*Electronic Supporting Information*

# Catalytic oxidation of alkanes by a (salen)osmium(VI) nitrido complex using $H_2O_2$ as the terminal oxidant

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## Experimental Section

**Materials.** All chemicals were of reagent grade unless otherwise specified. [**1**]$PF_6$ was synthesized according to a literature method.[1] All organic substrates were obtained from Sigma Aldrich and purified according to literature methods.[2] Hydrogen peroxide (35%, Sigma Aldrich) was used as received and standardized by iodometry.[3] 2-Methyl-1-phenyl-2-propyl hydroperoxide (MPPH) was prepared according to a literature method,[4] and its purity was determined to be >99% by NMR spectroscopy. Active MPPH levels were further measured by iodometric titrations, which showed >99% peroxide activity. Cyclohexane-$d_{12}$ (99.6 atom % D) was purchased from Sigma Aldrich and used as received. Bromotrichloromethane was purchased from Aldrich and was purified by passing through a short column of neutral alumina prior to use.

**Instrumentation.** Gas chromatographic analyses of organic products were performed on a HP5890 GC/FID equipped with a DB-FFAP column (30 m × 0.25 mm i.d.). GC/MS measurements were carried out on an Agilent 6890N gas chromatograph interfaced to a 5975 mass selective detector.

**Catalytic Oxidation of Alkanes.** The oxidant (0.5 M) was added into a yellow solution of **1** (0.625 mM) in $CH_2Cl_2/CH_3CO_2H$ (5:2, v/v) containing a substrate (1.2 M) at 23 $^oC$. The mixture was vigorously stirred under argon. Chlorobenzene was then added as an internal standard, and the organic products were identified and quantified by GC/FID and GC/MS at various time intervals.

Catalytic oxidation of cyclohexane was also carried out by slow addition of $H_2O_2$. A solution of $H_2O_2$ (0.17 M) in $CH_2Cl_2/CH_3CO_2H$ (5:2, v/v) was slowly added within

3 h into a solution of **1** (0.045 mM) in $CH_2Cl_2/CH_3CO_2H$ (5:2, v/v) containing cyclohexane (0.69 M or 1.37 M) at 23 °C. The mixture was vigorously stirred for 24 h. Chlorobenzene was then added as an internal standard, and the organic products were analyzed by GC/FID and GC/MS.

When MPPH was used as the oxidant, $PPh_3$ (5 M) was added into the reaction mixture before product analysis in order to consume all unreacted MPPH since MPPH will decompose in the GC injection port to give a variety of products. The amount of unreacted MPPH was determined based on the amount of $PPh_3$=O generated. When no $PPh_3$=O could be detected, it was assumed that all MPPH was consumed.

Kinetic isotope effects (KIEs) were investigated by using an equimolar mixture of cyclohexane and cyclohexane-$d_{12}$ as the substrate. The organic products were identified and quantified by GC/FID and GC/MS. The KIE value was calculated by taking the ratio of the corresponding peak areas of non deuterated and deuterated organic products from GC measurements.

**Theoretical method.** All optimizations and frequency calculations were done at B3LYP (Becke three-parameter Lee–Yang–Parr hybrid functional) level[5] using LanL2DZ basis set[6] for Os and Fe, and 6-31G(d) basis set for nonmetal atoms. The solvent effect of $CH_3CO_2H$ (acetic acid) is taken into account by the polarizable continuum model.[7] The geometries were fully optimized without symmetry or geometry constraint. The nature of all stationary points was confirmed by vibrational frequencies calculations. All reactants, intermediates, and products have no imaginary frequency while all transition states have only one imaginary frequency. The connectivity of transition state structures were confirmed by intrinsic reaction coordinate calculations.

**Table S1.** Effects of various solvents on catalytic oxidation of cyclohexane by **1**/$H_2O_2$[a]

| Entry | Various solvents | Products yield [b] | | | Total yield |
|---|---|---|---|---|---|
| | | Cy-OH | Cy=O | Cy-Cl | |
| 1 | $CH_2Cl_2/CH_3CO_2H$ (5:2, v/v) | 61% | 12% | 2% | 75% |
| 2 | $CH_2Cl_2/CF_3CH_2OH$ (5:2, v/v) | 63% | 6% | 1% | 70% |
| 3 | $CF_3CH_2OH$ with 1.4% $CH_3CO_2H$ | 53% | 3% | n.d. | 56% |
| 4 | $CF_3CH_2OH$ | 51% | 3% | n.d. | 54% |
| 5 | $CH_3CN$ | n.d. | n.d. | n.d. | 0% |

[a]Reaction conditions: **1** (0.625 mM), cyclohexane (1.2 M), $H_2O_2$ (50 mM, 80 eq.), T = 23 °C, time = 3 h, under argon.

[b]Product yields were calculated based on $H_2O_2$ acting as a two-electron oxidant.

**Table S2.** Catalytic oxidation of cyclohexane by **1** with slow addition of $H_2O_2$[a]

| Entry | Cyclohexane | Products yield [b] | | | Total yield | TON | Time |
|---|---|---|---|---|---|---|---|
| | | Cy-OH | Cy=O | Cy-Cl | | | |
| 1 | 0.69 M | 16% | 4% | 1% | 21% | 787 | 15 min |
| | | 18% | 5% | 1% | 24% | 918 | 1.5 h |
| | | 20% | 6% | 1% | 27% | 1025 | 2.5 h |
| | | 22% | 8% | 1% | 31% | 1183 | 3.5 h |
| | | 31% | 26% | 1% | 58% | 2230 | 20 h |
| 2 | 1.37 M | 10% | 1% | tr. | 11% | 415 | 15 min |
| | | 24% | 4% | 1% | 29% | 1083 | 16.5 h |

[a] Reaction conditions: **1** (0.045 mM), $CH_2Cl_2/CH_3CO_2H$ (5:2), $H_2O_2$ (0.17 M) was slowly added within 3 h using syringe pump, T = 23 °C, under argon. [b] Products yields were calculated based on $H_2O_2$ acting as a two-electron oxidant.

**Table S3.** KIE for catalytic oxidation of cyclohexane by **1**/$H_2O_2$

| KIE for cyclohexanol | KIE for cyclohexanone | KIE for chlorocyclohexane | Overall K. I. E. |
|---|---|---|---|
| 4.12 | 9.74 | 1.69 | 4.16 |

Reaction conditions: **1** (0.625 mM), cyclohexane/cyclohexane-$d_{12}$ (1:1) (1.2 M), $CH_2Cl_2$/$CH_3CO_2H$ (5:2, v/v), $H_2O_2$ (50 mM, 80 equiv.), T = 23 $^oC$, time = 3 h, under argon.

**Table S4.** Catalytic oxidation of cyclohexane by **1**/$H_2O_2$ under various conditions[a]

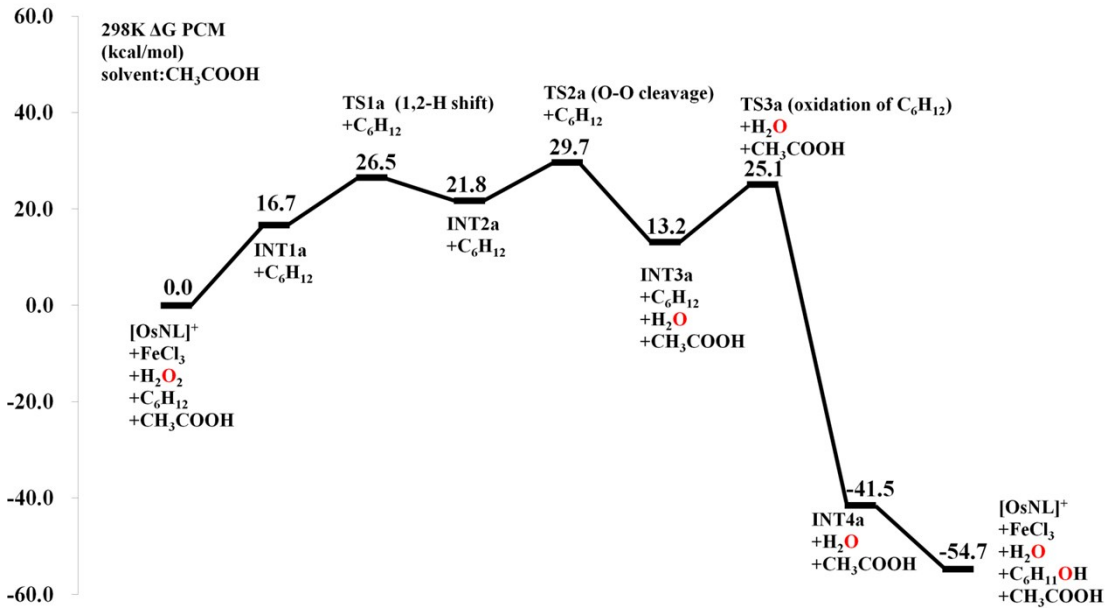
| Entry | Cyclohexane | $H_2O_2$ | Products yield[b] | | | Total yield | Alcohol/ ketone ratio |
|---|---|---|---|---|---|---|---|
| | | | Cy-OH | Cy=O | Cy-Cl | | |
| 1 | 1.2 M | 25 mM | 35% | 3% | 2% | 40% | 11.7 |
| 2 | 1.2 M | 50 mM | 61% | 12% | 2% | 75% | 5.1 |
| 3 | 1.2 M | 100 mM | 30% | 20% | 3% | 53% | 1.5 |
| 4 | 2.4 M | 50 mM | 62% | 8% | 2% | 72% | 7.8 |

[a]Reaction conditions: **1** (0.625 mM), $CH_2Cl_2$/$CH_3CO_2H$ (5:2, v/v), T = 23 $^oC$, time = 3 h, under argon. [b]Products yields were calculated based on $H_2O_2$ acting as a two-electron oxidant.

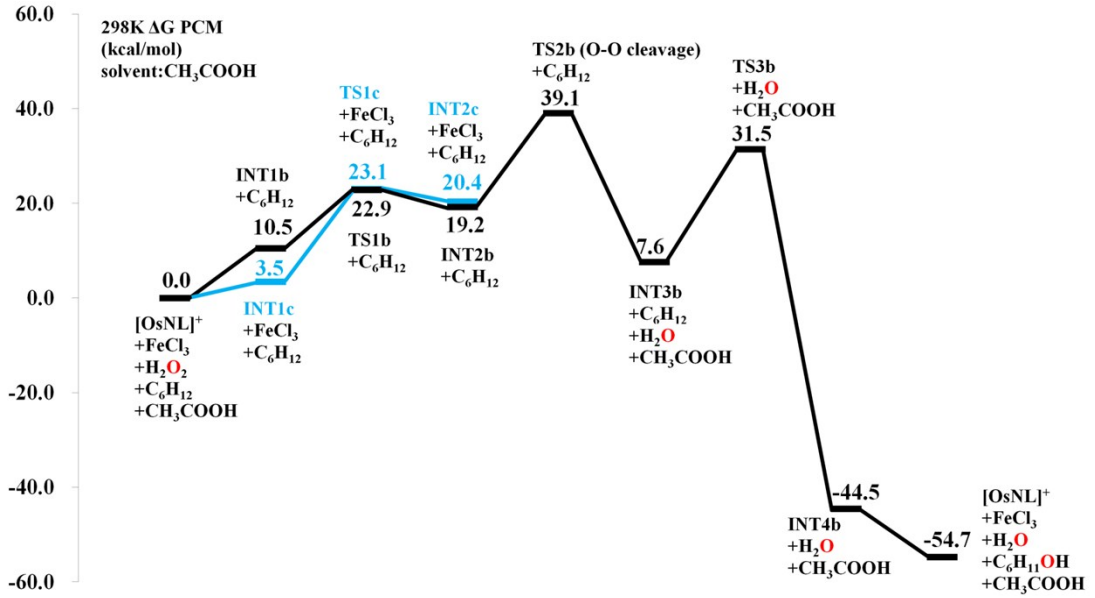
**Table S5** Catalytic oxidation of cyclohexane by **1**/$H_2{}^{18}O_2$[a]

| Products | Products yield[b] | % $^{18}$O-labeled |
|---|---|---|
| Cy-OH | 30% | 100% |
| Cy=O | 5% | 12% |

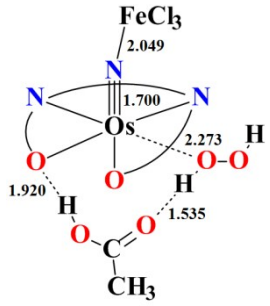
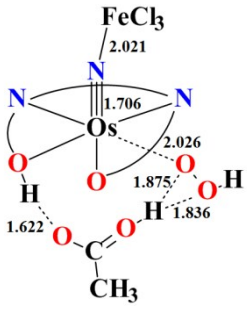
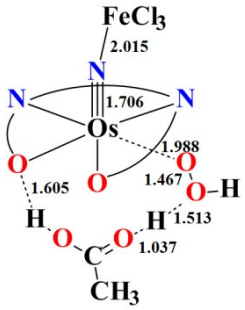
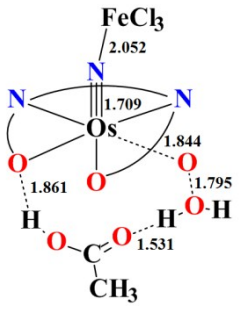
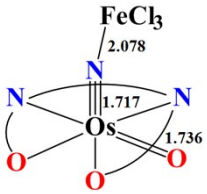
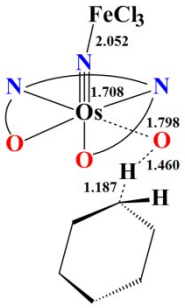
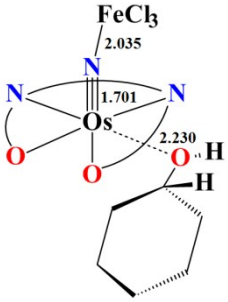
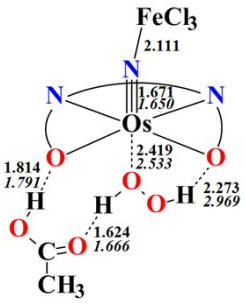
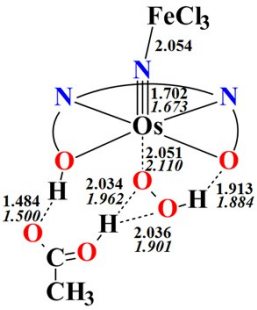
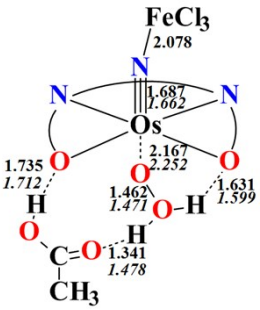
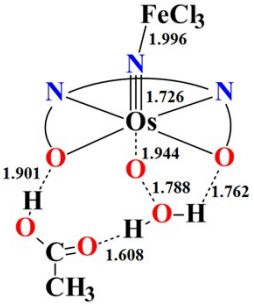
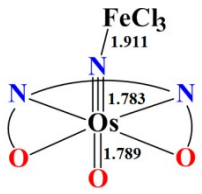
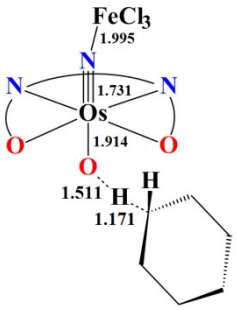
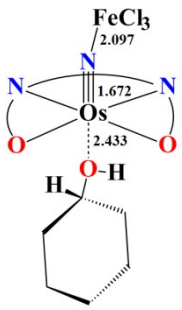
[a]Reaction conditions: **1** (0.625 mM), cyclohexane (1.2 M), $CH_2Cl_2/CH_3CO_2H$ (5:2 v/v), $H_2{}^{18}O_2$ (0.165 M), T = 23 °C, time = 5 h, under argon. [b] Product yield = mmol of product / mmol of $H_2{}^{18}O_2$.




