

SUPPORTING INFORMATION

Spectroscopic Characterization of $\mu\text{-}\eta^1\text{:}\eta^1$ -Peroxo Ligands Formed by Reaction of Dioxygen with Electron-Rich Iridium Clusters

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Supplementary data

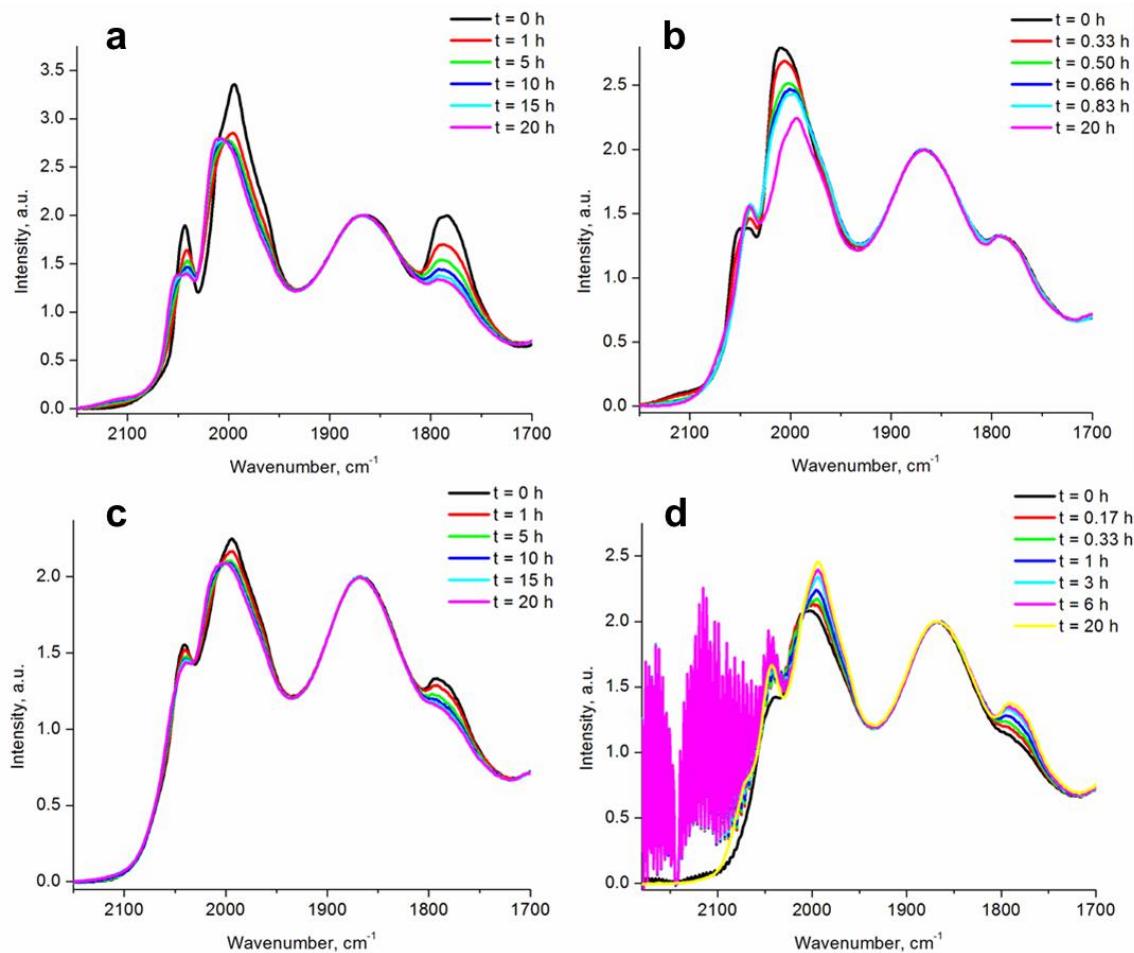
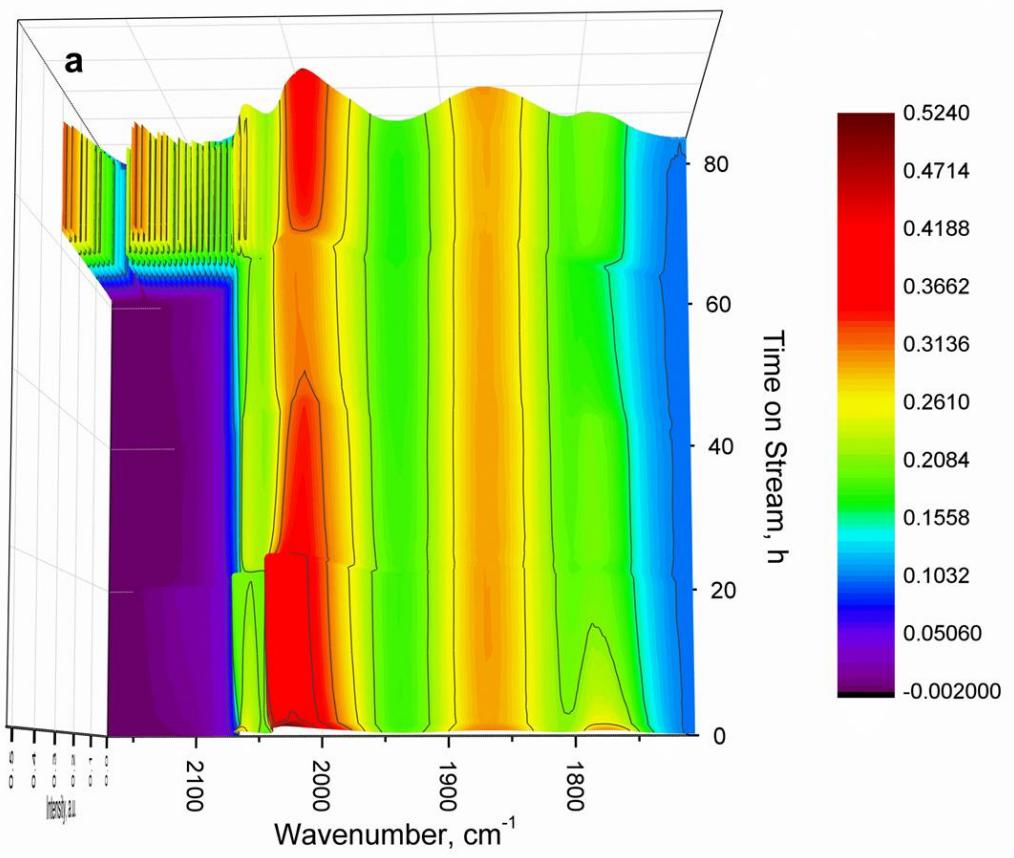
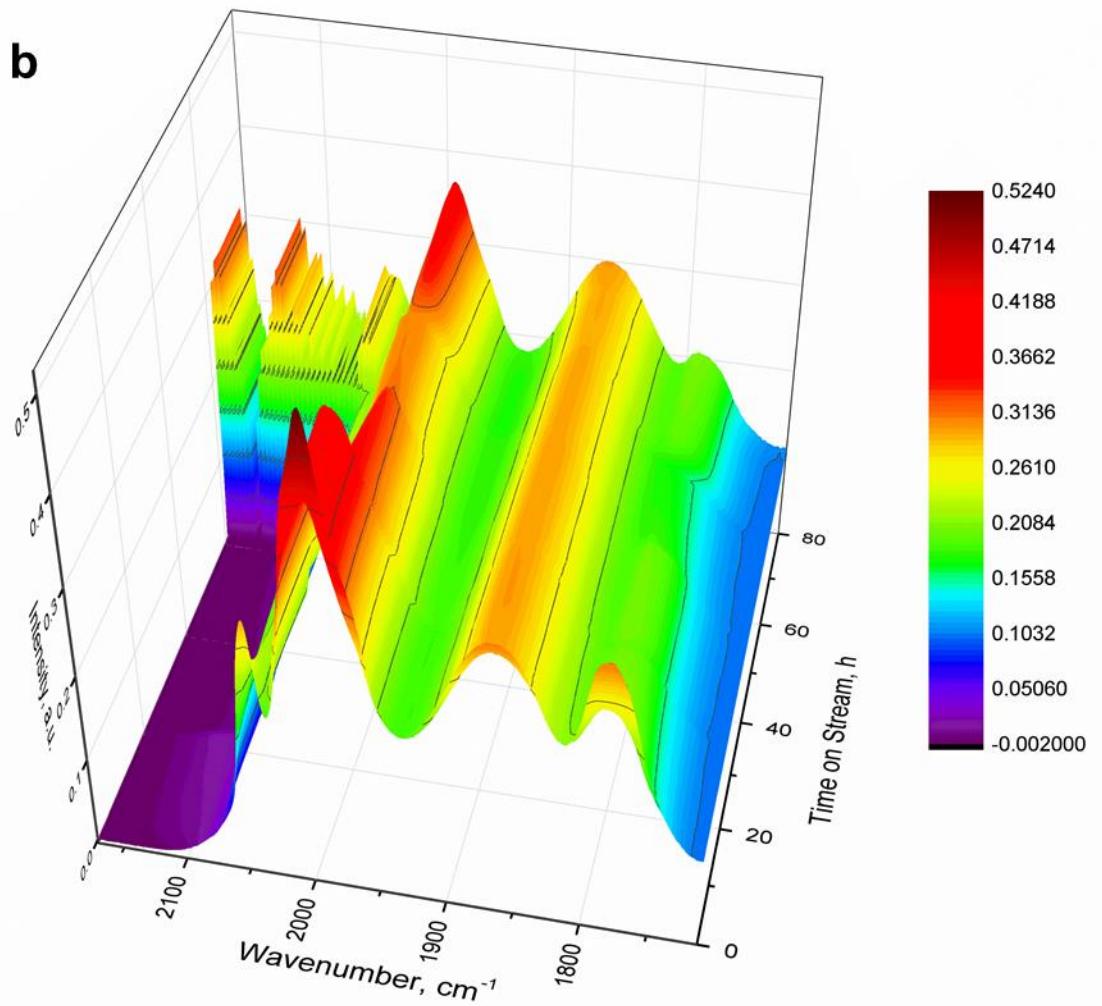


Figure S1. FTIR spectra in the ν_{CO} region characterizing the terminal and bridging CO starting with **2** and (a) during first H_2 treatment, (b) during subsequent O_2 treatment of sample resulting in (a), (c) during second H_2 treatment of sample resulting in (b), and (d) during recarbonylation by CO flow of sample resulting in (c). H_2 treatment: H_2 flowrate = 10 mL/min, He flowrate = 50 mL/min; O_2 treatment: 50 mL/min of 20% O_2 , He flowrate = 10 mL/min; CO treatment: CO flowrate = 20 mL/min; all treatments were done at 323 K and 1 bar.





