

Supporting Information

Mechanism and Selectivity of Rhodium-Catalyzed 1:2 Coupling of Aldehydes and Allenes

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Table of Contents:

| | |
|--|------------|
| 1. Complete reference of Gaussian 03----- | S2 |
| 2. Results of the [RhCl(dppe)]-catalyzed Reaction ----- | S3 |
| 3. Results of the [Rh(dppe)⁺]-catalyzed Reaction ----- | S16 |
| 4. Table of calculated energies ----- | S24 |
| 5. Cartesian coordinates ----- | S26 |

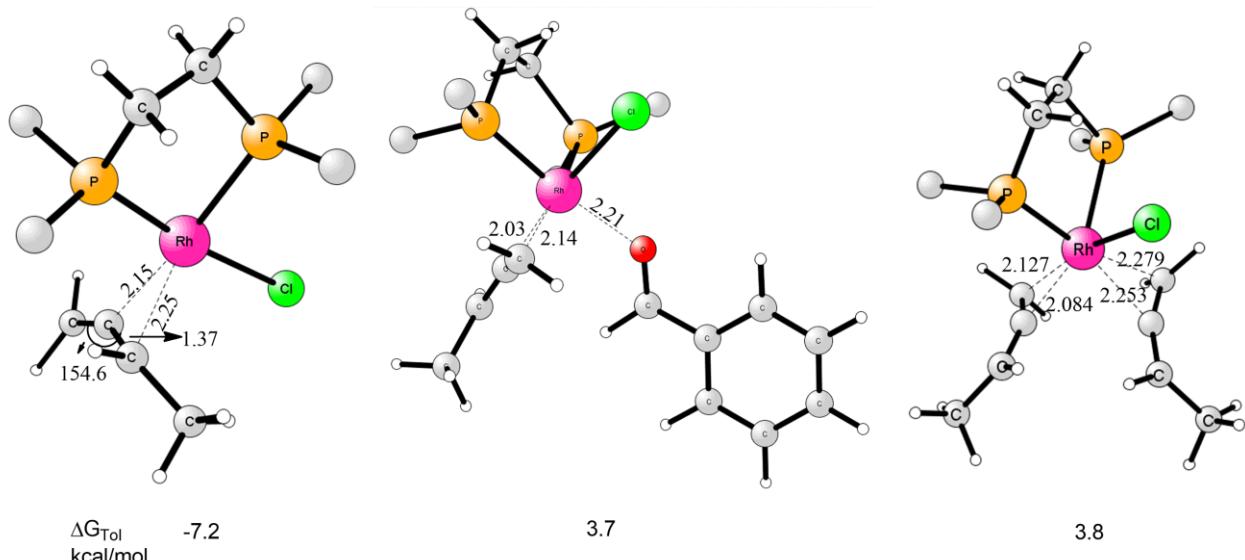
1. Complete reference of Gaussian 03

Gaussian 03, Revision D.01: Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P.Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A., Gaussian, Inc., Wallingford CT, **2004**.

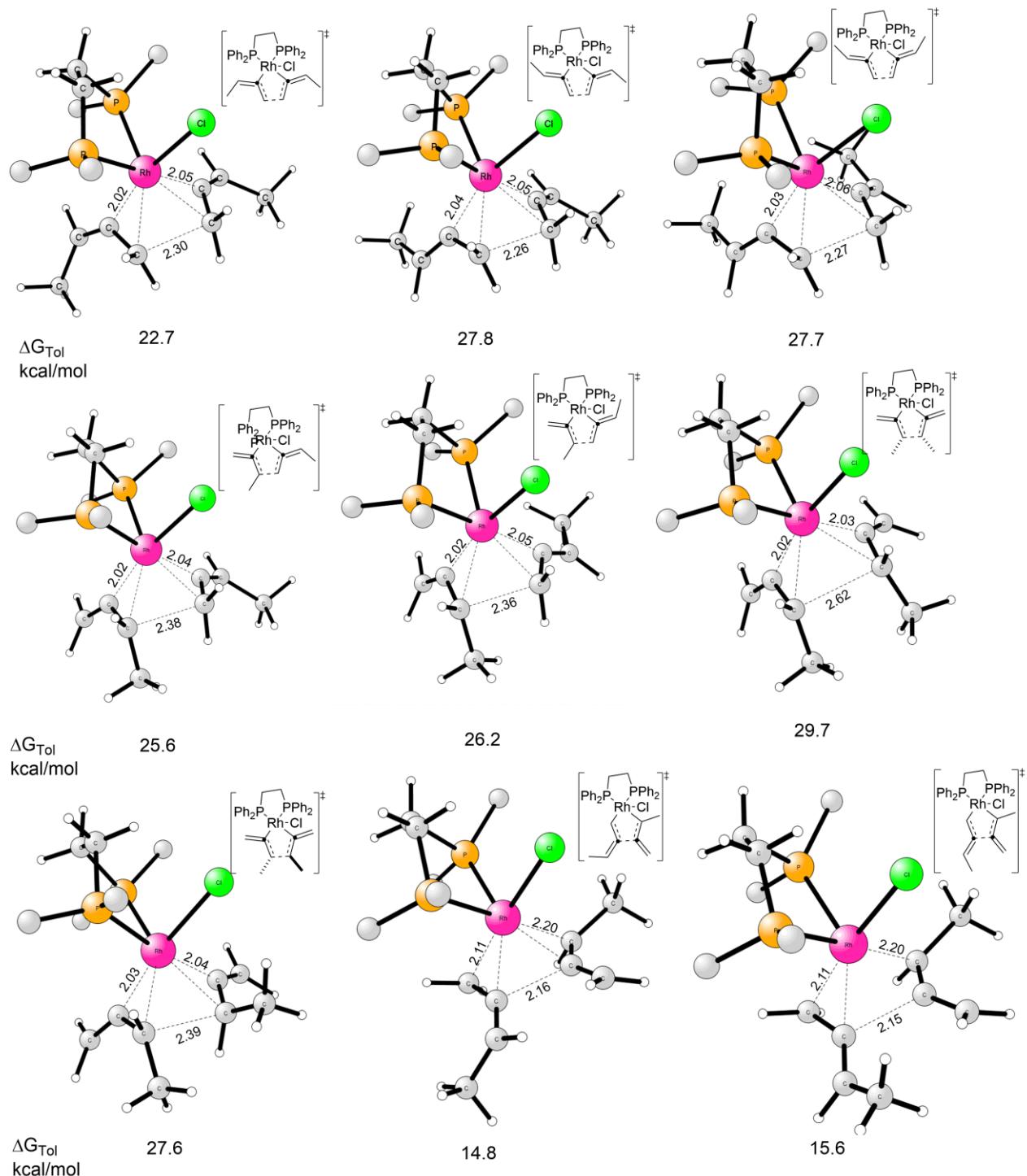
2. Results of the [RhCl(dppe)]-catalyzed reaction

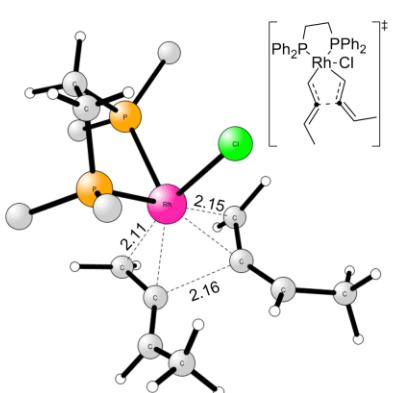
2.1. Other possible intermediates formed between catalyst and substrates

(Distances and angles are given in Å and degrees, respectively; Energies are given in kcal/mol relative to the global zero, which is the sum of the energies of the free reactants and catalyst.)

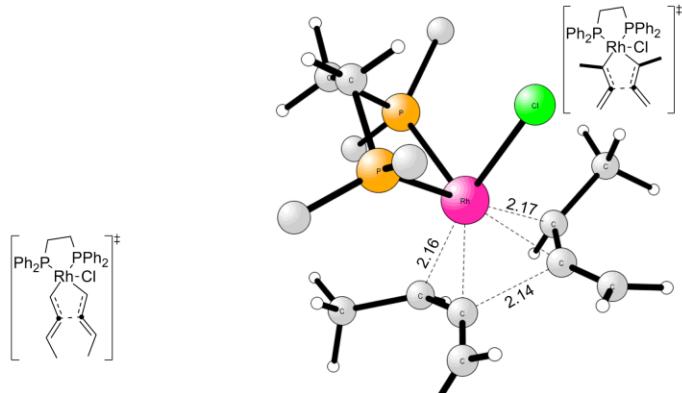


2.2. Other possibilities for allene-allene oxidative coupling



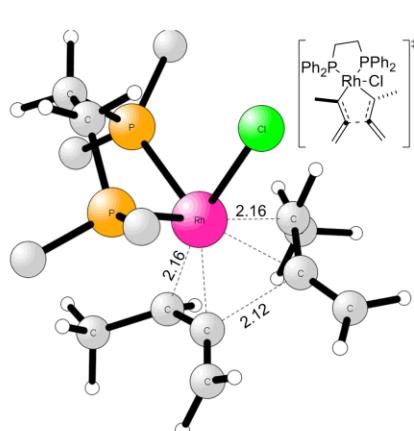


ΔG_{Tol}
kcal/mol
15.0

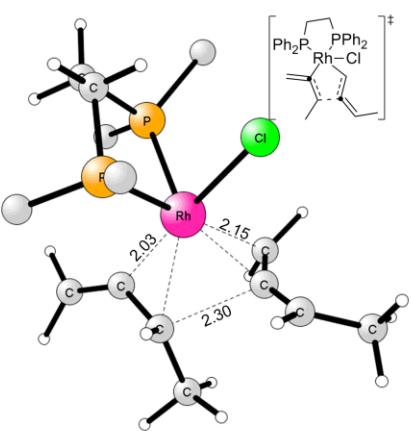


Not observed

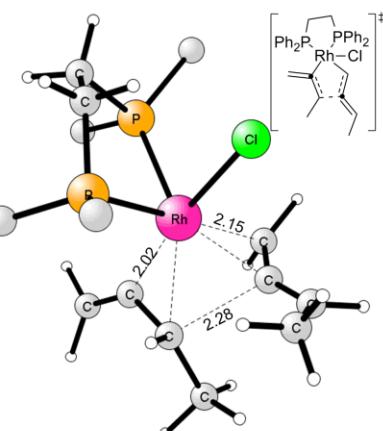
18.6



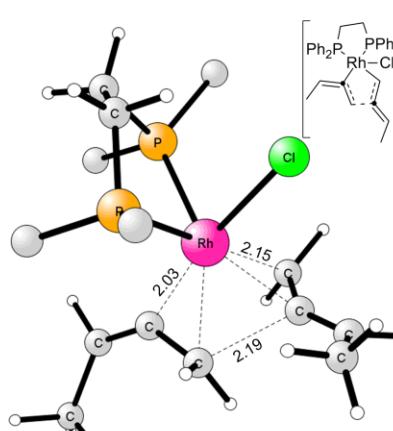
ΔG_{Tol}
kcal/mol
20.7



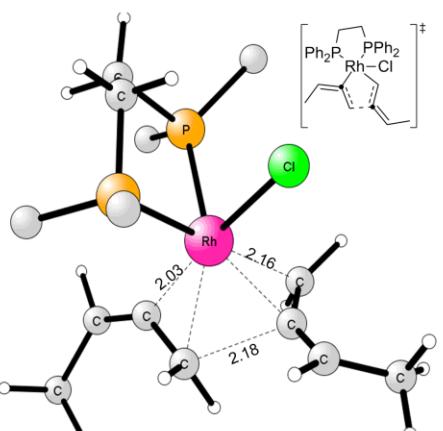
19.1



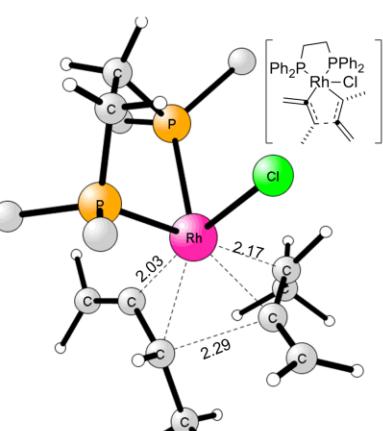
18.8



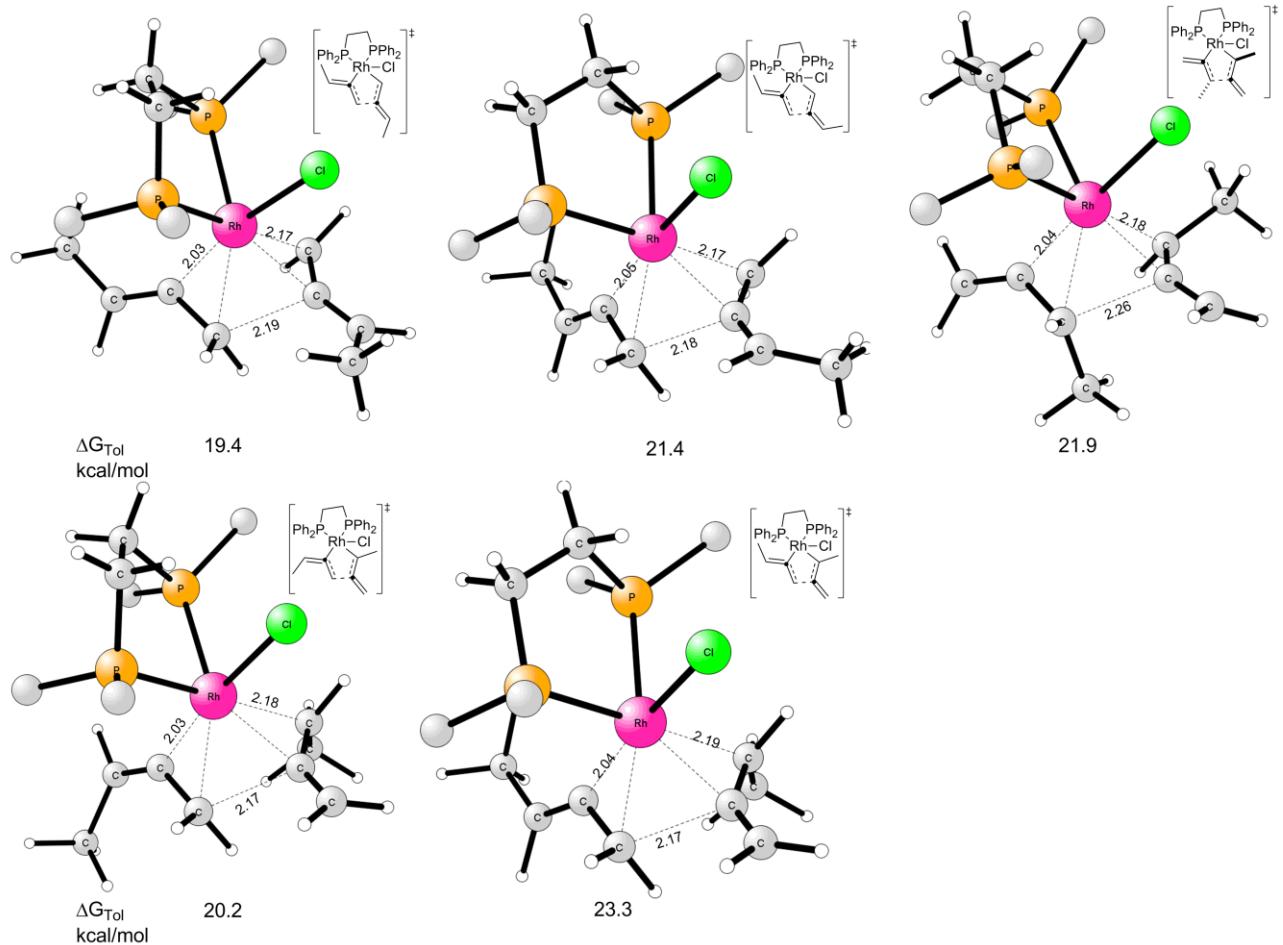
ΔG_{Tol}
kcal/mol
16.8



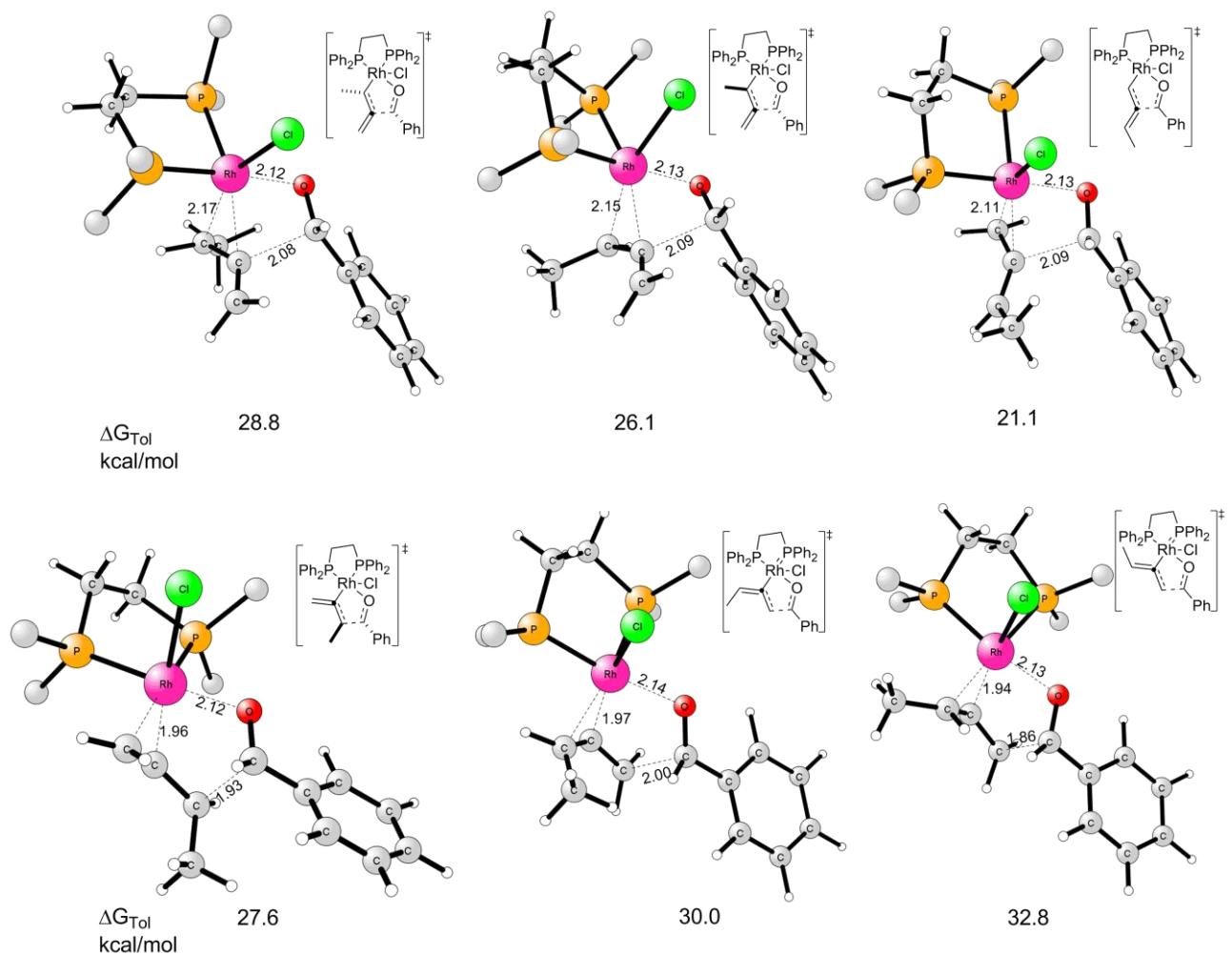
18.8



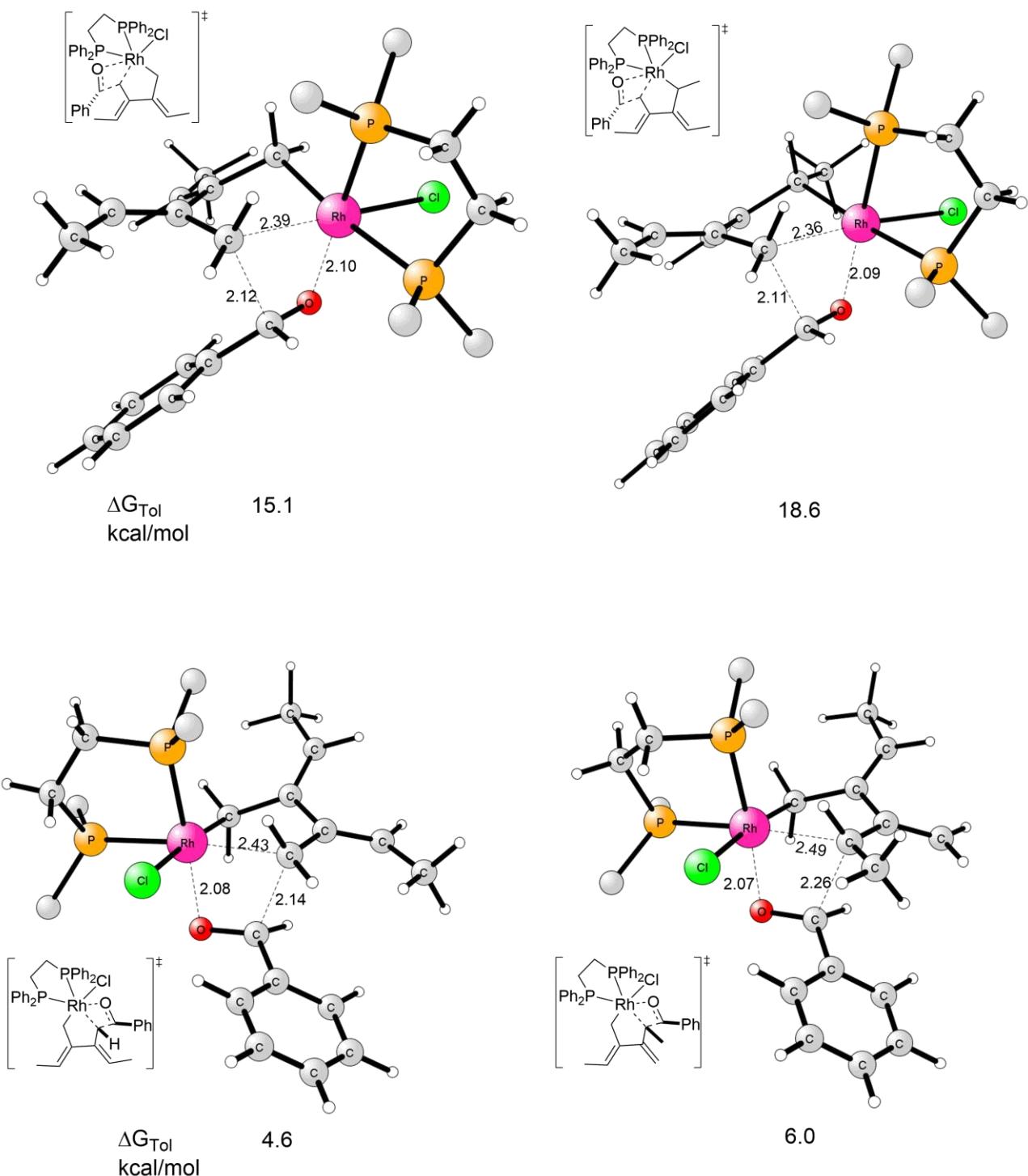
22.3



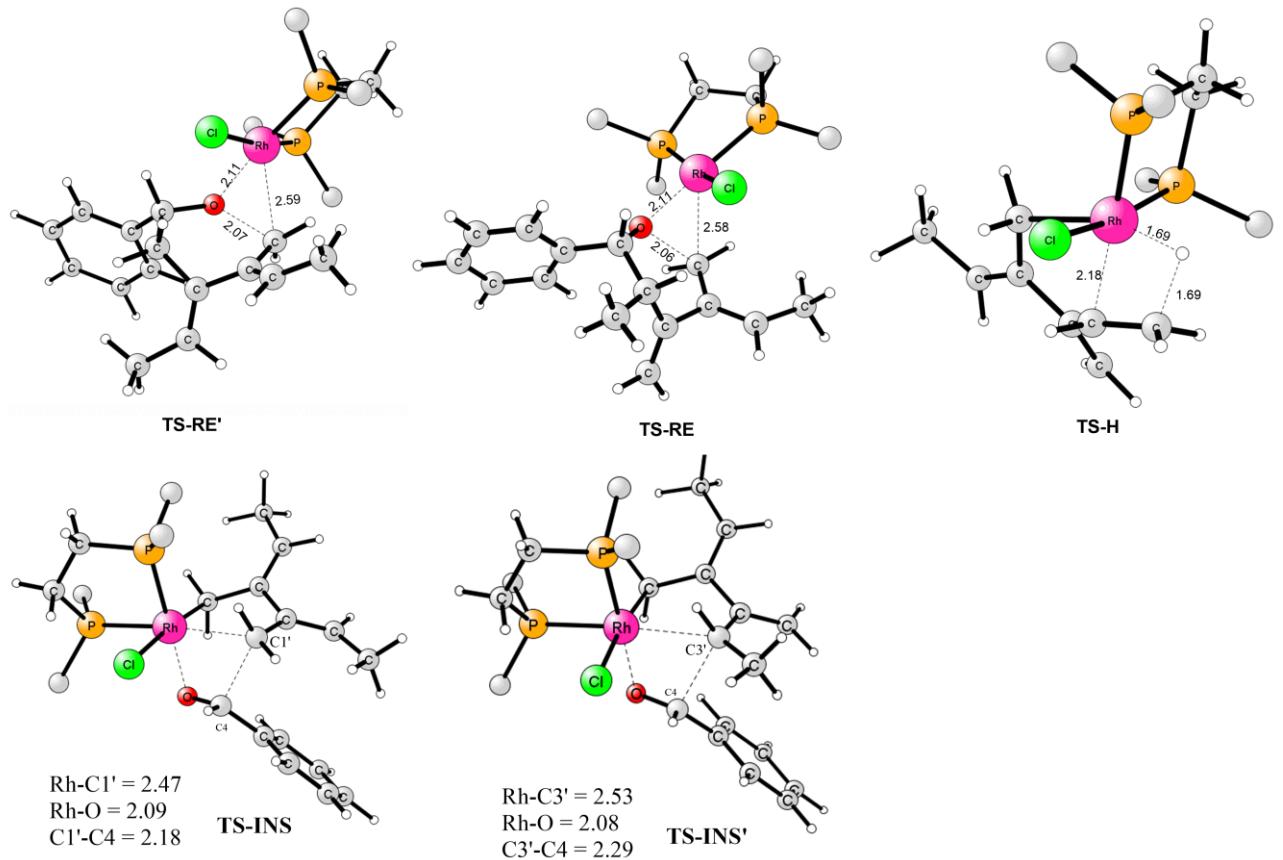
2.3. Other possibilities for aldehyde-allene oxidative coupling



2.4. Other possibilities for the migratory Insertion

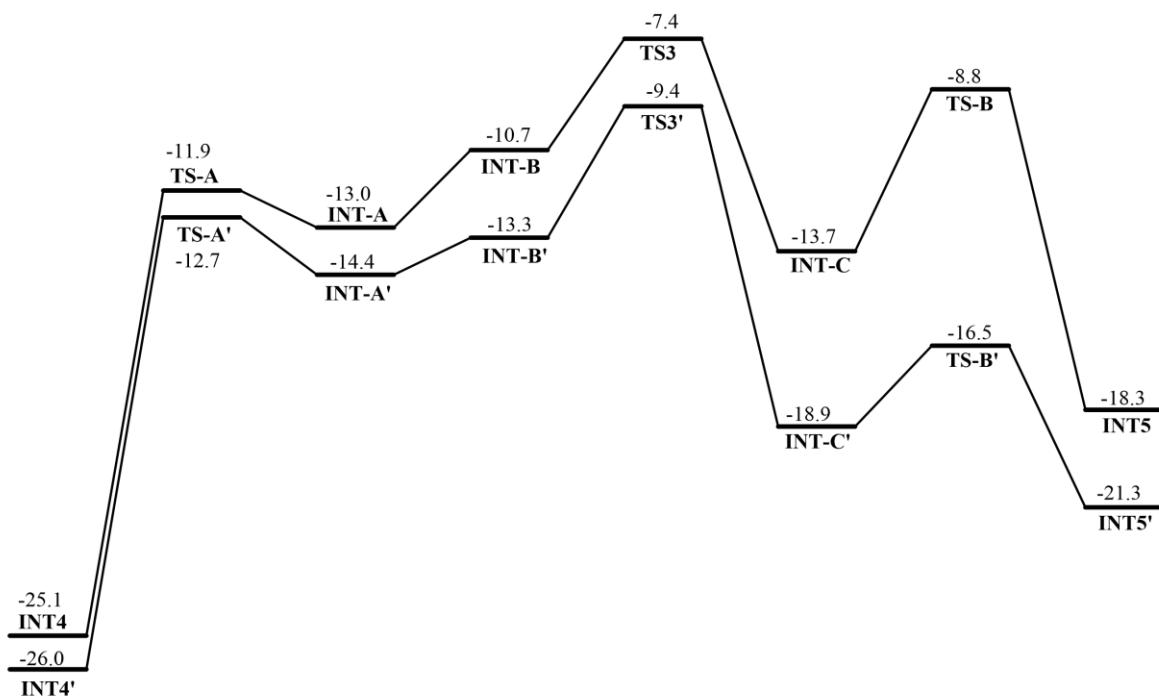


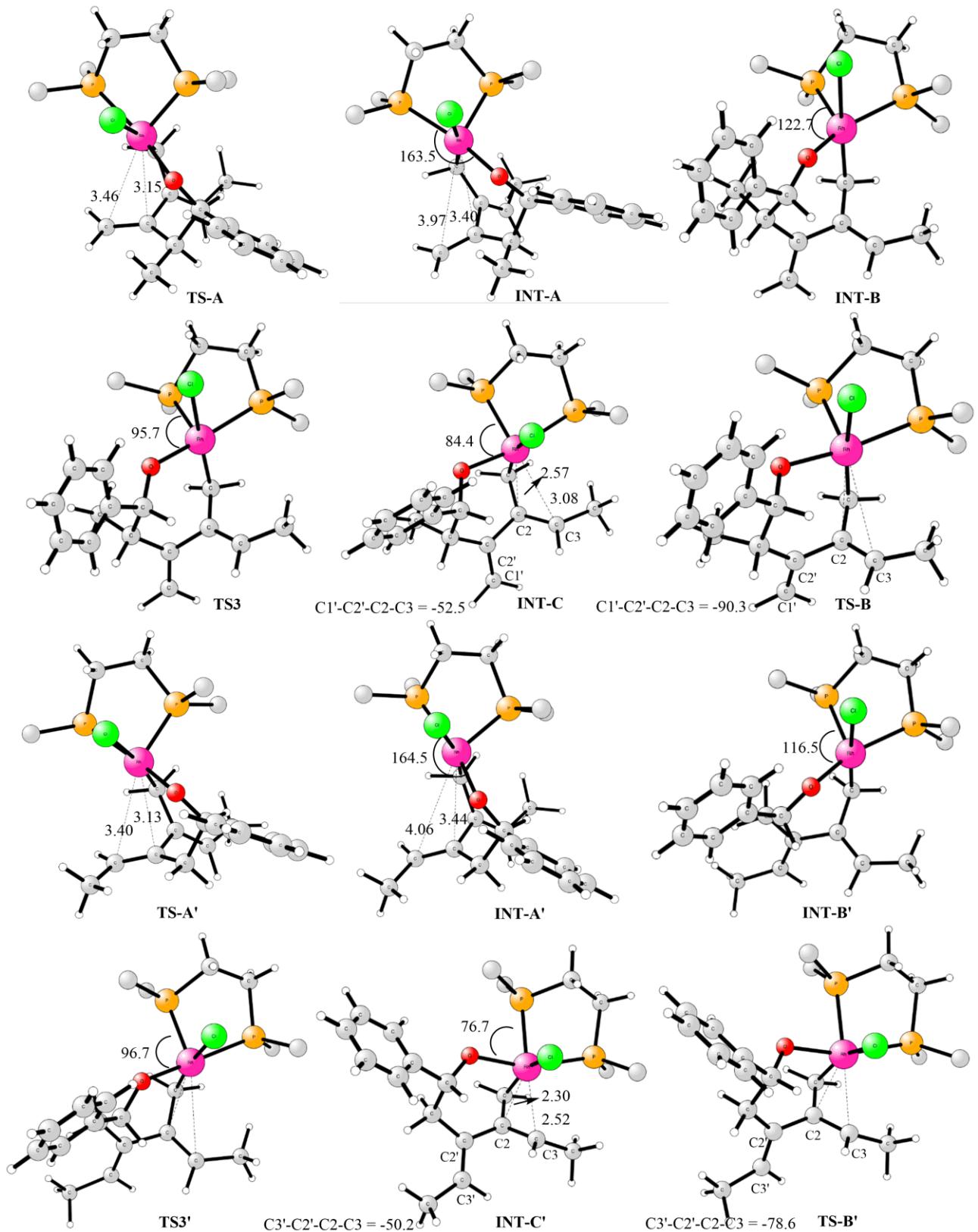
2.5. Optimized structures of TS-RE, TS-RE', TS-INS, TS-INS' and TS-H



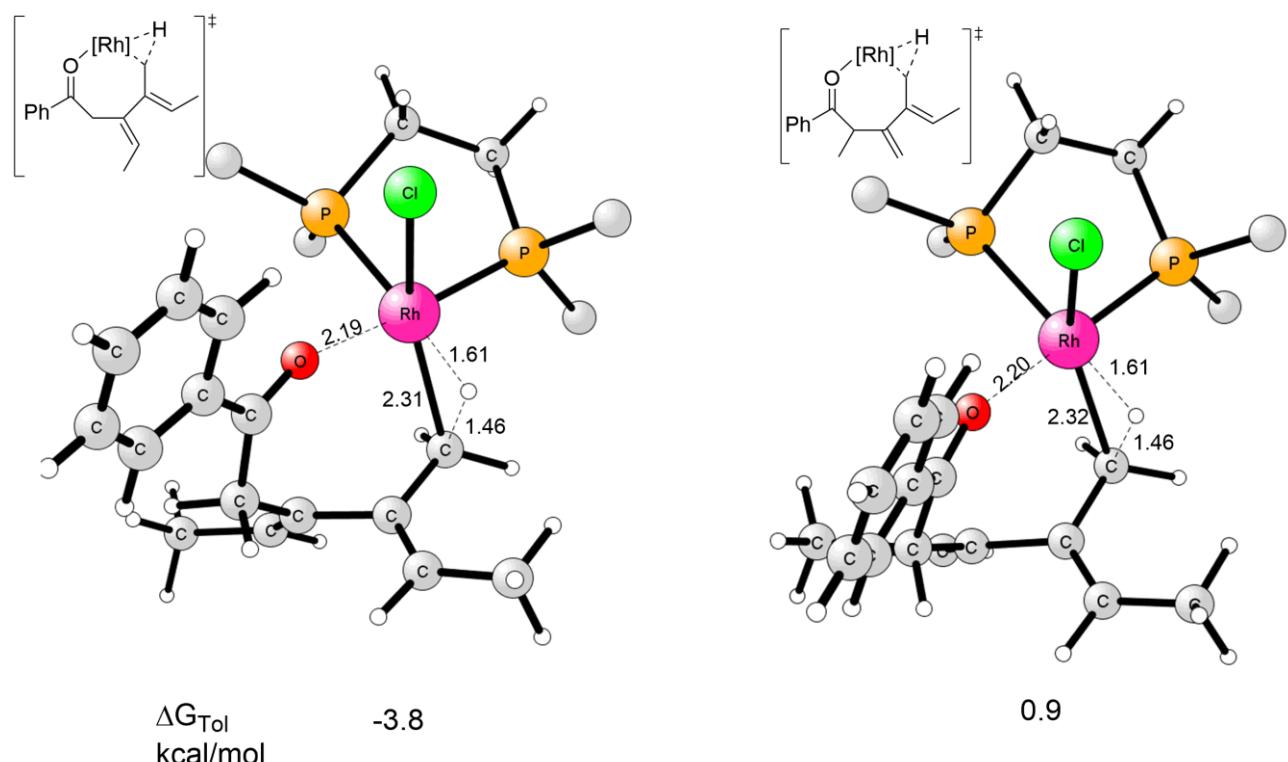
2.6. Isomerization of INT4 to INT5 (and INT4' to INT5')

The isomerization of **INT4** to **INT5** (and **INT4'** to **INT5'**) was found to take place through a series of steps (see the figures below for the calculated free energy profiles and optimized structures). First, the C-C double bond dissociates from the Rh center via **TS-A** to form a five-coordinated complex **INT-A**, having octahedral structure with a vacant coordination site. In order for the double bond of the allyl ligand to associate to the metal, and thus form the η^3 structure, the empty coordination site needs to relocate to the other side of the octahedron, *trans* to the other phosphorus atom. Therefore, the alkoxide ligand and the vacant site must switch places. This takes place via an initial isomerization of **INT-A** to **INT-B**, which has a trigonal bipyramidal geometry. An energy scan shows there is no transition state for this transformation. By further decreasing of the P-Rh-O angle **INT-B** isomerizes to the desired octahedral complex **INT-C**. The conversion of **INT-B** into **INT-C** requires passing transition state **TS3**, which is the highest point in the profile, and the corresponding barrier is 17.7 kcal/mol relative to **INT4** (16.6 kcal/mol for **TS3'** relative to **INT4'**). Finally, **INT5** and **INT5'** are formed by association of the double bond of the allyl ligand to the Rh-center (**TS-B** and **TS-B'**).



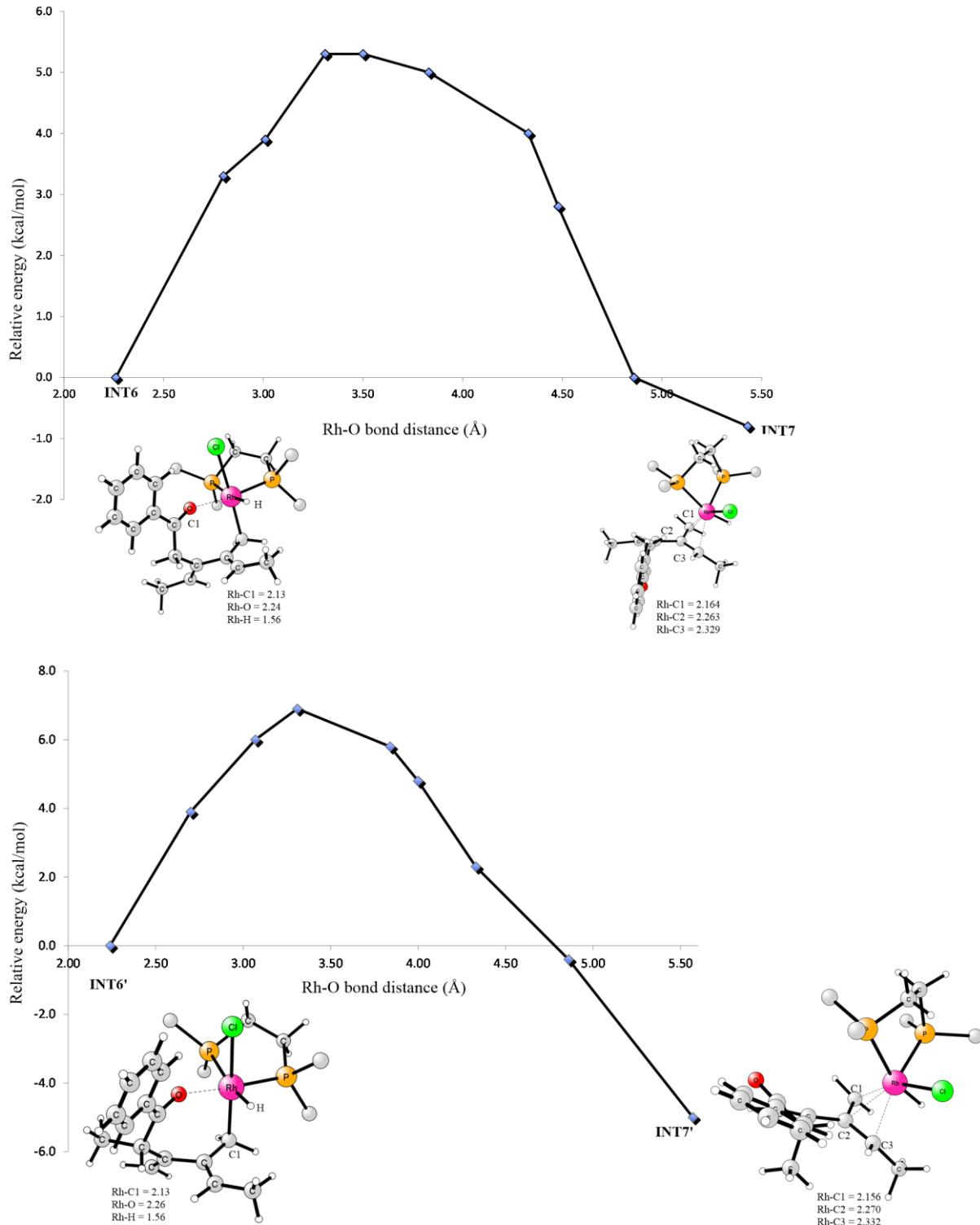


2.7. Direct reductive elimination from INT6 and INT6'

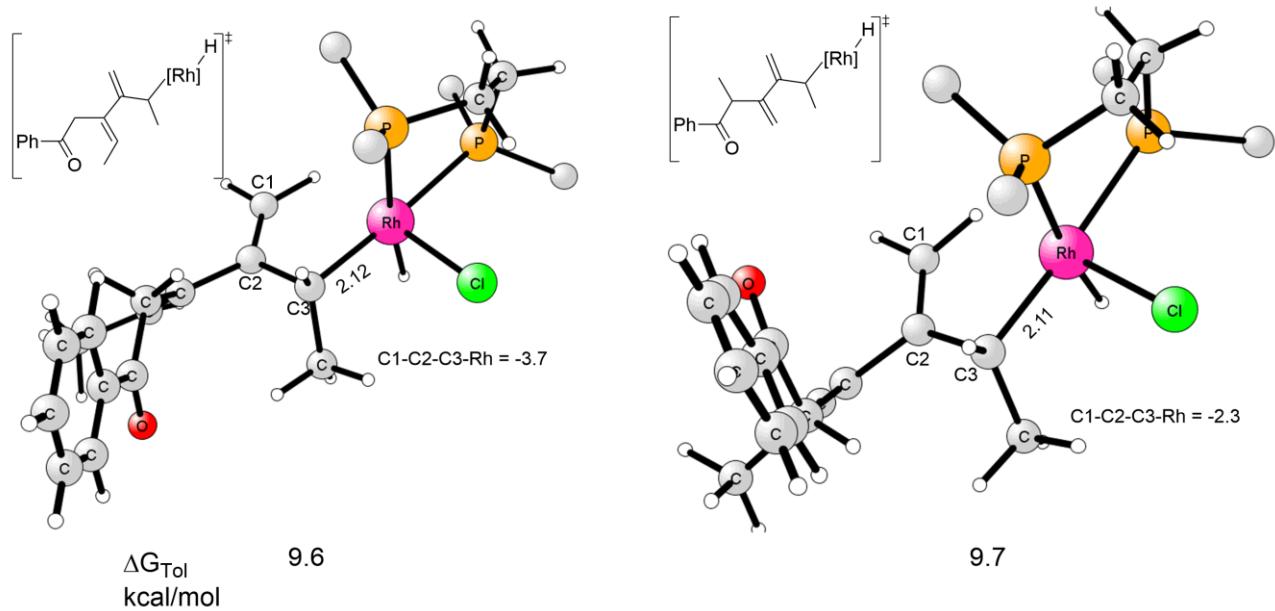


2.8. Energy scans for the isomerization from INT6 to INT7 (and INT6' to INT7')

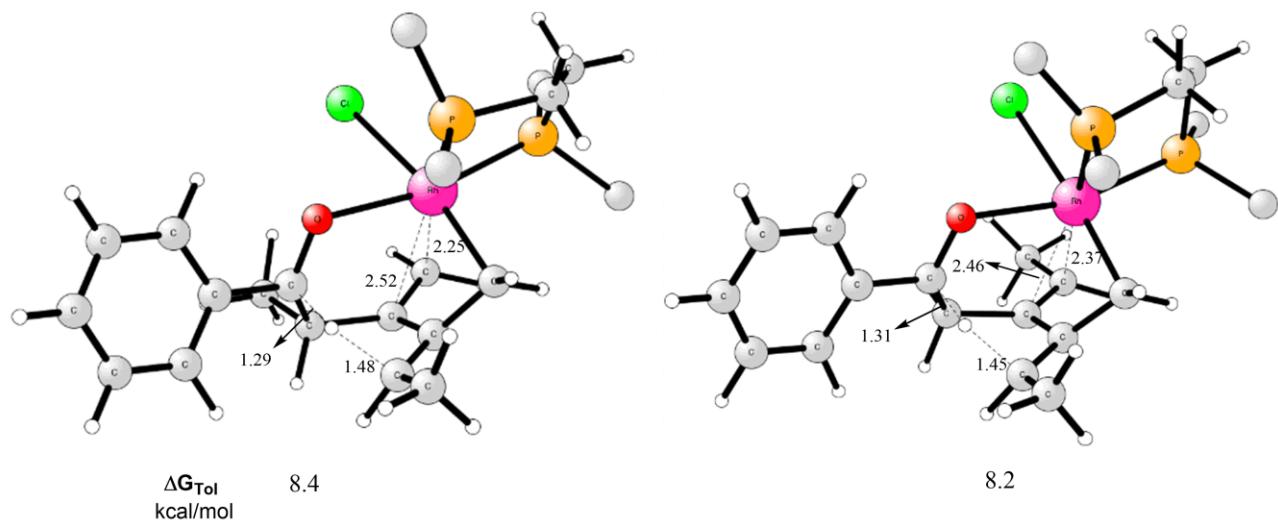
Geometries were optimized at the B3LYP/6-31G(*d,p*) (LANL2DZ for Rh) level. The final energies are single-point energies with large basis set [B3LYP/6-311+G(2*d,2p*) (LANL2DZ for Rh)] corrected for solvation and dispersion effects.