**Scheme S1**. Reaction mechanism ($H_2O_2$ is *cis* to the nitrido ligand) with $FeCl_3$ obtained at B3LYP level. ΔG (298K) free energies are in kcal/mol. Basis sets: LanL2DZ for Os and Fe, 6-31G(d) for non-metal. Solvent: $CH_3CO_2H$.




**Scheme S2**. Reaction mechanism ($H_2O_2$ is *trans* to the nitrido ligand) with $FeCl_3$ (in black) and without $FeCl_3$ (in blue) obtained at B3LYP level. ΔG (298K) free energies are in kcal/mol. Basis sets: LanL2DZ for Os and Fe, 6-31G(d) for non-metal. Solvent: $CH_3CO_2H$.

| | | | |
|---|---|---|---|
| **INT1a** | **TS1a** | **INT2a** | **TS2a** |
|  |  |  |  |
| **INT3a** | **TS3a** | **INT4a** | |
|  |  |  | |
| **INT1b, INT1c** | **TS1b, TS1c** | **INT2b, INT2c** | **TS2b** |
|  |  |  |  |
| **INT3b** | **TS3b** | **INT4b** | |
|  |  |  | |

**Scheme S3.** Structures of intermediates and transition states in Schemes S1 and S2.

## The Cartesian coordinates of all the structures in Scheme 1

**Reactant: $[OsNL]^+$**

| | | | |
|---|---|---|---|
| N | -0.112582 | -0.386047 | 2.138518 |
| N | -1.247515 | 1.045828 | -0.193874 |
| N | 1.367525 | 1.006339 | 0.106232 |
| O | -1.347817 | -1.823866 | -0.063809 |
| O | 1.233086 | -1.862475 | -0.079887 |
| C | -0.562805 | 2.342823 | -0.510979 |
| C | -1.365121 | 3.614141 | -0.204684 |
| C | 0.772189 | 2.360951 | 0.253637 |
| H | -0.335776 | 2.310000 | -1.585231 |
| C | -0.529686 | 4.853989 | -0.577767 |
| H | -1.627161 | 3.629510 | 0.861294 |
| H | -2.300569 | 3.634038 | -0.772321 |
| C | 1.628751 | 3.556231 | -0.167930 |
| H | 0.546534 | 2.455186 | 1.325092 |
| C | 0.846828 | 4.856701 | 0.100876 |
| H | -1.086478 | 5.756038 | -0.302570 |
| H | -0.401883 | 4.883207 | -1.668321 |
| H | 2.565056 | 3.572804 | 0.400439 |
| H | 1.884980 | 3.479821 | -1.233119 |
| H | 1.437653 | 5.709990 | -0.248333 |
| H | 0.723278 | 4.981867 | 1.184822 |
| C | -2.653279 | -1.626598 | -0.213053 |
| C | -3.259936 | -0.341497 | -0.382727 |
| C | -3.473814 | -2.771233 | -0.255316 |
| C | -4.666320 | -0.260569 | -0.586693 |
| C | -4.842330 | -2.652803 | -0.437814 |
| H | -3.001043 | -3.740404 | -0.137506 |
| C | -5.452097 | -1.392312 | -0.602896 |
| H | -5.113499 | 0.719786 | -0.726182 |
| H | -5.453188 | -3.550739 | -0.458257 |
| H | -6.524163 | -1.317249 | -0.748692 |
| C | 2.552366 | -1.736328 | -0.249646 |
| C | 3.250849 | -0.490913 | -0.310658 |
| C | 3.279118 | -2.927343 | -0.428890 |
| C | 4.650983 | -0.495268 | -0.553397 |

| | | | |
|---|---|---|---|
| C | 4.647717 | -2.895142 | -0.654849 |
| H | 2.736094 | -3.865454 | -0.388101 |
| C | 5.346897 | -1.675245 | -0.717679 |
| H | 5.170042 | 0.457956 | -0.603294 |
| H | 5.184124 | -3.830142 | -0.788154 |
| H | 6.416559 | -1.663603 | -0.896193 |
| C | -2.520971 | 0.872224 | -0.453932 |
| C | 2.621075 | 0.783998 | -0.180620 |
| H | -3.076621 | 1.749035 | -0.781175 |
| H | 3.256166 | 1.652774 | -0.342684 |
| Os | -0.023115 | -0.434886 | 0.493579 |

**Reactant: $H_2O_2$**

| | | | |
|---|---|---|---|
| O | 0.196598 | 0.034102 | -0.761265 |
| H | -0.396258 | -0.703832 | -0.994168 |
| O | 0.149051 | -0.037216 | 0.689272 |
| H | -0.400662 | 0.743210 | 0.886811 |

**Reactant: $C_6H_{12}$**

| | | | |
|---|---|---|---|
| C | 0.505747 | 1.377467 | -0.233862 |
| C | -0.938010 | 1.126754 | 0.232036 |
| C | -1.445578 | -0.251127 | -0.224275 |
| C | -0.503249 | -1.377560 | 0.231390 |
| C | 0.940508 | -1.126847 | -0.234507 |
| C | 1.448076 | 0.251034 | 0.221805 |
| H | -2.460097 | -0.427327 | 0.156497 |
| H | -0.976245 | 1.179020 | 1.330607 |
| H | -1.600512 | 1.918408 | -0.141672 |
| H | 0.523963 | 1.440053 | -1.332402 |
| H | 0.862818 | 2.345885 | 0.140243 |
| H | 1.603009 | -1.918502 | 0.139198 |
| H | 0.978743 | -1.179110 | -1.333079 |
| H | 1.519160 | 0.263082 | 1.319913 |
| H | 2.462596 | 0.427234 | -0.158963 |
| H | -1.516665 | -0.263175 | -1.322382 |
| H | -0.521464 | -1.440148 | 1.329930 |
| H | -0.860321 | -2.345976 | -0.142717 |

**Reactant: $CH_3COOH$**

| | | | |
|---|---|---|---|
| C | 0.136967 | 1.390136 | -0.001391 |
| H | 0.716399 | 1.671536 | -0.886834 |
| H | 0.728233 | 1.666019 | 0.877948 |
| H | -0.811821 | 1.927055 | 0.006666 |
| C | -0.119044 | -0.095355 | -0.004306 |
| O | 1.037689 | -0.799261 | -0.014388 |
| H | 0.793316 | -1.744887 | -0.015530 |
| O | -1.207800 | -0.631863 | 0.001724 |

**INT1:**

| | | | |
|---|---|---|---|
| N | -0.359098 | -0.326169 | -1.897013 |
| N | 0.585858 | -1.830656 | 0.280637 |
| N | 2.055667 | 0.155174 | -0.582692 |
| O | -1.836904 | -0.140684 | 0.542066 |
| O | 0.457398 | 1.139604 | 1.366413 |
| C | 2.020436 | -2.172763 | 0.006555 |
| C | 2.273597 | -3.609758 | -0.467552 |
| C | 2.548593 | -1.162907 | -1.040781 |
| H | 2.562354 | -1.992796 | 0.944943 |
| C | 3.776887 | -3.811815 | -0.739973 |
| H | 1.687957 | -3.797382 | -1.376979 |
| H | 1.948841 | -4.333422 | 0.286791 |
| C | 4.055336 | -1.331616 | -1.240088 |
| H | 2.041275 | -1.360948 | -1.993850 |
| C | 4.340642 | -2.768771 | -1.715399 |
| H | 3.934714 | -4.821429 | -1.134016 |
| H | 4.323633 | -3.756267 | 0.211185 |
| H | 4.418666 | -0.609839 | -1.980320 |
| H | 4.589813 | -1.142433 | -0.299762 |
| H | 5.421643 | -2.903913 | -1.826941 |
| H | 3.899500 | -2.915521 | -2.710099 |
| C | -2.327541 | -1.259816 | 1.080872 |
| C | -1.583056 | -2.470703 | 1.254780 |
| C | -3.660249 | -1.221692 | 1.536284 |
| C | -2.218167 | -3.584562 | 1.872766 |
| C | -4.246343 | -2.330851 | 2.126568 |

| | | | |
|---|---|---|---|
| H | -4.219684 | -0.300946 | 1.414360 |
| C | -3.527611 | -3.527751 | 2.299661 |
| H | -1.642463 | -4.496437 | 2.004129 |
| H | -5.276726 | -2.266433 | 2.463979 |
| H | -3.994180 | -4.388820 | 2.765478 |
| C | 1.291536 | 2.160708 | 1.427734 |
| C | 2.465441 | 2.230694 | 0.611500 |
| C | 1.051286 | 3.204437 | 2.348819 |
| C | 3.351263 | 3.325241 | 0.749341 |
| C | 1.921392 | 4.283161 | 2.434095 |
| H | 0.170629 | 3.137360 | 2.979578 |
| C | 3.076304 | 4.353980 | 1.631931 |
| H | 4.251013 | 3.350913 | 0.140203 |
| H | 1.708442 | 5.082252 | 3.138563 |
| H | 3.749376 | 5.200558 | 1.715868 |
| C | -0.216252 | -2.664869 | 0.884345 |
| C | 2.848137 | 1.113390 | -0.198718 |
| H | 0.205267 | -3.631846 | 1.152356 |
| H | 3.902834 | 1.023775 | -0.454072 |
| Os | 0.002680 | 0.014969 | -0.305345 |
| O | -0.597754 | 2.136327 | -0.936303 |
| H | -1.337709 | 2.029527 | -1.632430 |
| C | -5.037213 | 1.879901 | -2.781761 |
| H | -5.698324 | 2.505476 | -2.173381 |
| H | -5.554039 | 0.930716 | -2.956546 |
| H | -4.827586 | 2.371359 | -3.731384 |
| C | -3.755956 | 1.629781 | -2.038965 |
| O | -3.946756 | 1.054265 | -0.858096 |
| O | -2.649258 | 1.930079 | -2.489857 |
| O | -1.346898 | 2.881187 | 0.060794 |
| H | -0.676661 | 3.543874 | 0.317596 |
| H | -3.098660 | 0.829777 | -0.397765 |

**TS1:**

| | | | |
|---|---|---|---|
| N | 0.434880 | 0.532026 | -1.978188 |
| N | -0.657437 | 1.720922 | 0.303658 |
| N | -1.999849 | -0.258688 | -0.765928 |
| O | 1.903748 | 0.149786 | 0.434519 |

| | | | |
|---|---|---|---|
| O | -0.445170 | -1.027728 | 1.394037 |
| C | -2.084164 | 2.030296 | -0.019290 |
| C | -2.366596 | 3.485501 | -0.416024 |
| C | -2.530315 | 1.070750 | -1.157321 |
| H | -2.667266 | 1.771407 | 0.874437 |
| C | -3.861538 | 3.656389 | -0.749376 |
| H | -1.745110 | 3.748517 | -1.281771 |
| H | -2.099761 | 4.168812 | 0.396914 |
| C | -4.035090 | 1.198618 | -1.398372 |
| H | -2.003036 | 1.353519 | -2.076370 |
| C | -4.348162 | 2.651806 | -1.804828 |
| H | -4.034740 | 4.680633 | -1.096628 |
| H | -4.449227 | 3.532679 | 0.170374 |
| H | -4.349245 | 0.506247 | -2.187465 |
| H | -4.595906 | 0.945414 | -0.489183 |
| H | -5.427593 | 2.759319 | -1.954906 |
| H | -3.872011 | 2.868369 | -2.770238 |
| C | 2.331644 | 1.276259 | 1.114938 |
| C | 1.452820 | 2.344797 | 1.427169 |
| C | 3.661969 | 1.304744 | 1.528899 |
| C | 1.979838 | 3.418389 | 2.186368 |
| C | 4.143675 | 2.385985 | 2.264577 |
| H | 4.316022 | 0.480418 | 1.269160 |
| C | 3.300830 | 3.448430 | 2.602792 |
| H | 1.318704 | 4.242446 | 2.437023 |
| H | 5.182781 | 2.389480 | 2.578279 |
| H | 3.672718 | 4.287251 | 3.180753 |
| C | -1.298415 | -2.019439 | 1.529278 |
| C | -2.413384 | -2.213617 | 0.641214 |
| C | -1.154067 | -2.919150 | 2.613776 |
| C | -3.309473 | -3.292688 | 0.863850 |
| C | -2.024199 | -3.982847 | 2.777120 |
| H | -0.327756 | -2.759194 | 3.299874 |
| C | -3.109897 | -4.183038 | 1.897260 |
| H | -4.158317 | -3.409430 | 0.195191 |
| H | -1.872737 | -4.670719 | 3.604457 |
| H | -3.787837 | -5.016782 | 2.045888 |
| C | 0.063027 | 2.500181 | 1.039399 |

| | | | |
|---|---|---|---|
| C | -2.775541 | -1.207473 | -0.300198 |
| H | -0.406348 | 3.407439 | 1.418647 |
| H | -3.824945 | -1.155637 | -0.586040 |
| Os | 0.011332 | -0.096522 | -0.492956 |
| O | 0.331423 | -2.038476 | -0.911586 |
| H | 2.237334 | -2.181415 | -1.795851 |
| C | 5.312979 | -1.601792 | -2.573323 |
| H | 5.687335 | -2.629006 | -2.505023 |
| H | 6.046472 | -0.913771 | -2.153966 |
| H | 5.147195 | -1.383319 | -3.632408 |
| C | 4.018718 | -1.496378 | -1.821837 |
| O | 3.900267 | -0.822888 | -0.792449 |
| O | 3.037430 | -2.195000 | -2.367072 |
| O | 1.427231 | -2.559239 | -0.090717 |
| H | 1.060884 | -2.457642 | 0.811051 |
| H | 2.680584 | -0.375114 | -0.014605 |

