Electronic Supplementary Information

Homogeneous Oxidation of C–H bonds with *m*-CPBA Catalyzed by a Co/Fe System: Mechanistic Insights from the Point of View of the Oxidant

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Materials and methods

All chemicals were of reagent grade and used as received. Labeled dioxygen (99% of ^{18}O) was purchased from CortecNet. Labeled water (97% of ^{18}O) and deuterated reagents were purchased from Eurisotop (Cambridge Isotope Laboratories, Inc.) and Sigma-Aldrich. All experiments were carried out in air, unless stated otherwise. The coordination compound $[Co^{III}_4Fe^{III}_2O(Sae)_8]\cdot 4DMF\cdot H_2O$ (**1**) (H_2Sae = salicylidene-2-ethanolamine) was synthesized according to a published protocol.[S1] Elemental analyses for CHN and for metals (atomic absorption spectroscopy) were performed by the Microanalytical Service of the Instituto Superior Técnico. ESI-MS mass spectra were obtained using LCQ Fleet mass spectrometer with an ESI source (Thermo Scientific).

Synthesis and crystal structure of [Co(HSae)(Sae)]·CH₃OH·H₂O (2).

Et_3N (0.28 mL, 2 mmol), 2-aminoethanol (0.12 mL, 2 mmol) and salicylic aldehyde (0.21 mL, 2 mmol) were added to 20 mL of methanol in this order and stirred for 5 min at 40 °C in a glass beaker. Then $Co(NO_3)_2\cdot 6H_2O$ (0.29 g, 1 mmol) dissolved in methanol (20 mL) was added dropwise upon stirring, affording a dark red solution. A dark red precipitate started to form in 5 min. The mixture was stirred for 1 h, then the precipitate was filtered off producing the powdered complex **2** (yield: 0.27 g, 62%). X-ray quality brown crystals of **2** (20 mg) were deposited from the filtrate in three days. The latter crystalline fraction was used for catalytic studies. The complex **2** slowly absorbs moisture if exposed in air. Calcd. (%) for $[Co(HSae)(Sae)]\cdot CH_3OH\cdot 1.9H_2O$: C, 50.42; H, 5.98; N, 6.12. Found (%): C, 50.5; H, 5.5; N, 6.2.

The crystal structure of **2** was reported earlier (R_1 = 0.1361), where **2** was obtained as a reaction by-product.[S2] Re-investigation of the structure of **2** (Figure S1, a) with higher data quality (R_1 = 0.0512) revealed the details of H-bonding in this structure (Figure S1, b). The molecules of the complex are bridged by strong O–H···O bonds into hexanuclear supramolecular moieties, bridged by the uncoordinated methanol and water molecules into a 1D chain (Figure S1, b).

Catalytic oxidation of alkanes

The reactions were typically carried out in air in thermostated cylindrical vials with vigorous stirring. Pre-catalyst **1** and the co-catalyst (nitric acid) were introduced into the reaction mixture in the form of stock solutions in acetonitrile (typically with [**1**] = 5×10^{-5} M and $[HNO_3]$ = 0.5 M). Firstly, the solution of **1** was added to a solution of CH_3CN and CH_3NO_2 (GC internal standard, final $[CH_3NO_2]$ = 0.2 M). Then the solution of nitric acid in acetonitrile (typically $[HNO_3]_0$ = 0.5 M) was added under stirring, with the subsequent addition of alkane. Solid oxidant (*m*-CPBA) was dissolved in CH_3CN (typically 30 mg in 1 mL of CH_3CN) and dropwise added to a hot (50 °C) solution of other components. (*CAUTION. The combination of m-CPBA with organic compounds at elevated temperatures may be explosive!*). Samples were quenched at room temperature with excess of solid PPh_3, according to developed methods,[S3] and directly analyzed by

GC and GC-MS techniques. A test with addition of the GC internal standard (CH_3NO_2) only after quenching a sample with PPh_3 revealed the same results as the above procedure, showing that CH_3NO_2 is not oxidized or decomposed during the reaction.

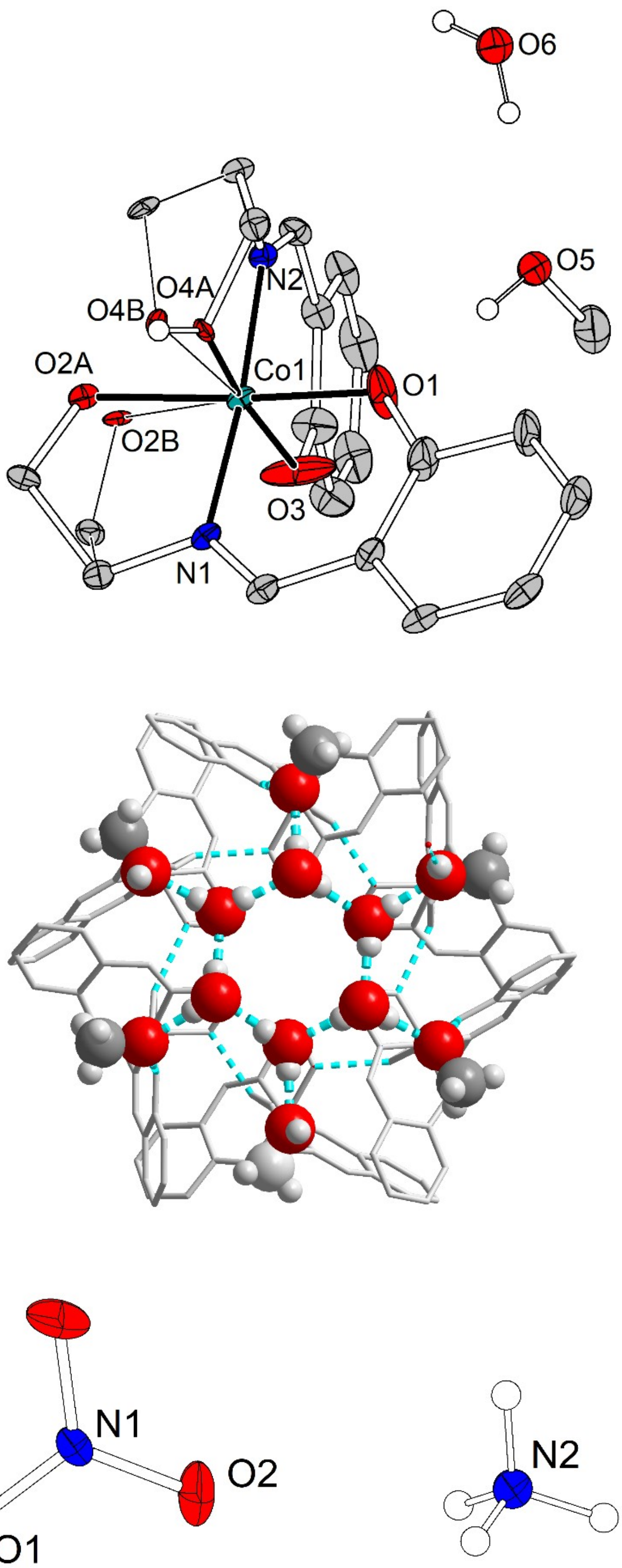
WARNING. Nitric acid stock solution in acetonitrile must not be kept for more than one week even at low temperature because of gradual change of its concentration. After staying for a prolonged time, colorless crystals of **3** start to precipitate, found to be ammonium nitrate, NH_4NO_3 (Figure S1).

X-ray crystallography

The X-ray diffraction data for **2** and **3** were collected using a Bruker D8 Quest diffractometer with graphite-monochromated Mo Kα radiation. Cell parameters were retrieved and refined using Bruker SAINT on all the observed reflections. Absorption corrections were applied using SADABS.[S4] The structure was solved by direct methods and refined against F^2 using the programs package SHELX-2018/3.[S5] All atoms were localized in the difference Fourier map and refined freely. The ethyl groups in **2** were found to be disordered over two positions, each with 0.5 occupation (Figure S1). The unit cell parameters of the structures **2** and **3** are consistent with those reported earlier for the respective crystal structures CCDC 724129 (for **2**) and CCDC 1592576, 1593832, 1600070, 1603205, 1603206, 1607970, 1612970, 1639855 and 1931542 (for NH_4NO_3, **3**).

Crystal data for **2**: $C_{19}H_{25}CoN_2O_6$, M = 436.34, a = 17.5321(14) Å, b = 17.5321(14) Å, c = 10.9885(10) Å, V = 2925.1(5) Å^3, T = 150(2) K, space group $P\text{–}3$, Z = 6, Mo$K\alpha$, 36719 reflections measured, 3445 independent reflections (R_{int} = 0.1651), R_1 = 0.0512 ($I > 2\sigma(I)$, 2393 reflections), $wR(F^2)$ = 0.1081, GoF (F^2) = 1.131. CCDC deposition number 2113995.

Crystal data for **3**: $H_4N_2O_3$, M = 80.05, a = 5.4460(6) Å, b = 5.7605(8) Å, c = 4.9406(6) Å, V = 154.99(3) Å^3, T = 296(2) K, space group $Pmmn$, Z = 2, Mo$K\alpha$, 1535 reflections measured, 259 independent reflections (R_{int} = 0.0310), R_1 = 0.0458 ($I > 2\sigma(I)$, 234 reflections), $wR(F^2)$ = 0.1114, GoF (F^2) = 1.268. CCDC deposition number 2017735.



a

b

c

Figure S1. (*a*) Molecular structure of **2** showing the numbering scheme. N–H and N–H hydrogen atoms are omitted for clarity. (*b*) Fragment of the crystal structure of **2**, featuring six-membered supramolecular moiety, capped by a layer constructed from the uncoordinated methanol and water molecules. (*c*) The structure of the compound **3**, showing the numbering scheme. Thermal ellipsoids are shown at 30% probability level.

Gas chromatography

A Perkin-Elmer Clarus 600 gas chromatograph, equipped with two non-polar capillary columns (pairs of SGE BPX5, 30 m × 0.22 mm × 25 µm or Phenomenex ZB-5, 30 m × 0.25 mm × 25 µm), one having an EI-MS (electron impact) detector and the other one with a FID detector, was used for analyses of the reaction mixtures. The following GC conditions have been used: 50 °C (3 min), 50–120 °C (8 degrees per minute), 120–300 °C (35 degrees per minute), 300 °C (3.11 min), 20 min total run time; 200 °C injector temperature. For analysis of oxidation products of highly-boiling compounds, such as adamantane or *cis*-decahydronaphthalene, a different program was employed: 50 °C (3 min), 50–150 °C (30 degrees per minute), 150–300 °C (14 degrees per minute), 300 °C (2.95 min), 20 min total run time; 200 °C injector temperature. Initial isothermal step (50 °C for 3 min) is important for clear separation of CH_3NO_2 (internal standard) from CH_3CN (solvent). Helium was used as the carrier gas (1 mL per minute flow). All EI mass spectra were recorded with 70 eV energy.

Mass-spectrometry

The identification of peaks at the chromatograms was made on the basis of comparison of respective EI mass-spectra with those from the NIST database v. 2.2 (PerkinElmer TurboMass v. 5.4.2.1617 software was used). However, the patterns of mass-spectra of the main products, tertiary *cis*- and *trans*-1,2-dimethylcyclohexanol, were not found in the NIST database of the version used. The identification of these products was made by comparing the chromatograms obtained from the oxidation of *cis*- and *trans*-substrates and their mixture. The EI mass-spectra of *cis*- and *trans*-alcohols were found to be nearly equal (Figure S5), in contrast to mass-spectra of respective *cis*- and *trans*-alkanes. Further, the mass-spectrum of *trans*-alcohol was already reported elsewhere[S6-S8] and found to be identical to that obtained within the present studies.

Electrospray mass spectra (ESI-MS) were obtained using an LCQ Fleet mass spectrometer with an ESI source (Thermo Scientific).

HF-EPR Spectroscopy

High-frequency EPR spectra were recorded with a home-built spectrometer at the EMR facility of NHMFL (National High Magnetic Field Laboratory, Florida State University). The instrument is a transmission-type device in which waves are propagated in cylindrical light-pipes. The microwaves were generated by a phase-locked oscillator (Virginia Diodes) operating at a frequency of 13 ± 1 GHz and generating its harmonics, of which the 4th, 8th, 12th, 16th, 24th, and 32nd were available. A superconducting magnet (Oxford Instruments) capable of reaching a field of 17 T was employed.

Computational details

The full geometry optimization of all structures and transition states was carried out at the DFT/HF hybrid level of theory by using the B3LYP* [S9-S12] with the help of the Gaussian 09[S13] program package. It was shown that while the popular pure functionals such as BP86 underestimate the relative stability of high spin states and many hybrid functionals with a high contribution of the Hartree-Fock term overestimate the relative stability of high spin states, the modified B3LYP functional (B3LYP*) correctly describes the relative energies of the low and high spin states in a number of transition metal complexes.[S11, S12] Since the relative stability of the high and low spin states is a crucial issue for the description of Co catalysed reactions, namely the B3LYP* functional was selected for the calculations. The B3LYP* functional was constructed using the keywords blyp, IOp(3/76=1000001500), IOp(3/77=0720008500) and IOp(3/78=0810010000).

The geometry optimization was carried out by using a relativistic Stuttgart pseudopotential that describes 10 core electrons (MDF10) and the appropriate contracted basis set[S14] for the cobalt atom and the 6-31G* basis set for other atoms. Single-point calculations were then performed on the basis of the equilibrium geometries found by using the 6-311+G** basis set for nonmetal atoms. Cartesian d and f functions (6d and 10f) were used for all calculations. No symmetry operations were applied. The stability test was performed for key structures using the keyword STABLE(Opt).

The Hessian matrix was calculated analytically for the optimized structures to prove the location of correct minima (no imaginary frequencies) or saddle points (only one imaginary frequency) and to estimate the thermodynamic parameters, with the latter calculated at 25 °C. The nature of all transition states was investigated by analysis of the vectors associated with the imaginary frequency and by the calculations of the intrinsic reaction coordinates (IRC) by using the method developed by Gonzalez and Schlegel.[S15-S17]

The total energies corrected for solvent effects E_s were estimated at the single-point calculations on the basis of gas-phase geometries at the CPCM-B3LYP*/6-311+G**//gas-B3LYP*/6-31G* level of theory using the polarizable continuum model in the CPCM version[S18, S19] with CH_3CN as solvent. The UAKS model was applied for the molecular cavity and dispersion, cavitation, and repulsion terms were taken into account. The entropic term in CH_3CN solution (S_s) was calculated according to the procedure described by Wertz[S20] and Cooper and Ziegler[S21] using eqn. 1–4:

$$\Delta S_1 = R \ln V^{s}_{m,liq}/V_{m,gas} \quad (1)$$

$$\Delta S_2 = R \ln V^{\circ}_{m}/V^{s}_{m,liq} \quad (2)$$

$$\alpha = [S^{\circ,s}_{liq} - (S^{\circ,s}_{gas} + \Delta S_1)]/[S^{\circ,s}_{gas} + \Delta S_1] \quad (3)$$

$$S_s = S_g + \Delta S_{sol} = S_g + [\Delta S_1 + \alpha(S_g + \Delta S_1) + \Delta S_2] =$$
$$S_g + [(-12.04\ \text{cal/mol}\bullet\text{K}) - 0.233(S_g - 12.04\ \text{cal/mol}\bullet\text{K}) + 5.87\ \text{cal/mol}\bullet\text{K}] \quad (4)$$

where S_g is the gas-phase entropy of solute, ΔS_{sol} is the solvation entropy, $S^{o,s}_{liq}$, $S^{o,s}_{gas}$ and $V^{s}_{m,liq}$ are the standard entropies and molar volume of the solvent in the liquid or gas phases (149.6 and 245.5 J/mol•K and 52.16 mL/mol, respectively, for CH_3CN), $V_{m,gas}$ is the molar volume of the ideal gas at 25 °C (24450 mL/mol), V^{o}_{m} is the molar volume of the solution that correspond to the standard conditions (1000 mL/mol). The enthalpies and Gibbs free energies in solution (H_s and G_s, respectively) were estimated using the expressions 5 and 6

$$H_s = E_s(6\text{-}311\text{+}G^{**}) + H_g(6\text{-}31G^{*}) - E_g(6\text{-}31G^{*}) \quad (5)$$

$$G_s = H_s - TS_s \quad (6)$$

where E_s and E_g are the total energies in solution and the gas phase and H_g is the gas-phase enthalpy calculated at the corresponding level. In this work, energies are discussed in terms of Gibbs free energies in solution.

Estimate of rate constants of cyclohexane and cyclohexanol oxidation

Oxidation of cyclohexane was considered a two-step irreversible reaction (rate constants k_1 and k_2):

$$k_1 \qquad A \rightarrow B \quad (9)$$

$$k_2 \qquad B \rightarrow C \quad (10)$$

where A is cyclohexane, B is cyclohexanol and C is cyclohexanone. Analytical expressions[S22] describing this process have the following form:

$$B(t) = \frac{A_0 k_1 (e^{-k_1 t} - e^{-k_2 t})}{k_2 - k_1} \quad (11)$$

$$C(t) = A_0 \left(1 - \frac{k_2 e^{-k_1 t}}{k_2 - k_1} - \frac{k_1 e^{-k_2 t}}{k_1 - k_2} \right) \quad (12)$$

where $B(t)$ and $C(t)$ are concentrations of cyclohexanol and cyclohexanone after reaction time t and A_0 is the initial concentration of cyclohexane. Equations (11) and (12) were used to fit the experimental data in the quasi-stationary region $t = 0 \ldots n$ min, where dependence $B(t) + C(t)$ on t is linear.

Under the conditions of experiment, cyclohexanol quantitatively oxidizes to cyclohexanone with selectivity close to 100%. Hence, the following expressions were applied simultaneously to fit the whole range experimental data when using cyclohexanol as a substrate (B and C have the same meaning as above):

$$B(t) = A_0 e^{-kt} \quad (13)$$

$$C(t) = A_0 - A_0 e^{-kt} \quad (14)$$

Experiments with $^{18}O_2$ and $H_2{}^{18}O$ and under inert conditions

In the experiments under $^{16}O_2$, $^{18}O_2$ or N_2 atmosphere, the catalytic reaction mixtures freshly prepared in Schlenk flask (at room temperature) were frozen with liquid nitrogen, the gas atmosphere was pumped and filled with N_2 a few times in order to remove air. The frozen mixtures were left to warm up in vacuum until becoming liquid and the above procedure was repeated. Then the frozen mixtures were pumped again, the vacuum pump was turned off, and the Schlenk flasks were filled with the desired gas ($^{16}O_2$, $^{18}O_2$ or N_2) using a syringe through a septum and heated up to 50 °C with a possibility of gas escape to compensate excessive pressure. In the experiments with $H_2{}^{18}O$, a reduced reaction volume was used (2.5 mL) and labeled water was added prior to the addition of the oxidant (*m*-CPBA).

The $^{16}O/^{18}O$ oxygenated products were determined by the relative abundances of mass peaks at m/z = 57/59 for cyclohexanol, 61/63 for deuterated cyclohexanol (see below for details) and at m/z = $M^+/M^+ + 2$ molecular ion peaks for other compounds. The MS data for 130 m/z molecular ion peaks of weakly ^{18}O-enriched tertiary alcohols were corrected as described earlier.[S23] The H/D compositions of chlorobenzene were determined by the relative abundances of mass peaks at m/z = 112/113. The isotopic enrichment (*IE*) was calculated by considering the natural ratio *R* of the normal (*A*) and enriched (B) m/z peaks ($R = B / A$):

$$IE(\%) = \frac{B - AR}{B + A(1 - R)} \times 100 \tag{15}$$

Blank tests: checking of a non-catalytic *m*-CPBA activity

There are indications that *m*-CPBA may selectively oxidize tertiary C–H bonds of organic substrates via a metal-free radical mechanism,[S24-26] including hydroxylation of dimethylcyclohexanes and decahydronaphthalenes with a RC index of 50 – 90%.[S27] High loadings of oxidant and substrate ($[m\text{-CPBA}]_0$ and $[\text{alkane}]_0 > 1$ M) were used, along with elevated temperatures (ca. 50 °C) and long reaction time (6 – 24 h). Also, high amounts of chlorobenzene were typically formed.[S24, 25, 27] We attempted to reproduce these results reacting 1 M *cis*-decahydronaphthalene (which is less volatile than *cis*-1,2-DMCH) with 1 M of *m*-CPBA in CH_3CN or $CHCl_3$ at 50 °C. After 3 h reaction time the *cis*/*trans* ratios of tertiary alcohols formed were 1.3 and 6.2 for CH_3CN and $CHCl_3$, respectively. Probes taken after 24 h revealed *cis*/*trans* ratios of 2.6 and 6.3, respectively. Observed amounts of chlorobenzene, as a reaction product, were comparable to that for tertiary alcohols. Hence, although some stereoselectivity can be observed using non-catalytic hydroxylation with *m*-CPBA, the stereopurity of the alcohols formed is low. If the reaction is performed under conditions of our experiment (Entry 7, Table 1), only traces of tertiary alcohols are seen in the course of *cis*-1,2-DMCH oxidation, with a *cis*/*trans* ratio nearly 1 : 1.

Calculation of ^{18}O incorporation levels into normal and deuterated cyclohexanols

The mass-spectra of normal and deuterated cyclohexanols are depicted at Figure S2. The molecular ions of these compounds (100 and 111 *m/z*, respectively) are too weak for reliable determination of their $^{18}O/^{16}O$ compositions when the incorporation of ^{18}O is relatively low. Thus, this isotopic composition for C_6H_{11}–OH is determined by the ratio of 59/57 *m/z* peaks, corresponding to the oxygen-containing species $C_3H_4{=}^{18}OH^+$ / $C_3H_4{=}^{16}OH^+$.[S28, 29] Intensities of these signal are sufficient even for species labeled at level of few percent, while the 102 *m/z* peak (M + 2 labeled molecular ion) is not seen under such conditions (Figure S2). The $^{18}O/^{16}O$ composition of deuterated cyclohexanol, C_6D_{11}–OH, can be determined from the ratio of 63/61 *m/z* peaks ($C_3D_4{=}^{18}OH^+$ / $C_3D_4{=}^{16}OH^+$ ratio). However, the respective peak at 63 *m/z* ($C_3D_4{=}^{18}OH^+$) already has high intensity, being probably overlapped with some other fragmentation products.

The 59/57 and 63/61 natural ratios were estimated as 0.0093(5) and 0.119(6) from 20 and 12 measurements, respectively (Figure S3). These natural ratios were accounted during the calculations of $^{18}O/^{16}O$ compositions of normal and labeled cyclohexanols (eqn. (3)).

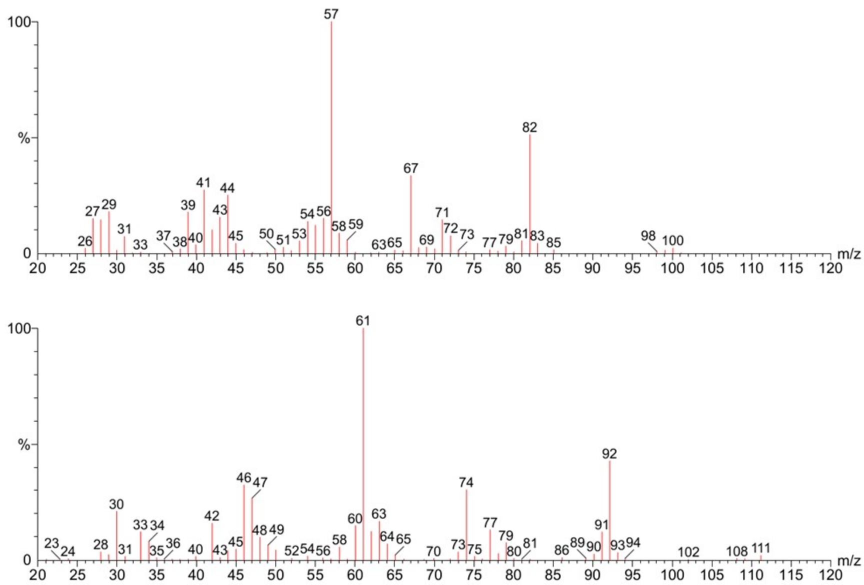


Figure S2. EI mass spectra of C_6H_{11}–OH (top) and C_6D_{11}–OH (bottom), both enriched with 4.5% of ^{18}O.

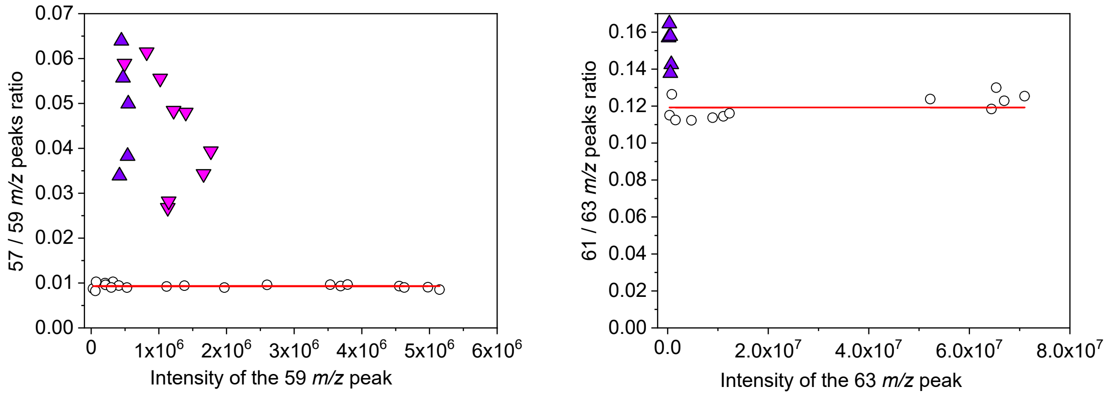


Figure S3. Changes of the mass spectra upon ^{18}O-incorportation into cyclohexanols. Left: empty circles and solid red line show the dependence of 59/57 *m/z* intensities ratio on the 59 *m/z* peak intensity for non-labeled cyclohexanol. Top- (△) and bottom- (▽) oriented triangles show the 59/57 *m/z* intensities ratios for the oxidation of C_6H_{12} and C_6H_{12}/C_6D_{12} mixture in the presence of $H_2{}^{18}O$, respectively. Right: the same dependence for 63/61 *m/z* ratio observed for C_6D_{11}–OH. Top-oriented triangles show the 63/61 *m/z* ratio for oxidation of C_6H_{12}/C_6D_{12} mixture in the presence of $H_2{}^{18}O$.

Estimate of D incorporation levels into chlorobenzene

The typical mass spectra of normal and deuterated chlorobenzene are depicted in the Figure S4. Statistical distribution of the 113/112 *m/z* peaks for normal chlorobenzene gave the ratio of 0.06(1). Deviations from this ratio, exhibited by D-enriched species, are shown in the Figure S5.

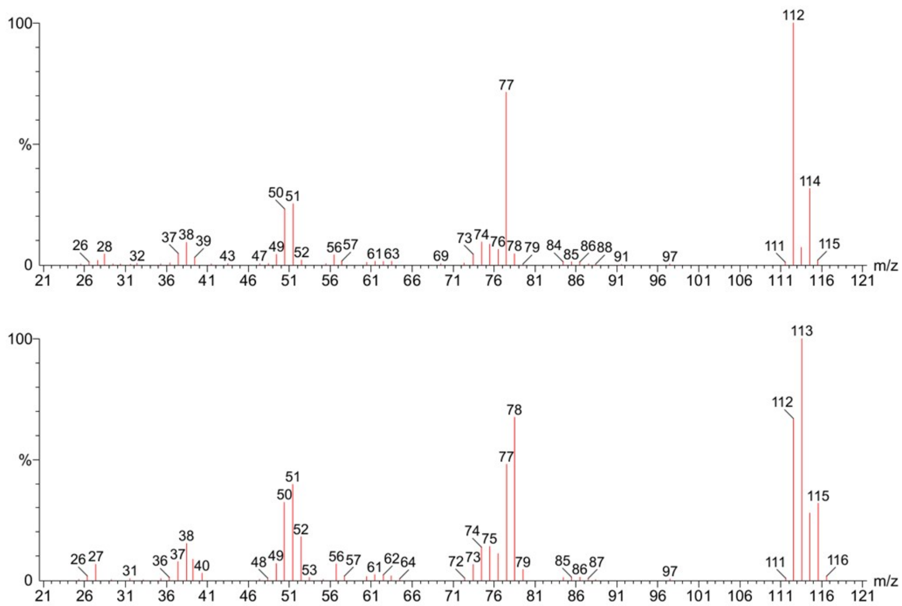


Figure S4. EI mass spectra of normal (top) and deuterated chlorobenzene (bottom, 59% of D-enrichment).

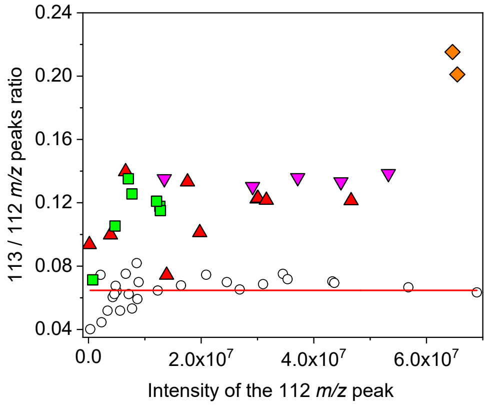


Figure S5. Changes of the mass spectra upon D-incorporation into chlorobenzene. Empty circles and solid red line show the data for non-labeled cyclohexanol. Squares (□), top- (△) and bottom- (▽) oriented triangles show the ratios for oxidation of 0.1 M of methylcyclohexane, while rhombs (◇) correspond to its 0.2 M concentration.

Oxygen exchange between water and tertiary 1,2-dimethylcyclohexane-1-oles and other alcohols in the presence of nitric acid and pre-catalyst 1

The possibility of a direct oxygen exchange between tertiary alcohols and water, under the conditions of experiment, was studied in the following way. The typical catalytic reaction system (Entry 5, Table 1) was initiated and stirred for 24 h at 50 °C to ensure complete consumption of *m*-CPBA. Then $H_2{}^{18}O$ was added dropwise (the final concentration was 0.5 M) and the mixture was stirred further. The aliquots were taken before addition of $H_2{}^{18}O$, after 1 h and 24 h. The observed 130/128 *m/z* ratios are depicted at Figure S6. The mass spectra of normal and partially labeled tertiary alcohols are shown in Figures S7–9. No incorporation of ^{18}O into the tertiary alcohols was observed after 1h of stirring. After 24h of stirring the *cis*-alcohol was found to contain 0.8% of labeled oxygen, while the *trans*-alcohol accumulated higher level of 21%.

A series of alcohols was tested for oxygen exchange using simplified conditions (stirring of 0.05 M acetonitrile solution of alcohol, in the presence of 0.005 M of HNO_3, with 0.5 M of $H_2{}^{18}O$ at 50 °C). No oxygen exchange (after 24 h) was observed for cyclohexanol, 2,6-dimethylcyclohexanol, cycloheptanol, cyclooctanol and triphenylmethanol. Cumyl alcohol (2-phenyl-2-propanol) exhibited strong and fast exchange, leading to >50% ^{18}O enrichment after 1 h; 2,3-dimethyl-2-butanol revealed slow exchange, showing *ca*. 1% of ^{18}O-labeling after 1 h of treatment and 12% after 24 h. The ^{18}O labeling of 1-indanol was found to be >90% after 1 h of time.