2.9. η^3 - η^1 - η^3 Isomerization of INT7 and INT7'

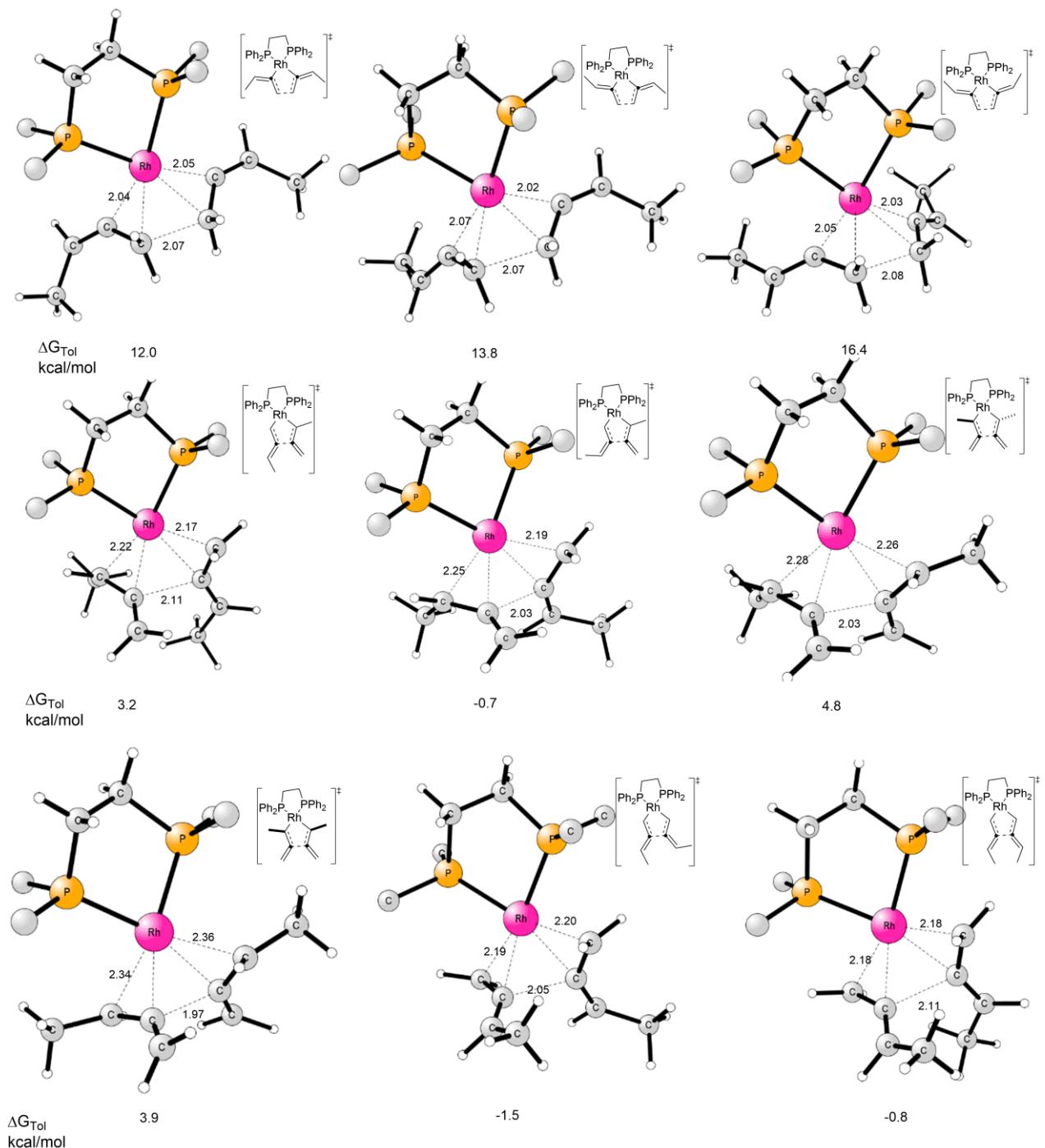


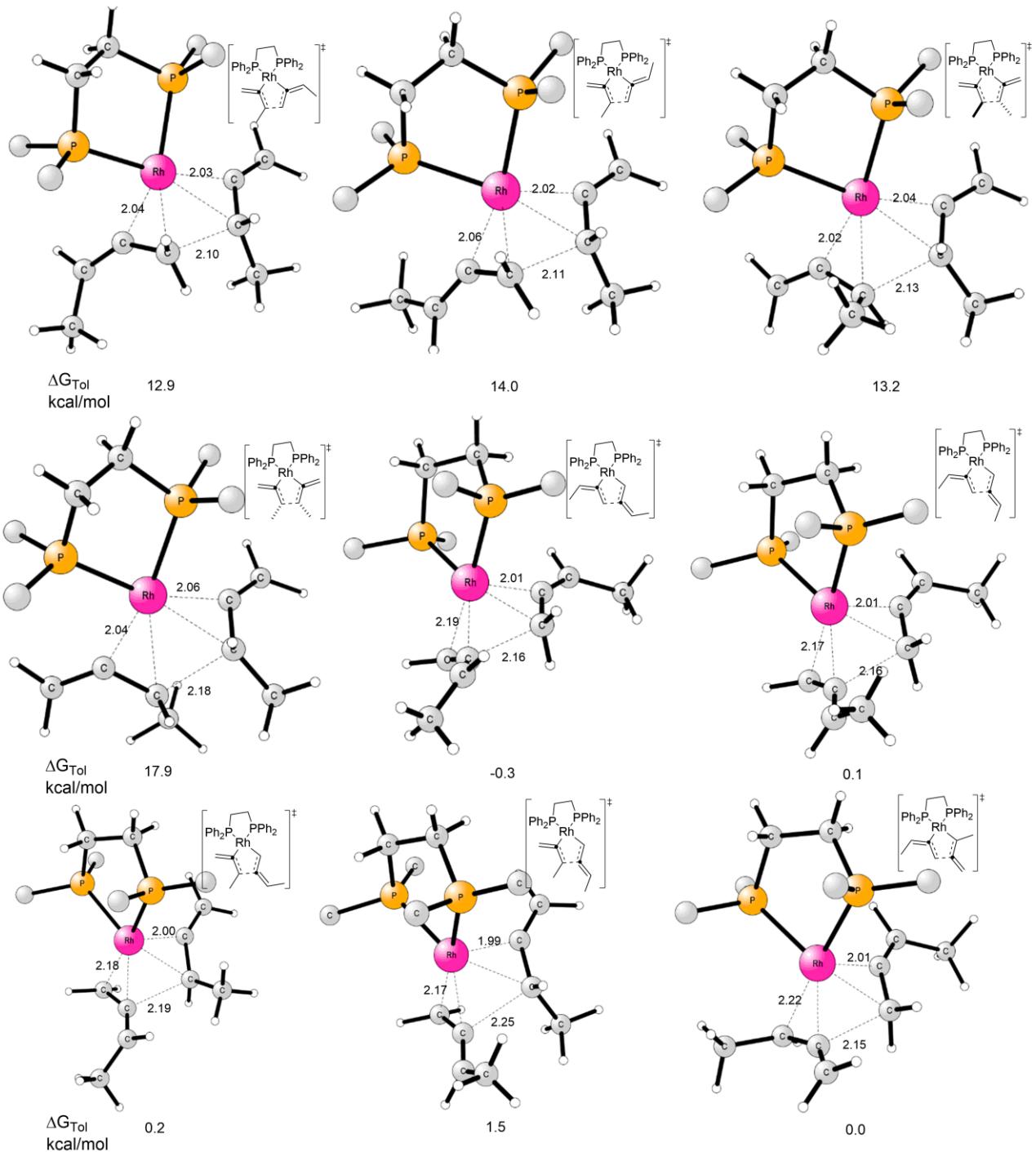
2.10. Alkoxide oxidation from INT4 and INT4'

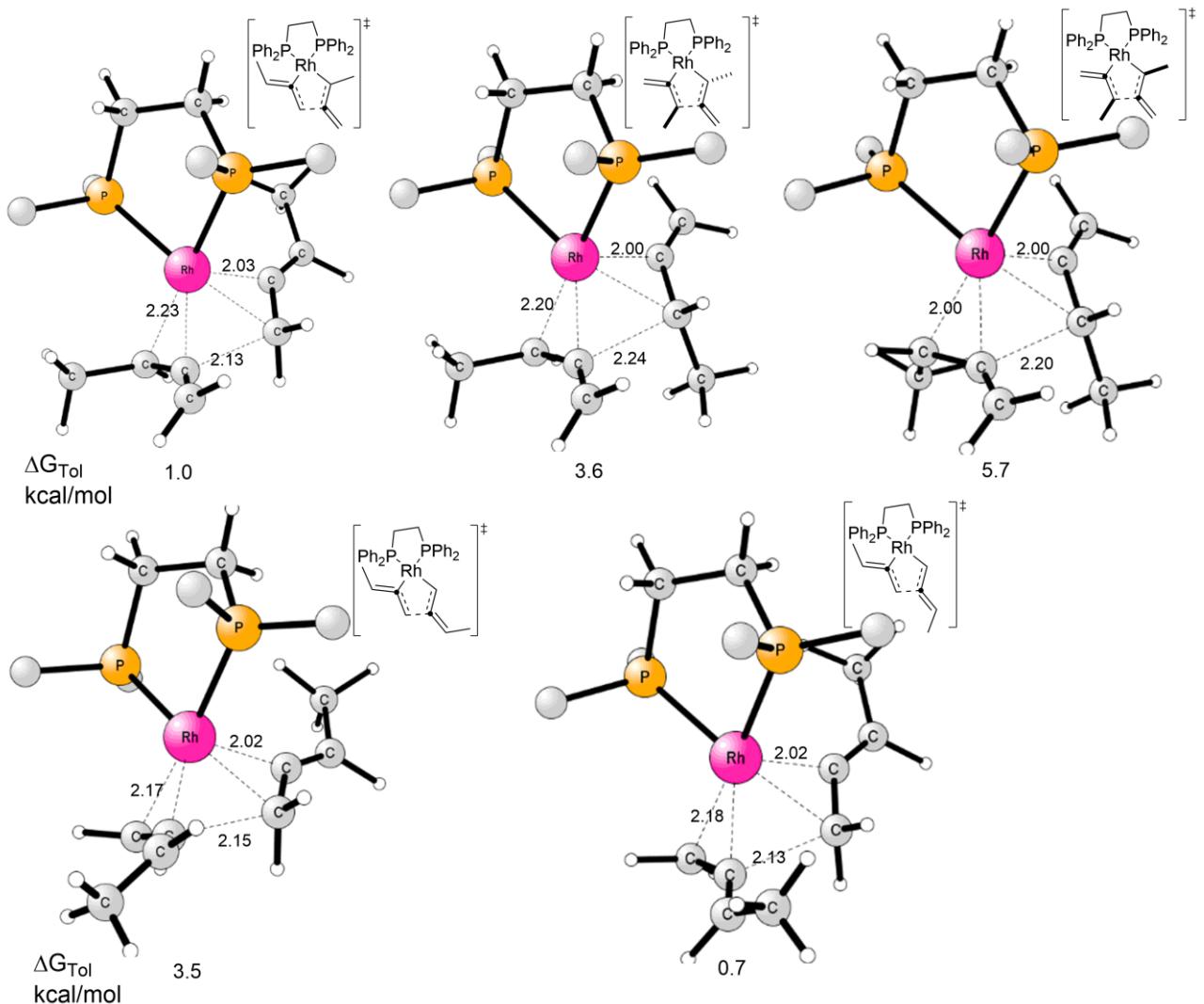


3. Results of the $[\text{Rh}(\text{dppe})^+]$ -catalyzed reaction.

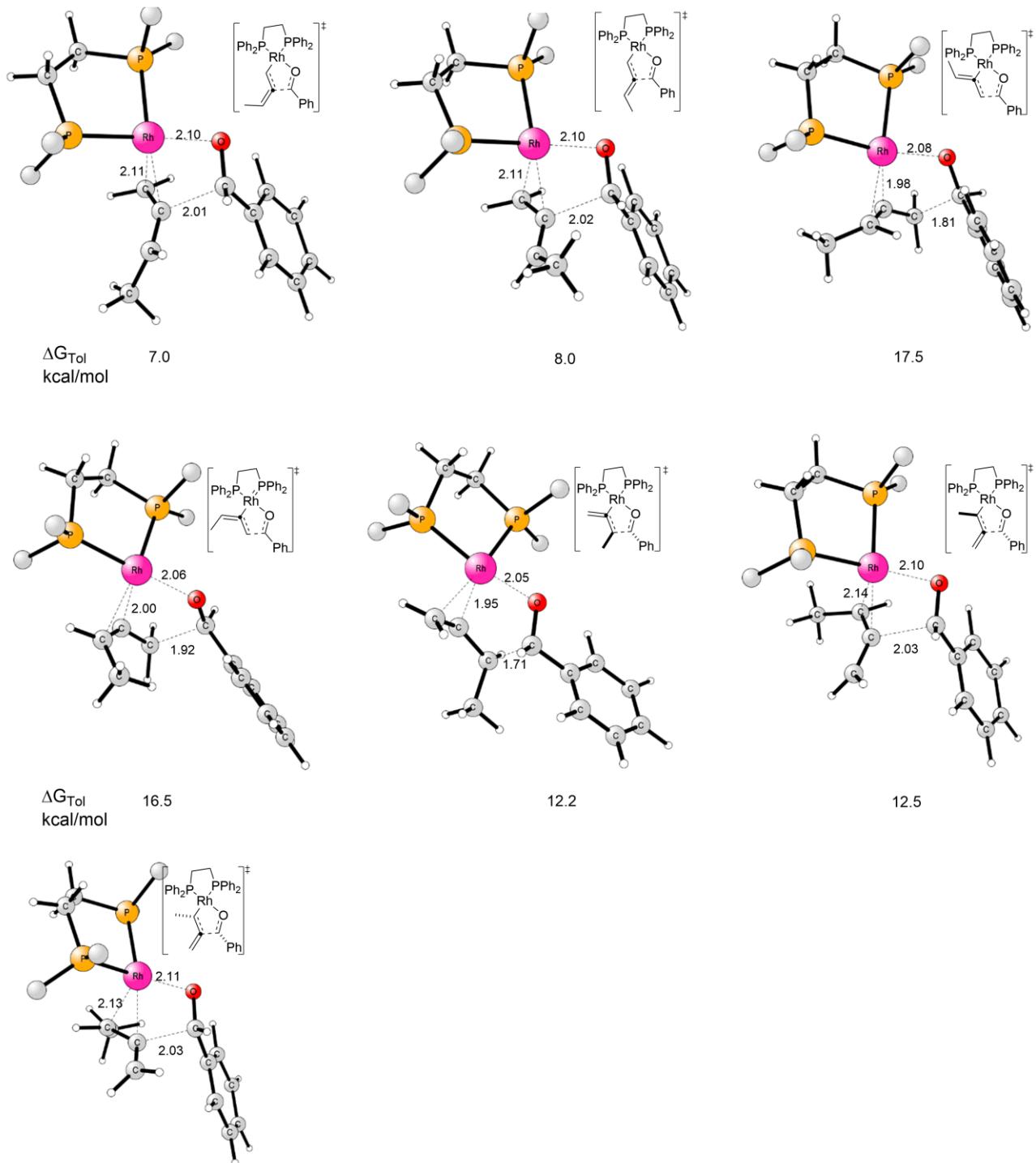
3.1. Other possibilities for allene-allene oxidative coupling



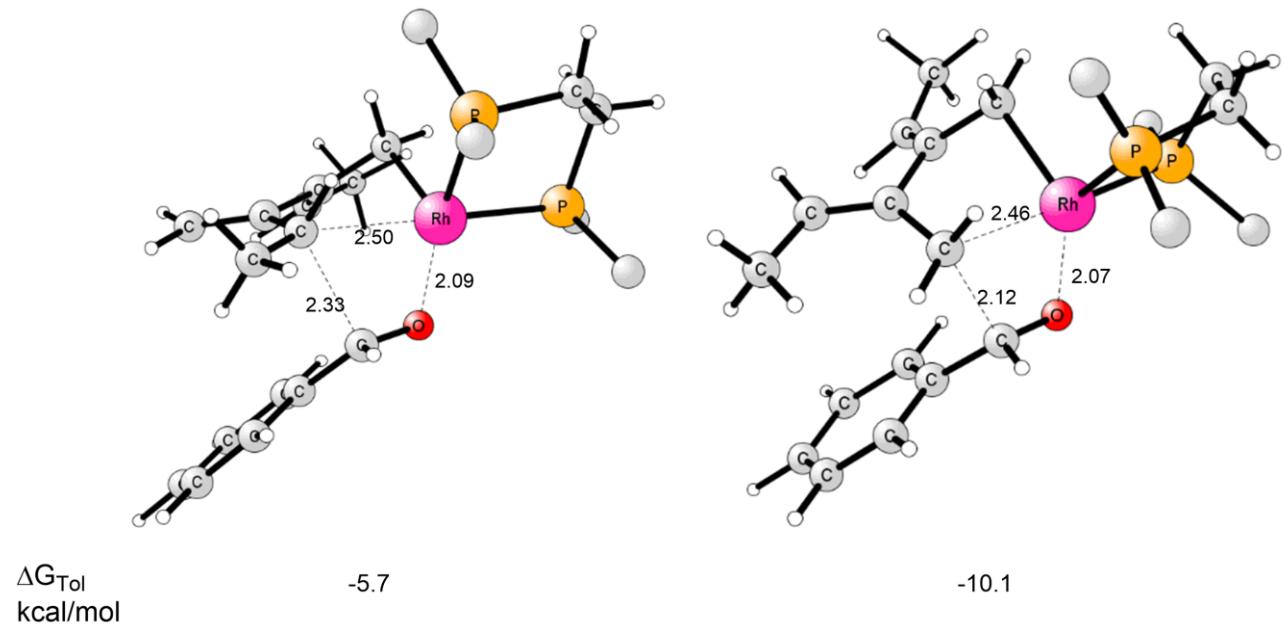




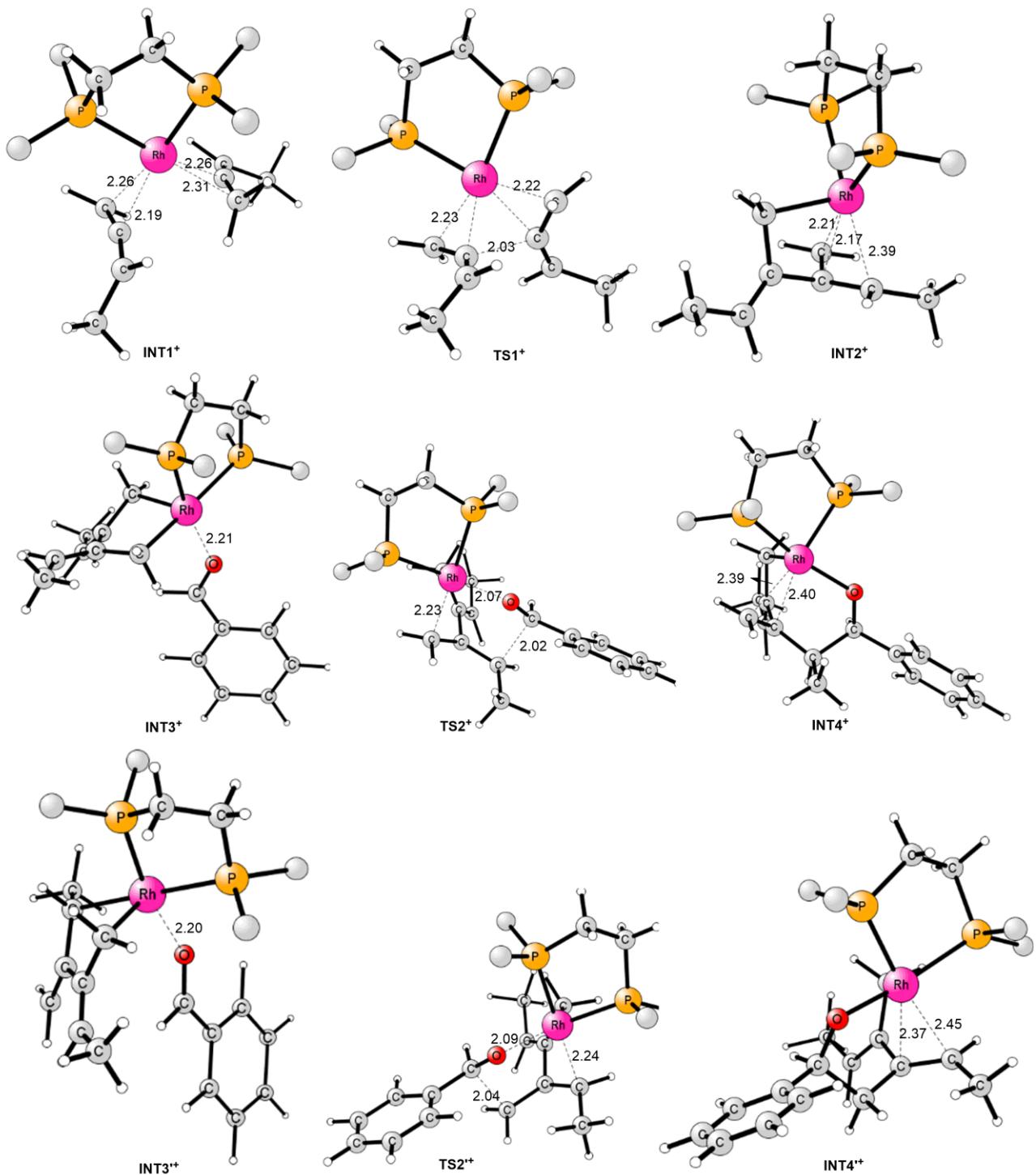
3.2. Possibilities for aldehyde-allene oxidative coupling



3.3. Migratory insertion from INT3⁺ and INT3^{’+}

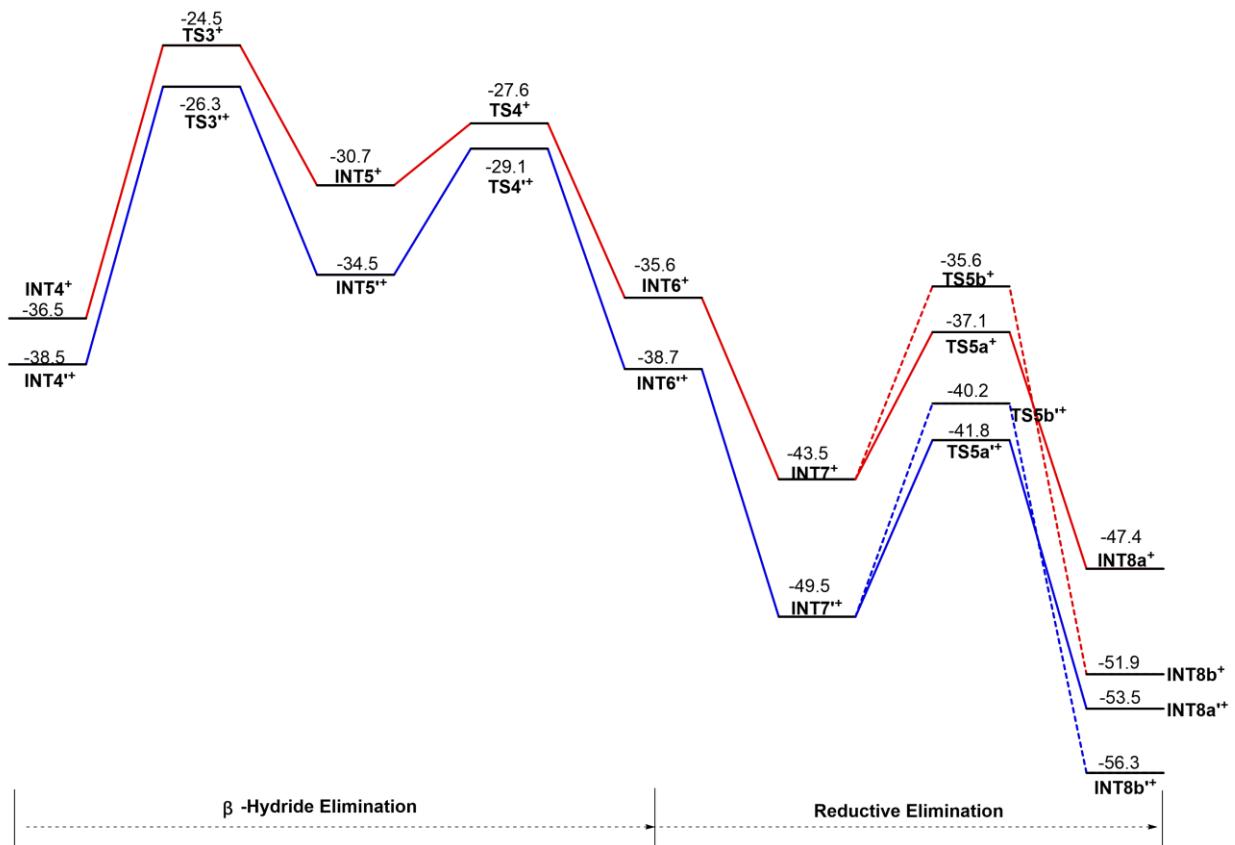


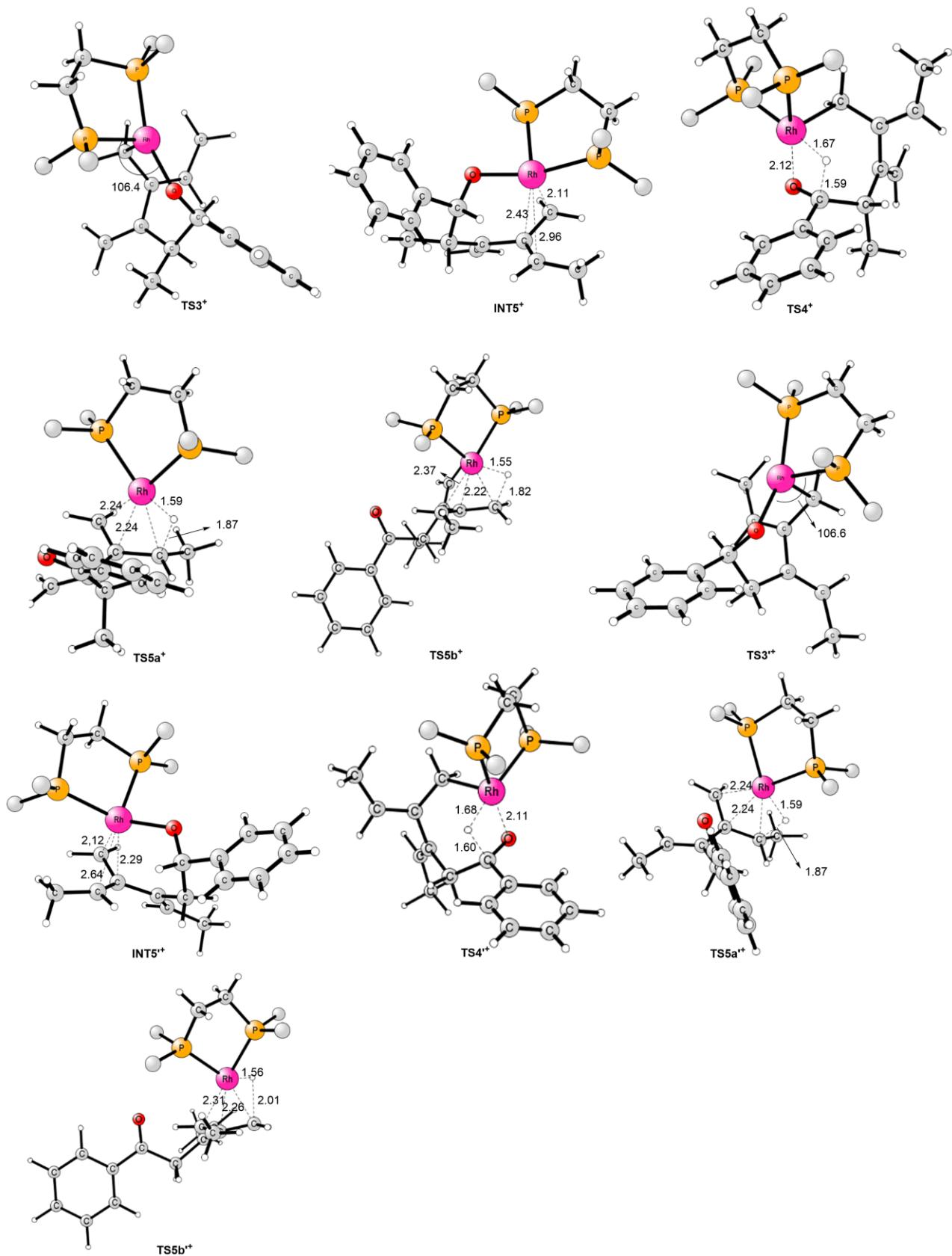
3.4. Structures of selected intermediates and TSs in Figure 10



3.5. β -Hydride elimination from INT4⁺ and INT4⁺⁺

In the case of the reaction catalyzed by the cationic rhodium catalyst, a pathway similar to the one established for the neutral chloride-containing catalyst was also considered. The corresponding calculated free energy profile and optimized structures are shown in the figures below.





4. Table of calculated energies

Energies and energy corrections of the stationary points.

| Stationary point | Single-point energy 6-311+G(2d,2p), lanl2dz (a.u.) | Thermal correction to Gibbs free energy at 298.15 K (a.u.) | Optimization energy 6-31G(d,p) , lanl2dz (a.u.) | Solvation energy (Tol) (a.u.) | Dispersion correction (kcal/mol) |
|-------------------|---|--|--|-------------------------------------|----------------------------------|
| RhCl(dppe) | -2258.125286 | 0.362255 | -2257.747445 | -0.017224 | -58.009422 |
| 1 | -345.680878 | 0.079549 | -345.575499 | -0.005615 | -6.835528 |
| 2 | -156.030029 | 0.057275 | -155.981278 | -0.001305 | -2.834755 |
| INT1 | -2414.178421 | 0.443052 | -2413.757781 | -0.016041 | -71.539806 |
| TS1 | -2570.177152 | 0.526675 | -2569.715171 | -0.013515 | -91.471668 |
| TS1a | -2603.786703 | 0.460526 | -2603.308110 | -0.017352 | -75.933841 |
| TS1b | -2759.818209 | 0.548809 | -2759.299497 | -0.018033 | -93.226569 |
| INT2 | -2570.246019 | 0.532237 | -2569.787161 | -0.013077 | -93.083239 |
| INT2a | -2603.789310 | 0.462150 | -2603.313355 | -0.018367 | -77.020712 |
| INT2b | -2759.852977 | 0.553598 | -2759.336346 | -0.017760 | -95.603989 |
| TS-H | -2570.184551 | 0.530213 | -2569.723966 | -0.014630 | -96.474537 |
| INT3 | -2915.932083 | 0.632190 | -2915.373710 | -0.015573 | -107.341346 |
| TS2 | -2915.907036 | 0.637497 | -2915.350069 | -0.016497 | -115.255915 |
| INT4 | -2915.924649 | 0.638575 | -2915.367845 | -0.015922 | -116.484181 |
| TS3 | -2915.898094 | 0.639494 | -2915.339741 | -0.018020 | -114.756689 |
| TS-INS | -2915.883222 | 0.636975 | -2915.326153 | -0.016682 | -114.640145 |
| INT5' | -2915.921700 | 0.637966 | -2915.365337 | -0.014892 | -114.836812 |
| TS4' | -2915.903948 | 0.633221 | -2915.345609 | -0.016088 | -112.156742 |
| TS-RE' | -2915.888186 | 0.632367 | -2915.329120 | -0.015703 | -104.939921 |
| INT6' | -2915.928475 | 0.632398 | -2915.370529 | -0.016757 | -107.597837 |
| INT7' | -2915.932975 | 0.631815 | -2915.374062 | -0.016696 | -109.800630 |
| TS5a' | -2915.918468 | 0.629100 | -2915.358190 | -0.016345 | -107.348379 |
| TS5b' | -2915.909119 | 0.628527 | -2915.349372 | -0.017199 | -110.081560 |
| INT8a' | -2915.966169 | 0.629594 | -2915.405528 | -0.015774 | -103.078817 |
| INT8b' | -2915.933697 | 0.631252 | -2915.374384 | -0.018295 | -108.763593 |
| INT3' | -2915.924508 | 0.634215 | -2915.365778 | -0.015155 | -111.018996 |
| TS2' | -2915.905496 | 0.637588 | -2915.348389 | -0.016089 | -115.889329 |
| INT4' | -2915.929072 | 0.638794 | -2915.372383 | -0.015577 | -115.037803 |
| TS3' | -2915.905389 | 0.639397 | -2915.347216 | -0.018435 | -111.836221 |
| TS-INS' | -2915.877180 | 0.636944 | -2915.318890 | -0.016351 | -116.674098 |
| INT5 | -2915.915372 | 0.640804 | -2915.359389 | -0.014763 | -117.718704 |
| TS4 | -2915.897684 | 0.635092 | -2915.339539 | -0.015879 | -115.446254 |

| | | | | | |
|-----------------------------|--------------|----------|--------------|-----------|-------------|
| TS-RE | -2915.882093 | 0.635989 | -2915.323471 | -0.015374 | -107.820595 |
| INT6 | -2915.921645 | 0.633865 | -2915.363888 | -0.016409 | -109.567491 |
| INT7 | -2915.918741 | 0.633525 | -2915.361043 | -0.015589 | -112.734106 |
| TS5a | -2915.910617 | 0.632718 | -2915.351038 | -0.014601 | -111.253836 |
| TS5b | -2915.898251 | 0.631392 | -2915.339134 | -0.016322 | -111.811419 |
| INT8a | -2915.958517 | 0.634696 | -2915.399724 | -0.013736 | -108.577583 |
| INT8b | -2915.924712 | 0.632332 | -2915.366600 | -0.016970 | -109.067132 |
| 3 | -657.831039 | 0.243771 | -657.642973 | -0.005170 | -27.704756 |
| 4 | -657.835421 | 0.242845 | -657.646753 | -0.005795 | -27.265911 |
| 5 | -657.826454 | 0.245999 | -657.638777 | -0.004814 | -29.914985 |
| 6 | -657.829311 | 0.245247 | -657.640999 | -0.005593 | -29.776911 |
| Rh(dppe)⁺ | -1797.636883 | 0.364735 | -1797.301771 | -0.049281 | -55.734391 |
| INT1⁺ | -2109.755634 | 0.524104 | -2109.335274 | -0.033812 | -83.830856 |
| TS1⁺ | -2109.731687 | 0.527191 | -2109.310730 | -0.034282 | -84.462044 |
| INT2⁺ | -2109.789441 | 0.530970 | -2109.372920 | -0.034456 | -85.456334 |
| INT3⁺ | -2455.479989 | 0.629889 | -2454.965000 | -0.034446 | -100.067122 |
| TS2⁺ | -2455.457686 | 0.634399 | -2454.944311 | -0.035224 | -106.168603 |
| INT4⁺ | -2455.473785 | 0.638953 | -2454.960551 | -0.036276 | -108.123291 |
| INT3'⁺ | -2455.474109 | 0.630448 | -2454.959302 | -0.035023 | -103.316085 |
| TS2'⁺ | -2455.457452 | 0.634926 | -2454.943725 | -0.035029 | -106.276715 |
| INT4'⁺ | -2455.479141 | 0.638579 | -2454.965801 | -0.035934 | -106.706045 |
| TS6⁺ | -2455.452131 | 0.637867 | -2454.940717 | -0.035555 | -111.322989 |
| TS6'⁺ | -2455.453357 | 0.637208 | -2454.941701 | -0.035552 | -110.280057 |
| INT9⁺ | -2455.519340 | 0.638382 | -2455.006377 | -0.034090 | -106.689806 |
| INT9'⁺ | -2455.523470 | 0.639251 | -2455.010857 | -0.034128 | -106.871712 |

5. Cartesian coordinates

RhCl(dppe)

| | | | | | | | |
|---|-------------|-------------|-------------|----------|-------------|-------------|-------------|
| P | 1.53980400 | 0.08543000 | -0.43069200 | C | -2.00282500 | 3.19477200 | 0.24579800 |
| C | 0.64555900 | 0.10853100 | -2.07479500 | C | -2.79196300 | 4.29963100 | 0.55863500 |
| C | -0.60467400 | 0.98727200 | -1.95689000 | H | -4.18046000 | 4.16734200 | 0.64496300 |
| P | -1.46323700 | 0.52620900 | -0.35321400 | H | -4.77258100 | 2.92516100 | 0.41815500 |
| H | 1.29809600 | 0.41800700 | -2.89683400 | H | -3.98511900 | 1.81776700 | 0.09392800 |
| H | 0.36405400 | -0.93241500 | -2.26566800 | H | -0.92130700 | 3.29835800 | 0.21488500 |
| H | -0.33253200 | 2.04512500 | -1.88270000 | H | -2.32235100 | 5.26076000 | 0.74687500 |
| H | -1.26766800 | 0.86934800 | -2.81927800 | Rh | -4.79504700 | 5.02668400 | 0.89713500 |
| C | -2.56642000 | -0.86762600 | -0.85250300 | Cl | 0.09566900 | 0.09911700 | 1.21903300 |
| C | -2.59204700 | 1.94275000 | -0.00658700 | | 1.47079600 | -0.34103000 | 3.09270900 |
| C | 2.65387000 | 1.55607900 | -0.43459200 | 1 | | | |
| C | 2.68386400 | -1.34757300 | -0.58063300 | C | -1.29874000 | -0.47231900 | 1.59389900 |
| C | 3.32418100 | 1.86822700 | 0.76171500 | C | 0.10143400 | -0.45456800 | 1.59445100 |
| C | 4.19287800 | 2.95657700 | 0.81597400 | C | 0.79255300 | 0.75937500 | 1.59391800 |
| C | 4.39489800 | 3.75733400 | -0.31142900 | C | 0.08158600 | 1.95880800 | 1.59284400 |
| C | 3.72424200 | 3.46263200 | -1.49789600 | C | -1.31930100 | 1.94610500 | 1.59227800 |
| C | 2.85991700 | 2.36653900 | -1.56145500 | C | -2.00875900 | 0.72354100 | 1.59280900 |
| H | 3.14691500 | 1.26570700 | 1.64898700 | H | -1.82854400 | -1.42040700 | 1.59432400 |
| H | 4.70589000 | 3.18455100 | 1.74577100 | H | 0.65349900 | -1.39023100 | 1.59530400 |
| H | 5.06679800 | 4.60953300 | -0.26275600 | H | 1.87842300 | 0.76824500 | 1.59435100 |
| H | 3.87079000 | 4.08289800 | -2.37779100 | H | 0.60869100 | 2.91035700 | 1.59243000 |
| H | 2.35184300 | 2.15883200 | -2.49765000 | H | -3.09407700 | 0.74208600 | 1.59234700 |
| C | 3.68240700 | -1.35834100 | -1.56879900 | C | -2.06754700 | 3.22372600 | 1.59110800 |
| C | 4.51452100 | -2.46722800 | -1.71382900 | H | -1.42660200 | 4.13411300 | 1.58987800 |
| C | 4.36337300 | -3.56974900 | -0.86841200 | O | -3.28045200 | 3.31589900 | 1.59137800 |
| C | 3.38256200 | -3.55798500 | 0.12365800 | | | | |
| C | 2.54292500 | -2.45139400 | 0.27043600 | 2 | | | |
| H | 3.82244100 | -0.49666700 | -2.21591800 | C | 0.33439000 | 1.40917300 | 0.04169800 |
| H | 5.28466800 | -2.46806800 | -2.48002700 | C | -0.94299900 | 1.15443100 | -0.07462600 |
| H | 5.01616600 | -4.43112400 | -0.97883500 | H | -1.30158900 | 0.22368600 | -0.50965700 |
| H | 3.27294200 | -4.40651100 | 0.79264600 | H | -1.69860400 | 1.86350000 | 0.25760700 |
| H | 1.79486900 | -2.42311400 | 1.05606100 | C | 1.61302300 | 1.66284000 | 0.16030900 |
| C | -3.43706200 | -0.78943300 | -1.95327300 | H | 2.11713800 | 2.17011300 | -0.66385600 |
| C | -4.22690300 | -1.88208500 | -2.31035800 | C | 2.45860000 | 1.30554100 | 1.35952000 |
| C | -4.15840100 | -3.06680100 | -1.57197100 | H | 3.28308200 | 0.64196400 | 1.07183100 |
| C | -3.29813800 | -3.15521200 | -0.47716600 | H | 2.90803100 | 2.20306800 | 1.80150100 |
| C | -2.50489500 | -2.06238500 | -0.12056900 | H | 1.86561000 | 0.80391800 | 2.12777300 |
| H | -3.50931200 | 0.12928700 | -2.52931600 | | | | |
| H | -4.89515600 | -1.80971900 | -3.16379900 | | | | |
| H | -4.77316000 | -3.91738100 | -1.85234400 | | | | |
| H | -3.23887400 | -4.07449500 | 0.09819500 | | | | |
| H | -1.81854900 | -2.12913900 | 0.71979600 | | | | |

TS1Imaginary frequency: -328.5 cm⁻¹

| | | | | | | | |
|---|-------------|-------------|--------------|----|-------------|-------------|-------------|
| P | 2.54469800 | -2.89840700 | -8.16927700 | C | 2.75945100 | 3.64433100 | -6.52328800 |
| C | 2.58864700 | -2.08632900 | -9.84679600 | C | 4.07809000 | 3.37486400 | -6.15475800 |
| C | 2.74521800 | -0.55972000 | -9.73813000 | H | 4.65058500 | 2.14942800 | -6.49936500 |
| P | 1.57730000 | 0.17540500 | -8.44858800 | H | 3.91329800 | 1.20328300 | -7.21221900 |
| H | 1.57730000 | 0.17540500 | -8.44858800 | H | 1.00189400 | 2.93301000 | -7.53043800 |
| H | 3.36466000 | -2.52158100 | -10.48597600 | H | 2.30074500 | 4.59199500 | -6.25533500 |
| H | 1.61507600 | -2.33579300 | -10.27892500 | H | 4.65275100 | 4.11057300 | -5.59958100 |
| H | 3.76641200 | -0.28732700 | -9.46004400 | H | 5.67308000 | 1.92380800 | -6.20971800 |
| H | 2.53641300 | -0.08690000 | -10.70202100 | Rh | 4.37492200 | 0.24751500 | -7.44129300 |
| C | 0.41002000 | 1.16944300 | -9.47838600 | C | 0.88364800 | -1.58581300 | -6.97397800 |
| C | 2.59281600 | 1.47262300 | -7.61062100 | C | 1.36429400 | -2.30034600 | -4.97697100 |
| C | 4.30411700 | -2.88179300 | -7.59312500 | H | 2.04476600 | -1.08947600 | -5.27676300 |
| C | 4.30411700 | -2.88179300 | -7.59312500 | H | 1.72108100 | -0.15300600 | -4.82593100 |
| C | 2.29440400 | -4.69165900 | -8.52224900 | H | 3.11831300 | -1.13708400 | -5.44981400 |
| C | 4.57975400 | -3.38235200 | -6.30808500 | C | 4.57975400 | -3.40874900 | -4.25430200 |
| C | 5.88239700 | -3.39876900 | -5.81142700 | H | 0.85826200 | -4.25897900 | -4.42489500 |
| C | 6.93765000 | -2.91186400 | -6.58677400 | Cl | 6.93765000 | -2.46434500 | -8.75191300 |
| C | 6.68033000 | -2.41522200 | -7.86410000 | C | -0.72887700 | -2.46434500 | -8.75191300 |
| C | 5.37501400 | -2.40241600 | -8.36453700 | H | 2.49979800 | -3.54637000 | -3.11976600 |
| H | 5.37501400 | -2.40241600 | -8.36453700 | H | 1.97935700 | -3.68232800 | -2.16211000 |
| H | 3.76523800 | -3.75974900 | -5.69815800 | H | 3.14130200 | -4.42794200 | -3.25221200 |
| H | 6.07322600 | -3.79122500 | -4.81659900 | H | 3.13909500 | -2.66374400 | -3.03488100 |
| H | 7.95210000 | -2.92280700 | -6.19873600 | C | -0.70486500 | -1.88756800 | -5.50014800 |
| H | 7.49444000 | -2.04181600 | -8.47909400 | C | -0.71334800 | -0.55318400 | -5.95444800 |
| H | 5.20591800 | -2.02550500 | -9.36762000 | H | -1.49033700 | -0.26742100 | -6.65856600 |
| C | 3.30381800 | -5.45525700 | -9.13152800 | H | -0.35298000 | 0.25024400 | -5.31486400 |
| C | 3.10500900 | -6.81104800 | -9.38919000 | C | -1.15962300 | -3.89914100 | -5.13389800 |
| C | 1.89921600 | -7.42051200 | -9.03382400 | H | -1.52368900 | -2.87437700 | -5.15626300 |
| C | 0.89382200 | -6.66842400 | -8.42551200 | C | -3.23124000 | -1.60611400 | -4.78269800 |
| C | 1.08636100 | -5.30909700 | -8.16953600 | H | -3.62631600 | -3.19574700 | -5.46450000 |
| H | 4.25305800 | -4.99662100 | -9.39278600 | H | -3.89264400 | -3.16907300 | -3.06090200 |
| H | 3.89264400 | -7.39166000 | -9.86134200 | H | -3.16907300 | -3.06090200 | -3.76555300 |
| H | 1.74603600 | -8.47795300 | -9.23117900 | | | | |
| H | -0.04785000 | -7.13621300 | -8.15273400 | | | | |
| H | 0.29425700 | -4.71341300 | -7.73004400 | | | | |
| C | 0.88912000 | 2.22124100 | -10.28130000 | | | | |
| C | 0.01561800 | 2.95908800 | -11.07775200 | | | | |
| C | -1.34909200 | 2.65612200 | -11.08479800 | | | | |
| C | -1.83048000 | 1.61098700 | -10.29804500 | | | | |
| C | -0.95783200 | 0.86756900 | -9.49779600 | | | | |
| H | 1.94549200 | 2.47511600 | -10.27519600 | | | | |
| H | 0.39898800 | 3.76967100 | -11.69123100 | | | | |
| H | -2.03007000 | 3.23090700 | -11.70638200 | | | | |
| H | -2.88745600 | 1.36110100 | -10.30913100 | | | | |
| H | -1.32536900 | 0.02263700 | -8.92736300 | | | | |
| C | 2.02248400 | 2.70261500 | -7.24305100 | | | | |