**INT2:**

| | | | |
|---|---|---|---|
| N | -0.459623 | -0.560726 | -1.955053 |
| N | 0.636591 | -1.708993 | 0.324048 |
| N | 1.999074 | 0.238536 | -0.769809 |
| O | -1.883548 | -0.076767 | 0.430059 |
| O | 0.505727 | 0.985736 | 1.402096 |
| C | 2.046641 | -2.052008 | -0.026289 |
| C | 2.282229 | -3.509215 | -0.445301 |
| C | 2.507182 | -1.096110 | -1.160673 |
| H | 2.652632 | -1.822182 | 0.860352 |
| C | 3.771847 | -3.718430 | -0.780831 |
| H | 1.653163 | -3.738372 | -1.315383 |
| H | 1.991352 | -4.196702 | 0.356142 |
| C | 4.008369 | -1.255580 | -1.404981 |
| H | 1.972872 | -1.370409 | -2.078435 |
| C | 4.288691 | -2.712918 | -1.821980 |
| H | 3.918470 | -4.741986 | -1.142579 |
| H | 4.361667 | -3.623670 | 0.141167 |
| H | 4.337672 | -0.566438 | -2.190939 |
| H | 4.575476 | -1.017941 | -0.495362 |
| H | 5.365889 | -2.846449 | -1.968642 |

| | | | |
|---|---|---|---|
| H | 3.811878 | -2.908024 | -2.791806 |
| C | -2.235003 | -1.080784 | 1.258419 |
| C | -1.406467 | -2.193068 | 1.600600 |
| C | -3.517443 | -0.997883 | 1.830326 |
| C | -1.918470 | -3.168980 | 2.495262 |
| C | -3.985949 | -1.975090 | 2.698272 |
| H | -4.136101 | -0.141238 | 1.583938 |
| C | -3.185544 | -3.075519 | 3.038547 |
| H | -1.282073 | -4.010982 | 2.752979 |
| H | -4.981847 | -1.875577 | 3.120073 |
| H | -3.550751 | -3.836896 | 3.719223 |
| C | 1.309239 | 2.010405 | 1.493705 |
| C | 2.415056 | 2.214615 | 0.591499 |
| C | 1.150058 | 2.940942 | 2.554529 |
| C | 3.286795 | 3.319250 | 0.780471 |
| C | 1.993360 | 4.029070 | 2.681965 |
| H | 0.330496 | 2.778884 | 3.247746 |
| C | 3.071231 | 4.232354 | 1.790651 |
| H | 4.129370 | 3.438690 | 0.103673 |
| H | 1.829459 | 4.736819 | 3.490504 |
| H | 3.729953 | 5.085649 | 1.914383 |
| C | -0.063649 | -2.435563 | 1.134409 |
| C | 2.784509 | 1.187468 | -0.325908 |
| H | 0.404595 | -3.337814 | 1.528208 |
| H | 3.834701 | 1.127404 | -0.609958 |
| Os | -0.032973 | 0.086381 | -0.475843 |
| O | -0.296636 | 2.011185 | -0.951463 |
| H | -2.534813 | 2.403262 | -1.377922 |
| C | -5.059893 | 1.014124 | -3.061458 |
| H | -5.402819 | 1.977968 | -3.438127 |
| H | -5.881959 | 0.443056 | -2.626666 |
| H | -4.648656 | 0.435651 | -3.898171 |
| C | -3.977592 | 1.204888 | -2.055405 |
| O | -3.799051 | 0.259656 | -1.206568 |
| O | -3.286430 | 2.274214 | -2.112012 |
| O | -1.531307 | 2.567346 | -0.353749 |
| H | -1.264582 | 3.499530 | -0.238085 |
| H | -3.003598 | 0.298323 | -0.538463 |

**TS2:**

| | | | |
|---|---|---|---|
| N | -0.498744 | -0.632111 | -1.899301 |
| N | 0.571841 | -1.679484 | 0.419399 |
| N | 1.989177 | 0.116631 | -0.821456 |
| O | -1.831055 | 0.066465 | 0.486277 |
| O | 0.616031 | 1.026728 | 1.372072 |
| C | 1.939037 | -2.130347 | 0.030362 |
| C | 2.064785 | -3.616726 | -0.329304 |
| C | 2.407345 | -1.259476 | -1.163944 |
| H | 2.595562 | -1.903031 | 0.880571 |
| C | 3.526402 | -3.930011 | -0.706118 |
| H | 1.390863 | -3.844119 | -1.165355 |
| H | 1.761750 | -4.247627 | 0.513030 |
| C | 3.885990 | -1.514995 | -1.455841 |
| H | 1.822878 | -1.543566 | -2.047763 |
| C | 4.062894 | -3.005299 | -1.810718 |
| H | 3.599136 | -4.975449 | -1.024735 |
| H | 4.154700 | -3.829698 | 0.189355 |
| H | 4.221169 | -0.884839 | -2.287332 |
| H | 4.501326 | -1.268704 | -0.580961 |
| H | 5.124222 | -3.210155 | -1.986983 |
| H | 3.540491 | -3.214723 | -2.753544 |
| C | -2.184422 | -0.814374 | 1.441705 |
| C | -1.407651 | -1.939307 | 1.848411 |
| C | -3.422715 | -0.584948 | 2.065674 |
| C | -1.921143 | -2.787907 | 2.863004 |
| C | -3.894844 | -1.438299 | 3.054250 |
| H | -3.998789 | 0.281566 | 1.758132 |
| C | -3.144402 | -2.552168 | 3.461310 |
| H | -1.324319 | -3.642769 | 3.168773 |
| H | -4.855369 | -1.232170 | 3.517320 |
| H | -3.515567 | -3.215634 | 4.234833 |
| C | 1.465065 | 2.016751 | 1.382850 |
| C | 2.540495 | 2.132135 | 0.426017 |
| C | 1.392577 | 2.997589 | 2.407548 |
| C | 3.465592 | 3.207118 | 0.527868 |
| C | 2.283749 | 4.052279 | 2.447264 |
| H | 0.597886 | 2.901821 | 3.140540 |

| | | | |
|---|---|---|---|
| C | 3.329872 | 4.170911 | 1.501722 |
| H | 4.282075 | 3.259675 | -0.187784 |
| H | 2.184780 | 4.801826 | 3.228021 |
| H | 4.026192 | 5.000904 | 1.559195 |
| C | -0.115117 | -2.298088 | 1.326273 |
| C | 2.833952 | 1.044969 | -0.443483 |
| H | 0.330035 | -3.191755 | 1.764159 |
| H | 3.869475 | 0.916835 | -0.757388 |
| Os | -0.050603 | 0.119360 | -0.472701 |
| O | -0.189541 | 1.921379 | -0.992037 |
| H | -2.310800 | 2.407107 | -1.245570 |
| C | -5.081059 | 0.645923 | -3.261827 |
| H | -5.188221 | 1.493975 | -3.937467 |
| H | -6.030895 | 0.438755 | -2.759474 |
| H | -4.808358 | -0.250181 | -3.829498 |
| C | -4.017721 | 0.931145 | -2.241947 |
| O | -3.890801 | -0.024467 | -1.335105 |
| O | -3.332273 | 1.958294 | -2.263386 |
| O | -1.638251 | 2.739336 | -0.527527 |
| H | -1.329605 | 3.622911 | -0.812068 |
| H | -3.155648 | 0.159281 | -0.692021 |

**INT3:**

| | | | |
|---|---|---|---|
| N | 0.860082 | 0.407609 | -2.069272 |
| N | 0.916358 | 1.066054 | 0.536230 |
| N | -1.424153 | 0.826936 | -0.613038 |
| O | 1.600778 | -1.548660 | -0.237292 |
| O | -0.814856 | -1.351040 | 0.957100 |
| C | -0.018893 | 2.193652 | 0.759876 |
| C | 0.629280 | 3.565996 | 0.986353 |
| C | -0.967748 | 2.227311 | -0.472135 |
| H | -0.632014 | 1.927632 | 1.630855 |
| C | -0.447546 | 4.661266 | 1.094787 |
| H | 1.310619 | 3.785504 | 0.153910 |
| H | 1.223289 | 3.557893 | 1.906158 |
| C | -2.055881 | 3.288802 | -0.304927 |
| H | -0.371171 | 2.452562 | -1.365083 |
| C | -1.392300 | 4.664359 | -0.113694 |

| | | | |
|---|---|---|---|
| H | 0.045989 | 5.633854 | 1.193191 |
| H | -1.029279 | 4.508377 | 2.013854 |
| H | -2.708964 | 3.295114 | -1.184394 |
| H | -2.675639 | 3.065752 | 0.572805 |
| H | -2.172471 | 5.421377 | 0.017657 |
| H | -0.837338 | 4.934805 | -1.021725 |
| C | 2.841209 | -1.201273 | 0.155769 |
| C | 3.126178 | 0.052425 | 0.752864 |
| C | 3.846595 | -2.167822 | 0.028128 |
| C | 4.442043 | 0.300807 | 1.205171 |
| C | 5.135524 | -1.883447 | 0.466515 |
| H | 3.596446 | -3.124428 | -0.417125 |
| C | 5.440828 | -0.647202 | 1.056658 |
| H | 4.659933 | 1.256954 | 1.672271 |
| H | 5.911150 | -2.634344 | 0.350968 |
| H | 6.448211 | -0.438300 | 1.399988 |
| C | -2.073869 | -1.617692 | 0.958724 |
| C | -3.042037 | -0.804508 | 0.229483 |
| C | -2.575960 | -2.698774 | 1.742245 |
| C | -4.432313 | -1.131895 | 0.296254 |
| C | -3.916495 | -3.000682 | 1.739350 |
| H | -1.858479 | -3.289090 | 2.301846 |
| C | -4.860363 | -2.219913 | 1.009141 |
| H | -5.140385 | -0.504122 | -0.236617 |
| H | -4.270760 | -3.852264 | 2.313271 |
| H | -5.912439 | -2.481577 | 1.038874 |
| C | 2.132839 | 1.074431 | 0.971021 |
| C | -2.653772 | 0.444833 | -0.279870 |
| H | 2.466868 | 1.929950 | 1.557016 |
| H | -3.418384 | 1.213032 | -0.377856 |
| Os | 0.111175 | -0.481436 | -0.851347 |
| O | -0.847722 | -1.697527 | -1.655455 |

**TS3:**

| | | | |
|---|---|---|---|
| N | -0.784253 | 0.680597 | -2.132259 |
| N | -2.040349 | 0.947399 | 0.282636 |
| N | -1.604915 | -1.478951 | -0.610395 |
| O | 0.771534 | 1.613649 | 0.037820 |

| | | | |
|---|---|---|---|
| O | 0.090182 | -0.704601 | 1.385685 |
| C | -3.227197 | 0.047742 | 0.275746 |
| C | -4.582241 | 0.740676 | 0.081097 |
| C | -2.989039 | -1.010685 | -0.837849 |
| H | -3.220110 | -0.484323 | 1.236242 |
| C | -5.711407 | -0.305269 | 0.017261 |
| H | -4.556462 | 1.331547 | -0.843822 |
| H | -4.784018 | 1.431074 | 0.906621 |
| C | -4.092870 | -2.068881 | -0.834713 |
| H | -2.989222 | -0.496098 | -1.806720 |
| C | -5.452311 | -1.378572 | -1.048893 |
| H | -6.658574 | 0.206704 | -0.183691 |
| H | -5.814851 | -0.783957 | 1.000586 |
| H | -3.907358 | -2.802215 | -1.627289 |
| H | -4.106739 | -2.607958 | 0.121189 |
| H | -6.246144 | -2.132661 | -1.025079 |
| H | -5.477558 | -0.924103 | -2.048324 |
| C | 0.349410 | 2.811967 | 0.461836 |
| C | -1.000330 | 3.101676 | 0.812057 |
| C | 1.326071 | 3.812484 | 0.601222 |
| C | -1.314662 | 4.398464 | 1.290015 |
| C | 0.979588 | 5.076066 | 1.060653 |
| H | 2.350152 | 3.569840 | 0.338632 |
| C | -0.347378 | 5.379205 | 1.408006 |
| H | -2.344244 | 4.613078 | 1.562948 |
| H | 1.750107 | 5.835797 | 1.153321 |
| H | -0.609035 | 6.367953 | 1.769034 |
| C | 0.391254 | -1.956630 | 1.511032 |
| C | -0.204903 | -2.990858 | 0.682727 |
| C | 1.286054 | -2.376722 | 2.537962 |
| C | 0.133291 | -4.357606 | 0.902143 |
| C | 1.620610 | -3.704706 | 2.685376 |
| H | 1.714891 | -1.609601 | 3.174344 |
| C | 1.049978 | -4.711925 | 1.861641 |
| H | -0.341940 | -5.116421 | 0.286284 |
| H | 2.331205 | -3.991696 | 3.455817 |
| H | 1.323577 | -5.751363 | 2.008083 |
| C | -2.081063 | 2.152425 | 0.755678 |

| | | | |
|---|---|---|---|
| C | -1.326287 | -2.668885 | -0.119363 |
| H | -3.029065 | 2.506037 | 1.158587 |
| H | -2.070003 | -3.446230 | -0.288548 |
| Os | -0.298300 | 0.109819 | -0.634493 |
| O | 1.167429 | -0.902021 | -1.023426 |
| C | 4.034229 | 0.077096 | 0.521612 |
| C | 5.534567 | 0.483805 | 0.526218 |
| C | 6.344015 | -0.362165 | -0.464756 |
| C | 5.759997 | -0.284526 | -1.881157 |
| C | 4.261254 | -0.696737 | -1.894239 |
| C | 3.508599 | 0.159644 | -0.896656 |
| H | 7.388869 | -0.025873 | -0.474510 |
| H | 5.619893 | 1.546468 | 0.261516 |
| H | 5.924837 | 0.375829 | 1.545662 |
| H | 3.943290 | -0.950942 | 0.895211 |
| H | 3.460970 | 0.727000 | 1.189944 |
| H | 3.848418 | -0.584661 | -2.902548 |
| H | 4.181289 | -1.755225 | -1.614993 |
| H | 3.372763 | 1.190302 | -1.242188 |
| H | 2.377535 | -0.280288 | -0.887916 |
| H | 6.352495 | -1.409001 | -0.129821 |
| H | 5.853894 | 0.739967 | -2.265669 |
| H | 6.310026 | -0.937248 | -2.569903 |