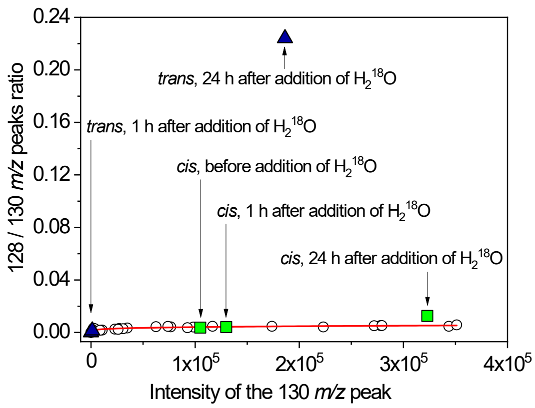


Figure S6. EI mass spectra (Figures S7-S9), shown as a dependence of 130/128 *m/z* peaks ratio on the intensity of 130 *m/z* peak. Empty circles and solid red line: dependence of 130/128 *m/z* intensities ratio on the 130 m/z peak intensity for non-labeled tertiary 1,2-DMCH alcohols. Green squares (□) and dark blue triangles (△) show the 130/128 *m/z* intensities ratios for tertiary *cis*- and *trans*-alcohol in the test for oxygen exchange with $H_2{}^{18}O$ under non-catalytic conditions.

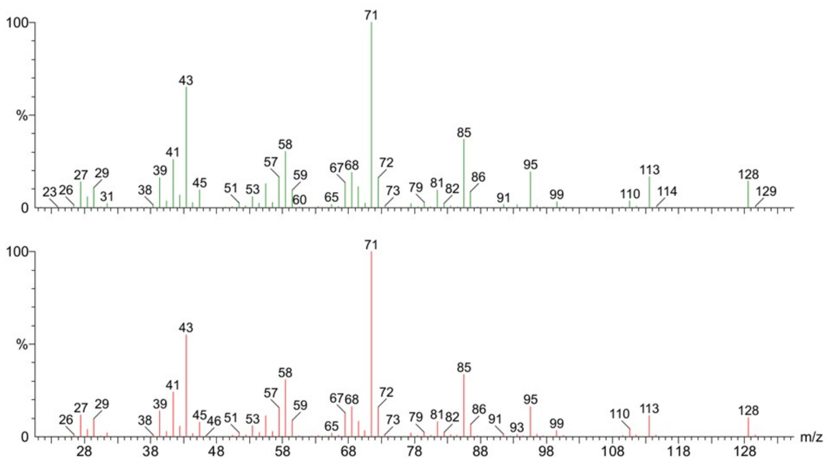


Figure S7. EI mass spectra of the non-labeled tertiary *trans*- (top) and *cis*- (bottom) tertiary alcohols (aliquots taken before addition of $H_2{}^{18}O$).

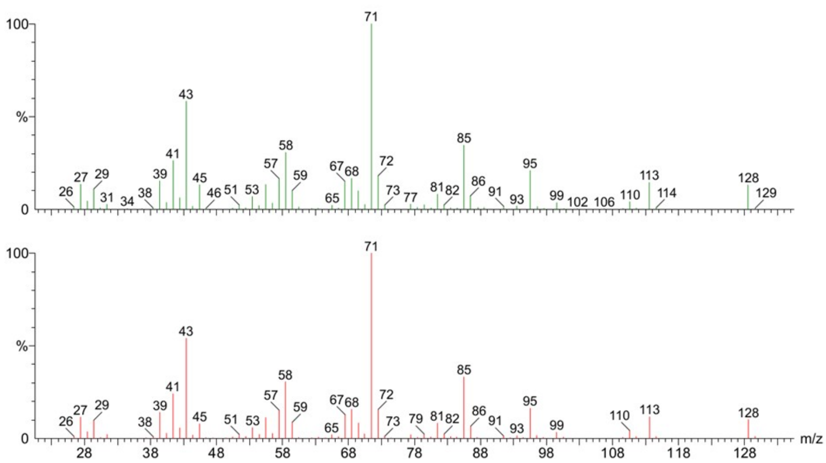


Figure S8. EI mass spectra of the tertiary *trans*- (top) and *cis*- (bottom) alcohols, measured 1 h after addition of $H_2{}^{18}O$.

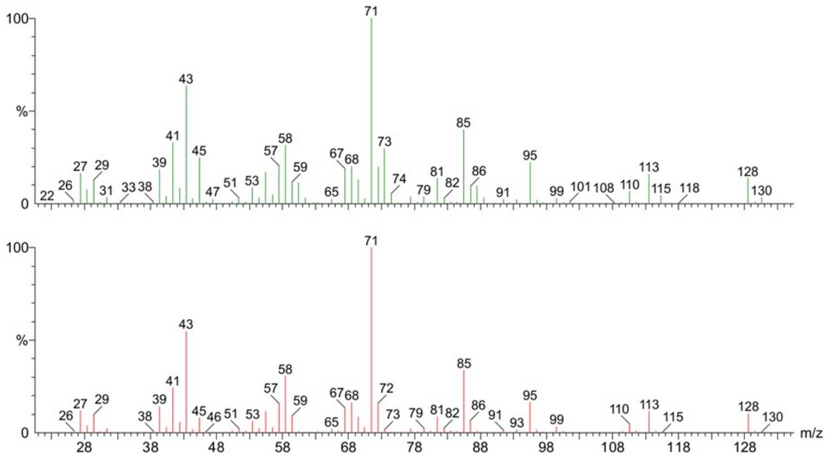


Figure S9. EI mass spectra of the tertiary *trans*- (top) and *cis*- (bottom) alcohols, measured 24 h after addition of $H_2{}^{18}O$.

Incorporation of ^{18}O from $H_2{}^{18}O$ in the course of a catalyst-free oxidation

The Entry 7 (Table 1) reveals the possibility of a catalyst-free oxidation of *cis*-1,2-DMCH with *m*-CPBA, although with very low yields and selectivity. The same test performed in the presence of 0.5 M of $H_2{}^{18}O$ suggested the incorporation of ^{18}O into the tertiary alcohols, but too weak intensities of the 128 and 130 *m/z* signals did not allow reliable determination of ^{18}O levels. When the concentrations of $H_2{}^{18}O$ and *m*-CPBA were increased up 1.0 and 0.14 M (all other conditions as in Entry 7) the pronounced incorporation of ^{18}O into tertiary *cis*-alcohol of 6.2% after 6 h was observed (Figure S10). In the case of tertiary *trans*-alcohol the 130 *m/z* signals were too weak for reliable determination of the ^{18}O levels. The chromatograms recorded before and after addition of solid PPh_3 to aliquots show difference in *c/t* ratios as well as in the chlorobenzene yield (Figure S11).

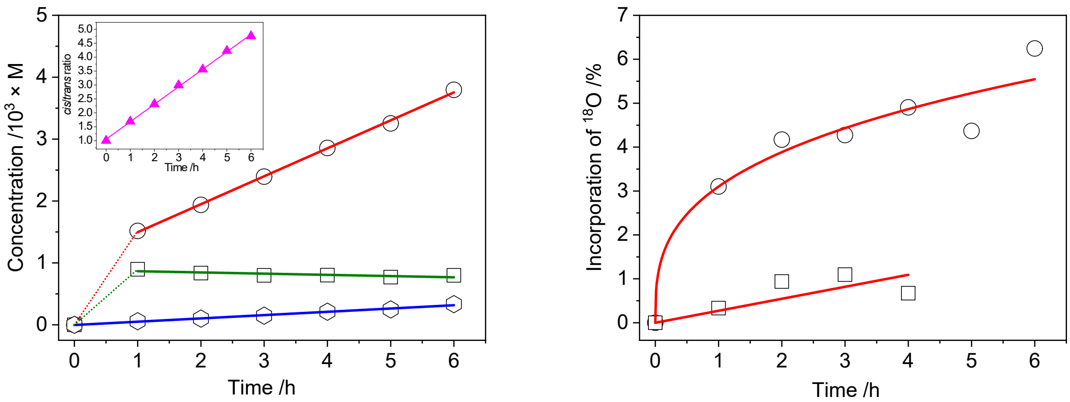


Figure S10. Left: accumulations of the *cis*- (○) and *trans*- (□) tertiary alcohols and chlorobenzene (⬡) in the course of *cis*-1,2-DMCH (0.1 M) oxidation with *m*-CPBA (0.14 M) in the presence of HNO_3 (5.5×10^{-3} M) and $H_2{}^{18}O$ (1 M) and absence of the metal catalyst, at 50 °C in acetonitrile. Inset shows the growth of *cis*/*trans* ratio with the time. Right: incorporations of ^{18}O into tertiary *cis*-alcohol from $H_2{}^{18}O$ for the reaction conducted in the presence (○) or absence (□) of nitric acid promoter.

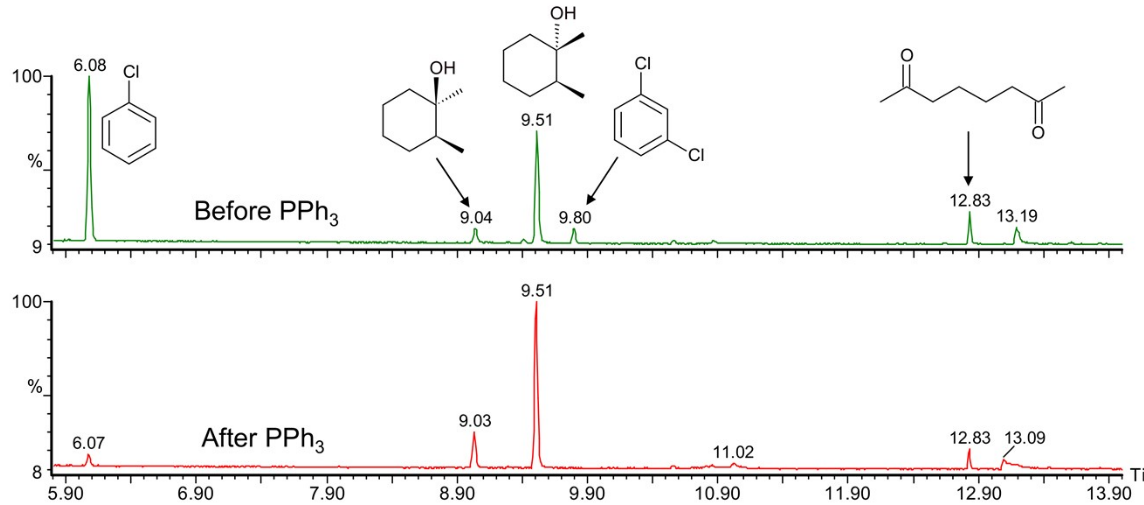


Figure S11. Fragments of the chromatograms showing the main reaction products from the catalyst-free oxidation of *cis*-1,2-DMCH (conditions are as those in Figure S10 caption) recorded at 5 h before (top) and after (bottom) addition of PPh_3. 6.08 min: chlorobenzene; 9.04 min: tertiary *trans*-alcohol; 9.51 min: tertiary *trans*-alcohol; 9.80 min: 1,3-chloronenzene; 12.83 min: 2,7-octanedione; 13.19 min (only before PPh_3): 1,3-chlorophenol.

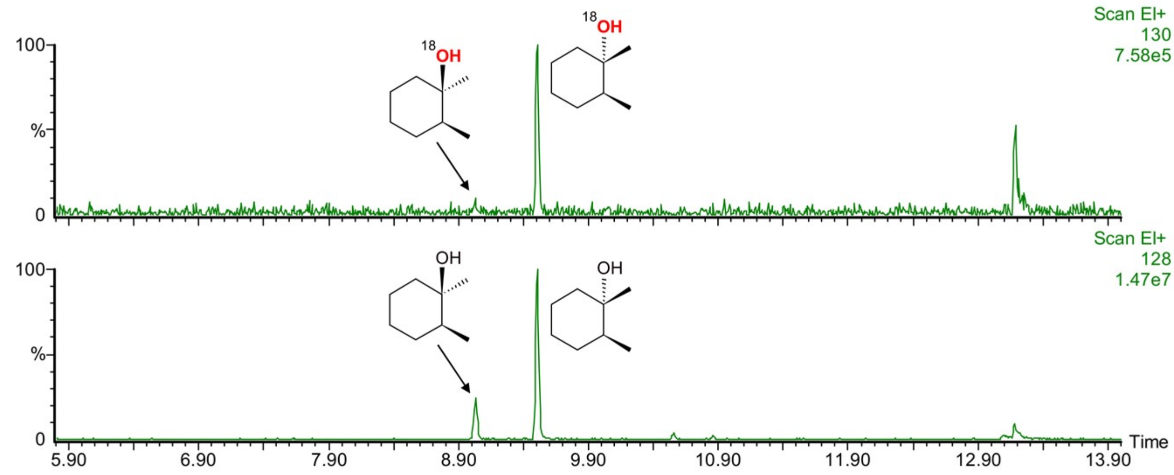


Figure S12. Fragments of the chromatograms showing the intensities of the signals 128 and 130 *m/z*, corresponding to normal and labeled tertiary alcohols in the course of the catalyst-free oxidation of *cis*-1,2-DMCH (Figure S10). Under these conditions, the expected intensity of the 130 *m/z* signal for non-labeled tertiary *cis*-alcohol is ca. 7×10^4.

Estimate of ^{18}O levels in the course of *cis*-1,2-DMCH oxidation under $^{18}O_2$ or in the presence of $H_2{}^{18}O$

The observed levels of ^{18}O incorporations for tertiary *trans*- and *cis*-alcohols are depicted at Figure S13. As can be seen, in the case of $^{18}O_2$ test (Figure S13, left) the 130/128 *m/z* ratios of *cis*-alcohol are close to those expected for non-labeled species, while *trans*-alcohol shows more than 100 fold increase. Although 130/128 *m/z* ratios for *trans*-alcohol suggested the presence of ^{18}O (Figure S13, right, blue squares), the absolute intensity of the respective 130 *m/z* signals were very low (lower than 10^4), thus falling into the non-reliable region.[S23]

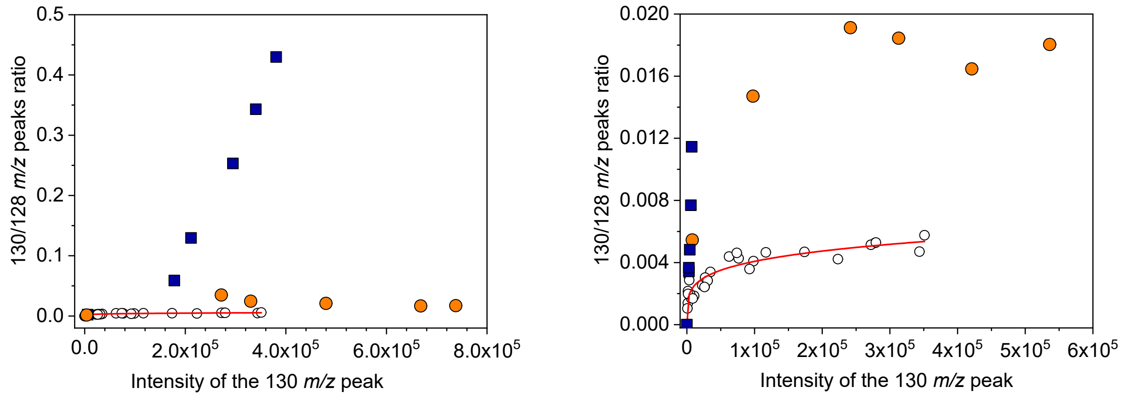


Figure S13. Dependence of 130/128 *m/z* intensities ratios on the 130 *m/z* peak intensities for non-labeled tertiary 1,2-DMCH alcohols (empty circles and red line), and labeled *trans*- (blue squares) and *cis*- (orange circles) alcohols in the course of reaction under $^{18}O_2$ (left) and in the presence of $H_2{}^{18}O$ (right).

Oxidation of cyclohexane in the presence of $H_2{}^{18}O$ and oxidation of cyclohexanol

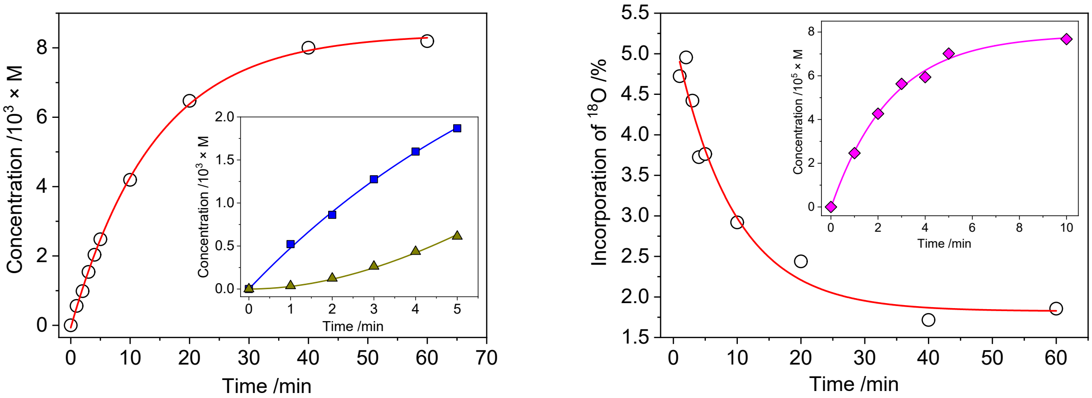


Figure S14. Left: accumulation of the products (sum of cyclohexanol and cyclohexanone) with time in the course of cyclohexane (0.1 M) oxidation with *m*-CPBA (0.027 M) catalyzed by **1** ($[\mathbf{1}_{\mathbf{Co}}]_0 = 1.1 \times 10^{-5}$ M) in the presence of HNO_3 (5.5×10^{-3} M) and $H_2{}^{18}O$ (0.5 M) in acetonitrile at 50 °C. Inset shows accumulations of particular products, cyclohexanol (□) and cyclohexanone (△). The fit (solid lines) was obtained using the equations 11 and 12 with $k_1 = 8.47 \times 10^{-5}$ and $k_2 = 2.03 \times 10^{-3}$ s^{-1}. Right: incorporation of ^{18}O into cyclohexanol in the same reaction shown as a function of time. Inset shows accumulation of ^{18}O-enriched cyclohexanol with time.

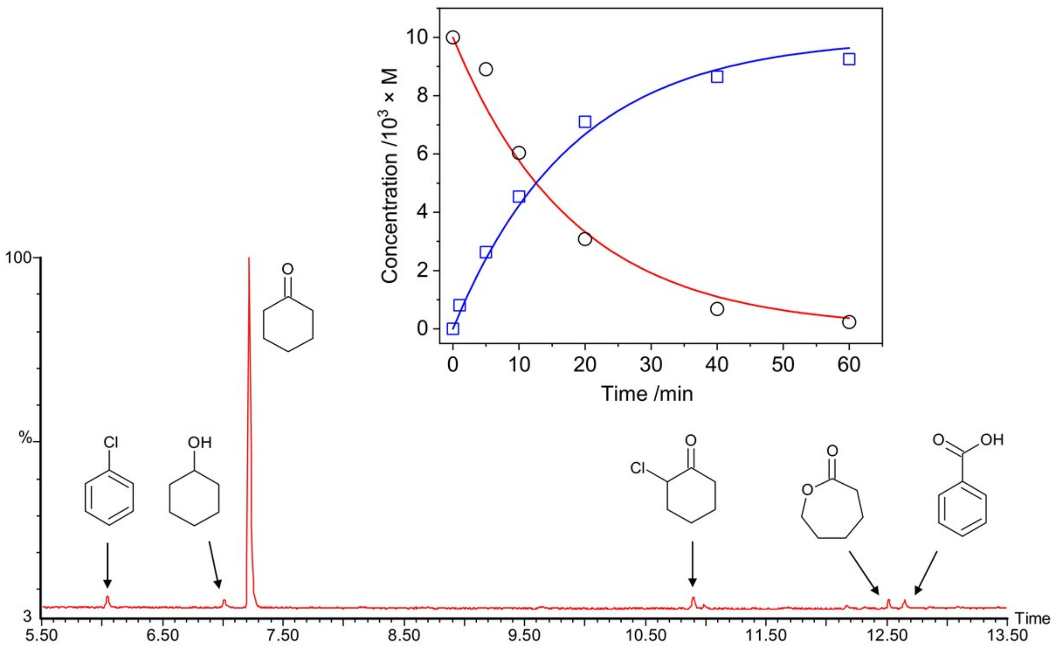


Figure S15. Fragment of the chromatogram showing the main reaction products in the course of cyclohexanol (0.01 M) oxidation with *m*-CPBA (0.027 M) catalyzed by **1** ($[\mathbf{1}_{\mathbf{Co}}]_0 = 1.1 \times 10^{-5}$ M) in the presence of HNO_3 (5.5×10^{-3} M) in acetonitrile at 50 °C, 1 h. Inset shows consumption of cyclohexanol (○) and accumulation of cyclohexanone (□). The fit (solid lines) gave $k = 9.2 \times 10^{-4}$ s^{-1}.

Kinetic isotope effect and D-labeled species

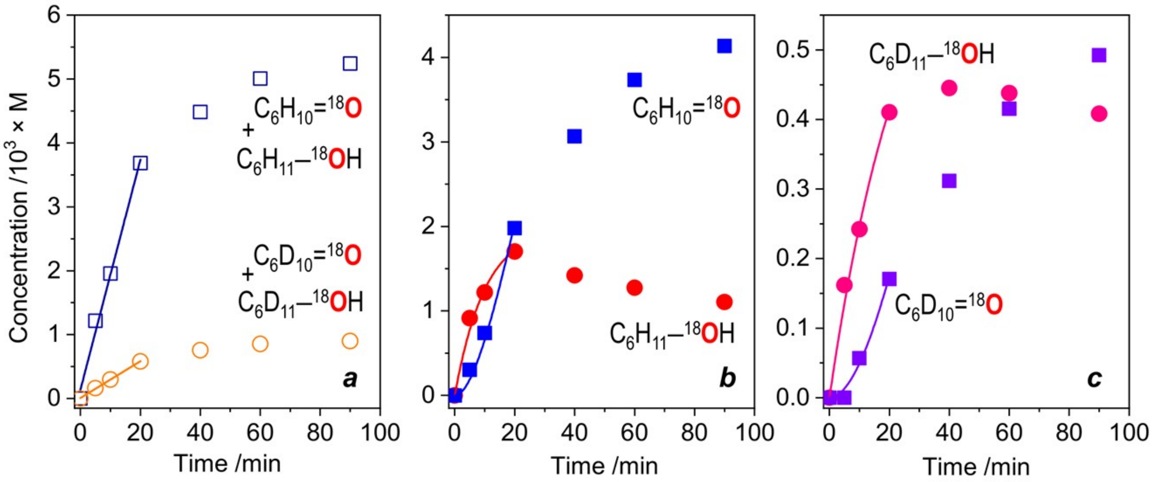


Figure S16. Accumulations of products (normal and deuterated cyclohexanol and cyclohexanone) in the course of oxidation of equimolar mixture of C_6H_{12} and C_6D_{12} (0.05 each) with *m*-CPBA (0.027 M) catalyzed by **1** ($[\mathbf{1_{Co}}]_0 = 1.1 \times 10^{-5}$ M) in the presence of HNO_3 (5.5×10^{-3} M) in acetonitrile at 50 °C.

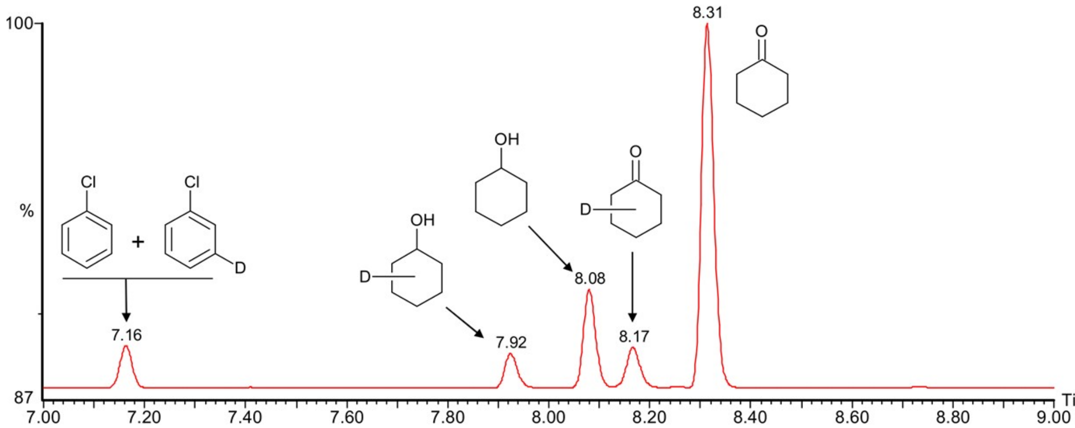


Figure S17. Fragment of the chromatogram showing the main reaction products in the course of competitive oxidation of equimolar mixture of normal and deuterated cyclohexane (conditions are stated in Figure S16 caption) after 90 min.

Table S1. Rate constants calculated for oxidation of normal and deuterated cyclohexane.

	Substrate	
k, s^{-1}	C_6H_{12}	C_6D_{12}
k_1, CyH → CyOH	6.5×10^{-5}	9.9×10^{-6}
k_2, CyOH → Cy=O	15.1×10^{-4}	6.2×10^{-4}
k_2 / k_1	23	63

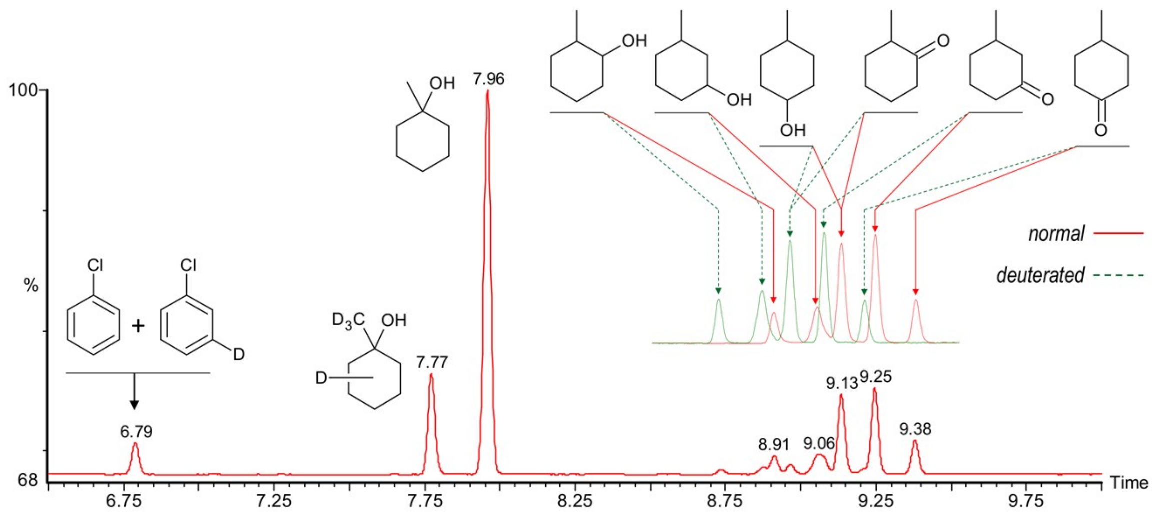


Figure S18. Fragment of the chromatogram showing the main reaction products in the course of competitve oxidation of equimolar mixture of normal and deuterated methylcyclohexane (0.05 each) with *m*-CPBA (0.027 M) catalyzed by **1** ([$\mathbf{1_{Co}}$]$_0$ = 1.1 × 10^{-5} M) in the presence of HNO_3 (5.5 × 10^{-3} M) in acetonitrile at 50 °C. Peaks of secondary alcohols and ketones overlap, resulting in a complex pattern which does not allow estimate of particular concentrations. From the intensities of 112 and 124 *m/z* peaks, corresponding to normal and deuterated methylcyclohexanones, one could expect KIE of 7.7 for oxidation of secondary C–H bonds.

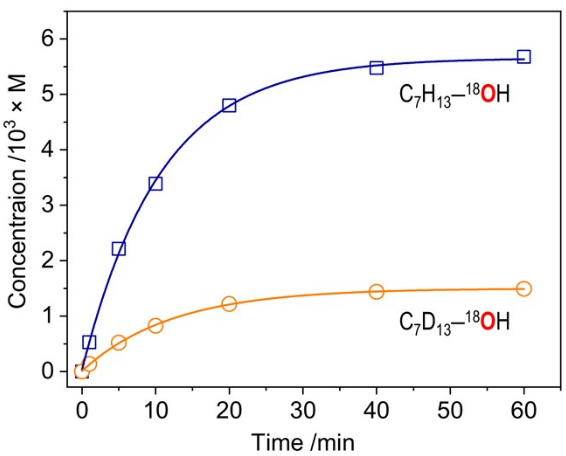


Figure S19. Accumulations of products (normal and deuterated tertiary methylcyclohexanols) in the course of oxidation of equimolar mixture of C_7H_{14} and C_7D_{14} (0.05 each) with *m*-CPBA (0.027 M) catalyzed by **1** ([$\mathbf{1_{Co}}$]$_0$ = 1.1 × 10^{-5} M) in the presence of HNO_3 (5.5 × 10^{-3} M) in acetonitrile at 50 °C.

Reactions at different temperatures

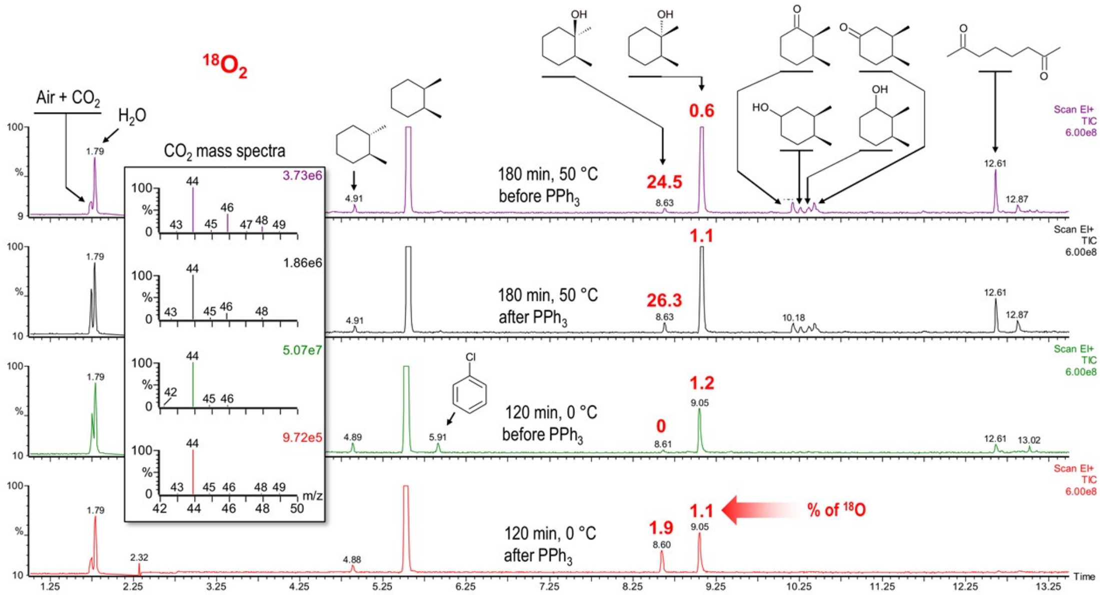


Figure S20. Fragments of the chromatograms showing the main reactions products, along with substrates, in the course of *cis*-1,2-DMCH (0.1 M) oxidation with *m*-CPBA (0.027 M) catalyzed by **1** ([$\mathbf{1_{Co}}$]$_0$ = 1.1 × 10^{-5} M) in the presence of HNO_3 (5.5 × 10^{-3} M) in acetonitrile under $^{18}O_2$ atmosphere. The reaction was initiated and continued at 0 °C for the first 2 h. Then the reaction mixture was heated until 50 °C and continued at this temperature. The inset shows the EI spectra of (labeled) CO_2 present in the reaction solution. Analysis of the headspace atmosphere of the Schlenk tube revealed similar spectra.