TS1aImaginary frequency: -463.9 cm⁻¹

| | | | | | | | |
|---|-------------|-------------|-------------|----|-------------|-------------|-------------|
| P | 2.36233400 | 1.35551800 | -4.39646700 | C | -4.17835700 | -0.01904600 | -3.37476000 |
| C | 1.48414800 | 0.17459500 | -5.55180600 | C | -4.53292500 | -0.42821200 | -2.08991300 |
| C | 0.01270900 | 0.07578700 | -5.12045000 | C | -3.54153000 | -0.84031400 | -1.19545800 |
| P | -0.05234700 | -0.41650800 | -3.31474100 | H | -2.20215100 | -0.84144600 | -1.57983700 |
| H | 1.56566600 | 0.50728400 | -6.59120400 | H | -2.58639500 | 0.29889800 | -4.77326400 |
| H | 1.96368600 | -0.80600900 | -5.46932200 | H | -4.94248500 | 0.30327700 | -4.07633900 |
| H | -0.47756300 | 1.04993200 | -5.22667400 | H | -5.57557200 | -0.42482300 | -1.78540300 |
| H | -0.52943600 | -0.64878100 | -5.73728700 | Rh | 1.32223600 | 1.07379400 | -2.20152700 |
| C | 0.41018200 | -2.19940000 | -3.43772400 | Cl | 2.51746200 | 3.08302200 | -1.49265900 |
| C | -1.83660700 | -0.43277400 | -2.87501500 | C | 4.21495500 | -0.57906300 | 1.93897000 |
| C | 2.08128900 | 2.97965300 | -5.22037700 | C | 4.16723200 | 0.62778000 | 2.64257700 |
| C | 4.15358300 | 1.00996900 | -4.59277300 | C | 3.23428000 | 1.60417300 | 2.28898300 |
| C | 1.20121200 | 3.90904700 | -4.64840500 | C | 2.36444200 | 1.39315800 | 1.21928300 |
| C | 0.92526400 | 5.11013300 | -5.30653200 | C | 2.40595700 | 0.18372700 | 0.51812800 |
| C | 1.53185300 | 5.39664300 | -6.52926800 | C | 3.32498700 | -0.80956100 | 0.89294900 |
| C | 2.42180900 | 4.48085700 | -7.09740500 | H | 4.93504700 | -1.34428700 | 2.21502300 |
| C | 2.69564700 | 3.27874000 | -6.44726800 | H | 4.85431900 | 0.80468700 | 3.46548500 |
| H | 0.76510500 | 3.70770700 | -3.67573900 | H | 3.19077800 | 2.54063600 | 2.83718600 |
| H | 0.24615300 | 5.82569600 | -4.85236500 | H | 1.66369000 | 2.16326300 | 0.92138600 |
| H | 1.32141800 | 6.33456300 | -7.03544200 | H | 3.32717200 | -1.75645000 | 0.36248000 |
| H | 2.90659700 | 4.70568400 | -8.04324000 | C | 1.41912600 | -0.16433100 | -0.55844800 |
| H | 3.40034300 | 2.57934500 | -6.88868000 | H | 0.39573700 | 1.11020400 | -0.88664300 |
| C | 4.66843500 | 0.24552800 | -5.65197600 | O | 0.87251700 | -1.25172700 | -0.54818900 |
| C | 6.04200200 | 0.01459800 | -5.75126100 | | | | |
| C | 6.91152900 | 0.54457900 | -4.79712000 | | | | |
| C | 6.40473900 | 1.30437100 | -3.74029700 | | | | |
| C | 5.03367100 | 1.53545600 | -3.63096700 | | | | |
| H | 4.00779400 | -0.17491900 | -6.40393200 | | | | |
| H | 6.42947400 | -0.57947500 | -6.57414100 | | | | |
| H | 7.97973600 | 0.36307800 | -4.87519700 | | | | |
| H | 7.07674100 | 1.71491000 | -2.99234200 | | | | |
| H | 4.63624400 | 2.11672200 | -2.80282600 | | | | |
| C | -0.52589200 | -3.16649100 | -3.83350500 | | | | |
| C | -0.13756600 | -4.49528800 | -4.00856200 | | | | |
| C | 1.18972300 | -4.87166500 | -3.79388100 | | | | |
| C | 2.12703200 | -3.91589000 | -3.39844600 | | | | |
| C | 1.73916300 | -2.58791300 | -3.21525400 | | | | |
| H | -1.56221100 | -2.88507800 | -3.99551000 | | | | |
| H | -0.87305600 | -5.23624000 | -4.30885400 | | | | |
| H | 1.49051000 | -5.90683000 | -3.92802100 | | | | |
| H | 3.15912600 | -4.20427900 | -3.22097300 | | | | |
| H | 2.46367300 | -1.85071000 | -2.88314000 | | | | |
| C | -2.83754700 | -0.02146300 | -3.76773100 | | | | |

TS1bImaginary frequency: -350.3 cm⁻¹

| | | | | | | | |
|---|-------------|-------------|--------------|----|-------------|-------------|-------------|
| P | 2.98330900 | -2.65708300 | -8.48237000 | C | 2.37816200 | 3.07112700 | -5.67158700 |
| C | 2.91039700 | -1.74376200 | -10.10408600 | C | 3.39762500 | 3.86251100 | -6.20611900 |
| C | 2.85509500 | -0.21811100 | -9.89800400 | C | 3.92292500 | 3.55798300 | -7.46193800 |
| P | 1.65409000 | 0.22853500 | -8.52822600 | H | 3.43169200 | 2.46735600 | -8.18350900 |
| H | 3.73899500 | -2.02943100 | -10.76118800 | H | 1.10536500 | 1.35471800 | -5.96610100 |
| H | 1.97911700 | -2.09835100 | -10.55639800 | H | 1.96428800 | 3.30330800 | -4.69438000 |
| H | 3.83666300 | 0.16283000 | -9.60539100 | H | 3.78034000 | 4.71131300 | -5.64669600 |
| H | 2.56889100 | 0.27955800 | -10.82901800 | Rh | 4.71409100 | 4.17035300 | -7.88557000 |
| C | 0.21340200 | 1.01866800 | -9.36123900 | C | 2.25979900 | 2.25979900 | -9.16506700 |
| C | 2.41397300 | 1.66261600 | -7.65140600 | C | -1.65036500 | -3.00339200 | -1.91500000 |
| C | 4.72820900 | -2.49872800 | -7.89243000 | C | -1.49904900 | -1.80329900 | -1.21337200 |
| C | 2.93250700 | -4.44264500 | -8.93847700 | C | -0.99422400 | -0.67624300 | -1.86580600 |
| C | 5.09307900 | -3.18714100 | -6.72190200 | C | -0.63451400 | -0.74689800 | -3.21130300 |
| C | 6.39219800 | -3.11035400 | -6.22366600 | C | -0.77191000 | -1.94945200 | -3.91678900 |
| C | 7.35452700 | -2.34440400 | -6.88652700 | H | -1.29022900 | -3.07415100 | -3.25853500 |
| C | 7.00901500 | -1.66496600 | -8.05355100 | H | -2.05525700 | -3.87898400 | -1.41526000 |
| C | 5.70639800 | -1.74287900 | -8.55451000 | H | -1.78121500 | -1.74635300 | -0.16580100 |
| H | 4.35622900 | -3.79416200 | -6.20530000 | H | -0.88681100 | 0.26054200 | -1.32588700 |
| H | 6.65414900 | -3.65095100 | -5.31865200 | H | -0.26114900 | 0.12552700 | -3.73620800 |
| H | 8.36677500 | -2.28306200 | -6.49778200 | C | -1.41307600 | -4.00464800 | -3.80767000 |
| H | 7.75238700 | -1.07489600 | -8.58203500 | C | -0.41916500 | -2.03024500 | -5.36645900 |
| H | 5.47010000 | -1.21727100 | -9.47326400 | H | -0.83478100 | -2.90440500 | -5.88566700 |
| C | 4.01549800 | -5.01845600 | -9.62476100 | O | 1.55285700 | -2.67741500 | -5.29958200 |
| C | 3.99001600 | -6.36623000 | -9.97928100 | C | -0.28550400 | -0.92211500 | -6.03200900 |
| C | 2.88839600 | -7.15639600 | -9.64155300 | C | 1.52400000 | -2.67741500 | -5.29958200 |
| C | 1.81309400 | -6.59182300 | -8.95554200 | H | -0.88681100 | 0.26054200 | -1.32588700 |
| C | 1.82930000 | -5.23972300 | -8.60544400 | C | -1.49904900 | -1.80329900 | -1.21337200 |
| H | 4.88670600 | -4.41910100 | -9.87321700 | H | -0.96310200 | -4.68260300 | -5.18795800 |
| H | 4.83105400 | -6.79961000 | -10.51312700 | Cl | -0.34044300 | -2.68577500 | -8.90791800 |
| H | 2.87015400 | -8.20794000 | -9.91431800 | C | 2.72410000 | -4.42659000 | -3.88194500 |
| H | 0.95110100 | -7.20015400 | -8.69724500 | H | 2.23924100 | -4.72079000 | -2.94048100 |
| H | 0.97725900 | -4.78737400 | -8.11223900 | H | 3.24277800 | -5.31955500 | -4.25485100 |
| C | 0.39746100 | 2.03700500 | -10.31094800 | H | 3.46281300 | -3.65419500 | -3.65346100 |
| C | -0.70210700 | 2.65252100 | -10.90578400 | H | 1.98033300 | -0.58956800 | -4.88322100 |
| C | -1.99625700 | 2.26465500 | -10.54709200 | | | | |
| C | -2.18391300 | 1.26402700 | -9.59421400 | | | | |
| C | -1.08545800 | 0.63697800 | -9.00020100 | | | | |
| H | 1.39844800 | 2.36460300 | -10.57997600 | | | | |
| H | -0.55013500 | 3.43606300 | -11.64291500 | | | | |
| H | -2.85393500 | 2.74483500 | -11.01009700 | | | | |
| H | -3.18777500 | 0.95868100 | -9.31395800 | | | | |
| H | -1.22818600 | -0.15414800 | -8.27395600 | | | | |
| C | 1.89192700 | 1.97639700 | -6.38505300 | | | | |

| INT2 | | | | C | 4.29351500 | 3.14136400 | -6.21468600 |
|-------------|-------------|-------------|--------------|----|-------------|-------------|-------------|
| P | 2.34471200 | -2.99207800 | -8.24270600 | C | 4.75955700 | 1.87340200 | -6.56594500 |
| C | 2.41726900 | -2.13648100 | -9.89846400 | C | 3.92524500 | 0.97729100 | -7.23446800 |
| C | 2.55775100 | -0.61097600 | -9.76286900 | H | 1.13854100 | 2.91434300 | -7.45608000 |
| P | 1.48033700 | 0.11573400 | -8.38881100 | H | 2.60794800 | 4.48551400 | -6.25921900 |
| H | 3.20245800 | -2.55168200 | -10.53938400 | H | 4.94334300 | 3.83823100 | -5.69327000 |
| H | 1.45059500 | -2.37872900 | -10.34893100 | H | 5.77362000 | 1.57518300 | -6.31504500 |
| H | 3.59237100 | -0.33324100 | -9.54589600 | H | 4.30622700 | -0.01191800 | -7.46981300 |
| H | 2.28473800 | -0.12799800 | -10.70495300 | Rh | 0.73042300 | -1.66661900 | -7.05501500 |
| C | 0.29192600 | 1.21865000 | -9.26507100 | C | 1.01710600 | -1.71157600 | -4.35692900 |
| C | 2.61228200 | 1.33901600 | -7.58168600 | C | 1.90206100 | -1.06822900 | -5.37773900 |
| C | 4.07784300 | -3.00862700 | -7.60748900 | H | 1.88563300 | 0.02382400 | -5.34907200 |
| C | 2.06381000 | -4.76641800 | -8.68945500 | H | 2.93398600 | -1.41965200 | -5.39002400 |
| C | 4.29458100 | -3.43024100 | -6.28335600 | C | 1.26862900 | -2.13824200 | -3.11351600 |
| C | 5.58199700 | -3.47349200 | -5.74874800 | H | 0.47271900 | -2.66437900 | -2.58467200 |
| C | 6.67683400 | -3.08146500 | -6.52276000 | Cl | -0.93827200 | -2.15703300 | -8.97079000 |
| C | 6.47666000 | -2.65674000 | -7.83636400 | C | 2.55497600 | -1.94267000 | -2.36234200 |
| C | 5.18790400 | -2.62570600 | -8.37634100 | H | 2.39180900 | -1.36330300 | -1.44417200 |
| H | 3.44915800 | -3.72926900 | -5.67004900 | H | 2.98684200 | -2.90287100 | -2.05025800 |
| H | 5.72891100 | -3.80702800 | -4.72555300 | H | 3.29949500 | -1.41321800 | -2.96298600 |
| H | 7.67883200 | -3.10837000 | -6.10443800 | C | -0.25120500 | -1.99322600 | -5.12025200 |
| H | 7.32287100 | -2.35585700 | -8.44761400 | C | -0.86491900 | -0.86544600 | -5.76208300 |
| H | 5.05843600 | -2.31059500 | -9.40652700 | H | -1.80730800 | -0.99373000 | -6.28457400 |
| C | 3.08382000 | -5.72848000 | -8.61170000 | H | -0.69374300 | 0.11956000 | -5.33796600 |
| C | 2.83354300 | -7.05673800 | -8.96192400 | C | -0.40037200 | -3.29756400 | -5.61659500 |
| C | 1.56588300 | -7.44213800 | -9.39805500 | H | 0.31251400 | -4.02008900 | -5.22450800 |
| C | 0.54728700 | -6.49078700 | -9.48111400 | C | -1.63061600 | -3.89076100 | -6.24166300 |
| C | 0.78688200 | -5.16281000 | -9.12607100 | H | -2.27946100 | -3.14721000 | -6.70251800 |
| H | 4.07686400 | -5.44928400 | -8.27800000 | H | -1.36387500 | -4.61686700 | -7.01395300 |
| H | 3.63428400 | -7.78806900 | -8.89419000 | H | -2.19736300 | -4.42795900 | -5.46675200 |
| H | 1.37315800 | -8.47601500 | -9.67085700 | | | | |
| H | -0.44327300 | -6.78016700 | -9.82090200 | | | | |
| H | -0.01089100 | -4.42769800 | -9.19008200 | | | | |
| C | 0.74563200 | 2.12257700 | -10.24113600 | | | | |
| C | -0.14674100 | 2.98280800 | -10.87907200 | | | | |
| C | -1.50290300 | 2.95611800 | -10.54353200 | | | | |
| C | -1.95955600 | 2.06715600 | -9.57082900 | | | | |
| C | -1.06859600 | 1.19912900 | -8.93515600 | | | | |
| H | 1.80092700 | 2.17081000 | -10.49531400 | | | | |
| H | 0.21662100 | 3.67478300 | -11.63358300 | | | | |
| H | -2.19895500 | 3.62574700 | -11.04093600 | | | | |
| H | -3.01376400 | 2.03646900 | -9.31148900 | | | | |
| H | -1.42709200 | 0.48296100 | -8.20678400 | | | | |
| C | 2.15032000 | 2.61135400 | -7.20867700 | | | | |
| C | 2.98428900 | 3.50372800 | -6.53242400 | | | | |

| INT2a | | | | C | -4.87580200 | -0.53803100 | -2.77535300 |
|-------|-------------|-------------|-------------|----|-------------|-------------|-------------|
| P | 2.31440200 | 1.53059200 | -4.00429400 | C | -4.04366100 | -0.65388400 | -1.65821800 |
| C | 1.66322100 | 0.19792300 | -5.14840700 | C | -2.65942700 | -0.59123600 | -1.80340000 |
| C | 0.14160700 | 0.05223700 | -4.96868500 | H | -2.51570200 | -0.17546900 | -5.18961700 |
| P | -0.26243400 | -0.34398400 | -3.18480200 | H | -4.96047800 | -0.26920800 | -4.91313800 |
| H | 1.90051400 | 0.42635400 | -6.19234500 | H | -5.95477200 | -0.57954700 | -2.65716600 |
| H | 2.15612700 | -0.74541100 | -4.89236000 | H | -4.47354500 | -0.78539200 | -0.66960900 |
| H | -0.36365500 | 0.99078100 | -5.22427200 | H | -2.01059900 | -0.66937700 | -0.93546300 |
| H | -0.24740900 | -0.73208800 | -5.62687000 | Rh | 0.73819000 | 1.30761900 | -1.91041000 |
| C | 0.27335900 | -2.10997800 | -3.08035700 | Cl | 1.30249300 | 3.44749400 | -0.95012700 |
| C | -2.09162300 | -0.42112400 | -3.07856500 | C | 4.30441200 | -1.49039400 | 0.99743600 |
| C | 1.99582100 | 3.05230400 | -5.00627800 | C | 5.19223500 | -0.41046100 | 0.98794600 |
| C | 4.14519900 | 1.36886200 | -4.06558000 | C | 4.77079000 | 0.82800400 | 0.50359900 |
| C | 1.12267800 | 4.03682300 | -4.52254500 | C | 3.47553100 | 0.99430000 | 0.00971800 |
| C | 0.84195300 | 5.16810200 | -5.29526900 | C | 2.58142600 | -0.08365100 | 0.01808900 |
| C | 1.43292500 | 5.32856000 | -6.54740000 | C | 3.00568400 | -1.32755800 | 0.52511600 |
| C | 2.31612800 | 4.35773200 | -7.03051000 | H | 4.62187000 | -2.45530900 | 1.38321400 |
| C | 2.59687400 | 3.22822800 | -6.26503500 | H | 6.20459900 | -0.53425500 | 1.36281400 |
| H | 0.69192900 | 3.93895900 | -3.53091900 | H | 5.45150800 | 1.67437500 | 0.50904900 |
| H | 0.16726100 | 5.92573100 | -4.90750400 | H | 3.14350800 | 1.96311400 | -0.34484200 |
| H | 1.21619100 | 6.21010400 | -7.14421900 | H | 2.29799900 | -2.14903100 | 0.54655700 |
| H | 2.78894100 | 4.48451500 | -8.00044600 | C | 1.14876000 | -0.02855300 | -0.47014700 |
| H | 3.29888200 | 2.48860600 | -6.64129300 | H | -0.53063500 | 1.41064900 | -1.04896600 |
| C | 4.82768200 | 0.41154400 | -4.83050400 | O | 0.33836400 | -0.82412300 | -0.04741300 |
| C | 6.22318000 | 0.34699700 | -4.80115300 | | | | |
| C | 6.95085900 | 1.23752300 | -4.01223900 | | | | |
| C | 6.27898600 | 2.19346600 | -3.24572800 | | | | |
| C | 4.88726100 | 2.25568800 | -3.26522100 | | | | |
| H | 4.28238800 | -0.28673200 | -5.45747400 | | | | |
| H | 6.73888200 | -0.39873400 | -5.39968000 | | | | |
| H | 8.03562400 | 1.18653300 | -3.99210000 | | | | |
| H | 6.83958400 | 2.88850000 | -2.62732700 | | | | |
| H | 4.37013300 | 2.99497700 | -2.65915000 | | | | |
| C | -0.60029000 | -3.15767000 | -3.40911400 | | | | |
| C | -0.15378500 | -4.47978300 | -3.40008900 | | | | |
| C | 1.16928300 | -4.77278700 | -3.06512000 | | | | |
| C | 2.04520700 | -3.73771300 | -2.73479500 | | | | |
| C | 1.59937300 | -2.41519300 | -2.73782500 | | | | |
| H | -1.63295600 | -2.94353100 | -3.66478600 | | | | |
| H | -0.84307700 | -5.28105700 | -3.65076700 | | | | |
| H | 1.51360100 | -5.80293700 | -3.05508200 | | | | |
| H | 3.07364300 | -3.95603000 | -2.46222500 | | | | |
| H | 2.28344300 | -1.62197800 | -2.45395800 | | | | |
| C | -2.93088200 | -0.30897400 | -4.19594000 | | | | |
| C | -4.31873900 | -0.36384600 | -4.04188600 | | | | |

| INT2b | | | | C | 3.17295600 | 3.27118900 | -5.50860500 |
|--------------|-------------|-------------|--------------|----|-------------|-------------|-------------|
| P | 3.11233400 | -2.88529200 | -8.49994700 | C | 3.85972000 | 3.00430900 | -6.69241400 |
| C | 2.92111400 | -1.85640700 | -10.04125100 | C | 3.42118300 | 1.99005400 | -7.54823100 |
| C | 2.77122600 | -0.36382400 | -9.69925300 | H | 0.72791500 | 0.91435400 | -5.77091700 |
| P | 1.58296400 | -0.10819300 | -8.27372600 | H | 1.50020200 | 2.71701000 | -4.25896400 |
| H | 3.74532100 | -2.02668100 | -10.74176500 | H | 3.51772900 | 4.05883700 | -4.84477800 |
| H | 1.99967600 | -2.23483800 | -10.49318100 | H | 4.73883800 | 3.58537200 | -6.95658300 |
| H | 3.73673700 | 0.05707300 | -9.41216800 | H | 3.96941500 | 1.81319100 | -8.46784700 |
| H | 2.41031500 | 0.19319200 | -10.56807600 | Rh | 1.23219100 | -2.13619800 | -7.22552900 |
| C | 0.11005800 | 0.71743400 | -9.00521500 | C | -0.67590600 | -1.17071400 | -1.37182200 |
| C | 2.28922700 | 1.23048500 | -7.22394800 | C | -1.23192000 | 0.10914200 | -1.44124800 |
| C | 4.83038600 | -2.51439600 | -7.90983600 | C | -1.51465000 | 0.66955800 | -2.68805900 |
| C | 3.27965900 | -4.62006700 | -9.11349400 | C | -1.23651600 | -0.04060200 | -3.85850000 |
| C | 5.27540900 | -3.08230700 | -6.70389500 | C | -0.67267000 | -1.31939100 | -3.79727200 |
| C | 6.56093000 | -2.84059300 | -6.22257600 | C | -0.40356400 | -1.88025100 | -2.54184300 |
| C | 7.43543500 | -2.02094900 | -6.93870300 | H | -0.45391300 | -1.61618300 | -0.40561500 |
| C | 7.01661800 | -1.46102200 | -8.14453500 | H | -1.44527200 | 0.66211600 | -0.53060300 |
| C | 5.72907800 | -1.70913100 | -8.62765300 | H | -1.95629000 | 1.66088200 | -2.75077800 |
| H | 4.61938200 | -3.73843100 | -6.14437500 | H | -1.45775600 | 0.38075500 | -4.83356500 |
| H | 6.87887100 | -3.29425200 | -5.28838300 | H | 0.02729100 | -2.87708500 | -2.47895500 |
| H | 8.43573000 | -1.82701700 | -6.56305700 | C | -0.41396500 | -2.10207200 | -5.08163200 |
| H | 7.69203200 | -0.83317700 | -8.71875400 | H | -1.19902200 | -2.87847500 | -5.15920600 |
| H | 5.44406400 | -1.27800000 | -9.58041600 | O | -0.39793200 | -1.29635500 | -6.22671900 |
| C | 4.52544300 | -5.12876600 | -9.51916100 | C | 0.95082200 | -2.81845200 | -5.11221200 |
| C | 4.63098600 | -6.43038000 | -10.00910000 | C | 2.07886900 | -1.92123200 | -5.26738900 |
| C | 3.49783500 | -7.24184200 | -10.09375300 | H | 3.08842700 | -2.31377500 | -5.19165500 |
| C | 2.25807600 | -6.74405400 | -9.69090800 | C | 0.98406700 | -4.14683700 | -5.49119000 |
| C | 2.14360100 | -5.44111200 | -9.20175100 | H | 0.01733400 | -4.62645900 | -5.63730900 |
| H | 5.41640000 | -4.51335300 | -9.45117000 | Cl | -0.21803700 | -2.98719400 | -9.12690000 |
| H | 5.59984100 | -6.81011500 | -10.32108500 | C | 2.15866100 | -5.08017600 | -5.45666400 |
| H | 3.58215500 | -8.25664900 | -10.47247000 | H | 1.96379700 | -5.87063900 | -4.71932900 |
| H | 1.37096700 | -7.36717600 | -9.75885900 | H | 2.32190100 | -5.58078000 | -6.41600600 |
| H | 1.17442600 | -5.04148300 | -8.92042600 | H | 3.08036400 | -4.57914500 | -5.15639300 |
| C | 0.29404000 | 1.87570700 | -9.78018100 | H | 1.97060800 | -0.91784300 | -4.86866900 |
| C | -0.80199400 | 2.53065400 | -10.33750800 | | | | |
| C | -2.09213800 | 2.04172500 | -10.11403200 | | | | |
| C | -2.27837300 | 0.90349000 | -9.33069300 | | | | |
| C | -1.18432600 | 0.23497700 | -8.77403300 | | | | |
| H | 1.29054300 | 2.27979200 | -9.94050400 | | | | |
| H | -0.65014100 | 3.42219400 | -10.93941200 | | | | |
| H | -2.94786200 | 2.55204500 | -10.54755200 | | | | |
| H | -3.27971400 | 0.52275200 | -9.15194500 | | | | |
| H | -1.32641900 | -0.64721100 | -8.16263700 | | | | |
| C | 1.60014800 | 1.50799200 | -6.02986700 | | | | |
| C | 2.04077700 | 2.52056200 | -5.18032800 | | | | |

TS-HImaginary frequency: -856.7 cm⁻¹

| | | | | | | | |
|---|-------------|-------------|--------------|----|-------------|-------------|--------------|
| P | 2.37772400 | -3.04628500 | -8.95847600 | C | 1.10455100 | 3.08436500 | -5.68114000 |
| C | 2.04672600 | -1.55325100 | -10.02070300 | C | 2.42548900 | 3.08047400 | -5.23562800 |
| C | 1.93378900 | -0.31215100 | -9.13600100 | H | 3.23248000 | 1.96898600 | -5.48609000 |
| P | 0.83550400 | -0.59093300 | -7.63870600 | H | 2.71624700 | 0.86789800 | -6.16701000 |
| H | 2.80060100 | -1.42510200 | -10.80420400 | H | 0.46900800 | 3.94614100 | -5.49795700 |
| H | 1.10003400 | -1.77654500 | -10.52192500 | H | 2.82502200 | 3.93695700 | -4.70024200 |
| H | 2.91423400 | -0.05662000 | -8.72451800 | H | 4.26357800 | 1.95308700 | -5.14532000 |
| H | 1.58475500 | 0.56856400 | -9.68480500 | Rh | 3.35285900 | 0.00764500 | -6.34232500 |
| C | -0.85350200 | -0.11236700 | -8.21795100 | C | 1.03777700 | -2.86222900 | -7.05427900 |
| C | 1.38851400 | 0.86280000 | -6.62719600 | C | 1.56824200 | -1.73659900 | -4.26836000 |
| C | 4.19349600 | -3.03270300 | -8.63529000 | H | 2.36575200 | -2.45257800 | -5.34616400 |
| C | 2.13926000 | -4.42386500 | -10.15596000 | H | 4.29932000 | -1.94547900 | -5.59649500 |
| C | 2.469731700 | -3.96468200 | -7.70996700 | H | 2.61303000 | -3.47502400 | -5.04644900 |
| C | 6.05953700 | -3.99692300 | -7.41557400 | C | 4.69731700 | -1.04638700 | -3.23481500 |
| C | 6.93707700 | -3.09592900 | -8.02427100 | H | 1.40383500 | -0.60947000 | -2.50956200 |
| C | 6.44512500 | -2.16063400 | -8.93410600 | Cl | 1.48785000 | -5.29124400 | -6.73379400 |
| C | 5.08179600 | -2.13011400 | -9.24022800 | C | 3.79216800 | 0.24252800 | -2.93857800 |
| H | 4.01303000 | -4.65267000 | -7.22102100 | H | 3.54525500 | -0.82810500 | -2.94493400 |
| H | 6.43468900 | -4.72543900 | -6.70250900 | H | 3.80602500 | -1.21182900 | -1.94951700 |
| H | 7.99708500 | -3.12089200 | -7.78778900 | C | 4.19185800 | -1.32357400 | -3.67277300 |
| H | 7.11881600 | -1.45381600 | -9.41057200 | C | 0.09260400 | -1.88604500 | -4.44646600 |
| H | 4.72633600 | -1.39604300 | -9.95651500 | H | -0.85581700 | -1.06514800 | -3.95852000 |
| C | 3.12231100 | -4.72204800 | -11.11243200 | H | -1.91128100 | -1.27903300 | -4.09902200 |
| C | 2.89569900 | -5.71082300 | -12.07009700 | H | -0.60432100 | -0.17575900 | -3.38878000 |
| C | 1.68881400 | -6.41318000 | -12.07821500 | C | -0.22167600 | -3.07911000 | -5.28247800 |
| C | 0.71191000 | -6.12773200 | -11.12310800 | H | 0.16366000 | -4.01584500 | -4.88607600 |
| C | 0.93549300 | -5.14123400 | -10.16158500 | C | -1.16867400 | -3.20595100 | -6.32831700 |
| H | 4.06914200 | -4.19028100 | -11.10537100 | H | -1.82510100 | -2.38154600 | -6.58481500 |
| H | 3.66369000 | -5.93556800 | -12.80491000 | H | -0.41164200 | -3.24014000 | -7.84140000 |
| H | 1.51531300 | -7.18724400 | -12.82060500 | H | -1.55757700 | -4.19750200 | -6.53746600 |
| H | -0.22114500 | -6.68378700 | -11.11442400 | H | 0.19436400 | -4.93784900 | -9.39643000 |
| H | -3.18121900 | 0.37734300 | -7.69163200 | C | -1.16013200 | 0.03476800 | -9.57918500 |
| C | -3.47222700 | 0.51936000 | -9.04964500 | C | -2.45800500 | 0.34533200 | -9.99079600 |
| C | -1.88688300 | 0.05869700 | -7.27908400 | C | -3.18121900 | 0.37734300 | -7.69163200 |
| H | -0.39448900 | -0.09192900 | -10.33603900 | H | -2.67198000 | 0.45286500 | -11.05028000 |
| H | -4.48063800 | 0.76295900 | -9.37087000 | H | -3.96235400 | 0.51218800 | -6.94886600 |
| H | -1.67406100 | -0.05156400 | -6.22008400 | C | 0.58951700 | 1.98769500 | -6.37648200 |

| INT3 | | | | C | 3.42019800 | 4.30497800 | -7.57484200 |
|-------------|-------------|-------------|--------------|----|-------------|-------------|-------------|
| P | 3.60796000 | -2.39658800 | -8.25588000 | C | 4.23528400 | 3.27677400 | -8.04941000 |
| C | 2.90953500 | -1.98299200 | -9.93268600 | C | 3.69222300 | 2.02308200 | -8.33479300 |
| C | 2.51338200 | -0.50086800 | -10.01657200 | H | 0.45444400 | 2.65064000 | -7.50333700 |
| P | 1.57825600 | 0.11711000 | -8.49168000 | H | 1.41775200 | 4.85497400 | -6.99109700 |
| H | 3.58826900 | -2.25243600 | -10.74864500 | H | 3.84237100 | 5.28228600 | -7.35902700 |
| H | 2.01865700 | -2.61294800 | -10.01203000 | H | 5.29810200 | 3.44529900 | -8.19756500 |
| H | 3.39712600 | 0.12782800 | -10.14817300 | H | 4.35581100 | 1.23706700 | -8.67976200 |
| H | 1.86723600 | -0.32936000 | -10.88173200 | Rh | 1.74644900 | -1.44502800 | -6.83762000 |
| C | -0.07056400 | 0.56797400 | -9.19977800 | C | 2.04710100 | 0.52939200 | -4.63544600 |
| C | 2.31967200 | 1.78010500 | -8.16462100 | C | 2.92807100 | -0.24590800 | -5.57649400 |
| C | 5.27123300 | -1.58850900 | -8.23393500 | H | 3.66136200 | 0.36767400 | -6.10202800 |
| C | 4.03278500 | -4.19291300 | -8.38629900 | H | 3.45074600 | -1.04081900 | -5.02900200 |
| C | 5.88829900 | -1.37165300 | -6.99004200 | C | 2.33722300 | 1.71290300 | -4.05952700 |
| C | 7.14675300 | -0.77433100 | -6.90903300 | H | 1.56825700 | 2.15931000 | -3.42852400 |
| C | 7.80737700 | -0.36991800 | -8.07064200 | Cl | 0.13113800 | -3.10518000 | -8.04724400 |
| C | 7.20699700 | -0.57685300 | -9.31366000 | C | 3.61976600 | 2.48651600 | -4.16346600 |
| C | 5.95284500 | -1.18639300 | -9.39471600 | H | 3.44847100 | 3.49313600 | -4.56624600 |
| H | 5.37708100 | -1.66777800 | -6.07989500 | H | 4.07576600 | 2.61968100 | -3.17217100 |
| H | 7.60658000 | -0.61800700 | -5.93741900 | H | 4.35508000 | 1.99312500 | -4.80340100 |
| H | 8.78363200 | 0.10223200 | -8.00796900 | C | 0.74627000 | -0.15576600 | -4.41784600 |
| H | 7.71632100 | -0.27101100 | -10.22334000 | C | 0.15682600 | -0.61816300 | -5.71409000 |
| H | 5.51499700 | -1.35445100 | -10.37347300 | H | -0.59849900 | -1.40458800 | -5.62582500 |
| C | 5.35798200 | -4.65602500 | -8.41169600 | H | -0.28621200 | 0.22385500 | -6.25510400 |
| C | 5.62981800 | -6.02288300 | -8.49734600 | C | 0.24611200 | -0.36778900 | -3.18347700 |
| C | 4.58512700 | -6.94504800 | -8.56178000 | H | 0.83715400 | -0.01161400 | -2.33935600 |
| C | 3.26427800 | -6.49280500 | -8.53365400 | C | -1.05396900 | -1.03345600 | -2.83077000 |
| C | 2.98429600 | -5.12933900 | -8.43904000 | H | -1.60763900 | -1.36281800 | -3.71367900 |
| H | 6.18325000 | -3.95388900 | -8.36748200 | H | -0.89669800 | -1.90625700 | -2.18223300 |
| H | 6.66148300 | -6.36361500 | -8.51644800 | H | -1.70602000 | -0.34897900 | -2.27027400 |
| H | 4.79846400 | -8.00816800 | -8.63116600 | C | 1.17320900 | -3.87910300 | -5.01421700 |
| H | 2.44348500 | -7.20324700 | -8.58128900 | O | 1.97692600 | -2.96583100 | -5.22125800 |
| H | 1.95392600 | -4.78521800 | -8.40427100 | C | 1.33494700 | -4.84955500 | -3.92627600 |
| C | -0.14620300 | 1.59348400 | -10.16108600 | C | 0.38355300 | -5.87244800 | -3.78871000 |
| C | -1.36471900 | 1.92542100 | -10.74965700 | C | 2.41495300 | -4.77049800 | -3.02999200 |
| C | -2.52678200 | 1.23987400 | -10.38499300 | C | 0.50979600 | -6.81068600 | -2.76632300 |
| C | -2.45872900 | 0.21926100 | -9.43835200 | H | -0.44810600 | -5.92568400 | -4.48657800 |
| C | -1.23798400 | -0.12090700 | -8.84796700 | C | 2.53659800 | -5.70730800 | -2.01041400 |
| H | 0.74638800 | 2.14383700 | -10.44386400 | H | 3.13774900 | -3.97047700 | -3.15137000 |
| H | -1.40703400 | 2.72022700 | -11.48910400 | C | 1.58534800 | -6.72688800 | -1.87886800 |
| H | -3.47777700 | 1.50012200 | -10.84147800 | H | -0.22490100 | -7.60290100 | -2.65978800 |
| H | -3.35515900 | -0.32593400 | -9.15756100 | H | 3.36851200 | -5.64938500 | -1.31490700 |
| H | -1.18315500 | -0.94466800 | -8.14749000 | H | 1.68447700 | -7.45710300 | -1.08062600 |
| C | 1.51540900 | 2.81434700 | -7.65811800 | H | 0.30249900 | -3.98897600 | -5.67841300 |
| C | 2.06024600 | 4.06621800 | -7.37173300 | | | | |

TS-INSImaginary frequency: -384.6 cm⁻¹

| | | | | | | | |
|---|-------------|-------------|--------------|----|-------------|-------------|-------------|
| P | 3.82427200 | -2.53716400 | -8.41876900 | C | 1.79819800 | 3.69075700 | -7.02248600 |
| C | 3.23722500 | -1.95358200 | -10.08151500 | C | 3.11868900 | 4.08184800 | -7.25116900 |
| C | 2.61832700 | -0.54614900 | -10.02735400 | H | 3.60047300 | 1.87980200 | -8.13191100 |
| P | 1.66839400 | -0.19939800 | -8.42941700 | H | 1.08995000 | 4.38791000 | -6.58419100 |
| H | 4.03267700 | -2.01562600 | -10.83185100 | H | 3.44349600 | 5.08719300 | -6.99895500 |
| H | 2.46670400 | -2.68517400 | -10.33755000 | H | 5.05596100 | 3.45259100 | -7.96031700 |
| H | 3.38231500 | 0.22722500 | -10.13229000 | H | 4.33103900 | 1.18698800 | -8.53553800 |
| H | 1.91649100 | -0.41599500 | -10.85503100 | Rh | 2.04921500 | -2.05367200 | -6.99823700 |
| C | -0.04071300 | 0.18602700 | -9.02036400 | C | 2.31143300 | -0.28189700 | -4.59863900 |
| C | 2.26439700 | 1.48866200 | -7.94943800 | C | 3.18876900 | -1.04467100 | -5.54052300 |
| C | 5.45461000 | -1.73281300 | -8.12006200 | H | 3.96807700 | -0.42706900 | -5.98542800 |
| C | 4.29341100 | -4.29791500 | -8.66123900 | H | 3.63944700 | -1.91008200 | -5.04427600 |
| C | 6.12321500 | -2.01010900 | -6.91475700 | C | 2.59129700 | 0.95565000 | -4.12946100 |
| C | 7.36525500 | -1.43881300 | -6.64437700 | H | 1.84717600 | 1.41466400 | -3.47928200 |
| C | 7.96107400 | -0.57879300 | -7.57059000 | Cl | 0.54451000 | -3.41940300 | -8.61737100 |
| C | 7.31076000 | -0.30004100 | -8.77234500 | C | 3.83659000 | 1.76766600 | -4.33129500 |
| C | 6.06642900 | -0.87460900 | -9.04650600 | H | 3.60417900 | 2.75723100 | -4.74110700 |
| H | 5.67145700 | -2.68008500 | -6.18980800 | H | 4.33693300 | 1.93769800 | -3.36705900 |
| H | 7.86821800 | -1.66525200 | -5.70885300 | H | 4.55933700 | 1.28954900 | -4.99547900 |
| H | 8.92843500 | -0.13338900 | -7.35759100 | C | 1.06882700 | -0.98262700 | -4.15835200 |
| H | 7.77181100 | 0.35792200 | -9.50355600 | C | 0.36304400 | -1.72452700 | -5.22113200 |
| H | 5.58780900 | -0.65875500 | -9.99613600 | H | -0.57869400 | -2.19582600 | -4.95119700 |
| C | 5.52018100 | -4.62029200 | -9.26850100 | H | 0.15020100 | -1.09904900 | -6.09553400 |
| C | 5.86266900 | -5.95137200 | -9.49939100 | C | 0.68837800 | -0.93762500 | -2.85755900 |
| C | 4.99045800 | -6.97365700 | -9.11763300 | H | 1.35540300 | -0.41998100 | -2.16995100 |
| C | 3.77537300 | -6.65894300 | -8.50964800 | C | -0.56733200 | -1.47366100 | -2.23657600 |
| C | 3.42059300 | -5.32788400 | -8.28014800 | H | -1.26360900 | -1.88951600 | -2.96807400 |
| H | 6.21179900 | -3.83510200 | -9.55769600 | H | -0.34816800 | -2.26067100 | -1.50380400 |
| H | 6.81127400 | -6.18904100 | -9.97246400 | H | -1.09172100 | -0.67555600 | -1.69278500 |
| H | 5.26032400 | -8.01144700 | -9.29290600 | C | 1.07891500 | -3.77467600 | -5.33944600 |
| H | 3.09436200 | -7.44983600 | -8.20930900 | O | 2.30012600 | -3.73320500 | -5.78474500 |
| H | 2.47532800 | -5.08237500 | -7.81530800 | C | 0.84606200 | -4.24362600 | -3.95167100 |
| C | -0.23424700 | 1.24043300 | -9.93197000 | C | -0.38880600 | -4.82306100 | -3.62122000 |
| C | -1.50993800 | 1.54955000 | -10.39888900 | C | 1.85055700 | -4.16709200 | -2.97614800 |
| C | -2.61345500 | 0.81579800 | -9.95495100 | C | -0.61922500 | -5.31574400 | -2.33880800 |
| C | -2.43071000 | -0.23052100 | -9.05272000 | H | -1.16314100 | -4.89624300 | -4.38155000 |
| C | -1.15118900 | -0.55055400 | -8.59002200 | C | 1.61867900 | -4.65780200 | -1.69210700 |
| H | 0.61125400 | 1.83200400 | -10.27120500 | H | 2.80814800 | -3.73631600 | -3.24506100 |
| H | -1.64248400 | 2.36413400 | -11.10524500 | C | 0.38470100 | -5.22985800 | -1.36933900 |
| H | -3.60886500 | 1.05817000 | -10.31629400 | H | -1.57547600 | -5.76985700 | -2.09479400 |
| H | -3.28126800 | -0.81390700 | -8.71285300 | H | 2.40113000 | -4.59717400 | -0.94064500 |
| H | -1.01181800 | -1.40216400 | -7.93672500 | H | 0.20879700 | -5.61572500 | -0.36893600 |
| C | 1.37585900 | 2.40580900 | -7.36346000 | H | 0.28920000 | -4.03978000 | -6.05220700 |

TS2Imaginary frequency: -381.9 cm⁻¹

| | | | | | | | |
|---|-------------|-------------|-------------|----|-------------|-------------|-------------|
| P | -2.57491300 | 2.02293100 | -0.89235400 | C | -1.02133300 | -3.29293400 | 0.41365900 |
| C | -2.63377400 | 1.32305000 | -2.61698000 | C | 0.21283300 | -3.94329100 | 0.46408200 |
| C | -1.82387400 | 0.02107500 | -2.73406400 | C | 1.31500900 | -3.37892300 | -0.17928200 |
| P | -0.19890700 | 0.11840600 | -1.78391400 | H | 1.18322900 | -2.17930700 | -0.88037500 |
| H | -3.66532700 | 1.19176700 | -2.96041100 | H | -2.11848700 | -1.59099000 | -0.28050300 |
| H | -2.16827400 | 2.10660900 | -3.22165100 | H | -1.88400400 | -3.71872500 | 0.91834200 |
| H | -2.38552200 | -0.83300200 | -2.34711400 | H | 0.31529200 | -4.87985800 | 1.00458400 |
| H | -1.59977300 | -0.18756000 | -3.78336700 | Rh | 2.28133200 | -3.87375100 | -0.14208900 |
| C | 1.11314400 | 0.03655400 | -3.06890000 | C | -0.31009500 | 2.00182100 | -0.35634600 |
| C | -0.05691500 | -1.52372000 | -0.95053600 | C | -0.31139400 | 1.86408200 | 2.58943900 |
| C | -3.72773500 | 0.97574400 | 0.10584300 | C | -0.49912800 | 0.89640700 | 1.44101800 |
| C | -3.51534200 | 3.61207400 | -0.99793400 | H | 0.32304100 | 0.17381800 | 1.39530800 |
| C | -3.83772000 | 1.22191400 | 1.48590600 | C | -1.42716700 | 0.32626400 | 1.50868300 |
| C | -4.71799900 | 0.48264300 | 2.27474000 | H | -0.59514900 | 1.66891000 | 3.88806600 |
| C | -5.50177800 | -0.52238400 | 1.70269100 | C | -0.37980900 | 2.48124900 | 4.58333400 |
| C | -5.40404100 | -0.77725500 | 0.33542900 | C | 0.28061000 | 3.13871800 | 2.07757500 |
| C | -4.52689900 | -0.03111500 | -0.45747100 | H | -0.48169600 | 3.76479600 | 1.05730400 |
| H | -3.22748800 | 1.99058300 | 1.95043500 | H | -0.08428300 | 4.65314100 | 0.57594000 |
| H | -4.78814500 | 0.69021000 | 3.33841700 | C | -1.55672300 | 3.79156600 | 1.20747600 |
| H | -6.18484800 | -1.09995300 | 2.31868600 | C | 1.64137200 | 3.41610200 | 2.33231600 |
| H | -6.01406500 | -1.55123800 | -0.12163100 | C | 2.25103900 | 4.74653400 | 1.94413200 |
| H | -4.48530400 | -0.23680100 | -1.52165900 | H | 1.75159000 | 5.58030900 | 2.45324100 |
| C | -4.90920900 | 3.63604800 | -0.81464600 | H | 3.31128000 | 4.77957400 | 2.20652300 |
| C | -5.61694200 | 4.83272700 | -0.92695900 | C | 2.17039200 | 4.92056400 | 0.86640600 |
| C | -4.94418400 | 6.02050500 | -1.21848900 | H | -1.18352100 | 0.42577500 | 4.49231400 |
| C | -3.56143200 | 6.00381400 | -1.40370100 | H | -0.47737800 | -0.03938100 | 5.19349600 |
| C | -2.84571500 | 4.81025400 | -1.29473500 | H | -2.08769400 | 0.65326400 | 5.07170500 |
| H | -5.44822300 | 2.72467300 | -0.58011500 | C | -1.43961400 | -0.31892400 | 3.73483200 |
| H | -6.69370900 | 4.83474100 | -0.78251000 | C | 2.38071100 | 2.01107800 | 1.04696200 |
| H | -5.49596600 | 6.95283300 | -1.30108900 | O | 1.77608200 | 2.18566800 | -0.08385700 |
| H | -3.03027700 | 6.92249800 | -1.63549000 | H | 2.02629200 | 2.96326300 | 3.24539400 |
| H | -1.77443500 | 4.79435900 | -1.46719700 | C | 3.85712900 | 2.22968600 | 1.07117200 |
| C | 1.04174000 | -0.92516400 | -4.09196100 | C | 4.63307400 | 1.70019400 | 2.11267900 |
| C | 2.04498500 | -1.00560100 | -5.05586400 | C | 4.48699100 | 2.96001300 | 0.05234700 |
| C | 3.13451300 | -0.13203400 | -5.00183600 | H | 6.01321000 | 1.89449800 | 2.13757000 |
| C | 3.21584200 | 0.81558300 | -3.98219300 | C | 4.14968800 | 1.13058400 | 2.90371500 |
| C | 2.20961600 | 0.90756300 | -3.01659600 | H | 5.86753700 | 3.15183500 | 0.07682500 |
| H | 0.21111400 | -1.62476200 | -4.13310400 | C | 3.87745600 | 3.36367900 | -0.74953900 |
| H | 1.97816500 | -1.74972000 | -5.84453200 | H | 6.63417200 | 2.62178600 | 1.11834700 |
| H | 3.91671800 | -0.19324700 | -5.75346900 | H | 6.60527000 | 1.47619100 | 2.94689100 |
| H | 4.06063600 | 1.49657500 | -3.93725500 | H | 6.34809400 | 3.71711600 | -0.71705500 |
| H | 2.26395500 | 1.65063800 | -2.22972300 | H | 7.70988700 | 2.77317100 | 1.13564300 |
| C | -1.15398100 | -2.08930000 | -0.27891000 | Cl | 2.06492600 | 1.19285600 | 1.70422200 |