**INT4:**

| | | | |
|---|---|---|---|
| N | 0.384445 | -0.297081 | -1.961841 |
| N | 2.173200 | 0.616040 | -0.017337 |
| N | -0.195544 | 1.708076 | -0.058454 |
| O | 1.076068 | -2.100198 | 0.169672 |
| O | -0.341911 | -0.404319 | 1.691064 |
| C | 2.171238 | 2.113733 | -0.067258 |
| C | 3.349366 | 2.747224 | -0.820005 |
| C | 0.833383 | 2.552845 | -0.708413 |
| H | 2.171867 | 2.462145 | 0.974436 |
| C | 3.201444 | 4.280970 | -0.822645 |
| H | 3.371018 | 2.360496 | -1.847273 |
| H | 4.301991 | 2.481978 | -0.350599 |
| C | 0.671652 | 4.071304 | -0.630598 |

| | | | |
|---|---|---|---|
| H | 0.846468 | 2.254655 | -1.764253 |
| C | 1.843759 | 4.737413 | -1.376043 |
| H | 4.014971 | 4.716962 | -1.412268 |
| H | 3.322088 | 4.653830 | 0.203611 |
| H | -0.282147 | 4.370897 | -1.079521 |
| H | 0.666251 | 4.404016 | 0.415276 |
| H | 1.751280 | 5.825671 | -1.295274 |
| H | 1.778704 | 4.493129 | -2.444588 |
| C | 2.357917 | -2.417882 | 0.273283 |
| C | 3.434115 | -1.472055 | 0.294235 |
| C | 2.666377 | -3.788359 | 0.408519 |
| C | 4.766641 | -1.947057 | 0.454391 |
| C | 3.976760 | -4.212846 | 0.550968 |
| H | 1.843095 | -4.494826 | 0.396661 |
| C | 5.043132 | -3.291572 | 0.574895 |
| H | 5.574223 | -1.220223 | 0.475619 |
| H | 4.181805 | -5.275185 | 0.648534 |
| H | 6.065010 | -3.636531 | 0.689490 |
| C | -1.382016 | 0.218045 | 2.210430 |
| C | -1.847681 | 1.480833 | 1.719569 |
| C | -2.048474 | -0.351841 | 3.320337 |
| C | -2.949850 | 2.115388 | 2.346392 |
| C | -3.143221 | 0.279129 | 3.890335 |
| H | -1.680807 | -1.298580 | 3.703285 |
| C | -3.607750 | 1.517872 | 3.403428 |
| H | -3.274890 | 3.084054 | 1.975500 |
| H | -3.646422 | -0.187956 | 4.732387 |
| H | -4.461532 | 2.002151 | 3.865312 |
| C | 3.272090 | -0.057612 | 0.198807 |
| C | -1.098195 | 2.204938 | 0.739706 |
| H | 4.180454 | 0.528061 | 0.325775 |
| H | -1.251210 | 3.282710 | 0.705682 |
| Os | 0.377097 | -0.280274 | -0.297689 |
| O | -1.563807 | -1.419571 | -0.440757 |
| C | -2.866024 | -1.160319 | -2.480492 |
| C | -4.215830 | -0.714176 | -3.072418 |
| C | -5.394718 | -1.412077 | -2.377072 |
| C | -5.348359 | -1.204008 | -0.855649 |

| | | | |
|---|---|---|---|
| C | -3.995211 | -1.646973 | -0.268806 |
| C | -2.848308 | -0.925748 | -0.973833 |
| H | -6.344551 | -1.038035 | -2.777532 |
| H | -4.319935 | 0.375030 | -2.963793 |
| H | -4.226021 | -0.922440 | -4.148289 |
| H | -2.710629 | -2.231320 | -2.666223 |
| H | -2.037889 | -0.623928 | -2.955351 |
| H | -3.963131 | -1.443245 | 0.810000 |
| H | -3.868057 | -2.729552 | -0.406494 |
| H | -2.893924 | 0.147263 | -0.755575 |
| H | -1.690623 | -1.749743 | 0.467733 |
| H | -5.360467 | -2.488422 | -2.597472 |
| H | -5.512436 | -0.141946 | -0.624988 |
| H | -6.154832 | -1.759855 | -0.364239 |

**Product: $H_2O$**

| | | | |
|---|---|---|---|
| O | 0.000000 | 0.000000 | -0.142354 |
| H | 0.000000 | -0.760425 | 0.459018 |
| H | 0.000000 | 0.760425 | 0.459018 |

**Product: $C_6H_{11}OH$**

| | | | |
|---|---|---|---|
| C | -1.159297 | -1.268827 | -0.208856 |
| C | 0.332563 | -1.265206 | 0.165983 |
| C | 1.040913 | -0.000005 | -0.335225 |
| C | 0.332597 | 1.265251 | 0.165886 |
| C | -1.159266 | 1.268883 | -0.208945 |
| C | -1.867579 | 0.000054 | 0.291373 |
| H | 0.433415 | -1.308523 | 1.262174 |
| H | 0.840900 | -2.150081 | -0.236058 |
| H | -1.256515 | -1.329850 | -1.302802 |
| H | -1.645872 | -2.164483 | 0.197068 |
| H | 0.433452 | 1.308649 | 1.262074 |
| H | 0.840953 | 2.150084 | -0.236223 |
| H | -1.645814 | 2.164579 | 0.196922 |
| H | -1.256488 | 1.329835 | -1.302894 |
| H | -1.875499 | 0.000092 | 1.391464 |
| H | -2.916859 | 0.000057 | -0.030077 |
| H | 1.028576 | -0.000046 | -1.433424 |

| | | | |
|---|---|---|---|
| O | 2.432353 | -0.000013 | 0.002040 |
| H | 2.490730 | 0.000170 | 0.972093 |

## The Cartesian coordinate of all the structures on Scheme S1, S2, and S3

**Reactant: $FeCl_3$**

| | | | |
|---|---|---|---|
| Fe | 0.035131 | -0.020283 | -0.180547 |
| Cl | 1.936374 | -1.117958 | 0.086100 |
| Cl | -0.063854 | 2.165878 | 0.091186 |
| Cl | -1.907652 | -1.027637 | 0.091185 |

**INT1a**

| | | | |
|---|---|---|---|
| N | 0.751133 | 0.513979 | -0.613009 |
| N | -0.695291 | 0.911536 | 1.738403 |
| N | -2.033692 | 0.866699 | -0.502304 |
| O | 0.601738 | -1.679205 | 1.200362 |
| O | -2.007115 | -1.597597 | 0.532044 |
| C | -1.615053 | 2.080264 | 1.522075 |
| C | -1.155347 | 3.404362 | 2.146845 |
| C | -1.800395 | 2.244308 | -0.006058 |
| H | -2.583634 | 1.786413 | 1.948470 |
| C | -2.166399 | 4.517974 | 1.809204 |
| H | -0.160391 | 3.658210 | 1.760886 |
| H | -1.077610 | 3.316188 | 3.235179 |
| C | -2.863235 | 3.298929 | -0.312760 |
| H | -0.845302 | 2.567733 | -0.436046 |
| C | -2.421242 | 4.641139 | 0.300549 |
| H | -1.791017 | 5.466758 | 2.206734 |
| H | -3.113814 | 4.312701 | 2.325625 |
| H | -2.986750 | 3.402289 | -1.396665 |
| H | -3.832205 | 3.000680 | 0.108740 |
| H | -3.192562 | 5.394563 | 0.109852 |
| H | -1.509170 | 4.986168 | -0.203247 |
| C | 1.108558 | -1.473692 | 2.420128 |
| C | 0.818570 | -0.328187 | 3.230626 |
| C | 1.955923 | -2.470168 | 2.938424 |
| C | 1.410790 | -0.233752 | 4.521611 |

| | | | |
|---|---|---|---|
| C | 2.521318 | -2.336918 | 4.197903 |
| H | 2.164819 | -3.341847 | 2.328890 |
| C | 2.254210 | -1.212876 | 5.001236 |
| H | 1.184687 | 0.636659 | 5.130754 |
| H | 3.177672 | -3.119439 | 4.566688 |
| H | 2.700957 | -1.121405 | 5.984978 |
| C | -3.067906 | -1.856571 | -0.219874 |
| C | -3.627213 | -0.867708 | -1.087693 |
| C | -3.690110 | -3.115818 | -0.120370 |
| C | -4.784819 | -1.178389 | -1.836577 |
| C | -4.808608 | -3.399345 | -0.890768 |
| H | -3.264720 | -3.849309 | 0.555745 |
| C | -5.357912 | -2.435905 | -1.759147 |
| H | -5.218438 | -0.415145 | -2.476292 |
| H | -5.269470 | -4.379871 | -0.818336 |
| H | -6.235423 | -2.673856 | -2.350598 |
| C | -0.056294 | 0.736855 | 2.866962 |
| C | -3.164957 | 0.485817 | -1.022698 |
| H | -0.216347 | 1.495022 | 3.629731 |
| H | -3.852940 | 1.263040 | -1.350285 |
| Os | -0.493854 | -0.333655 | 0.176077 |
| O | -0.332339 | -1.719910 | -1.617601 |
| H | 0.660620 | -1.758547 | -1.887258 |
| C | 4.214049 | -3.232883 | -1.992162 |
| H | 4.426295 | -4.227459 | -1.593557 |
| H | 4.984428 | -2.547123 | -1.619947 |
| H | 4.243688 | -3.236431 | -3.081977 |
| C | 2.877750 | -2.745150 | -1.518990 |
| O | 2.598104 | -3.101676 | -0.271718 |
| O | 2.128459 | -2.059635 | -2.220517 |
| O | -0.540041 | -3.117908 | -1.286437 |
| H | -1.082140 | -3.395179 | -2.050616 |
| H | 1.759810 | -2.696028 | 0.054927 |
| Fe | 2.247867 | 1.601938 | -1.493970 |
| Cl | 1.930310 | 1.606883 | -3.689659 |
| Cl | 1.857074 | 3.647495 | -0.658314 |
| Cl | 4.140952 | 0.758026 | -0.675702 |

**TS1a**

| | | | |
|---|---|---|---|
| N | 0.911452 | 0.509723 | -0.632664 |
| N | -0.664033 | 0.950753 | 1.606285 |
| N | -1.867782 | 1.098493 | -0.710914 |
| O | 0.451496 | -1.754228 | 0.979015 |
| O | -2.201106 | -1.240716 | 0.569506 |
| C | -1.414392 | 2.220975 | 1.368513 |
| C | -0.823450 | 3.472547 | 2.031971 |
| C | -1.512645 | 2.432488 | -0.167408 |
| H | -2.433220 | 2.054779 | 1.743687 |
| C | -1.688143 | 4.700401 | 1.686009 |
| H | 0.206932 | 3.613972 | 1.682550 |
| H | -0.786336 | 3.353811 | 3.119787 |
| C | -2.443083 | 3.602384 | -0.486849 |
| H | -0.512298 | 2.663620 | -0.550969 |
| C | -1.879063 | 4.876345 | 0.172134 |
| H | -1.222957 | 5.595405 | 2.112577 |
| H | -2.669278 | 4.594534 | 2.168942 |
| H | -2.516330 | 3.738379 | -1.571715 |
| H | -3.453395 | 3.406128 | -0.104586 |
| H | -2.556650 | 5.713532 | -0.026175 |
| H | -0.918585 | 5.129053 | -0.295554 |
| C | 0.781558 | -1.690636 | 2.282135 |
| C | 0.493260 | -0.582546 | 3.140483 |
| C | 1.435589 | -2.811014 | 2.824235 |
| C | 0.898549 | -0.655865 | 4.499612 |
| C | 1.820663 | -2.842016 | 4.157818 |
| H | 1.635454 | -3.658816 | 2.178278 |
| C | 1.556283 | -1.758242 | 5.009171 |
| H | 0.678442 | 0.188385 | 5.146593 |
| H | 2.327912 | -3.722423 | 4.540949 |
| H | 1.857783 | -1.786513 | 6.050447 |
| C | -3.263737 | -1.420486 | -0.184732 |
| C | -3.668461 | -0.460339 | -1.175003 |
| C | -4.073534 | -2.561844 | 0.017119 |
| C | -4.845839 | -0.688154 | -1.928521 |
| C | -5.194560 | -2.773339 | -0.767113 |
| H | -3.775032 | -3.270951 | 0.782206 |

| | | | |
|---|---|---|---|
| C | -5.586236 | -1.840291 | -1.751820 |
| H | -5.154218 | 0.058976 | -2.654616 |
| H | -5.788023 | -3.670354 | -0.615189 |
| H | -6.473758 | -2.019754 | -2.349132 |
| C | -0.196865 | 0.624235 | 2.773377 |
| C | -3.048508 | 0.826283 | -1.200788 |
| H | -0.344353 | 1.336914 | 3.583580 |
| H | -3.647381 | 1.665325 | -1.551357 |
| Os | -0.489136 | -0.266499 | -0.044533 |
| O | -0.754179 | -1.487120 | -1.639278 |
| H | 0.781163 | -2.401227 | -2.208586 |
| C | 3.739972 | -3.761367 | -2.044737 |
| H | 4.071693 | -4.513903 | -1.328467 |
| H | 4.476324 | -2.947629 | -2.061596 |
| H | 3.658420 | -4.174774 | -3.050555 |
| C | 2.441554 | -3.183355 | -1.616116 |
| O | 2.185013 | -3.164926 | -0.362537 |
| O | 1.669947 | -2.719509 | -2.531419 |
| O | -0.699831 | -2.907083 | -1.247804 |
| H | -1.448415 | -3.253555 | -1.768762 |
| H | 1.363564 | -2.676535 | 0.004127 |
| Fe | 2.609230 | 1.497238 | -1.109473 |
| Cl | 1.918390 | 3.298178 | -2.235692 |
| Cl | 3.421864 | 1.940074 | 0.931055 |
| Cl | 3.891231 | 0.069293 | -2.257798 |