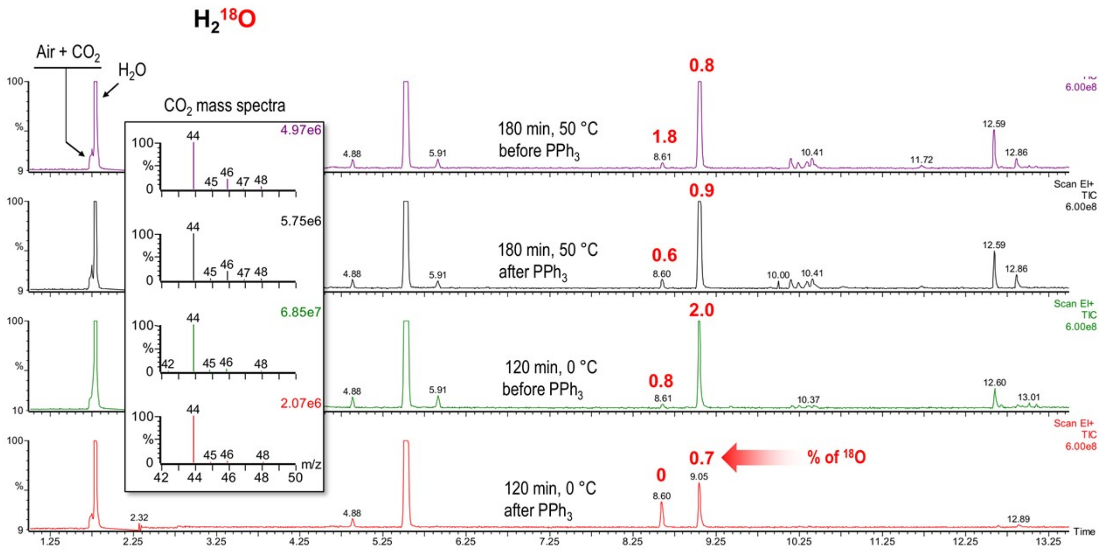


Figure S21. Fragments of the chromatograms showing the main reactions products, along with substrates, in the course of *cis*-1,2-DMCH (0.1 M) oxidation with *m*-CPBA (0.027 M) catalyzed by **1** ([$\mathbf{1_{Co}}$]$_0$ = 1.1 × 10^{-5} M) in the presence of HNO_3 (5.5 × 10^{-3} M) in acetonitrile in the presence of $H_2{}^{18}O$ (0.5 M). The reaction was initiated and continued at 0 °C for the first 2 h. Then the reaction mixture was heated until 50 °C and continued at this temperature. The inset shows the EI spectra of (labeled) CO_2 present in the reaction solution. Analysis of the headspace atmosphere of the Schlenk tube revealed similar spectra.

Search for alkyl hydroperoxides

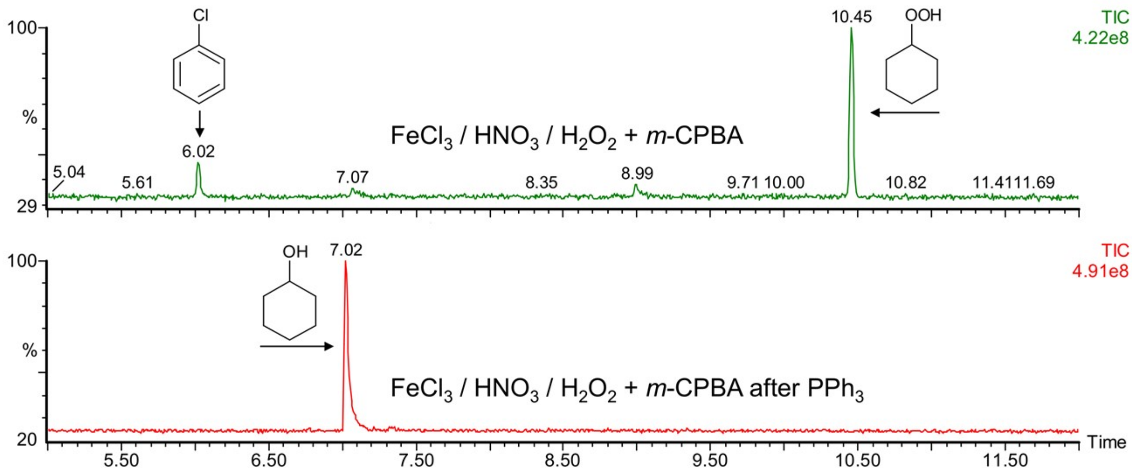


Figure S22. Fragments of the chromatograms (recorded before and after addition of PPh_3) illustrating persistence of cyclohexyl hydroperoxide in the presence of *m*-CPBA. Cyclohexyl hydroperoxide was obtained by reacting H_2O_2 (1 M) with cyclohexane (0.37 M) in the presence of HNO_3 (4×10^{-3} M) and $FeCl_3$ (6×10^{-4} M) as a catalyst in acetonitrile at 50 °C. After 1 h the solution of *m*-CPBA in acetonitrile was added to reach its final concentration of 0.027 M and the mixture was stirred for another 1 h before being analyzed.

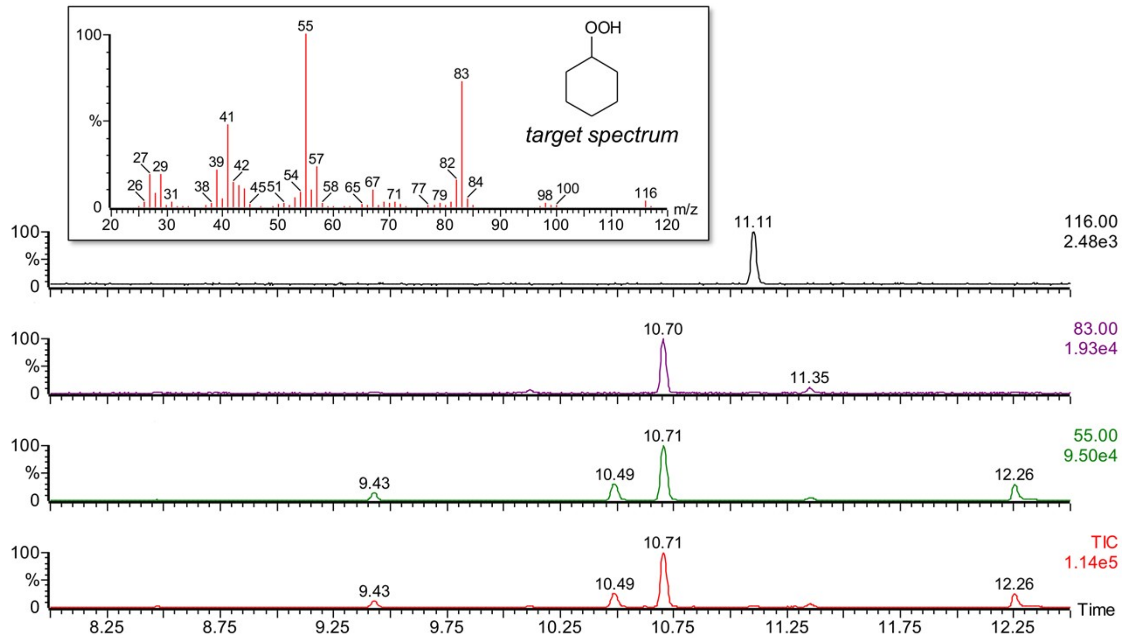


Figure S23. Fragments of the chromatograms showing the region where cyclohexyl hydroperoxide, CyOOH, is expected (ca. 10.5 min) in the course of cyclohexane (0.2 M) oxidation with *m*-CPBA (0.027 M) catalyzed by **1** ($[\mathbf{1}_{\mathbf{Co}}]_0 = 1.1 \times 10^{-5}$ M) in the presence of HNO_3 (5.5×10^{-3} M) in acetonitrile at 0 °C after 2 h. The full MS chromatogram is shown in bottom, while the other chromatograms demonstrate the intensities of particular *m/z* signals designated in the right. No signs for CyOOH are seen since no coinciding 55, 83 and 116 *m/z* peaks are observed.

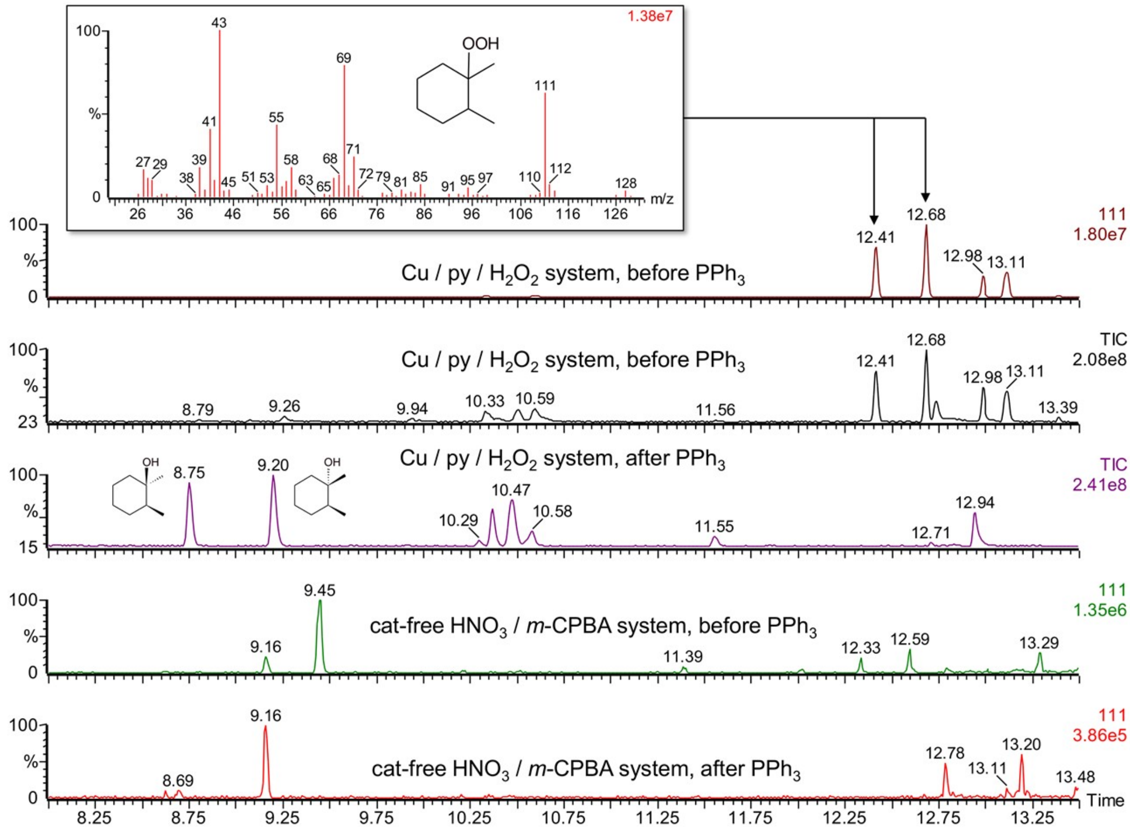


Figure S24. Fragments of the chromatograms showing the main reactions products in the course of *cis*-1,2-DMCH (0.1 M) oxidation with two different catalytic systems (both in acetonitrile at 50 °C): (a) [Cu(L)] / Pyridine / H_2O_2 (where L = 2,4-methoxy-1,3,5-triazapentadiene), known to attack C–H bonds with HO• radicals and form alkyl hydroperoxides as main products,[S30] and (b) catalyst-free oxidation with *m*-CPBA (0.027 M) in the presence of HNO_3 (5.5×10^{-3} M). The weak peaks at 12.3 and 12.6 min observed for (b) reveal MS spectra corresponding to tertiary alkyl hydroperoxides (see the inset).

Stability of complex catalytic species under catalytic conditions

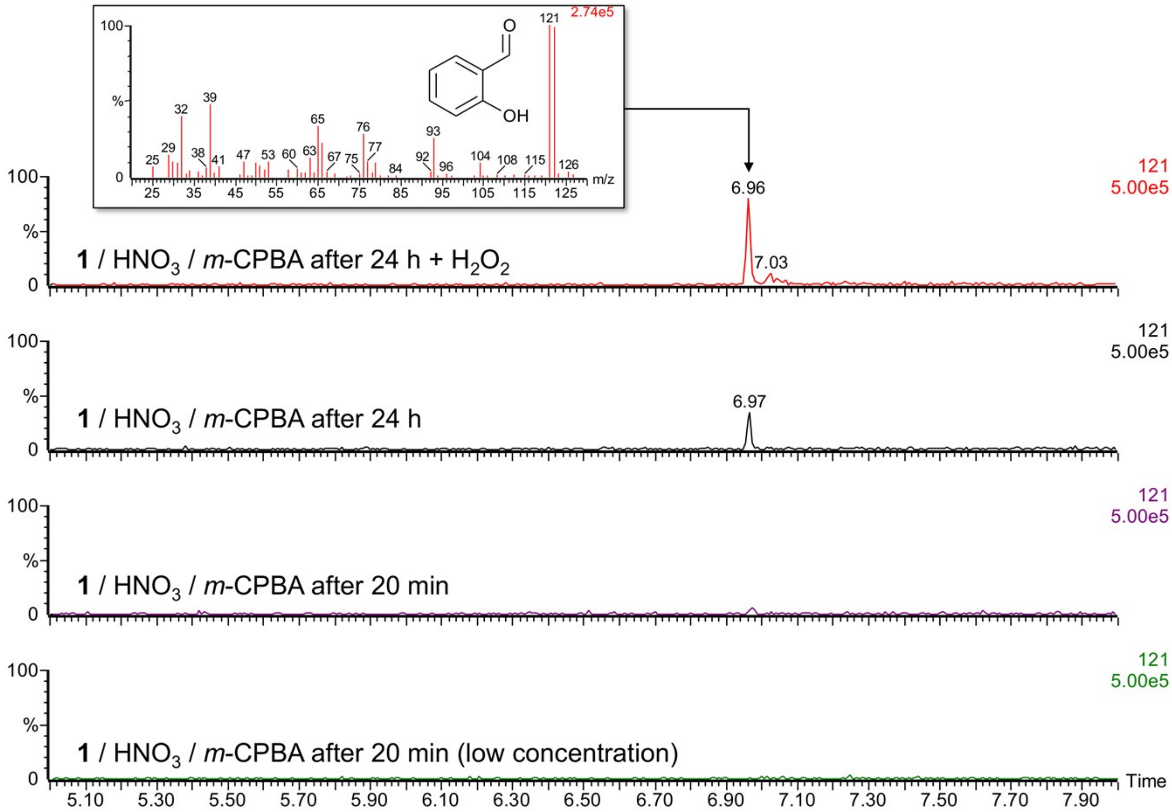


Figure S25. Fragments of the chromatograms showing the 121 *m/z* signal, corresponding to salicylic aldehyde (formed from the degradation of Schiff base ligand H_2Sae), for $[\mathbf{1}]_0 = 2.7 \times 10^{-6}$ M and $[m\text{-CPBA}]_0 = 0.027$ M (bottom) and $[\mathbf{1}]_0 = 1 \times 10^{-5}$ M and $[m\text{-CPBA}]_0 = 0.1$ M (other chromatograms), in the presence of HNO_3 (5.5×10^{-3} M) in acetonitrile. The peak of salicylic aldehyde becomes clearly visible only after treatment of **1** with *m*-CPBA for 24 h and enhances after addition of H_2O_2 (1 M).

Reaction by-products

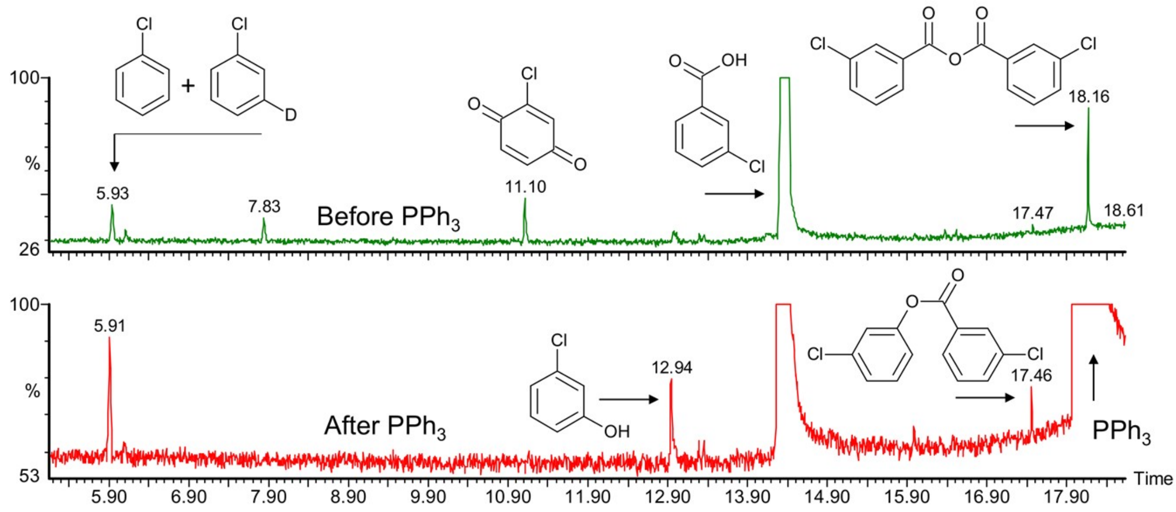


Figure S26. Fragments of chromatograms recorded before and after addition of PPh_3, in the course of substrate-free decomposition of 0.027 M of *m*-CPBA, catalyzed by **1** ([$\mathbf{1_{Co}}$]$_0$ = 1.1×10^{-5} M) in the presence of HNO_3 (5.5×10^{-3} M) in deuterated acetonitrile (CD_3CN) at 50 °C, after 1 h.

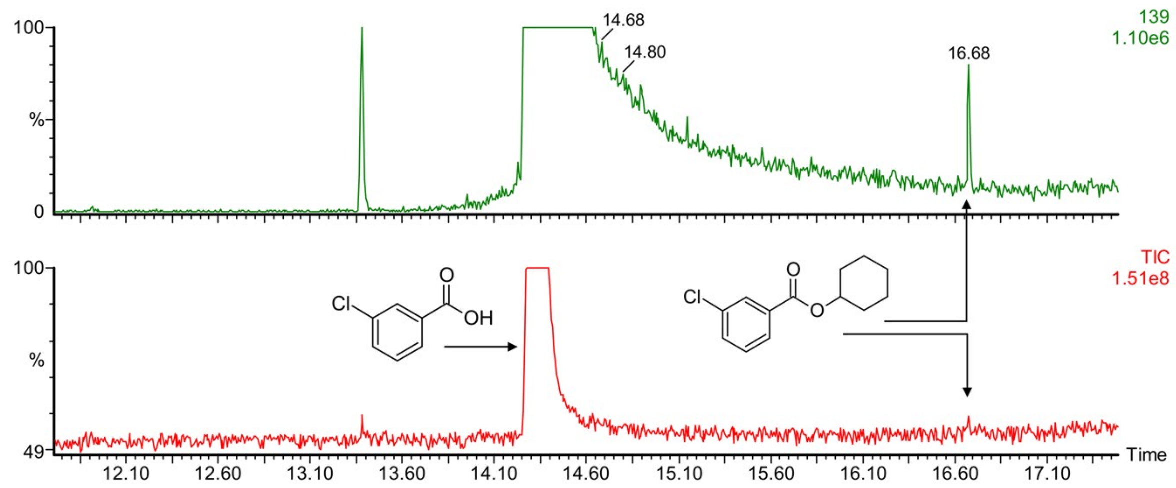


Figure S27. Fragments of the chromatograms showing the peak of cyclohexyl *m*-chlorobenzoate ester observed in the course of cyclohexane (0.2 M) oxidation with *m*-CPBA (0.027 M) catalyzed by **1** ([$\mathbf{1_{Co}}$]$_0$ = 1.1×10^{-5} M) in the presence of HNO_3 (5.5×10^{-3} M) in acetonitrile at 0 °C after 2 h.

Accumulation of ^{18}O-labeled $OPPh_3$ and tertiary alcohols

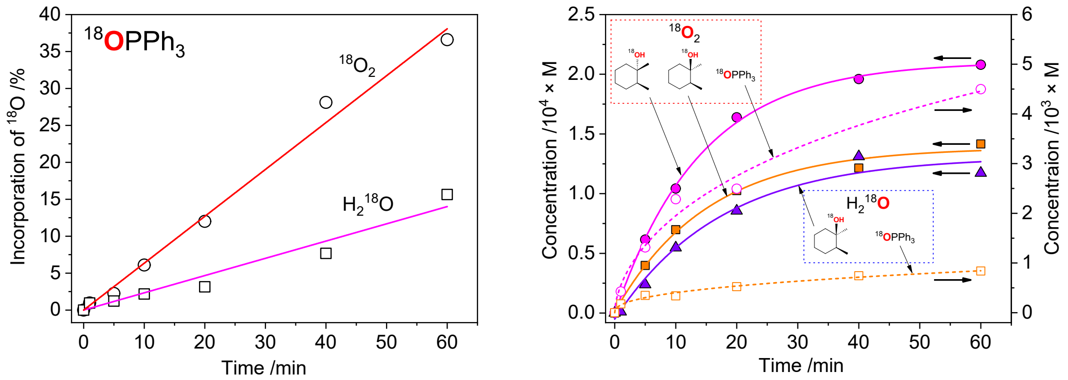


Figure S28. Left: incorporation of ^{18}O into $^{18}OPPh_3$, observed after treatment of the reaction probe with PPh_3 for oxidations of *cis*-1,2-DMCH under $^{18}O_2$ or in the presence of 0.5 M $H_2{}^{18}O$ (conditions are as those for Entry 5, Table 1). Right: accumulations of ^{18}O-labeled tertiary alcohols and $^{18}OPPh_3$ for the same reactions.

HF-EPR spectra of cobalt species before and after interaction with *m*-CPBA

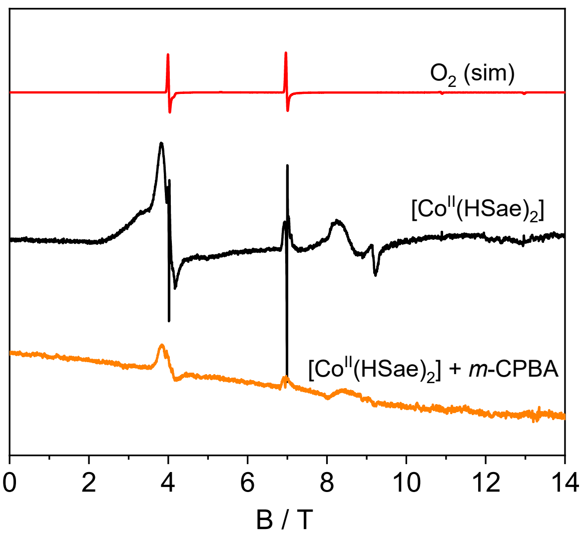


Figure S29. HF-EPR spectra (256 GHz, 5 K) of 20 mM solution of [Co(HSae)$_2$] complex in acetonitrile, formed *in situ* (black line). After addition of 1 equivalent of *m*-CPBA (at room temperature) the deep green color of the initial solution immediately turned to dark brown one. This solution was frozen, and the spectrum recorded under the same conditions (orange line). The sharp lines, visible in the spectrum of the pure complex, correspond to frozen oxygen (red line).

ESI-MS spectra of catalytic solutions

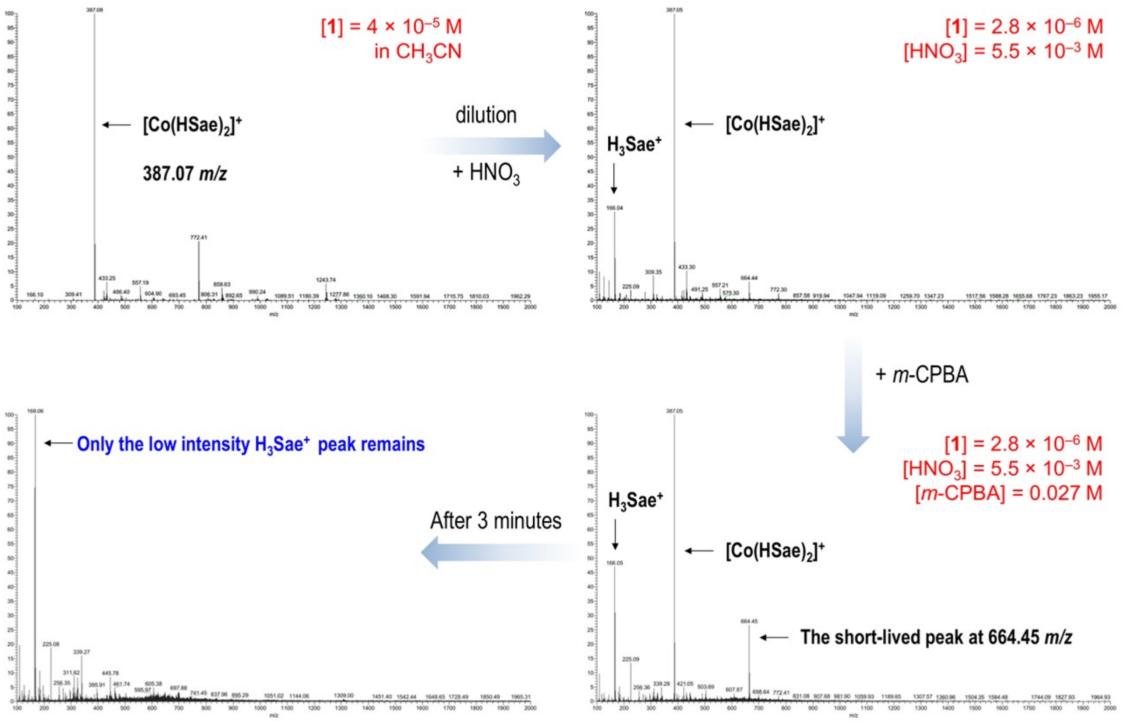
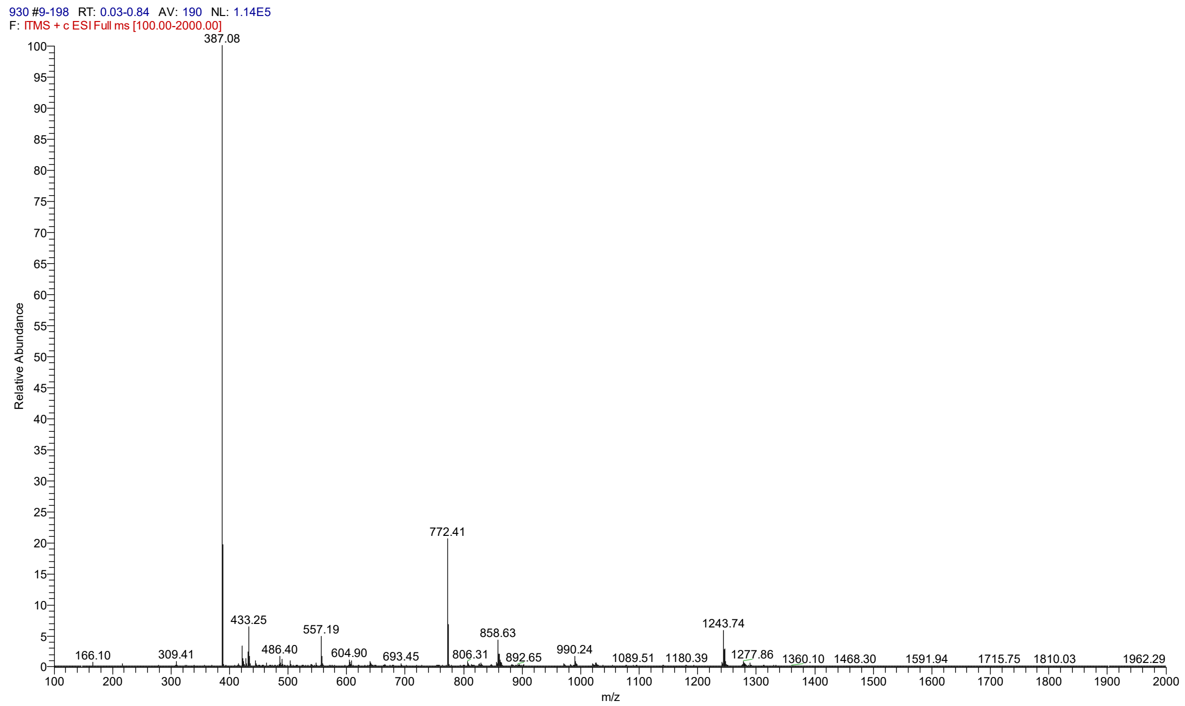
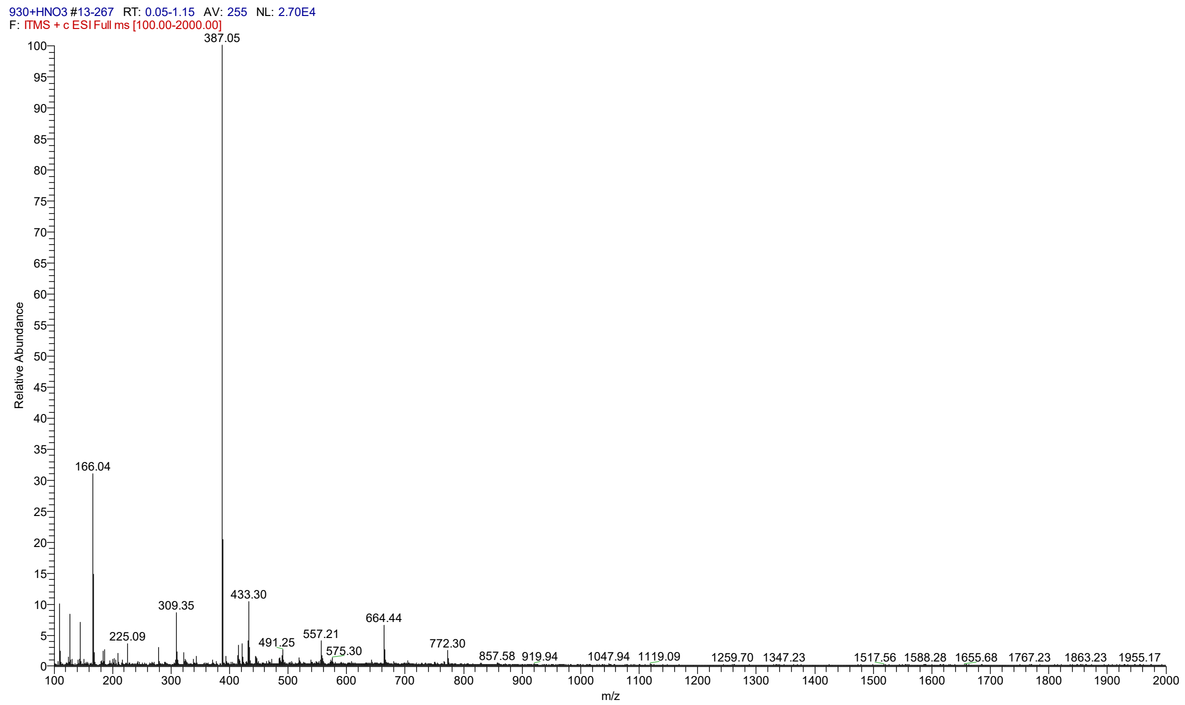
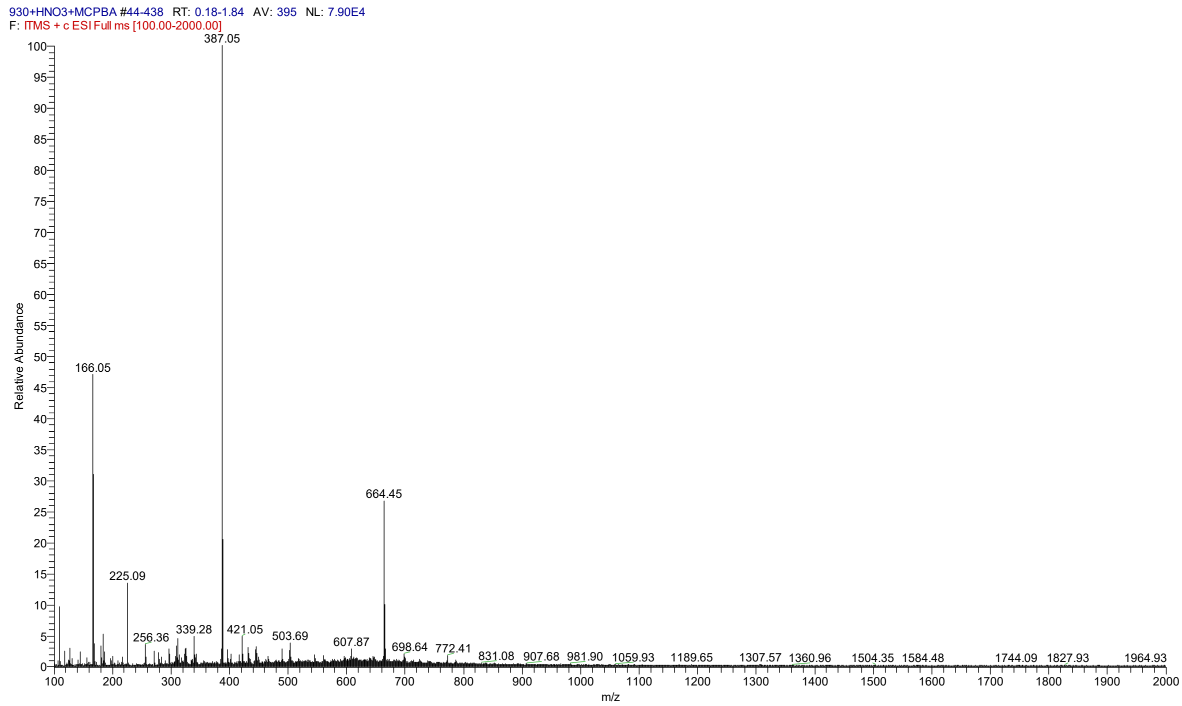


Figure S30. Evolution of the ESI-MS spectra of the complex **1** in the presence of other components of the catalytic system, in acetonitrile at room temperature. The detailed spectra are shown in Figure S31 in the same order.