INT4

| | | | | | | | |
|---|-------------|-------------|-------------|----|-------------|-------------|-------------|
| P | -2.59797500 | 2.08205400 | -0.81796400 | C | 0.44839500 | -3.82006900 | 0.48512600 |
| C | -2.56433700 | 1.43951500 | -2.56363400 | C | 1.35097500 | -1.90923600 | -0.69498000 |
| C | -1.75167800 | 0.13850700 | -2.66160700 | H | -2.04459400 | -1.71401600 | -0.44574300 |
| P | -0.14150800 | 0.24441400 | -1.69432300 | H | -1.69613300 | -3.84746600 | 0.71366900 |
| H | -3.57325700 | 1.31647900 | -2.97085900 | H | 0.59887000 | -4.75990200 | 1.00845100 |
| H | -2.06538300 | 2.23720100 | -3.12197300 | H | 2.54943000 | -3.49729200 | 0.11720300 |
| H | -2.32258400 | -0.71214500 | -2.28211600 | H | 2.20819700 | -1.36655200 | -1.07845500 |
| H | -1.50420600 | -0.07717300 | -3.70421900 | Rh | -0.27579000 | 2.01983500 | -0.22532200 |
| C | 1.16642000 | 0.22871800 | -2.98349400 | C | -0.35450200 | 1.87995500 | 2.55285400 |
| C | 0.05673000 | -1.39629600 | -0.88366200 | C | -0.48371800 | 0.81882800 | 1.49790200 |
| C | -3.74190700 | 0.95139500 | 0.09457500 | H | 0.36110400 | 0.12811300 | 1.46738800 |
| C | -3.59460900 | 3.63925100 | -0.90655100 | H | -1.41269600 | 0.24909400 | 1.54600300 |
| C | -3.85082800 | 1.09174900 | 1.48933200 | C | -0.72728500 | 1.85063100 | 3.84040800 |
| C | -4.72212700 | 0.28638600 | 2.22218300 | H | -0.57566600 | 2.75143900 | 4.43693000 |
| C | -5.49599200 | -0.68102400 | 1.57715700 | C | 0.21982800 | 3.10832100 | 1.88923500 |
| C | -5.39869700 | -0.83158300 | 0.19409000 | C | -0.63813300 | 3.96057200 | 1.25169000 |
| C | -4.53207400 | -0.01864200 | -0.54202900 | H | -0.28030800 | 4.82657700 | 0.70790200 |
| H | -3.24661900 | 1.83011400 | 2.00846900 | H | -1.70782500 | 3.89483300 | 1.41063400 |
| H | -4.79166500 | 0.41200600 | 3.29862600 | C | 1.73015400 | 3.27534800 | 1.89238400 |
| H | -6.17122400 | -1.31100300 | 2.14878700 | C | 2.21908300 | 4.56956100 | 1.23788500 |
| H | -6.00202800 | -1.57561800 | -0.31827100 | H | 1.75613200 | 5.44759000 | 1.70055500 |
| H | -4.49241300 | -0.14078500 | -1.61920200 | H | 3.30134100 | 4.66279700 | 1.35576900 |
| C | -4.97910400 | 3.63251100 | -0.66214400 | H | 1.99169000 | 4.57549600 | 0.16810300 |
| C | -5.72065800 | 4.81031500 | -0.75882300 | C | -1.32154100 | 0.67295500 | 4.56027900 |
| C | -5.09265300 | 6.00962200 | -1.09778200 | H | -0.65572300 | 0.32880500 | 5.36273800 |
| C | -3.71907600 | 6.02398700 | -1.34333300 | H | -2.27305100 | 0.93642100 | 5.04017600 |
| C | -2.96921100 | 4.85064700 | -1.24767900 | H | -1.49740400 | -0.17097300 | 3.88854500 |
| H | -5.48516300 | 2.71189600 | -0.39436300 | C | 2.32540800 | 1.98355000 | 1.22324600 |
| H | -6.78964700 | 4.78764400 | -0.56637500 | O | 1.78081200 | 1.82373500 | -0.04766800 |
| H | -5.67110400 | 6.92647800 | -1.16976000 | H | 2.03077600 | 3.26361400 | 2.95140600 |
| H | -3.22180600 | 6.95184200 | -1.61120900 | C | 3.84983500 | 1.99780700 | 1.16990200 |
| H | -1.90366600 | 4.86218400 | -1.45724800 | C | 4.59257700 | 1.62148100 | 2.29720300 |
| C | 1.15484700 | -0.80236100 | -3.94062800 | C | 4.53741000 | 2.39233200 | 0.01613100 |
| C | 2.12337600 | -0.84471200 | -4.94110700 | C | 5.98759400 | 1.64829500 | 2.27972300 |
| C | 3.11560200 | 0.13843800 | -4.99106700 | H | 4.07114200 | 1.29821200 | 3.19628900 |
| C | 3.13533900 | 1.15540000 | -4.03767000 | C | 5.93308700 | 2.41424900 | -0.00713500 |
| C | 2.16571900 | 1.20769900 | -3.03235800 | H | 3.96309800 | 2.67596400 | -0.85810900 |
| H | 0.39980800 | -1.58329800 | -3.90120700 | C | 6.66392800 | 2.04521500 | 1.12400900 |
| H | 2.10532800 | -1.64362800 | -5.67690200 | H | 6.54594100 | 1.35219100 | 3.16405600 |
| H | 3.87103000 | 0.10730600 | -5.77139200 | H | 6.45194700 | 2.72105800 | -0.91175500 |
| H | 3.90546000 | 1.92028300 | -4.07332100 | H | 7.75026300 | 2.06219700 | 1.10449200 |
| H | 2.16959300 | 1.99456700 | -2.29055900 | H | 2.06296300 | 1.15218900 | 1.90242800 |
| C | -1.03499700 | -2.10159000 | -0.35344200 | Cl | 0.10059000 | 3.69227800 | -2.16789700 |
| C | -0.83948000 | -3.30935700 | 0.31797600 | | | | |

INT5'

| | | | | | | | |
|---|--------------|-------------|--------------|----|-------------|-------------|-------------|
| P | 3.48829400 | -2.30163200 | -7.86011600 | C | 3.78865200 | 4.52891500 | -7.85474300 |
| C | 3.16090900 | -1.89360400 | -9.63959100 | C | 4.54244400 | 3.35486900 | -7.80189800 |
| C | 2.92463900 | -0.39302500 | -9.84035300 | H | 3.93464900 | 2.11883400 | -8.02192500 |
| P | 1.77885100 | 0.36023900 | -8.53842100 | H | 0.75157100 | 3.18420700 | -8.56810200 |
| H | 3.95531700 | -2.26431900 | -10.29672800 | H | 1.82407700 | 5.36123400 | -8.16369100 |
| H | 2.24892300 | -2.45530900 | -9.86508000 | H | 4.26202000 | 5.49116600 | -7.68272700 |
| H | 3.86770500 | 0.15707000 | -9.79502900 | H | 5.60579800 | 3.39701900 | -7.58416500 |
| H | 2.48867800 | -0.20323500 | -10.82476700 | Rh | 4.54039000 | 1.22013500 | -7.95197200 |
| C | 0.26214300 | 0.76251100 | -9.51906100 | C | 1.77350300 | -1.19095400 | -6.64065900 |
| C | 2.56128100 | 2.03135000 | -8.31425900 | C | 1.60537600 | -0.18554400 | -4.62498900 |
| C | 5.20081600 | -1.73756200 | -7.48331300 | H | 2.79363200 | 0.22332300 | -5.30933500 |
| C | 3.65371400 | -4.13397600 | -7.85342100 | H | 2.82021300 | 1.16960100 | -5.83644900 |
| C | 5.61435400 | -1.81452200 | -6.14097900 | C | 3.74564800 | -0.09695600 | -4.90094800 |
| C | 6.89826600 | -1.41748600 | -5.77242700 | C | 0.35683500 | 0.05571600 | -5.25222600 |
| C | 7.78647200 | -0.92636900 | -6.73417600 | H | -0.47662200 | -0.53727100 | -4.88099300 |
| C | 7.38610100 | -0.84381200 | -8.06733500 | Cl | 0.06115200 | -2.54849600 | -7.90702600 |
| C | 6.10183600 | -1.25215200 | -8.44201400 | C | -0.06824100 | 1.39864100 | -5.79680000 |
| H | 4.92063500 | -2.18911000 | -5.39277400 | H | -0.78058000 | 1.30473900 | -6.61926800 |
| H | 7.20626200 | -1.48869700 | -4.73316200 | H | -0.57810900 | 1.95675000 | -4.99760000 |
| H | 8.78529000 | -0.61263700 | -6.44479700 | C | 0.77080200 | 2.01112900 | -6.13005600 |
| H | 8.07275200 | -0.46949300 | -8.82151300 | C | 1.70293400 | -1.05507100 | -3.41893700 |
| H | 5.81732900 | -1.19945400 | -9.48840300 | C | 0.77265700 | -2.23811600 | -3.31834500 |
| C | 4.86885500 | -4.73280000 | -8.22837500 | H | 1.02544200 | -2.82803400 | -2.43586700 |
| C | 4.98265900 | -6.12156000 | -8.28128500 | H | -0.26592600 | -1.90924300 | -3.17402200 |
| C | 3.88879300 | -6.92513000 | -7.95238800 | C | 2.58311200 | -0.68872500 | -2.46706000 |
| C | 2.68256900 | -6.33506100 | -7.57455400 | H | 3.18826700 | 0.19645400 | -2.66107000 |
| C | 2.55904400 | -4.94546000 | -7.52290600 | C | 2.82503900 | -1.32210800 | -1.12737200 |
| H | 5.73088100 | -4.12011700 | -8.47311200 | H | 2.24326200 | -2.23125700 | -0.96594200 |
| H | 5.92677100 | -6.57339000 | -8.57293700 | H | 3.88640900 | -1.57603900 | -1.00907600 |
| H | 3.98011600 | -8.00745400 | -7.98569700 | C | 2.58292700 | -0.62158900 | -0.31716700 |
| H | 1.83199400 | -6.95284800 | -7.30290200 | C | 0.88304200 | -3.13023800 | -4.60964800 |
| H | 1.62540700 | -4.48600200 | -7.22806400 | O | 2.02388700 | -2.78668900 | -5.34926500 |
| C | 0.37571400 | 1.51338600 | -10.70412600 | C | 0.94698200 | -4.60648400 | -4.23431600 |
| C | -0.75280100 | 1.82486600 | -11.46036000 | C | -0.18119100 | -5.42480800 | -4.35841400 |
| C | -2.01438100 | 1.39255700 | -11.04314000 | C | 2.13301600 | -5.16756600 | -3.73884800 |
| C | -2.136662900 | 0.64625400 | -9.87228700 | C | -0.13366000 | -6.77150800 | -3.98723300 |
| C | -1.00661100 | 0.32829400 | -9.11356100 | H | -1.10154000 | -5.00572200 | -4.75813800 |
| H | 1.34605900 | 1.87382200 | -11.03391900 | C | 2.18501800 | -6.51106800 | -3.37099400 |
| H | -0.64670200 | 2.40562800 | -12.37225400 | H | 3.01689700 | -4.54195300 | -3.66295700 |
| H | -2.89459700 | 1.63366300 | -11.63245200 | C | 1.05003900 | -7.31885500 | -3.49123400 |
| H | -3.11158200 | 0.29430300 | -9.54818100 | H | -1.01993100 | -7.39209300 | -4.09169700 |
| H | -1.10095600 | -0.29946300 | -8.23629800 | C | 3.11327000 | -6.93259400 | -2.99347000 |
| C | 1.81315800 | 3.21905800 | -8.35052600 | H | 1.09108600 | -8.36632600 | -3.20469000 |
| C | 2.42236500 | 4.45540000 | -8.12455300 | H | -0.02425000 | -2.99283900 | -5.21442100 |

TS4'Imaginary frequency: -584.1 cm⁻¹

| | | | | | | | |
|---|-------------|-------------|--------------|----|-------------|-------------|-------------|
| P | 3.78411700 | -2.70802600 | -8.13448900 | C | 1.16207400 | 3.53389200 | -8.12945900 |
| C | 3.23159600 | -2.42271600 | -9.88768900 | C | 2.48587900 | 3.95688100 | -8.25243000 |
| C | 2.45624700 | -1.10490800 | -10.06698100 | C | 3.49465800 | 3.01110000 | -8.44207700 |
| P | 1.43191500 | -0.58568000 | -8.56156100 | H | 3.17897200 | 1.65401000 | -8.52198500 |
| H | 4.07131200 | -2.48360200 | -10.58804400 | H | 0.36934900 | 4.26022600 | -7.97417400 |
| H | 2.56361200 | -3.26606000 | -10.07208100 | H | 2.73070100 | 5.01349600 | -8.19508100 |
| H | 3.13297800 | -0.27717900 | -10.29184300 | H | 4.53098700 | 3.32593300 | -8.52504100 |
| H | 1.76923700 | -1.19442300 | -10.91254300 | Rh | 3.98567700 | 0.93941600 | -8.65142400 |
| C | -0.30767500 | -0.52393500 | -9.16374400 | C | 1.89141400 | -2.03881900 | -6.82938100 |
| C | 1.84654900 | 1.21776500 | -8.42794300 | C | 2.36695400 | -0.20153800 | -4.36312500 |
| C | 5.39666100 | -1.83033900 | -7.95229400 | C | 3.02242600 | -0.70400500 | -5.60188700 |
| C | 4.30185400 | -4.46924600 | -8.07825400 | H | 3.40596000 | 0.10225400 | -6.22575200 |
| C | 6.12034200 | -2.01431400 | -6.76070000 | H | 3.84415400 | -1.36810000 | -5.32137800 |
| C | 7.33614700 | -1.36421400 | -6.55727400 | C | 2.15531000 | 1.09397200 | -4.03904300 |
| C | 7.85190800 | -0.51388600 | -7.53864900 | H | 1.69734800 | 1.28083200 | -3.06722700 |
| C | 7.14698300 | -0.32492300 | -8.72673100 | Cl | 0.66612300 | -3.75752900 | -8.32991600 |
| C | 5.92880700 | -0.97899800 | -8.93275900 | C | 2.50697000 | 2.32897700 | -4.81302000 |
| H | 5.73673000 | -2.68198000 | -5.99446200 | H | 1.61103600 | 2.91314400 | -5.05775400 |
| H | 7.88165900 | -1.52230200 | -5.63149100 | H | 3.14833400 | 2.98582000 | -4.20923500 |
| H | 8.79905800 | -0.00691600 | -7.37902300 | C | 3.02749300 | 2.11776400 | -5.74708900 |
| H | 7.54550100 | 0.32471700 | -9.50103400 | C | 1.99570600 | -1.23108300 | -3.33639100 |
| H | 5.40863000 | -0.82958200 | -9.87356300 | H | 0.72543000 | -1.99868500 | -3.59369100 |
| C | 5.36898100 | -4.92683100 | -8.86885500 | H | 0.51036000 | -2.69397900 | -2.77472000 |
| C | 5.74895500 | -6.26707700 | -8.82756100 | C | -0.11867700 | -1.30066200 | -3.63188400 |
| C | 5.07405600 | -7.15765300 | -7.98823500 | H | 2.75414000 | -1.37757400 | -2.23791200 |
| C | 4.01983900 | -6.70493400 | -7.19478500 | C | 3.62393100 | -0.72513700 | -2.15855800 |
| C | 3.62678300 | -5.36502100 | -7.23796400 | C | 2.57830100 | -2.32978000 | -1.08803900 |
| H | 5.90990400 | -4.23673000 | -9.51067600 | H | 1.71809700 | -2.99398200 | -1.19834200 |
| H | 6.57208000 | -6.61503000 | -9.44533800 | H | 3.46854800 | -2.96093900 | -0.97274200 |
| H | 5.37298700 | -8.20168500 | -7.95328300 | C | 2.45932800 | -1.78367200 | -0.14282600 |
| H | 3.49526500 | -7.39554000 | -6.54080600 | O | 0.72877600 | -2.88003200 | -4.85294500 |
| H | 2.80146300 | -5.00909400 | -6.63165000 | C | 1.84421300 | -3.44728400 | -5.17768200 |
| C | -0.60778700 | 0.13265500 | -10.36944600 | C | 2.80146300 | -3.61957300 | -5.09506500 |
| C | -1.92236200 | 0.20418100 | -10.82830700 | C | -1.81803800 | -2.99689600 | -4.95002600 |
| C | -2.95396400 | -0.37230000 | -10.08333200 | C | -0.52175000 | -4.98544100 | -5.39617700 |
| C | -2.66377800 | -1.02011400 | -8.88271400 | C | -2.99553900 | -3.72761500 | -5.10357800 |
| C | -1.34707200 | -1.10097300 | -8.42507200 | H | -1.87608000 | -1.93397700 | -4.73338900 |
| H | 0.18106200 | 0.60469600 | -10.94862400 | C | -1.69903000 | -5.71888800 | -5.53461200 |
| H | -2.14005400 | 0.71132200 | -11.76395000 | H | 0.44558700 | -5.45529500 | -5.52261900 |
| H | -3.97845000 | -0.31806000 | -10.44074900 | C | -2.93838100 | -5.09367000 | -5.39048300 |
| H | -3.45759300 | -1.48192600 | -8.30322600 | H | -3.95635900 | -3.23198500 | -4.99526600 |
| H | -1.12193500 | -1.63987300 | -7.51313000 | H | -1.64797500 | -6.77858700 | -5.76749300 |
| C | 0.84454100 | 2.17712900 | -8.21311100 | H | -3.85529800 | -5.66497400 | -5.50535300 |

TS-RE'Imaginary frequency: -371.9 cm⁻¹

| | | | | | | | |
|---|-------------|-------------|--------------|----|-------------|-------------|-------------|
| P | 3.55122100 | -1.96892200 | -8.37976900 | C | 1.75212900 | 4.49391100 | -7.05941100 |
| C | 3.82642400 | -1.10747800 | -10.02222400 | C | 2.65463000 | 5.30566100 | -7.74968400 |
| C | 3.67575200 | 0.41144400 | -9.87711100 | H | 3.42924600 | 4.76096400 | -8.77416500 |
| P | 2.16521300 | 0.80141200 | -8.83493900 | H | 3.30001600 | 3.41104800 | -9.10793400 |
| H | 4.79394300 | -1.37694900 | -10.45866000 | H | 0.92857000 | 2.50811500 | -6.83981000 |
| H | 3.04917500 | -1.49841200 | -10.68689100 | H | 1.14447000 | 4.91140300 | -6.26134000 |
| H | 4.53742800 | 0.83806900 | -9.35286400 | H | 2.75455700 | 6.35612500 | -7.49088600 |
| H | 3.61490900 | 0.88843100 | -10.86094400 | Rh | 4.13455800 | 5.38419800 | -9.31702500 |
| C | 0.80071200 | 0.81239600 | -10.08030400 | C | 3.90991600 | 3.01308000 | -9.91245300 |
| C | 2.39595700 | 2.58658000 | -8.41712200 | C | 2.01607800 | -0.77834700 | -7.19851600 |
| C | 5.24254400 | -2.24839100 | -7.69003700 | H | 3.41666500 | -0.76558600 | -5.02039400 |
| C | 5.24254400 | -2.24839100 | -7.69003700 | H | 3.76684000 | 0.02897000 | -5.67140400 |
| C | 3.06046400 | -3.67231700 | -8.88685700 | H | 4.05257200 | -1.63874300 | -5.01958500 |
| C | 5.44395100 | -3.30599200 | -6.78570100 | C | 2.87042700 | 0.92547500 | -3.32455900 |
| C | 6.68811000 | -3.49835100 | -6.18488700 | H | 2.44976400 | 1.11246200 | -2.33687200 |
| C | 7.75104400 | -2.63941100 | -6.47400300 | Cl | 7.75104400 | -2.63941100 | -6.47400300 |
| C | 7.56084800 | -1.58393400 | -7.36648000 | C | -0.00586900 | 0.25931000 | -6.26144000 |
| C | 6.31537300 | -1.38747300 | -7.96699600 | H | 3.43792500 | 2.12888000 | -4.01130600 |
| H | 6.31537300 | -1.38747300 | -7.96699600 | H | 2.71422900 | 2.95110800 | -3.97659800 |
| H | 4.62504200 | -3.98101200 | -6.55621800 | H | 4.33936800 | 2.48299800 | -3.49258000 |
| H | 6.82803700 | -4.32436300 | -5.49323700 | H | 3.69656000 | 1.95723500 | -5.05753200 |
| H | 8.71996600 | -2.79244300 | -6.00771500 | C | 2.12971400 | -1.40491400 | -2.94359000 |
| H | 8.38213200 | -0.91212800 | -7.60009100 | C | 2.12971400 | -1.40491400 | -2.94359000 |
| H | 8.38213200 | -0.91212800 | -7.60009100 | C | 0.82614300 | -1.84521200 | -3.56536800 |
| H | 6.19213700 | -0.55904200 | -8.65813300 | H | 0.25322400 | -0.94237300 | -3.80244100 |
| C | 3.83131100 | -4.40134200 | -9.80875600 | C | 2.63400700 | -1.80641800 | -1.76560500 |
| C | 3.43338200 | -5.67601400 | -10.20806400 | H | 2.10380700 | -2.23080900 | -5.67180600 |
| C | 3.43338200 | -5.67601400 | -10.20806400 | H | 3.57371400 | -1.35252300 | -1.44800000 |
| C | 2.26850200 | -6.24227600 | -9.68165800 | C | 0.98279300 | -2.63776100 | -4.89748700 |
| C | 1.50520600 | -5.53030700 | -8.75692600 | O | 2.10380700 | -2.23080900 | -5.67180600 |
| C | 1.89571700 | -4.24776900 | -8.36331000 | C | 2.10380700 | -2.23080900 | -5.67180600 |
| H | 4.74879300 | -3.97879900 | -10.20971600 | C | 1.11154500 | -4.13554500 | -4.64337900 |
| H | 4.03371400 | -6.22993700 | -10.92441200 | C | -0.01648600 | -4.95995100 | -4.74400800 |
| H | 1.96279400 | -7.23839500 | -9.98929800 | C | 2.33453700 | -4.71665800 | -4.27968700 |
| H | 0.60886600 | -5.97089300 | -8.33076900 | H | 0.06874000 | -6.32931400 | -4.48077400 |
| H | 1.31353300 | -3.69233500 | -7.63748100 | H | -0.97072100 | -4.52385900 | -5.03166800 |
| C | 0.80624400 | 1.69122200 | -11.17576500 | C | 2.42299900 | -6.08369500 | -4.01542700 |
| C | -0.21542100 | 1.64526400 | -12.12304300 | C | 3.21563000 | -4.08785000 | -4.21075300 |
| C | -1.25841100 | 0.72537600 | -11.98278800 | H | 1.29047400 | -6.89614400 | -4.11489900 |
| C | -1.25841100 | 0.72537600 | -11.98278800 | H | -0.81783200 | -6.95222500 | -4.56630100 |
| C | -1.27847600 | -0.14146300 | -10.89027500 | H | 3.37849200 | -6.51843700 | -3.73298500 |
| C | -0.25506800 | -0.09871600 | -9.94018300 | H | 1.36137300 | -7.96136100 | -3.91291300 |
| H | 1.60036200 | 2.42528700 | -11.28410900 | H | 0.05698100 | -2.46236900 | -5.46048600 |
| H | -0.20188000 | 2.33033900 | -12.96623300 | C | 2.06094200 | -2.81697300 | -0.81291800 |
| H | -2.05584100 | 0.69252600 | -12.72000000 | H | 1.84651700 | -2.35819000 | 0.16139700 |
| H | -2.09427300 | -0.84830700 | -10.76906400 | H | 1.14093500 | -3.27488500 | -1.18131600 |
| H | -0.27721000 | -0.75152000 | -9.07351400 | H | 2.78012600 | -3.62438600 | -0.62631100 |
| C | 1.62289100 | 3.14286000 | -7.38401200 | H | 0.23095500 | -2.44739900 | -2.87418900 |

| INT6' | | | | C | 3.21789600 | 4.17482500 | -8.21949900 |
|-------|-------------|-------------|--------------|----|-------------|-------------|-------------|
| P | 3.43963900 | -2.62447600 | -8.03386500 | C | 4.07670800 | 3.07448000 | -8.19640400 |
| C | 3.15618600 | -2.35027700 | -9.85515400 | C | 3.58364700 | 1.79322400 | -8.44271800 |
| C | 2.81674800 | -0.88512400 | -10.17411900 | H | 0.31138000 | 2.57236600 | -8.94971300 |
| P | 1.56571800 | -0.11944200 | -8.98406400 | H | 1.18319900 | 4.83252400 | -8.49787900 |
| H | 4.00310000 | -2.69316200 | -10.45965200 | H | 3.60244000 | 5.17216300 | -8.02629500 |
| H | 2.29638800 | -2.98851600 | -10.07810800 | H | 5.13251600 | 3.20988200 | -7.97980900 |
| H | 3.71375200 | -0.26164900 | -10.13994300 | H | 4.26602600 | 0.95053800 | -8.38946200 |
| H | 2.40670900 | -0.80600500 | -11.18489100 | Rh | 1.36701400 | -1.43745800 | -7.17006800 |
| C | 0.06626100 | 0.17702100 | -10.01203000 | C | 1.66693400 | -0.22941000 | -4.47066300 |
| C | 2.22414000 | 1.59179700 | -8.73315500 | C | 2.23704300 | -0.03164700 | -5.83373300 |
| C | 5.12195900 | -1.93036300 | -7.70370700 | H | 2.06051100 | 0.97704500 | -6.19970600 |
| C | 3.73996100 | -4.44281700 | -7.90283700 | H | 3.31103800 | -0.23137700 | -5.85194700 |
| C | 5.53318700 | -1.84559900 | -6.36179700 | C | 0.64426600 | 0.49231200 | -3.96006900 |
| C | 6.78377700 | -1.32792600 | -6.02686600 | H | 0.31193900 | 0.26188100 | -2.94665600 |
| C | 7.64588000 | -0.87203400 | -7.02713700 | Cl | 0.05707700 | -3.16844300 | -8.59293100 |
| C | 7.25021800 | -0.94428000 | -8.36281500 | C | -0.11747700 | 1.59680600 | -4.63183700 |
| C | 6.00012200 | -1.47225500 | -8.69895700 | H | -1.16485000 | 1.30431800 | -4.79158500 |
| H | 4.86282800 | -2.18405500 | -5.57698800 | H | -0.13695900 | 2.49947100 | -4.00690800 |
| H | 7.08365000 | -1.27434900 | -4.98394800 | H | 0.29783600 | 1.86614100 | -5.60461800 |
| H | 8.61805100 | -0.46337900 | -6.76681500 | C | 2.25485500 | -1.32485300 | -3.62286600 |
| H | 7.91565600 | -0.59655800 | -9.14825800 | C | 1.29133400 | -2.40346000 | -3.18450500 |
| H | 5.72250200 | -1.53259800 | -9.74648700 | H | 1.76739300 | -3.14343800 | -2.53308100 |
| C | 4.98706100 | -5.01976300 | -8.19393300 | H | 0.47677200 | -1.96770900 | -2.58855700 |
| C | 5.16942200 | -6.39877600 | -8.08967700 | C | 3.55287800 | -1.30771300 | -3.27539800 |
| C | 4.11027400 | -7.21721000 | -7.69099000 | H | 4.14014700 | -0.46016800 | -3.62879100 |
| C | 2.86880200 | -6.65101400 | -7.39861800 | C | 4.32206900 | -2.28954300 | -2.43501900 |
| C | 2.68067400 | -5.27113000 | -7.49986400 | H | 3.73559400 | -3.15841200 | -2.12659400 |
| H | 5.82132800 | -4.39306200 | -8.49422700 | H | 5.20014000 | -2.66486500 | -2.97677500 |
| H | 6.13928100 | -6.83274700 | -8.31741300 | H | 4.70343100 | -1.80818300 | -1.52492400 |
| H | 4.25407300 | -8.29110500 | -7.60821200 | C | 0.64311300 | -3.14901600 | -4.34409100 |
| H | 2.04006300 | -7.28220200 | -7.09037400 | O | 0.88718300 | -2.86894400 | -5.51558800 |
| H | 1.71022300 | -4.83174100 | -7.29569300 | C | -0.32299800 | -4.25001800 | -4.06497500 |
| C | 0.19259800 | 0.83096900 | -11.25047400 | C | -0.58586600 | -4.71574600 | -2.76574400 |
| C | -0.93032500 | 1.08011200 | -12.03768900 | C | -0.99801200 | -4.82714500 | -5.15706100 |
| C | -2.19449900 | 0.68327500 | -11.59415200 | C | -1.50233400 | -5.74558900 | -2.56107400 |
| C | -2.32736100 | 0.03793100 | -10.36512900 | H | -0.07888900 | -4.28110300 | -1.91047700 |
| C | -1.20382300 | -0.21896100 | -9.57551400 | C | -1.91390900 | -5.85370600 | -4.94500600 |
| H | 1.16655600 | 1.16416700 | -11.59884200 | H | -0.79696100 | -4.44926800 | -6.15661800 |
| H | -0.81851100 | 1.58533900 | -12.99285900 | C | -2.16617700 | -6.31585100 | -3.64983800 |
| H | -3.07055700 | 0.87576200 | -12.20728500 | H | -1.69855500 | -6.10263300 | -1.55436900 |
| H | -3.30616700 | -0.28112300 | -10.01931000 | H | -2.43451300 | -6.29215300 | -5.79120400 |
| H | -1.30089900 | -0.75246900 | -8.63791900 | H | -2.88119500 | -7.11777800 | -3.48806800 |
| C | 1.36711200 | 2.70320600 | -8.73814900 | H | 0.05864000 | -0.63716200 | -6.88456100 |
| C | 1.86153100 | 3.98414600 | -8.48443700 | | | | |

| INT7' | | | | C | 4.15316000 | 4.18696900 | -9.00476700 |
|-------|-------------|-------------|--------------|----|-------------|-------------|-------------|
| P | 2.75771400 | -2.27665000 | -7.27683400 | C | 4.73669000 | 2.93687900 | -8.79111700 |
| C | 2.24583400 | -2.34609000 | -9.07704400 | C | 3.94541100 | 1.78876000 | -8.74737100 |
| C | 2.40712300 | -0.96888000 | -9.73761700 | H | 0.90592900 | 3.22151100 | -9.27636600 |
| P | 1.49516700 | 0.36284800 | -8.76962300 | H | 2.30483300 | 5.24792400 | -9.33343800 |
| H | 2.81761600 | -3.10319500 | -9.62302500 | H | 4.77001100 | 5.08040000 | -9.03743600 |
| H | 1.19386900 | -2.64538400 | -9.07225700 | H | 5.81114900 | 2.85157400 | -8.65456900 |
| H | 3.46406600 | -0.69402100 | -9.79844500 | H | 4.42257200 | 0.83344200 | -8.55330900 |
| H | 2.01645400 | -0.98682900 | -10.75912200 | Rh | 1.09961300 | -0.36625500 | -6.58834200 |
| C | 0.05134800 | 0.75836000 | -9.84708100 | C | 1.78342300 | 0.02620900 | -4.46684500 |
| C | 2.55535100 | 1.86849700 | -8.93302400 | C | 2.14924900 | 1.08584600 | -5.37457300 |
| C | 4.59082200 | -2.02952200 | -7.43657400 | H | 1.55597100 | 1.99398500 | -5.40813600 |
| C | 2.64112100 | -4.04864100 | -6.74815700 | H | 3.20387800 | 1.25347200 | -5.56967700 |
| C | 5.22711700 | -1.07471800 | -6.63082700 | C | 0.41608700 | -0.30920800 | -4.36242900 |
| C | 6.60169200 | -0.84354200 | -6.74328600 | H | 0.19355600 | -1.27902300 | -3.92641800 |
| C | 7.35891400 | -1.56202900 | -7.66799700 | Cl | -0.73496100 | -1.97279400 | -7.22134100 |
| C | 6.73915100 | -2.52069200 | -8.47448400 | C | -0.74261400 | 0.65142500 | -4.24247900 |
| C | 5.36942100 | -2.75403100 | -8.35742200 | H | -1.61587000 | 0.27718200 | -4.78364100 |
| H | 4.64335700 | -0.52448900 | -5.90206200 | H | -1.01959800 | 0.73168900 | -3.18120500 |
| H | 7.07664200 | -0.10119400 | -6.10792700 | H | -0.50976200 | 1.65384600 | -4.60701100 |
| H | 8.42615300 | -1.38109800 | -7.75949300 | C | 2.81115000 | -0.81350400 | -3.78693900 |
| H | 7.32359200 | -3.08877300 | -9.19283900 | C | 2.47162400 | -2.24791100 | -3.44811200 |
| H | 4.90895300 | -3.51574900 | -8.97927000 | H | 1.76770900 | -2.66240700 | -4.17485500 |
| C | 3.73215800 | -4.73302300 | -6.18571700 | H | 3.36490800 | -2.87981200 | -3.52890400 |
| C | 3.60178000 | -6.05846000 | -5.76499900 | C | 3.94582000 | -0.22789500 | -3.35681400 |
| C | 2.38101000 | -6.72184800 | -5.90000200 | H | 4.08327900 | 0.82919100 | -3.57687800 |
| C | 1.28602500 | -6.04390700 | -6.44098100 | C | 5.03356300 | -0.84744100 | -2.53043400 |
| C | 1.40728800 | -4.71655300 | -6.85558200 | H | 4.95291200 | -1.93395600 | -2.45199700 |
| H | 4.69185300 | -4.23795300 | -6.08267200 | H | 6.02200700 | -0.60915600 | -2.94219700 |
| H | 4.45878000 | -6.57207000 | -5.33796000 | H | 5.00832800 | -0.44535600 | -1.50976000 |
| H | 2.28374800 | -7.75702500 | -5.58446400 | C | 1.91571500 | -2.44280000 | -2.02883100 |
| H | 0.32778500 | -6.54608600 | -6.54017800 | O | 1.94095300 | -1.53849700 | -1.20869900 |
| H | 0.53933200 | -4.18724500 | -7.23599900 | C | 1.36117800 | -3.78860700 | -1.66398600 |
| C | 0.25954700 | 1.12476100 | -11.18947900 | C | 1.34753200 | -4.87796800 | -2.54887200 |
| C | -0.81996700 | 1.42214800 | -12.01858900 | C | 0.83936400 | -3.95125800 | -0.36973400 |
| C | -2.12332200 | 1.35829700 | -11.51715500 | C | 0.82161000 | -6.10493400 | -2.14329000 |
| C | -2.33793900 | 0.99560400 | -10.18840700 | H | 1.74380500 | -4.78481200 | -3.55387000 |
| C | -1.25772700 | 0.69520400 | -9.35341100 | C | 0.31248800 | -5.17451800 | 0.03123800 |
| H | 1.26890300 | 1.19519100 | -11.58628800 | H | 0.85958700 | -3.09809400 | 0.30003200 |
| H | -0.64473900 | 1.70604900 | -13.05246700 | C | 0.30269800 | -6.25532800 | -0.85647500 |
| H | -2.96579700 | 1.58883200 | -12.16329100 | H | 0.81564800 | -6.93976200 | -2.83761100 |
| H | -3.34854000 | 0.93496500 | -9.79530300 | H | -0.09152600 | -5.28929600 | 1.03303000 |
| H | -1.42938300 | 0.37752400 | -8.33171500 | H | -0.10987100 | -7.21100700 | -0.54505600 |
| C | 1.97804000 | 3.13187900 | -9.13621000 | H | 0.04124800 | 0.74970100 | -6.63022700 |
| C | 2.77102900 | 4.28017000 | -9.17129600 | | | | |

TS5a'Imaginary frequency: -617.9 cm⁻¹

| | | | | | | | |
|---|-------------|-------------|--------------|----|-------------|-------------|-------------|
| P | 3.05668200 | -1.85037700 | -7.45513000 | C | 1.06940700 | 4.52050000 | -9.04256900 |
| C | 2.43043800 | -1.94489300 | -9.21345200 | C | 2.43056100 | 4.81240700 | -8.95559900 |
| C | 2.05503800 | -0.56512500 | -9.77758600 | H | 2.90317400 | 2.45388700 | -8.68640900 |
| P | 0.97455000 | 0.39724600 | -8.56915700 | H | 0.34722800 | 5.32120900 | -9.17592600 |
| H | 3.14939100 | -2.46057400 | -9.85968300 | H | 2.77577300 | 5.84020200 | -9.02108300 |
| H | 1.53978800 | -2.57822400 | -9.14181100 | H | 4.40810800 | 3.98846600 | -8.69748500 |
| H | 2.94716700 | 0.03412800 | -9.97640300 | H | 3.63109900 | 1.66525700 | -8.51834800 |
| H | 1.52178000 | -0.67769800 | -10.72604400 | Rh | 1.31227500 | -0.49505300 | -6.37990600 |
| C | -0.68350100 | 0.37993900 | -9.37785800 | C | 1.97541700 | -0.06386800 | -4.37583300 |
| C | 1.53582400 | 2.14524600 | -8.79598700 | C | 2.59817700 | 0.85670200 | -5.30556900 |
| C | 4.75843800 | -1.13936600 | -7.59735500 | H | 2.22574100 | 1.87317600 | -5.39604100 |
| C | 3.42103300 | -3.62608400 | -7.06116800 | H | 3.66354500 | 0.76723500 | -5.48867200 |
| C | 5.47308100 | -0.88993400 | -6.41168900 | C | 0.54330400 | 0.09059300 | -4.30228500 |
| C | 6.76142400 | -0.35745100 | -6.45179800 | H | -0.01012200 | -0.76059500 | -3.91501300 |
| C | 7.36157000 | -0.05804700 | -7.67696400 | Cl | -0.37252900 | -2.41424400 | -6.55763900 |
| C | 6.66814200 | -0.30700000 | -8.86095000 | C | -0.12245100 | 1.41391200 | -3.96121400 |
| C | 5.37995800 | -0.84805100 | -8.82196900 | H | -1.17727700 | 1.41590500 | -4.24944300 |
| H | 5.02105800 | -1.12156400 | -5.45177300 | H | -0.07147300 | 1.53480700 | -2.87159800 |
| H | 7.29654800 | -0.17544600 | -5.52406700 | H | 0.36888400 | 2.27218900 | -4.42301100 |
| H | 8.36343000 | 0.36031600 | -7.70784500 | C | 2.68871700 | -1.09369000 | -3.58355000 |
| H | 7.12922600 | -0.08877300 | -9.82012800 | C | 1.97769900 | -2.40566100 | -3.32009000 |
| H | 4.87389200 | -1.05338900 | -9.75878500 | H | 1.29293200 | -2.63752600 | -4.14833500 |
| C | 4.71089200 | -4.16799300 | -7.18986200 | H | 2.69909500 | -3.22862900 | -3.30466100 |
| C | 4.94510800 | -5.51578600 | -6.91165800 | C | 3.90729900 | -0.81291300 | -3.07845900 |
| C | 3.89699400 | -6.34269200 | -6.50595700 | H | 4.31588600 | 0.17583900 | -3.28143200 |
| C | 2.61150500 | -5.81295900 | -6.38068500 | C | 4.75884500 | -1.68704700 | -2.20310800 |
| C | 2.37030900 | -4.46431100 | -6.65025700 | H | 4.37004200 | -2.70256000 | -2.09743400 |
| H | 5.53899800 | -3.54358800 | -7.50595100 | H | 5.78302200 | -1.75914700 | -2.59154100 |
| H | 5.94954000 | -5.91705300 | -7.01504600 | H | 4.83824400 | -1.26110500 | -1.19425800 |
| H | 4.08098800 | -7.39182500 | -6.29135100 | C | 1.17330900 | -2.43739500 | -2.01887500 |
| H | 1.78602400 | -6.44964400 | -6.07382400 | O | 0.97559900 | -1.42209000 | -1.36675700 |
| H | 1.36784700 | -4.05728200 | -6.55010100 | C | 0.61438800 | -3.75410200 | -1.56323800 |
| C | -0.84209900 | 0.77401400 | -10.71912100 | C | 0.71677800 | -4.93200300 | -2.31988000 |
| C | -2.10028900 | 0.75952400 | -11.31782600 | C | -0.04515200 | -3.79263100 | -0.32392200 |
| C | -3.21810600 | 0.35100400 | -10.58396500 | C | 0.17101600 | -6.12364200 | -1.84185500 |
| C | -3.06981700 | -0.04278400 | -9.25494500 | H | 1.20947100 | -4.92614700 | -3.28656500 |
| C | -1.80882400 | -0.03054400 | -8.65129000 | C | -0.58350300 | -4.98305700 | 0.15399500 |
| H | 0.01599300 | 1.11231600 | -11.29388800 | H | -0.12002500 | -2.87079200 | 0.24312800 |
| H | -2.20982500 | 1.06927000 | -12.35343500 | C | -0.47601700 | -6.15236400 | -0.60527200 |
| H | -4.19898400 | 0.33823000 | -11.05111100 | H | 0.24912700 | -7.02914900 | -2.43641300 |
| H | -3.93253300 | -0.37183300 | -8.68307400 | H | -1.08877000 | -5.00292100 | 1.11540200 |
| H | -1.68819800 | -0.37738700 | -7.63093000 | H | -0.89805700 | -7.08240900 | -0.23475100 |
| C | 0.62440100 | 3.19898400 | -8.96416400 | H | 0.04129800 | 0.33935100 | -5.90574000 |