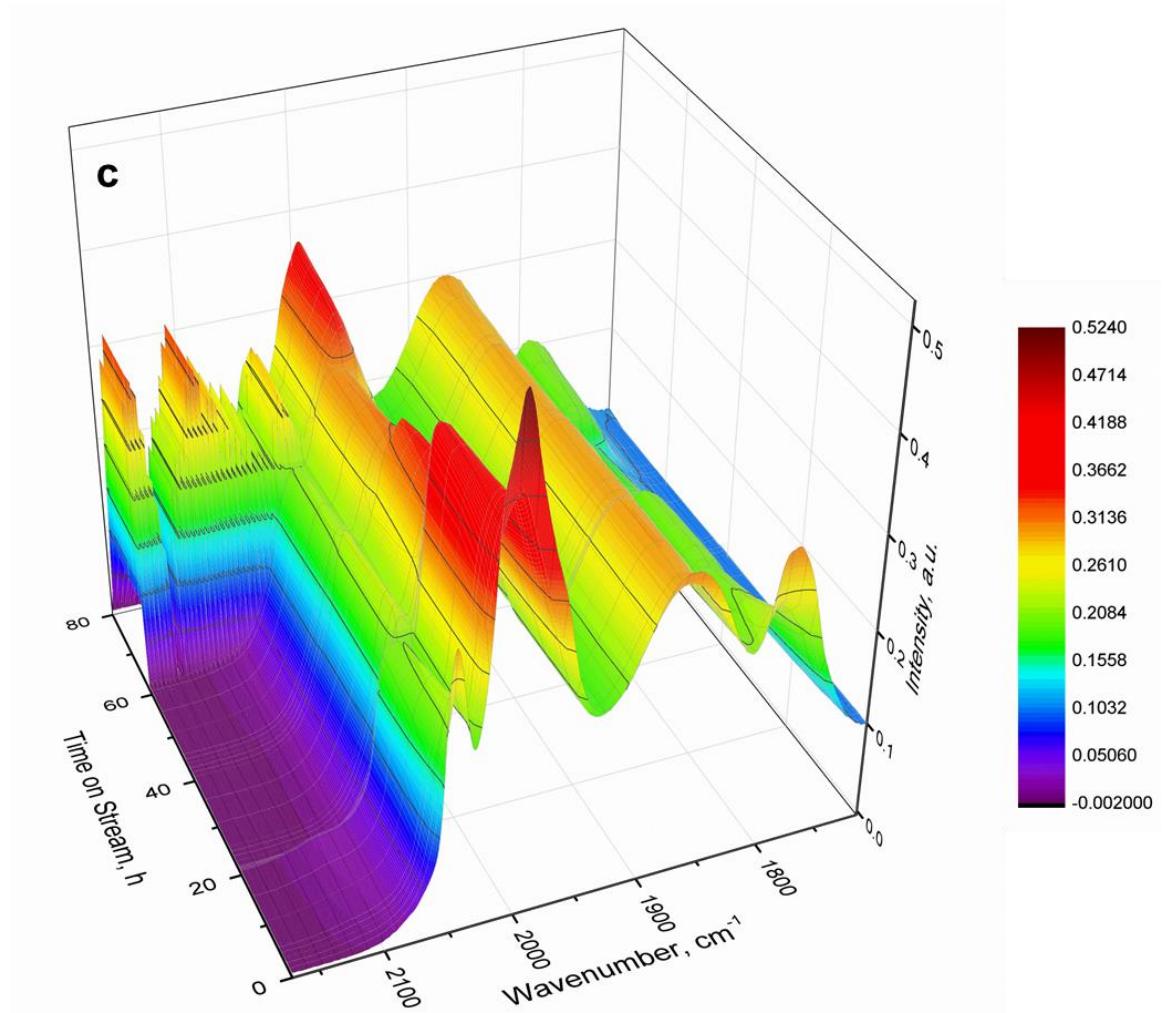


Figure S2. FTIR spectra of supported clusters in the ν_{CO} stretching region as a function of time on stream during the following treatments, starting with silica-supported cluster **2**: first H_2 treatment (0–20 h), dioxygen treatment (20–40 h), second H_2 treatment (40–60 h), and recarbonylation in flowing CO (60–80 h). The spectra are represented as a 3D mesh plots ((a) top view, (b) bridging carbonyl side view, and (c) terminal carbonyl side view) to show transitions between the four treatments stated above as a function of time on stream. Dark purple regions represent bands of low intensity, and red regions represent bands of high intensity. Data are supplementary to ease viewing of the hydride band formation and removal (a and c) at 2110 cm^{-1} from dark purple to light purple; blue shift ($t = \text{time on stream} = 0\text{--}20 \text{ h}$ and $t = 40\text{--}60 \text{ h}$) of terminal carbonyl band at 1994 cm^{-1} (a, b, and c), and decarbonylation and recarbonylation trends of terminal (2043 cm^{-1} and 1994 cm^{-1}) and bridging carbonyl bands (1776 cm^{-1}). Gas-flow treatment conditions are as follows: H_2 treatment: H_2 flowrate = 10 mL/min, He flowrate = 50 mL/min; O_2 treatment, 50 mL/min of 20% O_2 , He flowrate = 10 mL/min; CO treatment: CO flowrate = 20 mL/min; all treatments were performed at 323 K and 1 bar.

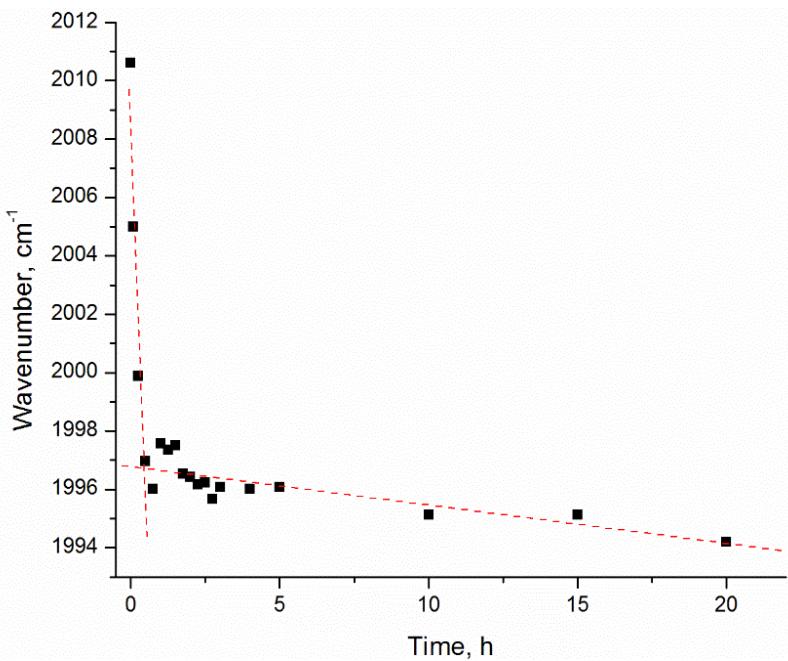


Figure S3. Red shift of terminal carbonyl band for SiO_2 -supported cluster $\text{Ir}_4\text{L}_3(\text{CO})_9$ **2** that had been previously treated with flowing H_2 for 20 h, during subsequent reaction with flowing O_2 (323 K, 1 bar, 50 mL/min of 20% O_2 , 10 mL/min of He).

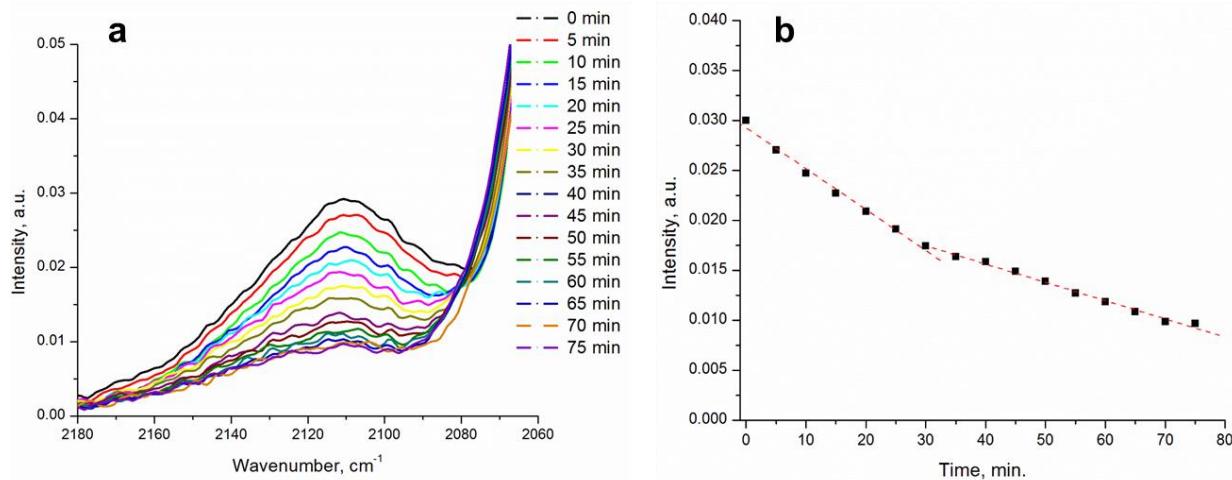


Figure S4. (a) FTIR spectrum showing a decrease in hydride band intensity at 2110 cm^{-1} and (b) hydride band intensity as a function of time on stream for SiO_2 -supported $\text{Ir}_4\text{L}_3(\text{CO})_9$ cluster **2** that had been previously treated in flowing H_2 for 20 h, during treatment in flowing O_2 (323 K, 1 bar, 50 mL/min of 20% O_2 , 10 mL/min of He). Terminally bonded M-H stretching absorptions occur in the region of $1900 \pm 300 \text{ cm}^{-1}$. For hydridometal complexes with hydrogen in a position bridging two metals, the M-H bond is shifted to lower frequencies, around $1100 \pm 300 \text{ cm}^{-1}$, and the band is considerably broadened, with a peak full width at half maximum of approximately 100 cm^{-1} .¹ Thus, both the frequency and the narrowness of our M-H stretching band in Figure S4A correspond to a terminally bonded M-H bond—not bridging.