930 #9-198 RT: 0.03-0.84 AV: 190 NL: 1.14E5
F: ITMS + c ESI Full ms [100.00-2000.00]
387.08
772.41
433.25
557.19
858.63
1243.74
486.40
604.90
693.45
806.31
892.65
990.24
1089.51
1180.39
1277.86
1360.10
1468.30
1591.94
1715.75
1810.03
1962.29
166.10
309.41
Relative Abundance
m/z


930+HNO3 #13-267 RT: 0.05-1.15 AV: 255 NL: 2.70E4
F: ITMS + c ESI Full ms [100.00-2000.00]
387.05
166.04
309.35
433.30
225.09
664.44
491.25
557.21
575.30
772.30
857.58
919.94
1047.94
1119.09
1259.70
1347.23
1517.56
1588.28
1655.68
1767.23
1863.23
1955.17
Relative Abundance
m/z



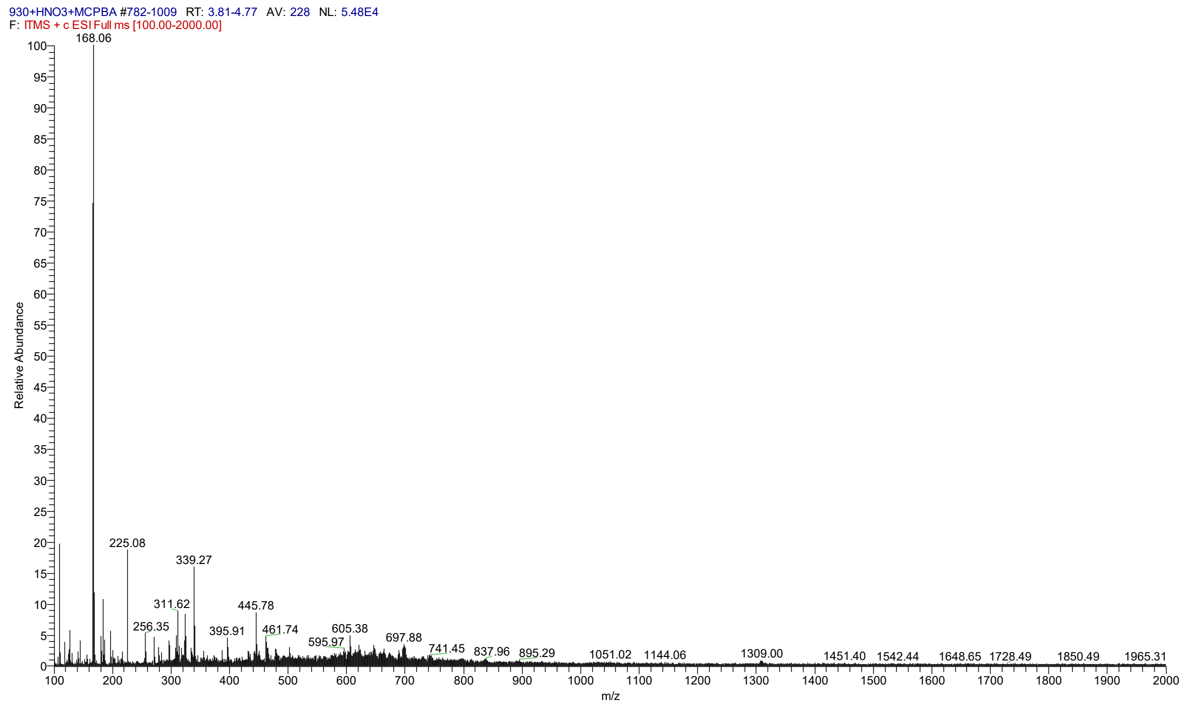
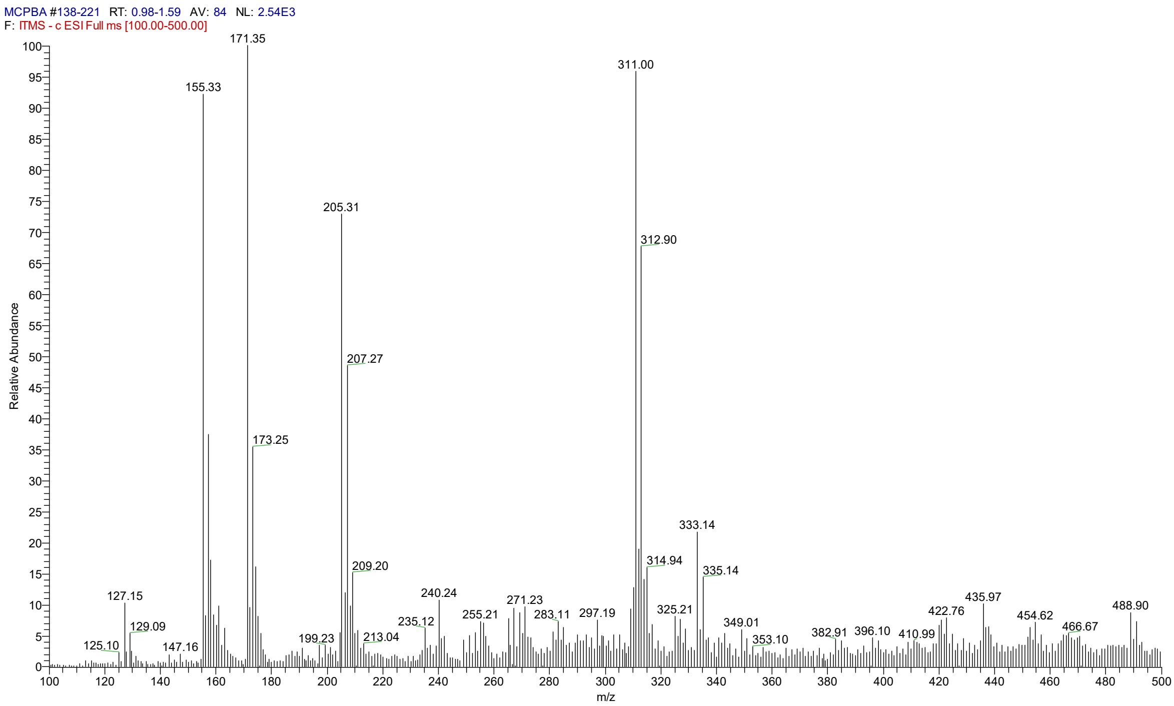


Figure S31. ESI-MS spectra corresponding to those shown in Figure S30 in the same order.



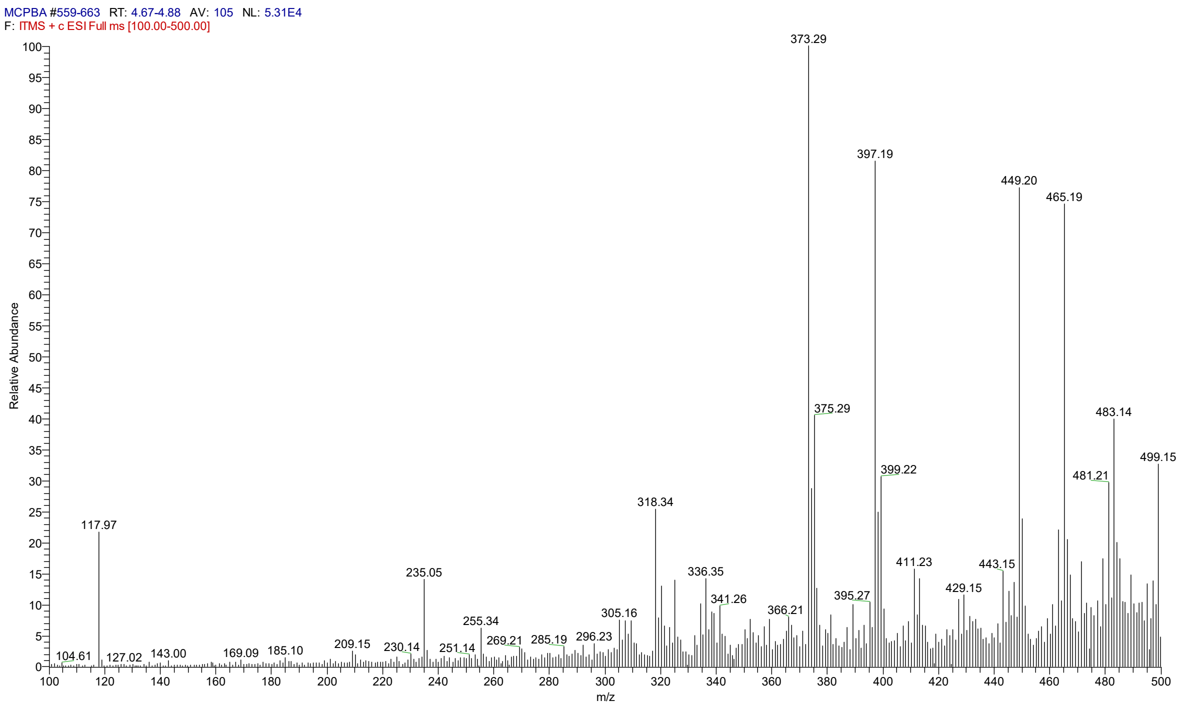
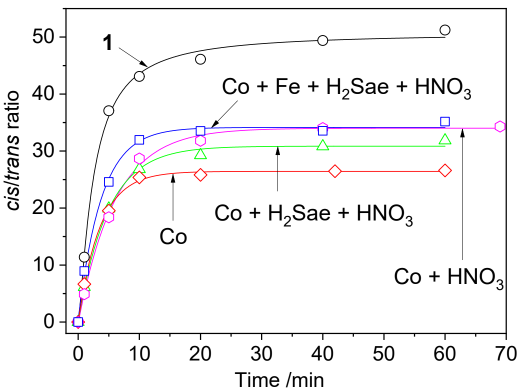


Figure S32. ESI-MS spectra recorded in negative (top) and positive (bottom) modes of the 0.03 M solution of *m*-CPBA in acetonitrile.

In situ catalytic systems



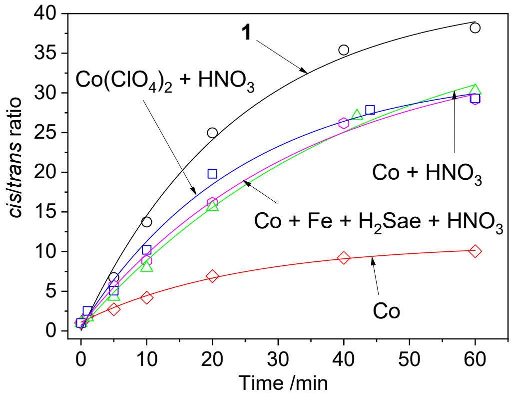


Figure S33. The *c*/*t* ratios as function of time shown for catalytic systems using pre-catalyst **1** and respective mixtures of salts and ligand H_2Sae (*in situ* systems) in the presence or absence of HNO_3 (5.5 × 10^{-3} M) for $[Co]_0$ = 1.2 × 10^{-4} M (left) and 1.1 × 10^{-5} M (right). The salts are nitrates, unless stated otherwise. Concentration of the iron salt was twice lower than the cobalt one.

Reaction mass balance for 1 and 2

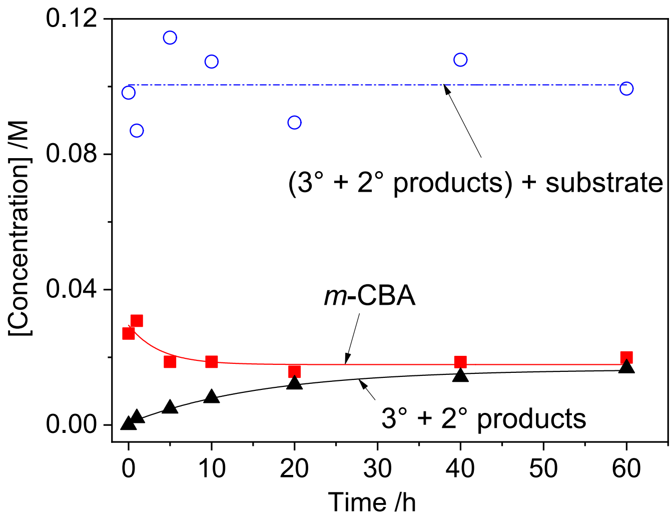


Figure S34. Accumulation of the sums of tertiary and secondary hydroxylation products (△, black line), amount of *m*-chlorobenzoic acid (*m*-CBA) as a function of time after reduction of the samples with PPh_3 (□, red line) and mass balance of the *cis*-1,2-DMCH oxidation (sum of hydroxylation products and substrate, where the latter was corrected for evaporation, ○, blue line). The data correspond to the Entry 5, Table 1. The amounts of *m*-CBA were obtained by averaging four independent tests made under the same conditions and corrected for the "ballast" amount of *m*-CBA contained in the commercial *m*-CPBA oxidant (0.009 M under conditions of Entry 5).

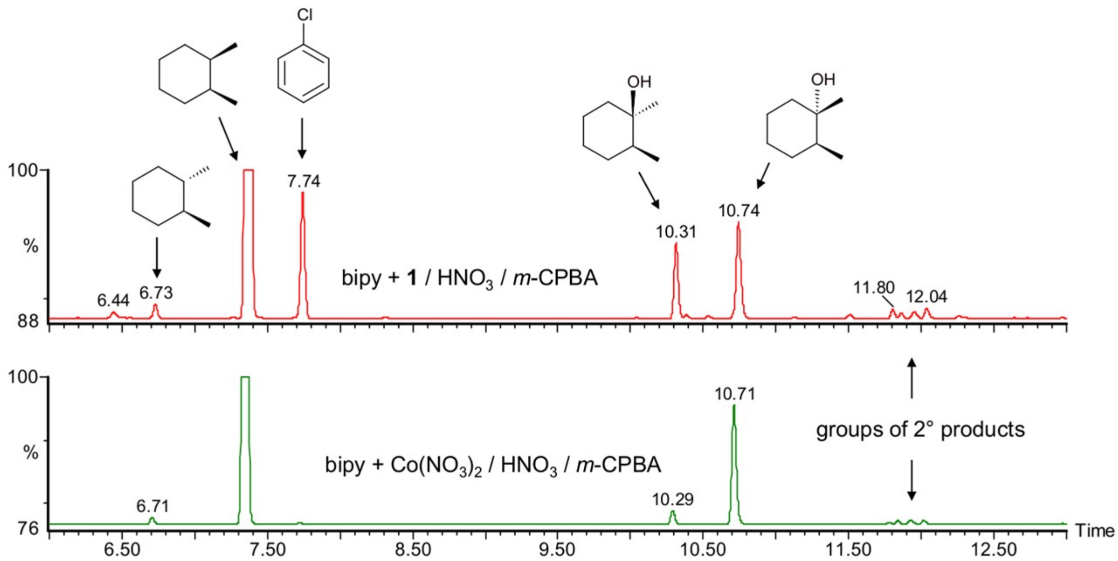


Figure S35. Fragments of the chromatograms showing the main reactions products, along with substrates, in the course of *cis*-1,2-DMCH (0.1 M) oxidation with *m*-CPBA (0.027 M) catalyzed by **1** ([$\mathbf{1_{Co}}$]$_0$ = 1 × 10^{-5} M, top) or $Co(NO_3)_2$ (1 × 10^{-5} M, bottom) in the presence of HNO_3 (5.5 × 10^{-3} M) and 2,2′-bipyridine (1.5 × 10^{-5} M for **1** or 1 × 10^{-5} M for $Co(NO_3)_2$) in acetonitrile at 50 °C after 1 h. The bipyridine was added prior in a form of stock solution in acetonitrile after addition of the catalyst solution.

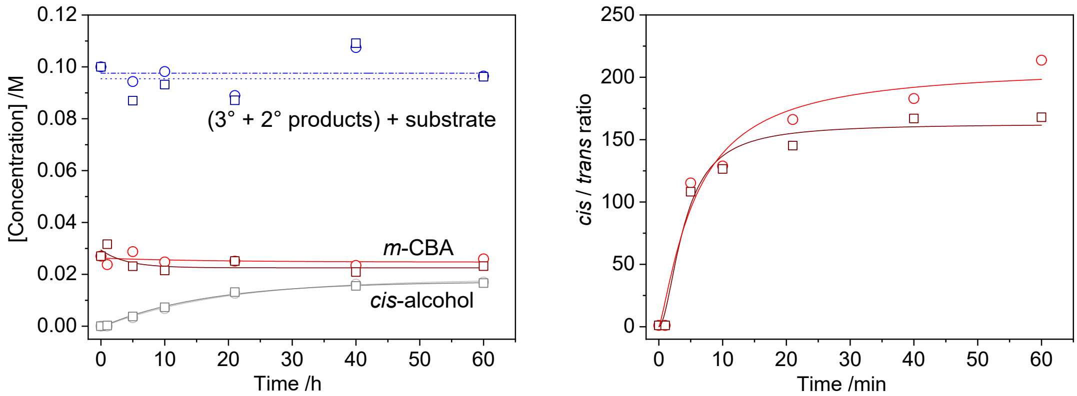


Figure S36. Left: Accumulation of the tertiary *cis*-alcohols, amount of *m*-chlorobenzoic acid (*m*-CBA) as a function of time after reduction of the samples with PPh_3 and mass balance of the *cis*-1,2-DMCH oxidation (sum of hydroxylation products and substrate, where the latter was corrected for evaporation. The data correspond to the Entries 15 (○) and 16 (□), Table 1. The amounts of *m*-CBA were obtained by averaging four independent tests made under the same conditions and corrected for the "ballast" amount of *m*-CBA contained in the commercial *m*-CPBA oxidant (0.009 M under conditions of Entries 15 and 16). Right: *cis* / *trans* ratio as a function of time under the same conditions.

Theoretical calculations: alternative reaction mechanisms

Besides the mechanisms discussed in the main text, several other possibilities were considered. First pathway is similar to the non-radical mechanism based on **TS1**. However, it affects the peroxo oxygen atom which is not bonded to the metal center (Scheme S1A). Second pathway is also concerted nonradical and it involves simultaneous formation of the C–O(1) bond and hydrogen transfer assisted by water which inevitably exists in the reaction mixture (or by any other possible proton shuttle) (Scheme S1B). However, careful analysis of the potential energy surface (PES) revealed that the corresponding transition states for these both pathways do not exist.

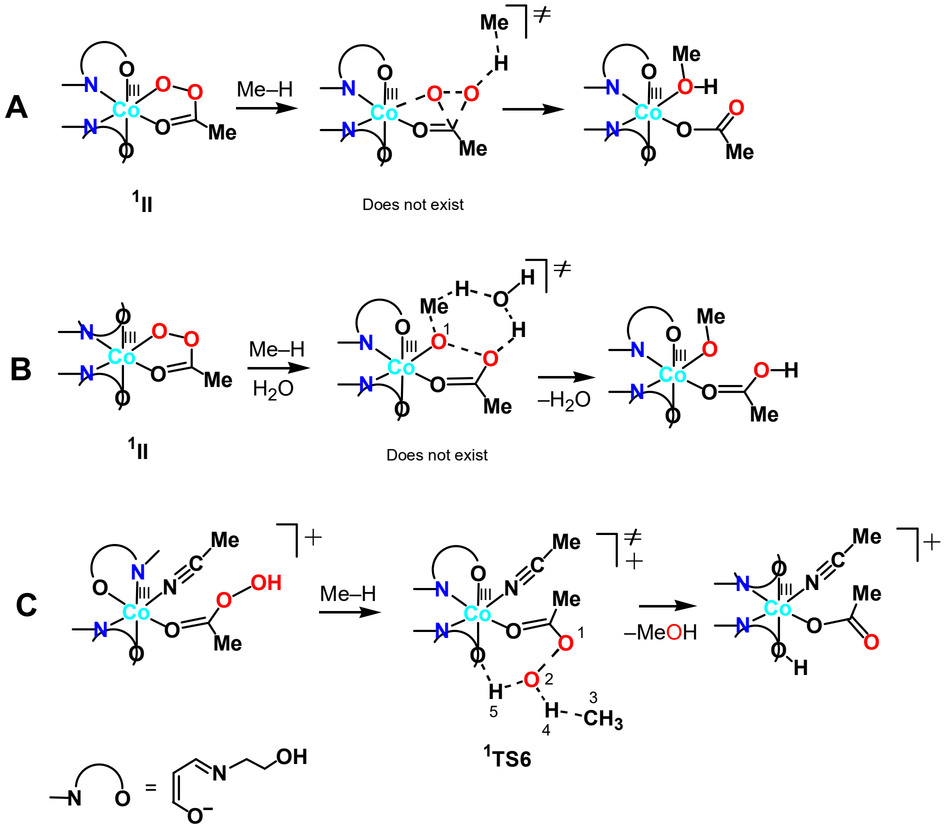
Search of PES for the system $[Co(Sae)_2(NCMe)\{\underline{O}{=}C(Me)OOH\}]^+$ + CH_4 with protonated peroxoacetic acid allowed the location of transition state ^{1}**TS6** (Scheme S1C) which corresponds to the simultaneous cleavage of the O(1)–O(2) and C(3)–H(4) bonds, transfer of the protons H(4) and H(5) and formation of the C(3)O(2) bond. However, the calculated activation energy of this pathway is 41.6 kcal/mol relative to $[Co(Sae)_2(NCMe)\{\underline{O}{=}C(Me)OOH\}]^+$ and CH_4. Thus, this mechanism is not the most plausible one.

For the model reaction of the methane oxidation with peroxoacetic acid and catalyst **II**, another possible transition state (^{1}**TS4**) with the η^2-coordinated peroxoacetate was also found for the concerted closed-shell non-radical mechanism (Scheme S3). However, ^{1}**TS4** is significantly less stable than ^{1}**TS1** (by 11.8 kcal/mol) and this possibility may be ruled out.

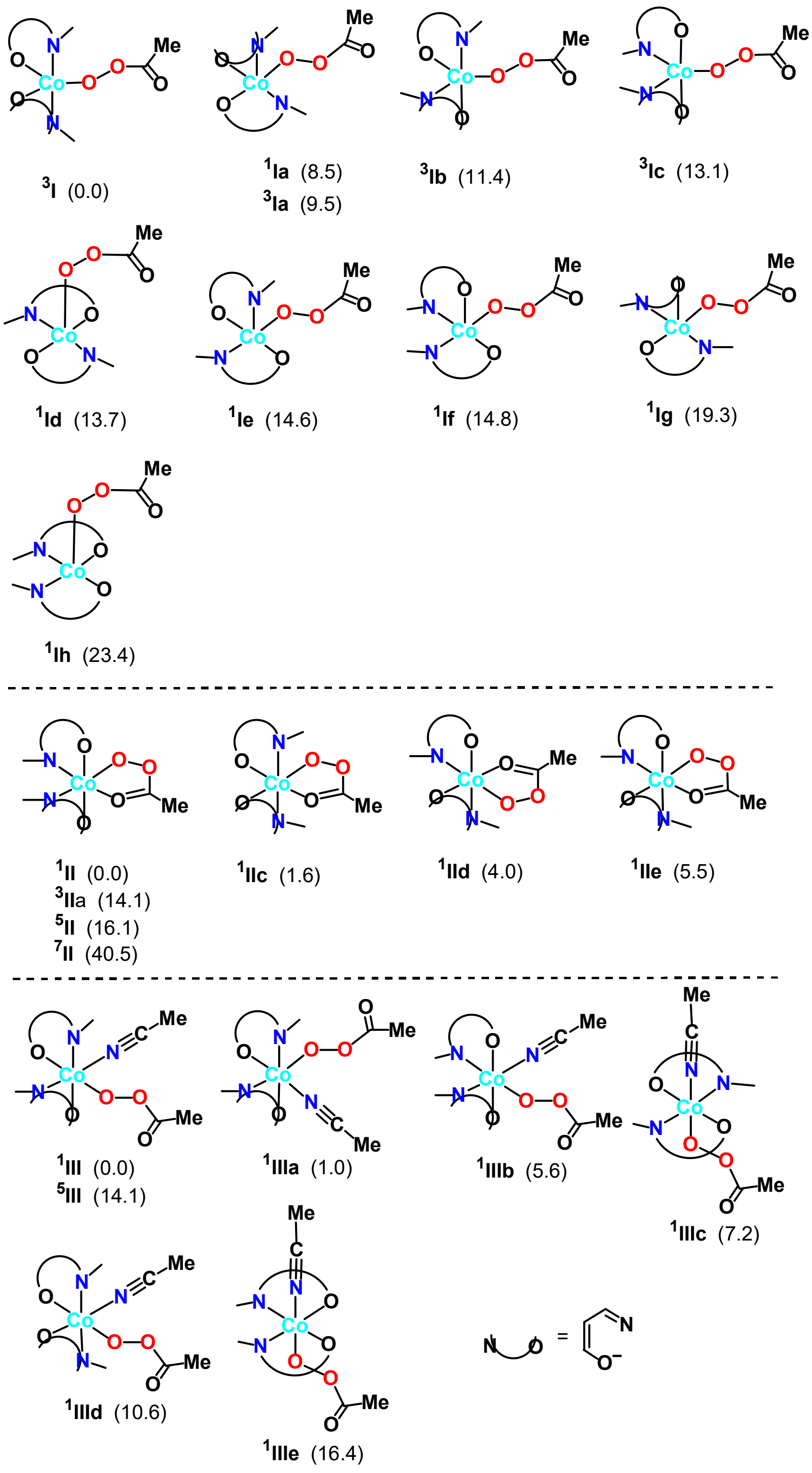
Besides the mechanism based on complex ^{3}**V**, another pathway including an H-abstraction by alkane from ^{3}**IIb** via ^{3}**TS5** to give the hydroxo complex $[Co(HL)_2(OH)\{OC(O)Me\}]$ (^{3}**VI**) and methyl radical loosely bound to the hydroxo ligand is possible (Scheme S3,B). The hydrogen abstraction by complex ^{3}**V** (via ^{3}**TS2**) is more favourable than that by complex ^{3}**IIb** (via ^{3}**TS5**) by 6.4 kcal/mol. Similar rebound pathway $^{5/7}$**IIb** + CH_4 → $^{5/7}$**TS5** → $^{5/7}$**VI** was found for the quintet and septet surfaces. However, they are more energy demanding that the route on the triplet surface (by 4.8–18.8 kcal/mol).