TS5b'Imaginary frequency: -753.1 cm⁻¹

| | | | | | | | |
|---|-------------|-------------|--------------|----|-------------|-------------|--------------|
| P | 2.59691400 | -1.91796400 | -7.85414200 | C | 3.56090700 | 4.60964600 | -8.40520600 |
| C | 2.35781700 | -1.81422200 | -9.70644900 | C | 4.93835000 | 4.38116100 | -8.43976500 |
| C | 2.70117200 | -0.39814600 | -10.19634500 | C | 5.41302400 | 3.09824100 | -8.71106200 |
| P | 1.88557500 | 0.91222300 | -9.11558500 | H | 4.52138200 | 2.04917100 | -8.94759000 |
| H | 2.96456500 | -2.56335200 | -10.22531400 | H | 1.60235200 | 3.76389300 | -8.63406600 |
| H | 1.29951400 | -2.03138400 | -9.87616700 | H | 3.17744200 | 5.60454600 | -8.19661700 |
| H | 3.78344900 | -0.24628600 | -10.18415800 | H | 5.63345300 | 5.19547500 | -8.25686400 |
| H | 2.36359300 | -0.25369900 | -11.22660600 | Rh | 6.48197600 | 2.90622000 | -8.73979100 |
| C | 0.66233200 | 1.71324100 | -10.24440100 | C | 4.92520900 | 1.06072700 | -9.13422200 |
| C | 3.13566800 | 2.26716500 | -8.92869200 | C | 1.13530800 | -0.11124900 | -7.09646500 |
| C | 4.44184200 | -1.76761500 | -7.72815300 | C | 1.46572200 | 0.28729700 | -4.97040800 |
| C | 2.28317500 | -3.69402100 | -7.44824900 | H | 0.10214900 | 1.95995700 | -5.30335300 |
| C | 5.00577200 | -0.77634600 | -6.91406100 | H | 1.81864600 | 2.28881100 | -5.78258800 |
| C | 6.39367100 | -0.62005300 | -6.83828900 | C | 0.48313800 | -0.75586200 | -5.07310100 |
| C | 7.23411500 | -1.44539500 | -7.58429200 | Cl | 0.81591400 | -1.75048500 | -4.78770100 |
| C | 6.68398200 | -2.43133600 | -8.40892600 | C | -0.82238900 | -1.34031700 | -8.34239200 |
| C | 5.30076300 | -2.59126400 | -8.47951200 | H | -1.00914800 | -0.58162800 | -4.89695900 |
| H | 4.35603000 | -0.11821000 | -6.34681900 | H | -1.54684100 | -1.27730200 | -5.54570900 |
| H | 6.81266000 | 0.15281700 | -6.20020900 | H | -1.28957800 | -0.79232600 | -3.85438800 |
| H | 8.31210900 | -1.32266800 | -7.52829800 | C | -1.36091500 | 0.42357900 | -5.14126900 |
| H | 7.33240700 | -3.07558100 | -8.99608500 | C | 2.77981300 | 0.11863200 | -4.29749300 |
| H | 4.88851700 | -3.36970400 | -9.11494400 | H | 3.18823500 | -1.28934700 | -3.91524700 |
| C | 2.84217400 | -2.01247500 | -4.64416500 | C | 3.42712000 | -1.38357200 | -3.93027100 |
| C | 3.24748300 | -4.51250600 | -6.83669500 | H | 4.28111800 | 1.19212400 | -3.90773000 |
| C | 2.95827900 | -5.84501900 | -6.52986800 | C | 5.09704200 | 2.17964200 | -4.12205400 |
| C | 1.70209400 | -6.37665200 | -6.82324600 | H | 0.73169400 | -5.56409600 | -7.41378000 |
| C | 1.01149400 | -4.23215200 | -7.71976600 | C | 5.29082300 | 0.23453000 | -3.11732900 |
| H | 4.23232900 | -4.12119700 | -6.60670500 | H | 5.48483200 | 1.93870200 | -3.56868400 |
| H | 3.72160500 | -6.46549000 | -6.06810100 | H | 4.60858700 | 1.49931200 | -2.10168100 |
| H | 1.48043100 | -7.41494200 | -6.59208000 | C | 2.76210600 | -1.66327700 | -2.48268600 |
| H | -0.25352400 | -5.96432100 | -7.63561000 | O | 2.72539800 | -0.80309200 | -1.61634600 |
| H | 0.23870000 | -3.59789100 | -8.14544400 | C | 2.72539800 | -0.80309200 | -2.13988500 |
| C | 1.10233400 | 2.38040800 | -11.40222300 | C | 2.43554400 | -4.13404300 | -3.07815300 |
| C | 0.18639800 | 2.98144900 | -12.26314900 | C | 2.15989100 | -3.38043400 | -0.79518900 |
| C | -1.18086500 | 2.92814800 | -11.97582500 | C | 2.16419300 | -2.44465800 | -11.62456500 |
| C | -1.62390000 | 2.26808000 | -10.83075100 | H | 2.12883300 | -5.43568900 | -2.67989500 |
| C | -0.70931700 | 1.65932900 | -9.96586200 | C | 2.65305300 | -3.95200400 | -4.12404100 |
| H | 2.16419300 | 2.44465800 | -11.62456500 | C | 1.85696700 | -4.67831900 | -0.39933500 |
| H | 0.53845700 | 3.49463300 | -13.15368500 | H | 2.17555300 | -2.56269900 | -0.08273000 |
| H | -1.89528300 | 3.39817600 | -12.64601800 | H | 1.83962300 | -5.71070800 | -1.34317300 |
| H | -2.68554000 | 2.21397300 | -10.60787500 | H | 2.10995300 | -6.22852900 | -3.42124400 |
| H | -1.05660800 | 1.10453700 | -9.10114200 | H | 1.63155700 | -4.88919400 | 0.64219700 |
| C | 2.66996300 | 3.56496800 | -8.64705600 | H | 1.59873700 | -6.72470600 | -1.03621700 |
| | | | | H | 0.19520500 | 1.16185300 | -6.90436600 |

| INT8a' | | | | C | -0.84817500 | 4.36368900 | -8.78767800 |
|--------|--------------|-------------|--------------|----|-------------|-------------|--------------|
| P | 3.95096500 | -1.06085100 | -8.05117900 | C | 0.14704500 | 4.13143100 | -7.83637700 |
| C | 3.40675500 | -0.77965800 | -9.83376900 | C | 0.72214300 | 2.86585600 | -7.71660400 |
| C | 2.36382900 | 0.33717900 | -9.90002100 | H | -1.03561300 | 1.25545700 | -10.15228200 |
| P | 1.17232600 | 0.19676100 | -8.46443700 | H | -2.05018000 | 3.49913500 | -10.35674000 |
| H | 4.27237400 | -0.57298700 | -10.47102800 | H | -1.30032300 | 5.34786900 | -8.87382900 |
| H | 2.97112400 | -1.72741200 | -10.16504600 | H | 0.46648700 | 4.93153000 | -7.17478500 |
| H | 2.82933100 | 1.31952800 | -9.77184400 | H | 1.46937800 | 2.66969100 | -6.95488600 |
| H | 1.84258200 | 0.36253000 | -10.86260700 | Rh | 2.33089700 | -0.38064200 | -6.62335200 |
| C | -0.101110600 | -1.02894400 | -9.00226200 | C | 3.13637800 | -1.06737900 | -3.96657000 |
| C | 0.31050300 | 1.82192600 | -8.55739300 | C | 4.09219400 | -0.91578500 | -4.92862500 |
| C | 5.59725500 | -0.21814600 | -7.95864000 | H | 4.63384100 | 0.01989400 | -5.02967400 |
| C | 4.38276000 | -2.85816000 | -8.08959200 | H | 4.51769300 | -1.79028500 | -5.40701800 |
| C | 6.69151800 | -0.79349800 | -7.29349800 | C | 2.76481100 | 0.09452800 | -3.06894800 |
| C | 7.89608700 | -0.09823800 | -7.16568500 | H | 1.68103900 | 0.14078200 | -2.93407200 |
| C | 8.02944300 | 1.18271200 | -7.70090100 | Cl | 0.38048600 | 0.39791200 | -5.32373900 |
| C | 6.94756200 | 1.76841800 | -8.36207200 | C | 3.46314200 | -0.01586500 | -1.69863200 |
| C | 5.74282500 | 1.07728300 | -8.48370800 | H | 3.17960900 | 0.83166900 | -1.06611500 |
| H | 6.61222900 | -1.79427800 | -6.88210300 | H | 3.18322400 | -0.93708100 | -1.18075600 |
| H | 8.73070200 | -0.56329100 | -6.64865000 | H | 4.55286600 | -0.00431200 | -1.81011000 |
| H | 8.96697000 | 1.72214000 | -7.60279700 | C | 2.57856800 | -2.40944700 | -3.62838300 |
| H | 7.03934900 | 2.76653300 | -8.78094900 | C | 1.08659000 | -2.49142500 | -3.37745700 |
| H | 4.91006300 | 1.55945200 | -8.98639300 | H | 0.58908500 | -1.65944500 | -3.88064200 |
| C | 5.40637200 | -3.36958400 | -8.90566900 | H | 0.67538700 | -3.39837600 | -3.84351800 |
| C | 5.63929900 | -4.74311500 | -8.96991500 | C | 3.40442500 | -3.46575100 | -3.50141900 |
| C | 4.85249000 | -5.62342800 | -8.22188900 | H | 4.46901500 | -3.29522600 | -3.65374600 |
| C | 3.83197900 | -5.12581000 | -7.41122700 | C | 3.03459800 | -4.86750900 | -3.11887200 |
| C | 3.59697300 | -3.75004400 | -7.34545800 | H | 1.95597800 | -5.03735700 | -3.10375200 |
| H | 6.02847800 | -2.69484800 | -9.48684200 | H | 3.48983700 | -5.58880800 | -3.80947600 |
| H | 6.43409700 | -5.12684200 | -9.60346000 | H | 3.41390400 | -5.10145600 | -2.11671200 |
| H | 5.03583200 | -6.69299300 | -8.27313900 | C | 0.67365900 | -2.55962400 | -1.90431800 |
| H | 3.21582900 | -5.80557000 | -6.82968900 | O | 1.47014300 | -2.87827300 | -1.03205300 |
| H | 2.80264000 | -3.35448900 | -6.71845500 | C | -0.76079400 | -2.28557000 | -1.55551000 |
| C | -0.13939500 | -1.58802300 | -10.28876900 | C | -1.68169400 | -1.72981800 | -2.45831900 |
| C | -1.11954900 | -2.52424100 | -10.62953300 | C | -1.18397300 | -2.59969800 | -0.25258400 |
| C | -2.07728800 | -2.90839100 | -9.69205600 | C | -3.00006400 | -1.50027300 | -2.06169200 |
| C | -2.04814500 | -2.35596800 | -8.40877200 | H | -1.37628800 | -1.44753400 | -3.46017700 |
| C | -1.06623100 | -1.42983400 | -8.06084300 | C | -2.49989600 | -2.37525100 | 0.13766800 |
| H | 0.59038400 | -1.30458200 | -11.04018900 | H | -0.45579700 | -3.01873700 | 0.43381200 |
| H | -1.13153500 | -2.94940500 | -11.62932000 | C | -3.41221000 | -1.82510700 | -0.76856700 |
| H | -2.83978100 | -3.63517300 | -9.95769900 | H | -3.70244100 | -1.05978600 | -2.76322100 |
| H | -2.79015800 | -2.65136000 | -7.67221700 | H | -2.81754000 | -2.62539200 | 1.14601100 |
| H | -1.03201200 | -1.01393100 | -7.05778000 | H | -4.43983700 | -1.64571800 | -0.46442900 |
| C | -0.69384700 | 2.05973500 | -9.50745900 | H | 3.04498000 | 1.03070700 | -3.56065300 |
| C | -1.26960000 | 3.32591900 | -9.62114100 | | | | |

INT8b'

| | | | | | | | |
|---|-------------|-------------|--------------|----|-------------|-------------|-------------|
| P | 2.32748300 | -1.88789700 | -7.91419900 | C | 5.14216100 | 4.16899400 | -8.30277800 |
| C | 2.22305500 | -1.81820600 | -9.77743600 | C | 5.55584800 | 2.89371500 | -8.68443200 |
| C | 2.68846100 | -0.43646500 | -10.26941400 | H | 4.61499000 | 1.90723000 | -8.99308700 |
| P | 1.90728100 | 0.92562200 | -9.22381500 | H | 1.78043400 | 3.71735300 | -8.50378000 |
| H | 2.81293100 | -2.62285600 | -10.22970000 | H | 3.43954300 | 5.44466000 | -7.93935200 |
| H | 2.81293100 | -2.62285600 | -10.22970000 | H | 5.87464600 | 4.93451500 | -8.06360400 |
| H | 1.16612100 | -1.97209100 | -10.01396500 | H | 6.61498300 | 2.65902100 | -8.74589000 |
| H | 3.77759400 | -0.36440700 | -10.21408300 | H | 4.97263100 | 0.92276200 | -9.27201900 |
| H | 2.40425500 | -0.28442000 | -11.31412200 | Rh | 0.98809600 | -0.22641400 | -7.26693800 |
| C | 0.85617700 | 1.85333700 | -10.43419000 | C | 1.22023800 | 0.18098100 | -5.15662400 |
| C | 3.24123500 | 2.18144800 | -8.93558000 | C | 0.50739800 | 1.49891300 | -5.38624000 |
| C | 4.15647200 | -1.87025300 | -7.63341800 | H | -0.25126700 | 1.70183600 | -4.61899000 |
| C | 1.79178600 | -3.58047100 | -7.43405400 | H | 1.18232200 | 2.34990700 | -5.46408700 |
| C | 4.74372300 | -0.84013000 | -6.88776100 | C | 0.39645000 | -0.98923400 | -5.34551000 |
| C | 6.13129500 | -0.78779300 | -6.72105500 | H | 0.85799700 | -1.93973400 | -5.09251500 |
| C | 6.94575800 | -1.75621000 | -7.30703100 | Cl | -1.11825700 | -1.00347300 | -8.62880600 |
| C | 6.37103500 | -2.78180000 | -8.06390400 | C | -1.10295900 | -1.02987900 | -5.13512200 |
| C | 4.98753500 | -2.83892900 | -8.22668600 | H | -1.54064800 | -1.85826400 | -5.69657500 |
| H | 4.11151800 | -0.07748300 | -6.44475300 | H | -1.32449800 | -1.17988700 | -4.06760700 |
| H | 6.57112400 | 0.01733200 | -6.13962300 | H | -1.61476000 | -0.12290100 | -5.46336000 |
| H | 8.02382900 | -1.71327700 | -7.18018000 | C | 2.47990600 | 0.15780700 | -4.36947100 |
| H | 7.00017200 | -3.53653500 | -8.52722800 | C | 3.02600600 | -1.20000300 | -3.97824600 |
| H | 4.55437700 | -3.64723000 | -8.80890600 | H | 2.89073300 | -1.92897300 | -4.78363000 |
| C | 2.58915200 | -4.42721000 | -6.64727300 | H | 4.10851300 | -1.15104400 | -3.82573300 |
| C | 2.12044600 | -5.68518300 | -6.26381600 | C | 3.08177900 | 1.28709300 | -3.93370800 |
| C | 0.85476600 | -6.11237400 | -6.66538600 | H | 2.63827000 | 2.24289900 | -4.19697200 |
| C | 0.05200300 | -5.27052500 | -7.43889800 | C | 4.29642800 | 1.41789800 | -3.06001000 |
| C | 0.50614500 | -4.00646100 | -7.81379200 | H | 4.80340800 | 0.47221900 | -2.85596300 |
| H | 3.57842600 | -4.11264300 | -6.33328200 | H | 5.02783100 | 2.10167500 | -3.51014000 |
| H | 2.74504000 | -6.32511500 | -5.64728200 | H | 4.02344600 | 1.85430300 | -2.08978400 |
| H | 0.49094900 | -7.09196300 | -6.36832400 | C | 2.39917000 | -1.78154600 | -2.70580400 |
| H | -0.94096200 | -5.59023500 | -7.74141800 | O | 1.53712300 | -1.18175800 | -2.08465800 |
| H | -0.14863200 | -3.33242800 | -8.36064300 | C | 2.88165900 | -3.12492800 | -2.23279900 |
| C | 1.44833500 | 2.51053600 | -11.52821900 | C | 3.91444300 | -3.83593100 | -2.86362500 |
| C | 0.66403600 | 3.21147100 | -12.44173400 | C | 2.26441300 | -3.68116300 | -1.10100700 |
| C | -0.72230300 | 3.27292700 | -12.27004600 | C | 4.31990300 | -5.07702400 | -2.37157600 |
| C | -1.31591700 | 2.62501600 | -11.18813100 | H | 4.41200000 | -3.42588100 | -3.73634100 |
| C | -0.53386300 | 1.91430900 | -10.27212000 | C | 2.66674800 | -4.92045200 | -0.61245000 |
| H | 2.52682700 | 2.48689500 | -11.65915600 | H | 1.46950200 | -3.11669300 | -0.62525600 |
| H | 1.13347700 | 3.71400100 | -13.28298500 | C | 3.69660500 | -5.62147800 | -1.24721700 |
| H | -1.33374500 | 3.82248700 | -12.98053800 | H | 5.12361300 | -5.61715400 | -2.86384200 |
| H | -2.39331100 | 2.65985600 | -11.05439400 | H | 2.18038100 | -5.34238100 | 0.26232300 |
| H | -1.00342300 | 1.36723000 | -9.46147700 | H | 4.01266300 | -6.58833800 | -0.86565600 |
| C | 2.83811800 | 3.47269500 | -8.54552600 | H | -0.08436400 | 1.46993600 | -6.33421800 |
| C | 3.77607400 | 4.45409300 | -8.23242900 | | | | |

| INT3' | | | | C | 3.44557000 | 4.14559500 | -7.54439200 |
|-------|-------------|-------------|--------------|----|-------------|-------------|-------------|
| P | 3.55444800 | -2.57446900 | -8.07416800 | C | 4.25084800 | 3.09365300 | -7.98166200 |
| C | 2.90059000 | -2.17022700 | -9.76913400 | C | 3.69461200 | 1.83775200 | -8.22996500 |
| C | 2.50381000 | -0.68998600 | -9.87207100 | H | 0.46144100 | 2.52718100 | -7.43197000 |
| P | 1.55228600 | -0.04211100 | -8.36760400 | H | 1.44745600 | 4.73479100 | -6.98416300 |
| H | 3.60157400 | -2.44310500 | -10.56475400 | H | 3.87741000 | 5.12495500 | -7.35916700 |
| H | 2.01203000 | -2.79947100 | -9.86823600 | H | 5.31612900 | 3.24521000 | -8.13041300 |
| H | 3.38676400 | -0.06124600 | -10.00694000 | H | 4.35135300 | 1.03493900 | -8.54803400 |
| H | 1.86379600 | -0.53167900 | -10.74412400 | Rh | 1.66591800 | -1.59442400 | -6.68317700 |
| C | -0.06979300 | 0.43436000 | -9.11938100 | C | 2.03783600 | 0.44758200 | -4.55171200 |
| C | 2.31852300 | 1.61528000 | -8.06021400 | C | 2.88219400 | -0.40070700 | -5.45361300 |
| C | 5.22517800 | -1.78285500 | -8.01917000 | H | 3.64666700 | 0.15685600 | -5.99718900 |
| C | 3.97157400 | -4.37558100 | -8.17887200 | H | 3.36212900 | -1.19677000 | -4.87027700 |
| C | 5.82805300 | -1.58375000 | -6.76521400 | C | 2.36193600 | 1.64561600 | -4.02776400 |
| C | 7.09253400 | -1.00254900 | -6.66165600 | H | 1.61184100 | 2.13302200 | -3.40451400 |
| C | 7.77366200 | -0.59581500 | -7.81042900 | Cl | 0.12031900 | -3.26461100 | -8.01202300 |
| C | 7.18775900 | -0.78518100 | -9.06307700 | C | 3.66184400 | 2.38169100 | -4.17368900 |
| C | 5.92799300 | -1.37933600 | -9.16671000 | H | 3.50984900 | 3.38223800 | -4.59758900 |
| H | 5.30227300 | -1.88292200 | -5.86447500 | H | 4.13784900 | 2.52558700 | -3.19330600 |
| H | 7.54080900 | -0.86081700 | -5.68246100 | H | 4.37237800 | 1.85305300 | -4.81334500 |
| H | 8.75450700 | -0.13602200 | -7.73042000 | C | 0.73235100 | -0.20244900 | -4.27683800 |
| H | 7.71317200 | -0.47830400 | -9.96320300 | C | 0.06322500 | -0.70066100 | -5.52423700 |
| H | 5.50277900 | -1.53386900 | -10.15308500 | H | -0.24671500 | 0.16842200 | -6.11602200 |
| C | 5.28360200 | -4.85332900 | -8.02862000 | C | 0.27226400 | -0.37243200 | -3.02363500 |
| C | 5.55312700 | -6.22171400 | -8.09379500 | H | 0.84448700 | -0.01710300 | -2.17161200 |
| C | 4.52015900 | -7.13312700 | -8.31291900 | C | 1.28564700 | -4.18398600 | -5.02331200 |
| C | 3.21206300 | -6.66746300 | -8.45922800 | O | 1.88889000 | -3.10764700 | -5.07157100 |
| C | 2.93311500 | -5.30240600 | -8.38610500 | C | 1.46923400 | -5.14596200 | -3.93192500 |
| H | 6.10210500 | -4.16139500 | -7.86484200 | C | 0.77173000 | -6.36322500 | -3.98097300 |
| H | 6.57519800 | -6.57175600 | -7.97731100 | C | 2.32035600 | -4.86712200 | -2.84826000 |
| H | 4.73234400 | -8.19728600 | -8.36742700 | C | 0.92593300 | -7.29759700 | -2.95894200 |
| H | 2.39935200 | -7.36858300 | -8.62868500 | H | 0.11383100 | -6.56830500 | -4.82152600 |
| H | 1.90936600 | -4.95110200 | -8.47952000 | C | 2.47004300 | -5.80119400 | -1.82995200 |
| C | -0.11341100 | 1.46001500 | -10.08261500 | H | 2.84304100 | -3.91662000 | -2.82526600 |
| C | -1.31507000 | 1.80112000 | -10.69989800 | C | 1.77465500 | -7.01571600 | -1.88576500 |
| C | -2.49144300 | 1.12544600 | -10.36321400 | H | 0.38791500 | -8.23986300 | -2.99599400 |
| C | -2.45465900 | 0.10397500 | -9.41587800 | H | 3.12423700 | -5.58950200 | -0.98951000 |
| C | -1.25031000 | -0.24506400 | -8.79797000 | H | 1.89462800 | -7.74271200 | -1.08743200 |
| H | 0.78984600 | 2.00309300 | -10.34421800 | H | 0.58222700 | -4.44051300 | -5.83032800 |
| H | -1.33334000 | 2.59581400 | -11.44045300 | H | -0.67395200 | -0.85901100 | -2.81060700 |
| H | -3.42899700 | 1.39388100 | -10.84214600 | C | -1.14164700 | -1.60353500 | -5.29314900 |
| H | -3.36175700 | -0.43400200 | -9.15632400 | H | -0.88643500 | -2.46547100 | -4.66778500 |
| H | -1.21535400 | -1.06905200 | -8.09832600 | H | -1.93985700 | -1.05541400 | -4.77060800 |
| C | 1.52494000 | 2.67349700 | -7.58695600 | H | -1.55157000 | -1.99095300 | -6.22636800 |
| C | 2.08257200 | 3.92767600 | -7.33775300 | | | | |

TS-INS'Imaginary frequency: -329.3 cm⁻¹

| | | | | | | | |
|---|-------------|-------------|--------------|----|-------------|-------------|-------------|
| P | 3.79331900 | -2.54317400 | -8.42458500 | C | 1.82354500 | 3.68665500 | -7.02366300 |
| C | 3.21050400 | -1.97041100 | -10.09203100 | C | 3.15660700 | 4.05439300 | -7.21500800 |
| C | 2.61922100 | -0.55046900 | -10.04984700 | H | 0.34068000 | 2.15484700 | -7.25313100 |
| P | 1.65503100 | -0.18747500 | -8.46563300 | H | 1.11852700 | 4.39202700 | -6.59333900 |
| H | 4.00123100 | -2.05522700 | -10.84509500 | H | 3.49496500 | 5.04928900 | -6.94024500 |
| H | 2.42491200 | -2.69027600 | -10.33672300 | H | 5.09688500 | 3.39772900 | -7.89031600 |
| H | 3.39989000 | 0.20744700 | -10.14512300 | H | 4.34234700 | 1.15523500 | -8.51472100 |
| H | 1.93201100 | -0.40875800 | -10.88784700 | Rh | 2.01025400 | -2.04424200 | -7.02162600 |
| C | -0.03921300 | 0.22431000 | -9.07683500 | C | 2.26170000 | -0.31658900 | -4.57175700 |
| C | 2.26937300 | 1.48771700 | -7.96765700 | C | 3.13914400 | -1.02371500 | -5.55957900 |
| C | 5.42267200 | -1.73835300 | -8.12659800 | H | 3.88302500 | -0.36322400 | -6.00444400 |
| C | 4.25320000 | -4.30983100 | -8.63798900 | H | 3.63709700 | -1.87867400 | -5.09195500 |
| C | 6.07585900 | -1.98770000 | -6.90676700 | C | 2.53012400 | 0.90010700 | -4.04759000 |
| C | 7.31625200 | -1.41311200 | -6.63543900 | H | 1.79604500 | 1.30645300 | -3.35251300 |
| C | 7.92582600 | -0.57807900 | -7.57533800 | Cl | 0.46823900 | -3.39543500 | -8.60177600 |
| C | 7.29156400 | -0.32839400 | -8.79213100 | C | 3.74720200 | 1.75384300 | -4.24842800 |
| C | 6.04907200 | -0.90618700 | -9.06728400 | H | 3.47442200 | 2.75614800 | -4.59894700 |
| H | 5.61412400 | -2.63970800 | -6.17204100 | H | 4.27601600 | 1.88922000 | -3.29411300 |
| H | 7.80705600 | -1.61761400 | -5.68847600 | H | 4.45789100 | 1.33100400 | -4.96123400 |
| H | 8.89176700 | -0.12999800 | -7.36155700 | C | 1.02931400 | -1.04339800 | -4.13999000 |
| H | 7.76400400 | 0.30904900 | -9.53412000 | C | 0.27468500 | -1.69278700 | -5.22146800 |
| H | 5.58337500 | -0.71396600 | -10.02827900 | H | 0.30542600 | -1.04989600 | -6.11394200 |
| C | 5.51813400 | -4.65590500 | -9.14606400 | C | 0.67316400 | -1.10087500 | -2.83658300 |
| C | 5.85297300 | -5.99367800 | -9.34871700 | H | 1.29292300 | -0.65346100 | -2.06718100 |
| C | 4.93468600 | -6.99928800 | -9.03808900 | C | 1.10397900 | -3.82578800 | -5.31417800 |
| C | 3.68075600 | -6.66129100 | -8.52932300 | O | 2.29831000 | -3.70966700 | -5.80828400 |
| C | 3.33452800 | -5.32390700 | -8.32681200 | C | 0.95927300 | -4.29889200 | -3.92422400 |
| H | 6.24525500 | -3.88480500 | -9.37952700 | C | -0.19691800 | -5.00117400 | -3.54234300 |
| H | 6.83190900 | -6.24927500 | -9.74431200 | C | 1.98159300 | -4.10755600 | -2.97951200 |
| H | 5.19861300 | -8.04211200 | -9.19109400 | C | -0.33021600 | -5.49864900 | -2.24722500 |
| H | 2.96323200 | -7.43892000 | -8.28449800 | H | -0.98024000 | -5.17535600 | -4.27502800 |
| H | 2.35857000 | -5.06067200 | -7.94071600 | C | 1.84901100 | -4.61036000 | -1.68685300 |
| C | -0.20258600 | 1.25957300 | -10.01567400 | H | 2.87881900 | -3.58029700 | -3.28133600 |
| C | -1.46882400 | 1.59009300 | -10.49343600 | C | 0.69376300 | -5.30353400 | -1.31640600 |
| C | -2.59210200 | 0.89752600 | -10.03287300 | H | -1.22518200 | -6.04691400 | -1.96687100 |
| C | -2.43913000 | -0.12832000 | -9.10194700 | H | 2.64688000 | -4.46063700 | -0.96473600 |
| C | -1.16926800 | -0.46963500 | -8.62796500 | H | 0.59358400 | -5.69512800 | -0.30784000 |
| H | 0.65892900 | 1.82041600 | -10.36698100 | H | 0.28967800 | -4.09086900 | -5.99713600 |
| H | -1.57887500 | 2.38948000 | -11.22071500 | H | -0.23522200 | -1.59419200 | -2.50869900 |
| H | -3.58008200 | 1.15643000 | -10.40303400 | C | -1.17124600 | -2.10382000 | -5.02133900 |
| H | -3.30572000 | -0.67854000 | -8.74766500 | H | -1.30752200 | -2.76248600 | -4.15988800 |
| H | -1.05394200 | -1.30342200 | -7.94809900 | H | -1.80527200 | -1.22088800 | -4.85801600 |
| C | 1.38448600 | 2.41493000 | -7.39214400 | H | -1.55322900 | -2.62705700 | -5.90448400 |

TS2'Imaginary frequency: -377.4 cm⁻¹

| | | | | | | | |
|---|-------------|-------------|-------------|----|-------------|-------------|-------------|
| P | -2.54938400 | 2.01181800 | -0.87978100 | C | -1.16346400 | -3.32204200 | 0.36349300 |
| C | -2.61465300 | 1.34988800 | -2.62015700 | C | 0.06066300 | -3.98491200 | 0.46453800 |
| C | -1.82372100 | 0.03873900 | -2.76462200 | C | 1.19363400 | -3.43220100 | -0.13419800 |
| P | -0.20814700 | 0.08398300 | -1.79490100 | H | 1.10269400 | -2.23155700 | -0.83962000 |
| H | -3.64693900 | 1.24299200 | -2.96870300 | H | -2.21488400 | -1.61110400 | -0.37613400 |
| H | -2.13350800 | 2.13562000 | -3.20872300 | H | -2.05074200 | -3.73906800 | 0.83149000 |
| H | -2.40463800 | -0.81659100 | -2.41009400 | H | 0.13150700 | -4.92245200 | 1.00839800 |
| H | -1.58892000 | -0.14133100 | -3.81683000 | Rh | 2.15224200 | -3.93769900 | -0.05911600 |
| C | 1.12301100 | -0.04547800 | -3.05681100 | C | -0.27921000 | 1.97438400 | -0.36249700 |
| C | -0.12652600 | -1.56197100 | -0.95952100 | C | -0.35934300 | 1.81102800 | 2.57657200 |
| C | -3.70778300 | 0.94511800 | 0.08965700 | C | -0.46230400 | 0.85084300 | 1.42050400 |
| C | -3.47348400 | 3.61349800 | -0.96836700 | H | 0.40712700 | 0.18407200 | 1.38281300 |
| C | -3.77302100 | 1.09712100 | 1.48588800 | H | -1.35089400 | 0.21870000 | 1.45810600 |
| C | -4.66693800 | 0.34065400 | 2.24422000 | C | -0.75107800 | 1.62822000 | 3.84895700 |
| C | -5.50504100 | -0.58913300 | 1.62513500 | C | -0.57989700 | 2.44369900 | 4.55270100 |
| C | -5.45066200 | -0.75052000 | 0.24100000 | C | 0.29786500 | 3.07397200 | 2.11553600 |
| C | -4.56398800 | 0.01491900 | -0.52085500 | H | -0.39477200 | 3.77595800 | 1.08612500 |
| H | -3.12190700 | 1.80730200 | 1.98642500 | C | -1.47603100 | 3.77333400 | 1.21657000 |
| H | -4.70310500 | 0.47563200 | 3.32107800 | C | 1.64620700 | 3.27855000 | 2.43380900 |
| H | -6.19684500 | -1.18091800 | 2.21748400 | H | -1.38658700 | 0.39255300 | 4.42084800 |
| H | -6.10284200 | -1.46560500 | -0.25227600 | H | -0.72563100 | -0.07675300 | 5.16233900 |
| H | -4.55764400 | -0.11597100 | -1.59731100 | H | -2.31981500 | 0.62943800 | 4.94816400 |
| C | -4.74165000 | 3.77326200 | -0.38512000 | C | -1.60551800 | -0.35362800 | 3.65331500 |
| C | -5.42303500 | 4.98671200 | -0.49456900 | O | 2.45342700 | 1.99397100 | 1.00462000 |
| C | -4.85270500 | 6.05357100 | -1.18890900 | H | 1.80765400 | 2.19706500 | -0.08780200 |
| C | -3.59446400 | 5.90117900 | -1.77380800 | C | 2.03723500 | 2.79194600 | 3.32240300 |
| C | -2.90320400 | 4.69437500 | -1.66394100 | C | 3.90222700 | 2.34331900 | 1.03503400 |
| H | -5.20665500 | 2.95703100 | 0.15460400 | C | 4.74089800 | 1.79388700 | 2.01529600 |
| H | -6.40201900 | 5.09314800 | -0.03569500 | C | 4.44380600 | 3.21596800 | 0.07900900 |
| H | -5.38488000 | 6.99707800 | -1.27260600 | C | 6.09809300 | 2.11111500 | 2.04382600 |
| H | -3.14041600 | 6.72561700 | -2.31616800 | H | 4.32529300 | 1.11380400 | 2.75583500 |
| H | -1.91883700 | 4.58235900 | -2.11053800 | C | 5.80094200 | 3.53038400 | 0.10767600 |
| C | 1.03832600 | -1.00621900 | -4.07930200 | H | 3.78611500 | 3.63032300 | -0.67859600 |
| C | 2.05875000 | -1.12562300 | -5.02110000 | C | 6.63134800 | 2.98129700 | 1.08954200 |
| C | 3.17892000 | -0.29367500 | -4.94403300 | H | 6.74021900 | 1.67801000 | 2.80573700 |
| C | 3.27300900 | 0.65306300 | -3.92447100 | H | 6.21418700 | 4.20574700 | -0.63646500 |
| C | 2.24926500 | 0.78496900 | -2.98234300 | H | 7.68884900 | 3.22945000 | 1.11021600 |
| H | 0.18302000 | -1.67414300 | -4.13764000 | Cl | 2.19616000 | 1.13368300 | 1.63382800 |
| H | 1.98133700 | -1.86812800 | -5.81033200 | H | 0.11889600 | 3.38509500 | -2.49753100 |
| H | 3.97478700 | -0.38596300 | -5.67793400 | C | 2.12002100 | 4.21753900 | 2.16551400 |
| H | 4.14102900 | 1.30278300 | -3.86211700 | H | 0.20387600 | 5.84658700 | 1.30064900 |
| H | 2.31283500 | 1.53074300 | -2.19834900 | H | 1.16073500 | 4.93171100 | 0.11214400 |
| C | -1.25549800 | -2.11712100 | -0.33386900 | H | -0.47086200 | 5.43682900 | -0.28645900 |

| INT4' | | | | | C | 0.20565000 | -3.96775400 | 0.49831000 |
|-------|-------------|-------------|-------------|--|----|-------------|-------------|-------------|
| P | -2.54070000 | 2.03400800 | -0.83628600 | | C | 1.33796900 | -3.36004000 | -0.04607000 |
| C | -2.49428700 | 1.40595000 | -2.58587500 | | C | 1.22836600 | -2.14354100 | -0.72067000 |
| C | -1.72803500 | 0.07738000 | -2.66622900 | | H | -2.12471000 | -1.64972300 | -0.34939200 |
| P | -0.12704300 | 0.12986500 | -1.67803500 | | H | -1.92387600 | -3.80736900 | 0.80351200 |
| H | -3.49642200 | 1.32051000 | -3.01757100 | | H | 0.29212800 | -4.91749600 | 1.01825100 |
| H | -1.95022300 | 2.18169400 | -3.13160600 | | H | 2.31105700 | -3.83282500 | 0.05008900 |
| H | -2.33379300 | -0.74936600 | -2.28690300 | | H | 2.11465300 | -1.68198600 | -1.14233800 |
| H | -1.47744700 | -0.15248600 | -3.70484700 | | Rh | -0.22159300 | 1.91556700 | -0.22553900 |
| C | 1.20514800 | 0.05766200 | -2.94069100 | | C | -0.37356400 | 1.83274500 | 2.52295900 |
| C | -0.02071900 | -1.51780000 | -0.86150200 | | C | -0.41832400 | 0.73572000 | 1.50600600 |
| C | -3.73307800 | 0.92060300 | 0.03501900 | | H | 0.46511600 | 0.09409700 | 1.50329900 |
| C | -3.48578300 | 3.62153200 | -0.94862600 | | H | -1.31364100 | 0.11403400 | 1.54959600 |
| C | -3.78466900 | 0.94344500 | 1.43966200 | | C | -0.86046900 | 1.85138500 | 3.77404500 |
| C | -4.69077200 | 0.14014900 | 2.13392600 | | H | -0.77260000 | 2.78043000 | 4.33900700 |
| C | -5.55297700 | -0.70976800 | 1.43892900 | | C | 0.24260200 | 3.05557000 | 1.88269600 |
| C | -5.51198600 | -0.74338100 | 0.04467900 | | C | -0.58446900 | 3.99657900 | 1.33091100 |
| C | -4.61490800 | 0.06983100 | -0.65147500 | | H | -1.65252600 | 3.86023300 | 1.48880600 |
| H | -3.11265300 | 1.58981400 | 1.99591200 | | C | 1.75023600 | 3.15927500 | 1.90381000 |
| H | -4.71541400 | 0.17457100 | 3.21903500 | | C | -1.48908200 | 0.69505600 | 4.49981100 |
| H | -6.25293800 | -1.33999000 | 1.97980500 | | H | -0.88456600 | 0.40608800 | 5.36978400 |
| H | -6.18330300 | -1.39632000 | -0.50583800 | | H | -2.48194900 | 0.95721600 | 4.88870200 |
| H | -4.61816900 | 0.03962200 | -1.73570600 | | H | -1.59095300 | -0.18507200 | 3.86008200 |
| C | -4.68922000 | 3.81840100 | -0.25134000 | | C | 2.39958800 | 1.92470900 | 1.22136100 |
| C | -5.38585400 | 5.02300500 | -0.36538900 | | O | 1.82334700 | 1.71735300 | -0.03236000 |
| C | -4.89681200 | 6.04396500 | -1.18008300 | | H | 2.08406100 | 3.22849600 | 2.94837800 |
| C | -3.70061200 | 5.85687200 | -1.87529300 | | C | 3.90342000 | 2.12180400 | 1.06842300 |
| C | -2.99272600 | 4.66009000 | -1.75991800 | | C | 4.80487800 | 1.52611900 | 1.95699200 |
| H | -5.09436500 | 3.03459800 | 0.37800100 | | C | 4.40460400 | 2.93583000 | 0.04260800 |
| H | -6.31481200 | 5.15689800 | 0.18177100 | | C | 6.17966900 | 1.74176300 | 1.83374400 |
| H | -5.44215400 | 6.97917700 | -1.27070000 | | H | 4.42695600 | 0.88514300 | 2.75093800 |
| H | -3.30785100 | 6.64711800 | -2.50877800 | | C | 5.77662100 | 3.15069700 | -0.08467800 |
| H | -2.04526300 | 4.53629200 | -2.27618300 | | H | 3.70433800 | 3.38581600 | -0.65495300 |
| C | 1.12736600 | -0.91995400 | -3.94922400 | | C | 6.66950900 | 2.55558300 | 0.81145200 |
| C | 2.12128300 | -1.00858800 | -4.92156500 | | H | 6.86643100 | 1.26984600 | 2.53170400 |
| C | 3.20607700 | -0.12798100 | -4.88990400 | | H | 6.15206400 | 3.78337700 | -0.88495900 |
| C | 3.29302400 | 0.83196900 | -3.88258900 | | H | 7.73856400 | 2.72240000 | 0.71044700 |
| C | 2.29768900 | 0.93319800 | -2.90661900 | | H | 2.25651200 | 1.06329000 | 1.90069500 |
| H | 0.30079700 | -1.62530500 | -3.97340400 | | Cl | 0.20886600 | 3.52462800 | -2.21313800 |
| H | 2.05063400 | -1.76445100 | -5.69856800 | | H | 2.08499100 | 4.06086400 | 1.38642400 |
| H | 3.98188800 | -0.19592300 | -5.64764200 | | C | -0.19943100 | 5.31197100 | 0.71897900 |
| H | 4.13796900 | 1.51338300 | -3.85014400 | | H | -0.36206500 | 6.11568700 | 1.45100200 |
| H | 2.36257100 | 1.66640500 | -2.11319300 | | H | 0.83835100 | 5.34176400 | 0.38862000 |
| C | -1.15074700 | -2.12570900 | -0.29053200 | | H | -0.82588800 | 5.52256000 | -0.15026100 |
| C | -1.03812300 | -3.34610400 | 0.37613400 | | | | | |

| INT5 | | | | C | 4.09895400 | 4.38061100 | -7.60237600 |
|-------------|-------------|-------------|--------------|----|-------------|-------------|-------------|
| P | 3.20971000 | -2.39005600 | -8.02537500 | C | 4.71882600 | 3.13305100 | -7.50888500 |
| C | 2.95322600 | -1.82793100 | -9.77467900 | C | 4.00361200 | 1.97051600 | -7.79584600 |
| C | 2.87212200 | -0.30138900 | -9.84887400 | H | 1.00216500 | 3.37181800 | -8.57009100 |
| P | 1.75117900 | 0.44162300 | -8.52051500 | H | 2.26466900 | 5.41971800 | -8.05339900 |
| H | 3.72243300 | -2.22321200 | -10.44724100 | H | 4.65514200 | 5.28588500 | -7.37718000 |
| H | 1.99854500 | -2.28120900 | -10.06176100 | H | 5.75965800 | 3.06052700 | -7.20689400 |
| H | 3.86122000 | 0.14093100 | -9.70944200 | H | 4.50126200 | 1.01010700 | -7.69682100 |
| H | 2.50773200 | 0.02092200 | -10.82788500 | Rh | 1.64777200 | -1.20482300 | -6.72252300 |
| C | 0.27936300 | 0.98535600 | -9.49901400 | C | 1.40179800 | -0.30796200 | -4.68613600 |
| C | 2.65586000 | 2.03260400 | -8.19448400 | C | 2.70571700 | -0.02860200 | -5.23370600 |
| C | 4.95340400 | -2.01541800 | -7.57844900 | H | 2.92345700 | 0.95227100 | -5.64338100 |
| C | 3.18725800 | -4.22628200 | -8.14702300 | H | 3.54960300 | -0.53251300 | -4.77589500 |
| C | 5.32734900 | -2.23397200 | -6.23975700 | C | 0.26508100 | 0.21914000 | -5.31706300 |
| C | 6.63135600 | -1.97085400 | -5.82412700 | H | -0.67970200 | -0.25959200 | -5.07003900 |
| C | 7.57578000 | -1.47916100 | -6.73049000 | Cl | -0.31741700 | -2.38742900 | -7.80595900 |
| C | 7.21341400 | -1.26230100 | -8.05968200 | C | 0.11110800 | 1.63483800 | -5.80331300 |
| C | 5.90942600 | -1.53506000 | -8.48490300 | H | -0.52244100 | 1.70562800 | -6.69101300 |
| H | 4.58418900 | -2.61432600 | -5.54422600 | H | -0.39177900 | 2.21078500 | -5.01260200 |
| H | 6.91184700 | -2.14933800 | -4.78994700 | H | 1.06164700 | 2.12670100 | -6.00713100 |
| H | 8.59006100 | -1.27105600 | -6.40196000 | C | 1.21425900 | -1.31239500 | -3.58909600 |
| H | 7.94416100 | -0.88854200 | -8.77142700 | C | 0.33053900 | -2.50954400 | -3.88896700 |
| H | 5.65335600 | -1.38123400 | -9.52864800 | H | -0.47404800 | -2.16712600 | -4.54881200 |
| C | 4.38752200 | -4.94347800 | -8.27750900 | C | 1.80470700 | -1.07332300 | -2.41084300 |
| C | 4.36754500 | -6.32884400 | -8.44399800 | H | 2.44720400 | -0.20944700 | -2.26463500 |
| C | 3.15245000 | -7.01291300 | -8.48018200 | C | 1.16873800 | -3.50840400 | -4.78095200 |
| C | 1.95691200 | -6.30438500 | -8.34980100 | O | 2.14867300 | -2.81727500 | -5.50279700 |
| C | 1.96738700 | -4.91968900 | -8.18087600 | C | 1.87476100 | -4.59478500 | -3.97425700 |
| H | 5.34129100 | -4.42873700 | -8.24512100 | C | 1.36533700 | -5.89917600 | -3.95332600 |
| H | 5.30437400 | -6.87048100 | -8.54004000 | C | 3.04029300 | -4.32327400 | -3.24161500 |
| H | 3.13797300 | -8.09209200 | -8.60535700 | C | 1.98911800 | -6.90494000 | -3.21207900 |
| H | 1.00637000 | -6.82984200 | -8.37210800 | H | 0.47287700 | -6.12905900 | -4.53060100 |
| H | 1.03580500 | -4.37457200 | -8.07034900 | C | 3.66585000 | -5.32526400 | -2.49913000 |
| C | 0.44798400 | 1.77228100 | -10.65395700 | H | 3.44864400 | -3.31921000 | -3.25974700 |
| C | -0.65386000 | 2.17949600 | -11.40366900 | C | 3.14249500 | -6.62060000 | -2.47982500 |
| C | -1.94230200 | 1.80549100 | -11.01192800 | H | 1.57765700 | -7.91099500 | -3.21279100 |
| C | -2.11885700 | 1.02181500 | -9.87300200 | H | 4.56676600 | -5.09623600 | -1.93514400 |
| C | -1.01617100 | 0.61036000 | -9.11848300 | H | 3.63301600 | -7.40144800 | -1.90485400 |
| H | 1.44120900 | 2.08522100 | -10.96344500 | H | 0.45016600 | -4.01130600 | -5.44753500 |
| H | -0.50666000 | 2.78824200 | -12.29128200 | H | 1.65623700 | -1.72157700 | -1.55404300 |
| H | -2.80137600 | 2.12066700 | -11.59746000 | C | -0.33574100 | -3.15374000 | -2.66984800 |
| H | -3.11542900 | 0.71418100 | -9.57039100 | H | -0.96163200 | -3.99596800 | -2.98277900 |
| H | -1.15503000 | -0.04385200 | -8.26583800 | H | 0.39294800 | -3.54378100 | -1.95469000 |
| C | 2.04206500 | 3.29227200 | -8.27374800 | H | -0.97597300 | -2.43304000 | -2.15012900 |
| C | 2.75889000 | 4.45502400 | -7.98167500 | | | | |

TS4Imaginary frequency: -599.2 cm⁻¹

| | | | | | | | |
|---|-------------|-------------|--------------|----|-------------|-------------|-------------|
| P | 3.79023800 | -2.71255000 | -8.12601300 | C | 1.16967000 | 3.54197700 | -8.20014100 |
| C | 3.23939400 | -2.42605700 | -9.87941000 | C | 2.49963800 | 3.95464000 | -8.28275400 |
| C | 2.46499000 | -1.10803600 | -10.05778600 | C | 3.50818100 | 2.99972100 | -8.42325900 |
| P | 1.43619400 | -0.58825900 | -8.55544800 | H | 3.18607900 | 1.64382800 | -8.49369300 |
| H | 4.08041300 | -2.48530100 | -10.57837500 | H | 0.37708300 | 4.27562900 | -8.08343600 |
| H | 2.57228300 | -3.26945300 | -10.06612900 | H | 2.74956800 | 5.01040300 | -8.23218400 |
| H | 3.14365700 | -0.28000800 | -10.27571700 | H | 4.54886200 | 3.30677800 | -8.47482000 |
| H | 1.78239400 | -1.19408300 | -10.90731000 | Rh | 3.99130800 | 0.92144500 | -8.58541400 |
| C | -0.30451600 | -0.53958000 | -9.15301100 | C | 1.90711200 | -2.03047000 | -6.81495500 |
| C | 1.84797100 | 1.21722300 | -8.43750700 | C | 2.35010400 | -0.20901000 | -4.37272500 |
| C | 5.40471300 | -1.83885200 | -7.94135900 | C | 3.02399000 | -0.66195500 | -5.61826200 |
| C | 4.30439800 | -4.47493600 | -8.07167500 | H | 3.34971000 | 0.16933000 | -6.24215800 |
| C | 6.12667200 | -2.02721100 | -6.74934500 | H | 3.88580900 | -1.28042300 | -5.35573100 |
| C | 7.34333700 | -1.37966600 | -6.54290400 | C | 2.03098300 | 1.06134300 | -4.04064100 |
| C | 7.86144500 | -0.52745600 | -7.52146100 | H | 1.57285000 | 1.20661800 | -3.06162700 |
| C | 7.15795000 | -0.33383100 | -8.70961200 | Cl | 0.67773600 | -3.74892900 | -8.31799700 |
| C | 5.93886700 | -0.98536400 | -8.91878600 | C | 2.26379300 | 2.32320300 | -4.81654100 |
| H | 5.74082600 | -2.69610600 | -5.98517500 | H | 1.31669100 | 2.81986000 | -5.06259600 |
| H | 7.88759100 | -1.54113400 | -5.61697100 | H | 2.83967100 | 3.03855000 | -4.21354400 |
| H | 8.80920000 | -0.02239500 | -7.35940900 | C | 2.80292400 | 2.15996900 | -5.74955200 |
| H | 7.55811100 | 0.31767100 | -9.48149400 | C | 2.07993800 | -1.26988000 | -3.34682100 |
| H | 5.41943000 | -0.83175300 | -9.85933700 | C | 0.79053600 | -2.05509700 | -3.50513100 |
| C | 5.37430300 | -4.93119900 | -8.85936600 | H | -0.02493700 | -1.32101200 | -3.54949700 |
| C | 5.75180700 | -6.27224900 | -8.82181600 | C | 2.93546600 | -1.44461800 | -2.33371600 |
| C | 5.07162200 | -7.16504300 | -7.98916700 | H | 3.82612800 | -0.82824400 | -2.25427500 |
| C | 4.01464400 | -6.71365500 | -7.19863600 | C | 0.76031200 | -2.88352600 | -4.81721600 |
| C | 3.62405500 | -5.37291200 | -7.23805300 | O | 1.86223600 | -3.45686300 | -5.17127100 |
| H | 5.91927300 | -4.23951600 | -9.49603500 | C | -0.55587100 | -3.57874700 | -5.09968300 |
| H | 6.57709900 | -6.61904400 | -9.43734900 | C | -1.78592100 | -2.91706300 | -4.96841700 |
| H | 5.36856500 | -8.20972700 | -7.95713900 | C | -0.54687100 | -4.93766900 | -5.43148000 |
| H | 3.48592900 | -7.40598000 | -6.54983600 | H | -2.98350000 | -3.60308800 | -5.16546300 |
| H | 2.79651000 | -5.01813900 | -6.63427700 | H | -1.81081700 | -1.85833000 | -4.72471600 |
| C | -0.61224000 | 0.08851400 | -10.37174400 | C | -1.74500300 | -5.62690900 | -5.61530100 |
| C | -1.93014000 | 0.15079900 | -10.82268700 | H | 0.40650200 | -5.43780500 | -5.54735400 |
| C | -2.95702200 | -0.40657400 | -10.05707000 | C | -2.96550600 | -4.96357000 | -5.48451500 |
| C | -2.65904900 | -1.02616300 | -8.84344500 | H | -3.92947700 | -3.07791600 | -5.06566000 |
| C | -1.33932400 | -1.09754900 | -8.39352300 | H | -1.72388400 | -6.68177800 | -5.87326500 |
| H | 0.17264900 | 0.54557500 | -10.96802300 | H | -3.89812400 | -5.50032700 | -5.63415300 |
| H | -2.15390300 | 0.63566600 | -11.76864400 | C | 0.57320200 | -1.67482900 | -5.87837100 |
| H | -3.98388700 | -0.35974900 | -10.40865300 | H | 0.49976000 | -3.01369900 | -2.33284200 |
| H | -3.44883900 | -1.47392600 | -8.24767700 | H | 1.25302600 | -3.80525100 | -2.27741700 |
| H | -1.10847500 | -1.61434900 | -7.47027900 | H | 0.50916100 | -2.46145200 | -1.38912000 |
| C | 0.84576700 | 2.18584900 | -8.27306200 | H | -0.47953600 | -3.48271300 | -2.44410800 |
| | | | | H | 2.79455200 | -2.19440600 | -1.56265400 |