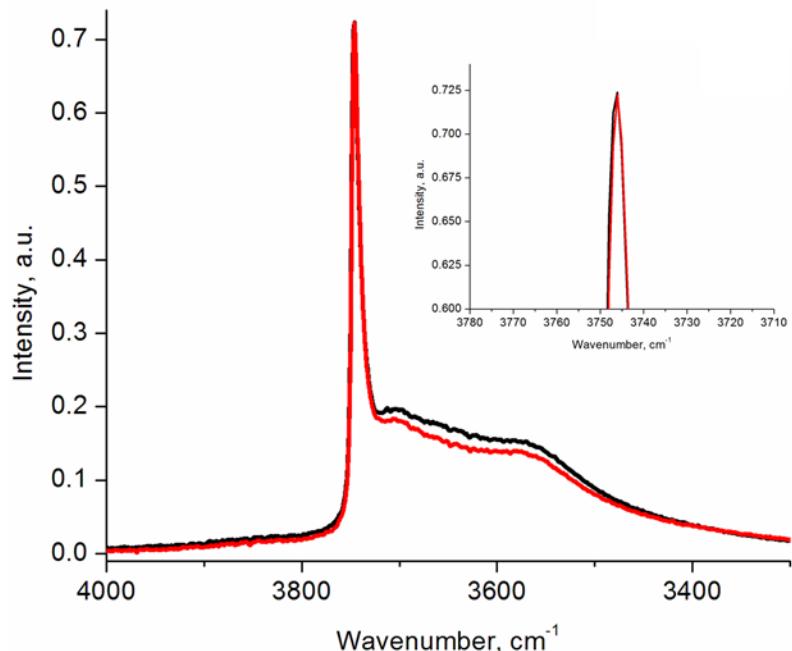


Figure S5. FTIR spectra characterizing silanols in the v_{OH} region for silica-supported $\text{Ir}_4\text{L}_3(\text{CO})_9$ **2** after its treatment with H_2 for 20 h (H_2 flowrate = 10 mL/min; He flowrate = 50 mL/min) (black) and subsequent 20 h of treatment in flowing O_2 (50 mL/min of 20% O_2 , 10 mL/min of He) (red) under flow at 323 K and 1 bar.

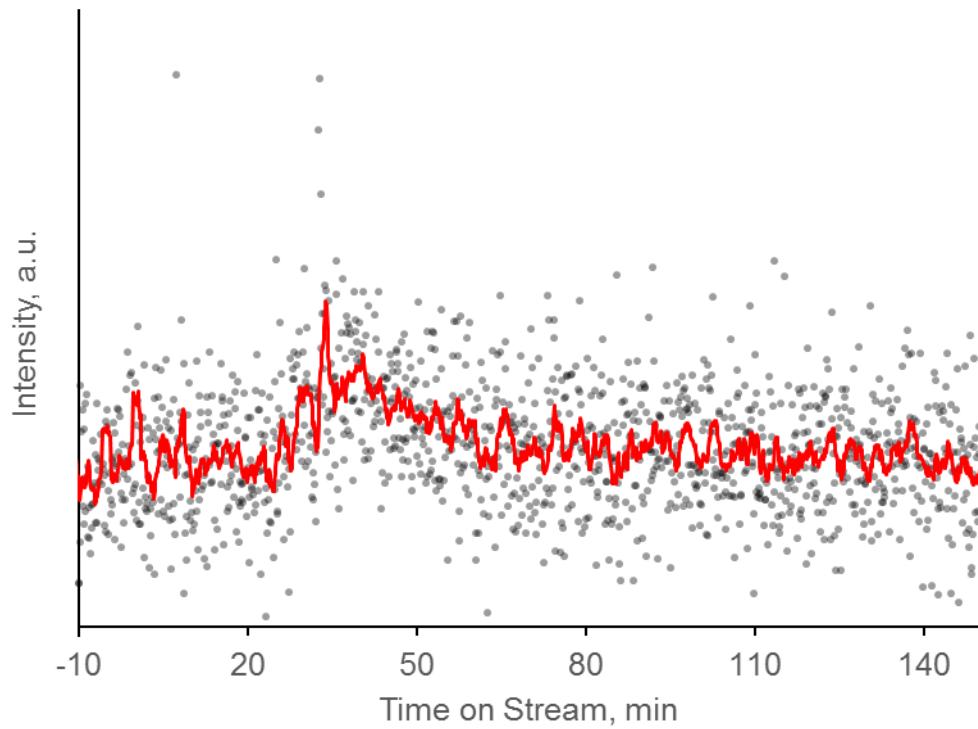


Figure S6. Signal of mass to charge ratio of 44 for silica-supported $\text{Ir}_4\text{L}_3(\text{CO})_9$ **2** after 20 h of H_2 treatment characterizing CO_2 during treatment in flowing O_2 at 323 K, 1 bar, 50 mL/min of O_2 (20% O_2 balance He) and 10 mL/min of He. Red line represents a moving average for the CO_2 signal.

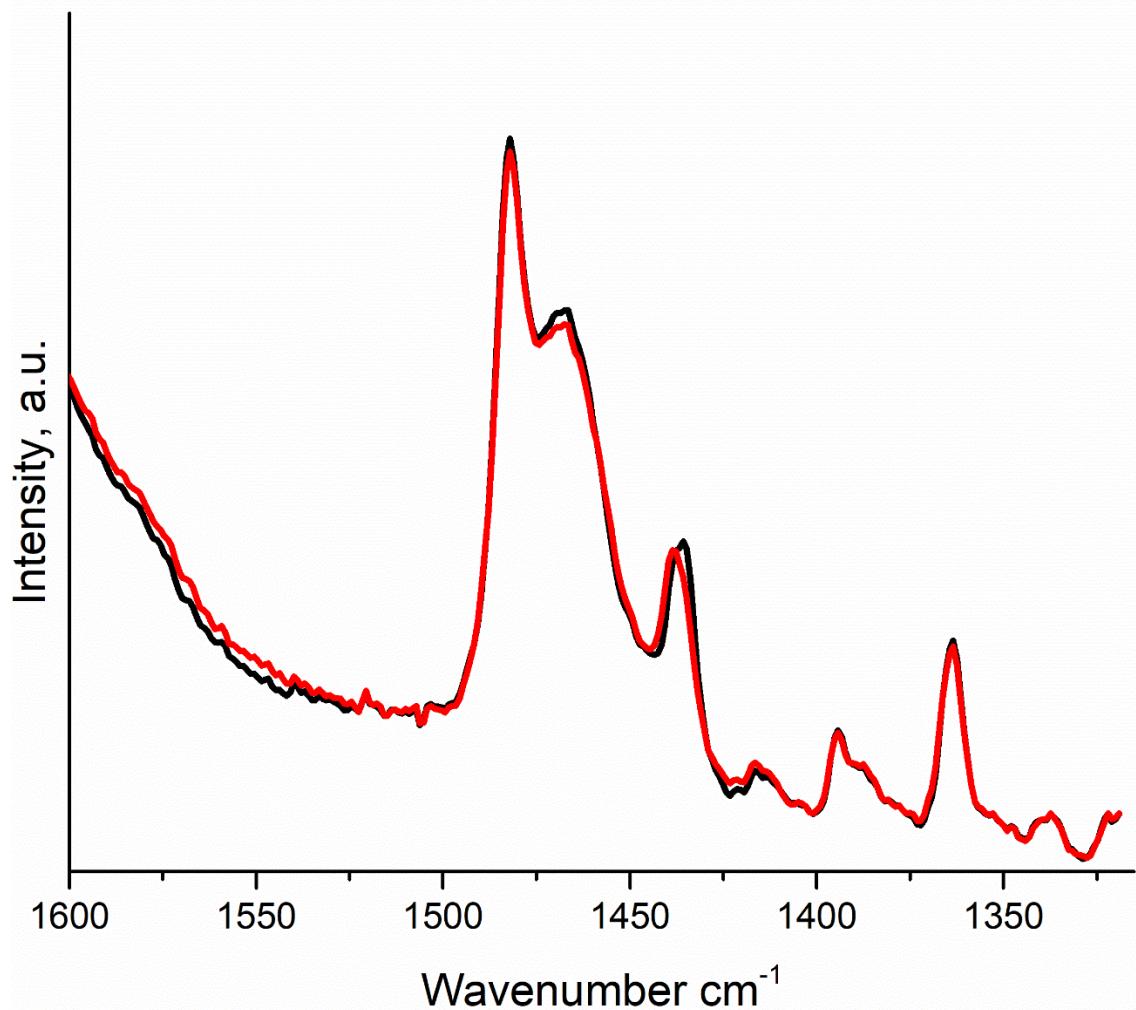


Figure S7. FTIR spectra of **2** (tetrairidium cluster supported on silica) after treatment in flowing gases. Sample **2** following 20 h of flowing H₂ (black) and after an additional 20 h in O₂ (red) at 323 K. A comparison of the spectra show a lack of bands growing in at 1584 cm⁻¹ and 1485 cm⁻¹ upon reaction with O₂, which would have otherwise been indicative of bound carbonate ligands.