Computational details of the radical rebound mechanism

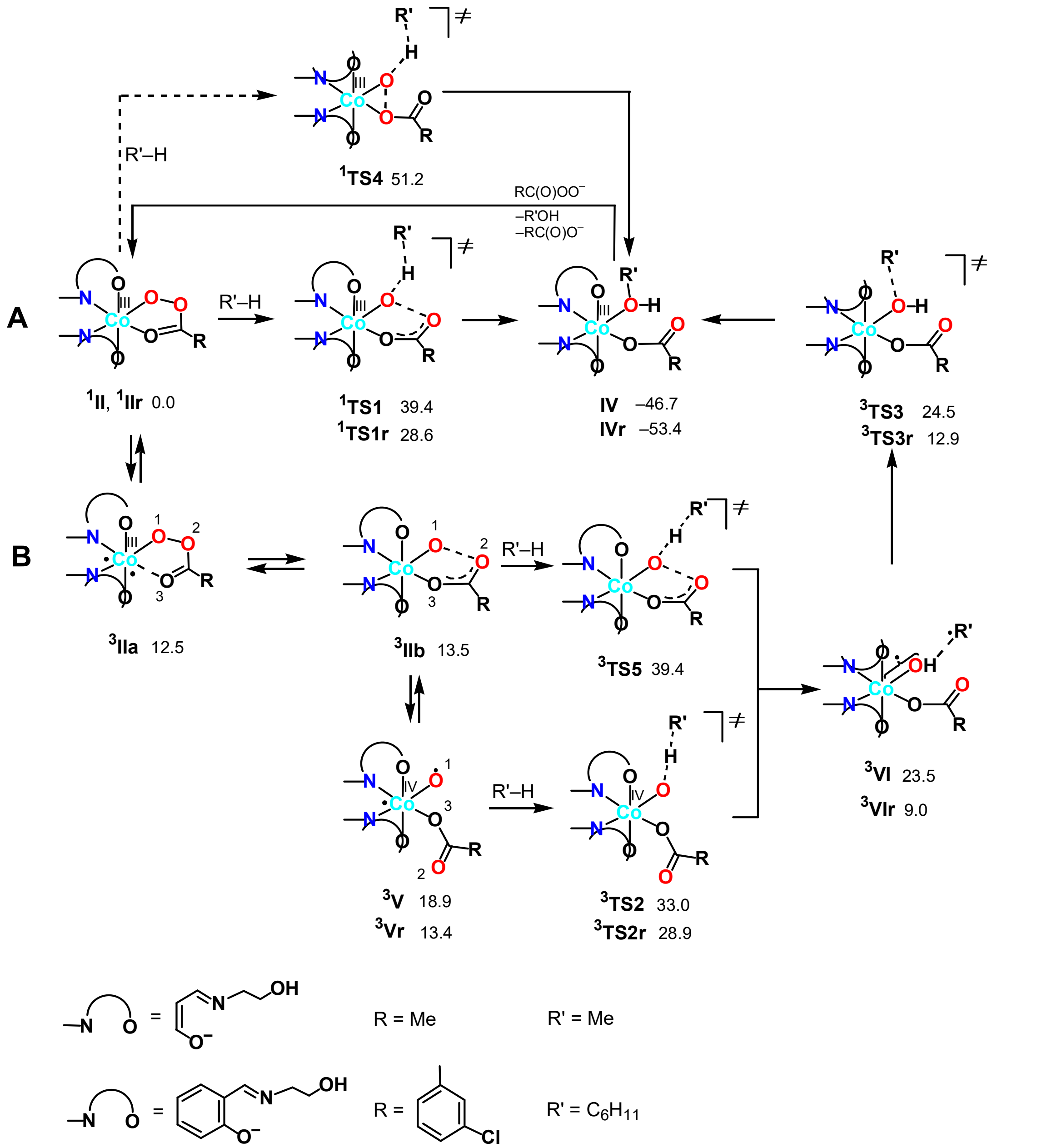
To investigate the radical rebound mechanism in more detail, calculations of the methane oxidation with peroxoacetic acid and catalyst **II** via this mechanism were carried out. The homolytic O–O bond cleavage requires the initial spin conversion of **II** from singlet to triplet state. Two structures of the triplet model complex ^{3}**II** were found (Scheme S3). In the first one (^{3}**IIa**), spin density is mostly localized at the Co atom (1.75 e, Figure S37), and the Co–O(3) bond is significantly elongated (to 2.540 Å). In the second complex (^{3}**IIb**), spin density is localized at the O(1), O(2) and Co atoms (1.35, 0.28 and 0.26 e, respectively). The O(1)–O(2) distance is 2.223 Å that corresponds to the spontaneous O–O bond rupture upon formation of ^{3}**IIb**. Finally, a simple rotation of the acetate ligand around the Co–O(3) bond leads to the oxo-complex [Co(HL)$_2$(O){OC(O)Me}] (^{3}**V**). Therefore, complex ^{3}**V** (or ^{3}**Vr** which corresponds to the real species used in this work) may be considered as an active catalytic species for this mechanism.



Scheme S1. Alternative mechanisms of hydroxylation.



Scheme S2. The calculated structures of various isomers of complexes **I**–**III** with relative energies (in kcal/mol) and spin states (the upper index) indicated.



Scheme S3. The possible mechanisms of the alkane (R′H) hydroxylation on the singlet (A) and triplet (B) surfaces (Gibbs free energies in CH_3CN solution are indicated relative to **¹II** or **¹IIr** in kcal/mol).

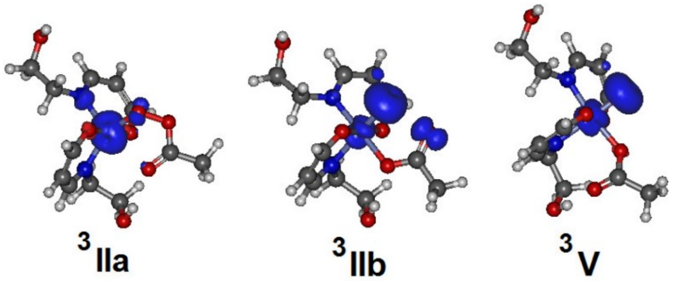


Figure S37. Spin density distribution in **³IIa**, **³IIb** and **³V**.

Table S2. Calculated total energies (E_g, E_s), enthalpies (H_g, H_s), Gibbs free energies (G_g, G_s) (in Hartree) and entropies (S_g, S_s) (in cal/mol•K) in gas phase and acetonitrile solution.

	E_g	E_s	H_g	H_s	S_g	S_s	G_g	G_s
MeCN	–132.667040	–132.718468	–132.617182	–132.668610	60.14	42.78	–132.645754	–132.688934
CH_4	–40.483901	–40.498456	–40.435148	–40.449703	46.67	32.40	–40.457323	–40.465099
C_6H_{12}	–235.703449	–235.770012	–235.526794	–235.593357	74.68	53.97	–235.562275	–235.619001
^{3}I	–1249.930822	–1250.327156	–1249.586141	–1249.982475	174.53	130.86	–1249.669065	–1250.044649
^{1}Ia	–1249.917271		–1249.571902		166.14		–1249.650840	
^{3}Ia	–1249.915644		–1249.571705		172.21		–1249.653529	
^{3}Ib	–1249.912592		–1249.568369		175.72		–1249.651860	
^{3}Ic	–1249.909998		–1249.565956		180.79		–1249.651856	
^{1}Id	–1249.908942		–1249.563842		170.37		–1249.644791	
^{1}Ie	–1249.907563		–1249.562475		168.87		–1249.642710	
^{1}If	–1249.907201		–1249.562025		167.00		–1249.641370	
^{1}Ig	–1249.900104		–1249.555345		169.67		–1249.635963	
^{1}Ih	–1249.893547		–1249.548952		168.62		–1249.629067	
^{1}II	–1249.941218	–1250.338466	–1249.595186	–1249.992434	161.53	120.85	–1249.671931	–1250.049852
^{3}IIa	–1249.918714	–1250.313184	–1249.574074	–1249.968544	172.40	129.22	–1249.655988	–1250.029939
^{3}IIb	–1249.915844	–1250.314687	–1249.571230	–1249.970073	163.95	122.71	–1249.649127	–1250.028376
^{5}IIb	–1249.915625	–1250.309179	–1249.571982	–1249.965536	176.16	132.11	–1249.655680	–1250.028306
^{7}IIa	–1249.818101		–1249.477671		179.63		–1249.563020	
^{7}IIb	–1249.876673	–1250.280800	–1249.535246	–1249.939373	179.94	135.02	–1249.620742	–1250.003526
^{1}IIc	–1249.938725		–1249.593099		160.95		–1249.669571	
^{1}IId	–1249.934875		–1249.588920		159.40		–1249.664655	
^{1}IIe	–1249.932381		–1249.587223		165.34		–1249.665783	
^{1}III	–1382.604801	–1383.038291	–1382.206935	–1382.640425	183.37	137.66	–1382.294061	–1382.705833
^{5}III	–1382.582265		–1382.187510		196.94		–1382.281082	
^{1}IIIa	–1382.603285		–1382.205876		183.13		–1382.292886	
^{1}IIIb	–1382.595926		–1382.198587		185.22		–1382.286592	
^{1}IIIc	–1382.593310		–1382.196351		196.42		–1382.289677	
^{1}IIId	–1382.587940		–1382.190917		191.14		–1382.281735	

¹IIIe	–1382.578741		–1382.181964		186.18		–1382.270424	
¹IIr	–2208.134411	–2208.673559	–2207.642148	–2208.181296	207.72	156.41	–2207.740845	–2208.255613
¹IV	–1290.502940	–1290.926150	–1290.103313	–1290.526523	176.29	132.21	–1290.187073	–1290.589341
³IV	–1290.481659	–1290.900998	–1290.084158	–1290.503497	187.83	141.10	–1290.173403	–1290.570537
⁷IV	–1290.380420		–1289.986891		195.55		–1290.079801	
¹IVr	–2443.943040	–2444.545463	–2443.271126	–2443.873549	240.00	181.27	–2443.385156	–2443.959675
³V	–1249.903907	–1250.304343	–1249.559864	–1249.960300	167.24	125.24	–1249.639322	–1250.019807
⁵V	–1249.898936	–1250.305107	–1249.556655	–1249.962826	175.28	131.43	–1249.639937	–1250.025274
⁷V	–1249.879047	–1250.286474	–1249.538378	–1249.945805	182.29	136.83	–1249.624991	–1250.010818
³Vr	–2208.105269	–2208.647105	–2207.615130	–2208.156966	215.73	162.58	–2207.717630	–2208.234213
³VI	–1290.378610	–1290.799692	–1289.987074	–1290.408156	193.92	145.79	–1290.079209	–1290.477424
³VIr	–2443.813195	–2444.430464	–2443.146805	–2443.764074	267.47	202.42	–2443.273887	–2443.860250
¹TS1	–1290.366360	–1290.782246	–1289.975401	–1290.391287	170.84	128.02	–1290.056574	–1290.452111
¹TS1r	–2443.793610	–2444.405196	–2443.129431	–2443.741017	245.10	185.20	–2443.245883	–2443.829009
¹TS4	–1290.349771	–1290.761680	–1289.958951	–1290.370860	175.50	131.60	–1290.042336	–1290.433389
³TS4	–1290.331117		–1289.941618		180.05		–1290.027164	
³TS5	–1290.336830	–1290.770963	–1289.950285	–1290.384418	189.62	142.48	–1290.040379	–1290.452113
⁵TS5	–1290.350912	–1290.752590	–1289.964556	–1290.366234	185.72	139.47	–1290.052798	–1290.432502
⁷TS5	–1290.341794	–1290.751376	–1289.956729	–1290.366311	192.16	144.43	–1290.048032	–1290.434935
³TS2	–1290.368120	–1290.784875	–1289.980820	–1290.397575	181.88	136.52	–1290.067236	–1290.462438
⁵TS2	–1290.352140	–1290.771438	–1289.966952	–1290.386250	191.80	144.15	–1290.058081	–1290.454742
⁷TS2	–1290.341233	–1290.757279	–1289.957336	–1290.373382	195.66	147.13	–1290.050302	–1290.443287
³TS2r	–2443.798025	–2444.400487	–2443.136095	–2443.738557	250.75	189.55	–2443.255233	–2443.828616
³TS3	–1290.373676	–1290.798560	–1289.983074	–1290.407958	190.40	143.08	–1290.073540	–1290.475938
³TS3r	–2443.811357	–2444.427523	–2443.146379	–2443.762545	254.52	192.45	–2443.267309	–2443.853984
¹TS6	–1423.424468	–1423.925820	–1422.969637	–1423.470989	201.36	151.52	–1423.065311	–1423.542979

Table S3. Cartesian atomic coordinates (in Å) of the calculated equilibrium structures (atomic symbols or nuclear charges are given in the first column).

MeCN

N		-1.081372	-1.530901	0.993099
C		-1.610684	-2.347075	1.630271
C		-2.275390	-3.372502	2.431481
H		-2.580113	-4.213916	1.797663
H		-3.168090	-2.959122	2.916015
H		-1.598685	-3.747934	3.208486

CH_4

C	0.000000	0.000000	0.000000
H	0.632101	0.000000	0.893988
H	0.632101	0.000000	-0.893988
H	-0.632101	0.893988	0.000000
H	-0.632101	-0.893988	0.000000

C_6H_{12}

H	-2.852985	-0.112215	1.178848
C	-2.023257	-0.531906	1.771286
C	-1.572054	0.506329	2.811717
C	-0.873868	-0.917114	0.825287
H	-2.420411	-1.426470	2.272734
C	-0.954912	1.744873	2.140893
C	-0.256927	0.321491	0.154400
C	0.194443	1.359604	1.194878
H	-0.093551	-1.441763	1.401006
H	-1.228619	-1.626559	0.063570
H	0.589372	0.028063	-0.483589
H	-1.005483	0.781098	-0.512013
H	1.024142	0.939718	1.787230
H	0.591705	2.254176	0.693539
H	-1.735092	2.269699	1.565161
H	-0.600095	2.454191	2.902704
H	-2.418518	0.799887	3.449441
H	-0.823709	0.046768	3.478377

^{3}I

H	1.845313	-2.213470	-3.114181
C	1.849868	-3.021584	-2.380155
C	3.097529	-3.877645	-2.588653
N	1.782077	-2.431740	-1.035031
Co	2.205220	-0.542960	-0.844964
C	1.432968	-3.220704	-0.051676
O	2.192971	-0.638853	1.066105
N	2.618183	1.361450	-0.648270
C	3.408264	1.996201	-1.471014
O	3.737858	-0.865018	-1.984530
C	1.925074	2.144304	0.383506
H	2.362171	3.153056	0.399180
C	0.408709	2.274944	0.168751
H	0.958354	-3.641414	-2.554614
H	2.112834	1.671234	1.354369
H	3.470568	3.082239	-1.349521
O	0.099466	2.892632	-1.059334
H	0.030500	2.899733	0.996098
H	-0.068596	1.289567	0.255363
H	-0.278124	2.198444	-1.638260
H	3.163419	-4.133114	-3.661226
O	2.977774	-5.060067	-1.795944
H	3.981769	-3.288815	-2.314587
H	3.869795	-5.407744	-1.637458
H	1.164777	-4.245533	-0.317889
H	1.089231	-3.631636	2.038581
C	1.402582	-2.877035	1.323849
C	1.805204	-1.645208	1.783479
H	1.815192	-1.456002	2.865293
H	5.117472	-0.313872	-3.346110
C	4.379629	0.061475	-2.623070
C	4.234953	1.419814	-2.470794
H	4.838140	2.084460	-3.081559
O	0.782007	0.081854	-1.860183
O	-0.219350	-0.879766	-2.283159

C	-1.398500	-0.250749	-2.508983
C	-2.421482	-1.247734	-3.009346
O	-1.607657	0.933909	-2.345559
H	-2.037089	-2.271466	-3.016284
H	-2.720732	-0.963630	-4.025445
H	-3.311201	-1.189289	-2.372303

^{1}Ia

1	-0.651356	-0.013688	-0.850035
6	-1.420108	-0.690011	-0.476014
6	-1.638809	-1.805227	-1.496413
7	-0.991182	-1.212088	0.835483
27	0.888195	-1.369119	1.302098
6	-1.965454	-1.644674	1.615516
8	0.535153	-2.654346	2.654581
7	1.144832	0.047999	2.517893
6	2.300054	0.206979	3.126505
8	2.642312	-2.060497	1.358876
6	0.111241	1.069603	2.715803
1	0.408185	1.669323	3.587519
6	-0.056824	2.006576	1.496286
1	-2.361723	-0.132125	-0.360671
1	-0.843373	0.585532	2.955295
1	2.356234	1.064689	3.802760
8	1.179043	2.404498	0.942022
1	-0.573424	2.913508	1.839449
1	-0.697546	1.529792	0.743271
1	1.479339	1.649034	0.395282
1	-1.829973	-1.338419	-2.478446
8	-2.756549	-2.587277	-1.076319
1	-0.724151	-2.407523	-1.579874
1	-2.704394	-3.448439	-1.520997
1	-2.986150	-1.473363	1.265152
1	-2.705876	-2.587694	3.401312
6	-1.815420	-2.333739	2.834314
6	-0.591238	-2.840513	3.240029

1	-0.549902	-3.496980	4.120031
1	4.495191	-2.230509	2.112760
6	3.557728	-1.659732	2.156456
6	3.458995	-0.584987	3.025737
1	4.311957	-0.326305	3.644713
8	1.420391	-0.230745	-0.085178
8	1.484455	-1.151309	-1.214616
6	2.716715	-1.217297	-1.828323
6	3.771685	-0.239946	-1.383878
8	2.825656	-2.032635	-2.714894
1	3.419135	0.790112	-1.515706
1	4.664744	-0.408315	-1.990936
1	3.998721	-0.368646	-0.321863

³Ia

1	2.975576	1.938056	0.270762
6	3.743040	1.181932	0.450270
6	4.494233	1.526563	1.733740
7	3.097677	-0.136765	0.531358
27	1.362081	-0.334158	1.399267
6	3.809057	-1.167605	0.119642
8	1.793877	-2.115203	1.940065
7	0.202365	-1.037010	-0.181207
6	-0.895298	-1.680246	0.115758
8	-0.003467	-0.452658	2.691884
6	0.496169	-0.804228	-1.593269
1	-0.302548	-1.242116	-2.212488
6	0.621498	0.698480	-1.915777
1	4.456867	1.184863	-0.386680
1	1.442012	-1.302484	-1.855737
1	-1.489631	-2.079301	-0.717653
8	-0.465184	1.455230	-1.419620
1	0.635058	0.815287	-3.007943
1	1.578901	1.079496	-1.529583
1	-0.278082	1.589645	-0.469754
1	4.866702	2.562343	1.648446

8	5.569061	0.601010	1.875990
1	3.801050	1.487219	2.587074
1	5.865207	0.622255	2.800157
1	4.740047	-0.941451	-0.408129
1	4.163136	-3.280986	-0.083165
6	3.515526	-2.525191	0.350091
6	2.588138	-2.900564	1.309891
1	2.541291	-3.951809	1.625116
1	-1.547637	-1.453192	3.500427
6	-0.988113	-1.281540	2.571247
6	-1.427721	-1.900185	1.416885
1	-2.314616	-2.523471	1.491230
8	0.966130	1.440312	1.079857
8	1.189210	2.138345	2.336752
6	0.060030	2.725743	2.873524
6	-1.211124	2.671912	2.068693
8	0.208897	3.273822	3.939687
1	-1.073987	3.160103	1.095886
1	-1.987850	3.193524	2.633420
1	-1.509057	1.635412	1.883308

^{3}Ib

1	-0.205768	-3.205012	1.136307
6	0.507160	-3.417063	0.332882
6	-0.267648	-3.828088	-0.932555
7	1.355888	-2.247511	0.081276
27	0.613591	-0.399056	-0.090016
6	2.627157	-2.512652	-0.183520
8	2.141805	0.220192	-1.051980
7	-1.010827	-0.808168	0.896805
6	-2.215702	-0.777647	0.373369
8	-0.313505	-0.259056	-1.812704
6	-0.836891	-0.905742	2.356936
1	-0.700948	0.109372	2.757961
6	-1.923552	-1.642391	3.146703
1	1.136342	-4.261582	0.651669

1	0.116740	-1.420315	2.535508
1	-3.052686	-0.889234	1.066913
8	-3.171059	-0.957457	3.236503
1	-1.518470	-1.850442	4.151704
1	-2.154465	-2.608686	2.680195
1	-3.008446	-0.102337	3.672041
1	-0.783061	-4.777256	-0.735293
8	0.594783	-4.056945	-2.035585
1	-1.032481	-3.072761	-1.166815
1	0.880775	-3.184143	-2.356795
1	2.952411	-3.545591	-0.018746
1	4.617898	-1.981046	-0.779275
6	3.599090	-1.624080	-0.667338
6	3.289223	-0.338907	-1.095087
1	4.080471	0.278002	-1.541899
1	-1.931518	-0.231840	-3.012497
6	-1.585931	-0.360618	-1.976235
6	-2.531367	-0.605665	-0.995145
1	-3.578481	-0.643458	-1.280687
8	0.678047	1.051638	1.039616
8	1.933914	1.762877	1.096667
6	1.973049	2.901272	0.323449
6	0.736421	3.271002	-0.453509
8	3.010727	3.522992	0.346786
1	0.537739	2.521613	-1.228578
1	0.910284	4.245686	-0.916585
1	-0.141861	3.308163	0.200152

^{3}Ic

1	0.461965	0.578931	-1.330811
6	1.029383	-0.251806	-1.758278
6	2.504927	0.132138	-1.813498
7	0.807541	-1.453619	-0.946427
27	0.817508	-1.363460	1.062386
6	0.650280	-2.584517	-1.599015
8	0.948365	-3.254416	1.236944

7	2.534241	-1.146992	2.076446
6	2.906134	0.005030	2.593890
8	0.550050	0.507378	0.930629
6	3.331724	-2.318564	2.452690
1	4.393353	-2.030426	2.540895
6	2.863203	-2.934843	3.779286
1	0.676235	-0.426544	-2.785652
1	3.255231	-3.068899	1.661451
1	3.809500	0.002472	3.212169
8	3.082115	-2.074272	4.892729
1	3.365663	-3.908268	3.917347
1	1.784741	-3.111454	3.734253
1	4.036879	-2.067856	5.077563
1	2.595385	1.092178	-2.352771
8	3.202975	-0.909576	-2.490394
1	2.884499	0.277486	-0.790172
1	4.155192	-0.752120	-2.384979
1	0.617793	-2.525466	-2.692434
1	0.347893	-4.711905	-1.697231
6	0.525822	-3.870968	-1.034248
6	0.700854	-4.115602	0.314889
1	0.656819	-5.153227	0.673214
1	0.714466	2.413872	1.514613
6	1.148872	1.411392	1.621056
6	2.262076	1.247378	2.424879
1	2.669473	2.115608	2.933047
8	-0.744761	-1.609099	2.011830
8	-1.409238	-0.421298	2.490310
6	-2.556568	-0.117712	1.802563
6	-2.970236	-1.043696	0.685993
8	-3.156519	0.872042	2.158448
1	-2.211947	-1.058861	-0.105631
1	-3.922511	-0.685537	0.286651
1	-3.070026	-2.071550	1.052050

[1]Id

1	0.655920	0.871265	-1.258280
6	0.922059	0.080026	-1.961395
6	2.177551	0.489268	-2.726322
7	1.097505	-1.176306	-1.214633
27	1.555942	-1.120357	0.705942
6	0.835939	-2.271120	-1.887766
8	1.411745	-3.002022	0.857110
7	2.200329	-1.092538	2.570157
6	2.702538	-0.022555	3.146091
8	2.224354	0.610753	0.361180
6	2.006466	-2.265741	3.454372
1	2.982449	-2.757170	3.611380
6	1.343317	-1.989127	4.809964
1	0.099287	-0.033904	-2.681972
1	1.385630	-2.979435	2.916456
1	2.951177	-0.111943	4.206296
8	2.190987	-1.370366	5.785928
1	0.953116	-2.945369	5.195178
1	0.489920	-1.318568	4.672895
1	2.886385	-2.012104	6.012333
1	2.029133	1.510710	-3.120136
8	2.372757	-0.443695	-3.789634
1	3.031321	0.505571	-2.035527
1	3.288893	-0.360205	-4.099169
1	0.560377	-2.148604	-2.938258
1	0.654875	-4.413902	-2.063835
6	0.871697	-3.593571	-1.386660
6	1.151244	-3.865171	-0.066980
1	1.161468	-4.908245	0.276607
1	2.934850	2.444785	0.777443
6	2.696261	1.462893	1.208228
6	2.938509	1.233137	2.540762
1	3.345986	2.032498	3.152150
8	-0.151432	-0.582848	1.083503
8	-0.612829	-1.224595	2.288449

6	-1.653717	-2.100419	2.087925
6	-2.247320	-2.184534	0.706433
8	-2.025107	-2.716152	3.062668
1	-2.534178	-1.190530	0.346384
1	-3.120289	-2.840631	0.755089
1	-1.515764	-2.585827	-0.003680

[1]Ie

1	-0.059560	-2.294189	-2.303044
6	0.916892	-2.769046	-2.180521
6	1.627660	-2.835044	-3.530304
7	1.696371	-2.033854	-1.173605
27	1.528207	-0.067463	-0.990581
6	2.481403	-2.770782	-0.420133
8	2.914800	0.016140	0.301513
7	-0.009285	-0.115202	0.075766
6	-1.211544	0.035753	-0.423258
8	0.660101	0.056592	-2.649547
6	0.241689	-0.142060	1.522281
1	0.760678	0.791109	1.788253
6	-0.967627	-0.354824	2.436580
1	0.745809	-3.799483	-1.834627
1	0.947028	-0.958106	1.725220
1	-2.023917	0.119724	0.300412
8	-1.942568	0.681275	2.408976
1	-0.573357	-0.500665	3.457279
1	-1.503021	-1.271870	2.159679
1	-1.489993	1.526178	2.579359
1	0.931742	-3.268033	-4.271303
8	2.783506	-3.655817	-3.372942
1	1.886829	-1.817805	-3.854458
1	3.387281	-3.471761	-4.110228
1	2.462705	-3.850746	-0.594492
1	3.963541	-3.036335	1.118979
6	3.366275	-2.306943	0.580192
6	3.550643	-0.963856	0.841930

1	4.308759	-0.662616	1.577788
1	-0.943202	0.314155	-3.836636
6	-0.614477	0.179000	-2.798789
6	-1.555950	0.140895	-1.791094
1	-2.603409	0.266669	-2.044868
8	1.733032	1.768012	-0.867776
8	0.635151	2.530573	-1.424871
6	0.967808	3.225687	-2.554578
6	2.400798	3.162929	-3.022511
8	0.080992	3.856920	-3.090128
1	3.092029	3.406938	-2.209219
1	2.515172	3.864657	-3.852948
1	2.643188	2.147702	-3.357385

[1]If

1	-0.811938	-0.862663	-1.757384
6	-1.348231	-1.504061	-1.055594
6	-1.725734	-2.810338	-1.755235
7	-0.511192	-1.719223	0.134661
27	1.435268	-1.399377	0.174994
6	-1.184037	-2.049639	1.223798
8	1.628604	-2.393687	1.773765
7	1.474249	-0.633202	-1.602507
6	1.579567	0.658293	-1.788275
8	1.336430	0.186173	1.115030
6	1.718169	-1.501469	-2.759022
1	1.466366	-0.938800	-3.670150
6	3.192654	-1.979187	-2.842321
1	-2.278377	-0.988345	-0.774128
1	1.050652	-2.373498	-2.712670
1	1.722113	1.003012	-2.816753
8	4.095381	-0.931891	-2.573006
1	3.374940	-2.329152	-3.867650
1	3.350836	-2.827865	-2.163057
1	4.063829	-0.838630	-1.593474
1	-2.197650	-2.566583	-2.723754

8	-2.622359	-3.525803	-0.912751
1	-0.814724	-3.396846	-1.958355
1	-2.656087	-4.448355	-1.213428
1	-2.273215	-2.064831	1.140810
1	-1.322210	-2.659981	3.278963
6	-0.642394	-2.425721	2.465621
6	0.715334	-2.631347	2.640674
1	1.076340	-3.061283	3.584869
1	1.347513	2.169389	1.288772
6	1.394290	1.350677	0.559799
6	1.506070	1.649472	-0.780273
1	1.560915	2.692076	-1.076220
8	3.324541	-1.292858	0.124369
8	3.758316	-2.679462	0.156193
6	4.469537	-3.010342	1.290535
6	4.820579	-1.896044	2.239774
8	4.787722	-4.172031	1.400249
1	5.352742	-1.094954	1.714422
1	5.447398	-2.312955	3.032472
1	3.909694	-1.457178	2.657525

^{1}Ig

1	1.769885	-3.564914	2.858461
6	2.740305	-3.072188	2.724414
6	3.660637	-3.971970	1.903493
7	2.509513	-1.770438	2.100301
27	1.027726	-1.616599	0.850873
6	3.292251	-0.772232	2.396218
8	1.072936	0.221166	0.718012
7	-0.492006	-1.733178	-0.364358
6	-1.739768	-1.872785	0.026979
8	-0.047019	-1.920625	2.388108
6	-0.215509	-1.545236	-1.802326
1	0.321523	-2.434079	-2.165545
6	-1.388614	-1.224138	-2.726558
1	3.183652	-2.940336	3.722848

1	0.501882	-0.723283	-1.884761
1	-2.501840	-1.944713	-0.750342
8	-2.340565	-2.276284	-2.900368
1	-0.962146	-0.921015	-3.697765
1	-1.961416	-0.369771	-2.344342
1	-1.858620	-3.052934	-3.233806
1	3.641630	-4.985870	2.339833
8	4.973253	-3.414516	1.963859
1	3.297522	-4.027778	0.866128
1	5.525905	-3.870099	1.307611
1	4.115860	-0.963945	3.091153
1	3.879328	1.295316	2.176210
6	3.142109	0.548532	1.899631
6	2.067808	0.938397	1.132263
1	1.991771	1.985942	0.816446
1	-1.744801	-2.117994	3.453286
6	-1.333734	-2.000034	2.441568
6	-2.191163	-1.977192	1.363660
1	-3.259044	-2.072168	1.536980
8	2.239795	-1.995972	-0.521634
8	2.637111	-0.857111	-1.338186
6	3.967196	-0.838620	-1.650253
6	4.819444	-1.987137	-1.175507
8	4.354378	0.097346	-2.316845
1	4.818147	-2.049306	-0.081705
1	5.834393	-1.827083	-1.549507
1	4.422094	-2.936115	-1.555948

[1]Ih

1	1.709851	0.392782	-1.154263
6	2.191614	-0.456449	-1.643614
6	3.611543	-0.055613	-2.044024
7	2.055700	-1.624247	-0.743770
27	0.559948	-1.611565	0.513956
6	2.708986	-2.720557	-1.077544
8	0.351401	-3.511902	0.425696