**INT2a**

| | | | |
|---|---|---|---|
| N | 0.857282 | 0.771464 | -0.412307 |
| N | -0.976870 | 0.721613 | 1.674619 |
| N | -1.968908 | 1.009397 | -0.726289 |
| O | 0.559624 | -1.717908 | 0.878492 |
| O | -2.085139 | -1.499948 | 0.263912 |
| C | -1.844771 | 1.924287 | 1.496012 |
| C | -1.462142 | 3.147643 | 2.340130 |
| C | -1.836868 | 2.301956 | -0.010481 |
| H | -2.866088 | 1.609500 | 1.749643 |
| C | -2.438075 | 4.303826 | 2.045950 |
| H | -0.431542 | 3.441807 | 2.104408 |

| | | | |
|---|---|---|---|
| H | -1.497295 | 2.907903 | 3.407891 |
| C | -2.878843 | 3.384259 | -0.291010 |
| H | -0.844458 | 2.691849 | -0.265713 |
| C | -2.530184 | 4.629947 | 0.547360 |
| H | -2.119992 | 5.190519 | 2.604470 |
| H | -3.434309 | 4.034629 | 2.422610 |
| H | -2.883895 | 3.634326 | -1.357764 |
| H | -3.883281 | 3.030143 | -0.024320 |
| H | -3.288870 | 5.401164 | 0.377632 |
| H | -1.575194 | 5.043884 | 0.198080 |
| C | 0.661490 | -1.826915 | 2.217743 |
| C | 0.125046 | -0.894174 | 3.159427 |
| C | 1.342098 | -2.957367 | 2.703388 |
| C | 0.324515 | -1.138403 | 4.543998 |
| C | 1.520693 | -3.159713 | 4.065337 |
| H | 1.727872 | -3.676289 | 1.988701 |
| C | 1.013339 | -2.245189 | 5.000670 |
| H | -0.084766 | -0.426148 | 5.254549 |
| H | 2.055505 | -4.042356 | 4.403170 |
| H | 1.153119 | -2.406594 | 6.063858 |
| C | -3.047854 | -1.716934 | -0.604111 |
| C | -3.506239 | -0.698240 | -1.511312 |
| C | -3.706447 | -2.968840 | -0.611481 |
| C | -4.583214 | -0.978203 | -2.388803 |
| C | -4.725869 | -3.220797 | -1.512529 |
| H | -3.371628 | -3.725146 | 0.090921 |
| C | -5.169174 | -2.227714 | -2.413659 |
| H | -4.936778 | -0.192248 | -3.050350 |
| H | -5.199574 | -4.198302 | -1.520028 |
| H | -5.977189 | -2.441644 | -3.105070 |
| C | -0.636034 | 0.285101 | 2.848039 |
| C | -3.065096 | 0.649056 | -1.342438 |
| H | -0.971222 | 0.861629 | 3.709681 |
| H | -3.741793 | 1.443765 | -1.652895 |
| Os | -0.478533 | -0.237878 | -0.085863 |
| O | -0.493320 | -1.197556 | -1.827266 |
| H | 1.406607 | -2.686108 | -2.058568 |
| C | 4.680686 | -2.789550 | -1.576213 |

| | | | |
|---|---|---|---|
| H | 4.842365 | -3.503667 | -2.384761 |
| H | 5.212111 | -3.083693 | -0.670560 |
| H | 5.054685 | -1.809718 | -1.899512 |
| C | 3.227329 | -2.645024 | -1.302156 |
| O | 2.881733 | -2.338569 | -0.103546 |
| O | 2.413532 | -2.813868 | -2.270313 |
| O | -0.062406 | -2.594784 | -1.708074 |
| H | -0.618689 | -3.011573 | -2.394826 |
| H | 1.895229 | -2.183585 | 0.120006 |
| Fe | 2.537824 | 1.766930 | -0.907815 |
| Cl | 3.289410 | 0.640489 | -2.697172 |
| Cl | 1.973669 | 3.878099 | -1.364008 |
| Cl | 3.847811 | 1.544010 | 0.883331 |

**TS2a**

| | | | |
|---|---|---|---|
| N | 0.956312 | 0.687892 | -0.245398 |
| N | -0.975412 | 0.485313 | 1.748365 |
| N | -1.783009 | 1.232984 | -0.608802 |
| O | 0.358278 | -1.906782 | 0.663919 |
| O | -2.232659 | -1.358935 | 0.029777 |
| C | -1.703045 | 1.787678 | 1.724341 |
| C | -1.241541 | 2.820636 | 2.761469 |
| C | -1.562981 | 2.380678 | 0.300128 |
| H | -2.763861 | 1.552588 | 1.883711 |
| C | -2.075918 | 4.107800 | 2.607918 |
| H | -0.175576 | 3.031923 | 2.610548 |
| H | -1.357037 | 2.429406 | 3.777445 |
| C | -2.464801 | 3.603611 | 0.136202 |
| H | -0.522656 | 2.690749 | 0.152327 |
| C | -2.042313 | 4.662029 | 1.175081 |
| H | -1.701420 | 4.860588 | 3.309517 |
| H | -3.115201 | 3.897962 | 2.895710 |
| H | -2.367722 | 4.007192 | -0.877596 |
| H | -3.517369 | 3.334235 | 0.291409 |
| H | -2.706381 | 5.528782 | 1.092775 |
| H | -1.030413 | 5.014842 | 0.937703 |
| C | 0.311967 | -2.279144 | 1.957488 |
| C | -0.209996 | -1.474681 | 3.012979 |

| | | | |
|---|---|---|---|
| C | 0.827240 | -3.550593 | 2.255388 |
| C | -0.175319 | -1.986398 | 4.334712 |
| C | 0.847690 | -4.018114 | 3.563526 |
| H | 1.209193 | -4.157257 | 1.441516 |
| C | 0.346639 | -3.235860 | 4.615413 |
| H | -0.573824 | -1.371987 | 5.136780 |
| H | 1.253663 | -5.004458 | 3.766353 |
| H | 0.363701 | -3.606924 | 5.634210 |
| C | -3.148798 | -1.350799 | -0.910136 |
| C | -3.429602 | -0.177314 | -1.700634 |
| C | -3.942374 | -2.503722 | -1.117361 |
| C | -4.465117 | -0.217427 | -2.670471 |
| C | -4.911785 | -2.518726 | -2.103154 |
| H | -3.744275 | -3.375900 | -0.503406 |
| C | -5.177102 | -1.376237 | -2.893617 |
| H | -4.681240 | 0.680983 | -3.241559 |
| H | -5.487239 | -3.425116 | -2.267904 |
| H | -5.949982 | -1.408968 | -3.653914 |
| C | -0.804262 | -0.176751 | 2.850892 |
| C | -2.876096 | 1.075842 | -1.313591 |
| H | -1.164747 | 0.287149 | 3.768590 |
| H | -3.448788 | 1.975316 | -1.533911 |
| Os | -0.454171 | -0.271840 | -0.146816 |
| O | -0.518641 | -0.929753 | -1.868552 |
| H | 1.022423 | -2.604043 | -2.132018 |
| C | 4.853829 | -2.745685 | -1.548476 |
| H | 5.039212 | -3.218058 | -2.512972 |
| H | 5.310998 | -3.322622 | -0.740487 |
| H | 5.303705 | -1.746406 | -1.543244 |
| C | 3.378443 | -2.606127 | -1.323186 |
| O | 3.062552 | -2.297050 | -0.070127 |
| O | 2.544206 | -2.750921 | -2.218695 |
| O | -0.010022 | -2.635213 | -2.103745 |
| H | -0.313558 | -2.652114 | -3.033233 |
| H | 2.086683 | -2.196915 | 0.039180 |
| Fe | 2.616326 | 1.812797 | -0.680875 |
| Cl | 3.394658 | 0.765688 | -2.484254 |
| Cl | 1.793040 | 3.844551 | -1.114611 |

| | | | |
|---|---|---|---|
| Cl | 3.900580 | 1.812580 | 1.137337 |

**INT3a**

| | | | |
|---|---|---|---|
| N | -0.880622 | -0.222338 | -0.915863 |
| N | 0.015901 | 0.063281 | 1.588355 |
| N | 1.588144 | -1.178720 | -0.097101 |
| O | -0.126339 | 2.287652 | -0.111484 |
| O | 2.341417 | 1.401579 | 0.353254 |
| C | 0.592341 | -1.210718 | 2.077192 |
| C | -0.250904 | -1.977687 | 3.105033 |
| C | 0.854547 | -2.082313 | 0.813668 |
| H | 1.571250 | -0.967502 | 2.510793 |
| C | 0.393699 | -3.337381 | 3.433647 |
| H | -1.261838 | -2.125003 | 2.704835 |
| H | -0.338479 | -1.392885 | 4.026969 |
| C | 1.553134 | -3.392922 | 1.178901 |
| H | -0.106666 | -2.302423 | 0.334236 |
| C | 0.672766 | -4.168384 | 2.174948 |
| H | -0.271275 | -3.885529 | 4.109105 |
| H | 1.332179 | -3.174035 | 3.979863 |
| H | 1.724893 | -3.986743 | 0.274592 |
| H | 2.527656 | -3.190711 | 1.641902 |
| H | 1.178564 | -5.101704 | 2.442751 |
| H | -0.271675 | -4.447556 | 1.690043 |
| C | -1.146739 | 2.674723 | 0.676249 |
| C | -1.549670 | 1.923556 | 1.811280 |
| C | -1.756856 | 3.899003 | 0.374819 |
| C | -2.598065 | 2.430005 | 2.610538 |
| C | -2.801032 | 4.354969 | 1.171098 |
| H | -1.410723 | 4.458347 | -0.487011 |
| C | -3.228207 | 3.621992 | 2.290345 |
| H | -2.908000 | 1.864715 | 3.484236 |
| H | -3.287386 | 5.292463 | 0.920562 |
| H | -4.040297 | 3.991238 | 2.906836 |
| C | 3.517680 | 1.063764 | -0.086374 |
| C | 3.799558 | -0.270897 | -0.592001 |
| C | 4.585682 | 1.994027 | -0.016210 |
| C | 5.114484 | -0.585458 | -1.048585 |

| | | | |
|---|---|---|---|
| C | 5.829417 | 1.658177 | -0.505321 |
| H | 4.378327 | 2.977792 | 0.389921 |
| C | 6.102483 | 0.365946 | -1.034371 |
| H | 5.314011 | -1.588849 | -1.412152 |
| H | 6.624882 | 2.397147 | -0.482251 |
| H | 7.095528 | 0.134566 | -1.403296 |
| C | -0.897273 | 0.710381 | 2.236016 |
| C | 2.886462 | -1.311360 | -0.336985 |
| H | -1.219693 | 0.321470 | 3.200615 |
| H | 3.275381 | -2.324947 | -0.263402 |
| Os | 0.594793 | 0.553304 | -0.504080 |
| Fe | -2.727365 | -1.091336 | -1.306243 |
| Cl | -3.729704 | 0.550947 | -2.412880 |
| Cl | -2.086930 | -2.878000 | -2.464769 |
| Cl | -3.507016 | -1.520917 | 0.745092 |
| O | 1.434620 | 0.810418 | -2.001057 |

**TS3a**

| | | | |
|---|---|---|---|
| N | 0.740161 | -0.818395 | -0.750605 |
| N | 1.545749 | 0.576368 | 1.451865 |
| N | 0.916500 | 1.944021 | -0.696662 |
| O | -1.016810 | -0.739114 | 1.439403 |
| O | -0.953124 | 1.971550 | 1.255008 |
| C | 2.558035 | 1.576710 | 1.011040 |
| C | 4.016976 | 1.231940 | 1.338725 |
| C | 2.375111 | 1.767771 | -0.521531 |
| H | 2.285710 | 2.525667 | 1.491866 |
| C | 4.961450 | 2.304248 | 0.762145 |
| H | 4.255985 | 0.245585 | 0.921729 |
| H | 4.162803 | 1.177895 | 2.422574 |
| C | 3.274959 | 2.887221 | -1.045359 |
| H | 2.639224 | 0.829836 | -1.024317 |
| C | 4.741614 | 2.531700 | -0.739375 |
| H | 5.996285 | 1.999872 | 0.950795 |
| H | 4.807626 | 3.248706 | 1.301185 |
| H | 3.128002 | 3.009131 | -2.124264 |
| H | 3.023648 | 3.839817 | -0.560896 |
| H | 5.387092 | 3.340995 | -1.096232 |

| | | | |
|---|---|---|---|
| H | 5.023763 | 1.631062 | -1.300052 |
| C | -0.513558 | -1.381032 | 2.503091 |
| C | 0.787434 | -1.136735 | 3.028714 |
| C | -1.355681 | -2.313736 | 3.128971 |
| C | 1.200356 | -1.865068 | 4.170107 |
| C | -0.910535 | -3.020412 | 4.238464 |
| H | -2.346429 | -2.471525 | 2.717470 |
| C | 0.373142 | -2.801564 | 4.765032 |
| H | 2.190024 | -1.677285 | 4.575953 |
| H | -1.569046 | -3.748250 | 4.702481 |
| H | 0.711083 | -3.356087 | 5.633557 |
| C | -1.475149 | 2.997772 | 0.641267 |
| C | -0.919724 | 3.528863 | -0.588424 |
| C | -2.580745 | 3.672880 | 1.218808 |
| C | -1.509375 | 4.675836 | -1.190006 |
| C | -3.151486 | 4.753073 | 0.577699 |
| H | -2.978074 | 3.291842 | 2.153438 |
| C | -2.624058 | 5.260907 | -0.638315 |
| H | -1.065857 | 5.074526 | -2.097773 |
| H | -4.020888 | 5.232483 | 1.018257 |
| H | -3.088161 | 6.118736 | -1.112515 |
| C | 1.702702 | -0.155232 | 2.510339 |
| C | 0.366489 | 3.101497 | -0.999017 |
| H | 2.618015 | -0.022862 | 3.084840 |
| H | 0.992669 | 3.809337 | -1.538603 |
| Os | -0.120415 | 0.374437 | 0.117866 |
| O | -1.594977 | 0.639431 | -0.876823 |
| Fe | 1.807181 | -2.257077 | -1.752455 |
| Cl | 0.311474 | -3.894454 | -1.944774 |
| Cl | 2.440338 | -1.171406 | -3.595625 |
| Cl | 3.486494 | -2.688947 | -0.342766 |
| C | -4.851255 | 0.134732 | -1.058372 |
| C | -6.227017 | -0.581791 | -0.955037 |
| C | -6.140002 | -2.024127 | -1.468842 |
| C | -5.053056 | -2.819858 | -0.736294 |
| C | -3.672420 | -2.111578 | -0.838426 |
| C | -3.809594 | -0.690688 | -0.325730 |
| H | -7.111074 | -2.521215 | -1.344897 |

| | | | |
|---|---|---|---|
| H | -6.554512 | -0.580047 | 0.093255 |
| H | -6.966433 | -0.004735 | -1.523696 |
| H | -4.577914 | 0.229226 | -2.117195 |
| H | -4.920731 | 1.144596 | -0.639492 |
| H | -2.921214 | -2.667561 | -0.268008 |
| H | -3.355302 | -2.103682 | -1.889137 |
| H | -3.937544 | -0.648981 | 0.762293 |
| H | -2.774100 | -0.140236 | -0.510260 |
| H | -5.924420 | -2.016775 | -2.546435 |
| H | -5.323308 | -2.929249 | 0.322776 |
| H | -4.958534 | -3.831186 | -1.149855 |