TS-REImaginary frequency: -381.7 cm⁻¹

| | | | | | | | |
|---|-------------|-------------|--------------|----|-------------|-------------|-------------|
| P | 3.53824900 | -1.98097900 | -8.37119000 | C | 1.79341700 | 4.47928800 | -7.02284900 |
| C | 3.81102000 | -1.11669400 | -10.01263400 | C | 2.67094900 | 5.29513500 | -7.74012600 |
| C | 3.66104700 | 0.40184200 | -9.86904300 | C | 3.41012400 | 4.75538800 | -8.79362100 |
| P | 2.15288200 | 0.79449900 | -8.82645700 | H | 3.27000000 | 3.40654400 | -9.12848400 |
| H | 4.77948400 | -1.38325200 | -10.44840900 | H | 0.97874600 | 2.49185300 | -6.78543300 |
| H | 3.03441600 | -1.50606500 | -10.67858200 | H | 1.21263400 | 4.89308400 | -6.20297700 |
| H | 4.52342900 | 0.83102900 | -9.34850000 | H | 2.77871000 | 6.34486700 | -7.48065900 |
| H | 3.59757900 | 0.87679100 | -10.85363100 | Rh | 4.09640000 | 5.38144000 | -9.35769100 |
| C | 0.78818000 | 0.80258800 | -10.07053900 | C | 3.85318900 | 3.01209400 | -9.95455100 |
| C | 2.39112700 | 2.57850700 | -8.40992600 | C | 1.99849000 | -0.78354600 | -7.18770700 |
| C | 5.23347000 | -2.24464800 | -7.68165200 | C | 2.86367000 | -0.37995500 | -3.77016100 |
| C | 3.06953700 | -3.69074200 | -8.87439300 | C | 3.43193300 | -0.80467100 | -5.03863500 |
| C | 5.45624900 | -3.31641900 | -6.80054200 | H | 3.79173900 | -0.01522200 | -5.69042000 |
| C | 6.70270800 | -3.49579900 | -6.20047800 | H | 4.05377400 | -1.68709200 | -5.04287400 |
| C | 7.74785200 | -2.60868900 | -6.46720600 | Cl | 2.93435300 | 0.90091300 | -3.33250800 |
| C | 7.53649400 | -1.53798000 | -7.33665700 | C | 2.52307000 | 1.09191900 | -2.34087600 |
| C | 6.28823600 | -1.35501900 | -7.93548400 | H | -0.01415000 | 0.27098700 | -6.25438800 |
| H | 4.65343900 | -4.01452800 | -6.58731300 | C | 2.68121000 | 2.83352900 | -4.19499300 |
| H | 6.85827200 | -4.33365100 | -5.52683800 | H | 4.22710000 | 2.60885300 | -3.38485900 |
| H | 8.71871600 | -2.75118800 | -6.00152500 | C | 3.95490000 | 1.89869600 | -4.98519300 |
| H | 8.34341300 | -0.84337900 | -7.55320500 | C | 2.16073200 | -1.40840200 | -2.94056600 |
| H | 6.14966300 | -0.51370900 | -8.60742700 | C | 0.81805900 | -1.80893200 | -3.52547200 |
| C | 3.75987900 | -4.35191500 | -9.90501800 | H | 0.35056300 | -0.87012400 | -3.84573300 |
| C | 3.39693000 | -5.64504200 | -10.28044300 | C | 2.66233400 | -1.83004300 | -1.77406600 |
| C | 2.35429500 | -6.29920500 | -9.61651000 | H | 3.61986800 | -1.46776000 | -1.41079700 |
| C | 1.67479800 | -5.65349200 | -8.58471700 | C | 0.95918400 | -2.62369100 | -4.85836600 |
| C | 2.02260800 | -4.35102000 | -8.22159300 | O | 2.07748000 | -2.23133100 | -5.64993400 |
| H | 4.58730800 | -3.86398600 | -10.41345200 | C | 1.08539500 | -4.12762700 | -4.64665000 |
| H | 3.93202800 | -6.14504800 | -11.08359300 | C | 0.00049500 | -4.96979700 | -4.92080900 |
| H | 2.07990900 | -7.31087700 | -9.90263500 | C | 2.28067300 | -4.70449800 | -4.19500900 |
| H | 0.87902300 | -6.16064600 | -8.04888000 | C | 0.09785000 | -6.35207100 | -4.73732400 |
| H | 1.50353200 | -3.84941100 | -7.41619900 | H | -0.93029200 | -4.53822700 | -5.28134700 |
| C | 0.79846100 | 1.66997500 | -11.17463500 | C | 2.38169400 | -6.08222700 | -4.00907600 |
| C | -0.22329800 | 1.61917600 | -12.12236400 | H | 3.13062400 | -4.06453900 | -3.98914400 |
| C | -1.27055700 | 0.70489100 | -11.97268100 | C | 1.29113100 | -6.91287900 | -4.28004100 |
| C | -1.29356400 | -0.15048900 | -10.87130700 | H | -0.75702200 | -6.98789200 | -4.95327700 |
| C | -0.27061800 | -0.10204700 | -9.92204600 | H | 3.31415800 | -6.51218800 | -3.65368500 |
| H | 1.59609100 | 2.39922600 | -11.29138900 | H | 1.37267000 | -7.98705500 | -4.13890300 |
| H | -0.20587200 | 2.29529900 | -12.97329200 | H | 0.02889100 | -2.43094500 | -5.40790600 |
| H | -2.06782500 | 0.66774600 | -12.71019700 | H | 2.13916600 | -2.54120900 | -1.14409300 |
| H | -2.11167000 | -0.85299600 | -10.74332400 | C | -0.13260700 | -2.48602800 | -2.53313900 |
| H | -0.29497400 | -0.74740000 | -9.05074900 | H | -1.09212200 | -2.70380000 | -3.01304700 |
| C | 1.65391800 | 3.12962400 | -7.34914100 | H | 0.26386500 | -3.43056800 | -2.15060400 |
| | | | | H | -0.32675700 | -1.82536100 | -1.68240700 |

| INT6 | | | | C | 3.04080500 | 4.12608300 | -8.33547800 |
|-------------|-------------|-------------|--------------|----|-------------|-------------|-------------|
| P | 3.57339700 | -2.63618100 | -8.07460600 | C | 3.94424800 | 3.06247900 | -8.29525200 |
| C | 3.26757900 | -2.40727600 | -9.89877600 | C | 3.50577200 | 1.75934300 | -8.52912800 |
| C | 2.85693800 | -0.96536500 | -10.23905700 | H | 0.20671100 | 2.39718700 | -9.06279100 |
| P | 1.57461600 | -0.24090300 | -9.05614300 | H | 0.98269100 | 4.69663300 | -8.63272700 |
| H | 4.12655100 | -2.71894300 | -10.50314500 | H | 3.38288200 | 5.14054600 | -8.15186800 |
| H | 2.43805900 | -3.08914700 | -10.10659000 | H | 4.99237500 | 3.24377700 | -8.07502600 |
| H | 3.72266800 | -0.29858700 | -10.21868400 | H | 4.22209400 | 0.94597100 | -8.46345300 |
| H | 2.43891600 | -0.92159800 | -11.24874100 | Rh | 1.44274500 | -1.54149300 | -7.22935000 |
| C | 0.06112600 | -0.02626600 | -10.08359700 | C | 1.68840700 | -0.30008900 | -4.53212000 |
| C | 2.15701300 | 1.49926200 | -8.82398900 | C | 2.21217300 | -0.06004400 | -5.90822800 |
| C | 5.22759600 | -1.86787100 | -7.77009900 | H | 1.93872200 | 0.92768900 | -6.27258400 |
| C | 3.94892500 | -4.43767300 | -7.91222800 | H | 3.29961000 | -0.16047400 | -5.94217000 |
| C | 5.64719900 | -1.74935000 | -6.43352300 | C | 0.61796800 | 0.32903800 | -3.99763800 |
| C | 6.87951900 | -1.17827200 | -6.11807100 | H | 0.33361500 | 0.07811100 | -2.97475200 |
| C | 7.71333200 | -0.70174200 | -7.13261600 | Cl | 0.21940400 | -3.35382700 | -8.61341000 |
| C | 7.30805600 | -0.80638100 | -8.46328800 | C | -0.25180700 | 1.36079000 | -4.65385400 |
| C | 6.07682300 | -1.38782200 | -8.78018700 | H | -1.28241600 | 0.99240100 | -4.75152400 |
| H | 4.99950300 | -2.10338900 | -5.63655000 | H | -0.30332300 | 2.27642500 | -4.04974300 |
| H | 7.18646900 | -1.10011300 | -5.07882500 | H | 0.09471000 | 1.63133200 | -5.65287600 |
| H | 8.67119300 | -0.25194800 | -6.88737800 | C | 2.39760300 | -1.33275400 | -3.70122600 |
| H | 7.95147400 | -0.44254300 | -9.25973200 | C | 1.54905900 | -2.49197600 | -3.18929800 |
| H | 5.79196200 | -1.47260100 | -9.82409100 | H | 0.84140400 | -2.08277400 | -2.45485200 |
| C | 5.21085100 | -4.97012100 | -8.22283500 | C | 3.69982800 | -1.21144700 | -3.41305700 |
| C | 5.45218800 | -6.33781600 | -8.09328400 | H | 4.26409600 | -0.35078700 | -3.75859600 |
| C | 4.43752000 | -7.18887800 | -7.64953500 | C | 0.71307300 | -3.09477200 | -4.32326700 |
| C | 3.18131000 | -6.66687800 | -7.33820000 | O | 1.03365600 | -2.93118700 | -5.49920100 |
| C | 2.93424100 | -5.29834800 | -7.46479500 | C | -0.49146800 | -3.92466900 | -4.02792600 |
| H | 6.01057800 | -4.31656400 | -8.55793200 | C | -0.99748100 | -4.11239100 | -2.72956100 |
| H | 6.43298800 | -6.73750700 | -8.33633200 | C | -1.16236100 | -4.51027600 | -5.11889800 |
| H | 4.62702800 | -8.25395400 | -7.54711700 | C | -2.14182600 | -4.88040000 | -2.52361900 |
| H | 2.38689600 | -7.32458800 | -6.99666200 | H | -0.50970800 | -3.65601700 | -1.87492300 |
| H | 1.95142200 | -4.89410300 | -7.24695200 | C | -2.30376400 | -5.27780100 | -4.90598700 |
| C | 0.15420900 | 0.61760000 | -11.33028200 | H | -0.78126200 | -4.33880000 | -6.12247100 |
| C | -0.98083700 | 0.80302800 | -12.11778600 | C | -2.79374300 | -5.46736500 | -3.61057500 |
| C | -2.22392700 | 0.35211700 | -11.66643200 | H | -2.52594400 | -5.01797500 | -1.51718100 |
| C | -2.32391200 | -0.28363900 | -10.42934000 | H | -2.81521500 | -5.72485200 | -5.75322200 |
| C | -1.18797000 | -0.47690200 | -9.63943600 | H | -3.68564900 | -6.06619400 | -3.44806400 |
| H | 1.11057800 | 0.99228100 | -11.68510100 | H | 0.08881300 | -0.81814800 | -6.95426200 |
| H | -0.89503600 | 1.30099600 | -13.07942700 | C | 2.35080300 | -3.61756200 | -2.49956000 |
| H | -3.10915900 | 0.49522900 | -12.27988400 | H | 3.09421500 | -4.03518100 | -3.18507400 |
| H | -3.28583900 | -0.64447100 | -10.07729000 | H | 2.87298200 | -3.23074900 | -1.62038200 |
| H | -1.25768300 | -1.00242500 | -8.69493300 | H | 1.69854500 | -4.43038400 | -2.17338100 |
| C | 1.25487100 | 2.57398800 | -8.84690800 | H | 4.24413200 | -1.93790100 | -2.81970300 |
| C | 1.69503600 | 3.87696100 | -8.60559800 | | | | |

INT7

| | | | | | | | |
|---|-------------|-------------|--------------|----|-------------|-------------|--------------|
| P | 2.86653100 | -2.48479600 | -7.69758000 | C | 3.93206200 | 4.15041800 | -8.49943800 |
| C | 2.55860500 | -2.38098600 | -9.54146500 | C | 4.51728000 | 2.91349500 | -8.21877300 |
| C | 2.66198000 | -0.93387800 | -10.03970400 | H | 3.79543500 | 1.73582700 | -8.40869600 |
| P | 1.52697800 | 0.19778700 | -9.05654500 | H | 0.87856400 | 3.07698600 | -9.53705500 |
| H | 3.23976900 | -3.03429300 | -10.09588600 | H | 2.15205600 | 5.15695600 | -9.18222000 |
| H | 1.54190900 | -2.76003300 | -9.68148500 | H | 4.49444000 | 5.06758500 | -8.34970500 |
| H | 3.68589500 | -0.56152600 | -9.94567400 | H | 5.53652900 | 2.86248500 | -7.84643900 |
| H | 2.38623400 | -0.87022100 | -11.09633000 | Rh | 4.25848600 | 0.78670800 | -8.15666900 |
| C | 0.19490100 | 0.61274100 | -10.26167800 | C | 0.93376600 | -0.80427300 | -7.03782000 |
| C | 1.28023900 | -0.53107700 | -4.81090600 | C | 2.47941900 | 1.77352600 | -8.90003600 |
| C | 1.69641500 | 0.60715700 | -5.59697200 | C | 4.66414100 | -2.03820700 | -7.58014400 |
| C | 1.05644300 | 1.48190000 | -5.66034500 | C | 2.89059900 | -4.31760800 | -7.43191200 |
| C | 2.75567600 | 0.84436900 | -5.62530800 | C | 5.13823700 | -1.43256300 | -6.40651200 |
| C | -0.05827500 | -0.96350500 | -4.93318200 | C | 6.48466500 | -1.08182300 | -6.27614100 |
| C | -0.26953800 | -1.97279400 | -4.59110500 | H | 7.37740100 | -1.32083400 | -7.32051300 |
| C | -0.67052200 | -2.46435100 | -8.03751300 | Cl | 6.92077300 | -1.92698200 | -8.49335800 |
| C | -1.29388000 | -0.09349500 | -4.93730000 | C | 5.57916600 | -2.28746500 | -8.61920200 |
| C | -2.04060600 | -0.48133000 | -5.63532100 | H | 4.45967900 | -1.25221500 | -5.58132300 |
| H | -1.74073800 | -0.11179900 | -3.93185800 | H | 6.83121600 | -0.62490000 | -5.35364800 |
| H | -1.08405500 | 0.94686700 | -5.19288300 | C | 8.42311600 | -1.04326900 | -7.22182200 |
| H | 2.26262200 | -1.29690300 | -3.98227900 | C | 7.61009900 | -2.12513500 | -9.30950400 |
| H | 1.95952800 | -2.74383600 | -3.60504400 | C | 5.25284700 | -2.77378100 | -9.53273800 |
| C | 1.28060500 | -3.16509000 | -4.35327500 | C | 4.02630000 | -4.99030500 | -6.95437300 |
| C | 3.26759200 | -0.62021300 | -3.39892800 | C | 4.00942400 | -6.37654700 | -6.78701900 |
| C | 3.41142300 | 0.43979600 | -3.57893200 | C | 2.86241300 | -7.10848900 | -7.09253900 |
| C | 3.17574100 | -3.68915000 | -3.55922000 | C | 1.72299800 | -6.44446100 | -7.55241300 |
| C | 4.32908500 | -3.28837600 | -3.60643800 | O | 1.72842000 | -5.05904600 | -7.71524100 |
| C | 2.91485100 | -5.16153900 | -3.38019100 | H | 4.92580100 | -4.43689800 | -6.70865700 |
| H | 1.68582300 | -5.77946300 | -3.65851700 | C | 4.89601400 | -6.88079700 | -6.41342700 |
| H | 3.97990700 | -5.94933700 | -2.91245300 | C | 2.85324000 | -8.18728500 | -6.96486700 |
| H | 1.52649100 | -7.15197300 | -3.46694700 | C | 0.82100000 | -7.00426300 | -7.78443800 |
| H | 0.85235600 | -5.20392600 | -4.04624600 | C | 0.82952400 | -4.54894200 | -8.04882500 |
| C | 3.81665100 | -7.31624800 | -2.70988300 | C | 0.52923800 | 1.13436300 | -11.52506900 |
| C | 4.92804800 | -5.46188600 | -2.71216500 | C | -0.46580200 | 1.44393400 | -12.45014800 |
| C | 2.58702600 | -7.92124000 | -2.98610400 | C | -1.80941400 | 1.23441500 | -12.12643700 |
| C | 0.57341100 | -7.61926700 | -3.69599500 | H | -2.14883400 | 0.71404100 | -10.87852700 |
| H | 4.64501300 | -7.91158700 | -2.33642900 | C | -1.15368500 | 0.40211900 | -9.94771700 |
| H | 2.45728500 | -8.98846900 | -2.82947800 | H | 1.56902400 | 1.31542400 | -11.78395400 |
| H | -0.20259200 | 0.22715500 | -7.13576700 | C | -0.19358500 | 1.84890100 | -13.42075100 |
| C | 1.24534700 | -2.78771200 | -2.22413800 | H | -2.58563500 | 1.47335000 | -12.84807900 |
| H | 1.91833700 | -2.42554500 | -1.44157800 | H | -3.19013200 | 0.53779300 | -10.62524200 |
| H | 0.92406500 | -3.79855000 | -1.96277500 | C | -1.41733000 | -0.03866800 | -8.99346800 |
| C | 3.96428400 | -1.10647700 | -2.72889700 | C | 1.89636500 | 3.02123500 | -9.16625300 |
| C | 2.61906400 | 4.19995500 | -8.96703000 | | | | |

TS5aImaginary frequency: -517.9 cm⁻¹

| | | | | | | | |
|---|-------------|-------------|--------------|----|-------------|-------------|--------------|
| P | 3.11134900 | -1.88633900 | -7.49977200 | C | 0.10004100 | 4.45211500 | -8.79909000 |
| C | 2.74000500 | -1.62584800 | -9.31976000 | C | 1.34145200 | 5.05922400 | -8.60716800 |
| C | 2.34672900 | -0.18394000 | -9.66250900 | C | 2.47261900 | 4.26401000 | -8.41210800 |
| P | 0.98781400 | 0.40901900 | -8.51439300 | H | 2.36183000 | 2.87351600 | -8.41078000 |
| H | 3.58472700 | -1.96827500 | -9.92732600 | H | -0.98345800 | 2.60497300 | -8.96505400 |
| H | 1.90322200 | -2.30096900 | -9.53077800 | H | -0.78768300 | 5.06080300 | -8.94669400 |
| H | 3.19411900 | 0.49671500 | -9.54591200 | H | 1.42714700 | 6.14196000 | -8.60469600 |
| H | 2.01271100 | -0.11255100 | -10.70236300 | Rh | 3.44362200 | 4.72538600 | -8.25506400 |
| C | -0.54172100 | 0.02644400 | -9.47336300 | C | 3.25035500 | 2.27536900 | -8.23119200 |
| C | -0.54172100 | 0.02644400 | -9.47336300 | C | 1.11963500 | 2.24970900 | -8.62291000 |
| C | 4.88932600 | -1.40854500 | -7.32254700 | H | 2.93580700 | 0.85336200 | -5.52417300 |
| C | 3.21098700 | -3.72987400 | -7.43724800 | H | 2.65501900 | 1.88587700 | -5.71211000 |
| C | 5.56375100 | -1.77681700 | -6.14394500 | H | 3.96884700 | 0.62125300 | -5.76274600 |
| C | 6.89867900 | -1.41973800 | -5.95191100 | C | 0.90768600 | 0.41117900 | -4.30813400 |
| C | 7.58244500 | -0.68486700 | -6.92260400 | Cl | 0.31333600 | -0.32494900 | -3.77088400 |
| C | 6.92328100 | -0.31290600 | -8.09409500 | C | -0.36526000 | -2.26910000 | -5.91753000 |
| C | 5.58810200 | -0.67312100 | -8.29312800 | H | 6.89867900 | -1.41973800 | -5.95191100 |
| H | 5.05726100 | -2.34725300 | -5.37213100 | H | 0.37903000 | 1.82676900 | -4.13783900 |
| H | 7.40217800 | -1.72003100 | -5.03758900 | H | 0.54103200 | 2.12928500 | -3.09439100 |
| H | 8.62146800 | -0.40762600 | -6.76882500 | C | 0.88094000 | 2.55240700 | -4.77978400 |
| H | 7.44687500 | 0.25160000 | -8.86075100 | C | 3.01620500 | -0.86170800 | -3.58048000 |
| H | 5.10716900 | -0.38620700 | -9.22168300 | H | 2.24527100 | -2.07740600 | -3.07744900 |
| C | 5.10716900 | -0.38620700 | -9.22168300 | C | 4.31699100 | -4.40528900 | -7.98357100 |
| C | 4.31699100 | -4.40528900 | -7.98357100 | C | 4.27298500 | -0.58999800 | -3.18984400 |
| C | 4.35890800 | -5.79813200 | -7.98902300 | H | 4.77725300 | 0.31450500 | -3.51447300 |
| C | 3.30186700 | -6.53303800 | -7.44537400 | C | 2.98803900 | -3.41739200 | -3.24023300 |
| C | 2.20367700 | -5.86874400 | -6.90137200 | O | 4.19980800 | -3.48530200 | -3.39701400 |
| C | 2.15224400 | -4.47196000 | -6.89670800 | C | 2.19103000 | -4.68722600 | -3.11744900 |
| H | 5.15136500 | -3.84526800 | -8.39438800 | C | 0.80512800 | -4.76021900 | -3.33317600 |
| H | 5.21971700 | -6.30896200 | -8.41172000 | C | 2.89567800 | -5.85971800 | -2.79515400 |
| H | 3.33980500 | -7.61897400 | -7.44326500 | C | 0.14333300 | -5.98447100 | -3.22150900 |
| H | 1.38408000 | -6.43158100 | -6.46469400 | H | 0.24155700 | -3.88479100 | -3.63841800 |
| H | 1.29141500 | -3.95809200 | -6.47952700 | C | 0.04218000 | 1.11726200 | -11.25349700 |
| C | -0.71475000 | 0.48917600 | -10.79123300 | H | 0.22781200 | 0.46117100 | -5.91863200 |
| C | -1.86448700 | 0.16638500 | -11.50859200 | C | -3.75221300 | -0.87723600 | -11.48001800 |
| C | -1.86448700 | 0.16638500 | -11.50859200 | H | -2.69240800 | -1.08616200 | -9.61457800 |
| C | -2.85656300 | -0.62413400 | -10.91932800 | H | -1.54058300 | -0.76433500 | -8.88893700 |
| C | -2.85656300 | -0.62413400 | -10.91932800 | H | -0.92588900 | -6.03243600 | -3.40579300 |
| C | -2.69240800 | -1.08616200 | -9.61457800 | H | -0.92588900 | -6.03243600 | -3.40579300 |
| C | -1.54058300 | -0.76433500 | -8.88893700 | H | -0.92588900 | -6.03243600 | -3.40579300 |
| H | 0.04218000 | 1.11726200 | -11.25349700 | H | 0.04218000 | 1.11726200 | -11.25349700 |
| H | -1.98824600 | 0.53118100 | -12.52451300 | H | 0.482852400 | -1.26681600 | -2.55349600 |
| H | -3.75221300 | -0.87723600 | -11.48001800 | C | 1.85480100 | -1.92414800 | -1.58266100 |
| H | -3.45709000 | -1.70416500 | -9.15304000 | H | 1.25325400 | -2.77017400 | -1.23899200 |
| H | -1.40680800 | -1.14426100 | -7.87958000 | H | 1.27289200 | -1.00907400 | -1.43754100 |
| C | -0.01141500 | 3.06027100 | -8.80764000 | H | 1.27289200 | -1.00907400 | -1.43754100 |

TS5bImaginary frequency: -740.3 cm⁻¹

| | | | | | | | |
|---|-------------|-------------|--------------|----|-------------|-------------|-------------|
| P | 2.58256100 | -1.94580400 | -7.65389500 | C | 3.22877800 | 4.80316600 | -8.58916600 |
| C | 2.54416800 | -1.78182200 | -9.51878100 | C | 4.58573200 | 4.67357800 | -8.28793500 |
| C | 3.00165300 | -0.36438500 | -9.89558200 | C | 5.15856800 | 3.40178300 | -8.23309500 |
| P | 1.94011900 | 0.90140000 | -9.00513300 | H | 4.38333100 | 2.26770200 | -8.47713500 |
| H | 3.18547100 | -2.53688300 | -9.98557600 | H | 1.40355400 | 3.79212400 | -9.09196800 |
| H | 3.18547100 | -2.53688300 | -9.98557600 | H | 2.77050200 | 5.78722800 | -8.63408900 |
| H | 1.50894900 | -1.95240500 | -9.82567400 | H | 5.19063600 | 5.55505100 | -8.09662800 |
| H | 4.04324900 | -0.21746100 | -9.59505000 | H | 6.21271600 | 3.28747900 | -7.99681500 |
| H | 2.94336000 | -0.19896600 | -10.97528100 | Rh | 4.85108200 | 1.29099300 | -8.40063900 |
| C | 0.77174400 | 1.48463000 | -10.31276800 | C | 1.11086500 | -0.09368800 | -6.99705100 |
| C | 3.02142800 | 2.38608500 | -8.79719100 | C | 1.39465800 | 0.47006800 | -4.90421900 |
| C | 4.41124900 | -1.89377800 | -7.36060300 | H | 0.90697800 | 1.63300900 | -5.62198200 |
| C | 2.16754300 | -3.70780400 | -7.29865900 | H | -0.09104500 | 1.99860500 | -5.38477400 |
| C | 2.16754300 | -3.70780400 | -7.29865900 | H | 1.59917900 | 2.43202200 | -5.86460200 |
| C | 4.97694800 | -0.83395300 | -6.64252900 | C | 0.47649200 | -0.64010800 | -4.95016200 |
| C | 6.36342700 | -0.74831200 | -6.47027200 | H | 0.86396000 | -1.59439300 | -4.60267400 |
| C | 7.19764000 | -1.71698900 | -7.02470000 | Cl | -0.76756900 | -1.45284200 | -8.20952100 |
| C | 6.64461100 | -2.77773700 | -7.74934200 | C | -0.76756900 | -1.45284200 | -8.20952100 |
| C | 5.26401300 | -2.86809400 | -7.91261200 | H | -1.02709400 | -0.55111900 | -4.79582500 |
| H | 4.33236800 | -0.07757400 | -6.20533000 | H | -1.50573400 | -1.35668400 | -5.35828600 |
| H | 6.77686000 | 0.06353700 | -5.88027100 | H | -1.30942800 | -0.65333500 | -3.73677800 |
| H | 8.27366600 | -1.65409800 | -6.88868600 | C | -1.44692100 | 0.38728500 | -5.16534500 |
| H | 7.28990200 | -3.53650700 | -8.18341900 | C | 2.69506900 | 0.48891500 | -4.16456500 |
| H | 4.84670200 | -3.70525600 | -8.46449400 | H | 3.06915100 | -0.77972200 | -3.39683500 |
| C | 2.83136800 | -4.40175000 | -6.27230200 | C | 2.64172100 | -1.63898500 | -3.91843400 |
| C | 2.47014600 | -5.71013600 | -5.94682900 | H | 3.37698500 | 1.63743200 | -3.99649100 |
| C | 1.44035200 | -6.34664200 | -6.63992000 | C | 3.04203700 | 2.56916500 | -4.43661500 |
| C | 0.76598900 | -5.66069800 | -7.65117800 | O | 4.56295400 | -1.08680100 | -3.20860900 |
| C | 1.11604800 | -4.34903200 | -7.97624800 | C | 5.43549100 | -0.23223000 | -3.26591100 |
| H | 3.64472100 | -3.93027000 | -5.73184400 | C | 4.95291100 | -2.50578700 | -2.87432700 |
| H | 3.00288900 | -6.23007900 | -5.15531700 | C | 4.04484500 | -3.57338900 | -2.79361900 |
| H | 1.16146100 | -7.36675300 | -6.39017400 | C | 6.31297900 | -2.75676700 | -2.62271100 |
| H | -0.04814200 | -6.14193300 | -8.18578400 | H | 4.48577400 | -4.85497600 | -2.46143700 |
| H | 0.53590100 | -3.80468200 | -8.71072900 | H | 2.98907100 | -3.42154800 | -2.98897700 |
| C | 1.27217100 | 2.03325600 | -11.50799300 | C | 6.75314900 | -4.03528700 | -2.29593000 |
| C | 0.40374000 | 2.48174100 | -12.50048900 | H | 7.00474200 | -1.92419900 | -2.68801900 |
| C | -0.97856400 | 2.39459300 | -12.30944500 | H | 5.83886400 | -5.08947500 | -2.21257400 |
| C | -1.48243300 | 1.85754900 | -11.12601700 | H | 3.76864300 | -5.66772300 | -2.39317100 |
| C | -0.61444200 | 1.40314700 | -10.12782200 | H | 7.80734600 | -4.21250400 | -2.10298500 |
| H | 2.34484200 | 2.12486000 | -11.65889000 | H | 6.17964400 | -6.08796800 | -1.95411300 |
| H | 0.80336300 | 2.90205900 | -13.41918800 | H | 0.09283400 | 1.12174500 | -6.94373100 |
| H | -1.65654000 | 2.74401200 | -13.08324900 | C | 4.29116600 | 1.66483500 | -3.42182700 |
| H | -2.55514200 | 1.77954100 | -10.97477700 | H | 2.42188200 | -0.71680200 | -1.98295900 |
| H | -1.00925900 | 0.94321400 | -9.22919100 | H | 2.58384200 | -1.63756400 | -1.41583500 |
| C | 2.45395500 | 3.67152600 | -8.84487900 | H | 2.84803500 | 0.11753100 | -1.41919800 |
| | | | | H | 1.34493500 | -0.55250000 | -2.07411900 |

| INT8a | | | | C | -0.90603500 | 3.99484100 | -9.13192900 |
|--------------|-------------|-------------|--------------|----|-------------|-------------|--------------|
| P | 4.04750500 | -1.21318700 | -7.89738500 | C | 0.12194900 | 3.89549400 | -8.19221000 |
| C | 3.47427200 | -1.13195000 | -9.69182500 | C | 0.73612500 | 2.66618400 | -7.95157000 |
| C | 2.43505200 | -0.02172300 | -9.85277300 | H | -1.04105200 | 0.74978300 | -10.13723100 |
| P | 1.24697000 | -0.05547000 | -8.40938600 | H | -2.12607000 | 2.92950400 | -10.55674100 |
| H | 4.32884100 | -0.99330300 | -10.36121900 | H | -1.38874300 | 4.95132900 | -9.31242500 |
| H | 3.02791900 | -2.10604200 | -9.91499100 | H | 0.43676500 | 4.77240000 | -7.63364600 |
| H | 2.90606300 | 0.96515000 | -9.80730400 | H | 1.51013700 | 2.57538600 | -7.19649100 |
| H | 1.91508900 | -0.07535600 | -10.81470700 | Rh | 2.44728500 | -0.37248300 | -6.52118800 |
| C | 0.02637800 | -1.37855300 | -8.82211000 | C | 3.38601500 | -0.57299700 | -3.91692700 |
| C | 0.33255900 | 1.52447900 | -8.65871200 | C | 4.31288300 | -0.41977100 | -4.90741000 |
| C | 5.67798300 | -0.32985400 | -7.93745100 | H | 4.70609500 | 0.56194700 | -5.15453800 |
| C | 4.48273300 | -2.99658600 | -7.72585700 | H | 4.87410900 | -1.27603500 | -5.26251900 |
| C | 6.89579800 | -0.93742500 | -7.59905600 | C | 2.88209200 | 0.63516900 | -3.15056400 |
| C | 8.08517300 | -0.20306800 | -7.60805000 | H | 1.82116700 | 0.52790200 | -2.91350500 |
| C | 8.07733300 | 1.14632700 | -7.95797300 | Cl | 0.46333300 | 0.43905100 | -5.28719400 |
| C | 6.86886500 | 1.76579000 | -8.28762400 | C | 3.69359300 | 0.84722200 | -1.85729500 |
| C | 5.68060700 | 1.03754300 | -8.26611400 | H | 3.29938000 | 1.70323400 | -1.30004700 |
| H | 6.92252300 | -1.98726000 | -7.32815900 | H | 3.65252400 | -0.03012700 | -1.20397100 |
| H | 9.01784800 | -0.69155600 | -7.33987000 | H | 4.74763200 | 1.04430900 | -2.07989100 |
| H | 9.00277700 | 1.71491200 | -7.96652900 | C | 3.05786000 | -1.92686400 | -3.37058200 |
| H | 6.84978500 | 2.81958800 | -8.55114300 | C | 1.59123700 | -2.24690900 | -3.09741000 |
| H | 4.74406400 | 1.54188200 | -8.48616600 | H | 0.99386000 | -1.43368700 | -3.51518500 |
| C | 5.32570900 | -3.65615800 | -8.63892700 | C | 4.04824000 | -2.77933100 | -3.06428400 |
| C | 5.56745200 | -5.02362400 | -8.51338100 | H | 5.08913700 | -2.50969400 | -3.21453600 |
| C | 4.96963800 | -5.75014700 | -7.47836100 | C | 1.10361200 | -3.55541800 | -3.74651700 |
| C | 4.12736100 | -5.10687500 | -6.57202000 | O | 1.86540200 | -4.47131100 | -4.02685000 |
| C | 3.88363900 | -3.73708500 | -6.69843200 | C | -0.37720200 | -3.73777500 | -3.94623000 |
| H | 5.79723400 | -3.10288800 | -9.44659600 | C | -1.29763900 | -2.67686900 | -3.95747600 |
| H | 6.21999200 | -5.52344200 | -9.22401200 | C | -0.84537200 | -5.04958000 | -4.13467500 |
| H | 5.15945100 | -6.81597200 | -7.38555500 | C | -2.65813000 | -2.93107200 | -4.14328100 |
| H | 3.64585200 | -5.65219700 | -5.76662200 | H | -0.96236700 | -1.64980700 | -3.86342200 |
| H | 3.21724000 | -3.24592300 | -5.99886700 | C | -2.20219300 | -5.30077400 | -4.31155700 |
| C | -0.08144300 | -1.95853500 | -10.09608300 | H | -0.12043900 | -5.85653700 | -4.13605000 |
| C | -1.01329100 | -2.97052600 | -10.33975900 | C | -3.11392700 | -4.23997700 | -4.31279100 |
| C | -1.84992500 | -3.41321500 | -9.31550300 | H | -3.36004000 | -2.10239200 | -4.15746300 |
| C | -1.75137300 | -2.84149600 | -8.04483300 | H | -2.55228800 | -6.32027600 | -4.44656600 |
| C | -0.81862900 | -1.83542700 | -7.79603400 | H | -4.17469400 | -4.43368100 | -4.44728900 |
| H | 0.55680800 | -1.63327000 | -10.91118800 | H | 2.95757300 | 1.52247100 | -3.78479400 |
| H | -1.08051100 | -3.41167400 | -11.33043600 | H | 3.84600000 | -3.76459800 | -2.66202400 |
| H | -2.57111400 | -4.20338400 | -9.50497900 | C | 1.28550200 | -2.33717300 | -1.57813800 |
| H | -2.39083000 | -3.18571800 | -7.23750700 | H | 0.22440400 | -2.53203100 | -1.39933500 |
| H | -0.73396300 | -1.39824300 | -6.80588300 | H | 1.86750400 | -3.13800000 | -1.11229200 |
| C | -0.70475600 | 1.62943000 | -9.59673100 | H | 1.54628000 | -1.39699000 | -1.08494700 |
| C | -1.32017900 | 2.85994200 | -9.83139100 | | | | |

| INT8b | | | | C | 4.87596100 | 4.36130900 | -8.18649700 |
|-------|-------------|-------------|--------------|----|-------------|-------------|-------------|
| P | 2.60626700 | -1.98619600 | -7.92797500 | C | 5.32529000 | 3.03969000 | -8.18783900 |
| C | 2.46323900 | -1.80194500 | -9.77848300 | C | 4.44988600 | 1.99773200 | -8.49580200 |
| C | 2.83842700 | -0.36476400 | -10.17758700 | H | 1.63671300 | 3.82239000 | -9.06133200 |
| P | 1.90446600 | 0.87667500 | -9.10755100 | H | 3.17810900 | 5.65542700 | -8.49331500 |
| H | 3.08988300 | -2.53572800 | -10.29613200 | H | 5.55763300 | 5.17150100 | -7.94420300 |
| H | 1.41489200 | -2.00696000 | -10.01442700 | H | 6.35931900 | 2.81376000 | -7.94288100 |
| H | 3.91300500 | -0.20261200 | -10.05412100 | H | 4.82110900 | 0.97931100 | -8.46007600 |
| H | 2.59786000 | -0.18421000 | -11.22878600 | Rh | 1.18350000 | -0.42759700 | -7.15721200 |
| C | 0.72574000 | 1.65666100 | -10.30046400 | C | 1.43155400 | 0.06410800 | -5.09713100 |
| C | 3.10950000 | 2.25706900 | -8.82669800 | C | 0.40487900 | 1.15535100 | -5.35237300 |
| C | 4.43056500 | -1.91046500 | -7.65300800 | H | -0.45926900 | 1.08031600 | -4.68063100 |
| C | 2.18017100 | -3.73447100 | -7.53923500 | H | 0.83223200 | 2.15492900 | -5.29299400 |
| C | 4.96052000 | -1.09519200 | -6.64692400 | C | 0.92068900 | -1.28268200 | -5.20045700 |
| C | 6.34090500 | -1.03815700 | -6.42935600 | H | 1.64354100 | -2.06390300 | -4.96349800 |
| C | 7.20465600 | -1.78364000 | -7.23054600 | Cl | -0.90761900 | -1.35306600 | -8.44734500 |
| C | 6.68707400 | -2.59633600 | -8.24424200 | C | -0.50361600 | -1.71696400 | -4.91614200 |
| C | 5.31040200 | -2.66573900 | -8.45106100 | H | -0.71861000 | -2.65570800 | -5.43298500 |
| H | 4.29739300 | -0.48980900 | -6.04106600 | H | -0.65602800 | -1.88495500 | -3.83761300 |
| H | 6.72097500 | -0.41581200 | -5.62571500 | H | -1.24960000 | -0.99748100 | -5.25847700 |
| H | 8.27785800 | -1.73730700 | -7.06771100 | C | 2.66652000 | 0.45029600 | -4.33878500 |
| H | 7.35546100 | -3.18155500 | -8.86960600 | C | 3.00931700 | -0.39447000 | -3.10553800 |
| H | 4.92397500 | -3.32195200 | -9.22513000 | H | 2.33743800 | -1.25163100 | -3.10090300 |
| C | 3.07134600 | -4.57528400 | -6.85251700 | C | 3.37272100 | 1.55221900 | -4.64283200 |
| C | 2.71198800 | -5.89115700 | -6.55475800 | H | 3.13025800 | 2.15305400 | -5.51433100 |
| C | 1.46397900 | -6.38180100 | -6.93953500 | C | 4.45910600 | -0.90149400 | -3.04568000 |
| C | 0.56873300 | -5.54634200 | -7.61131300 | O | 5.39256000 | -0.17810000 | -3.36807900 |
| C | 0.91430500 | -4.22687700 | -7.90321100 | C | 4.74085800 | -2.27937100 | -2.51035900 |
| H | 4.04662700 | -4.21107500 | -6.54968900 | C | 3.74765100 | -3.18203800 | -2.09629200 |
| H | 3.41135500 | -6.52984600 | -6.02258200 | C | 6.08893900 | -2.66844300 | -2.41457600 |
| H | 1.18709900 | -7.40720100 | -6.71039700 | C | 4.09544300 | -4.43980200 | -1.60185100 |
| H | -0.41037800 | -5.91628600 | -7.90187000 | H | 2.69794600 | -2.91666500 | -2.15034500 |
| H | 0.19278700 | -3.56485600 | -8.37478000 | C | 6.43494900 | -3.92309900 | -1.92534000 |
| C | 1.19478300 | 2.26524600 | -11.47915500 | H | 6.84666800 | -1.96064700 | -2.73196200 |
| C | 0.30597400 | 2.85907600 | -12.37291300 | C | 5.43695400 | -4.81355200 | -1.51681700 |
| C | -1.06524300 | 2.85724800 | -12.09924400 | H | 3.31664500 | -5.12712200 | -1.28511500 |
| C | -1.53875200 | 2.25556700 | -10.93455700 | H | 7.48052500 | -4.20982500 | -1.85904600 |
| C | -0.65016700 | 1.65468700 | -10.03739700 | H | 5.70491200 | -5.79401700 | -1.13332800 |
| H | 2.26008200 | 2.29081100 | -11.69290500 | H | -0.07336700 | 1.05931000 | -6.36970500 |
| H | 0.68188300 | 3.32558000 | -13.27933600 | H | 4.23368100 | 1.85281900 | -4.05968100 |
| H | -1.75880500 | 3.32033600 | -12.79576200 | C | 2.74791600 | 0.39738000 | -1.79686600 |
| H | -2.60384400 | 2.23899900 | -10.72231000 | H | 2.92231000 | -0.22741400 | -0.91412000 |
| H | -1.02749200 | 1.13934500 | -9.16098400 | H | 3.40747300 | 1.26712100 | -1.73969500 |
| C | 2.66710100 | 3.59140300 | -8.81156700 | H | 1.71193700 | 0.74701000 | -1.77032900 |
| C | 3.54174000 | 4.63155500 | -8.49381100 | | | | |

| 3 | | | | | H | | | |
|----------|---|-------------|-------------|-------------|----------|-------------|-------------|-------------|
| | C | 3.26377900 | -1.02207400 | -3.87776300 | | H | -1.44630900 | -0.24597900 |
| | C | 4.03442300 | -0.88990500 | -4.96722000 | C | 2.34901400 | 0.19657800 | -4.14043900 |
| | H | 4.54033100 | 0.04537300 | -5.19305600 | C | 2.97502200 | -1.13788900 | -3.79090600 |
| | H | 4.17889000 | -1.70992900 | -5.66387100 | H | 2.78499100 | -1.86849000 | -4.58381600 |
| | C | 3.05744700 | 0.13411700 | -2.91513600 | H | 4.06658200 | -1.04760700 | -3.74571000 |
| | H | 1.98595800 | 0.26819900 | -2.71206400 | C | 2.97379700 | 1.35373700 | -3.83703300 |
| | C | 3.79221500 | -0.06465400 | -1.57708600 | H | 2.48605800 | 2.28553700 | -4.10966500 |
| | H | 3.61257700 | 0.78385500 | -0.90819500 | C | 4.27089500 | 1.54910800 | -3.10764700 |
| | H | 3.45103000 | -0.97444900 | -1.07688000 | H | 4.80215300 | 0.62033700 | -2.88874500 |
| | H | 4.87206800 | -0.14578200 | -1.73974400 | H | 4.94657700 | 2.19893500 | -3.67866900 |
| | C | 2.60399600 | -2.32258600 | -3.55986800 | H | 4.09320400 | 2.05236400 | -2.14813900 |
| | C | 1.10518800 | -2.29412400 | -3.32195500 | C | 2.52847600 | -1.72184900 | -2.44499800 |
| | H | 0.66727400 | -1.39378700 | -3.76842500 | O | 1.88342700 | -1.06046400 | -1.64842300 |
| | H | 0.62566200 | -3.13298000 | -3.84365600 | C | 2.93578300 | -3.13015700 | -2.10896100 |
| | C | 3.32280000 | -3.45706500 | -3.50395000 | C | 3.72378000 | -3.92707500 | -2.95388000 |
| | H | 4.39611800 | -3.37158200 | -3.66484800 | C | 2.50784400 | -3.65782500 | -0.87980600 |
| | C | 2.82510800 | -4.84028400 | -3.20275300 | C | 4.07494700 | -5.22371800 | -2.57665300 |
| | H | 1.73489100 | -4.91052200 | -3.17074200 | H | 4.07188200 | -3.54226500 | -3.90674900 |
| | H | 3.18925700 | -5.55707100 | -3.94930700 | C | 2.85533900 | -4.95194400 | -0.50528900 |
| | H | 3.20082100 | -5.17958600 | -2.22915500 | H | 1.90278800 | -3.02656300 | -0.23766700 |
| | C | 0.66156400 | -2.37170200 | -1.85538300 | C | 3.64061500 | -5.73840800 | -1.35396100 |
| | O | 1.46475400 | -2.53868000 | -0.95092300 | H | 4.68657800 | -5.83137100 | -3.23723200 |
| | C | -0.80582100 | -2.25680800 | -1.55273100 | H | 2.51715800 | -5.35043800 | 0.44697100 |
| | C | -1.78597000 | -2.10321000 | -2.54575700 | H | 3.91322500 | -6.74884200 | -1.06245200 |
| | C | -1.20258200 | -2.31339400 | -0.20657600 | H | -0.40568200 | 1.41394500 | -5.91197300 |
| | C | -3.13370100 | -2.00810500 | -2.19843300 | | | | |
| | H | -1.50667700 | -2.05934000 | -3.59316200 | 5 | | | |
| | C | -2.54670200 | -2.21643600 | 0.13938400 | C | 2.53664800 | -0.59416800 | -3.75004100 |
| | H | -0.43266100 | -2.43456000 | 0.54792300 | C | 2.52514200 | -0.40109000 | -5.07772700 |
| | C | -3.51580700 | -2.06361500 | -0.85690000 | H | 2.52620400 | 0.59926800 | -5.50340200 |
| | H | -3.88433900 | -1.89050500 | -2.97444900 | H | 2.51069200 | -1.23481000 | -5.77258700 |
| | H | -2.84248500 | -2.26010600 | 1.18360200 | C | 2.55535300 | 0.57677600 | -2.78339200 |
| | H | -4.56562700 | -1.98820200 | -0.58790700 | H | 1.80003200 | 0.43103100 | -2.00027200 |
| | H | 3.39665300 | 1.06079200 | -3.39154600 | C | 3.93015300 | 0.77893900 | -2.12166600 |
| | | | | | H | 3.90041900 | 1.60790200 | -1.40709200 |
| 4 | | | | | H | 4.25232600 | -0.11944300 | -1.58633600 |
| | C | 1.02757400 | 0.19374000 | -4.82522500 | H | 4.69138800 | 1.00559400 | -2.87491000 |
| | C | 0.51482300 | 1.52192100 | -5.33869600 | C | 2.55818900 | -1.97544400 | -3.18439500 |
| | H | 0.30600100 | 2.21225300 | -4.51273800 | C | 1.47992100 | -2.34235500 | -2.14789400 |
| | H | 1.25398600 | 2.00799700 | -5.98509800 | H | 0.69351700 | -1.58094300 | -2.18943100 |
| | C | 0.31429200 | -0.94569200 | -4.95782900 | C | 3.48462200 | -2.86865300 | -3.56033800 |
| | H | 0.72613400 | -1.86185600 | -4.54197000 | H | 4.27389700 | -2.59770700 | -4.25392200 |
| | C | -1.03403200 | -1.14582300 | -5.58841500 | C | 0.84571100 | -3.69120200 | -2.52956000 |
| | H | -0.98786800 | -1.92468900 | -6.36092900 | O | 1.19315700 | -4.71530400 | -1.95798400 |