7	1.019214	0.130144	1.273731
6	0.131694	0.899462	1.890096
8	-0.860715	-1.791004	1.774349
6	2.410518	0.580864	1.407257
1	2.459993	1.678901	1.343049
6	3.013117	0.136292	2.753371
1	1.613811	-0.645429	-2.558673
1	3.021862	0.156079	0.609902
1	0.464507	1.903227	2.174282
8	2.336811	0.681412	3.874137
1	4.047112	0.501035	2.811414
1	3.042183	-0.966098	2.794289
1	1.494601	0.204889	3.971630
1	3.573176	0.982364	-2.416243
8	4.090696	-0.933258	-3.065629
1	4.279876	-0.072138	-1.165342
1	5.002770	-0.674646	-3.280566
1	3.489270	-2.611125	-1.835104
1	3.116870	-4.825663	-0.886652
6	2.449983	-4.019669	-0.595928
6	1.267330	-4.331741	0.055024
1	1.045994	-5.387156	0.268787
1	-2.462316	-1.118748	2.784521
6	-1.530421	-0.824119	2.283622
6	-1.156992	0.513368	2.288123
1	-1.818200	1.249754	2.733269
8	-0.450166	-1.214608	-0.968946
8	-1.584466	-0.404294	-0.650498
6	-2.778837	-1.103826	-0.686358
6	-2.729065	-2.548816	-1.103610
8	-3.769321	-0.475904	-0.390137
1	-2.272926	-2.649170	-2.094889
1	-3.754059	-2.928595	-1.116943
1	-2.111509	-3.127823	-0.407811

[1]II

H	-1.791040	0.568972	0.734648
C	-1.554679	-0.167576	-0.040796
C	-0.447506	0.392961	-0.966408
N	-1.151183	-1.433376	0.578284
Co	0.198040	-1.463428	2.016114
C	-1.551148	-2.523396	-0.030363
O	0.331951	-3.381120	2.058319
N	-1.104315	-1.424034	3.438889
C	-1.282813	-0.366897	4.193924
O	0.416712	0.435589	1.952416
C	-1.821342	-2.672168	3.733975
H	-1.099676	-3.401251	4.133037
C	-3.038106	-2.591930	4.658138
H	-2.463744	-0.342272	-0.635587
H	-2.171670	-3.086873	2.780593
H	-1.933131	-0.489252	5.062044
O	-2.752455	-2.267801	6.017461
H	-3.560724	-3.562041	4.590850
H	-3.737088	-1.820116	4.311599
H	-2.082265	-2.897718	6.335774
H	-0.890685	1.166224	-1.608296
O	0.089185	-0.601777	-1.825243
H	0.336410	0.855094	-0.355078
H	0.697263	-1.125808	-1.272028
H	-2.244159	-2.390809	-0.867973
H	-1.618872	-4.654040	-0.323122
C	-1.183988	-3.856700	0.272017
C	-0.273020	-4.183431	1.257775
H	-0.025313	-5.244134	1.410901
H	0.414127	2.260707	2.783129
C	0.060096	1.226991	2.901902
C	-0.717102	0.913818	3.996617
H	-0.944040	1.690569	4.720162
O	1.567354	-1.489569	3.308547
O	2.850957	-1.483644	2.612604

C	2.759396	-1.495225	1.313777
C	4.079905	-1.501502	0.598949
O	1.665160	-1.503169	0.701064
H	4.125817	-0.638293	-0.075519
H	4.152043	-2.409432	-0.012020
H	4.912387	-1.465642	1.305781

^{3}IIa

1	-1.619044	0.451646	0.547028
6	-1.380598	-0.289692	-0.223418
6	-0.176090	0.206451	-1.056218
7	-1.127853	-1.592180	0.407081
27	0.030359	-1.722061	2.023102
6	-1.525625	-2.643035	-0.278224
8	-0.180701	-3.638231	2.116221
7	-1.222366	-1.527521	3.647643
6	-1.147671	-0.483036	4.434287
8	0.432096	0.121471	1.981614
6	-2.110318	-2.644046	3.995242
1	-1.492737	-3.472424	4.377514
6	-3.265215	-2.373537	4.962168
1	-2.255193	-0.386533	-0.883917
1	-2.545892	-3.013084	3.057514
1	-1.722646	-0.492631	5.364403
8	-2.876682	-2.110449	6.310139
1	-3.949393	-3.238879	4.915942
1	-3.834019	-1.490865	4.642906
1	-2.336998	-2.861876	6.612139
1	-0.517720	1.045796	-1.678799
8	0.330263	-0.791609	-1.923241
1	0.601546	0.577657	-0.377750
1	0.956858	-1.313293	-1.384472
1	-2.064530	-2.444292	-1.210240
1	-1.726815	-4.757981	-0.611597
6	-1.339824	-3.998320	0.060192
6	-0.689761	-4.394137	1.215527

1	-0.591697	-5.469264	1.423893
1	0.790397	1.886645	2.860086
6	0.304473	0.911359	2.999127
6	-0.378505	0.681434	4.172821
1	-0.387940	1.471955	4.917682
8	1.643455	-2.133008	2.862827
8	2.762214	-1.365727	2.373600
6	2.800657	-1.317501	1.037231
6	4.053101	-0.637160	0.546454
8	1.911190	-1.758714	0.316741
1	3.772244	0.251760	-0.030981
1	4.584927	-1.318574	-0.128117
1	4.708794	-0.350012	1.372707

^{3}IIb

H	-0.022427	-1.300604	-2.573572
C	0.516420	-1.987186	-1.911911
C	2.044447	-1.792366	-2.097729
N	0.103372	-1.762695	-0.522718
Co	0.095874	0.092302	0.235499
C	0.054383	-2.827754	0.238987
O	-0.325543	-0.506564	2.018657
N	-1.789799	0.373368	-0.138691
C	-2.153459	1.450179	-0.787020
O	0.604134	0.823443	-1.449154
C	-2.785721	-0.505853	0.484488
H	-2.863869	-0.245529	1.551297
C	-4.178780	-0.529910	-0.150288
H	0.248488	-3.017006	-2.191566
H	-2.386044	-1.525478	0.448870
H	-3.219607	1.689879	-0.802909
O	-4.942361	0.662945	0.022597
H	-4.716934	-1.400153	0.262666
H	-4.101693	-0.675304	-1.234962
H	-5.047873	0.811193	0.978745
H	2.339153	-2.266358	-3.043727

O	2.793126	-2.407565	-1.065836
H	2.265756	-0.720144	-2.165102
H	2.657227	-1.830810	-0.284670
H	0.194908	-3.794460	-0.256045
H	-0.204154	-3.835919	2.122733
C	-0.170264	-2.866303	1.635627
C	-0.329695	-1.733029	2.406242
H	-0.502995	-1.852197	3.485232
H	0.547589	2.437512	-2.638808
C	-0.001556	1.873376	-1.873461
C	-1.270080	2.295038	-1.506223
H	-1.668386	3.202783	-1.948461
O	0.151571	1.681148	0.949340
O	2.350233	1.996624	0.847950
C	2.736794	0.817108	0.768194
C	4.216690	0.494338	0.918043
O	1.974961	-0.213984	0.576780
H	4.516000	-0.238535	0.159983
H	4.384616	0.045492	1.905635
H	4.816852	1.403638	0.831260

^{5}IIb

H	-1.918366	0.476973	0.407086
C	-1.539778	-0.218532	-0.349338
C	-0.331873	0.427935	-1.073142
N	-1.168439	-1.485075	0.291432
Co	-0.038661	-1.494820	2.021234
C	-1.310584	-2.546918	-0.482899
O	-0.162528	-3.535780	2.023902
N	-1.249630	-1.394219	3.668959
C	-1.318951	-0.335033	4.456928
O	0.027653	0.555253	1.982422
C	-1.897934	-2.638288	4.118004
H	-1.120106	-3.312833	4.510859
C	-3.047000	-2.538154	5.123937
H	-2.339089	-0.404764	-1.082891

H	-2.283600	-3.137940	3.221726
H	-1.822401	-0.453253	5.419809
O	-2.665094	-2.174840	6.451215
H	-3.572847	-3.508894	5.124894
H	-3.770449	-1.776001	4.807134
H	-1.986319	-2.807931	6.743770
H	-0.709468	1.221189	-1.732717
O	0.368950	-0.497051	-1.889091
H	0.329135	0.883287	-0.326032
H	0.929079	-1.012722	-1.277861
H	-1.773389	-2.383248	-1.462262
H	-1.140206	-4.630351	-0.951608
C	-0.946880	-3.876713	-0.192949
C	-0.410470	-4.286343	1.025009
H	-0.204772	-5.361301	1.162652
H	0.118075	2.366140	2.867639
C	-0.193390	1.314196	2.980761
C	-0.801489	0.946554	4.180136
H	-0.925818	1.711411	4.942379
O	1.542377	-1.551066	3.167819
O	2.822781	-1.576064	2.518749
C	2.743033	-1.558928	1.202159
C	4.087970	-1.571110	0.530149
O	1.662993	-1.537565	0.596800
H	4.178007	-0.681572	-0.104797
H	4.157145	-2.453062	-0.117790
H	4.899069	-1.586068	1.262671

[7]**IIa**

1	-1.824837	0.654231	0.164811
6	-1.451840	-0.152272	-0.482227
6	-0.173446	0.378583	-1.186480
7	-1.198624	-1.335407	0.317723
27	0.033798	-1.313950	2.011276
6	-1.728481	-2.513224	-0.198311
8	0.251407	-3.316116	1.961839

7	-1.245111	-1.368448	3.581478
6	-1.346447	-0.374171	4.448462
8	-0.164418	0.740139	1.978295
6	-1.879406	-2.658704	3.886851
1	-1.075149	-3.384767	4.082701
6	-2.925343	-2.713633	5.000481
1	-2.211446	-0.371468	-1.247320
1	-2.357409	-3.005781	2.960050
1	-1.829981	-0.576491	5.406833
8	-2.417612	-2.489189	6.315084
1	-3.427111	-3.694628	4.935541
1	-3.694928	-1.945921	4.848099
1	-1.698746	-3.127414	6.466734
1	-0.484625	1.171448	-1.881137
8	0.495292	-0.608362	-1.945253
1	0.487680	0.823358	-0.431111
1	1.013600	-1.125254	-1.300482
1	-2.453681	-2.418289	-1.006092
1	-1.745521	-4.613082	-0.385457
6	-1.301396	-3.785651	0.170988
6	-0.347517	-4.162325	1.163002
1	-0.107487	-5.222048	1.293025
1	-0.153609	2.502044	2.960713
6	-0.369355	1.422691	3.026670
6	-0.883631	0.939691	4.239457
1	-1.020169	1.652979	5.048339
8	1.568988	-1.130941	3.169040
8	2.843419	-1.410969	2.567929
6	2.794166	-1.459629	1.246913
6	4.134171	-1.726939	0.621019
8	1.745374	-1.310837	0.609405
1	4.328339	-0.968964	-0.146370
1	4.105306	-2.705899	0.126839
1	4.932522	-1.717887	1.367500

[7]IIb

H	0.006613	-2.118797	-2.302520
C	0.621433	-2.522717	-1.488640
C	2.117635	-2.198167	-1.763919
N	0.190927	-1.944542	-0.216337
Co	-0.026490	0.128921	-0.018560
C	0.289629	-2.742287	0.824445
O	-0.655285	-0.150798	1.888382
N	-1.972180	0.322602	-0.725555
C	-2.320917	0.906241	-1.856703
O	0.618693	0.586144	-1.931425
C	-3.023161	-0.137452	0.194493
H	-2.938373	0.468958	1.110066
C	-4.473865	-0.164836	-0.288092
H	0.489728	-3.615519	-1.463766
H	-2.753410	-1.157124	0.502834
H	-3.381375	1.097117	-2.033188
O	-5.039876	1.113326	-0.566524
H	-5.064084	-0.701263	0.475090
H	-4.561462	-0.735160	-1.221903
H	-4.949435	1.659872	0.233531
H	2.457227	-2.845498	-2.584296
O	2.933854	-2.457015	-0.641484
H	2.203017	-1.153157	-2.088071
H	2.785315	-1.688841	-0.044252
H	0.583767	-3.781495	0.636140
H	0.187615	-3.187902	2.919228
C	0.050100	-2.404197	2.178525
C	-0.387211	-1.157315	2.624066
H	-0.558152	-1.029498	3.704923
H	0.531834	1.533110	-3.710366
C	-0.043356	1.154775	-2.849911
C	-1.434801	1.331614	-2.869627
H	-1.868855	1.821828	-3.737558
O	0.167701	1.956806	0.385119
O	2.328053	2.194044	0.553152

C	2.755331	1.012236	0.600846
C	4.255131	0.827111	0.822353
O	2.052653	-0.046360	0.497953
H	4.625641	0.043436	0.151606
H	4.420152	0.493935	1.855110
H	4.797123	1.761484	0.656486

^{1}IIc

1	0.717453	2.329101	1.811542
6	0.640099	2.809297	0.828417
6	2.060562	3.132201	0.280843
7	-0.134221	1.955486	-0.072418
27	0.186261	0.011583	-0.201094
6	-1.032046	2.551349	-0.812224
8	-0.867748	-0.220790	-1.744359
7	0.487096	-1.941358	-0.303135
6	0.004567	-2.754614	0.604409
8	-1.304971	-0.148411	0.974439
6	1.130146	-2.534313	-1.479376
1	1.875002	-3.284064	-1.156133
6	0.139418	-3.197725	-2.447539
1	0.091129	3.752358	0.962344
1	1.661794	-1.739679	-2.008931
1	0.259565	-3.814066	0.505185
8	-0.489803	-4.362186	-1.915975
1	0.671230	-3.428974	-3.387309
1	-0.664100	-2.491240	-2.669338
1	0.185275	-5.060795	-1.864309
1	2.376016	4.098938	0.695686
8	2.102056	3.245729	-1.122760
1	2.787658	2.386026	0.640448
1	1.979063	2.331450	-1.457644
1	-1.172091	3.624871	-0.645735
1	-2.563220	2.588898	-2.325184
6	-1.837142	1.963690	-1.815336
6	-1.683252	0.658011	-2.219654

1	-2.293334	0.283291	-3.052484
1	-2.260420	-1.021855	2.499800
6	-1.487586	-1.171027	1.732100
6	-0.857552	-2.400852	1.666401
1	-1.144113	-3.169359	2.377833
8	1.752334	0.344160	-1.246906
8	2.917422	-0.025705	-0.430702
6	2.628104	-0.115029	0.845739
6	3.809216	-0.402599	1.726228
8	1.470757	0.019689	1.289907
1	3.656814	-1.369447	2.220729
1	3.867256	0.365804	2.505757
1	4.738466	-0.420533	1.151527

[1]IId

1	0.385909	-2.880681	-1.146690
6	0.195078	-3.324500	-0.161730
6	1.544939	-3.505416	0.593520
7	-0.772698	-2.504447	0.571988
27	-0.629626	-0.546972	0.653306
6	-1.630258	-3.161304	1.317731
8	-1.863660	-0.340095	2.057961
7	-2.052236	-0.279000	-0.670783
6	-2.705975	0.859660	-0.752391
8	-0.314203	1.341802	0.858137
6	-2.448677	-1.396757	-1.536367
1	-3.047567	-2.117723	-0.954315
6	-3.189949	-1.063574	-2.835215
1	-0.252641	-4.315948	-0.324096
1	-1.534822	-1.929348	-1.824789
1	-3.574236	0.881721	-1.415073
8	-4.532235	-0.607621	-2.672032
1	-3.163727	-1.965076	-3.472145
1	-2.669678	-0.263493	-3.376203
1	-5.015206	-1.289096	-2.172624
1	1.996755	-4.448712	0.257374

8	1.388141	-3.583393	1.989547
1	2.243639	-2.701304	0.316020
1	1.188606	-2.661306	2.266939
1	-1.610408	-4.253362	1.239626
1	-3.253621	-3.291806	2.721945
6	-2.578628	-2.614731	2.207803
6	-2.606075	-1.271170	2.533156
1	-3.317378	-0.924297	3.295271
1	-0.943170	3.240085	0.969585
6	-1.197312	2.234042	0.604735
6	-2.380000	2.062851	-0.092984
1	-3.029229	2.920546	-0.240367
8	0.826549	-0.770079	1.884028
8	2.030814	-0.275598	1.218883
6	1.889747	-0.186298	-0.077671
6	3.114691	0.292017	-0.799504
8	0.821713	-0.460923	-0.670260
1	2.929867	1.309975	-1.165155
1	3.296922	-0.350374	-1.667909
1	3.986865	0.295055	-0.140925

^{1}IIe

1	0.920629	-2.664289	-1.031110
6	0.435684	-3.348010	-0.328857
6	1.479186	-3.888211	0.649530
7	-0.655916	-2.623593	0.332908
27	-0.700101	-0.652107	0.372335
6	-1.571009	-3.359904	0.923579
8	-1.992375	-0.600095	1.783317
7	-2.079015	-0.540298	-0.971626
6	-2.846356	0.522780	-1.080917
8	-0.598198	1.252604	0.627471
6	-2.256055	-1.662919	-1.902520
1	-2.806246	-2.475730	-1.399442
6	-2.924239	-1.362041	-3.247444
1	0.032579	-4.201943	-0.896772

1	-1.259277	-2.059284	-2.127751
1	-3.671218	0.452595	-1.793774
8	-4.322579	-1.081704	-3.182916
1	-2.734430	-2.223984	-3.910598
1	-2.465453	-0.480968	-3.712037
1	-4.753358	-1.840037	-2.751046
1	2.354632	-4.236130	0.072624
8	0.904962	-4.966627	1.387667
1	1.803177	-3.078586	1.318355
1	1.357784	-5.025051	2.243712
1	-1.483437	-4.442125	0.794148
1	-3.332950	-3.627489	2.127715
6	-2.635392	-2.898660	1.725840
6	-2.736632	-1.578618	2.137126
1	-3.517709	-1.314818	2.865860
1	-1.434125	3.071285	0.715931
6	-1.560244	2.044777	0.341260
6	-2.690334	1.747199	-0.402399
1	-3.422959	2.528757	-0.578746
8	0.612921	-0.499391	-0.969597
8	1.870235	-0.089103	-0.342461
6	1.858649	-0.218122	0.961928
6	3.140433	0.200950	1.624331
8	0.871911	-0.633810	1.600125
1	3.950598	0.304514	0.897757
1	3.407979	-0.532514	2.392308
1	2.975264	1.164722	2.122505

^{1}IIr

H	-1.287955	-0.724555	2.899722
C	-0.707709	0.202632	2.901547
C	0.794185	-0.137974	3.070285
N	-0.947329	0.936119	1.651550
Co	-0.797034	0.000679	-0.081169
C	-0.996257	2.232950	1.755495
O	-0.905349	1.607879	-1.105600

N	-2.684847	-0.337838	-0.281804
C	-3.171846	-1.544372	-0.307265
O	-0.481563	-1.660379	0.785227
C	-3.555173	0.813941	-0.570475
H	-3.290777	1.195710	-1.566550
C	-5.066655	0.605548	-0.465312
H	-1.037039	0.827872	3.744152
H	-3.285125	1.608481	0.135109
H	-4.218138	-1.652321	-0.602795
O	-5.633059	-0.246203	-1.459386
H	-5.535115	1.604276	-0.493383
H	-5.329021	0.149043	0.497594
H	-5.393391	0.115532	-2.330596
H	0.967415	-0.423845	4.115697
O	1.637287	0.974059	2.801205
H	1.040447	-0.989213	2.426879
H	1.628676	1.079272	1.831741
H	-0.983864	2.649097	2.769424
O	-0.492696	-0.864310	-1.724407
O	0.945045	-1.013170	-1.897261
C	1.660809	-0.397630	-0.994916
O	1.145739	0.230442	-0.035357
C	3.681128	-0.936145	-2.385966
C	5.066152	-1.018794	-2.514383
C	3.124968	-0.504798	-1.171447
C	5.900582	-0.681307	-1.445484
C	3.950015	-0.162463	-0.088006
C	5.330671	-0.258123	-0.241781
H	3.029610	-1.195484	-3.215314
H	5.505228	-1.347120	-3.454022
H	6.981530	-0.744633	-1.539696
Cl	6.377262	0.159471	1.105089
H	3.518015	0.159024	0.855723
C	-1.029106	3.886103	-1.641058
C	-1.127226	5.209892	-1.252817

C	-0.987483	2.836261	-0.679219
C	-1.191297	5.571444	0.110498
C	-1.056161	3.204113	0.703496
C	-1.152995	4.572717	1.063686
H	-0.973999	3.603920	-2.690289
H	-1.152854	5.987232	-2.016073
H	-1.263710	6.616349	0.402570
H	-1.192602	4.825624	2.123741
C	-0.603845	-4.002021	0.943948
C	-1.301891	-5.184115	0.759104
C	-1.167231	-2.753604	0.569291
C	-2.596845	-5.190414	0.201986
C	-2.484674	-2.759060	0.015603
C	-3.173275	-3.984596	-0.153210
H	0.396884	-3.997707	1.370715
H	-0.836485	-6.126049	1.048095
H	-3.133280	-6.125692	0.060792
H	-4.179041	-3.959750	-0.573362

^{1}III

H	1.711208	-2.248261	-0.807971
C	1.371732	-2.742510	0.104434
C	2.599464	-2.891642	1.023811
N	0.249193	-1.988817	0.675947
Co	0.122158	-0.003916	0.601707
C	-0.619619	-2.697997	1.361092
O	-1.323210	0.102849	1.881741
N	-1.190957	-0.000526	-0.827901
C	-1.856670	1.094160	-1.122459
O	0.168269	1.914405	0.805406
C	-1.435423	-1.149784	-1.708253
H	-2.395706	-0.978558	-2.214918
C	-0.335522	-1.342157	-2.786358
H	1.008621	-3.747014	-0.172366
H	-1.536723	-2.062017	-1.112225
H	-2.599242	0.998272	-1.920452

O	0.146580	-0.121144	-3.301251
H	-0.775911	-1.903423	-3.622360
H	0.484532	-1.949161	-2.380914
H	0.736845	0.223403	-2.596608
H	3.304997	-3.579028	0.525448
O	2.302219	-3.328860	2.349158
H	3.102000	-1.930202	1.124587
H	1.992651	-4.249483	2.306524
H	-0.476641	-3.785445	1.343443
H	-2.373265	-2.978446	2.566201
C	-1.725986	-2.239722	2.103216
C	-1.983177	-0.896127	2.327369
H	-2.835723	-0.628376	2.969634
H	-0.631098	3.746943	0.666497
C	-0.722316	2.703460	0.331402
C	-1.730441	2.376706	-0.554090
H	-2.406078	3.155681	-0.893253
O	1.416411	0.177887	-0.790430
O	2.765625	-0.136872	-0.344175
C	3.557572	0.948084	-0.094046
C	3.106031	2.287127	-0.604690
O	4.586815	0.726710	0.517217
H	2.831082	2.227849	-1.663574
H	3.918884	3.002926	-0.456820
H	2.209731	2.600013	-0.058169
N	1.414727	0.001661	2.080077
C	2.243847	-0.111792	2.875187
C	3.349647	-0.322691	3.796112
H	4.268071	0.048696	3.324490
H	3.443457	-1.400578	3.978545
H	3.179548	0.201595	4.742908

^{1}IIIa

1	-0.236183	-3.397345	-0.405399
6	-0.078141	-3.473989	0.672416
6	1.264160	-4.158318	0.927491

7	-0.168547	-2.139731	1.269829
27	0.299976	-0.483320	0.274190
6	-0.551548	-2.095411	2.524541
8	0.441164	0.589646	1.873285
7	0.227286	-1.365490	-1.475679
6	-0.886343	-1.418449	-2.169219
8	-1.510386	0.016599	0.309563
6	1.450315	-1.733421	-2.196144
1	1.171640	-2.398091	-3.027266
6	2.195724	-0.501065	-2.775352
1	-0.869595	-4.118615	1.084650
1	2.118074	-2.294556	-1.529902
1	-0.816252	-1.849193	-3.173029
8	1.309923	0.429187	-3.349951
1	2.874116	-0.856110	-3.564237
1	2.807815	-0.032634	-1.991974
1	0.908005	0.879000	-2.569026
1	1.303236	-5.084752	0.326149
8	1.358785	-4.446290	2.319615
1	2.081915	-3.499690	0.596482
1	2.277066	-4.691353	2.517321
1	-0.863780	-3.044831	2.970534
1	-0.956177	-1.093998	4.381980
6	-0.577022	-0.967506	3.372494
6	-0.056355	0.259937	3.008787
1	-0.032951	1.061947	3.761400
1	-3.396981	0.035784	-0.339421
6	-2.380291	-0.305691	-0.577071
6	-2.166188	-0.992250	-1.756448
1	-3.005901	-1.160742	-2.423265
8	0.615505	1.145684	-0.731116
8	1.849553	1.789269	-0.317556
6	1.685035	2.908358	0.440029
6	0.313172	3.517070	0.515887
8	2.695222	3.348151	0.962612

1	-0.079611	3.697561	-0.491416
1	0.380890	4.454380	1.074477
1	-0.370306	2.818439	1.007330
7	2.245506	-0.770493	0.534882
6	3.269699	-0.315852	0.826324
6	4.490109	0.395608	1.167563
1	4.245389	1.469803	1.121530
1	5.285876	0.169613	0.448291
1	4.825203	0.133800	2.177558

[1]IIIb

1	-0.519613	-2.414307	0.683212
6	-0.336587	-1.691791	1.486394
6	0.822729	-2.210918	2.347866
7	-0.115538	-0.360802	0.916995
27	1.257074	-0.011321	-0.543911
6	-0.800128	0.615278	1.459577
8	1.098404	1.906636	-0.385843
7	-0.061812	-0.082990	-1.939854
6	-0.551124	-1.205952	-2.391728
8	1.705144	-1.865221	-0.657470
6	-0.325226	1.167773	-2.676184
1	0.592733	1.755642	-2.594377
6	-0.676944	1.000595	-4.163148
1	-1.250829	-1.668326	2.105800
1	-1.118520	1.742595	-2.174056
1	-1.295721	-1.144577	-3.185899
8	0.151986	0.095906	-4.862993
1	-0.642121	2.015655	-4.601430
1	-1.709811	0.644034	-4.294925
1	1.044938	0.099158	-4.463530
1	0.559514	-3.223788	2.701019
8	1.156066	-1.359714	3.446554
1	1.727345	-2.287930	1.741930
1	0.376164	-1.296975	4.024194
1	-1.536162	0.334865	2.224928

1	-1.358830	2.673443	1.726314
6	-0.697110	1.998768	1.191232
6	0.245953	2.536104	0.334521
1	0.297858	3.631121	0.238719
1	1.344454	-3.775644	-1.160560
6	0.983641	-2.743138	-1.269055
6	-0.151918	-2.513872	-2.013965
1	-0.650362	-3.356667	-2.482517
8	2.598459	0.451208	-1.800121
8	2.498720	-0.292950	-3.037134
6	3.570929	-1.104861	-3.294471
6	4.660928	-1.161937	-2.256251
8	3.558974	-1.704817	-4.347909
1	5.057685	-0.160340	-2.058367
1	5.449311	-1.821380	-2.629190
1	4.252849	-1.540892	-1.313278
7	2.623367	0.115025	0.883640
6	3.293400	0.177079	1.822052
6	4.086162	0.211118	3.042304
1	4.232105	1.246607	3.370894
1	5.065689	-0.252051	2.876582
1	3.538428	-0.344790	3.812848

^{1}IIIc

H	-1.850704	1.039550	-2.216646
C	-2.576510	1.132966	-1.405927
C	-3.703687	0.131353	-1.631624
N	-1.871068	0.939632	-0.133099
Co	-0.184617	-0.121460	-0.082136
C	-2.363816	1.549632	0.910933
O	0.354906	0.717228	1.560956
N	1.506270	-1.182637	-0.037283
C	1.730428	-2.175429	-0.860294
O	-0.835503	-0.985013	-1.666471
C	2.585728	-0.851153	0.913611
H	2.616102	-1.616692	1.711117

C	3.985732	-0.695793	0.306303
H	-3.001148	2.147119	-1.439930
H	2.320122	0.088694	1.393645
H	2.692511	-2.684860	-0.756439
O	4.636238	-1.929454	-0.029968
H	4.603799	-0.119115	1.013952
H	3.920127	-0.118181	-0.619673
H	4.807522	-2.397489	0.805549
H	-4.080366	0.263166	-2.661851
O	-4.735449	0.390435	-0.674971
H	-3.305566	-0.887804	-1.535084
H	-5.410263	-0.300567	-0.774283
H	-3.311805	2.078847	0.773635
H	-2.301496	2.136179	2.988759
C	-1.761146	1.632195	2.192918
C	-0.445978	1.273864	2.402325
H	0.014139	1.505788	3.374099
H	-0.850684	-2.367796	-3.116438
C	-0.290045	-1.996092	-2.245645
C	0.881349	-2.630678	-1.899547
H	1.216634	-3.470377	-2.501255
O	0.547990	1.190474	-1.169370
O	1.897674	1.498740	-0.759575
C	2.049937	2.754460	-0.243637
C	0.865584	3.686257	-0.292664
O	3.149564	3.034222	0.188809
H	0.463976	3.748494	-1.309844
H	1.196303	4.670324	0.050616
H	0.059037	3.315397	0.348614
N	-1.087687	-1.537648	1.000263
C	-1.612010	-2.351146	1.631947
C	-2.275610	-3.373331	2.431537
H	-2.577808	-4.212214	1.793708
H	-3.166081	-2.952226	2.912919
H	-1.595139	-3.744885	3.206642

[1]IIId

1	0.914425	1.534824	2.827474
6	1.016078	2.210561	1.971488
6	2.485060	2.582375	1.778232
7	0.419154	1.575532	0.798441
27	0.528890	-0.382138	0.554067
6	-0.232524	2.347428	-0.032399
8	-0.719336	-0.430006	-0.841088
7	0.568356	-2.352255	0.327414
6	-0.029537	-3.166602	1.156530
8	-0.887886	-0.431413	1.885806
6	1.239825	-2.863935	-0.872919
1	2.325229	-2.714976	-0.760748
6	0.951925	-4.306365	-1.283319
1	0.467759	3.131444	2.220933
1	0.945048	-2.213895	-1.703243
1	0.096390	-4.237901	0.981928
8	1.478382	-5.304531	-0.402231
1	1.346606	-4.445652	-2.304107
1	-0.128943	-4.489822	-1.323081
1	2.439242	-5.160639	-0.352630
1	2.919869	2.840247	2.761518
8	2.536104	3.703447	0.895418
1	3.033008	1.725219	1.362333
1	3.448132	3.794724	0.574174
1	-0.231754	3.420124	0.187660
1	-1.420807	2.685795	-1.796474
6	-0.955641	1.930136	-1.171646
6	-1.164872	0.599544	-1.469557
1	-1.795879	0.345045	-2.331215
1	-1.983703	-1.328960	3.305392
6	-1.249347	-1.498695	2.502816
6	-0.835922	-2.795935	2.263927
1	-1.255232	-3.591776	2.873144
8	2.069607	-0.164521	-0.545473

8	1.753510	-0.094472	-1.964942
6	2.408052	0.893002	-2.634633
6	3.348551	1.776527	-1.853742
8	2.200504	0.979493	-3.827891
1	2.791456	2.365716	-1.116098
1	3.850393	2.439063	-2.564659
1	4.083074	1.172801	-1.308618
7	1.825582	-0.654688	1.997366
6	2.537036	-1.014255	2.834264
6	3.428635	-1.477738	3.889180
1	4.451809	-1.566235	3.505385
1	3.096255	-2.459093	4.248012
1	3.422463	-0.772639	4.728729