**INT4a**

| | | | |
|---|---|---|---|
| N | 0.394012 | 1.055183 | -0.096248 |
| N | 1.957433 | -1.204635 | 0.351959 |
| N | -0.317807 | -1.068181 | 1.618033 |
| O | 0.677589 | -0.810466 | -2.256797 |
| O | -0.683391 | -2.427084 | -0.668757 |
| C | 2.043889 | -1.434164 | 1.832500 |
| C | 3.349354 | -0.979917 | 2.499013 |
| C | 0.835042 | -0.718020 | 2.481081 |
| H | 1.912384 | -2.514454 | 1.980263 |
| C | 3.276172 | -1.243853 | 4.016085 |
| H | 3.505685 | 0.087779 | 2.299162 |
| H | 4.206350 | -1.522645 | 2.087308 |
| C | 0.738412 | -1.058671 | 3.968162 |
| H | 0.974926 | 0.364641 | 2.377849 |
| C | 2.037219 | -0.610695 | 4.664858 |
| H | 4.186748 | -0.857939 | 4.486197 |
| H | 3.266376 | -2.328169 | 4.190665 |
| H | -0.123907 | -0.549916 | 4.412866 |
| H | 0.597242 | -2.138641 | 4.107370 |
| H | 1.988277 | -0.881689 | 5.724652 |
| H | 2.112270 | 0.483664 | 4.621461 |
| C | 1.921132 | -0.973206 | -2.698935 |
| C | 3.048742 | -1.234022 | -1.853623 |
| C | 2.114359 | -0.909953 | -4.091631 |
| C | 4.325362 | -1.415681 | -2.455190 |

| | | | |
|---|---|---|---|
| C | 3.376818 | -1.079464 | -4.638287 |
| H | 1.249097 | -0.720001 | -4.717580 |
| C | 4.495480 | -1.333746 | -3.820997 |
| H | 5.175743 | -1.619984 | -1.811288 |
| H | 3.500098 | -1.018387 | -5.715475 |
| H | 5.477166 | -1.468051 | -4.261641 |
| C | -1.796696 | -2.895674 | -0.129682 |
| C | -2.201010 | -2.537905 | 1.196208 |
| C | -2.575092 | -3.820106 | -0.855334 |
| C | -3.372915 | -3.109554 | 1.743125 |
| C | -3.738418 | -4.334746 | -0.304032 |
| H | -2.247100 | -4.099729 | -1.850868 |
| C | -4.148629 | -3.978146 | 0.996337 |
| H | -3.658465 | -2.851591 | 2.759014 |
| H | -4.339454 | -5.029569 | -0.882940 |
| H | -5.058254 | -4.396035 | 1.413976 |
| C | 2.990914 | -1.370537 | -0.434939 |
| C | -1.316136 | -1.792622 | 2.037834 |
| H | 3.922483 | -1.656258 | 0.048412 |
| H | -1.435756 | -1.906840 | 3.113794 |
| Os | 0.164046 | -0.611710 | -0.343997 |
| O | -1.800211 | -0.147602 | -1.292321 |
| Fe | 0.689119 | 2.999884 | 0.427117 |
| Cl | -0.080628 | 4.291452 | -1.220762 |
| Cl | -0.430861 | 3.167794 | 2.355143 |
| Cl | 2.900656 | 3.099368 | 0.719644 |
| C | -3.655852 | 1.102960 | -2.256718 |
| C | -4.593722 | 2.312820 | -2.087691 |
| C | -5.258380 | 2.313087 | -0.703204 |
| C | -4.210666 | 2.246138 | 0.418000 |
| C | -3.269400 | 1.038494 | 0.244153 |
| C | -2.622029 | 1.073121 | -1.133258 |
| H | -5.877508 | 3.210078 | -0.584808 |
| H | -4.018630 | 3.239424 | -2.220310 |
| H | -5.349798 | 2.295554 | -2.880587 |
| H | -4.237705 | 0.172056 | -2.223603 |
| H | -3.153475 | 1.145678 | -3.232297 |
| H | -2.501571 | 1.044224 | 1.025795 |

| | | | |
|---|---|---|---|
| H | -3.838084 | 0.104409 | 0.340878 |
| H | -1.946012 | 1.931483 | -1.217779 |
| H | -1.591473 | -0.257626 | -2.241437 |
| H | -5.933649 | 1.449165 | -0.624146 |
| H | -3.617847 | 3.171062 | 0.421600 |
| H | -4.697707 | 2.183819 | 1.397608 |

**INT1b**

| | | | |
|---|---|---|---|
| N | 0.972289 | -0.589042 | -0.900030 |
| N | -0.375846 | -1.135060 | 1.608035 |
| N | 1.002429 | 1.122154 | 1.336075 |
| O | -1.907232 | -0.556955 | -0.770775 |
| O | -0.656442 | 1.816095 | -0.948015 |
| C | 0.296415 | -0.651569 | 2.855639 |
| C | 0.745521 | -1.738422 | 3.838831 |
| C | 1.486792 | 0.226011 | 2.427510 |
| H | -0.443058 | -0.004433 | 3.343634 |
| C | 1.417144 | -1.081566 | 5.060036 |
| H | 1.441820 | -2.424145 | 3.338521 |
| H | -0.111685 | -2.326723 | 4.181602 |
| C | 2.124723 | 0.912366 | 3.637952 |
| H | 2.235003 | -0.420111 | 1.948731 |
| C | 2.569633 | -0.153300 | 4.657258 |
| H | 1.781324 | -1.866802 | 5.730738 |
| H | 0.663096 | -0.512297 | 5.619963 |
| H | 2.997277 | 1.497279 | 3.329160 |
| H | 1.404118 | 1.603187 | 4.095255 |
| H | 2.978373 | 0.346934 | 5.541411 |
| H | 3.386460 | -0.745381 | 4.224087 |
| C | -2.349186 | -1.816728 | -0.589030 |
| C | -1.955802 | -2.646776 | 0.504731 |
| C | -3.271981 | -2.310245 | -1.522788 |
| C | -2.513746 | -3.948252 | 0.612352 |
| C | -3.782599 | -3.596727 | -1.396534 |
| H | -3.571857 | -1.669892 | -2.344966 |
| C | -3.403852 | -4.427402 | -0.328334 |
| H | -2.219684 | -4.569494 | 1.453235 |
| H | -4.487888 | -3.959337 | -2.138242 |

| | | | |
|---|---|---|---|
| H | -3.811443 | -5.428280 | -0.239785 |
| C | 0.085152 | 2.940248 | -0.909608 |
| C | 1.066697 | 3.227022 | 0.088630 |
| C | -0.182162 | 3.896801 | -1.899829 |
| C | 1.735335 | 4.478494 | 0.048609 |
| C | 0.505137 | 5.105027 | -1.917852 |
| H | -0.933372 | 3.664637 | -2.647035 |
| C | 1.470783 | 5.404281 | -0.942234 |
| H | 2.473849 | 4.694871 | 0.814852 |
| H | 0.285702 | 5.826132 | -2.699453 |
| H | 1.998678 | 6.351215 | -0.963833 |
| C | -1.101035 | -2.220173 | 1.569095 |
| C | 1.412826 | 2.348246 | 1.164196 |
| H | -1.068581 | -2.866698 | 2.443691 |
| H | 2.103633 | 2.747125 | 1.903975 |
| Os | -0.204307 | 0.144533 | 0.032737 |
| Fe | 2.695521 | -1.383212 | -1.825418 |
| Cl | 2.165700 | -3.471933 | -2.340618 |
| Cl | 3.162910 | 0.026747 | -3.470725 |
| Cl | 4.071151 | -1.174637 | -0.073320 |
| O | -1.873414 | 2.555082 | 1.611328 |
| H | -1.859440 | 2.850702 | 0.678837 |
| O | -1.897753 | 1.118651 | 1.459960 |
| H | -2.843084 | 0.954806 | 1.133074 |
| C | -6.150273 | 1.749393 | -0.861169 |
| H | -6.083046 | 2.627879 | -1.510217 |
| H | -6.683045 | 1.997968 | 0.056351 |
| H | -6.698899 | 0.977592 | -1.411594 |
| C | -4.773155 | 1.247570 | -0.535906 |
| O | -4.024927 | 1.031602 | -1.614917 |
| H | -3.166516 | 0.611386 | -1.355089 |
| O | -4.378508 | 1.048741 | 0.613335 |

**TS1b**

| | | | |
|---|---|---|---|
| N | 0.623549 | -0.576741 | -1.019870 |
| N | -0.323074 | -0.913252 | 1.600532 |
| N | 1.463632 | 1.029546 | 1.070491 |
| O | -2.102174 | -0.194567 | -0.668345 |

| | | | |
|---|---|---|---|
| O | -0.301580 | 2.178111 | -0.941324 |
| C | 0.607111 | -0.575170 | 2.720006 |
| C | 0.938593 | -1.721938 | 3.679916 |
| C | 1.887295 | 0.015693 | 2.087622 |
| H | 0.101783 | 0.228641 | 3.270056 |
| C | 1.922979 | -1.234725 | 4.758476 |
| H | 1.373093 | -2.559181 | 3.118070 |
| H | 0.027340 | -2.084891 | 4.166903 |
| C | 2.853481 | 0.519522 | 3.163910 |
| H | 2.380984 | -0.776015 | 1.507791 |
| C | 3.185644 | -0.620998 | 4.143590 |
| H | 2.187931 | -2.077839 | 5.404964 |
| H | 1.422658 | -0.492918 | 5.394986 |
| H | 3.782423 | 0.872704 | 2.704718 |
| H | 2.402127 | 1.365008 | 3.699477 |
| H | 3.841550 | -0.234205 | 4.930461 |
| H | 3.752548 | -1.397324 | 3.612742 |
| C | -2.620741 | -1.454259 | -0.424511 |
| C | -2.146731 | -2.267852 | 0.636157 |
| C | -3.644163 | -1.894514 | -1.258077 |
| C | -2.751770 | -3.536447 | 0.809343 |
| C | -4.211431 | -3.153698 | -1.061151 |
| H | -3.987199 | -1.248249 | -2.058622 |
| C | -3.762211 | -3.982480 | -0.028068 |
| H | -2.405578 | -4.168443 | 1.621384 |
| H | -5.004384 | -3.486847 | -1.723155 |
| H | -4.201609 | -4.962357 | 0.122307 |
| C | 0.715844 | 3.051826 | -1.069649 |
| C | 1.887608 | 3.047257 | -0.254238 |
| C | 0.563948 | 4.051081 | -2.041693 |
| C | 2.860291 | 4.062127 | -0.450866 |
| C | 1.546111 | 5.018345 | -2.220445 |
| H | -0.335297 | 4.043320 | -2.648351 |
| C | 2.702845 | 5.030931 | -1.423625 |
| H | 3.746191 | 4.059798 | 0.177455 |
| H | 1.409273 | 5.775849 | -2.986351 |
| H | 3.460904 | 5.792975 | -1.566964 |
| C | -1.137186 | -1.920351 | 1.614599 |

| | | | |
|---|---|---|---|
| C | 2.154614 | 2.096567 | 0.783457 |
| H | -1.064006 | -2.604545 | 2.457209 |
| H | 3.040333 | 2.284206 | 1.385178 |
| Os | -0.183149 | 0.449063 | 0.072531 |
| Fe | 1.885600 | -1.992542 | -1.807708 |
| Cl | 1.417058 | -3.707818 | -0.457792 |
| Cl | 1.610127 | -2.347963 | -3.975608 |
| Cl | 3.842116 | -1.069201 | -1.261304 |
| O | -1.507473 | 2.858781 | 1.385218 |
| H | -1.280156 | 3.055710 | 0.449067 |
| O | -1.381331 | 1.422090 | 1.422576 |
| H | -3.332931 | 1.967927 | 1.246786 |
| C | -6.157795 | 2.324444 | -0.280870 |
| H | -6.530098 | 1.916631 | -1.220229 |
| H | -6.198961 | 3.418993 | -0.315788 |
| H | -6.782709 | 1.999365 | 0.555525 |
| C | -4.738077 | 1.896543 | -0.059857 |
| O | -4.050358 | 1.379467 | -0.949534 |
| H | -2.850895 | 0.520621 | -0.790656 |
| O | -4.297834 | 2.144208 | 1.161510 |

**INT2c**

| | | | |
|---|---|---|---|
| N | 0.714838 | -0.508182 | -0.984574 |
| N | -0.218701 | -1.235005 | 1.646176 |
| N | 1.470822 | 0.807235 | 1.340798 |
| O | -2.021035 | -0.228130 | -0.466398 |
| O | -0.444362 | 2.107254 | -0.479734 |
| C | 0.739533 | -1.025512 | 2.777348 |
| C | 1.150189 | -2.288517 | 3.541903 |
| C | 1.973614 | -0.302089 | 2.200881 |
| H | 0.232828 | -0.334474 | 3.462861 |
| C | 2.150699 | -1.920630 | 4.653496 |
| H | 1.598171 | -3.010539 | 2.846546 |
| H | 0.274846 | -2.763681 | 3.996065 |
| C | 2.952341 | 0.089995 | 3.310929 |
| H | 2.475350 | -0.992228 | 1.507470 |
| C | 3.365778 | -1.162273 | 4.106145 |
| H | 2.472709 | -2.836561 | 5.159928 |

| | | | |
|---|---|---|---|
| H | 1.640891 | -1.305577 | 5.407147 |
| H | 3.847265 | 0.553291 | 2.882675 |
| H | 2.480854 | 0.824480 | 3.977184 |
| H | 4.025185 | -0.861696 | 4.927130 |
| H | 3.952889 | -1.824427 | 3.456135 |
| C | -2.548540 | -1.455624 | -0.332372 |
| C | -2.127755 | -2.410648 | 0.649339 |
| C | -3.598696 | -1.804339 | -1.199755 |
| C | -2.806489 | -3.657644 | 0.728818 |
| C | -4.222575 | -3.041486 | -1.105642 |
| H | -3.909594 | -1.086786 | -1.950420 |
| C | -3.832662 | -3.980016 | -0.135351 |
| H | -2.491337 | -4.368012 | 1.487583 |
| H | -5.025568 | -3.280577 | -1.796564 |
| H | -4.329536 | -4.941365 | -0.066710 |
| C | 0.543060 | 3.044534 | -0.513299 |
| C | 1.709039 | 3.013825 | 0.304768 |
| C | 0.337804 | 4.123962 | -1.378749 |
| C | 2.618092 | 4.099300 | 0.226582 |
| C | 1.260047 | 5.164606 | -1.443431 |
| H | -0.555200 | 4.126712 | -1.994679 |
| C | 2.406815 | 5.159500 | -0.636699 |
| H | 3.503515 | 4.078808 | 0.855241 |
| H | 1.081125 | 5.988933 | -2.127084 |
| H | 3.120290 | 5.974562 | -0.688391 |
| C | -1.087427 | -2.208002 | 1.609902 |
| C | 2.065226 | 1.953735 | 1.210431 |
| H | -1.008974 | -2.964190 | 2.388032 |
| H | 2.945084 | 2.133379 | 1.824812 |
| Os | -0.160566 | 0.235252 | 0.251563 |
| Fe | 1.987084 | -1.408322 | -2.358956 |
| Cl | 0.689620 | -2.237975 | -3.947068 |
| Cl | 3.381829 | 0.201369 | -3.003419 |
| Cl | 2.908906 | -2.905735 | -0.977707 |
| O | -1.945506 | 2.360686 | 1.550638 |
| H | -1.497030 | 2.584361 | 0.671660 |
| O | -1.323195 | 1.077967 | 1.875072 |
| H | -3.005301 | 2.134577 | 1.324868 |

| | | | |
|---|---|---|---|
| C | -6.193820 | 2.269502 | -0.429181 |
| H | -6.780277 | 1.353608 | -0.563580 |
| H | -6.218422 | 2.815632 | -1.376395 |
| H | -6.627401 | 2.868009 | 0.371179 |
| C | -4.783786 | 1.898620 | -0.091912 |
| O | -4.109453 | 1.373967 | -1.091289 |
| H | -3.245673 | 0.950235 | -0.817956 |
| O | -4.315889 | 2.074179 | 1.047576 |