| | | | | | | | |
|----------|-------------|-------------|-------------|-----------------------|-------------|-------------|-------------|
| C | -0.20006200 | -3.74270900 | -3.60468800 | H | 6.47308300 | -4.91522800 | -3.25911700 |
| C | -0.55837900 | -2.63469800 | -4.38813400 | H | 5.26597800 | -5.83300000 | -1.28788700 |
| C | -0.84628000 | -4.97081800 | -3.82302600 | H | 1.39306300 | 1.34318200 | -6.37123500 |
| C | -1.54422000 | -2.75582100 | -5.36797900 | H | 3.07135900 | 2.60627000 | -3.16323300 |
| H | -0.05737000 | -1.68149500 | -4.25907300 | C | 3.60769200 | 0.77859900 | -1.53698400 |
| C | -1.83474400 | -5.08792400 | -4.79501800 | H | 4.02497700 | 0.12999400 | -0.76070900 |
| H | -0.55219000 | -5.81781800 | -3.21240100 | H | 4.42416400 | 1.38763000 | -1.93396800 |
| C | -2.18664100 | -3.97860500 | -5.57013800 | H | 2.87171100 | 1.43938000 | -1.07059200 |
| H | -1.80992500 | -1.89442500 | -5.97387800 | | | | |
| H | -2.33152500 | -6.04114100 | -4.95160400 | Rh(dppe) ⁺ | | | |
| H | -2.95784500 | -4.06813900 | -6.33015400 | P | 2.18889600 | -0.14828400 | -0.70977800 |
| H | 2.27134000 | 1.48855900 | -3.32006300 | C | 1.28267900 | 0.12491300 | -2.32054800 |
| H | 3.48413400 | -3.88534800 | -3.17794800 | C | 0.02373100 | 0.96989400 | -2.08082700 |
| C | 2.03566800 | -2.40033300 | -0.71530300 | P | -0.81752200 | 0.34204800 | -0.53905300 |
| H | 1.23702600 | -2.61401600 | 0.00184200 | H | 1.94645800 | 0.56706800 | -3.06948600 |
| H | 2.78177100 | -3.19226100 | -0.63078000 | H | 1.01121100 | -0.87363600 | -2.67733400 |
| H | 2.49928200 | -1.44882200 | -0.44106700 | H | 0.27449300 | 2.01905600 | -1.89918600 |
| | | | | H | -0.65294000 | 0.93383300 | -2.93959500 |
| 6 | | | | C | -1.83209100 | -1.08583700 | -1.07024500 |
| C | 1.34155100 | 0.00587900 | -4.67409500 | C | -1.95717900 | 1.64384400 | 0.04471600 |
| C | 0.65662800 | 0.83873500 | -5.73561600 | C | 3.44011100 | 1.17143900 | -0.52332600 |
| H | 0.01738300 | 0.23977300 | -6.38358700 | C | 3.12384400 | -1.70847100 | -0.89183500 |
| H | 0.03261900 | 1.61906000 | -5.28489800 | C | 4.41144600 | 1.03298600 | 0.48628500 |
| C | 1.15822800 | -1.32887600 | -4.58161500 | C | 5.34083400 | 2.04648000 | 0.71238400 |
| H | 1.68514600 | -1.87107300 | -3.80094900 | C | 5.31233600 | 3.20901500 | -0.06194000 |
| C | 0.30907600 | -2.22483300 | -5.43674400 | C | 4.35172100 | 3.35531800 | -1.06440300 |
| H | 0.92755300 | -2.99842600 | -5.91041800 | C | 3.41631300 | 2.34573200 | -1.29296100 |
| H | -0.43001500 | -2.75594200 | -4.82246400 | H | 4.45559600 | 0.12549000 | 1.08230900 |
| H | -0.23115900 | -1.70201000 | -6.22759300 | H | 6.08999200 | 1.92618600 | 1.48870100 |
| C | 2.24100200 | 0.73403400 | -3.73556200 | H | 6.03862600 | 3.99647400 | 0.11326300 |
| C | 2.95508600 | -0.06879800 | -2.64974500 | H | 4.33129700 | 4.25421200 | -1.67277600 |
| H | 2.20770300 | -0.70781900 | -2.16950800 | H | 2.67946200 | 2.48111100 | -2.07810500 |
| C | 2.41850800 | 2.06225900 | -3.83404900 | C | 4.37117400 | -1.73591200 | -1.53965100 |
| H | 1.92868600 | 2.65693100 | -4.59486500 | C | 5.03676200 | -2.94823500 | -1.71582400 |
| C | 4.06901300 | -0.95011800 | -3.25336700 | C | 4.47105600 | -4.13553000 | -1.24389700 |
| O | 4.75800900 | -0.52449700 | -4.16616400 | C | 3.23447300 | -4.11384700 | -0.59587600 |
| C | 4.35435200 | -2.30671000 | -2.66541000 | C | 2.56095300 | -2.90516800 | -0.41921400 |
| C | 3.67943300 | -2.83467800 | -1.55325200 | H | 4.82404000 | -0.81717300 | -1.89866800 |
| C | 5.36674300 | -3.07152800 | -3.26960100 | H | 5.99902400 | -2.96524300 | -2.21806900 |
| C | 4.00955500 | -4.09724900 | -1.05855200 | H | 4.99629900 | -5.07611300 | -1.37850400 |
| H | 2.89910000 | -2.26500400 | -1.06016000 | H | 2.79708700 | -5.03532300 | -0.22437800 |
| C | 5.69131600 | -4.33250900 | -2.78038000 | H | 1.59904800 | -2.88178600 | 0.08506300 |
| H | 5.88248500 | -2.64707100 | -4.12428100 | C | -2.65876800 | -1.00966600 | -2.20554700 |
| C | 5.01272800 | -4.84882400 | -1.67189200 | C | -3.42835900 | -2.10824900 | -2.58653500 |
| H | 3.48237600 | -4.49300400 | -0.19538400 | C | -3.38466600 | -3.28861600 | -1.83968600 |

| | | | | | | | |
|-------------------------|--------------|-------------|-------------|----|-------------|-------------|-------------|
| C | -2.57080900 | -3.37056100 | -0.70887100 | C | -0.97114800 | -4.11913500 | -2.69701500 |
| C | -1.79565700 | -2.27504500 | -0.32607500 | C | -0.56485300 | -3.12382700 | -1.80464500 |
| H | -2.71713600 | -0.09529800 | -2.78919400 | H | 2.12319600 | -1.93665700 | -3.53972500 |
| H | -4.06274000 | -2.04212000 | -3.46499000 | H | 1.38469400 | -3.68305000 | -5.11321600 |
| H | -3.98505500 | -4.14179800 | -2.14000900 | H | -0.59273800 | -5.09171700 | -4.58177700 |
| H | -2.536660900 | -4.28590900 | -0.12627500 | H | -1.83243000 | -4.73619000 | -2.45952800 |
| H | -1.15430100 | -2.33799600 | 0.54895900 | H | -1.10563600 | -2.97714000 | -0.87615000 |
| C | -1.41320500 | 2.88927500 | 0.41521800 | C | -2.12479400 | 2.68374100 | -2.30456800 |
| C | -2.24189600 | 3.90235800 | 0.89103100 | C | -3.20809300 | 2.64178800 | -3.18051500 |
| C | -3.61608100 | 3.67977900 | 1.01869100 | C | -4.11792600 | 1.58196900 | -3.12086100 |
| C | -4.15952100 | 2.44223200 | 0.67013300 | C | -3.94385300 | 0.56432600 | -2.18267300 |
| C | -3.33710100 | 1.42394300 | 0.18643000 | C | -2.85842300 | 0.60217400 | -1.30505500 |
| H | -0.34268000 | 3.06106300 | 0.34028400 | H | -1.43555800 | 3.52221200 | -2.35038300 |
| H | -1.81644300 | 4.86172600 | 1.16846800 | H | -3.34456400 | 3.43691500 | -3.90702300 |
| H | -4.26015000 | 4.46860300 | 1.39481400 | H | -4.96134200 | 1.55321800 | -3.80391600 |
| H | -5.22568300 | 2.26653400 | 0.77394200 | H | -4.65100900 | -0.25798200 | -2.13276300 |
| H | -3.77007100 | 0.46656500 | -0.08184400 | H | -2.71647700 | -0.18872600 | -0.57367200 |
| Rh | 0.75074300 | -0.04567400 | 0.97628500 | C | 0.56459400 | 3.80215000 | 1.28110900 |
| | | | | C | 0.49982500 | 4.99077000 | 2.00624600 |
| INT1⁺ | | | | C | -0.72033700 | 5.65319800 | 2.16078400 |
| P | 1.05896900 | -0.98576000 | -0.95265200 | C | -1.87528900 | 5.12310300 | 1.58545800 |
| C | 1.19972600 | 0.50688800 | -2.08738000 | C | -1.81408400 | 3.93797600 | 0.84997700 |
| C | 0.97016100 | 1.83138400 | -1.35105700 | H | 1.52083000 | 3.29700600 | 1.18504400 |
| P | -0.50210200 | 1.67454500 | -0.21768100 | H | 1.40217000 | 5.39948000 | 2.45078200 |
| H | 2.17052100 | 0.49943800 | -2.59152500 | H | -0.76900900 | 6.57805700 | 2.72717400 |
| H | 0.42897100 | 0.36873300 | -2.85182000 | H | -2.82664400 | 5.63301600 | 1.70198100 |
| H | 1.83347000 | 2.09833500 | -0.73524700 | H | -2.71779100 | 3.54572200 | 0.39528700 |
| H | 0.81362100 | 2.65138700 | -2.05901900 | Rh | -0.26769700 | -0.35921500 | 0.96375700 |
| C | -1.93865000 | 1.65957700 | -1.35889800 | C | -0.83689100 | -2.38544300 | 1.78252700 |
| C | -0.59061100 | 3.26889400 | 0.68348100 | C | 0.47706300 | -2.24030500 | 2.07020100 |
| C | 2.78986900 | -1.39825700 | -0.48174100 | H | 0.79132200 | -1.87816000 | 3.04577000 |
| C | 0.54786400 | -2.32366100 | -2.09907300 | H | 1.24849900 | -2.69606000 | 1.45640000 |
| C | 3.25839300 | -2.72071800 | -0.53379600 | C | -2.05753400 | -2.87491500 | 1.71826300 |
| C | 4.55526100 | -3.02752600 | -0.11493900 | H | -2.84403000 | -2.29005500 | 1.24274700 |
| C | 5.39854400 | -2.02195100 | 0.35717000 | C | -0.31919400 | 0.59571700 | 2.92889200 |
| C | 4.94006500 | -0.70336600 | 0.41442400 | C | -1.62843700 | 0.45171200 | 2.57540000 |
| C | 3.64370200 | -0.39414000 | 0.00593000 | H | -2.18960000 | 1.29512100 | 2.17983800 |
| H | 2.62035600 | -3.51142900 | -0.91463100 | H | -2.21570200 | -0.37725300 | 2.96121200 |
| H | 4.90520400 | -4.05406400 | -0.16573200 | C | 0.74134900 | 0.90471200 | 3.64608200 |
| H | 6.40754900 | -2.26175100 | 0.67774300 | H | 1.73224400 | 0.67378800 | 3.25776700 |
| H | 5.59250100 | 0.08493300 | 0.77776000 | C | 0.67259200 | 1.57829500 | 4.99673300 |
| H | 3.30351900 | 0.63480400 | 0.07103800 | H | 1.17758900 | 0.97034300 | 5.75591900 |
| C | 1.24991800 | -2.53626700 | -3.30002800 | H | 1.18213200 | 2.54841700 | 4.96663400 |
| C | 0.83775400 | -3.52730400 | -4.18837700 | H | -0.36014000 | 1.74099300 | 5.31179800 |
| C | -0.27436100 | -4.31949700 | -3.88814600 | C | -2.45157100 | -4.22420200 | 2.27392600 |

| | | | | | | | |
|---|-------------|-------------|--------------|-------------------------|-------------|-------------|--------------|
| H | -3.23779400 | -4.11097700 | 3.02899700 | H | -2.98189900 | 0.28956100 | -11.00513200 |
| H | -2.85591100 | -4.86441400 | 1.48146300 | H | -2.65249800 | -1.55637700 | -9.37565400 |
| H | -1.60151100 | -4.73383500 | 2.73199500 | H | -0.65223200 | -1.56818700 | -7.90230500 |
| | | | | C | 2.83040100 | 2.08879900 | -5.92207700 |
| TS1⁺ | | | | C | 2.90993500 | 3.26233300 | -5.17467700 |
| Imaginary frequency: -379.03 cm ⁻¹ | | | | | | | |
| P | 3.29184600 | -2.37617300 | -8.24867600 | C | 0.66977700 | 3.85307400 | -5.86005300 |
| C | 3.31107900 | -0.96487300 | -9.48496000 | C | 0.58752300 | 2.68175200 | -6.61695800 |
| C | 3.04944400 | 0.38063700 | -8.80588400 | H | 3.66948000 | 1.39821900 | -5.91772500 |
| P | 1.62563500 | 0.21844400 | -7.60778000 | H | 3.81267200 | 3.48320300 | -4.61321200 |
| H | 4.25818600 | -0.96457800 | -10.03260400 | H | 1.89202800 | 5.06154000 | -4.56025900 |
| H | 2.51414400 | -1.18631300 | -10.20157200 | H | -0.17531100 | 4.53419900 | -5.83421900 |
| H | 3.91567400 | 0.71602400 | -8.22848200 | H | -0.31944900 | 2.46687900 | -7.17134600 |
| H | 2.82987600 | 1.16106700 | -9.54101000 | Rh | 1.91750900 | -1.79255700 | -6.39805900 |
| C | 0.13997500 | 0.27534500 | -8.68271400 | C | 1.43649200 | -3.46490800 | -5.08486800 |
| C | 1.67300600 | 1.79402700 | -6.66505500 | C | 2.74056200 | -3.66675600 | -5.53609200 |
| C | 5.06015900 | -2.68952200 | -7.85023100 | H | 3.60319800 | -3.40129700 | -4.93123400 |
| C | 2.75109700 | -3.81455100 | -9.24846000 | H | 2.91419700 | -4.42914400 | -6.28916800 |
| C | 5.55337200 | -3.99814100 | -7.72335700 | C | 0.27489100 | -4.10656900 | -4.89925400 |
| C | 6.88332500 | -4.22038400 | -7.36155800 | H | -0.65235900 | -3.53838000 | -4.87395800 |
| C | 7.73649600 | -3.14327700 | -7.12018800 | C | 1.37585600 | -1.59187100 | -4.31042900 |
| C | 7.25431700 | -1.83813800 | -7.23991300 | C | 0.38702700 | -0.92084000 | -5.03090300 |
| C | 5.92553500 | -1.61242100 | -7.59691200 | H | 0.39793300 | 0.16433500 | -5.04401100 |
| H | 4.90899100 | -4.84737700 | -7.92522100 | H | -0.57643900 | -1.38328400 | -5.22872000 |
| H | 7.25168000 | -5.23812700 | -7.27526200 | C | 2.18761500 | -1.46909400 | -3.25175000 |
| H | 8.77117800 | -3.31854200 | -6.84248600 | H | 3.10512800 | -2.05212100 | -3.21439800 |
| H | 7.91270600 | -0.99440600 | -7.05678200 | C | 1.86328900 | -0.64553300 | -2.03745600 |
| H | 5.57097300 | -0.58968500 | -7.67661300 | H | 1.75129500 | -1.28511000 | -1.15265600 |
| C | 3.49635000 | -4.24461300 | -10.36074900 | H | 2.68213800 | 0.05068900 | -1.81948300 |
| C | 3.03472500 | -5.29766400 | -11.14860000 | H | 0.94194200 | -0.07378400 | -2.16720300 |
| C | 1.82916400 | -5.93233500 | -10.83565700 | C | 0.16842400 | -5.57455200 | -4.59378600 |
| C | 1.08417100 | -5.51124000 | -9.73390600 | H | -0.22139700 | -5.73245700 | -3.57998900 |
| C | 1.54102100 | -4.45463600 | -8.94297500 | H | -0.53787700 | -6.05908100 | -5.27879900 |
| H | 4.43992000 | -3.76660100 | -10.60725000 | H | 1.13441200 | -6.07837100 | -4.67091800 |
| H | 3.61577100 | -5.62435900 | -12.00557000 | | | | |
| H | 1.47350300 | -6.75328400 | -11.45079800 | INT2⁺ | | | |
| H | 0.14748700 | -6.00300600 | -9.48932000 | P | 2.65160600 | -2.83505000 | -8.10371500 |
| H | 0.96085200 | -4.11940800 | -8.08789400 | C | 3.10917500 | -1.71529900 | -9.53390900 |
| C | -0.05275800 | 1.31434800 | -9.61151900 | C | 3.31847400 | -0.26970000 | -9.06106700 |
| C | -1.17253700 | 1.31714400 | -10.44165300 | P | 1.82645300 | 0.29798400 | -8.09156500 |
| C | -2.11095700 | 0.28461900 | -10.35689800 | H | 3.98538500 | -2.08449600 | -10.07309600 |
| C | -1.92670400 | -0.75154500 | -9.44128200 | H | 2.26923300 | -1.76689900 | -10.23445200 |
| C | -0.80602900 | -0.75755300 | -8.60833500 | H | 4.18776600 | -0.20791600 | -8.39865400 |
| H | 0.66174300 | 2.12956300 | -9.68190300 | H | 3.50350400 | 0.39926400 | -9.90708000 |
| H | -1.31316000 | 2.12454900 | -11.15371400 | C | 0.55931400 | 0.63784200 | -9.37418500 |

| | | | | | | | |
|----|-------------|-------------|--------------|-------------------------|-------------|-------------|-------------|
| C | 2.28261600 | 1.92665900 | -7.38712800 | C | 2.56371800 | -0.96612200 | -5.16533600 |
| C | 4.22759100 | -3.46030900 | -7.40002100 | H | 2.57757000 | 0.12513100 | -5.15142900 |
| C | 1.85024500 | -4.27460600 | -8.91742300 | H | 3.55907800 | -1.37855300 | -5.33528900 |
| C | 4.22675700 | -3.92171100 | -6.07216200 | C | 2.13683200 | -2.08391100 | -2.89298000 |
| C | 5.38724100 | -4.44614400 | -5.50227600 | H | 1.38056000 | -2.57691800 | -2.28217900 |
| C | 6.56673100 | -4.50670300 | -6.24646200 | C | 3.50591700 | -1.96245800 | -2.29256300 |
| C | 6.58003100 | -4.04937200 | -7.56533400 | H | 3.48304700 | -1.31978000 | -1.40384500 |
| C | 5.41855300 | -3.53322000 | -8.14157500 | H | 3.87427800 | -2.93938700 | -1.95790200 |
| H | 3.31604200 | -3.86926200 | -5.48323000 | H | 4.23221300 | -1.53944800 | -2.99166500 |
| H | 5.37028000 | -4.80319200 | -4.47715000 | C | 0.39679500 | -1.81315700 | -4.71731700 |
| H | 7.47148200 | -4.90942800 | -5.80173700 | C | -0.20982300 | -0.63315900 | -5.25957500 |
| H | 7.49321700 | -4.09839000 | -8.15044800 | H | -1.21417400 | -0.67799000 | -5.67188800 |
| H | 5.45242000 | -3.20218200 | -9.17402600 | H | 0.06270900 | 0.32914400 | -4.83883400 |
| C | 2.40770500 | -5.56072700 | -8.90205300 | C | 0.15426200 | -3.08478200 | -5.27092400 |
| C | 1.73884500 | -6.62309600 | -9.51403500 | H | 0.81757200 | -3.87996200 | -4.94078100 |
| C | 0.51225100 | -6.41413900 | -10.14505800 | C | -1.11974500 | -3.54202200 | -5.93029300 |
| C | -0.05159400 | -5.13573500 | -10.16318000 | H | -1.74748400 | -2.71648900 | -6.27560300 |
| C | 0.60896200 | -4.07304300 | -9.54832200 | H | -0.90469000 | -4.19465800 | -6.78262100 |
| H | 3.36229300 | -5.73611900 | -8.41778300 | H | -1.71788200 | -4.13020500 | -5.22151000 |
| H | 2.18136300 | -7.61442200 | -9.49876700 | | | | |
| H | -0.00351000 | -7.24232700 | -10.62112500 | INT3⁺ | | | |
| H | -1.00517700 | -4.96697700 | -10.65447600 | P | -2.50120000 | 1.86109900 | -0.59292000 |
| H | 0.15777200 | -3.08322400 | -9.57161500 | C | -2.98272000 | 0.29602300 | -1.49118300 |
| C | 0.83407800 | 1.46491800 | -10.47697000 | C | -1.86958900 | -0.13737500 | -2.45712700 |
| C | -0.13829500 | 1.68251000 | -11.45179600 | P | -0.21321000 | -0.20818000 | -1.59237300 |
| C | -1.39436600 | 1.07927400 | -11.33844200 | H | -3.15254700 | -0.47483900 | -0.73352100 |
| C | -1.68001800 | 0.26123400 | -10.24503900 | H | -3.92997400 | 0.44883100 | -2.01809500 |
| C | -0.70753400 | 0.04314700 | -9.26660600 | H | -2.11236900 | -1.08776700 | -2.94244000 |
| H | 1.80034900 | 1.95239700 | -10.57010700 | H | -1.75336400 | 0.60350500 | -3.25526100 |
| H | 0.08193300 | 2.32555300 | -12.29832700 | C | 1.00200500 | -0.19444900 | -2.96974600 |
| H | -2.14927400 | 1.25246100 | -12.09918500 | C | -0.08057500 | -1.89997200 | -0.88481700 |
| H | -2.65782900 | -0.20082700 | -10.14929300 | C | -3.85564300 | 2.16641600 | 0.60058000 |
| H | -0.94023800 | -0.57774500 | -8.40460800 | C | -2.65557000 | 3.17506800 | -1.86508900 |
| C | 1.33092300 | 2.95850200 | -7.32782700 | C | -4.25780100 | 3.48431400 | 0.87388500 |
| C | 1.64916300 | 4.17702200 | -6.72858500 | C | -5.25559500 | 3.73625300 | 1.81482500 |
| C | 2.91603900 | 4.38106000 | -6.17802400 | C | -5.86091600 | 2.67967800 | 2.49779500 |
| C | 3.86588800 | 3.35955100 | -6.22588100 | C | -5.46543000 | 1.36721400 | 2.23631600 |
| C | 3.55211800 | 2.13718200 | -6.82164600 | C | -4.46772300 | 1.10975800 | 1.29565200 |
| H | 0.34541900 | 2.81675200 | -7.75945900 | H | -3.80267600 | 4.31444000 | 0.34380500 |
| H | 0.90685200 | 4.96866200 | -6.69640300 | H | -5.56278800 | 4.75919600 | 2.00982600 |
| H | 3.16222600 | 5.33172000 | -5.71533500 | H | -6.64001900 | 2.87792500 | 3.22739200 |
| H | 4.85391300 | 3.51249600 | -5.80259500 | H | -5.93497400 | 0.54056000 | 2.76051700 |
| H | 4.30772900 | 1.35793800 | -6.84599700 | H | -4.18197800 | 0.07961600 | 1.10803200 |
| Rh | 1.22246700 | -1.49898400 | -6.70299600 | C | -3.83814700 | 3.33437400 | -2.60766100 |
| C | 1.75486500 | -1.61440900 | -4.08693500 | C | -3.92322400 | 4.31789400 | -3.59164200 |

| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | -2.83152700 | 5.15323800 | -3.84533500 | H | 1.96493300 | -0.52151600 | 4.44641800 |
| C | -1.65518500 | 5.00772600 | -3.10955000 | H | 0.37272300 | -0.95939000 | 5.03797300 |
| C | -1.56810600 | 4.02416800 | -2.12215700 | H | 0.75128700 | -1.17399200 | 3.32792300 |
| H | -4.69949000 | 2.70279500 | -2.41000800 | C | 2.64971600 | 1.71520300 | 1.21035500 |
| H | -4.84177000 | 4.43499700 | -4.15840500 | O | 1.87636000 | 1.70079200 | 0.24100200 |
| H | -2.90155000 | 5.91902100 | -4.61174900 | H | -1.56519600 | 2.84129900 | 4.70241100 |
| H | -0.80877400 | 5.66103000 | -3.29767900 | C | 4.09537300 | 1.83003500 | 1.08631900 |
| H | -0.65578100 | 3.93123700 | -1.53731400 | C | 4.86784400 | 1.88487100 | 2.26088600 |
| C | 1.68546800 | 0.99928300 | -3.25002300 | C | 4.72323100 | 1.88528200 | -0.17387100 |
| C | 2.58014300 | 1.06706900 | -4.31978200 | C | 6.25244500 | 2.00040500 | 2.17917100 |
| C | 2.80745400 | -0.05980000 | -5.11145300 | H | 4.37675400 | 1.84149100 | 3.22958300 |
| C | 2.13910800 | -1.25486400 | -4.83317400 | C | 6.10520400 | 1.99675800 | -0.24871300 |
| C | 1.24089300 | -1.32441900 | -3.76869600 | H | 4.11501700 | 1.83108800 | -1.07084000 |
| H | 1.52446000 | 1.87282400 | -2.62475100 | C | 6.86814900 | 2.05606600 | 0.92567600 |
| H | 3.10061000 | 1.99645400 | -4.53160200 | H | 6.85078100 | 2.04654900 | 3.08321700 |
| H | 3.50567700 | -0.00930100 | -5.94148400 | H | 6.59693700 | 2.03739400 | -1.21546800 |
| H | 2.31758700 | -2.13358200 | -5.44558700 | H | 7.94851400 | 2.14458200 | 0.86057000 |
| H | 0.73339400 | -2.26026000 | -3.55455800 | H | 2.23437600 | 1.63478800 | 2.22825100 |
| C | -1.13318300 | -2.82667900 | -0.88326500 | | | | |
| C | -0.97686700 | -4.07739300 | -0.27939000 | | | | |
| C | 0.23115400 | -4.41830800 | 0.32754800 | | | | |
| C | 1.28738200 | -3.50269700 | 0.33181100 | | | | |
| C | 1.13169500 | -2.25206700 | -0.26289600 | | | | |
| H | -2.08085300 | -2.59155700 | -1.35682600 | | | | |
| H | -1.80025100 | -4.78522000 | -0.29073600 | | | | |
| H | 0.35175600 | -5.39165300 | 0.79295500 | | | | |
| H | 2.23310500 | -3.76424400 | 0.79702000 | | | | |
| H | 1.96105700 | -1.54961100 | -0.25684100 | | | | |
| Rh | -0.32000500 | 1.67863100 | 0.03554800 | | | | |
| C | -0.32057600 | 1.34522100 | 2.90315300 | | | | |
| C | -0.74175700 | 0.52769700 | 1.72969300 | | | | |
| H | -0.22001300 | -0.42226100 | 1.60257600 | | | | |
| H | -1.82186800 | 0.36758800 | 1.72653100 | | | | |
| C | 0.41514900 | 0.88869500 | 3.94280000 | | | | |
| H | 0.64725600 | 1.60910100 | 4.72733500 | | | | |
| C | -0.77070500 | 2.75572500 | 2.77694800 | | | | |
| C | -0.48441200 | 3.29639700 | 1.40173200 | | | | |
| H | 0.53699600 | 3.70007200 | 1.33838400 | | | | |
| H | -1.17475600 | 4.08678700 | 1.09496300 | | | | |
| C | -1.39124700 | 3.40052900 | 3.78311000 | | | | |
| C | -1.87183200 | 4.82132100 | 3.78996500 | | | | |
| H | -2.95268100 | 4.87169900 | 3.97143200 | | | | |
| H | -1.39482900 | 5.38506400 | 4.60223400 | | | | |
| H | -1.65687200 | 5.34390800 | 2.85472500 | | | | |
| C | 0.89965800 | -0.51182600 | 4.18472100 | | | | |

TS2⁺

Imaginary frequency: -377.1 cm⁻¹

| | | | |
|---|-------------|-------------|-------------|
| P | -2.74244600 | 1.73140300 | -0.71608800 |
| C | -3.10691200 | 0.07238800 | -1.48749700 |
| C | -1.92622300 | -0.36277900 | -2.36878200 |
| P | -0.28775500 | -0.13077900 | -1.49483600 |
| H | -3.26022200 | -0.64038900 | -0.67116600 |
| H | -4.03492300 | 0.11612300 | -2.06639800 |
| H | -2.04785600 | -1.39730800 | -2.70306500 |
| H | -1.87748000 | 0.26516000 | -3.26385200 |
| C | 0.93396800 | 0.09741100 | -2.84236000 |
| C | 0.13385700 | -1.74811700 | -0.73680600 |
| C | -4.16832100 | 2.09877000 | 0.37395700 |
| C | -2.87565700 | 2.91847600 | -2.10705300 |
| C | -4.49437700 | 3.44093700 | 0.63950200 |
| C | -5.53034100 | 3.75526000 | 1.51779200 |
| C | -6.25273700 | 2.73756900 | 2.14503900 |
| C | -5.93610300 | 1.40299500 | 1.89003300 |
| C | -4.89835300 | 1.08251800 | 1.01275900 |
| H | -3.94804900 | 4.24159600 | 0.15027500 |
| H | -5.77498500 | 4.79552500 | 1.70896700 |
| H | -7.06065100 | 2.98433800 | 2.82679600 |
| H | -6.49812400 | 0.60741900 | 2.36942100 |
| H | -4.67678100 | 0.03661600 | 0.82726700 |
| H | -4.07398700 | 3.05706700 | -2.82875900 |
| C | -4.14693700 | 3.94140600 | -3.90337000 |

| | | | | | | | | |
|----|-------------|-------------|-------------|-------------------------|-------------|-------------|-------------|--|
| C | -3.02843600 | 4.69694100 | -4.26765400 | H | 0.29469500 | -1.43782400 | 4.84189800 | |
| C | -1.83600500 | 4.56943700 | -3.55478000 | H | -1.33224100 | -0.92025900 | 5.24910700 | |
| C | -1.75980100 | 3.68397400 | -2.47769700 | H | -0.97929900 | -1.47792600 | 3.60640300 | |
| H | -4.95407200 | 2.48687600 | -2.54475400 | C | 2.11413700 | 1.74534100 | 1.50976000 | |
| H | -5.07666400 | 4.04455300 | -4.45438500 | O | 1.46532000 | 1.93503000 | 0.39257900 | |
| H | -3.08957000 | 5.38628400 | -5.10417900 | H | 1.70701300 | 2.38762300 | 3.75051500 | |
| H | -0.96734700 | 5.15839500 | -3.83214500 | C | 3.55763400 | 2.10328200 | 1.53613900 | |
| H | -0.82923300 | 3.59837500 | -1.92115400 | C | 4.39753600 | 1.54114600 | 2.51037200 | |
| C | 2.00424500 | 0.98847500 | -2.66734200 | C | 4.09899300 | 2.99405700 | 0.59642600 | |
| C | 2.94663500 | 1.15314800 | -3.68591000 | C | 5.75332800 | 1.86024500 | 2.54397200 | |
| C | 2.82541200 | 0.44103200 | -4.87900000 | H | 3.98563200 | 0.84697200 | 3.23950700 | |
| C | 1.76320700 | -0.45008000 | -5.05595500 | C | 5.45589400 | 3.30956900 | 0.62849500 | |
| C | 0.82242700 | -0.62571500 | -4.04314800 | H | 3.44631200 | 3.42687800 | -0.15455800 | |
| H | 2.10651100 | 1.53263100 | -1.73335700 | C | 6.28512000 | 2.74550400 | 1.60209600 | |
| H | 3.77574400 | 1.83962400 | -3.54318500 | H | 6.39626600 | 1.41713400 | 3.29843500 | |
| H | 3.55754100 | 0.57451200 | -5.66967100 | H | 5.86921800 | 3.99776700 | -0.10298800 | |
| H | 1.66996200 | -1.01114700 | -5.98080500 | H | 7.34178700 | 2.99423500 | 1.62686700 | |
| H | 0.01089500 | -1.33225800 | -4.19009400 | H | 1.87921200 | 0.83685400 | 2.07926100 | |
| C | -0.84616200 | -2.69839900 | -0.41044900 | | | | | |
| C | -0.48978900 | -3.89307200 | 0.21897300 | INT4⁺ | | | | |
| C | 0.84540800 | -4.14833100 | 0.53341400 | P | -2.74127300 | 1.75568100 | -0.65338800 | |
| C | 1.82623800 | -3.20498600 | 0.21670400 | C | -3.07254400 | 0.11706700 | -1.47700100 | |
| C | 1.47552700 | -2.01039700 | -0.41056700 | C | -1.87147700 | -0.25060500 | -2.35558400 | |
| H | -1.88992700 | -2.52589400 | -0.65433900 | P | -0.26354900 | -0.07589400 | -1.43008900 | |
| H | -1.25587800 | -4.62543000 | 0.45523900 | H | -3.21396500 | -0.62958800 | -0.68934700 | |
| H | 1.12169900 | -5.07956200 | 1.01819800 | H | -3.99381400 | 0.16158600 | -2.06614200 | |
| H | 2.86787800 | -3.40221200 | 0.45117000 | H | -1.97937700 | -1.25572700 | -2.77224900 | |
| H | 2.24813800 | -1.29062700 | -0.66358600 | H | -1.79995600 | 0.44082700 | -3.20056700 | |
| Rh | -0.56611200 | 1.65156900 | 0.08433000 | C | 0.99033000 | 0.17955900 | -2.74408700 | |
| C | -0.49784500 | 1.12822100 | 2.92252000 | C | 0.12594200 | -1.69504700 | -0.66685800 | |
| C | -1.17551300 | 0.49544900 | 1.72915200 | C | -4.20389400 | 2.07303800 | 0.40528700 | |
| H | -0.86883700 | -0.53656500 | 1.54941100 | C | -2.85205400 | 2.97937300 | -2.01375200 | |
| H | -2.26502500 | 0.55708800 | 1.78993300 | C | -4.59028200 | 3.39984800 | 0.66876500 | |
| C | -0.22595900 | 0.50128400 | 4.08462300 | C | -5.65729500 | 3.66842400 | 1.52520000 | |
| H | 0.26004800 | 1.08105700 | 4.86830500 | C | -6.35159100 | 2.62003700 | 2.13315800 | |
| C | -0.06951800 | 2.51401200 | 2.61480100 | C | -5.97605000 | 1.30040700 | 1.87996500 | |
| C | -0.90650600 | 3.19182200 | 1.66764500 | C | -4.90736400 | 1.02572900 | 1.02462900 | |
| H | -0.60821800 | 4.19208200 | 1.36250100 | H | -4.06804800 | 4.22430000 | 0.19304800 | |
| H | -1.97572600 | 3.10411600 | 1.84270900 | H | -5.94819700 | 4.69721800 | 1.71370800 | |
| C | 1.25247500 | 2.91069500 | 2.91058700 | H | -7.18337900 | 2.83121800 | 2.79788200 | |
| C | 1.71132700 | 4.33988100 | 2.71775000 | H | -6.51611500 | 0.48068100 | 2.34355500 | |
| H | 1.14397100 | 5.02912600 | 3.35384000 | H | -4.64178400 | -0.00984800 | 0.83885100 | |
| H | 2.76833000 | 4.44167800 | 2.97212800 | C | -4.05045400 | 3.16790900 | -2.72490300 | |
| H | 1.58993400 | 4.66879300 | 1.68084100 | C | -4.10388200 | 4.07762200 | -3.77915000 | |
| C | -0.58103800 | -0.90786800 | 4.44885500 | C | -2.96607700 | 4.80889100 | -4.13374000 | |

| | | | | | | | |
|----|-------------|-------------|-------------|-------------------------|--------------|-------------|-------------|
| C | -1.77345100 | 4.63048500 | -3.43236800 | H | -1.17281700 | -0.75893000 | 5.44995500 |
| C | -1.71614700 | 3.71928600 | -2.37558600 | H | -0.97309300 | -1.43579100 | 3.82692100 |
| H | -4.94474200 | 2.61695500 | -2.44760100 | C | 2.07175400 | 1.75956600 | 1.68686900 |
| H | -5.03324400 | 4.21926000 | -4.32216000 | O | 1.47708600 | 1.60497300 | 0.42359000 |
| H | -3.01228600 | 5.51831300 | -4.95427600 | H | 1.58496700 | 2.72394800 | 3.55800400 |
| H | -0.88920200 | 5.19882300 | -3.70340800 | C | 3.56260700 | 2.02725700 | 1.56143900 |
| H | -0.78483100 | 3.58779900 | -1.83009700 | C | 4.44190500 | 1.53468900 | 2.53443000 |
| C | 2.15131500 | 0.92565900 | -2.48931300 | C | 4.08694400 | 2.76887300 | 0.49408400 |
| C | 3.11147400 | 1.07701000 | -3.49207800 | C | 5.81271700 | 1.78229900 | 2.45089000 |
| C | 2.92456000 | 0.49277800 | -4.74490200 | H | 4.05135100 | 0.94690100 | 3.36258200 |
| C | 1.77311900 | -0.25627000 | -4.99932500 | C | 5.45816500 | 3.01212300 | 0.40417600 |
| C | 0.80927900 | -0.41623900 | -4.00547500 | H | 3.41299500 | 3.15142400 | -0.26555600 |
| H | 2.30085800 | 1.36263600 | -1.50798800 | C | 6.32503500 | 2.52134500 | 1.38294800 |
| H | 4.00979700 | 1.65138400 | -3.28688400 | H | 6.48031900 | 1.39178700 | 3.21340300 |
| H | 3.67422500 | 0.61427000 | -5.52094500 | H | 5.85112000 | 3.58786700 | -0.42916800 |
| H | 1.62564800 | -0.71989100 | -5.96993000 | H | 7.39193700 | 2.71073800 | 1.31238400 |
| H | -0.07092800 | -1.01382500 | -4.22045500 | H | 1.96103000 | 0.82677400 | 2.26398500 |
| C | -0.73913300 | -2.79716900 | -0.72365500 | INT3⁺ | | | |
| C | -0.37760700 | -4.00365100 | -0.11906900 | P | 0.00582100 | 0.62922000 | -1.59240300 |
| C | 0.84507000 | -4.11715900 | 0.54272600 | C | 0.69016900 | -0.95047500 | -2.32821100 |
| C | 1.70719600 | -3.01869000 | 0.60854700 | C | 1.32676300 | -1.84530600 | -1.25380300 |
| C | 1.35095600 | -1.80971500 | 0.01425000 | P | 2.49483200 | -0.85369800 | -0.18836500 |
| H | -1.69223200 | -2.73504900 | -1.23918400 | H | -0.057772100 | -1.49407700 | -2.88736800 |
| H | -1.05077400 | -4.85382500 | -0.17277700 | H | 1.45088100 | -0.63505800 | -3.04938400 |
| H | 1.12628600 | -5.05793600 | 1.00589200 | H | 0.55922400 | -2.25470600 | -0.58987600 |
| H | 2.65971900 | -3.10371700 | 1.12265800 | H | 1.86063400 | -2.68798700 | -1.70540600 |
| H | 2.01237700 | -0.95084200 | 0.08086200 | H | 3.90424900 | -0.47830400 | -1.30348200 |
| Rh | -0.53609100 | 1.59249300 | 0.21336700 | C | 3.16323500 | -2.03887100 | 1.03867500 |
| C | -0.55384100 | 1.08551900 | 2.89174700 | C | -1.76425000 | 0.28310300 | -1.23210400 |
| C | -1.23595000 | 0.36299600 | 1.76832100 | C | -0.05242400 | 1.78336700 | -3.01968500 |
| H | -0.90410300 | -0.66367500 | 1.61221900 | C | -2.63814300 | 1.37199800 | -1.06353800 |
| H | -2.32618800 | 0.42318800 | 1.79800400 | C | -3.97234800 | 1.16385400 | -0.71839200 |
| C | -0.19486500 | 0.57358600 | 4.08063100 | C | 0.34045300 | 1.22197900 | 4.77363600 |
| H | 0.34045300 | 1.22197900 | 4.77363600 | C | -4.45537400 | -0.13348600 | -0.52744800 |
| C | -0.17431000 | 2.45850900 | 2.41861200 | C | -3.59677900 | -1.22088100 | -0.68816900 |
| C | -1.13818700 | 3.25014800 | 1.83280400 | C | -2.27956000 | 2.38457400 | -1.22629000 |
| H | -0.89549500 | 4.24454600 | 1.47539900 | H | -4.63790700 | 2.01453900 | -0.60587800 |
| H | -2.19008700 | 3.03087300 | 1.96827200 | H | -5.49534700 | -0.29481200 | -0.26105000 |
| C | 1.28971400 | 2.85018300 | 2.50686300 | H | -3.96633900 | -2.23269400 | -0.55063800 |
| C | 1.58897100 | 4.29123900 | 2.08918200 | H | 0.98640700 | 5.00260500 | 2.66232100 |
| H | 0.98640700 | 5.00260500 | 2.66232100 | H | -1.61599000 | -1.88004100 | -1.16685200 |
| H | 2.64034300 | 4.52318200 | 2.26857400 | C | -0.80666700 | 1.49557100 | -4.17023600 |
| H | 1.39318100 | 4.45295900 | 1.02451600 | C | -0.79670000 | 2.37184900 | -5.25372100 |
| C | -0.50088500 | -0.80479100 | 4.58380600 | C | 0.41329200 | -1.30294500 | 4.92768000 |
| H | 0.41329200 | -1.30294500 | 4.92768000 | C | 0.70488200 | 3.84411200 | -4.05776400 |