[1]IIIe

1	-0.299033	0.430524	-0.453803
6	-0.874879	0.467225	-1.378810
6	0.001702	-0.004450	-2.539176
7	-2.125825	-0.287830	-1.151714
27	-2.690371	-0.716590	0.697440
6	-2.975050	-0.347756	-2.157024
8	-4.528485	-0.263726	0.288197
7	-0.915500	-1.401105	1.295153
6	-0.559697	-1.409439	2.567827
8	-3.435201	-1.001520	2.462332
6	0.036430	-2.013176	0.350692
1	0.938755	-1.389291	0.230272
6	0.490230	-3.430562	0.746518
1	-1.112115	1.527561	-1.540908
1	-0.464019	-2.068832	-0.618425
1	0.486648	-1.657489	2.786130
8	-0.591166	-4.324336	0.992542
1	1.161165	-3.394230	1.620982
1	1.065617	-3.862017	-0.082365
1	-1.129236	-3.906605	1.689289
1	1.011064	0.418411	-2.391963

8	-0.549988	0.451255	-3.777769
1	0.092558	-1.103664	-2.530643
1	-0.003708	0.094779	-4.498165
1	-2.578625	-0.092153	-3.143901
1	-4.928904	-0.712353	-2.985016
6	-4.356165	-0.621453	-2.066475
6	-5.039131	-0.445444	-0.869309
1	-6.139111	-0.407860	-0.896564
1	-3.379597	-1.058267	4.463687
6	-2.768893	-1.081656	3.549481
6	-1.391771	-1.213763	3.678969
1	-0.954185	-1.227110	4.671884
8	-2.303023	1.081494	0.963980
8	-1.929313	1.418951	2.314127
6	-2.888056	2.140991	2.978217
6	-4.127398	2.531311	2.215396
8	-2.648648	2.424228	4.133769
1	-3.862545	3.118014	1.328212
1	-4.761528	3.119792	2.884214
1	-4.654869	1.640924	1.857468
7	-3.147981	-2.598511	0.191120
6	-3.311315	-3.713125	-0.067246
6	-3.462614	-5.125875	-0.384598
1	-2.501174	-5.619142	-0.197417
1	-3.742868	-5.250387	-1.437106
1	-4.237383	-5.577534	0.245898

^{5}III

H	1.524834	-2.486598	-0.742535
C	1.236315	-2.885941	0.235194
C	2.513513	-2.949469	1.092674
N	0.175391	-2.053257	0.808550
Co	0.088835	0.038255	0.459154
C	-0.679543	-2.693249	1.576364
O	-1.397046	0.160239	1.840002
N	-1.275332	0.028651	-1.096312

C	-2.163705	0.992352	-1.204358
O	-0.056420	2.102162	0.565010
C	-1.367086	-1.048677	-2.078636
H	-2.252924	-0.889615	-2.712904
C	-0.105750	-1.146797	-2.979639
H	0.856475	-3.911662	0.079855
H	-1.495134	-2.004741	-1.547978
H	-2.957911	0.864366	-1.951697
O	0.387437	0.109782	-3.379324
H	-0.386868	-1.706373	-3.883110
H	0.672752	-1.725301	-2.462982
H	0.930960	0.411052	-2.617257
H	3.223268	-3.629319	0.590621
O	2.289676	-3.341501	2.445870
H	2.976163	-1.963667	1.129883
H	2.029957	-4.278459	2.453187
H	-0.570489	-3.784759	1.642819
H	-2.339026	-2.830048	2.925186
C	-1.732600	-2.143944	2.339778
C	-1.996858	-0.780687	2.451286
H	-2.797438	-0.471511	3.143602
H	-1.245234	3.727143	0.694555
C	-1.139248	2.699856	0.306403
C	-2.196057	2.201586	-0.476665
H	-3.043359	2.861104	-0.648450
O	1.523651	0.265147	-0.826407
O	2.838079	-0.193199	-0.397217
C	3.694016	0.818341	-0.074291
C	3.298951	2.220513	-0.450602
O	4.723073	0.495259	0.491655
H	3.056079	2.278427	-1.517841
H	4.132881	2.885959	-0.212252
H	2.396655	2.521272	0.094282
N	1.532364	0.242926	2.194526
C	2.435219	-0.010139	2.875902

C	3.604150	-0.390716	3.655884
H	4.501432	-0.128460	3.081255
H	3.576719	-1.476554	3.812735
H	3.617392	0.124128	4.623093

^{1}IV

H	-1.218256	-2.192062	1.671105
C	-1.028935	-2.825016	0.798720
C	-2.356746	-3.339047	0.209879
N	-0.225360	-2.071482	-0.173717
Co	-0.368228	-0.174764	-0.303121
C	0.556065	-2.751041	-0.970560
O	1.283878	0.061120	-1.242944
N	0.519700	0.011363	1.432179
C	-0.123318	0.367466	2.515833
O	-2.130802	-0.103923	0.410516
C	1.972998	-0.200042	1.474329
H	2.466996	0.641688	0.963513
C	2.622672	-0.423806	2.841957
H	-0.439718	-3.691092	1.133310
H	2.193206	-1.084471	0.864271
H	0.472926	0.557791	3.410703
O	2.632421	0.711613	3.705940
H	3.650138	-0.784849	2.662174
H	2.093235	-1.209725	3.395355
H	3.085744	1.434276	3.237765
H	-2.851567	-3.938954	0.988926
O	-2.139594	-4.160308	-0.914983
H	-3.001284	-2.485056	-0.034984
H	-2.127599	-3.531779	-1.672097
H	0.506247	-3.838720	-0.878623
O	-0.306932	1.891628	-0.469108
O	-2.220676	-2.014321	-2.585346
C	-1.894639	-0.843364	-2.799575
O	-1.167637	-0.060082	-2.056989
C	-2.377843	-0.147234	-4.074961

C	1.798604	-0.882143	-1.965086
C	1.478611	-2.218868	-1.911655
C	-2.412848	0.248548	1.616206
C	-1.526789	0.524776	2.638604
H	-3.136838	0.604202	-3.817761
H	-2.820575	-0.880404	-4.754847
H	-1.551484	0.375618	-4.570841
H	-1.923158	0.817189	3.606302
H	-3.490466	0.320762	1.820578
H	2.017934	-2.913472	-2.547970
H	2.594563	-0.551114	-2.644837
H	0.267795	1.846238	-1.260943
C	-1.500592	2.637519	-0.789736
H	-2.063840	2.734293	0.140017
H	-2.090640	2.104063	-1.540426
H	-1.213569	3.633565	-1.148712

^{3}IV

H	-0.631744	-2.683350	1.692659
C	-0.626954	-3.186720	0.715354
C	-2.065506	-3.594354	0.340080
N	-0.024754	-2.283656	-0.264229
Co	-0.415328	-0.243330	-0.248049
C	0.663277	-2.804786	-1.241295
O	1.274021	0.094692	-1.157931
N	0.383949	-0.015803	1.511389
C	-0.252696	0.534889	2.516048
O	-2.187415	-0.055748	0.409862
C	1.800498	-0.389121	1.642448
H	2.400808	0.334787	1.069798
C	2.366177	-0.540149	3.055826
H	-0.018822	-4.100358	0.802241
H	1.928481	-1.349256	1.128360
H	0.330372	0.756078	3.412615
O	2.468814	0.671493	3.801345
H	3.352216	-1.027289	2.964307

H	1.729392	-1.202026	3.656218
H	3.013521	1.291206	3.285282
H	-2.429965	-4.278271	1.121875
O	-2.102693	-4.267122	-0.896728
H	-2.708144	-2.702893	0.331703
H	-2.240080	-3.555197	-1.560097
H	0.714557	-3.897946	-1.308799
O	-0.207864	2.155462	-0.391390
O	-2.523122	-1.937442	-2.248990
C	-2.064561	-0.853697	-2.613994
O	-1.179903	-0.115331	-2.002099
C	-2.551669	-0.211254	-3.913831
C	1.694199	-0.714501	-2.086716
C	1.416559	-2.058878	-2.198527
C	-2.499358	0.490248	1.536399
C	-1.633605	0.845249	2.549922
H	-3.232680	0.617067	-3.675584
H	-3.090287	-0.951299	-4.512347
H	-1.713670	0.202754	-4.485934
H	-2.035521	1.298317	3.451002
H	-3.576458	0.656069	1.673969
H	1.895790	-2.610148	-3.003055
H	2.383682	-0.262382	-2.812862
H	0.476290	1.919199	-1.049334
C	-1.240136	2.909938	-1.038134
H	-1.981037	3.149759	-0.269866
H	-1.714834	2.322626	-1.833241
H	-0.839997	3.849049	-1.447311

^{7}IV

1	-0.913587	-2.562954	1.641091
6	-0.788597	-3.082606	0.680346
6	-2.193982	-3.599348	0.236691
7	-0.189808	-2.179871	-0.267913
27	-0.533002	-0.164323	-0.268160
6	0.602936	-2.757635	-1.264038

8	1.234432	0.241877	-1.147673
7	0.433875	0.039552	1.593070
6	-0.121348	0.550945	2.668150
8	-2.208604	0.010080	0.703122
6	1.858443	-0.324421	1.629845
1	2.427837	0.468013	1.119336
6	2.489499	-0.631003	2.989698
1	-0.139639	-3.960909	0.827731
1	1.970774	-1.213569	0.997063
1	0.515683	0.750689	3.534119
8	2.659592	0.498882	3.846716
1	3.456956	-1.128786	2.805147
1	1.863681	-1.334532	3.553375
1	3.219190	1.141811	3.377211
1	-2.550327	-4.264237	1.037449
8	-2.150984	-4.330454	-0.957707
1	-2.870153	-2.735696	0.162934
1	-2.212604	-3.654281	-1.668275
1	0.498548	-3.829826	-1.417868
8	-0.406536	2.129015	-0.454612
8	-2.426771	-2.027923	-2.416108
6	-2.086756	-0.887380	-2.745406
8	-1.368454	-0.059435	-2.037646
6	-2.519552	-0.316622	-4.092740
6	1.831306	-0.632076	-1.936728
6	1.517970	-2.026203	-2.000400
6	-2.454284	0.525000	1.852083
6	-1.501758	0.845378	2.808025
1	-3.127217	0.584509	-3.938788
1	-3.097867	-1.056609	-4.652511
1	-1.636122	-0.018616	-4.671490
1	-1.838586	1.267861	3.750777
1	-3.516608	0.690672	2.081294
1	2.109860	-2.592596	-2.720811
1	2.620565	-0.239688	-2.583130

1	0.368616	1.955540	-1.031797
6	-1.386609	2.884521	-1.179917
1	-2.237606	3.023811	-0.506932
1	-1.714005	2.340026	-2.072596
1	-0.984601	3.869997	-1.453664

[1]IVr

H	1.578153	1.063450	-3.255472
C	0.777465	1.767737	-3.015264
C	-0.562417	1.276746	-3.615590
N	0.657763	1.905458	-1.558719
Co	0.704725	0.332793	-0.426737
C	0.302393	3.077835	-1.118300
O	0.427537	1.293180	1.183052
N	2.638371	0.489223	-0.264150
C	3.450308	-0.395677	-0.767980
O	0.802389	-0.848892	-1.902351
C	3.175695	1.618969	0.513528
H	2.946948	1.449623	1.576044
C	4.659177	1.955189	0.344852
H	1.030442	2.750706	-3.437593
H	2.606506	2.510708	0.228669
H	4.509885	-0.296768	-0.519419
O	5.565818	0.989912	0.874973
H	4.825705	2.942978	0.807155
H	4.914427	2.045505	-0.718510
H	5.392845	0.912583	1.829327
H	-0.558024	1.471851	-4.695409
O	-1.658710	1.986588	-3.060151
H	-0.658412	0.198785	-3.445584
H	-1.736786	1.640259	-2.145921
H	0.235332	3.880033	-1.860197
C	-0.012966	3.461671	0.225078
C	0.053486	2.536380	1.314507
C	1.795200	-1.658666	-2.156908
C	3.110359	-1.496614	-1.616880

O	0.795781	-1.322534	0.673126
O	-1.653620	-1.733798	0.301297
C	-2.043839	-0.706828	-0.304585
O	-1.287799	0.269161	-0.688930
H	-0.184252	-1.634618	0.570838
C	-4.056392	0.156615	-1.633934
C	-5.438391	0.200156	-1.829708
C	-3.523888	-0.593435	-0.576770
C	-6.304672	-0.484196	-0.975230
C	-4.385988	-1.303652	0.273705
C	-5.760444	-1.230670	0.071812
H	-3.405407	0.686910	-2.321799
H	-5.847318	0.775293	-2.658404
H	-7.381651	-0.446397	-1.117120
Cl	-6.840188	-2.105292	1.158263
H	-3.969032	-1.904133	1.075688
C	-0.271423	3.020845	2.611498
C	-0.643546	4.339028	2.809093
C	-0.709289	5.251352	1.734644
C	-0.393668	4.806292	0.465567
H	-0.224491	2.316926	3.439562
H	-0.893021	4.675170	3.815014
H	-1.006625	6.283427	1.903600
H	-0.441043	5.489954	-0.382460
C	1.579142	-2.739684	-3.054314
C	2.603416	-3.611779	-3.379388
C	3.899420	-3.455216	-2.843117
C	4.138650	-2.402582	-1.981030
H	0.578416	-2.862866	-3.462152
H	5.133824	-2.251124	-1.562044
H	4.694286	-4.148014	-3.108806
H	2.400936	-4.437000	-4.061447
H	1.565575	-3.512201	1.950274
C	2.132703	-2.610277	2.227843
C	2.625458	-2.731835	3.680101

C	1.221417	-1.389229	2.055810
H	2.976021	-2.540434	1.527591
C	1.450062	-2.766458	4.670120
C	0.036189	-1.431090	3.026660
C	0.528051	-1.551403	4.480047
H	1.795300	-0.473619	2.245951
H	-0.574766	-0.531009	2.891526
H	-0.599263	-2.295330	2.780638
H	1.075115	-0.634773	4.756835
H	-0.333753	-1.613954	5.159009
H	0.870276	-3.689358	4.509158
H	1.822473	-2.805673	5.703826
H	3.249773	-3.629531	3.790275
H	3.273113	-1.871636	3.919527

^{3}V

H	-1.709859	2.305109	-1.419947
C	-1.290625	1.512451	-2.043354
C	0.173276	1.846101	-2.402634
N	-1.391869	0.227159	-1.342155
Co	-1.255586	0.139290	0.641179
C	-1.432663	-0.832866	-2.115924
O	-1.226511	-1.785961	0.652777
N	-3.227022	0.198467	0.810188
C	-3.762949	1.109874	1.581025
O	-1.130220	2.044143	0.740986
C	-4.035924	-0.905002	0.281615
H	-3.893078	-1.784927	0.928431
C	-5.532334	-0.635305	0.094269
H	-1.872654	1.453605	-2.974664
H	-3.624900	-1.175416	-0.696096
H	-4.820280	0.990673	1.831909
O	-6.279506	-0.498169	1.301410
H	-5.939833	-1.451482	-0.525948
H	-5.684021	0.302256	-0.454722
H	-6.202158	-1.332763	1.796124

H	0.170751	2.784837	-2.975608
O	0.758510	0.848497	-3.209766
H	0.742568	2.016757	-1.477518
H	1.085452	0.150272	-2.597030
H	-1.485721	-0.648927	-3.192017
O	-1.196472	0.027484	2.325195
O	1.452189	-0.881198	-1.137682
C	1.599977	-0.314366	-0.048511
O	0.682274	0.222713	0.704304
C	2.987094	-0.189781	0.584484
C	-1.264890	-2.551798	-0.381016
C	-1.402169	-2.182404	-1.702350
C	-1.887652	2.689078	1.551339
C	-3.092861	2.254207	2.081493
H	3.134718	0.808388	1.010501
H	3.754455	-0.404650	-0.164718
H	3.069747	-0.914113	1.405310
H	-3.631047	2.909547	2.759043
H	-1.536143	3.702582	1.785964
H	-1.424416	-2.956834	-2.462347
H	-1.197051	-3.619350	-0.131405

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H	-1.846952	2.287366	-1.175071
C	-1.364052	1.575219	-1.847827
C	0.104400	2.026365	-2.120145
N	-1.383939	0.242721	-1.264262
Co	-1.221921	0.027301	0.797173
C	-1.488746	-0.741215	-2.137989
O	-1.218088	-2.125777	0.488708
N	-3.211188	0.249460	0.690226
C	-3.827520	1.360424	1.048391
O	-0.927620	2.126139	1.028538
C	-3.968850	-0.971212	0.423348
H	-3.665198	-1.712113	1.181710
C	-5.496412	-0.886612	0.359364

H	-1.897952	1.573655	-2.809127
H	-3.627256	-1.385180	-0.538183
H	-4.914650	1.316952	1.128285
O	-6.131025	-0.502394	1.573188
H	-5.859003	-1.870523	0.014243
H	-5.813366	-0.147118	-0.387094
H	-5.847166	-1.120146	2.269545
H	0.044908	3.029948	-2.565262
O	0.745567	1.176277	-3.031509
H	0.635923	2.099743	-1.162319
H	1.114799	0.430902	-2.497517
H	-1.619669	-0.456100	-3.186046
O	-1.318099	-0.219102	2.395071
O	1.410999	-0.733252	-1.200484
C	1.615809	-0.423639	-0.011762
O	0.741524	-0.039770	0.858726
C	3.029272	-0.493732	0.567472
C	-1.207955	-2.721404	-0.609867
C	-1.419114	-2.122668	-1.882142
C	-1.860340	2.891865	1.386311
C	-3.240259	2.593307	1.387420
H	3.265084	0.429927	1.108021
H	3.756778	-0.664131	-0.231108
H	3.080897	-1.316249	1.292339
H	-3.918397	3.384913	1.696169
H	-1.572807	3.905930	1.715659
H	-1.459508	-2.785629	-2.743233
H	-1.038306	-3.812270	-0.596829

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H	-1.812204	2.432606	-1.760121
C	-1.253458	1.703530	-2.351367
C	0.264308	2.181584	-2.386740
N	-1.333766	0.404574	-1.749100
Co	-1.213539	0.314546	0.550826
C	-1.149114	-0.593775	-2.593533

O	-1.090401	-1.822930	0.143431
N	-3.310811	0.298936	0.841593
C	-3.960915	1.322119	1.375612
O	-1.279865	2.374166	0.562129
C	-3.974002	-1.008772	0.759319
H	-3.468704	-1.681289	1.468971
C	-5.488118	-1.087634	0.969824
H	-1.611004	1.691392	-3.391983
H	-3.759275	-1.415285	-0.239755
H	-4.968781	1.148905	1.759593
O	-5.929159	-0.772897	2.286918
H	-5.807441	-2.103957	0.678245
H	-6.009835	-0.383815	0.308431
H	-5.428712	-1.328100	2.910307
H	0.241396	3.152098	-2.903262
O	1.068360	1.303151	-3.100304
H	0.589684	2.313658	-1.348709
H	1.454633	0.651235	-2.446072
H	-1.094831	-0.368325	-3.663847
O	-1.338952	-0.028370	2.289082
O	2.026987	-0.460811	-1.269914
C	1.668466	-0.365177	-0.080846
O	0.753013	0.454414	0.337275
C	2.336471	-1.210055	0.992774
C	-0.963162	-2.477346	-0.908993
C	-0.994773	-1.947552	-2.237534
C	-2.201385	3.075653	1.071223
C	-3.464330	2.631275	1.501350
H	2.793734	-0.551863	1.742051
H	3.100588	-1.857606	0.553085
H	1.581926	-1.811828	1.514403
H	-4.129033	3.374195	1.935411
H	-1.996051	4.155871	1.161123
H	-0.852151	-2.659950	-3.047564
H	-0.815194	-3.568389	-0.821207

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H	-2.407767	-0.193524	2.286118
C	-1.529714	0.365084	2.624221
C	-0.580956	-0.584337	3.392246
N	-0.890457	0.993138	1.460660
Co	-1.036231	0.185166	-0.386174
C	-0.145522	2.030944	1.691923
O	-0.886531	1.953003	-1.074674
N	-3.006827	0.378117	-0.347748
C	-3.766786	-0.663082	-0.496887
O	-1.145900	-1.513852	0.417961
C	-3.563548	1.737859	-0.323546
H	-3.293302	2.228595	-1.268179
C	-5.064118	1.867824	-0.054037
H	-1.866539	1.157449	3.308177
H	-3.026551	2.288998	0.457495
H	-4.833282	-0.488854	-0.663782
O	-5.907120	1.347087	-1.078440
H	-5.272351	2.936422	0.123324
H	-5.341477	1.325678	0.858936
H	-5.707111	1.824505	-1.902668
H	-1.110226	-0.903004	4.302604
O	0.611927	0.063248	3.774104
H	-0.375722	-1.463440	2.772011
H	1.224365	-0.100821	3.023528
H	-0.006699	2.329949	2.735088
O	-1.187873	-0.445786	-1.927877
O	1.700050	-0.710811	1.390400
C	1.787608	-0.463615	0.182887
O	0.872379	0.017756	-0.609577
C	0.065868	2.768658	-0.670785
C	0.485114	2.848742	0.692277
C	-2.044959	-2.392712	0.046734
C	-3.337407	-2.033601	-0.452189
C	3.239106	-0.531249	-1.917093

C	4.469489	-0.774354	-2.529224
C	3.101388	-0.705550	-0.533451
C	5.570362	-1.188592	-1.774877
C	4.198306	-1.121926	0.232933
C	5.416784	-1.357136	-0.397046
H	2.379766	-0.209685	-2.497659
H	4.578107	-0.642127	-3.604384
H	6.532498	-1.379876	-2.243305
Cl	6.800280	-1.881633	0.564775
H	4.077045	-1.258333	1.303045
C	0.631489	3.673324	-1.600611
C	1.576416	4.604800	-1.193831
C	1.993015	4.681682	0.148515
C	1.436977	3.816324	1.077905
H	0.305261	3.608008	-2.635875
H	2.006444	5.282662	-1.930102
H	2.739079	5.412233	0.452110
H	1.737165	3.865684	2.124439
C	-4.263857	-3.047395	-0.790017
C	-3.938717	-4.386108	-0.659533
C	-2.669919	-4.738268	-0.154695
C	-1.744300	-3.770951	0.199682
H	-5.246436	-2.754062	-1.158922
H	-0.763165	-4.033310	0.587519
H	-2.408419	-5.789712	-0.044543
H	-4.654354	-5.157307	-0.934024

^{3}VI

H	-2.241723	-2.221930	-0.499084
C	-1.345002	-2.846562	-0.556849
C	-1.116644	-3.292603	-2.021586
N	-0.207245	-2.101224	-0.007367
Co	-0.153735	-0.150661	-0.051191
C	0.792729	-2.818005	0.452315
O	1.037565	-0.101547	1.459708
N	-1.758611	-0.065956	1.093777

C	-2.879938	0.437586	0.651736
O	-1.141490	-0.115681	-1.648920
C	-1.577736	-0.392808	2.510083
H	-0.867079	0.331428	2.936311
C	-2.830307	-0.476085	3.385429
H	-1.514399	-3.742396	0.058080
H	-1.074483	-1.367535	2.561680
H	-3.661342	0.645568	1.385399
O	-3.521963	0.755401	3.570810
H	-2.521900	-0.904601	4.354867
H	-3.564588	-1.162599	2.944902
H	-2.885072	1.406722	3.913481
H	-1.976722	-3.918147	-2.304216
O	0.056899	-4.059333	-2.162583
H	-1.092155	-2.408122	-2.668044
H	0.756678	-3.392884	-2.344521
H	0.734853	-3.899107	0.304445
O	-0.207877	1.650879	0.053476
O	1.460757	-1.753777	-2.546184
C	1.905893	-0.691892	-2.102659
O	1.469711	-0.000422	-1.086315
C	3.114849	-0.031690	-2.767930
C	1.904927	-1.018881	1.680456
C	1.897057	-2.310126	1.170990
C	-2.319804	0.389998	-1.741137
C	-3.171705	0.722143	-0.705713
H	2.807286	0.915075	-3.230387
H	3.525202	-0.694642	-3.534609
H	3.886339	0.200804	-2.023843
H	-4.142204	1.145995	-0.943771
H	-2.661899	0.526623	-2.775343
H	2.685351	-2.994962	1.468019
H	2.692446	-0.737508	2.393111
H	0.731735	1.930540	-0.025024
C	2.730773	3.164824	-0.030704

H	2.888884	3.308387	1.033365
H	2.422757	4.004032	-0.646097
H	2.943292	2.204033	-0.487596

^{3}VIr

H	2.325969	-1.960807	2.361564
C	1.399286	-2.543134	2.336668
C	0.461286	-2.075549	3.474013
N	0.788379	-2.404030	1.009184
Co	1.031630	-0.748093	-0.083282
C	-0.007965	-3.354017	0.628389
O	0.808205	-1.777581	-1.644595
N	2.974894	-0.993794	-0.168916
C	3.770462	-0.054488	0.231802
O	1.161996	0.270311	1.461816
C	3.484786	-2.163421	-0.895881
H	3.116688	-2.087284	-1.928132
C	4.993458	-2.409217	-0.871939
H	1.651490	-3.600564	2.501617
H	2.988577	-3.045657	-0.471464
H	4.827628	-0.127909	-0.034307
O	5.774699	-1.415216	-1.529491
H	5.168821	-3.405688	-1.312306
H	5.365676	-2.440308	0.160187
H	5.450717	-1.336836	-2.443983
H	0.965683	-2.308021	4.423903
O	-0.772952	-2.756137	3.444479
H	0.320324	-0.992074	3.400051
H	-1.350732	-2.184150	2.892297
H	-0.205024	-4.166308	1.334109
O	1.334417	0.716134	-1.109066
O	-1.752464	-0.790767	1.823467
C	-1.803823	-0.364563	0.662934
O	-0.850233	-0.342709	-0.220760
H	0.434144	1.059326	-1.297165
C	-1.637829	-3.906456	-3.244374

C	-2.119064	-4.670024	-2.162624
C	-0.662671	-2.939512	-3.058933
C	-1.595320	-4.454049	-0.896994
C	-0.140337	-2.675250	-1.766218
C	-0.619474	-3.461305	-0.669895
H	-2.038016	-4.076257	-4.243076
H	-2.884934	-5.425673	-2.320613
H	-1.938256	-5.050503	-0.051790
H	-0.283154	-2.345500	-3.887099
C	4.062188	3.146861	2.133376
C	2.800657	3.213200	2.757982
C	4.347353	2.082613	1.289820
C	1.840447	2.240735	2.531081
C	3.386706	1.086935	1.021342
C	2.098239	1.164425	1.640333
H	4.808583	3.915034	2.321402
H	2.574647	4.040894	3.428522
H	0.862508	2.280236	3.004455
H	5.327189	2.004045	0.819464
C	-5.405973	0.792014	0.584614
C	-4.190670	0.282465	1.032567
C	-5.576621	1.219462	-0.733818
C	-3.110861	0.202082	0.143002
C	-4.495465	1.130540	-1.614645
C	-3.266987	0.626840	-1.183505
Cl	-6.764329	0.899182	1.705891
H	-4.058853	-0.055195	2.055815
H	-2.424159	0.555660	-1.864106
H	-4.618803	1.457418	-2.645861
H	-6.536631	1.611217	-1.060254
H	1.586452	3.176757	-2.270525
C	0.697602	3.646766	-2.727330
C	0.900017	5.185842	-2.692829
C	-0.525081	3.255934	-1.954705
H	0.649465	3.289950	-3.764900

C	0.858088	5.717081	-1.250562
C	-0.651771	3.784855	-0.558921
C	-0.444976	5.323855	-0.535883
H	-1.414591	2.912124	-2.481644
H	-1.619720	3.516909	-0.116172
H	0.127930	3.334320	0.081699
H	-1.296455	5.810148	-1.036934
H	-0.438381	5.684572	0.503408
H	1.714890	5.308071	-0.689983
H	0.974894	6.810954	-1.247902
H	1.854741	5.448602	-3.172330
H	0.103893	5.668277	-3.281356

^{1}TS1

H	-0.028134	-2.216103	0.888022
C	-0.637847	-2.358187	-0.010569
C	-2.125957	-2.538857	0.389984
N	-0.454171	-1.223294	-0.920546
Co	-0.608958	0.627134	-0.258452
C	-0.487491	-1.500816	-2.201140
O	-0.425687	1.430652	-1.991229
N	1.319960	0.703837	0.054891
C	1.832631	0.771463	1.263165
O	-0.974859	0.034462	1.525257
C	2.207440	0.662721	-1.115832
H	2.142025	1.624715	-1.648546
C	3.679364	0.318670	-0.879743
H	-0.289367	-3.268895	-0.520183
H	1.805680	-0.087025	-1.807339
H	2.912763	0.914998	1.337187
O	4.431207	1.322587	-0.196453
H	4.130267	0.096922	-1.861924
H	3.770248	-0.586434	-0.266600
H	4.420190	2.123444	-0.748614
H	-2.254720	-3.552306	0.793379
O	-2.998045	-2.412028	-0.718401

H	-2.375364	-1.816893	1.176991
H	-2.989730	-1.454580	-0.931966
H	-0.518997	-2.561622	-2.469886
H	-0.492035	-0.979679	-4.288448
C	-0.475487	-0.582572	-3.278088
C	-0.453388	0.786910	-3.103000
H	-0.436702	1.428858	-3.995696
H	-0.668718	0.089660	3.503163
C	-0.206911	0.272167	2.522441
C	1.116034	0.677540	2.476310
H	1.658569	0.807824	3.407611
O	-0.985643	2.417018	0.383486
O	-2.961417	2.079148	0.826183
C	-3.314225	1.145408	0.077491
C	-4.793771	0.830438	-0.077771
O	-2.510019	0.405348	-0.603856
H	-4.948456	-0.252124	0.000577
H	-5.122891	1.146443	-1.076206
H	-5.381785	1.356715	0.678425
C	0.683175	3.699665	-0.100112
H	-0.001044	2.929334	0.701350
H	0.582355	3.405827	-1.139889
H	0.233842	4.665070	0.135203
H	1.674520	3.534693	0.332423

[1]TS1r

H	0.754844	1.425259	-3.436277
C	0.010428	2.100476	-3.005197
C	-1.412940	1.602426	-3.360941
N	0.177390	2.156282	-1.549521
Co	0.429917	0.480909	-0.511462
C	-0.118528	3.292508	-0.990002
O	0.462412	1.395812	1.171844
N	2.375382	0.643477	-0.704106
C	3.082268	-0.228281	-1.362941
O	0.299441	-0.570312	-2.091521