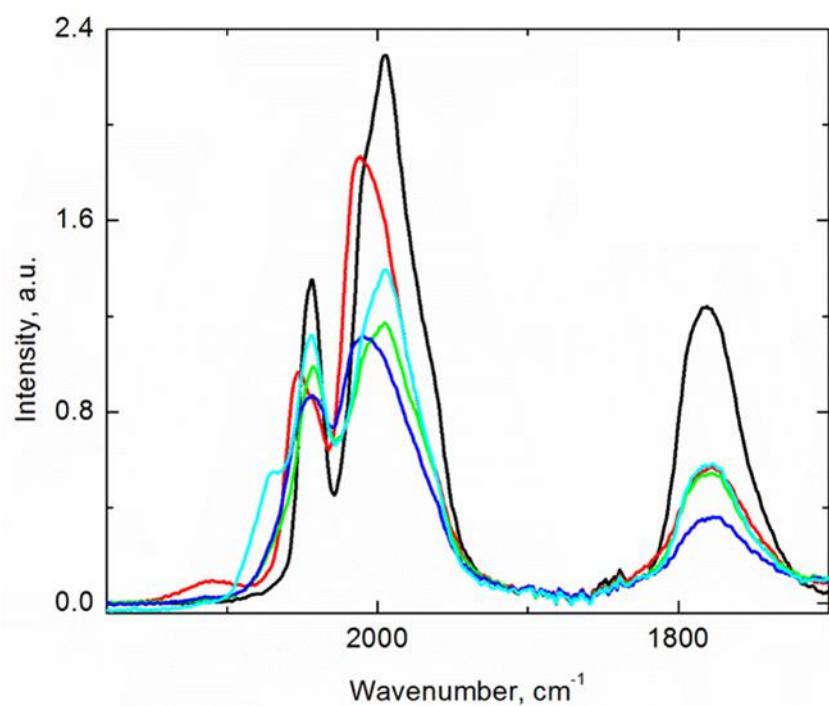


Figure S8. Difference FTIR spectra in the ν_{CO} region of silica-supported $\text{Ir}_4\text{L}_3(\text{CO})_9$ clusters whereby the SiO_2 features have been subtracted out for **2** prior to any treatment (black), during 20 h of treatment of **2** in flowing H_2 (red), followed by 20 h of O_2 treatment (green), then second H_2 treatment (dark blue), and finally recarbonylation by CO (light blue). All treatments were done with flowing gases at 323 K and 1 bar.

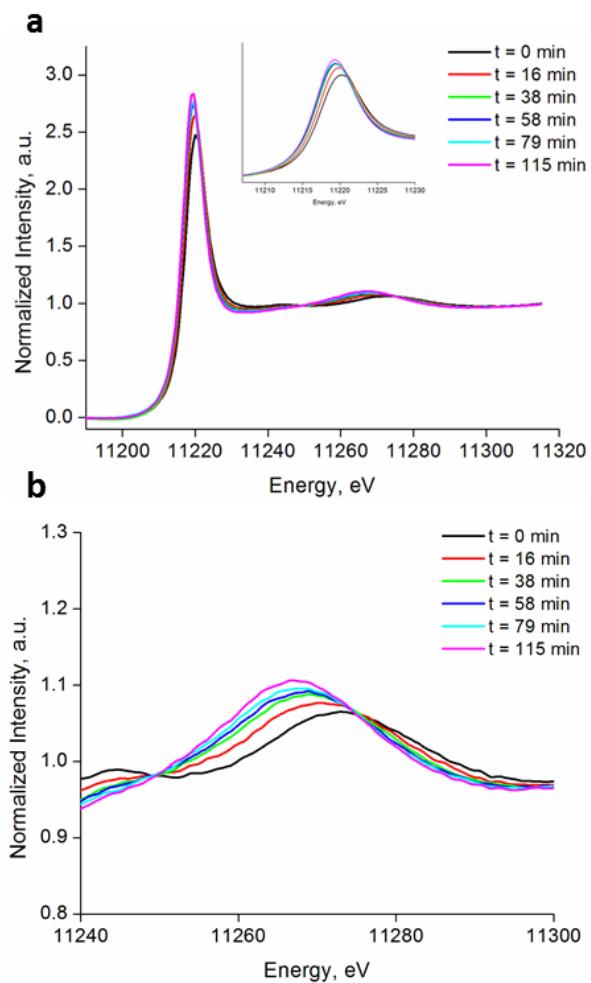


Figure S9 a) Ir L_{III} edge XAS in the (a) XANES region characterizing cluster **2** after 20 h of H₂ flow during O₂ treatment at 323 K, 1 bar, 50 mL/min of O₂ (20% of O₂ balance He) and 10 mL/min of He and (b) isosbestic points in the EXAFS region during O₂ flow for cluster **2** that had been allowed to react for 20 h in flowing H₂ (H₂ flowrate = 10 mL/min and He flowrate = 50 mL/min).

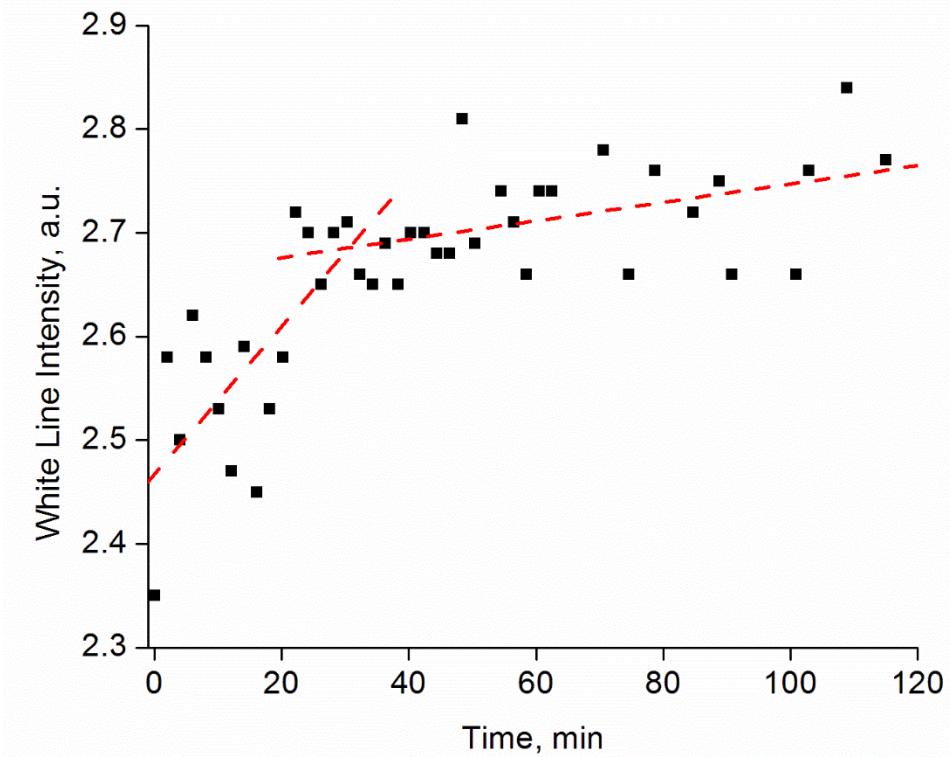
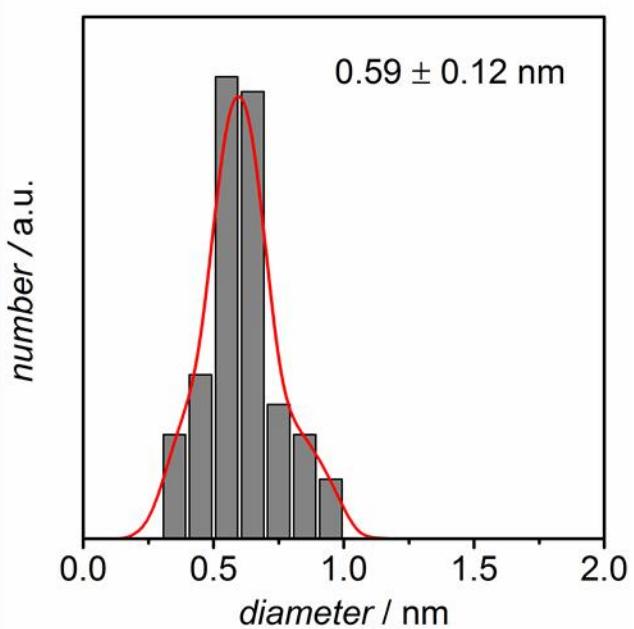
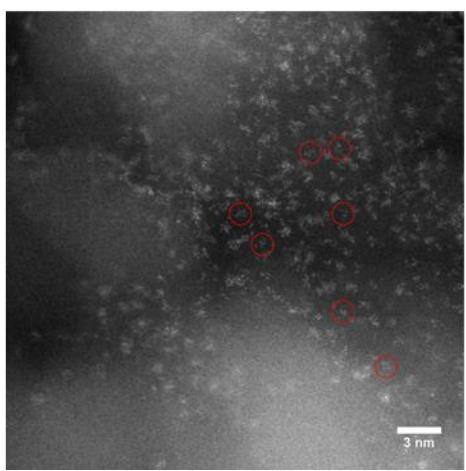
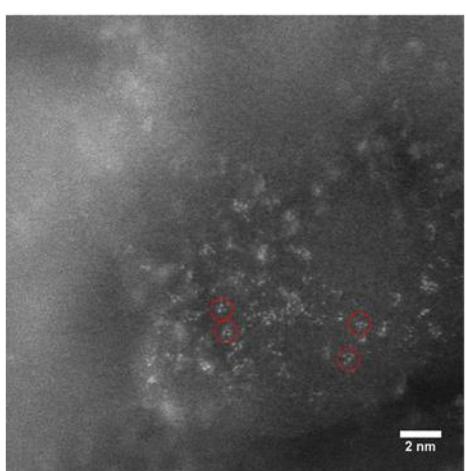
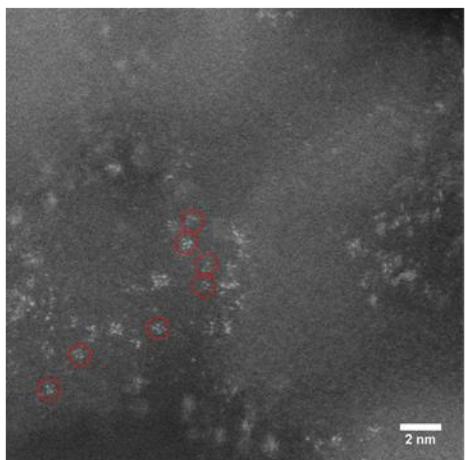


Figure S10. Increase in the whiteline intensity at the Ir L_{III} edge as a function of time on stream during O₂ treatment at 323 K, 1 bar, 50 mL/min of O₂ (20% of O₂ balance He) and 10 mL/min of He for supported Ir₄L₃(CO)₉ cluster **2** that had reacted for 20 h in flowing H₂ (H₂ flowrate = 10 mL/min and He flowrate = 50 mL/min).

