200 | 0.24850000 |
| | H | 0.72347600 | 0.19616600 | 0.14887300 |
| | H | 0.97473500 | -1.07685700 | 1.31427000 |
| | C | -6.56348700 | 0.79227400 | 0.85378500 |
| | H | -6.95432800 | -0.00242000 | 0.22006100 |
| | H | -6.36350200 | 0.35300400 | 1.82997400 |
| | H | -7.29963900 | 1.58067100 | 0.95014400 |
| | C | -5.29994300 | 1.34039900 | 0.26853400 |
| | C | -4.18639200 | 0.37005000 | 0.07412100 |
| | H | -4.37268300 | -0.65403500 | 0.35755500 |
| | C | -3.03195900 | 0.77890700 | -0.44340900 |
| | H | -2.95340700 | 1.82044800 | -0.72762800 |
| | C | -1.82725200 | -0.01584300 | -0.79669800 |
| | C | -1.50920200 | -1.37571600 | -0.18111300 |
| | C | -1.74933200 | -1.39519200 | 1.32652400 |
| | H | -1.30138000 | -0.53714800 | 1.82203900 |
| | H | -2.80285000 | -1.41287900 | 1.58451600 |
| | H | -1.29720100 | -2.29261000 | 1.74562000 |
| | C | -2.38292600 | -2.42386500 | -0.87382600 |
| | H | -2.17704600 | -3.40298900 | -0.44517000 |
| | H | -3.44543900 | -2.22927000 | -0.75996900 |
| | H | -2.16209700 | -2.46702900 | -1.93799900 |
| | O | -5.17811400 | 2.50261400 | -0.02935300 |
| | O | -1.09433800 | 0.47035200 | -1.62817300 |
| TS26 | C | -4.38390700 | -0.51800200 | 2.38207100 |
| | H | -5.46371400 | -0.43665700 | 2.39669600 |
| | H | -4.07610500 | -1.45561400 | 2.84215300 |
| | H | -3.94588700 | 0.28617800 | 2.97139800 |

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| | C | -3.88384200 | -0.44303200 | 0.97421500 |
| | C | -2.41540700 | -0.56734200 | 0.78477800 |
| | H | -1.80160500 | -0.74491400 | 1.65497400 |
| | C | -1.89961700 | -0.38075600 | -0.42446300 |
| | H | -2.56562500 | -0.12957700 | -1.24082000 |
| | C | -0.47051700 | -0.39206000 | -0.76883200 |
| | C | 4.62858400 | 0.70021300 | 0.86626400 |
| | C | 3.87476600 | 0.03738100 | -0.25654100 |
| | H | 3.79281400 | 0.73970400 | -1.08767900 |
| | H | 4.50690000 | -0.77541400 | -0.62586700 |
| | C | 2.51670700 | -0.48060900 | 0.15712700 |
| | H | 1.89320600 | 0.36613200 | 0.44102200 |
| | H | 2.63487400 | -1.08853100 | 1.05132400 |
| | C | 1.85055100 | -1.27667600 | -0.94985200 |
| | H | 1.91173500 | -0.72828100 | -1.88900100 |
| | H | 2.38931900 | -2.21414200 | -1.09924000 |
| | C | 0.38830300 | -1.63195800 | -0.68806600 |
| | C | 0.22911500 | -2.34680900 | 0.64892000 |
| | H | 0.44440100 | -1.69713200 | 1.49354200 |
| | H | -0.76877600 | -2.75818300 | 0.76746300 |
| | H | 0.93593000 | -3.17370800 | 0.68199400 |
| | C | -0.12571800 | -2.54736800 | -1.80498500 |
| | H | 0.43349300 | -3.48021000 | -1.78116100 |
| | H | -1.17979800 | -2.78337600 | -1.67507100 |
| | H | 0.01110500 | -2.09183900 | -2.78297300 |
| | O | -4.62360200 | -0.28854100 | 0.03303000 |
| | C | 5.85516200 | 1.47541200 | 0.48828000 |
| | H | 6.43698300 | 1.70461100 | 1.37326100 |
| | H | 6.46062500 | 0.92978100 | -0.23181200 |
| | H | 5.55233100 | 2.40685500 | 0.01164800 |
| | O | 0.00437000 | 0.62387500 | -1.26320700 |
| | O | -1.09747000 | 1.84179700 | -1.27943000 |
| | O | 4.26079800 | 0.61420700 | 2.01117700 |
| | N | -2.52010700 | 3.08868300 | -1.00773400 |
| | O | -3.16241100 | 2.92530800 | -0.08547100 |
| TS27 | C | 2.41663800 | 3.40932400 | -0.83472800 |
| | H | 3.11022900 | 4.19920300 | -0.57418900 |
| | H | 2.50041000 | 3.18079100 | -1.89618100 |
| | H | 1.39409400 | 3.74007500 | -0.65983300 |
| | C | 2.70586600 | 2.18701100 | -0.02150100 |
| | C | 1.82792700 | 1.01616300 | -0.25699300 |
| | H | 1.07495700 | 1.10039000 | -1.02284700 |
| | C | 1.93920300 | -0.05501300 | 0.53368000 |
| | H | 2.64984100 | -0.01792200 | 1.34827900 |
| | C | 1.20059000 | -1.29691900 | 0.45603000 |
| | C | -3.50504400 | 1.18469000 | 0.01111400 |
| | C | -2.95885500 | -0.21857000 | 0.05932300 |
| | H | -3.14195100 | -0.63528800 | 1.05074900 |
| | H | -3.56595100 | -0.81763500 | -0.62568100 |
| | C | -1.49405400 | -0.29295900 | -0.30464500 |
| | H | -0.92221300 | 0.23755700 | 0.45547400 |

| | | | |
|---|-------------|-------------|-------------|
| H | -1.35061100 | 0.24268800 | -1.24130900 |
| C | -1.00888200 | -1.72546700 | -0.40523400 |
| H | -1.20921900 | -2.24334300 | 0.53292500 |
| H | -1.55106400 | -2.25477400 | -1.19144400 |
| C | 0.49617200 | -1.90319900 | -0.71766100 |
| C | 0.86657400 | -1.33649500 | -2.08016600 |
| H | 0.46415300 | -0.34841300 | -2.26498000 |
| H | 1.94419800 | -1.29656700 | -2.21762800 |
| H | 0.45839300 | -1.99438900 | -2.84405200 |
| C | 0.80735200 | -3.40311900 | -0.71700000 |
| H | 0.22047500 | -3.87612500 | -1.50047400 |
| H | 1.85848000 | -3.58723900 | -0.92703700 |
| H | 0.55538600 | -3.86693700 | 0.23034500 |
| O | 3.60525600 | 2.14452000 | 0.78400300 |
| C | -4.85705200 | 1.40379700 | 0.61955900 |
| H | -5.24633200 | 2.37060800 | 0.32295300 |
| H | -5.54940100 | 0.61403600 | 0.33732200 |
| H | -4.76455000 | 1.37614800 | 1.70450900 |
| O | 1.18944500 | -2.02626100 | 1.51670900 |
| O | 0.64316600 | -0.94719900 | 2.30655800 |
| O | -2.88136100 | 2.08665000 | -0.49071600 |