C	3.022904	1.791562	-0.049303
H	2.695305	1.790026	0.997150
C	4.544905	1.888645	-0.110821
H	0.159886	3.108912	-3.418642
H	2.598158	2.702464	-0.493328
H	4.170027	-0.138979	-1.330242
O	5.217612	0.841577	0.594300
H	4.830664	2.877398	0.282968
H	4.912558	1.839224	-1.142988
H	5.087378	1.001123	1.544528
H	-1.622967	1.851573	-4.408894
O	-2.399879	2.246546	-2.568377
H	-1.451296	0.514750	-3.236407
H	-2.289379	1.858558	-1.674790
H	-0.346520	4.130852	-1.657988
C	-0.191152	3.595649	0.409268
C	0.087563	2.620059	1.419868
C	1.196139	-1.434298	-2.470165
C	2.585226	-1.328106	-2.133238
O	0.527077	-1.110956	0.479669
O	-1.478478	-1.767801	0.107113
C	-2.083086	-0.709420	-0.149655
O	-1.528053	0.421736	-0.436408
H	1.559874	-1.305482	0.827954
C	-4.391740	0.069991	-0.915283
C	-5.782547	-0.031370	-0.843835
C	-3.593021	-0.750414	-0.107313
C	-6.390861	-0.933152	0.031765
C	-4.192512	-1.676070	0.760153
C	-5.580613	-1.746672	0.826469
H	-3.938936	0.768051	-1.613346
H	-6.402487	0.600536	-1.477282
H	-7.473132	-1.010245	0.097184
Cl	-6.334363	-2.894071	1.934066
H	-3.568773	-2.325402	1.366271

C	-0.015980	3.038117	2.777336
C	-0.374786	4.333175	3.106664
C	-0.648444	5.292502	2.109220
C	-0.552897	4.913986	0.783617
H	0.184146	2.295733	3.547339
H	-0.451494	4.612877	4.157165
H	-0.933915	6.306392	2.379320
H	-0.764887	5.634222	-0.007363
C	0.806983	-2.508244	-3.318595
C	1.735537	-3.419001	-3.788837
C	3.104185	-3.313243	-3.456155
C	3.512354	-2.270501	-2.647108
H	-0.247638	-2.591976	-3.570138
H	4.566346	-2.155096	-2.390332
H	3.822343	-4.035495	-3.837253
H	1.401244	-4.236269	-4.427312
H	2.019455	-3.491877	1.565364
C	2.900352	-2.834201	1.587155
C	3.827554	-3.268145	2.761155
C	2.462210	-1.415120	1.833053
H	3.417893	-2.935306	0.626073
C	3.142004	-3.062407	4.119169
C	1.743674	-1.174813	3.126453
C	2.668399	-1.612324	4.297372
H	3.183463	-0.649021	1.532941
H	1.445531	-0.125351	3.214925
H	0.827147	-1.779845	3.144432
H	3.541745	-0.942620	4.348378
H	2.123914	-1.491087	5.243825
H	2.277006	-3.739278	4.196383
H	3.830682	-3.337199	4.930932
H	4.107125	-4.320572	2.614414
H	4.759173	-2.683208	2.721838

[1]TS4

H	0.421718	-1.314977	-2.706081

C	1.383255	-1.515289	-2.225466
C	2.483168	-0.670723	-2.884067
N	1.264264	-1.264106	-0.779852
Co	0.030233	0.077855	-0.101487
C	1.999835	-2.019777	0.003527
O	0.124686	-0.587835	1.705966
N	-1.535467	-0.974645	-0.557768
C	-2.216719	-0.770189	-1.657443
O	0.086400	1.024560	-1.752191
C	-2.103100	-1.896145	0.446398
H	-1.682128	-1.604640	1.408291
C	-3.642236	-1.862737	0.561569
H	1.620692	-2.576872	-2.384590
H	-1.768441	-2.927122	0.244117
H	-3.131075	-1.351600	-1.784589
O	-4.184348	-0.565475	0.536799
H	-3.892209	-2.411033	1.490418
H	-4.119788	-2.418051	-0.259028
H	-3.625993	0.018708	1.098918
H	2.520422	-0.918962	-3.952444
O	3.777460	-0.966141	-2.365123
H	2.239531	0.395756	-2.786131
H	3.835914	-0.547589	-1.490580
H	2.667795	-2.728595	-0.496212
H	2.699616	-2.686275	1.928454
C	2.003243	-2.029040	1.416834
C	1.049829	-1.353514	2.157783
H	1.036786	-1.487128	3.248713
H	-0.642114	1.654389	-3.508986
C	-0.811169	0.964400	-2.670750
C	-1.907604	0.128530	-2.705239
H	-2.589557	0.188110	-3.547536
O	-0.877474	1.637441	0.620408
O	1.096478	1.563445	0.575094
C	-1.462544	1.728700	1.815702

C	-0.807976	2.696469	2.773062
O	-2.490770	1.117246	2.089215
H	0.175582	2.301445	3.054059
H	-1.431419	2.826247	3.661589
H	-0.639895	3.659956	2.278078
H	2.180901	1.286297	0.971390
C	3.266396	1.420666	0.351353
H	3.137198	1.498207	-0.724176
H	3.670237	2.332849	0.794576
H	3.760015	0.502349	0.686985

^{3}TS4

1	1.076635	-1.069768	-3.117839
6	1.898108	-1.313687	-2.435750
6	2.979819	-0.236050	-2.537443
7	1.386514	-1.409159	-1.063697
27	-0.003698	0.017906	-0.186569
6	1.701368	-2.498129	-0.405379
8	0.401955	-0.679913	1.546252
7	-1.580308	-1.103332	-0.429120
6	-2.165409	-1.251704	-1.592941
8	-0.208159	0.876373	-1.853187
6	-2.278171	-1.635971	0.763704
1	-1.811888	-1.175656	1.634401
6	-3.792360	-1.333703	0.810830
1	2.322741	-2.281327	-2.747885
1	-2.107953	-2.722515	0.831598
1	-3.045002	-1.900686	-1.625211
8	-4.111709	0.000221	0.525689
1	-4.134756	-1.653691	1.814376
1	-4.340209	-1.953018	0.085803
1	-3.606788	0.571134	1.158105
1	3.391515	-0.219092	-3.553965
8	4.075169	-0.500268	-1.662309
1	2.530829	0.747021	-2.331133
1	3.683914	-0.774687	-0.812847

1	2.260867	-3.276476	-0.943486
1	1.755275	-3.719333	1.365524
6	1.419487	-2.770148	0.958026
6	0.855286	-1.855957	1.823492
1	0.792231	-2.117307	2.889297
1	-0.818412	1.028491	-3.753509
6	-0.931694	0.451091	-2.826148
6	-1.819472	-0.608420	-2.799815
1	-2.388020	-0.840374	-3.694730
8	-1.059277	1.576196	0.776142
8	0.920063	1.697720	0.413401
6	-1.418957	1.713200	2.030735
6	-0.432575	2.349347	2.985747
8	-2.544595	1.355107	2.406153
1	0.406626	1.660566	3.138759
1	-0.923891	2.556190	3.940542
1	-0.025820	3.270092	2.553662
1	2.027117	1.571937	0.686446
6	2.992618	2.164618	0.024479
1	3.601955	1.341049	-0.352850
1	2.630797	2.835957	-0.746882
1	3.407866	2.691323	0.889091

^{3}TS5

H	0.234942	-1.373381	-1.804844
C	0.793384	-2.022267	-1.122106
C	2.288206	-1.632077	-1.135580
N	0.194930	-1.958584	0.222174
Co	-0.008269	-0.242471	1.169122
C	-0.027174	-3.116716	0.801966
O	-0.315126	-1.096357	2.870197
N	-2.127028	-0.057181	0.783503
C	-2.585241	0.391364	-0.349404
O	0.387768	0.788408	-0.406699
C	-3.041961	-0.360602	1.890038
H	-2.619629	0.117769	2.784849

C	-4.512001	0.041270	1.753112
H	0.696704	-3.054674	-1.487432
H	-2.999002	-1.443428	2.084530
H	-3.664564	0.497741	-0.488522
O	-4.717086	1.434935	1.549432
H	-5.035781	-0.316360	2.657542
H	-4.987339	-0.455104	0.897440
H	-4.271852	1.905254	2.275631
H	2.696724	-1.922627	-2.114294
O	3.030209	-2.303335	-0.137698
H	2.379466	-0.543026	-1.033923
H	2.892034	-1.764454	0.670128
H	0.141735	-4.006485	0.187474
H	-0.596259	-4.382095	2.443835
C	-0.432474	-3.354856	2.132884
C	-0.505751	-2.347596	3.076568
H	-0.732243	-2.611212	4.119545
H	0.068460	1.492662	-2.259167
C	-0.419595	1.033345	-1.386613
C	-1.781966	0.831470	-1.443582
H	-2.297246	1.143542	-2.348040
O	-0.077830	1.273403	2.220545
O	2.040046	1.648327	2.722489
C	2.631881	0.631506	2.259334
C	4.115387	0.511687	2.603734
O	2.111595	-0.290990	1.565202
H	4.658078	0.125951	1.734080
H	4.222565	-0.210403	3.423511
H	4.530337	1.471969	2.920793
H	-0.053904	2.359514	1.569782
C	-0.081218	3.502407	1.025692
H	-0.224611	4.186880	1.864622
H	-0.919253	3.469767	0.326579
H	0.894659	3.589566	0.546727

^{5}TS5

1	0.314234	-1.455402	-1.876392
6	0.912929	-2.019393	-1.154884
6	2.354369	-1.468805	-1.117086
7	0.253232	-2.000542	0.164403
27	-0.143921	-0.320565	1.091505
6	0.121055	-3.172017	0.746385
8	-0.437245	-1.189992	2.792489
7	-2.238136	-0.320436	0.629426
6	-2.674261	-0.120168	-0.585657
8	0.157594	0.759731	-0.507960
6	-3.252146	-0.487082	1.676369
1	-2.760306	-0.920637	2.551308
6	-3.939073	0.829292	2.080747
1	0.947440	-3.062853	-1.497950
1	-4.035009	-1.190005	1.344449
1	-3.750824	-0.247095	-0.775922
8	-3.063431	1.874635	2.447022
1	-4.635875	0.590202	2.906182
1	-4.551153	1.192244	1.239773
1	-2.179971	1.509605	2.665612
1	2.825794	-1.715185	-2.079567
8	3.125642	-2.055886	-0.089793
1	2.325590	-0.375721	-1.018176
1	2.902104	-1.529330	0.707381
1	0.400452	-4.042015	0.144988
1	-0.394028	-4.486589	2.365313
6	-0.313787	-3.448000	2.059559
6	-0.524409	-2.454127	2.995236
1	-0.776361	-2.737414	4.026908
1	-0.138109	1.287400	-2.424895
6	-0.594826	0.796323	-1.551852
6	-1.890506	0.324518	-1.681432
1	-2.381129	0.447218	-2.643073
8	-0.407137	1.192736	2.130933
8	1.612537	1.624205	2.900830

6	2.322496	0.723845	2.377082
6	3.785261	0.672371	2.809562
8	1.930221	-0.151969	1.541798
1	4.413349	0.429196	1.945775
1	3.900039	-0.127877	3.552315
1	4.098726	1.618617	3.258152
1	-0.308752	2.250034	1.532733
6	-0.329312	3.469670	1.049866
1	0.097402	4.047613	1.870731
1	-1.395338	3.627711	0.880330
1	0.289286	3.414394	0.154632

^{7}TS5

H	-0.069534	-2.173463	-1.431407
C	0.515436	-2.598506	-0.605872
C	2.016756	-2.279986	-0.837998
N	0.037595	-2.042983	0.662190
Co	-0.126609	0.022173	0.893869
C	0.009205	-2.886612	1.671364
O	-0.735277	-0.260141	2.802237
N	-2.056369	0.319959	0.234919
C	-2.377291	1.068689	-0.805732
O	0.482162	0.454975	-0.997910
C	-3.134897	-0.226854	1.073097
H	-3.226568	0.397747	1.976695
C	-4.514801	-0.420129	0.438389
H	0.374478	-3.690602	-0.604461
H	-2.794066	-1.207342	1.429052
H	-3.432796	1.314948	-0.949099
O	-5.232368	0.784425	0.170565
H	-5.099331	-1.081396	1.101431
H	-4.421119	-0.928269	-0.529687
H	-5.328516	1.262813	1.012503
H	2.379496	-2.924110	-1.650794
O	2.807538	-2.544593	0.304022
H	2.109949	-1.233939	-1.156562

H	2.619210	-1.795650	0.912503
H	0.250997	-3.934434	1.454748
H	-0.282268	-3.416680	3.728812
C	-0.305561	-2.594075	3.018895
C	-0.637535	-1.330663	3.494309
H	-0.859883	-1.230804	4.569444
H	0.479764	1.607404	-2.654457
C	-0.121686	1.218437	-1.817519
C	-1.472893	1.568135	-1.763674
H	-1.868314	2.207907	-2.548156
O	0.093427	1.983986	1.262679
O	2.280712	2.114888	1.250745
C	2.670456	0.923714	1.343090
C	4.174680	0.679833	1.422589
O	1.920760	-0.110104	1.396779
H	4.432156	-0.190132	0.807695
H	4.442206	0.448345	2.461951
H	4.733673	1.561443	1.098579
H	0.150584	2.242079	2.419291
C	0.256142	2.577203	3.713435
H	-0.776416	2.619126	4.062356
H	0.767214	3.539376	3.658612
H	0.844215	1.766325	4.141643

^{3}TS2

H	-1.370823	-2.404462	-0.942287
C	-0.427252	-2.931069	-0.771863
C	0.043867	-3.590936	-2.088503
N	0.554413	-1.989204	-0.218527
Co	0.450414	-0.074746	-0.578090
C	1.528015	-2.512484	0.490777
O	1.411488	0.341061	1.037421
N	-1.305398	-0.020989	0.345633
C	-2.420636	0.174654	-0.309557
O	-0.309034	-0.397957	-2.280689
C	-1.279337	-0.036731	1.810562

H	-0.783199	0.881907	2.159294
C	-2.613800	-0.216034	2.539627
H	-0.611067	-3.723111	-0.031363
H	-0.626719	-0.862853	2.120846
H	-3.318781	0.364560	0.282096
O	-3.531648	0.864990	2.402101
H	-2.380949	-0.400847	3.602666
H	-3.142399	-1.100809	2.162853
H	-3.081533	1.676680	2.694833
H	-0.713394	-4.341307	-2.361527
O	1.283390	-4.245045	-1.937328
H	0.091630	-2.830819	-2.876531
H	1.944887	-3.548888	-2.148138
H	1.575799	-3.603492	0.528760
O	0.180282	1.669010	-0.799913
O	2.500762	-1.894030	-2.567663
C	2.801105	-0.742864	-2.241221
O	2.182942	0.049300	-1.410437
C	4.040750	-0.074583	-2.840444
C	2.310037	-0.438093	1.519485
C	2.474680	-1.786892	1.247266
C	-1.535440	-0.153744	-2.579273
C	-2.569040	0.154270	-1.716857
H	3.730661	0.755490	-3.488208
H	4.607883	-0.802404	-3.427392
H	4.674597	0.343864	-2.049373
H	-3.556259	0.334743	-2.130168
H	-1.749794	-0.237948	-3.653066
H	3.262205	-2.332222	1.758036
H	2.965631	0.034176	2.264206
H	1.160384	2.289831	-0.569935
C	2.221711	3.095723	-0.361647
H	2.211793	3.262935	0.716046
H	1.988189	3.973770	-0.966331
H	3.039778	2.478208	-0.728672

^{5}TS2

1	-1.240042	-2.413225	-1.562790
6	-0.331908	-2.920655	-1.225997
6	0.560583	-3.262622	-2.458597
7	0.388659	-2.078806	-0.282817
27	0.383031	-0.028258	-0.571998
6	0.982646	-2.734190	0.697553
8	1.761338	0.102167	1.147542
7	-1.319672	-0.137760	0.443621
6	-2.507216	-0.076681	-0.120405
8	-0.610924	-0.239648	-2.442429
6	-1.168421	-0.073970	1.895186
1	-0.527878	0.797222	2.107128
6	-2.428318	-0.010915	2.761449
1	-0.612583	-3.868773	-0.744985
1	-0.587131	-0.951331	2.222851
1	-3.369169	0.008204	0.542474
8	-3.251121	1.126956	2.536748
1	-2.097172	-0.064585	3.813670
1	-3.072009	-0.882128	2.583719
1	-2.688800	1.919113	2.596178
1	-0.045732	-3.906381	-3.111936
8	1.710797	-3.971816	-2.084982
1	0.791717	-2.336449	-3.000262
1	2.377408	-3.289027	-1.832318
1	0.821563	-3.815954	0.733747
8	0.166162	1.697426	-0.478757
8	3.104365	-1.753654	-1.332600
6	2.976437	-0.616074	-1.821110
8	1.982027	0.192901	-1.655689
6	4.071169	-0.041248	-2.720263
6	2.221646	-0.848271	1.813179
6	1.825462	-2.209283	1.693528
6	-1.858845	-0.097062	-2.550636
6	-2.798095	-0.061964	-1.500398

1	3.655186	0.192173	-3.708283
1	4.891674	-0.756576	-2.823629
1	4.447213	0.897999	-2.296332
1	-3.845994	0.031293	-1.774442
1	-2.261265	-0.003139	-3.575025
1	2.267354	-2.919568	2.388652
1	2.994621	-0.622277	2.569815
1	1.101733	2.302051	-0.799634
6	2.125779	3.178933	-1.079293
1	2.924660	2.831200	-0.424388
1	1.701600	4.149758	-0.817336
1	2.298257	3.015502	-2.142205

^{7}TS2

H	-1.225018	-2.736279	-0.887784
C	-0.256600	-3.183443	-0.640272
C	0.460391	-3.577892	-2.000288
N	0.538181	-2.246925	0.104259
Co	0.515729	-0.038254	-0.526969
C	1.508844	-2.788862	0.811374
O	1.577806	0.158560	1.393319
N	-1.407189	0.043354	0.283787
C	-2.483142	0.232964	-0.446996
O	-0.275991	-0.464334	-2.319344
C	-1.488698	0.160140	1.743475
H	-1.007635	1.108555	2.034700
C	-2.859154	0.055183	2.416927
H	-0.407482	-4.113676	-0.071793
H	-0.853550	-0.632247	2.164385
H	-3.413343	0.499623	0.061829
O	-3.744401	1.142455	2.157940
H	-2.689223	-0.061671	3.502040
H	-3.388348	-0.842779	2.072629
H	-3.277940	1.964624	2.389345
H	-0.171418	-4.372518	-2.426715
O	1.751272	-4.053405	-1.799327

H	0.442378	-2.702207	-2.657379
H	2.358973	-3.302121	-2.065918
H	1.614032	-3.878378	0.813452
O	0.475812	1.795549	-0.596822
O	2.994762	-1.918520	-2.822811
C	2.764798	-0.766703	-2.413290
O	2.327680	-0.497042	-1.217115
C	3.020430	0.421990	-3.326580
C	2.398195	-0.654074	1.855654
C	2.436446	-2.063154	1.585831
C	-1.482679	-0.227848	-2.679281
C	-2.547504	0.121779	-1.857589
H	2.058699	0.894346	-3.566033
H	3.511331	0.100301	-4.249464
H	3.634620	1.174683	-2.817634
H	-3.512940	0.291010	-2.327400
H	-1.683289	-0.336668	-3.756755
H	3.217433	-2.630867	2.088158
H	3.153100	-0.277467	2.569375
H	1.550554	2.271456	-0.406817
C	2.768874	2.772726	-0.172953
H	2.734336	3.075056	0.875005
H	2.842490	3.602035	-0.879432
H	3.429171	1.931558	-0.383218

^{3}TS2r

H	2.742488	-1.438624	2.263642
C	1.882186	-2.113294	2.319752
C	0.983277	-1.704941	3.509494
N	1.175615	-2.085702	1.032942
Co	1.192721	-0.443244	-0.139782
C	0.461384	-3.126128	0.734166
O	0.998664	-1.590807	-1.638167
N	3.151379	-0.552740	-0.319398
C	3.901118	0.439282	0.045111
O	1.326894	0.625447	1.387145

C	3.714108	-1.703428	-1.039891
H	3.351891	-1.655443	-2.075539
C	5.232568	-1.879852	-1.003334
H	2.254993	-3.133154	2.493356
H	3.255396	-2.602535	-0.610952
H	4.952009	0.421617	-0.254813
O	5.973542	-0.867874	-1.681610
H	5.455675	-2.877061	-1.419405
H	5.599318	-1.869030	0.031007
H	5.664058	-0.840124	-2.603982
H	1.567128	-1.871687	4.427282
O	-0.186557	-2.490291	3.575647
H	0.741847	-0.640221	3.427543
H	-0.848094	-1.980477	3.057675
H	0.393691	-3.925004	1.478899
O	1.338463	0.951382	-1.204979
O	-1.411328	-0.625559	2.002363
C	-1.606958	-0.396500	0.801899
O	-0.729545	-0.284524	-0.149259
C	0.114134	-2.563075	-1.664005
C	-0.216947	-3.346844	-0.515489
C	2.217210	1.576989	1.505392
C	3.478770	1.568300	0.830133
H	0.267526	1.605341	-1.383634
C	-3.364358	-0.245666	-1.048009
C	-4.692622	-0.082774	-1.445726
C	-3.030842	-0.203869	0.312983
C	-5.697376	0.132533	-0.498920
C	-4.033667	-0.003827	1.271314
C	-5.350090	0.169607	0.853317
H	-2.581434	-0.425240	-1.778954
H	-4.954441	-0.125381	-2.501723
H	-6.733505	0.264947	-0.799515
Cl	-6.611790	0.437405	2.057301
H	-3.766396	0.008572	2.323531

C	-0.478365	-2.913618	-2.902862
C	-1.370142	-3.973315	-2.988584
C	-1.703176	-4.738439	-1.855105
C	-1.114170	-4.429156	-0.638919
H	-0.213991	-2.320746	-3.775679
H	-1.820741	-4.212993	-3.951134
H	-2.405833	-5.564578	-1.934402
H	-1.343431	-5.019330	0.248389
C	4.389634	2.627490	1.038813
C	4.080891	3.685705	1.877711
C	2.845506	3.685248	2.557010
C	1.935999	2.654466	2.387685
H	5.349929	2.597688	0.524290
H	0.980758	2.643822	2.906786
H	2.599024	4.508731	3.225893
H	4.786919	4.500190	2.021441
H	0.869333	3.709722	-2.550426
C	-0.094710	3.267196	-2.846112
C	-1.079852	4.407247	-3.205284
C	-0.649869	2.447503	-1.696495
H	0.096046	2.634904	-3.723580
C	-1.415227	5.261345	-1.972982
C	-0.972415	3.260284	-0.458148
C	-1.956479	4.401245	-0.820622
H	-1.465833	1.776763	-1.992852
H	-1.398536	2.621730	0.325013
H	-0.048458	3.701900	-0.053261
H	-2.923406	3.962820	-1.112734
H	-2.146288	5.019303	0.068783
H	-0.505813	5.786267	-1.637999
H	-2.145543	6.039121	-2.240005
H	-0.649989	5.029160	-4.003963
H	-2.006498	3.969355	-3.608693

^{3}TS3

H	-1.562631	-3.272516	0.589471

C	-1.448903	-3.585755	-0.453984
C	-2.814436	-4.062362	-1.005082
N	-0.893999	-2.471462	-1.226544
Co	-1.237766	-0.575476	-0.715198
C	-0.254142	-2.777765	-2.327872
O	0.389262	-0.042989	-1.568874
N	-0.334357	-0.831450	1.016883
C	-0.981164	-0.719258	2.145133
O	-2.930456	-1.018063	-0.019801
C	1.123871	-0.977910	0.988913
H	1.551448	-0.043727	0.594676
C	1.822633	-1.367670	2.292917
H	-0.745473	-4.431039	-0.481986
H	1.360932	-1.748707	0.244181
H	-0.388419	-0.682913	3.061791
O	1.768151	-0.385778	3.324987
H	2.868328	-1.616172	2.041870
H	1.367275	-2.269738	2.721202
H	2.140042	0.439898	2.968439
H	-3.106826	-4.950028	-0.424163
O	-2.735375	-4.426436	-2.364022
H	-3.560236	-3.274540	-0.848084
H	-2.919998	-3.591390	-2.849422
H	-0.241220	-3.829719	-2.625738
O	-1.460887	1.163730	-0.194928
O	-3.263458	-1.849662	-3.120668
C	-2.942420	-0.659720	-3.141124
O	-2.093657	-0.043242	-2.362974
C	-3.570837	0.289292	-4.162255
C	0.799635	-0.595088	-2.656423
C	0.476150	-1.858581	-3.120092
C	-3.248135	-0.871806	1.220315
C	-2.392574	-0.667514	2.281703
H	-4.281414	0.951744	-3.650142
H	-4.103003	-0.285400	-4.925462

H	-2.807071	0.922696	-4.627753
H	-2.808943	-0.567790	3.279246
H	-4.325738	-0.957189	1.412367
H	0.935890	-2.211896	-4.038056
H	1.531734	0.002726	-3.216437
H	-1.739995	1.560990	-1.045560
C	-1.632068	3.499053	0.734708
H	-1.765304	3.047350	1.709385
H	-2.501731	3.792796	0.156669
H	-0.639408	3.768773	0.393540

^{3}TS3r

H	0.963794	2.442267	2.579579
C	0.076878	1.956577	3.000139
C	-1.155133	2.872189	2.809867
N	-0.094005	0.647584	2.361210
Co	0.503255	0.319103	0.449174
C	-0.766466	-0.243888	3.017780
O	0.738013	-1.501879	0.903072
N	2.380367	0.708340	0.893543
C	3.017963	1.669789	0.304883
O	0.160935	2.088947	0.015871
C	3.080341	-0.246278	1.763028
H	2.931273	-1.241858	1.326635
C	4.564012	-0.002610	2.039046
H	0.242715	1.808247	4.077135
H	2.546059	-0.263361	2.723032
H	4.101519	1.718842	0.426791
O	5.398467	-0.068070	0.886508
H	4.875994	-0.737617	2.800553
H	4.730006	0.994156	2.467832
H	5.272911	-0.939648	0.470859
H	-0.977140	3.782099	3.402113
O	-2.337114	2.260697	3.275623
H	-1.238831	3.146341	1.752556
H	-2.695002	1.793629	2.488948

H	-1.190100	0.043955	3.985100
O	1.130616	-0.031647	-1.234264
O	-2.744138	1.188025	0.787904
C	-2.412896	0.342848	-0.050926
O	-1.234927	-0.182449	-0.230246
H	0.306483	-0.326056	-1.672222
C	2.774377	4.695852	-1.867985
C	1.378843	4.874461	-1.933648
C	3.285664	3.626869	-1.148434
C	0.514682	3.995215	-1.300017
C	2.432811	2.705987	-0.503325
C	1.017916	2.881318	-0.581097
H	3.442113	5.392770	-2.368965
H	0.969100	5.714862	-2.492112
H	-0.564201	4.121962	-1.345692
H	4.363222	3.482160	-1.072568
C	-0.179119	-2.181964	1.561055
C	-0.972881	-1.607580	2.601561
C	-0.330021	-3.564240	1.290110
C	-1.878858	-2.418102	3.316966
C	-1.244796	-4.330440	1.997676
C	-2.033193	-3.762945	3.015723
H	-2.467043	-1.962848	4.113524
H	-2.748467	-4.372436	3.562960
H	-1.353348	-5.387419	1.757771
H	0.285121	-3.996911	0.504528
C	-4.182061	-1.677863	-2.782192
C	-3.181873	-1.218449	-1.924135
C	-5.464068	-1.123901	-2.740401
C	-3.458938	-0.195469	-1.007609
C	-5.726607	-0.106365	-1.820691
C	-4.743861	0.361590	-0.953347
H	-3.967442	-2.474755	-3.492313
H	-2.186181	-1.650960	-1.951012
H	-4.948400	1.149891	-0.235578

Cl	-7.342543	0.599203	-1.758136
H	-6.248957	-1.472760	-3.406571
H	5.340343	-2.341099	-3.556752
C	5.119140	-1.955009	-2.550033
C	4.757936	-3.134499	-1.634591
C	3.958000	-0.935304	-2.632613
H	6.032331	-1.453174	-2.196823
C	3.477452	-3.838827	-2.108738
C	2.652260	-1.599087	-2.925558
C	2.289041	-2.850540	-2.196748
H	3.889006	-0.418464	-1.656417
H	4.179810	-0.154819	-3.372639
H	1.975611	-1.169037	-3.659302
H	1.976134	-2.582569	-1.168546
H	1.421002	-3.338856	-2.661852
H	3.662546	-4.278484	-3.101056
H	3.223115	-4.670204	-1.435530
H	5.591764	-3.849259	-1.583808
H	4.599863	-2.767277	-0.603057

^{1}TS6

H	-1.593413	-0.661762	2.270476
C	-2.340865	-0.171319	1.640602
C	-2.399720	1.313128	2.038515
N	-2.019822	-0.405905	0.226101
Co	-0.194863	-0.211779	-0.447704
C	-3.032955	-0.569090	-0.593874
O	-0.646221	-0.299120	-2.273182
N	0.112471	-2.135540	-0.508758
C	1.073662	-2.629287	-1.248180
O	1.612151	0.235022	-1.076614
C	-0.646870	-3.111220	0.291038
H	-0.549423	-4.088646	-0.198971
C	-0.120153	-3.227560	1.745403
H	-3.312823	-0.641866	1.855179
H	-1.706381	-2.843397	0.294177

H	1.135073	-3.719926	-1.294160
O	1.291945	-3.196354	1.809449
H	-0.440061	-4.195768	2.148456
H	-0.558878	-2.442887	2.376111
H	1.533106	-2.275965	1.599612
H	-2.682992	1.369830	3.101874
O	-3.278890	2.082488	1.222528
H	-1.412157	1.770687	1.935810
H	-4.192332	1.928297	1.517339
H	-4.023640	-0.629314	-0.132747
H	-3.915749	-0.882408	-2.527383
C	-2.988425	-0.691661	-1.997508
C	-1.825184	-0.543766	-2.726636
H	-1.865351	-0.623479	-3.820077
H	3.162159	-0.133751	-2.327583
C	2.301448	-0.584803	-1.817504
C	2.066302	-1.924305	-1.977074
H	2.731982	-2.499807	-2.612181
O	0.571495	-0.285248	1.374608
C	1.327858	0.607220	1.893587
C	2.193577	0.198928	3.060684
N	-0.576273	1.705414	-0.551857
O	1.339899	1.811100	1.472219
H	3.242531	0.402036	2.811010
H	2.069824	-0.857027	3.316524
H	1.948699	0.824776	3.927677
O	2.995126	2.015061	0.380702
H	2.456791	1.441463	-0.267104
C	4.614343	2.490716	-1.095031
H	4.058569	1.927860	-0.031716
H	3.893610	2.621323	-1.897892
H	4.981692	3.416487	-0.653527
H	5.359444	1.705709	-1.258867
C	-0.985975	2.778643	-0.669360
C	-1.527971	4.125911	-0.745688

H	-0.785767	4.852722	-0.395356
H	-2.415061	4.165706	-0.101778
H	-1.811279	4.366555	-1.776827

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