**TS2b**

| | | | |
|---|---|---|---|
| N | 0.240164 | -0.587094 | -1.040989 |
| N | 0.193965 | -1.203981 | 1.701601 |
| N | 2.203759 | 0.316660 | 0.757669 |
| O | -1.942843 | 0.328696 | 0.252284 |
| O | 0.338646 | 2.226996 | -0.464064 |
| C | 1.488936 | -1.333131 | 2.435367 |
| C | 1.758787 | -2.693090 | 3.086547 |
| C | 2.616018 | -0.945073 | 1.451404 |
| H | 1.444735 | -0.561445 | 3.214855 |
| C | 3.125819 | -2.669197 | 3.794465 |
| H | 1.739424 | -3.480217 | 2.321301 |
| H | 0.981329 | -2.924113 | 3.822048 |
| C | 3.969678 | -0.898871 | 2.169065 |
| H | 2.653291 | -1.707938 | 0.661309 |
| C | 4.253820 | -2.253186 | 2.844028 |
| H | 3.327844 | -3.661235 | 4.211508 |
| H | 3.080626 | -1.972816 | 4.642213 |
| H | 4.772402 | -0.684967 | 1.456502 |
| H | 3.962029 | -0.092898 | 2.914773 |
| H | 5.202463 | -2.188093 | 3.387032 |
| H | 4.384916 | -3.020628 | 2.069870 |
| C | -2.646153 | -0.707292 | 0.561449 |
| C | -2.143448 | -1.854337 | 1.319266 |
| C | -4.021164 | -0.715235 | 0.144365 |
| C | -3.031189 | -2.905978 | 1.592252 |
| C | -4.841264 | -1.784243 | 0.415736 |
| H | -4.379289 | 0.146588 | -0.406446 |
| C | -4.349863 | -2.893920 | 1.140611 |

| | | | |
|---|---|---|---|
| H | -2.676711 | -3.753251 | 2.171006 |
| H | -5.870757 | -1.776765 | 0.073591 |
| H | -5.000152 | -3.734600 | 1.355884 |
| C | 1.482748 | 2.778403 | -0.898397 |
| C | 2.788624 | 2.315296 | -0.542123 |
| C | 1.365718 | 3.914093 | -1.716195 |
| C | 3.921566 | 3.025386 | -1.025904 |
| C | 2.495322 | 4.574101 | -2.181178 |
| H | 0.369201 | 4.253497 | -1.978437 |
| C | 3.785666 | 4.133081 | -1.837759 |
| H | 4.910572 | 2.669809 | -0.751435 |
| H | 2.374580 | 5.444049 | -2.819847 |
| H | 4.661454 | 4.656321 | -2.205306 |
| C | -0.829575 | -1.973370 | 1.904318 |
| C | 3.061341 | 1.176787 | 0.278258 |
| H | -0.705503 | -2.806059 | 2.592499 |
| H | 4.109840 | 1.000967 | 0.506465 |
| Os | 0.227358 | 0.369778 | 0.395303 |
| Fe | -0.036123 | -1.878301 | -2.537219 |
| Cl | -1.987000 | -1.282846 | -3.456922 |
| Cl | 1.738452 | -1.615305 | -3.881193 |
| Cl | -0.086505 | -3.900648 | -1.556506 |
| O | -0.384463 | 3.076438 | 1.946260 |
| H | -0.138104 | 3.112967 | 0.982594 |
| O | -0.253593 | 1.295230 | 2.035628 |
| H | -1.399111 | 3.125206 | 1.961017 |
| C | -5.012453 | 4.245167 | 0.860467 |
| H | -5.898392 | 3.602322 | 0.891825 |
| H | -5.035981 | 4.787166 | -0.090047 |
| H | -5.032851 | 4.945987 | 1.694531 |
| C | -3.774364 | 3.398927 | 0.932287 |
| O | -3.643659 | 2.581301 | -0.112123 |
| H | -2.888404 | 1.959855 | 0.012484 |
| O | -2.969857 | 3.452287 | 1.859951 |

**INT3b**

| | | | |
|---|---|---|---|
| N | -0.301126 | -0.703467 | 0.626768 |
| N | -0.778068 | 1.567478 | -0.856702 |

| | | | |
|---|---|---|---|
| N | 1.740809 | 1.088314 | 0.022015 |
| O | -1.133051 | -1.213674 | -1.942487 |
| O | 1.734890 | -1.749827 | -0.944523 |
| C | 0.026150 | 2.771012 | -0.497472 |
| C | -0.770503 | 3.977621 | 0.007189 |
| C | 1.096763 | 2.330820 | 0.539608 |
| H | 0.550851 | 3.037412 | -1.424832 |
| C | 0.182995 | 5.132395 | 0.362813 |
| H | -1.355731 | 3.686380 | 0.889051 |
| H | -1.471603 | 4.314515 | -0.763750 |
| C | 2.047153 | 3.481416 | 0.880920 |
| H | 0.567466 | 2.010614 | 1.446973 |
| C | 1.246262 | 4.698449 | 1.377739 |
| H | -0.403754 | 5.966216 | 0.761784 |
| H | 0.669123 | 5.496689 | -0.552121 |
| H | 2.748856 | 3.168877 | 1.661608 |
| H | 2.632812 | 3.753083 | -0.007550 |
| H | 1.939224 | 5.522159 | 1.577706 |
| H | 0.765830 | 4.449192 | 2.332784 |
| C | -2.352188 | -0.844765 | -1.978615 |
| C | -2.858855 | 0.456482 | -1.526301 |
| C | -3.290945 | -1.801671 | -2.521783 |
| C | -4.226928 | 0.684360 | -1.618229 |
| C | -4.640029 | -1.532817 | -2.570220 |
| H | -2.876785 | -2.744800 | -2.860486 |
| C | -5.118658 | -0.290956 | -2.111680 |
| H | -4.627170 | 1.643972 | -1.306053 |
| H | -5.331546 | -2.271383 | -2.960470 |
| H | -6.179432 | -0.068417 | -2.147035 |
| C | 2.988528 | -1.629522 | -0.741673 |
| C | 3.659286 | -0.406943 | -0.287012 |
| C | 3.786821 | -2.809937 | -0.977993 |
| C | 5.041875 | -0.444688 | -0.136001 |
| C | 5.155261 | -2.787532 | -0.832363 |
| H | 3.253569 | -3.699987 | -1.292973 |
| C | 5.793213 | -1.602775 | -0.416271 |
| H | 5.560991 | 0.441360 | 0.215877 |
| H | 5.740793 | -3.678483 | -1.031086 |

| | | | |
|---|---|---|---|
| H | 6.870400 | -1.577924 | -0.293423 |
| C | -2.048869 | 1.576787 | -1.070414 |
| C | 3.000696 | 0.826603 | 0.110457 |
| H | -2.589378 | 2.508178 | -0.918498 |
| H | 3.652949 | 1.581720 | 0.543296 |
| Os | 0.383888 | -0.108338 | -0.908204 |
| Fe | -1.202670 | -1.099231 | 2.265072 |
| Cl | -2.669548 | -2.768890 | 1.904586 |
| Cl | 0.328499 | -1.621206 | 3.839331 |
| Cl | -2.239548 | 0.852856 | 2.787103 |
| O | 1.011556 | 0.342885 | -2.521402 |

**TS3b**

| | | | |
|---|---|---|---|
| N | -1.325243 | -0.398897 | -0.858044 |
| N | -0.845479 | 0.546757 | 1.692420 |
| N | 0.349599 | -1.755774 | 0.919179 |
| O | -0.114032 | 1.983671 | -0.908198 |
| O | 1.512285 | -0.467423 | -1.429502 |
| C | -0.680543 | -0.484097 | 2.758934 |
| C | -1.742234 | -0.474569 | 3.864226 |
| C | -0.597891 | -1.867657 | 2.072844 |
| H | 0.303510 | -0.269112 | 3.195953 |
| C | -1.441576 | -1.582633 | 4.889592 |
| H | -2.734389 | -0.624989 | 3.419363 |
| H | -1.750737 | 0.492241 | 4.377869 |
| C | -0.272102 | -2.960626 | 3.096522 |
| H | -1.575030 | -2.079797 | 1.617068 |
| C | -1.321001 | -2.957557 | 4.223391 |
| H | -2.235221 | -1.594554 | 5.643916 |
| H | -0.507802 | -1.343299 | 5.416043 |
| H | -0.272802 | -3.943749 | 2.615206 |
| H | 0.731635 | -2.791432 | 3.509218 |
| H | -1.048815 | -3.715786 | 4.965073 |
| H | -2.294082 | -3.254191 | 3.810440 |
| C | -0.819467 | 2.893115 | -0.368934 |
| C | -1.476953 | 2.804991 | 0.943131 |
| C | -0.967451 | 4.115707 | -1.132115 |
| C | -2.203126 | 3.908907 | 1.374533 |

| | | | |
|---|---|---|---|
| C | -1.710416 | 5.173864 | -0.661449 |
| H | -0.468467 | 4.143383 | -2.094451 |
| C | -2.335604 | 5.077303 | 0.595768 |
| H | -2.690901 | 3.875124 | 2.343529 |
| H | -1.814483 | 6.076441 | -1.253587 |
| H | -2.924215 | 5.903999 | 0.978173 |
| C | 2.115252 | -1.642034 | -1.549620 |
| C | 1.939484 | -2.750070 | -0.655335 |
| C | 3.003932 | -1.784532 | -2.636227 |
| C | 2.655583 | -3.949440 | -0.903085 |
| C | 3.675950 | -2.977560 | -2.852947 |
| H | 3.131275 | -0.936361 | -3.300096 |
| C | 3.507292 | -4.072097 | -1.984839 |
| H | 2.520158 | -4.783544 | -0.220305 |
| H | 4.344469 | -3.062881 | -3.704400 |
| H | 4.041560 | -4.999415 | -2.159896 |
| C | -1.414512 | 1.688033 | 1.875205 |
| C | 1.099378 | -2.737225 | 0.503043 |
| H | -1.901846 | 1.867594 | 2.831771 |
| H | 1.090893 | -3.650289 | 1.093160 |
| Os | 0.150380 | -0.001023 | -0.046141 |
| Fe | -3.212338 | -0.555508 | -1.484761 |
| Cl | -3.164170 | -1.093556 | -3.646712 |
| Cl | -4.029514 | -2.176965 | -0.157933 |
| Cl | -4.186656 | 1.423091 | -1.048119 |
| O | 1.509002 | 0.925649 | 0.932934 |
| C | 4.299574 | 1.908635 | -0.862345 |
| C | 5.814184 | 2.094598 | -1.126838 |
| C | 6.564484 | 2.453836 | 0.163172 |
| C | 6.321358 | 1.415029 | 1.266853 |
| C | 4.807678 | 1.225377 | 1.536083 |
| C | 4.091323 | 0.877374 | 0.238403 |
| H | 7.639913 | 2.537953 | -0.040353 |
| H | 6.223602 | 1.163582 | -1.543212 |
| H | 5.954985 | 2.872137 | -1.888012 |
| H | 3.871062 | 2.871296 | -0.551012 |
| H | 3.786606 | 1.604752 | -1.781401 |
| H | 4.654335 | 0.444317 | 2.290204 |

| | | | |
|---|---|---|---|
| H | 4.397919 | 2.159281 | 1.944398 |
| H | 4.345746 | -0.134468 | -0.103520 |
| H | 2.944834 | 0.833015 | 0.472853 |
| H | 6.232337 | 3.441601 | 0.513861 |
| H | 6.756653 | 0.451510 | 0.967114 |
| H | 6.819244 | 1.713086 | 2.197978 |

**INT4b**

| | | | |
|---|---|---|---|
| N | 1.717172 | 0.001689 | -0.478065 |
| N | -0.419629 | -0.984992 | 1.153623 |
| N | -0.019710 | 1.635883 | 0.989419 |
| O | -0.515545 | -1.222749 | -1.735236 |
| O | -0.366879 | 1.454272 | -1.906808 |
| C | -0.636845 | -0.228860 | 2.428953 |
| C | -0.338572 | -0.993360 | 3.723398 |
| C | 0.194599 | 1.067874 | 2.348943 |
| H | -1.696786 | 0.058979 | 2.424515 |
| C | -0.606795 | -0.081145 | 4.935687 |
| H | 0.705657 | -1.331386 | 3.717820 |
| H | -0.975023 | -1.880680 | 3.801630 |
| C | -0.108532 | 1.987989 | 3.534005 |
| H | 1.258098 | 0.790827 | 2.378506 |
| C | 0.169059 | 1.238947 | 4.850889 |
| H | -0.339124 | -0.618721 | 5.851304 |
| H | -1.683403 | 0.128259 | 4.995818 |
| H | 0.520524 | 2.883253 | 3.490538 |
| H | -1.156489 | 2.314461 | 3.494234 |
| H | -0.094786 | 1.886880 | 5.693266 |
| H | 1.245944 | 1.040393 | 4.930968 |
| C | -0.562516 | -2.521780 | -1.452939 |
| C | -0.543766 | -3.069755 | -0.126958 |
| C | -0.663479 | -3.403459 | -2.546746 |
| C | -0.614638 | -4.481805 | 0.034891 |
| C | -0.714950 | -4.774561 | -2.348648 |
| H | -0.685637 | -2.975595 | -3.543167 |
| C | -0.687674 | -5.326177 | -1.052385 |
| H | -0.606951 | -4.887892 | 1.042266 |
| H | -0.780259 | -5.431381 | -3.211047 |

| | | | |
|---|---|---|---|
| H | -0.730759 | -6.400680 | -0.912716 |
| C | -0.363573 | 2.791115 | -1.791119 |
| C | -0.271292 | 3.510646 | -0.558372 |
| C | -0.496575 | 3.513433 | -2.988995 |
| C | -0.324316 | 4.930094 | -0.588969 |
| C | -0.532138 | 4.901665 | -2.981163 |
| H | -0.566891 | 2.953548 | -3.915391 |
| C | -0.447000 | 5.622399 | -1.777226 |
| H | -0.259191 | 5.469193 | 0.351977 |
| H | -0.631075 | 5.433462 | -3.922831 |
| H | -0.478152 | 6.706348 | -1.781510 |
| C | -0.548033 | -2.286581 | 1.064018 |
| C | -0.138827 | 2.907412 | 0.732733 |
| H | -0.693098 | -2.832797 | 1.993661 |
| H | -0.130265 | 3.590526 | 1.579559 |
| Os | 0.055692 | 0.182418 | -0.433667 |
| Fe | 3.725286 | -0.497972 | -0.138072 |
| Cl | 4.548688 | -1.139597 | -2.095299 |
| Cl | 4.485166 | 1.435117 | 0.666684 |
| Cl | 3.477934 | -2.082593 | 1.414939 |
| O | -2.346700 | 0.565577 | -0.384076 |
| C | -4.564924 | 0.813170 | 0.620376 |
| C | -5.846784 | 0.075148 | 1.047018 |
| C | -6.454299 | -0.714750 | -0.122299 |
| C | -5.428007 | -1.674593 | -0.743145 |
| C | -4.143017 | -0.937890 | -1.164894 |
| C | -3.554705 | -0.161039 | 0.012723 |
| H | -7.334067 | -1.274037 | 0.217443 |
| H | -5.612451 | -0.612969 | 1.872190 |
| H | -6.570595 | 0.797974 | 1.440562 |
| H | -4.811827 | 1.576042 | -0.131505 |
| H | -4.111541 | 1.333545 | 1.472434 |
| H | -3.403152 | -1.642231 | -1.559253 |
| H | -4.379550 | -0.228714 | -1.972753 |
| H | -3.209567 | -0.862131 | 0.778959 |
| H | -2.494137 | 0.964435 | -1.260850 |
| H | -6.805051 | -0.011503 | -0.891045 |
| H | -5.171566 | -2.457963 | -0.015676 |