a

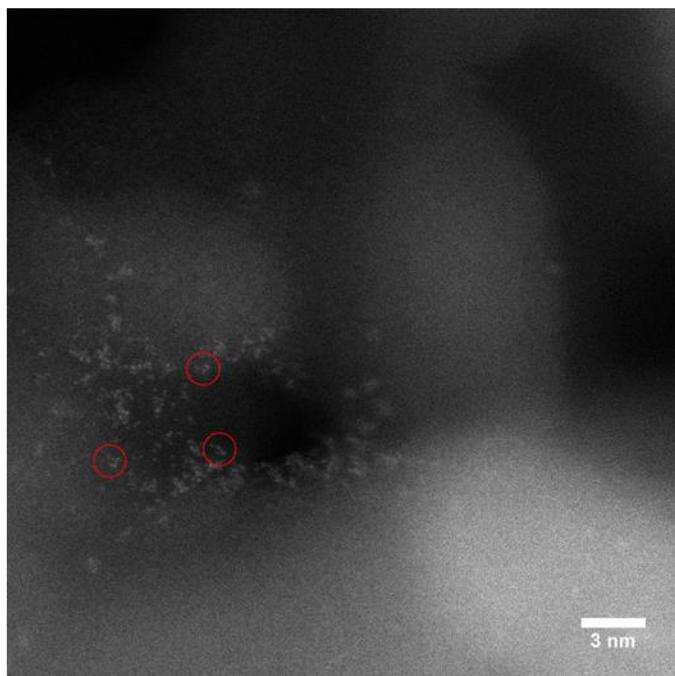
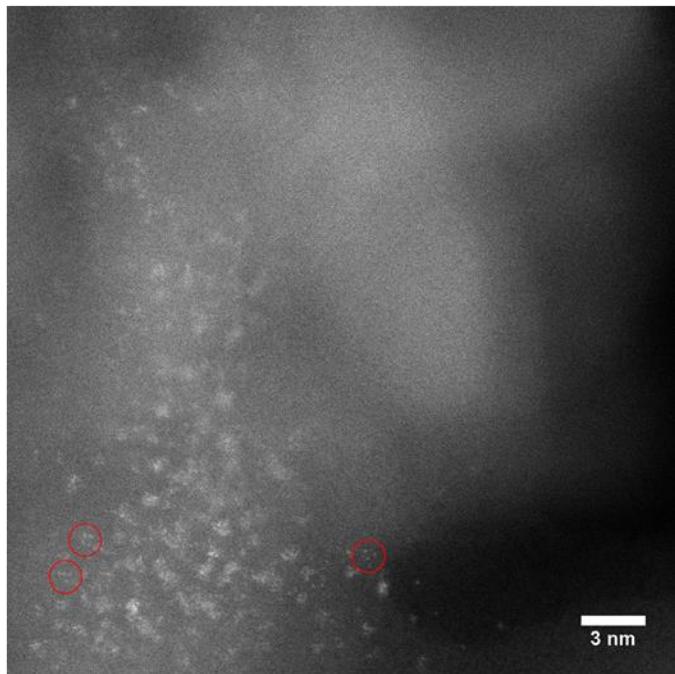
b

Figure S11. HAADF-STEM images and histograms characterizing silica-supported Ir_4 tetrahedral clusters (circled in red) (a) **2** after 20 h of H_2 treatment and (b) sample in (a) after 20 h of dioxygen treatment. The histogram for (b) is found in the main text. All treatments were done at 323 K and 1 bar.

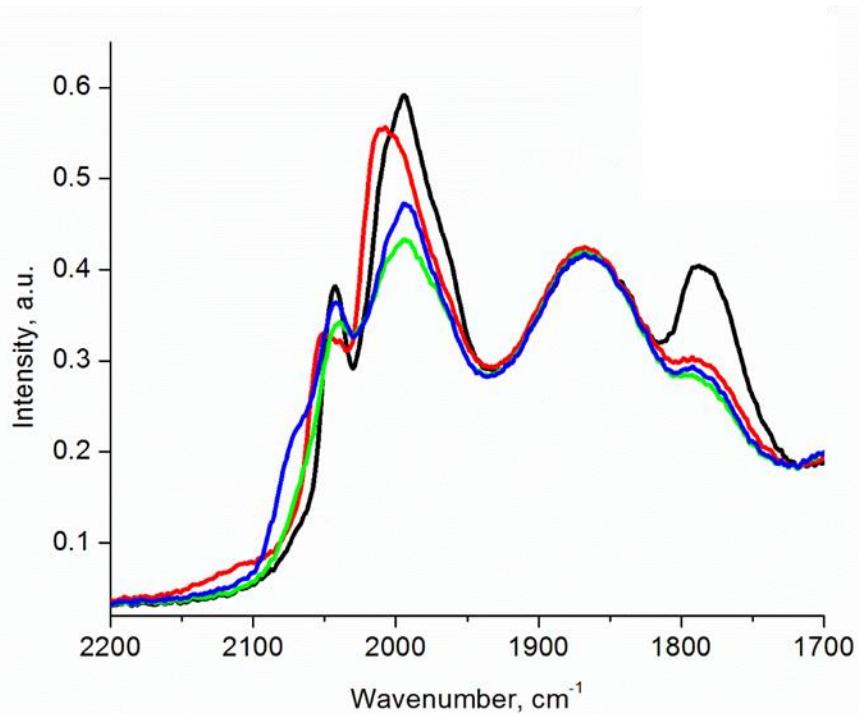


Figure S12. FTIR spectra in ν_{CO} stretching region for silica-supported $\text{Ir}_4\text{L}_3(\text{CO})_9$ **2** (black) during sequential H_2 treatment for 20 h (red), 20 h of treatment in flowing O_2 (green), and CO treatment (blue) at 323 K and 1 bar.

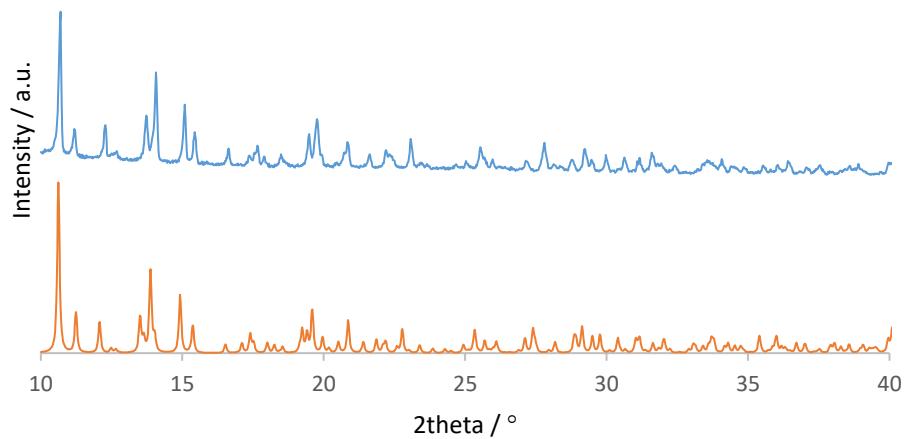


Figure S13. Observed (top) and simulated (bottom) powder X-ray diffraction pattern of **C2**. Simulated powder pattern was calculated using single crystal X-Ray diffraction data.²

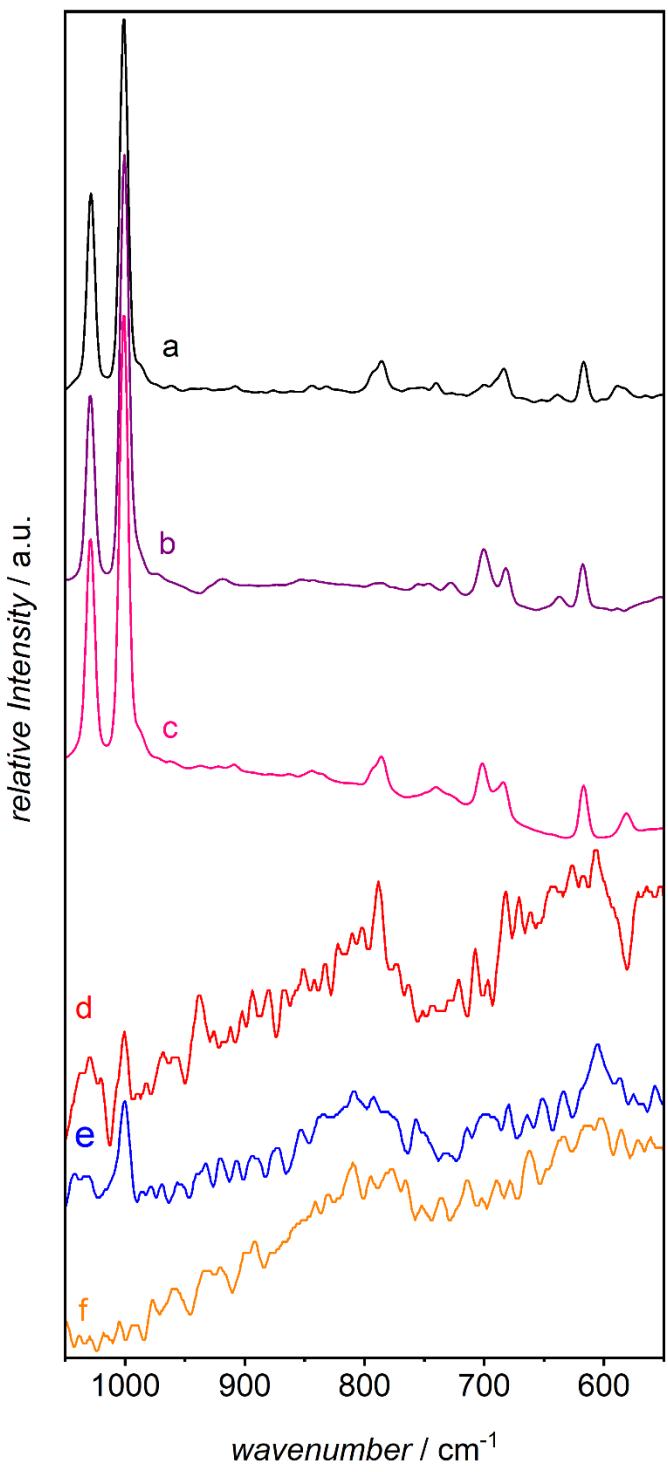


Figure S14: FT-Raman spectra of (a) **C2** (after treatment of **C1** with $^{16}\text{O}_2$), (b) **C1**, (c) cluster resulting from treatment of **C1** with $^{18}\text{O}_2$, (d) **2** (tetrairidium cluster supported on silica) after 20 h of exposure to H₂ and 20 h of exposure to $^{16}\text{O}_2$ at 323 K in a flow reactor, (e) **2**, (f) silica in a quartz tube as a control. Inset: zoomed-in region defining ^{16}O - ^{16}O and ^{18}O - ^{18}O stretches of bound bridging peroxy ligands.