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|----|-------------|-------------|-------------|--|-------------|-------------|-------------|
| C | 0.69846500 | 2.96694500 | -2.97059300 | O | 0.67992600 | 3.12298600 | 0.61669400 |
| H | -1.40945100 | 0.59303500 | -4.21614700 | H | 2.90362800 | 0.30937100 | 2.51082700 |
| H | -1.38098300 | 2.14166600 | -6.13951700 | H | -0.65287900 | -0.30825000 | 1.43079300 |
| H | -0.03465100 | 4.22721600 | -6.04464800 | H | 2.50978200 | 3.30842500 | 4.15302100 |
| H | 1.28784900 | 4.75920200 | -4.01159600 | H | -0.68838100 | 3.19040800 | 2.10035600 |
| H | 1.26433300 | 3.20674800 | -2.07498100 | C | -0.34831500 | 5.17618100 | 1.24452800 |
| C | 4.73157400 | -1.50341500 | -1.79352400 | C | -1.29356400 | 5.76054600 | 2.10650000 |
| C | 5.77228800 | -1.20633100 | -2.67199400 | C | 0.34620400 | 5.97654600 | 0.31733500 |
| C | 6.00094300 | 0.11412800 | -3.06909800 | C | -1.54450000 | 7.12820400 | 2.04218800 |
| C | 5.18574300 | 1.13885400 | -2.58765900 | H | -1.82370600 | 5.13861000 | 2.82310400 |
| C | 4.14147700 | 0.84356600 | -1.70915000 | C | 0.09272600 | 7.34054100 | 0.25724800 |
| H | 4.57378600 | -2.53103400 | -1.47938200 | H | 1.07553400 | 5.51272900 | -0.33812900 |
| H | 6.40760300 | -2.00448100 | -3.04349900 | C | -0.85170000 | 7.91539600 | 1.11834200 |
| H | 6.81461200 | 0.34222500 | -3.75072100 | H | -2.27285900 | 7.58141000 | 2.70674000 |
| H | 5.36202000 | 2.16593000 | -2.89194800 | H | 0.62597700 | 7.96337800 | -0.45396000 |
| H | 3.51035100 | 1.64703300 | -1.33792100 | H | -1.04551900 | 8.98269600 | 1.06819000 |
| C | 2.42111700 | -3.14540600 | 1.48388200 | | | | |
| C | 2.93723500 | -3.99353400 | 2.46541700 | TS2²⁺ | | | |
| C | 4.19356700 | -3.74470500 | 3.01851400 | Imaginary frequency: -388.0 cm ⁻¹ | | | |
| C | 4.93733500 | -2.64434300 | 2.58651800 | P | -0.02868300 | 0.55332000 | -1.64038400 |
| C | 4.42733200 | -1.79539200 | 1.60546300 | C | 0.66176700 | -1.01863800 | -2.37905700 |
| H | 1.44306000 | -3.36406400 | 1.06841200 | C | 1.31525400 | -1.90255100 | -1.30645300 |
| H | 2.35615800 | -4.84973900 | 2.79385100 | P | 2.44317700 | -0.86835100 | -0.23941500 |
| H | 4.59282700 | -4.40585200 | 3.78137200 | H | -0.10759900 | -1.57085000 | -2.92682400 |
| H | 5.91667900 | -2.44679100 | 3.01127000 | H | 1.41247600 | -0.69833700 | -3.10840600 |
| H | 5.02088100 | -0.95036200 | 1.27067600 | H | 0.55407800 | -2.33664600 | -0.65074600 |
| Rh | 1.40546300 | 1.05019900 | 0.44053700 | H | 1.87370000 | -2.72777800 | -1.75992000 |
| C | 0.20187300 | 0.92871400 | 3.02369000 | C | 3.87309200 | -0.49645000 | -1.32644300 |
| C | 0.30249300 | -0.01458700 | 1.86775600 | C | 3.09313000 | -2.00472900 | 1.04278900 |
| H | 0.88545200 | -0.90298400 | 2.12243800 | C | -1.79161600 | 0.21937400 | -1.25214700 |
| C | -0.91937200 | 1.08488900 | 3.76300300 | C | -0.06502900 | 1.75060700 | -3.02713900 |
| H | -0.87060600 | 1.76774700 | 4.61044100 | C | -2.64763700 | 1.31565200 | -1.04782100 |
| C | 1.46199000 | 1.71214000 | 3.22125100 | C | -3.98193300 | 1.11245900 | -0.69986800 |
| C | 1.58893900 | 2.74185100 | 4.07753300 | C | -4.47841600 | -0.18429500 | -0.54296300 |
| H | 0.79149700 | 3.04199300 | 4.75040000 | C | -3.63451400 | -1.27795100 | -0.73756300 |
| C | 2.53094900 | 1.30344100 | 2.24365100 | C | -2.29703700 | -1.07946900 | -1.08823800 |
| C | 3.69532600 | 2.26259100 | 2.04839500 | H | -2.27581900 | 2.32743800 | -1.18050600 |
| H | 4.27786100 | 2.38715000 | 2.97234300 | H | -4.63630800 | 1.96727700 | -0.55838100 |
| H | 4.38898100 | 1.89128200 | 1.28634500 | H | -5.51882600 | -0.34064800 | -0.27531100 |
| H | 3.35515000 | 3.25788400 | 1.74194100 | H | -4.01592400 | -2.28838400 | -0.62511800 |
| C | -2.23191200 | 0.37478100 | 3.61028700 | H | -1.66366900 | -1.94713800 | -1.24468500 |
| H | -2.37843200 | -0.34273100 | 4.42894700 | C | -0.43275600 | 1.34485700 | -4.32213900 |
| H | -3.06600200 | 1.08364700 | 3.67371000 | C | -0.46080400 | 2.27013500 | -5.36359200 |
| H | -2.32326600 | -0.17524900 | 2.67110100 | C | -0.13101400 | 3.60705200 | -5.12265500 |
| C | -0.11264100 | 3.74159600 | 1.34160300 | C | 0.22526800 | 4.01704200 | -3.83804200 |

| | | | | | | | |
|---|-------------|-------------|-------------|-------------------------|-------------|-------------|-------------|
| C | 0.26333000 | 3.09443800 | -2.78920500 | O | 0.71073300 | 3.06728400 | 0.44727700 |
| H | -0.70541800 | 0.31267400 | -4.52182200 | H | 2.74077900 | 0.44045400 | 2.45311600 |
| H | -0.74419700 | 1.94959400 | -6.36149300 | H | -0.80637600 | -0.15349900 | 1.32058700 |
| H | -0.15618700 | 4.32577600 | -5.93616500 | H | 1.83420400 | 3.97357900 | 3.15430700 |
| H | 0.47480600 | 5.05645500 | -3.64721200 | H | -0.84527200 | 3.09243300 | 1.78387200 |
| H | 0.52878300 | 3.41614900 | -1.78640500 | C | -0.12078700 | 5.10741900 | 1.38035000 |
| C | 4.72107000 | -1.51928600 | -1.78507400 | C | -1.19332400 | 5.70512600 | 2.05972900 |
| C | 5.77919400 | -1.22147000 | -2.64197300 | C | 0.78928500 | 5.91787500 | 0.68408100 |
| C | 6.00364400 | 0.09699700 | -3.04881700 | C | -1.35660700 | 7.08880600 | 2.04212100 |
| C | 5.16824700 | 1.11938700 | -2.59789500 | H | -1.90332400 | 5.08154500 | 2.59842400 |
| C | 4.10714800 | 0.82397600 | -1.73961800 | C | 0.62414400 | 7.30067400 | 0.66612600 |
| H | 4.56534800 | -2.54494600 | -1.46322400 | H | 1.61665300 | 5.45071700 | 0.15954700 |
| H | 6.43110400 | -2.01699600 | -2.98956200 | C | -0.44731100 | 7.88892700 | 1.34547700 |
| H | 6.83049600 | 0.32540600 | -3.71427900 | H | -2.19163200 | 7.54321100 | 2.56659100 |
| H | 5.34125900 | 2.14472300 | -2.90958100 | H | 1.33043900 | 7.92357600 | 0.12525600 |
| H | 3.46367700 | 1.62753800 | -1.38937900 | H | -0.57271800 | 8.96738700 | 1.33192100 |
| C | 2.35729100 | -3.11037000 | 1.50082300 | INT4⁺ | | | |
| C | 2.85686100 | -3.91615500 | 2.52585600 | P | -0.02985800 | 0.60641800 | -1.55706700 |
| C | 4.09017200 | -3.62578300 | 3.10952600 | C | 0.69914500 | -0.92053500 | -2.33762600 |
| C | 4.82815800 | -2.52680500 | 2.66378500 | C | 1.32412600 | -1.84204200 | -1.28479900 |
| C | 4.33479700 | -1.72021500 | 1.63944600 | P | 2.45166800 | -0.83742400 | -0.19120200 |
| H | 1.39833000 | -3.36310900 | 1.06071300 | H | -0.04339200 | -1.45258300 | -2.93868100 |
| H | 2.28145900 | -4.77266100 | 2.86337500 | H | 1.46779000 | -0.55844200 | -3.02724700 |
| H | 4.47686000 | -4.25416900 | 3.90577200 | H | 0.54692000 | -2.28009900 | -0.65072900 |
| H | 5.79081300 | -2.29848400 | 3.11069900 | H | 1.87692800 | -2.66238400 | -1.75326400 |
| H | 4.92499500 | -0.87746300 | 1.29288500 | Rh | 1.30682000 | 1.07243200 | 0.30104600 |
| C | 0.17599200 | 0.92857200 | 2.94601900 | C | 3.87863200 | -0.43560400 | -1.27078600 |
| C | 0.18585100 | 0.02592700 | 1.73770200 | C | -1.78651300 | 0.26074000 | -1.17209500 |
| H | 0.68803300 | -0.92506500 | 1.93274100 | C | -0.03542100 | 1.84435400 | -2.91001100 |
| C | -0.77331300 | 0.93336100 | 3.90386700 | C | -2.53933000 | 1.31164900 | -0.61788000 |
| H | -0.65858500 | 1.64099500 | 4.72393300 | C | -3.88561600 | 1.11911100 | -0.31488800 |
| C | 1.28684000 | 1.91069300 | 2.89537800 | C | -4.49036600 | -0.11953200 | -0.54802300 |
| C | 1.01552600 | 3.26111000 | 3.14668100 | C | -3.74397400 | -1.16852300 | -1.08491500 |
| H | 0.18726300 | 3.50934800 | 3.80256700 | C | -2.39512800 | -0.98218600 | -1.39754000 |
| C | 2.45866900 | 1.45838700 | 2.18502900 | H | -2.05992700 | 2.26601700 | -0.42047800 |
| C | 3.64451000 | 2.38283500 | 1.99192900 | H | -4.46417600 | 1.93737700 | 0.10297000 |
| H | 4.11276500 | 2.64600400 | 2.95082200 | H | -5.53987700 | -0.26560700 | -0.31156800 |
| H | 4.41309100 | 1.90411500 | 1.37737000 | H | -4.20909300 | -2.13243900 | -1.26755100 |
| H | 3.35932100 | 3.31536700 | 1.49691400 | H | -1.83754300 | -1.81130000 | -1.82119300 |
| C | -1.95489600 | 0.01770900 | 4.00379700 | C | -0.34051300 | 1.42897200 | -4.21902000 |
| H | -1.85873800 | -0.63899100 | 4.87813400 | C | -0.35895200 | 2.35470200 | -5.26020000 |
| H | -2.87740900 | 0.59177000 | 4.15204100 | C | -0.07844600 | 3.69987900 | -5.00618800 |
| H | -2.08142500 | -0.61490300 | 3.12226100 | C | 0.21300100 | 4.11688100 | -3.70757600 |
| C | 0.03315700 | 3.62935600 | 1.40143000 | C | 0.23632600 | 3.19726500 | -2.65626400 |

| | | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|--|
| H | -0.57447700 | 0.39062800 | -4.43396000 | H | 2.77223500 | 0.25015100 | 2.58038700 | |
| H | -0.59587000 | 2.02624400 | -6.26754900 | H | -0.93486400 | -0.19246200 | 1.38890400 | |
| H | -0.09495700 | 4.41939700 | -5.81925000 | H | 1.91950300 | 3.89516100 | 2.39563000 | |
| H | 0.41763900 | 5.16356400 | -3.50368500 | H | -1.00847500 | 3.13861900 | 1.99621600 | |
| H | 0.43039800 | 3.52410300 | -1.64073500 | C | -0.29399500 | 5.03549900 | 1.33036900 | |
| C | 4.72064900 | -1.44456800 | -1.77131700 | C | -1.43296400 | 5.68272500 | 1.82184500 | |
| C | 5.77067100 | -1.12058100 | -2.62837000 | C | 0.64955200 | 5.78219200 | 0.60992500 | |
| C | 5.99306700 | 0.21032500 | -2.99474700 | C | -1.62587800 | 7.04910700 | 1.60733500 | |
| C | 5.16331200 | 1.21832800 | -2.50338300 | H | -2.17513500 | 5.11383100 | 2.37742200 | |
| C | 4.11003200 | 0.89719700 | -1.64426300 | C | 0.45769900 | 7.14549800 | 0.38969100 | |
| H | 4.56564000 | -2.48021200 | -1.48277000 | H | 1.53189900 | 5.28617600 | 0.21518000 | |
| H | 6.41717900 | -1.90540200 | -3.00881800 | C | -0.68080900 | 7.78334400 | 0.88991500 | |
| H | 6.81320600 | 0.45889500 | -3.66127700 | H | -2.51458700 | 7.53753500 | 1.99618800 | |
| H | 5.33347200 | 2.25269400 | -2.78544900 | H | 1.19601800 | 7.71301300 | -0.16985700 | |
| H | 3.46638700 | 1.68685900 | -1.26500600 | H | -0.82981700 | 8.84544000 | 0.71972000 | |
| C | 2.31417500 | -3.09185700 | 1.52303700 | TS3 | | | | |
| C | 2.80404700 | -3.94418700 | 2.51420000 | Imaginary frequency: -75.6 cm ⁻¹ | | | | |
| C | 4.07699500 | -3.74215800 | 3.04838300 | P | -0.39586800 | 1.24337800 | -2.01482000 | |
| C | 4.86365900 | -2.68512200 | 2.58564400 | C | -0.56573300 | -0.29472100 | -3.04949800 | |
| C | 4.37967200 | -1.83184900 | 1.59462400 | C | -1.07090600 | -1.50365800 | -2.24820100 | |
| H | 1.32436400 | -3.27862400 | 1.11971400 | P | -0.44734900 | -1.47503600 | -0.47210000 | |
| H | 2.19007900 | -4.76854800 | 2.86353600 | H | -1.19120000 | -0.09630200 | -3.92598400 | |
| H | 4.45632300 | -4.40723600 | 3.81785400 | H | 0.45827200 | -0.47442800 | -3.38413600 | |
| H | 5.85795800 | -2.52660300 | 2.99168500 | H | 5.01030100 | -1.02626400 | 1.23168400 | |
| H | 5.01030100 | -1.02626400 | 1.23168400 | H | -2.16266100 | -1.53158300 | -2.20400000 | |
| Rh | 1.18927600 | 1.09364400 | 0.40125100 | H | -0.73865300 | -2.43073200 | -2.72190100 | |
| C | 0.22253300 | 0.87719600 | 2.91859800 | C | 0.57115300 | -2.99045800 | -0.25784000 | |
| C | 0.08260400 | -0.05998600 | 1.75809500 | C | -1.97121100 | -1.88426800 | 0.50339900 | |
| H | 0.57930100 | -1.02280500 | 1.89534900 | C | -2.08495000 | 1.97954000 | -1.91301000 | |
| C | -0.61117700 | 0.99696000 | 3.96378900 | C | 0.49123500 | 2.43224100 | -3.09114500 | |
| H | -0.40064400 | 1.77503500 | 4.69700400 | C | -2.24159600 | 3.25077600 | -1.33391200 | |
| C | 1.36559100 | 1.82015600 | 2.64836800 | C | -3.49751200 | 3.85078200 | -1.26355300 | |
| C | 1.03964600 | 3.29485900 | 2.63571100 | C | -4.61992200 | 3.19642600 | -1.77644000 | |
| H | 0.69913700 | 3.60450900 | 3.63150300 | C | -4.47686100 | 1.94060000 | -2.36545600 | |
| C | 2.61811100 | 1.30591000 | 2.37417900 | C | -3.21912400 | 1.33569300 | -2.43314500 | |
| C | 3.87952100 | 2.10108600 | 2.15591900 | H | -1.37788500 | 3.78090200 | -0.94769400 | |
| H | 4.38383900 | 2.27241600 | 3.11613800 | H | -3.59690200 | 4.83304000 | -0.81152300 | |
| H | 4.58192100 | 1.55454000 | 1.52050900 | H | -5.59760700 | 3.66616500 | -1.72322300 | |
| H | 3.69806200 | 3.07524200 | 1.69865600 | H | -5.34073900 | 1.42910800 | -2.78008300 | |
| C | -1.80018600 | 0.13097300 | 4.25390900 | H | -3.13389100 | 0.36484400 | -2.90827200 | |
| H | -1.65355000 | -0.42813900 | 5.18638200 | C | -0.13325000 | 2.85894200 | -4.27775700 | |
| H | -2.69975600 | 0.74145500 | 4.39715800 | C | 0.53658800 | 3.71696600 | -5.14691700 | |
| H | -1.99803400 | -0.59147800 | 3.45829700 | C | 1.82346500 | 4.16430600 | -4.83283000 | |
| C | -0.07213400 | 3.55554300 | 1.58991000 | C | 2.43554300 | 3.75295000 | -3.64958800 | |
| O | 0.26004700 | 2.89199800 | 0.38886500 | C | 1.77866200 | 2.88286000 | -2.77540100 | |

| | | | | | | | |
|----|-------------|-------------|-------------|----|------------|-------------|-------------|
| H | -1.14021100 | 2.53242200 | -4.52196600 | C | 2.50934500 | 2.72629200 | 1.27004900 |
| H | 0.05289700 | 4.03992700 | -6.06435400 | O | 2.04796400 | 2.06236200 | 0.13178700 |
| H | 2.34220600 | 4.83751700 | -5.50977500 | H | 2.08359000 | 4.48985200 | 2.44733200 |
| H | 3.43068400 | 4.10514500 | -3.39476500 | C | 3.91911500 | 3.27194400 | 0.96058400 |
| H | 2.23531800 | 2.57577000 | -1.84016700 | C | 4.55739400 | 4.21383700 | 1.78197700 |
| C | 0.13518300 | -4.22208500 | -0.77293800 | C | 4.63606600 | 2.75404900 | -0.12867900 |
| C | 0.89039400 | -5.37802400 | -0.57678600 | C | 5.85418700 | 4.65173900 | 1.50510400 |
| C | 2.08293800 | -5.31804600 | 0.14761700 | H | 4.05285300 | 4.61186800 | 2.65766300 |
| C | 2.51719600 | -4.10014200 | 0.67157200 | C | 5.93319600 | 3.19057200 | -0.40545500 |
| C | 1.76948900 | -2.93961000 | 0.46632100 | H | 4.16729200 | 1.98957800 | -0.73809600 |
| H | -0.80134800 | -4.28893400 | -1.31961800 | C | 6.54722200 | 4.14756800 | 0.40406700 |
| H | 0.54665300 | -6.32281500 | -0.98787100 | H | 6.32185400 | 5.38746400 | 2.15465100 |
| H | 2.67251600 | -6.21763600 | 0.29923900 | H | 6.46806500 | 2.77196100 | -1.25441900 |
| H | 3.44904700 | -4.04485000 | 1.22607800 | H | 7.55605800 | 4.48866400 | 0.18729000 |
| H | 2.13789000 | -1.99020900 | 0.83663500 | H | 2.64623700 | 2.01685600 | 2.10906900 |
| C | -3.12346700 | -1.09332200 | 0.34988500 | Cl | 2.45015700 | -0.46111200 | -1.65670600 |
| C | -4.27606000 | -1.35729000 | 1.08892300 | | | | |
| C | -4.29583000 | -2.40908800 | 2.00686400 | | | | |
| C | -3.15410600 | -3.19051700 | 2.18165500 | | | | |
| C | -2.00018400 | -2.93105800 | 1.43888800 | | | | |
| H | -3.12674800 | -0.25809300 | -0.34234000 | | | | |
| H | -5.15543000 | -0.73498600 | 0.95041900 | | | | |
| H | -5.19258600 | -2.61372900 | 2.58438100 | | | | |
| H | -3.15653700 | -4.00819900 | 2.89662500 | | | | |
| H | -1.12437800 | -3.55205600 | 1.58766800 | | | | |
| Rh | 0.66761000 | 0.59345600 | -0.12308800 | | | | |
| C | 0.06247300 | 1.75759600 | 2.51008400 | | | | |
| C | -0.69172200 | 1.39452300 | 1.28513900 | | | | |
| H | -1.43190900 | 0.61675500 | 1.47746900 | | | | |
| H | -1.19139100 | 2.26203800 | 0.85664700 | | | | |
| C | 0.39808900 | 0.88608100 | 3.49532000 | | | | |
| H | 0.95106400 | 1.29113400 | 4.34121900 | | | | |
| C | 0.45341600 | 3.19318600 | 2.68768800 | | | | |
| C | -0.10560300 | 3.90546700 | 3.67563200 | | | | |
| H | 0.17697400 | 4.94005800 | 3.85958800 | | | | |
| H | -0.86694500 | 3.48236200 | 4.32416400 | | | | |
| C | 1.52740500 | 3.81356100 | 1.79053200 | | | | |
| C | 0.97453700 | 4.67088400 | 0.64129700 | | | | |
| H | 0.26148400 | 5.41313500 | 1.01343300 | | | | |
| H | 1.79232400 | 5.19624300 | 0.13710100 | | | | |
| H | 0.48604400 | 4.04451400 | -0.10620400 | | | | |
| C | 0.07681600 | -0.57601100 | 3.58154000 | | | | |
| H | -0.53613700 | -0.92619100 | 2.75015000 | | | | |
| H | 0.99249700 | -1.18196000 | 3.60524300 | | | | |
| H | -0.46205200 | -0.79818200 | 4.51246300 | | | | |

TS3'

Imaginary frequency: -69.8 cm⁻¹

| | | | |
|---|-------------|-------------|-------------|
| P | -0.25369400 | 1.22579500 | -1.97548300 |
| C | -0.53181400 | -0.30040600 | -3.00212600 |
| C | -1.12389000 | -1.47611800 | -2.21285900 |
| P | -0.48673400 | -1.53604700 | -0.44200100 |
| H | -1.13652100 | -0.05476500 | -3.88166500 |
| H | 0.47940300 | -0.54763900 | -3.33447900 |
| H | -2.21336300 | -1.41201900 | -2.15686600 |
| H | -0.87883900 | -2.41857100 | -2.70909700 |
| C | 0.44912200 | -3.11199000 | -0.28414200 |
| C | -2.03498800 | -1.90883900 | 0.51248100 |
| C | -1.87043000 | 2.09597600 | -1.84418000 |
| C | 0.69255500 | 2.33181600 | -3.09204500 |
| C | -1.89045600 | 3.37509100 | -1.26220700 |
| C | -3.08321300 | 4.08707600 | -1.15416900 |
| C | -4.27612000 | 3.53516800 | -1.62846100 |
| C | -4.26736500 | 2.27125400 | -2.21752400 |
| C | -3.07193500 | 1.55475600 | -2.32546200 |
| H | -0.96557800 | 3.81839200 | -0.90552000 |
| H | -3.08034500 | 5.07445400 | -0.70229400 |
| H | -5.20521900 | 4.09115400 | -1.54484800 |
| H | -5.18766600 | 1.84077200 | -2.60169500 |
| H | -3.08661400 | 0.58048300 | -2.80272400 |
| C | 0.03826900 | 2.84956200 | -4.22550000 |
| C | 0.73949300 | 3.63379700 | -5.13873100 |
| C | 2.09032900 | 3.91976100 | -4.92097800 |
| C | 2.73503900 | 3.41773100 | -3.79132700 |

| | | | | | | | |
|----|--------------|-------------|-------------|----|-------------|-------------|-------------|
| C | 2.04582200 | 2.61783200 | -2.87645000 | C | 4.14523100 | 4.69277100 | 1.48955500 |
| H | -1.01598500 | 2.65059300 | -4.39511700 | C | 4.60310600 | 2.95687900 | -0.11039000 |
| H | 0.22998700 | 4.02638200 | -6.01411400 | C | 5.37191800 | 5.29259000 | 1.19223300 |
| H | 2.63401100 | 4.53829200 | -5.62979900 | H | 3.52124800 | 5.14504800 | 2.25433400 |
| H | 3.78028600 | 3.64785300 | -3.60810700 | C | 5.82852900 | 3.55387000 | -0.40767900 |
| H | 2.52890000 | 2.24057600 | -1.98519200 | H | 4.30728400 | 2.03224200 | -0.59360500 |
| C | -0.04821500 | -4.30328600 | -0.83719600 | C | 6.21743200 | 4.73048800 | 0.23648400 |
| C | 0.64441100 | -5.50270400 | -0.67386400 | H | 5.66436800 | 6.20093100 | 1.71306600 |
| C | 1.83496000 | -5.52735300 | 0.05594100 | H | 6.48562200 | 3.09193100 | -1.14045800 |
| C | 2.33029400 | -4.35016400 | 0.61726800 | H | 7.17076700 | 5.19741100 | 0.00389400 |
| C | 1.64553600 | -3.14622300 | 0.44426900 | H | 2.68351800 | 2.12613400 | 2.02534200 |
| H | -0.98551100 | -4.30523900 | -1.38651200 | Cl | 2.50381600 | -0.61385700 | -1.53614300 |
| H | 0.25310900 | -6.41560300 | -1.11355300 | H | 0.62570400 | 3.87445400 | 0.78917000 |
| H | 2.37531100 | -6.46106600 | 0.18297400 | C | 0.41579800 | 5.03874600 | 4.37967400 |
| H | 3.26094400 | -4.36089800 | 1.17651600 | H | -0.52540600 | 5.57357700 | 4.56446700 |
| H | 2.05999900 | -2.22791700 | 0.84297300 | H | 0.96901300 | 5.05190100 | 5.32805700 |
| C | -3.15823500 | -1.07576400 | 0.36538700 | H | 0.98701700 | 5.62068400 | 3.65306100 |
| C | -4.32486200 | -1.31180700 | 1.09200400 | | | | |
| C | -4.38818300 | -2.37768700 | 1.99136600 | | | | |
| C | -3.27540600 | -3.20110500 | 2.16044000 | | | | |
| C | -2.10789000 | -2.96930600 | 1.42995600 | P | -2.75749500 | 1.83877300 | -0.69272600 |
| H | -3.12782300 | -0.22821600 | -0.31161800 | C | -2.94408800 | 0.54642800 | -2.04602100 |
| H | -5.18103900 | -0.65682000 | 0.95871700 | C | -2.06298500 | -0.68136000 | -1.78402300 |
| H | -5.29590300 | -2.56082900 | 2.55889300 | P | -0.36108800 | -0.11001000 | -1.29910500 |
| H | -3.31161500 | -4.03047100 | 2.86093100 | H | -3.99526000 | 0.26624800 | -2.15944400 |
| H | -1.25520000 | -3.62309400 | 1.57333600 | H | -2.63364500 | 1.03782500 | -2.97325300 |
| Rh | 0.71883700 | 0.50405200 | -0.06877300 | H | -2.45472800 | -1.27367800 | -0.95078000 |
| C | 0.12075600 | 1.59831900 | 2.56296500 | H | -2.01550200 | -1.32755200 | -2.66648000 |
| C | -0.65737600 | 1.29402700 | 1.33734600 | C | 0.44672300 | 0.39856400 | -2.86241200 |
| H | -1.40368500 | 0.51823600 | 1.50720200 | C | 0.56151200 | -1.58577300 | -0.74170700 |
| H | -1.14945200 | 2.17938500 | 0.93718400 | C | -4.22838200 | 1.61471300 | 0.38956700 |
| C | 0.50466500 | 0.67313700 | 3.48192300 | C | -3.08257700 | 3.42038700 | -1.56920500 |
| H | 1.11059800 | 1.03234200 | 4.31215900 | C | -4.83323800 | 2.72345800 | 1.00607500 |
| C | 0.49433100 | 3.03062000 | 2.78171100 | C | -5.90842100 | 2.54915100 | 1.87879900 |
| C | 0.15016800 | 3.62662500 | 3.93864500 | C | -6.39322800 | 1.26866600 | 2.15033600 |
| H | -0.406668200 | 3.02491900 | 4.65665100 | C | -5.79748400 | 0.15967700 | 1.54682000 |
| C | 1.26528000 | 3.69672900 | 1.66292100 | C | -4.71944200 | 0.32989600 | 0.67725200 |
| C | 0.15865300 | -0.78513600 | 3.52625800 | H | -4.48181700 | 3.72683600 | 0.78708200 |
| H | -0.52133800 | -1.08398100 | 2.72761200 | H | -6.37115100 | 3.41653000 | 2.33958300 |
| H | 1.05711100 | -1.41301100 | 3.46020200 | H | -7.23252500 | 1.13544500 | 2.82575900 |
| H | -0.31966700 | -1.03563800 | 4.48295500 | H | -6.17289500 | -0.83882700 | 1.74917300 |
| C | 2.42495400 | 2.78466500 | 1.17219800 | H | -4.27329600 | -0.54742000 | 0.21827300 |
| O | 2.06174200 | 2.02448500 | 0.05893100 | C | -4.30054400 | 3.62551700 | -2.24165100 |
| H | 1.61858900 | 4.67589500 | 1.98635500 | C | -4.52258100 | 4.80674500 | -2.94735600 |
| C | 3.73131000 | 3.52629400 | 0.83188100 | C | -3.53644600 | 5.79667100 | -2.98746200 |

| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | -2.32654900 | 5.60262900 | -2.32096500 | H | 0.64965900 | -1.34290400 | 4.17635500 |
| C | -2.09924300 | 4.41866800 | -1.61538100 | H | 0.80773700 | -1.51394600 | 2.41856500 |
| H | -5.08043100 | 2.87036400 | -2.20695700 | C | 2.08407300 | 2.11093000 | 1.36018400 |
| H | -5.46602600 | 4.95647300 | -3.46338600 | O | 1.47351400 | 1.83383200 | 0.21276800 |
| H | -3.71400400 | 6.71677900 | -3.53579200 | H | 1.68891200 | 3.15260100 | 3.23584100 |
| H | -1.55949800 | 6.37070100 | -2.34737500 | C | 3.58206100 | 2.27008200 | 1.29107300 |
| H | -1.15744500 | 4.26763000 | -1.09589100 | C | 4.35036600 | 2.42927400 | 2.45588600 |
| C | 0.48583500 | 1.75253200 | -3.22785700 | C | 4.23173200 | 2.24338900 | 0.04848300 |
| C | 1.05227400 | 2.13528500 | -4.44490200 | C | 5.73556400 | 2.56218000 | 2.37921400 |
| C | 1.58280200 | 1.17182900 | -5.30360900 | H | 3.87014600 | 2.44533200 | 3.43099300 |
| C | 1.54981700 | -0.17817400 | -4.94464000 | C | 5.61860400 | 2.37476500 | -0.02592500 |
| C | 0.98851800 | -0.56605500 | -3.72916200 | H | 3.63535400 | 2.12886300 | -0.85004000 |
| H | 0.08055400 | 2.50446800 | -2.55909900 | C | 6.37457900 | 2.53457800 | 1.13686000 |
| H | 1.08163900 | 3.18562000 | -4.71816100 | H | 6.31663700 | 2.68562700 | 3.28824100 |
| H | 2.02527200 | 1.47090400 | -6.24894800 | H | 6.10930200 | 2.35896500 | -0.99482400 |
| H | 1.96682000 | -0.92922700 | -5.60853900 | H | 7.45358300 | 2.63990700 | 1.07724700 |
| H | 0.98225300 | -1.61604700 | -3.45293400 | H | 1.90513100 | 1.10982800 | 2.10243100 |
| C | -0.00316600 | -2.87033300 | -0.70856800 | | | | |
| C | 0.76309200 | -3.96255200 | -0.29401400 | | | | |
| C | 2.09381600 | -3.78253400 | 0.08454400 | | | | |
| C | 2.66057300 | -2.50502300 | 0.05559700 | P | -0.06769200 | 0.52295300 | -1.38516600 |
| C | 1.90093700 | -1.40869100 | -0.34895200 | C | 0.22716600 | -1.25855400 | -1.81726400 |
| H | -1.03065300 | -3.03744600 | -1.01451300 | C | 1.73829200 | -1.52315900 | -1.81786700 |
| H | 0.31934900 | -4.95327600 | -0.27584300 | P | 2.56799800 | -0.79697200 | -0.29509200 |
| H | 2.68817600 | -4.63462000 | 0.40001300 | H | -0.27233300 | -1.86139700 | -1.05242600 |
| H | 3.69575900 | -2.36103800 | 0.34996800 | H | -0.21791000 | -1.50473800 | -2.78657800 |
| H | 2.33363000 | -0.41270200 | -0.35342000 | H | 1.95902200 | -2.59166400 | -1.89643700 |
| Rh | -0.63119500 | 1.57868800 | 0.23067600 | H | 2.20558700 | -1.02981100 | -2.67567700 |
| C | -0.21869700 | 1.12363900 | 2.65526200 | C | 4.25838000 | -0.39539600 | -0.89235700 |
| C | -1.26710100 | 0.41138000 | 1.97989400 | C | 2.81288300 | -2.22068000 | 0.84530000 |
| H | -1.18561900 | -0.67231800 | 1.93272600 | C | -1.87081700 | 0.72771300 | -1.15004000 |
| H | -2.29212400 | 0.74891800 | 2.10515800 | C | 0.31431700 | 1.46384000 | -2.91038700 |
| C | 0.95647100 | 0.52512800 | 3.15975000 | C | -2.36347900 | 2.03056100 | -0.95124400 |
| H | 1.49848500 | 1.11454700 | 3.89911700 | C | -3.73105600 | 2.24195700 | -0.78714600 |
| C | -0.14595500 | 2.56423900 | 2.30870200 | C | -4.61910600 | 1.16264000 | -0.81072400 |
| C | -1.25549400 | 3.26414700 | 1.86939000 | C | -4.13569900 | -0.13245100 | -0.99872600 |
| H | -1.15684600 | 4.29106200 | 1.54275300 | C | -2.76655000 | -0.35279500 | -1.16904900 |
| H | -2.25899400 | 2.93471800 | 2.11043500 | H | -1.67430800 | 2.86851600 | -0.91342200 |
| C | 1.27202400 | 3.13802000 | 2.22041400 | H | -4.10395200 | 3.25117200 | -0.64088200 |
| C | 1.37442100 | 4.55370800 | 1.64757600 | H | -5.68420000 | 1.33143600 | -0.68462200 |
| H | 0.77920500 | 5.26351600 | 2.23008800 | H | -4.82158600 | -0.97380300 | -1.02153700 |
| H | 2.41468800 | 4.88669100 | 1.67664600 | H | -2.41562600 | -1.36683700 | -1.32972600 |
| H | 1.04177500 | 4.58721300 | 0.60629700 | C | -0.44287300 | 1.24026700 | -4.07367600 |
| C | 1.16776900 | -0.96040800 | 3.28768200 | C | -0.14368300 | 1.92991300 | -5.24669900 |
| H | 2.23030700 | -1.18407000 | 3.41372500 | C | 0.90407500 | 2.85510700 | -5.26698900 |

TS6⁺

Imaginary frequency: -875.4 cm⁻¹

| | | | | | | | |
|----|-------------|-------------|-------------|-------------------------|-------------|-------------|-------------|
| C | 1.65001700 | 3.09120000 | -4.11200400 | C | 0.33122100 | 3.65666300 | 1.40703300 |
| C | 1.35935000 | 2.39772200 | -2.93497500 | O | 0.58136300 | 2.99625000 | 0.27981700 |
| H | -1.27420700 | 0.54064000 | -4.06264500 | H | 2.70496800 | 0.09812700 | 2.71528300 |
| H | -0.73092100 | 1.75094400 | -6.14213200 | H | -0.81406100 | -0.52521800 | 1.71960800 |
| H | 1.13277600 | 3.39397900 | -6.18144200 | H | 2.34145700 | 3.80192700 | 2.18083200 |
| H | 2.45771300 | 3.81666600 | -4.12363400 | H | -0.63257900 | 3.04321600 | 1.95416300 |
| H | 1.92744300 | 2.59227200 | -2.03235200 | C | -0.14735900 | 5.07673500 | 1.25255700 |
| C | 5.14581100 | -1.40923000 | -1.29436000 | C | -0.53470500 | 5.84094500 | 2.36527100 |
| C | 6.39726000 | -1.08028000 | -1.81306300 | C | -0.22955500 | 5.65019900 | -0.02480900 |
| C | 6.77752900 | 0.25929200 | -1.93415100 | C | -0.98911500 | 7.14857300 | 2.20418200 |
| C | 5.90335300 | 1.27124400 | -1.53644700 | H | -0.48933900 | 5.41598800 | 3.36466100 |
| C | 4.64793400 | 0.94573100 | -1.01838700 | C | -0.68562600 | 6.95877900 | -0.18387500 |
| H | 4.86560300 | -2.45378900 | -1.19603100 | H | 0.07860600 | 5.06224000 | -0.88227700 |
| H | 7.07646700 | -1.86920900 | -2.12144800 | C | -1.06639600 | 7.71215900 | 0.92805400 |
| H | 7.75415500 | 0.51128800 | -2.33606800 | H | -1.28395500 | 7.72772800 | 3.07417200 |
| H | 6.19709000 | 2.31269700 | -1.62635300 | H | -0.73763500 | 7.39326700 | -1.17806000 |
| H | 3.96514700 | 1.73096100 | -0.70635400 | H | -1.41837700 | 8.73167000 | 0.80325600 |
| C | 1.86499900 | -3.25472800 | 0.92493800 | | | | |
| C | 2.01758900 | -4.29011600 | 1.84845000 | INT9⁺ | | | |
| C | 3.11392500 | -4.30381700 | 2.71226500 | P | -2.62174100 | 1.80325800 | -0.76075600 |
| C | 4.05943500 | -3.27880100 | 2.64701000 | C | -2.87331900 | 0.55987600 | -2.14340900 |
| C | 3.91101500 | -2.24385300 | 1.72289200 | C | -2.21059900 | -0.78365500 | -1.81828100 |
| H | 1.00480100 | -3.26720300 | 0.26231000 | P | -0.48575200 | -0.50452000 | -1.15157400 |
| H | 1.28129400 | -5.08705400 | 1.88909000 | H | -3.93890200 | 0.43841500 | -2.36042400 |
| H | 3.23240200 | -5.11020900 | 3.42923000 | H | -2.40647600 | 1.00213200 | -3.02900400 |
| H | 4.91898900 | -3.28683600 | 3.31034200 | H | -2.77151400 | -1.32241800 | -1.04954500 |
| H | 4.66660100 | -1.46622900 | 1.67020800 | H | -2.16986400 | -1.42694200 | -2.70271100 |
| Rh | 1.25551100 | 0.99672800 | 0.41763600 | C | 0.46401900 | -0.04945600 | -2.65894600 |
| C | 0.20506800 | 1.13204600 | 2.65982800 | C | 0.09765400 | -2.19792200 | -0.73075000 |
| C | 0.16496800 | -0.12035800 | 1.96606300 | C | -4.17140400 | 1.74484100 | 0.22964300 |
| H | 0.88406900 | -0.89088300 | 2.23064800 | C | -2.68251600 | 3.42511100 | -1.61725300 |
| C | -0.93345700 | 1.92077900 | 2.94490900 | C | -4.63301200 | 2.89813300 | 0.88619800 |
| H | -0.80083000 | 2.65501700 | 3.73971900 | C | -5.77148200 | 2.84727900 | 1.69105100 |
| C | 1.51402300 | 1.83992800 | 2.61014500 | C | -6.46353900 | 1.64590300 | 1.85634800 |
| C | 1.39559600 | 3.35506000 | 2.49205100 | C | -6.01162600 | 0.49372000 | 1.21130300 |
| H | 1.13089300 | 3.80072500 | 3.45717600 | C | -4.87225300 | 0.54100200 | 0.40654400 |
| C | 2.71482100 | 1.16269400 | 2.49549700 | H | -4.11555100 | 3.84328700 | 0.75341900 |
| C | 4.08872800 | 1.77702100 | 2.46850300 | H | -6.12126700 | 3.74986400 | 2.18314000 |
| H | 4.51220200 | 1.77302900 | 3.48214000 | H | -7.35119200 | 1.60893100 | 2.48020600 |
| H | 4.76798000 | 1.19799400 | 1.83723000 | H | -6.54797600 | -0.44312200 | 1.32893500 |
| H | 4.10001100 | 2.80669800 | 2.10866700 | H | -4.54259000 | -0.36747800 | -0.08755900 |
| C | -2.35490300 | 1.45072500 | 2.77822500 | C | -3.83605300 | 3.84358200 | -2.30372200 |
| H | -2.65393200 | 0.83012400 | 3.63249700 | C | -3.84139600 | 5.05529300 | -2.99195200 |
| H | -3.03660400 | 2.30470500 | 2.74676900 | C | -2.69906900 | 5.86127100 | -3.00071300 |
| H | -2.50173300 | 0.86878000 | 1.86645100 | C | -1.55200300 | 5.45355200 | -2.31964000 |

| | | | | | | | | |
|----|-------------|-------------|-------------|-------------------------|-------------|-------------|-------------|--|
| C | -1.54063100 | 4.23919600 | -1.62869600 | H | 1.71959600 | -1.75861200 | 1.61055600 | |
| H | -4.73229100 | 3.23007900 | -2.29232800 | C | 1.91882800 | 3.18085100 | 1.11785700 | |
| H | -4.73588900 | 5.37207200 | -3.51971700 | O | 1.30724700 | 2.93494600 | 0.07487300 | |
| H | -2.70669400 | 6.80566200 | -3.53663600 | H | 1.86605300 | 2.72131400 | 3.22045800 | |
| H | -0.66475000 | 6.07978000 | -2.32411200 | C | 3.33816500 | 3.62177900 | 1.07704000 | |
| H | -0.64641700 | 3.92199300 | -1.10015400 | C | 4.11368600 | 3.81788700 | 2.23483200 | |
| C | 1.20470800 | 1.14032900 | -2.70010000 | C | 3.92646200 | 3.84775000 | -0.18199500 | |
| C | 1.89745100 | 1.49380100 | -3.86173000 | C | 5.44145300 | 4.22716400 | 2.13299700 | |
| C | 1.85866600 | 0.66794300 | -4.98445300 | H | 3.69331400 | 3.65191100 | 3.22071000 | |
| C | 1.12736300 | -0.52291000 | -4.94819000 | C | 5.25084000 | 4.25762900 | -0.28078900 | |
| C | 0.43423400 | -0.88070300 | -3.79383900 | H | 3.32315200 | 3.69989500 | -1.07051600 | |
| H | 1.24769100 | 1.78705100 | -1.83040100 | C | 6.01150600 | 4.44781400 | 0.87741500 | |
| H | 2.46744300 | 2.41786200 | -3.88679300 | H | 6.03118100 | 4.37366000 | 3.03228300 | |
| H | 2.39714600 | 0.94635400 | -5.88533300 | H | 5.69356200 | 4.43156600 | -1.25657300 | |
| H | 1.09867600 | -1.17281600 | -5.81751800 | H | 7.04618300 | 4.76811600 | 0.80114100 | |
| H | -0.11556200 | -1.81741700 | -3.77470400 | H | 2.43510900 | 0.65008300 | 1.95467500 | |
| C | -0.73235600 | -3.08570000 | -0.02428100 | INT9⁺ | | | | |
| C | -0.27376100 | -4.35413100 | 0.33246300 | P | -0.46346200 | 0.05961600 | -1.30833600 | |
| C | 1.02192500 | -4.75152900 | -0.00314700 | C | 0.31331100 | -1.55012600 | -1.86065200 | |
| C | 1.85703900 | -3.87465900 | -0.69729100 | C | 1.83897400 | -1.42085600 | -1.87879600 | |
| C | 1.40134300 | -2.60565000 | -1.05816100 | P | 2.47006900 | -0.55292400 | -0.33515400 | |
| H | -1.74244900 | -2.79804200 | 0.25195500 | H | -0.00267700 | -2.32357700 | -1.15524400 | |
| H | -0.93026900 | -5.03147300 | 0.87017700 | H | -0.07197300 | -1.83341200 | -2.84501000 | |
| H | 1.37756000 | -5.73912600 | 0.27383200 | H | 2.31767900 | -2.39814500 | -1.98908100 | |
| H | 2.86524800 | -4.17772800 | -0.96310900 | H | 2.15192100 | -0.79829500 | -2.72270700 | |
| H | 2.05915400 | -1.93775800 | -1.60432900 | C | 4.02801500 | 0.22193700 | -0.92032100 | |
| Rh | -0.68798400 | 1.16715800 | 0.46883700 | C | 2.98134400 | -1.91694900 | 0.79452000 | |
| C | 0.31516100 | 0.66673200 | 2.38383600 | C | -2.26154900 | -0.33117700 | -1.28114800 | |
| C | -0.79482700 | -0.19840100 | 2.13594800 | C | -0.24248700 | 1.15856900 | -2.76517600 | |
| H | -0.58315000 | -1.24890000 | 1.97296800 | C | -3.19889300 | 0.53791000 | -1.86265200 | |
| H | -1.77480800 | -0.01095900 | 2.56791600 | C | -4.56311700 | 0.24585200 | -1.80851100 | |
| C | 1.73022700 | 0.17090000 | 2.64421000 | C | -5.01023900 | -0.91322000 | -1.17323600 | |
| H | 2.01324800 | 0.52416700 | 3.64734700 | C | -4.08706900 | -1.78211600 | -0.58764100 | |
| C | 0.01562200 | 2.09173500 | 2.40322300 | C | -2.72357800 | -1.49227800 | -0.63667300 | |
| C | -1.30147300 | 2.52710900 | 2.19975300 | H | -1.49046300 | 3.58271000 | 2.05143900 | |
| H | -2.16025000 | 1.95704300 | 2.53205500 | H | -2.86625600 | 1.43809500 | -2.36831700 | |
| C | 1.17405900 | 3.09222500 | 2.45853800 | H | -5.27493900 | 0.92516200 | -2.26761400 | |
| C | 0.75805300 | 4.52204000 | 2.87741000 | H | -6.07121800 | -1.13998300 | -1.13517900 | |
| H | 0.17881000 | 4.49299400 | 3.80377400 | H | -4.42708000 | -2.68748500 | -0.09396200 | |
| H | 1.64209400 | 5.14143300 | 3.04505000 | C | -2.02454300 | -2.18060200 | -0.17058200 | |
| H | 0.15572100 | 5.00953800 | 2.10633200 | C | -0.63116000 | 0.73349400 | -4.04876900 | |
| C | 1.93514600 | -1.34496700 | 2.59847200 | C | -0.44492000 | 1.56327200 | -5.15250200 | |
| H | 2.97590900 | -1.58220600 | 2.83648300 | C | 0.12949500 | 2.82709200 | -4.98888300 | |
| H | 1.30399300 | -1.85832400 | 3.33044400 | C | 0.51311300 | 3.25723500 | -3.71908100 | |

| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | -1.09633000 | -0.23788300 | -4.18965700 | H | 1.52368500 | -0.14465600 | 2.92637800 |
| H | -0.75009000 | 1.22574100 | -6.13833300 | H | -1.78058200 | -0.27953400 | 1.58501300 |
| H | 0.27387000 | 3.47258200 | -5.85002000 | H | 1.88650100 | 3.44953500 | 3.42852500 |
| H | 0.95664600 | 4.23984600 | -3.58896300 | H | -1.44818100 | 3.28898800 | 1.54161900 |
| H | 0.63464500 | 2.77297900 | -1.62525900 | C | 1.56829900 | 5.49242300 | 1.45465500 |
| C | 5.00596100 | -0.52252900 | -1.60515200 | C | 1.47360500 | 6.25397800 | 2.63334400 |
| C | 6.15985800 | 0.09938400 | -2.07905100 | C | 1.87220600 | 6.14001200 | 0.24304700 |
| C | 6.35059000 | 1.46942600 | -1.87745700 | C | 1.67683100 | 7.63167100 | 2.59803200 |
| C | 5.38264700 | 2.21597900 | -1.20591700 | H | 1.24486800 | 5.78084700 | 3.58238200 |
| C | 4.22374300 | 1.59737200 | -0.73022500 | C | 2.07274200 | 7.51524900 | 0.21062200 |
| H | 4.87291200 | -1.58894700 | -1.76340700 | H | 1.94653900 | 5.54420000 | -0.65994600 |
| H | 6.90908500 | -0.48369900 | -2.60600900 | C | 1.97505900 | 8.26331800 | 1.38844200 |
| H | 7.25045600 | 1.95143700 | -2.24756500 | H | 1.60252800 | 8.21231500 | 3.51196600 |
| H | 5.52521600 | 3.28187300 | -1.05466400 | H | 2.30522800 | 8.00791800 | -0.72833900 |
| H | 3.46192700 | 2.18429800 | -0.22725100 | H | 2.13170300 | 9.33749000 | 1.36326700 |
| C | 2.00275800 | -2.82390500 | 1.24088800 | | | | |
| C | 2.33665000 | -3.86158200 | 2.10991000 | | | | |
| C | 3.65035900 | -3.99953300 | 2.56536000 | | | | |
| C | 4.62469200 | -3.09516300 | 2.14448100 | | | | |
| C | 4.29615600 | -2.06053400 | 1.26414800 | | | | |
| H | 0.97198200 | -2.71566300 | 0.91618500 | | | | |
| H | 1.57095500 | -4.55971600 | 2.43514500 | | | | |
| H | 3.90988100 | -4.80491900 | 3.24546300 | | | | |
| H | 5.64740600 | -3.19295200 | 2.49620800 | | | | |
| H | 5.06995800 | -1.37368700 | 0.93950400 | | | | |
| Rh | 0.68945500 | 0.74138200 | 0.58934000 | | | | |
| C | -0.61671300 | 1.41509000 | 2.22648900 | | | | |
| C | -0.81545200 | 0.02950000 | 1.96960100 | | | | |
| H | -0.30697900 | -0.73978500 | 2.54581000 | | | | |
| C | -1.73457800 | 2.44798600 | 2.18359500 | | | | |
| H | -1.82194100 | 2.86592500 | 3.19822300 | | | | |
| C | 0.73392200 | 1.82477100 | 2.60912400 | | | | |
| C | 1.03831400 | 3.30469400 | 2.75101900 | | | | |
| H | 0.19468800 | 3.81341100 | 3.22659400 | | | | |
| C | 1.76838600 | 0.89016300 | 2.71067400 | | | | |
| C | 3.20692100 | 1.25128500 | 2.98224600 | | | | |
| H | 3.36458100 | 1.41955400 | 4.05692100 | | | | |
| H | 3.86500900 | 0.42911200 | 2.69237800 | | | | |
| H | 3.53620600 | 2.14615900 | 2.44978800 | | | | |
| C | -3.11350100 | 1.94042700 | 1.75890800 | | | | |
| H | -3.47680900 | 1.15214000 | 2.42531100 | | | | |
| H | -3.83461400 | 2.76183700 | 1.79646600 | | | | |
| H | -3.10917600 | 1.55057100 | 0.73840300 | | | | |
| C | 1.36594400 | 4.02137900 | 1.43868000 | | | | |
| O | 1.47537000 | 3.37424100 | 0.39634000 | | | | |