| | | | |
|---|---|---|---|
| H | -5.855513 | -2.185413 | -1.613347 |

**INT1c**

| | | | |
|---|---|---|---|
| N | 0.077021 | -0.553479 | -2.387617 |
| N | -0.436042 | -1.960900 | 0.088607 |
| N | 1.914690 | -0.756376 | -0.239175 |
| O | -1.829701 | 0.517366 | -0.483667 |
| O | 0.509674 | 1.773594 | -0.707405 |
| C | 0.732158 | -2.663924 | 0.704709 |
| C | 0.632893 | -4.192764 | 0.768736 |
| C | 1.997159 | -2.232634 | -0.064547 |
| H | 0.808738 | -2.258795 | 1.722500 |
| C | 1.903294 | -4.771257 | 1.419416 |
| H | 0.505086 | -4.591586 | -0.246267 |
| H | -0.237924 | -4.500640 | 1.355811 |
| C | 3.259733 | -2.773405 | 0.611064 |
| H | 1.933864 | -2.644893 | -1.081300 |
| C | 3.178989 | -4.308408 | 0.704767 |
| H | 1.842073 | -5.864709 | 1.413713 |
| H | 1.939627 | -4.462593 | 2.472895 |
| H | 4.149517 | -2.492716 | 0.037235 |
| H | 3.358520 | -2.338602 | 1.614335 |
| H | 4.064078 | -4.682386 | 1.230184 |
| H | 3.209892 | -4.732839 | -0.307612 |
| C | -2.912557 | -0.275000 | -0.415765 |
| C | -2.860916 | -1.666520 | -0.099354 |
| C | -4.163111 | 0.325213 | -0.636837 |
| C | -4.076306 | -2.395354 | -0.015836 |
| C | -5.330687 | -0.423577 | -0.566399 |
| H | -4.193430 | 1.385382 | -0.864295 |
| C | -5.295740 | -1.794248 | -0.258479 |
| H | -4.029295 | -3.449810 | 0.240881 |
| H | -6.283315 | 0.064727 | -0.749749 |
| H | -6.213533 | -2.369296 | -0.202345 |
| C | 1.745353 | 2.259641 | -0.582312 |
| C | 2.909079 | 1.480378 | -0.278129 |
| C | 1.888378 | 3.653125 | -0.727172 |
| C | 4.159090 | 2.142926 | -0.130025 |

| | | | |
|---|---|---|---|
| C | 3.126391 | 4.261956 | -0.585273 |
| H | 0.998030 | 4.230384 | -0.952861 |
| C | 4.276397 | 3.508695 | -0.284775 |
| H | 5.034777 | 1.543395 | 0.102483 |
| H | 3.203754 | 5.338503 | -0.707015 |
| H | 5.239622 | 3.994696 | -0.174874 |
| C | -1.661449 | -2.373007 | 0.244164 |
| C | 2.919114 | 0.058768 | -0.091837 |
| H | -1.803271 | -3.351666 | 0.699315 |
| H | 3.873382 | -0.373722 | 0.202428 |
| Os | 0.042588 | -0.171633 | -0.783072 |
| O | 1.011910 | 0.609539 | 2.542030 |
| H | 1.460308 | 1.339716 | 2.072025 |
| O | -0.129010 | 0.343821 | 1.691399 |
| H | -0.724110 | 1.136334 | 1.857748 |
| C | -2.524559 | 4.732237 | 1.912058 |
| H | -2.266185 | 4.882375 | 2.960123 |
| H | -3.610867 | 4.791276 | 1.785931 |
| H | -2.081396 | 5.521692 | 1.297052 |
| C | -2.037090 | 3.387001 | 1.448998 |
| O | -2.255126 | 3.174863 | 0.154641 |
| H | -1.964065 | 2.261689 | -0.101601 |
| O | -1.499491 | 2.571374 | 2.195622 |

**TS1c**

| | | | |
|---|---|---|---|
| N | -0.222531 | 0.233573 | -2.183177 |
| N | 0.522439 | 1.785538 | 0.072166 |
| N | -1.992401 | 0.829090 | -0.088948 |
| O | 1.815257 | -0.785453 | -0.675481 |
| O | -1.007345 | -1.904406 | -0.434698 |
| C | -0.513868 | 2.575161 | 0.799617 |
| C | -0.239139 | 4.074972 | 0.938200 |
| C | -1.867593 | 2.307425 | 0.101744 |
| H | -0.558071 | 2.117622 | 1.795724 |
| C | -1.397055 | 4.755515 | 1.689725 |
| H | -0.120209 | 4.524069 | -0.056869 |
| H | 0.692196 | 4.239898 | 1.490359 |
| C | -3.017181 | 2.976750 | 0.863280 |

| | | | |
|---|---|---|---|
| H | -1.814675 | 2.726973 | -0.912771 |
| C | -2.746738 | 4.484159 | 1.016349 |
| H | -1.206861 | 5.832857 | 1.739828 |
| H | -1.420713 | 4.389628 | 2.724932 |
| H | -3.961400 | 2.838047 | 0.326888 |
| H | -3.123615 | 2.508816 | 1.850953 |
| H | -3.558600 | 4.934902 | 1.596890 |
| H | -2.766523 | 4.957382 | 0.025413 |
| C | 2.890888 | 0.041909 | -0.933312 |
| C | 2.840494 | 1.439036 | -0.693659 |
| C | 4.049611 | -0.551688 | -1.427947 |
| C | 4.000733 | 2.196515 | -0.982438 |
| C | 5.172177 | 0.227024 | -1.706532 |
| H | 4.059505 | -1.623707 | -1.592131 |
| C | 5.148648 | 1.608744 | -1.491606 |
| H | 3.980324 | 3.266138 | -0.795459 |
| H | 6.065616 | -0.250251 | -2.096857 |
| H | 6.020468 | 2.215379 | -1.711155 |
| C | -2.318549 | -2.165418 | -0.524570 |
| C | -3.351776 | -1.195053 | -0.343111 |
| C | -2.682248 | -3.502855 | -0.760385 |
| C | -4.706950 | -1.617411 | -0.397845 |
| C | -4.017423 | -3.877212 | -0.824204 |
| H | -1.887591 | -4.229962 | -0.890807 |
| C | -5.043851 | -2.933715 | -0.642972 |
| H | -5.485903 | -0.874790 | -0.249239 |
| H | -4.267437 | -4.916970 | -1.014463 |
| H | -6.084338 | -3.236041 | -0.690376 |
| C | 1.740378 | 2.180148 | -0.103727 |
| C | -3.129185 | 0.194759 | -0.072271 |
| H | 1.991145 | 3.189446 | 0.217115 |
| H | -4.017618 | 0.778587 | 0.157533 |
| Os | -0.222518 | -0.035141 | -0.532130 |
| O | -0.415387 | -1.524260 | 2.176514 |
| H | -0.663219 | -2.084452 | 1.408798 |
| O | 0.207026 | -0.385616 | 1.503391 |
| H | 1.470831 | -1.585364 | 2.405020 |
| C | 3.979890 | -3.626352 | 2.514526 |

| | | | |
|---|---|---|---|
| H | 4.565320 | -3.062366 | 3.245992 |
| H | 4.625451 | -4.024856 | 1.732168 |
| H | 3.498829 | -4.454305 | 3.047478 |
| C | 2.919672 | -2.749430 | 1.914066 |
| O | 2.695043 | -2.719480 | 0.696783 |
| H | 2.081574 | -1.597780 | -0.088586 |
| O | 2.252750 | -2.043724 | 2.805695 |

**INT2c**

| | | | |
|---|---|---|---|
| N | 0.341141 | -0.226321 | -2.195159 |
| N | 0.139685 | -1.980223 | 0.092716 |
| N | 2.178480 | -0.256700 | -0.089813 |
| O | -1.860417 | 0.118135 | -0.525119 |
| O | 0.267382 | 1.981247 | -0.296044 |
| C | 1.416977 | -2.427618 | 0.729593 |
| C | 1.660265 | -3.940682 | 0.742849 |
| C | 2.571169 | -1.689349 | 0.019538 |
| H | 1.369555 | -2.058415 | 1.762201 |
| C | 3.012805 | -4.247891 | 1.411369 |
| H | 1.645643 | -4.323298 | -0.286473 |
| H | 0.866745 | -4.452855 | 1.296264 |
| C | 3.911910 | -1.974171 | 0.702459 |
| H | 2.613806 | -2.052673 | -1.017405 |
| C | 4.167736 | -3.491723 | 0.744046 |
| H | 3.194286 | -5.327280 | 1.372856 |
| H | 2.958916 | -3.974524 | 2.473767 |
| H | 4.727764 | -1.487616 | 0.157430 |
| H | 3.901239 | -1.562681 | 1.720489 |
| H | 5.104542 | -3.682511 | 1.278287 |
| H | 4.307538 | -3.862309 | -0.280410 |
| C | -2.660067 | -0.950116 | -0.625665 |
| C | -2.254245 | -2.294981 | -0.342639 |
| C | -3.996713 | -0.725410 | -1.010238 |
| C | -3.217003 | -3.336893 | -0.435192 |
| C | -4.902456 | -1.771771 | -1.108251 |
| H | -4.304270 | 0.290646 | -1.230860 |
| C | -4.519388 | -3.092636 | -0.819360 |
| H | -2.901348 | -4.349988 | -0.201996 |

| | | | |
|---|---|---|---|
| H | -5.923254 | -1.559536 | -1.413086 |
| H | -5.234422 | -3.904624 | -0.894144 |
| C | 1.424005 | 2.687173 | -0.390386 |
| C | 2.723508 | 2.128670 | -0.216234 |
| C | 1.295477 | 4.063775 | -0.613838 |
| C | 3.843806 | 2.996519 | -0.254146 |
| C | 2.417623 | 4.884690 | -0.662127 |
| H | 0.297738 | 4.469447 | -0.745019 |
| C | 3.702817 | 4.354352 | -0.479619 |
| H | 4.832845 | 2.570350 | -0.112266 |
| H | 2.289795 | 5.948229 | -0.840627 |
| H | 4.575088 | 4.998003 | -0.514174 |
| C | -0.947534 | -2.696162 | 0.089952 |
| C | 3.012281 | 0.731699 | -0.004776 |
| H | -0.865939 | -3.720810 | 0.447831 |
| H | 4.050868 | 0.496264 | 0.220370 |
| Os | 0.192006 | -0.048762 | -0.549030 |
| O | -0.436902 | 1.476541 | 2.083087 |
| H | -0.191191 | 1.983131 | 1.235585 |
| O | -0.125232 | 0.097363 | 1.675364 |
| H | -1.483629 | 1.527429 | 2.149330 |
| C | -4.770952 | 3.303891 | 1.663008 |
| H | -5.678759 | 2.765646 | 1.368071 |
| H | -4.726140 | 4.220386 | 1.067753 |
| H | -4.815603 | 3.539975 | 2.725847 |
| C | -3.575640 | 2.444644 | 1.374004 |
| O | -3.324513 | 2.299971 | 0.084795 |
| H | -2.655299 | 1.577192 | -0.097115 |
| O | -2.903115 | 1.919868 | 2.270855 |

The electronic energies (E, in hartress) and electronic energies with ΔH or ΔG correction at 298 K for all the intermediates and TSs are given below. The energy is obtained at B3LYP level with the basis sets of LanL2DZ for Os and Fe and 6-31G(d) for non-metals. Solvent is $CH_3CO_2H$.

| | E | E + ΔH | E + ΔG |
|---|---|---|---|
| $[OsNL]^+$ | -1179.83370 | -1179.43953 | -1179.51107 |
| $H_2O_2$ | -151.53568 | -151.50529 | -151.53176 |
| $C_6H_{12}$ | -235.87655 | -235.69895 | -235.73438 |
| $CH_3COOH$ | -229.08284 | -229.01547 | -229.04817 |
| $H_2O$ | -76.41276 | -76.38789 | -76.40933 |
| $C_6H_{11}OH$ | -311.08860 | -310.90570 | -310.94402 |
| $FeCl_3$ | -1504.14351 | -1504.13327 | -1504.17468 |
| | | | |
| INT1 | -1560.46696 | -1559.97100 | -1560.06443 |
| TS1 | -1560.44818 | -1559.95472 | -1560.04580 |
| INT2 | -1560.45251 | -1559.95984 | -1560.05207 |
| TS2 | -1560.44586 | -1559.95271 | -1560.04386 |
| INT3 | -1254.94185 | -1254.54452 | -1254.61868 |
| TS3 | -1490.80975 | -1490.23874 | -1490.33070 |
| INT4 | -1490.91920 | -1490.33953 | -1490.42957 |
| | | | |
| INT1a | -3064.63407 | -3064.12582 | -3064.23903 |
| TS1a | -3064.61796 | -3064.11236 | -3064.22338 |
| INT2a | -3064.62639 | -3064.12008 | -3064.23100 |
| TS2a | -3064.61269 | -3064.10725 | -3064.21838 |
| INT3a | -2759.10257 | -2758.69308 | -2758.78720 |
| TS3a | -2994.97536 | -2994.39124 | -2994.50255 |
| INT4a | -2995.09081 | -2994.49872 | -2994.60874 |
| | | | |
| INT1b | -3064.64485 | -3064.13581 | -3064.24889 |
| TS1b | -3064.62332 | -3064.11711 | -3064.22923 |
| INT2b | -3064.62631 | -3064.12085 | -3064.23505 |
| TS2b | -3064.59506 | -3064.09012 | -3064.20340 |
| INT3b | -2759.10881 | -2758.69962 | -2758.79603 |
| TS3b | -2994.96441 | -2994.38063 | -2994.49242 |
| INT4b | -2995.09542 | -2994.50479 | -2994.61343 |
| | | | |

| | | | |
|---|---|---|---|
| INT1c | -1560.48665 | -1559.99018 | -1560.08538 |
| TS1c | -1560.45581 | -1559.96217 | -1560.05423 |
| INT2c | -1560.46216 | -1559.96717 | -1560.05843 |

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