The broad absorption in the baseline between 900 cm^{-1} and 750 cm^{-1} can be assigned to the quartz tube, used as a sample holder and the silica used as a support material (Figure S14). We note that the $^{18}\text{O}_2$ -treated **C1** was measured in a quartz tube, in contrast to the $^{16}\text{O}_2$ -treated **C1** which was measured in a simple sample holder exposed to the atmosphere, accounting for some spectral differences when comparing $^{16}\text{O}_2$ -treated **C1** (i.e., cluster **C2**) and Cowie $^{18}\text{O}_2$ -treated **C1**.

Providing evidence of the effect of oxygen isotopic labelling, a broad Raman band centered at 756 cm^{-1} characterizing **C2** is evident in Figure 4b, and it is absent from the spectrum of **C3** in Figure 4c. This frequency is consistent with reported $^{16}\text{O}-^{16}\text{O}$ stretches in peroxy bands.³⁻⁷ The spectrum of **C3** in Figure 4c includes a shoulder at 729 cm^{-1} and evidence of a strong intensity gain at 701 cm^{-1} —in contrast to the results characterizing **C2**. We infer that the changes are a consequence of ^{18}O -labeling, resulting in a mean frequency red shift of 41 cm^{-1} from the 756 cm^{-1} band, and this shift coincides with DFT-calculated shifts based on a harmonic model with various functionals (Table S2, SI). We thus assign the 756 cm^{-1} band to bridging peroxy O–O stretching vibrations in **C2**. The manifestation of the ^{18}O -shifted band from a single band at 756 cm^{-1} in the spectrum of **C2** to two normal vibrations in that of **C3** implies that this O–O mode contributes to the potential energy distribution of two different normal modes.

To support the assignments above, we turned to electronic-structure calculations of **C2** and **C3** at the BP86 level. These Raman calculations (Table S3) show that the intense bands near 1000 cm^{-1} in Figure S14a are due to deformations of the phenyl rings. There are also weakly to moderately intense Raman deformations of the phenyl rings in the region of 710 to 660 cm^{-1} . The O–O stretch can lead to changes in these intensities as well as there are a large number of modes in these regions due to the number of phenyl rings. The O–O stretch for the ^{18}O labelled **C3** is predicted to be at 731 cm^{-1} . Again, this can couple with all of the modes in this region leading to changes in the Raman intensities.

Our assignment of a bridging peroxy species in **C2** with a Raman band at 756 cm^{-1} is supported by reported frequencies of such bands, which are lower than those of comparable mononuclear complexes,³⁻⁶ and our observed frequency is in the range observed for O–O vibrations assigned to bridging peroxy ligands, as reported for a number of compounds;^{3,8-10} examples are complexes of iron, copper, cobalt, and nickel (and platinum dimers). The bands are more than 80 cm^{-1} lower in frequency than that of an η^2 peroxy O–O stretch (expected to occur at about 840 cm^{-1} —and 885 cm^{-1} for atomic Ir).¹¹⁻¹⁶ Moreover, this range is red-shifted by more than 300 cm^{-1} relative to expectations for an O–O moiety with superoxide electronic structure (1100 cm^{-1}).¹⁷ Many of the reported mononuclear iridium and rhodium complexes incorporating peroxy ligands incorporate η^2 -peroxy ligands, but a dimeric iridium complex with a $\mu^1-\eta^1:\eta^1$ peroxy ligand is specific to the work of Cowie (Figure 1),² whereas other dinuclear iridium species have been reported with a μ -oxo bridge between the two Ir atoms.¹⁸⁻¹⁹

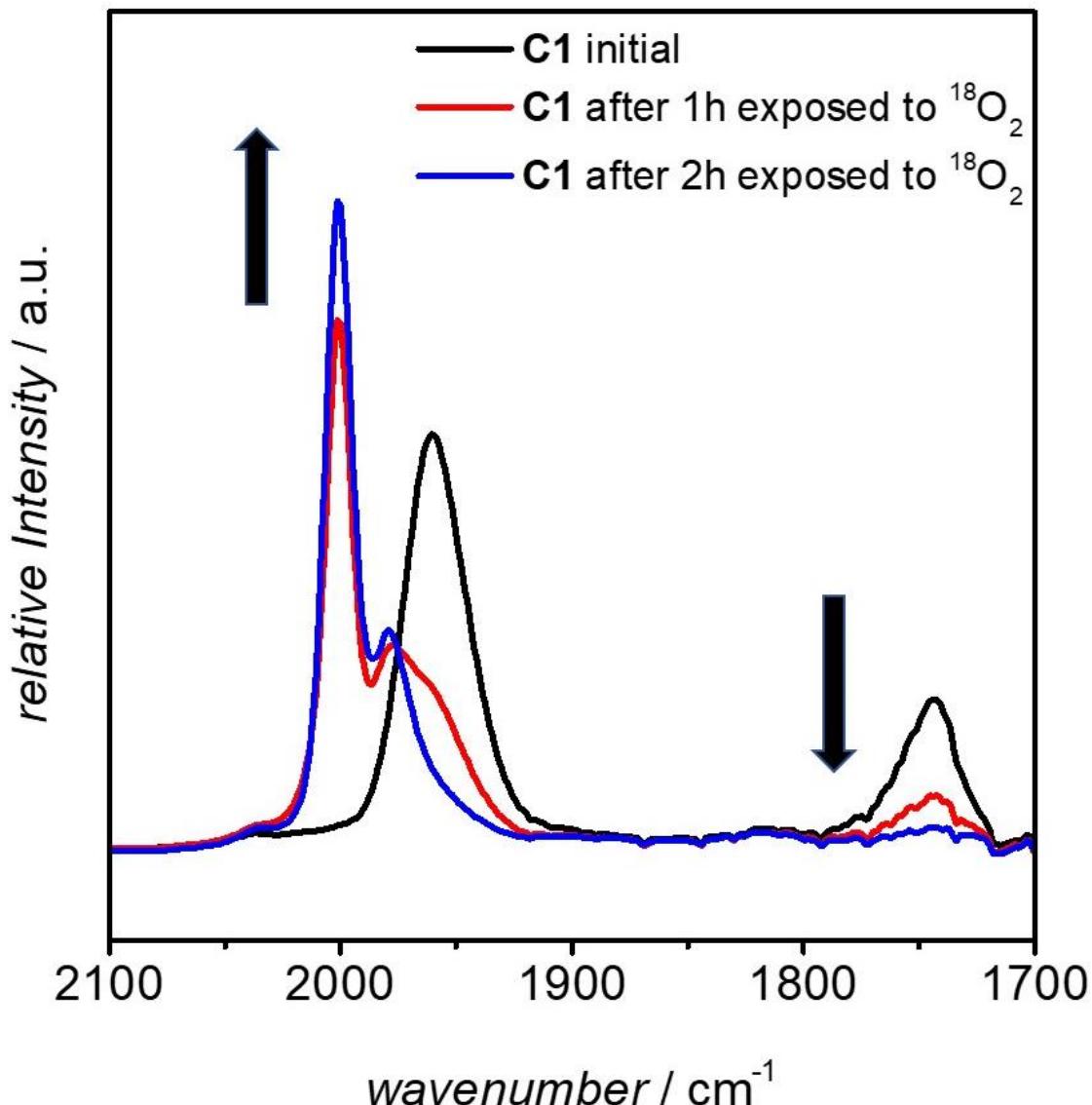


Figure S15. FTIR spectra of samples in dichloromethane solvent, which were used to monitor the progress of reaction of **C1** with ¹⁸O₂, to synthesize a pure compound consisting of ¹⁸O-labeled **C2**. During the 2-h reaction time used in our experimental procedure, more than 95% of the starting **C1** was converted to **C2**, as indicated by the disappearance of bridging CO bands at 1742 cm⁻¹ and the appearance of terminal CO bands at 2005 cm⁻¹. These correspond to bands previously reported for **C1** and **C2**.²

Comparison of the extended Raman spectrum region of diiridium clusters **C1**, **C2**, and **C3**:

Figure S16 below shows Raman spectra for **C1**, and its ¹⁶O₂ and ¹⁸O₂-treated derivatives **C2** and **C3**, respectively. Spectra corresponding to **C2** and **C3** show characteristic bands at 581 cm⁻¹ and 378 cm⁻¹, both of which are absent in the oxygen-free cluster **C1**. These differences are in addition to the presence of the 788 cm⁻¹ for **C2** and **C3** relative to **C1**, which is discussed in the text. In addition, a band at 253 cm⁻¹ occurs in the Raman spectrum of **C3** but is absent in spectra for

clusters **C1** and **C2**. The data above support that **C1**, **C2**, and **C3** are all distinct and separate chemical compounds, and are inconsistent with partial degradation of one of these compounds (i.e. **C3**) into another (i.e. **C1**) during the FT-Raman experiment. Such a conclusion is further reinforced with lack of absorbance of **C3** in the near-infrared region corresponding to the wavelength of the Raman laser in Figure S17.

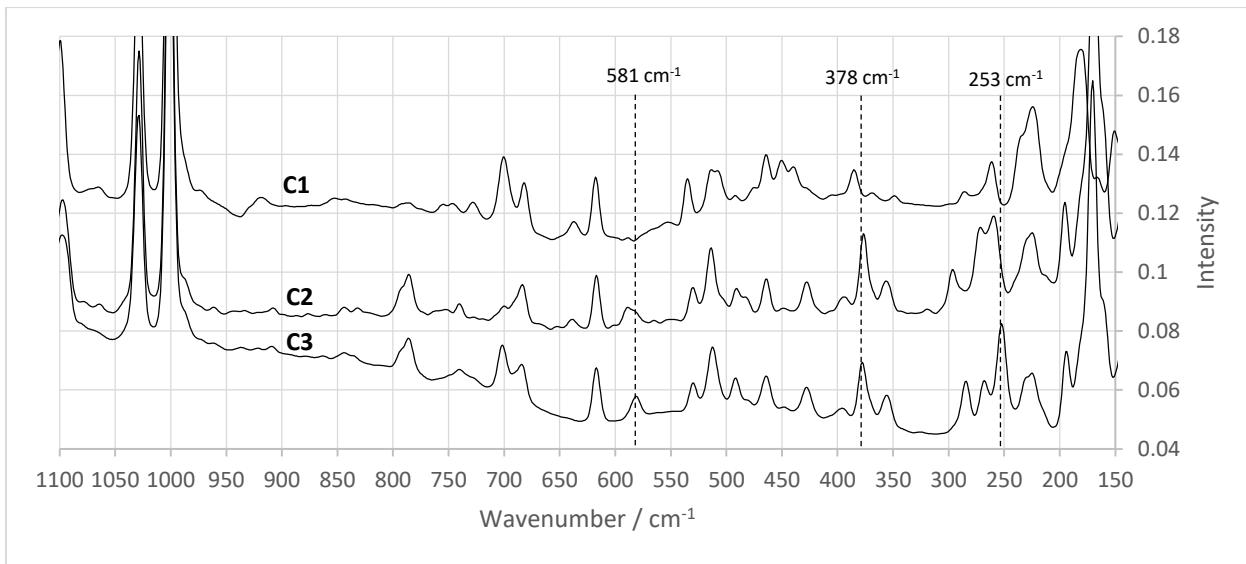


Figure S16. Solid-state FT-Raman spectra of **C1** (top spectrum), **C2** (middle spectrum), and **C3** (bottom spectrum) plotted in an extended wavelength range.

Near-infrared spectroscopy of cluster compound **C3**:

A near-infrared spectrum of cluster compound **C3** dissolved in dichloromethane solvent was recorded, and is shown in Figure S17. The observed absence of absorbance in the wavelength region around 1064 nm is consistent with the compound not absorbing laser radiation during the course of FT-Raman experiments, since the wavelength of the FT-Raman laser is 1064 nm.

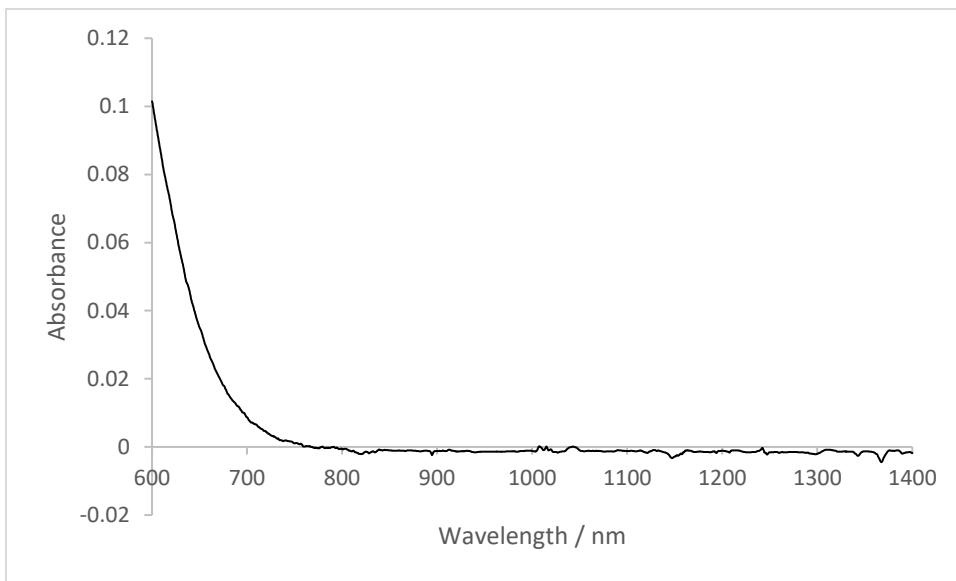


Figure S17. Near-IR spectrum of cluster compound **C3** dissolved in dichloromethane.

Experimental methods:

C1 was prepared according to a literature procedure.²⁰

C2 (with $^{16}\text{O}_2$) was prepared by a modified literature procedure;² 50 mg of **C1** was dissolved in 20 mL of dichloromethane and stirred at room temperature in air until all the solvent had evaporated (approximately 24 h).

Synthesis of C3 (C2 with $^{18}\text{O}_2$): **C1** (20 mg) was dissolved in 5 mL of dichloromethane under an Ar atmosphere. The headspace atmosphere was replaced twice with $^{18}\text{O}_2$, and the solution stirred for 2 h at room temperature. The solvent was removed by evacuation, and the product was stored under Ar. The reaction was monitored by IR spectroscopy, and results shown in Figure S14 demonstrate > 95% conversion of **C1** to **C2** during this procedure, based on the observed disappearance of the band at 1742 cm^{-1} and growth of the band at 2005 cm^{-1} , corresponding to bands reported for these compounds.^{2,20}

DFT Calculations

The calculations representing the tetrairidium cluster with two O_2 moieties (Table S1) show that there is some variation in the O-O bond distances as a function of the presence of vacancies and H or C_2H_5 moieties in the apical or radial positions of the Ir_4 clusters as well as the type of substituents on the P. The O-O distances do not show any real trends except that they tend to be longer for the structures with two vacancy sites. At the same computational level, an O_2^- diatomic anion is predicted to have a bond distance of 1.349 \AA and a frequency of 1229 cm^{-1} . The calculated bond distances are consistent with an O_2^- , but the frequencies are significantly lower. Thus the actual O_2 stretches are subtly influenced by their local environment and the amount of charge transfer between the iridium atoms and the oxygen atoms. The calculated CO stretching frequencies fall into two groups. The bridging CO stretches are significantly lower than the terminal CO stretches. The terminal CO stretches have a predicted range of about 100 cm^{-1} and are not strongly dependent on the substituents on the P or on the presence of vacancies. The bridging CO stretches are predicted to have a larger dependence on the presence of vacancies as well as the substituents on P with the $\text{P}(\text{CH}_3)(\text{C}_6\text{H}_5)_2$ having a broader range of values. In addition, the structures with a C_2H_5 and H present exhibit the strongest dependence on the substituents on P. The ^{18}O O_2 vibrational stretching frequencies show the expected harmonic red-shifts, further confirming the experimental assignment.

In order to better understand the role of charge transfer and computational method on the O_2 geometry and stretching frequencies in the tetrairidium cluster, additional calculations characterizing molecule **C2** with a known structure were done with the B3LYP,^{21,22} BP86,^{23,24} SVWN5,^{25,26} and CAM-B3LYP²⁷ functionals in addition to $\omega\text{B97X-D}$. The values in Table S2 show that there is significant dependence of the O-O stretch and the corresponding O-O bond distance on the functional. The functionals $\omega\text{B97X-D}$ and CAM-B3LYP have the largest O-O stretching frequencies and $\omega\text{B97X-D}$ has the shortest O-O bond distance. However, the local SVWN5 functional predicts an O-O bond distance that is essentially the same as that from CAM-B3LYP,

yet the SVWN5 O-O stretch is almost 100 cm^{-1} lower. The B3LYP functional predicts an O-O bond distance that is almost 0.02 Å longer than the SVWN5 value. Yet the SVWN5 O-O stretch is predicted to be at a lower frequency than the B3LYP value by $\sim 15\text{ cm}^{-1}$. The longest O-O bond distance is predicted at the BP86 level, and this corresponds to a stretching frequency of 784 cm^{-1} , consistent with the assigned band at 756 cm^{-1} in **C2**, considering the fact that the calculated values are harmonic frequencies and the experimental values, of course, include anharmonic terms.. The results show that the O₂ stretch is subtly influenced by the O-O bond distance and the interaction of the O₂ group with the Ir atoms. The corresponding ¹⁸O frequencies for the O₂ stretch for **C2** are given below. The calculated frequencies are harmonic values and do not include the effect of anharmonicity.

Table S1. Calculated O-O and C-O stretching frequencies for tetrairidium complexes (ν in cm^{-1} and IR intensity in parentheses in km/mol with ^{18}O shifts after the slash) and O-O bond distances ($R(\text{O-O})$ in \AA) at the $\omega\text{B97x-D/cc-pVDZ-PP}$ level. 1st ligand is apical and 2nd ligand is radial.

Ligands	$\nu(\text{CO})$ terminal	$\nu(\text{CO})$ bridging	$\nu(\text{O}_2)$	$R(\text{O}_2)$
$X_{\text{eq}} = \text{P}(\text{CH}_3)(\text{C}_6\text{H}_5)_2$				
C ₂ H ₅ ,v	2038(758) 2097(528) 2115(1763) 2126(225)	1738(939)	1080(366)/1021 1146(26)/1083	1.338 1.343
C ₂ H ₅ ,H	2055(336) 2082(527) 2102(1598) 2120(723) Ave 2090	1662(143)	993(73)/939 1063(56)/993	1.353 1.386
v,v	2057(791) 2092(524) 2116(1608) 2134(577)	1814(527)	984(193)/926 1074(86)/1012	1.353 1.385
CO,H	2057(704) 2074(460) 2095(648) 2113(983) 2140(477)	1888(353)	1013(133)/960 1074(9)/1012	1.354 1.368
$X_{\text{eq}} = \text{P}(\text{CH}_3)_3$				
C ₂ H ₅ ,v	2025(998) 2066(705) 2104(2149) 2116(72)	1747(501)	929(305)/863 1118(97)/1060	1.335 1.363

C ₂ H ₅ ,H	2030(1081) 2066(457) 2099(1805) 2113(646)	1808(540)	1039(405)/959 1118(6)/1063	1.343 1.353
v,v	2041(875) 2086(422) 2108(2050) 2125(630)	1776(468)	980(67)/927 1075(102)/1017	1.353 1.388
CO,H	2048(721) 2080(705) 2089(364) 2109(2027) 2130(584)	1773(489)	1201(53)/1133 1220(69)/1150	1.320 1.322

Table S2. Calculated O-O and C-O stretching frequencies for **C2** (ν in cm^{-1} and IR intensity in parentheses in km/mol) and relevant geometry parameters (bond distances in \AA and angles in degrees) with the cc-pVDZ-PP basis set and different DFT exchange-correlation functionals.

Value	Expt.	$\omega\text{B97X-D}$	B3LYP	BP86	SVWN5	CAM-B3LYP
$\nu(\text{CO})$	1979	2064(221)	2011(231)	1936(183)	1988(132)	2061(243)
	2005	2098(929)	2043(870)	1964(719)	2016(709)	2096(929)
$\nu(^{16}\text{O}_2)$		964(3)	866(4)	784(15)	849(9)	940(3)
$\nu(^{18}\text{O}_2)^*$		907(3)*	816(7)*	740(6)*	800(5)*	887(2)*
$\nu(\text{Ir-O})$		612(20)	505(6)	579(14)	599(15)	610(18)
		680(75)	661(57)	641(45)	662(31)	679(62)
R(O-O)	1.58(2)	1.446	1.475	1.493	1.456	1.458
R(Ir-Ir)	2.705	2.724	2.764	2.754	2.677	2.727
R(Ir-P)	2.377	2.384	2.408	2.393	2.337	2.385
R(Ir-O)	2.04	2.042	2.047	2.051	2.024	2.036
R(Ir-I)	2.83	2.807	2.871	2.852	2.758	2.819
Ir-Ir-O	71.7	71.1	70.9	71.3	71.6	71.1
Ir-O-O	102.0	107.2	107.4	106.9	106.5	107.0
O-Ir-Ir-O	-20.7	-10.4	-10.2	-10.5	-11.0	-11.0
Ir-O-O-Ir	-34.6	-19.5	-19.0	-19.3	-20.2	-20.5

*Indicates results of calculations for **C3**.

Table S3. Frequencies (cm⁻¹), IR Intensities (KM/mole) and Raman Activities (Å⁴/amu)

C1						C2						C3		
wB97xD			BP86			wB97xD			BP86			BP86		
Freq	IR	Raman	Freq	Intens	Raman	Freq	Intens	Raman	Freq	Intens	Raman	Freq	Int	Raman
14.1	0.3	0.7	11.7	0.1	0.1	11.6	0.0	0.3	11.4	0.0	0.3	11.4	0.0	0.3
21.0	0.5	0.4	19.3	0.2	0.3	21.8	0.1	0.2	18.3	0.1	0.3	18.3	0.1	0.3
25.4	0.2	0.2	22.2	0.2	0.5	25.1	0.8	0.1	22.5	0.8	0.3	22.5	0.8	0.3
27.9	0.1	1.8	27.1	0.6	0.5	34.0	0.3	1.4	28.7	0.1	2.2	28.7	0.1	2.2
34.2	0.6	0.5	31.2	0.5	0.6	34.5	0.2	2.3	33.3	0.0	1.3	33.3	0.0	1.3
37.8	0.1	5.4	33.0	0.0	3.0	38.9	0.4	3.5	34.7	0.1	2.4	34.7	0.1	2.4
38.4	0.2	3.1	34.1	0.1	3.3	42.0	0.1	4.2	36.5	0.3	0.7	36.5	0.3	0.7
41.2	0.1	6.0	37.1	0.2	3.9	43.3	0.5	3.2	36.9	0.4	2.8	36.9	0.4	2.8
44.0	0.5	7.6	38.4	0.3	3.4	45.2	0.3	4.7	39.9	0.4	2.0	39.9	0.4	2.0
47.6	0.3	3.9	41.6	0.3	9.2	48.7	0.3	4.8	43.1	0.3	9.3	43.1	0.3	9.3
49.2	0.3	5.1	43.3	0.3	5.9	50.4	0.1	5.5	44.7	0.2	5.0	44.7	0.2	5.0
49.5	0.3	2.4	47.9	0.2	4.6	52.4	0.1	3.0	47.3	0.2	5.3	47.3	0.2	5.3
51.5	0.1	3.9	50.4	0.1	11.6	55.1	0.2	10.2	49.2	0.2	8.7	49.2	0.2	8.7
53.9	0.3	3.6	51.4	0.1	4.0	56.5	0.2	0.9	51.5	0.2	4.4	51.5	0.2	4.4
57.4	0.0	4.0	52.9	0.0	2.1	57.1	0.5	4.5	53.7	0.6	1.4	53.7	0.6	1.4
58.9	0.3	2.7	54.3	0.2	2.7	62.5	0.0	2.8	55.2	0.3	2.8	55.2	0.3	2.8
64.7	0.1	2.3	56.2	0.1	3.2	66.2	0.1	1.3	56.0	0.1	15.8	56.0	0.1	15.8
65.5	0.1	2.0	56.7	0.4	3.5	69.0	0.2	4.2	58.4	0.0	2.3	58.4	0.0	2.3
67.5	0.1	1.9	57.5	0.2	3.5	71.9	0.6	3.2	60.3	0.5	4.1	60.3	0.5	4.1
69.9	0.2	3.9	60.1	0.1	2.6	74.2	0.2	5.2	62.0	0.3	2.0	62.0	0.3	2.0
73.0	0.3	1.4	61.2	0.1	1.7	78.3	0.3	2.6	63.7	0.6	2.6	63.7	0.6	2.7
77.7	0.9	2.3	64.4	0.1	1.4	79.7	0.6	2.7	66.3	0.4	5.2	66.3	0.5	5.2
81.6	0.1	1.2	66.9	0.1	1.9	82.0	0.4	0.6	70.7	0.3	1.1	70.7	0.3	1.1
84.1	0.8	3.1	70.1	0.5	4.4	84.7	0.3	1.5	74.4	0.2	4.3	74.4	0.2	4.3
87.9	0.8	2.1	72.6	0.6	2.9	88.6	0.9	5.6	76.3	0.2	2.7	76.3	0.2	2.7

89.2	0.2	1.2	80.2	0.6	2.7	94.3	2.1	4.0	82.3	1.7	2.5	82.3	1.7	2.5
90.3	0.0	3.3	81.9	0.4	1.7	94.9	0.1	2.7	84.3	0.5	3.8	84.2	0.5	3.8
98.2	2.4	3.8	83.4	0.4	0.8	100.2	1.7	1.7	85.0	0.2	1.3	84.9	0.2	1.2
101.3	1.7	2.4	88.1	1.7	0.2	101.3	0.6	1.6	86.6	0.4	1.6	86.6	0.4	1.6
103.7	0.2	1.8	90.2	0.0	1.7	102.7	1.8	1.0	91.3	1.0	1.1	91.3	1.0	1.1
107.0	1.4	1.9	91.5	0.4	1.0	106.7	1.9	1.5	94.4	1.3	5.2	94.4	1.3	5.2
111.4	2.7	5.8	97.9	1.7	7.6	111.7	1.4	18.6	100.4	0.8	12.9	100.3	0.8	13.0
119.4	0.4	0.7	98.8	0.6	2.8	118.4	6.0	2.6	107.2	3.7	2.1	107.1	3.6	2.1
123.6	8.2	2.8	106.6	0.0	0.1	126.5	3.2	0.8	113.4	10.5	1.1	113.3	10.5	1.1
129.7	9.0	3.5	114.6	10.0	4.6	129.7	8.1	3.3	115.6	1.5	3.7	115.4	1.5	3.8
131.7	0.2	1.2	118.3	9.5	5.2	132.3	1.1	1.3	116.7	0.1	0.2	116.5	0.1	0.2
136.0	0.2	0.5	122.4	0.1	0.5	140.5	1.0	0.6	121.9	1.9	1.2	121.8	1.8	1.2
137.7	0.2	0.1	125.9	0.1	0.5	143.2	1.0	0.3	127.9	3.0	0.4	127.4	3.1	0.4
155.4	4.8	1.0	149.2	2.5	1.4	162.0	3.8	0.6	147.5	1.8	0.5	147.5	1.8	0.5
165.4	3.1	1.9	150.5	1.8	1.6	170.4	0.1	18.0	152.7	0.3	17.6	152.7	0.3	17.6
171.6	0.3	11.7	156.6	0.2	18.0	179.7	2.1	1.2	155.9	1.1	7.6	155.9	1.0	7.4
184.9	0.9	0.5	166.6	0.9	3.7	183.0	0.4	0.5	162.9	0.3	2.0	162.7	0.2	2.0
188.4	1.0	0.1	168.3	1.7	2.3	188.9	0.9	1.9	165.8	0.2	0.8	165.7	0.2	0.9
191.6	0.2	3.2	174.0	0.9	1.3	190.1	0.6	0.4	168.9	0.7	0.9	168.8	0.7	1.0
193.5	1.1	2.5	174.7	0.3	0.6	192.8	0.4	0.6	171.3	0.6	3.9	171.2	0.6	3.8
195.7	1.3	0.9	181.5	1.2	2.7	196.1	0.6	2.2	180.0	0.1	4.2	180.0	0.1	4.1
202.0	1.0	0.8	182.0	0.1	0.6	217.6	10.1	2.8	199.1	2.2	3.3	198.9	3.4	3.4
215.3	2.1	1.0	201.0	1.3	0.7	220.0	1.8	1.9	205.0	1.5	0.8	201.6	7.8	0.9
218.2	0.3	0.9	202.2	1.8	0.2	222.4	2.1	2.3	205.5	5.2	0.8	204.8	1.7	0.7
224.0	1.0	1.5	208.6	0.2	0.1	224.3	0.2	2.3	210.6	0.5	4.3	209.0	1.9	5.0
228.3	0.7	4.6	212.0	2.2	1.2	228.7	0.8	2.4	211.8	3.5	1.9	210.3	1.1	2.2
230.4	0.8	5.7	214.1	0.2	7.3	231.7	2.2	1.4	215.4	2.1	4.7	214.4	1.9	3.7
232.0	1.1	2.3	215.2	2.1	5.4	234.1	0.6	4.2	217.3	1.0	4.7	216.8	1.7	5.4
233.9	1.2	3.2	217.0	1.1	6.9	235.3	2.0	1.5	221.9	3.2	1.9	220.2	2.3	2.2
234.4	0.7	4.0	218.1	0.4	3.0	238.3	1.8	1.3	226.0	3.8	1.6	223.6	1.0	1.9

256.9	3.9	0.5	235.0	0.9	0.2	258.7	3.0	3.1	236.3	1.0	12.5	227.3	1.1	11.5
272.9	0.3	1.4	246.3	0.1	2.1	262.3	5.8	2.0	240.5	1.6	4.8	240.3	1.2	4.0
276.1	0.8	0.3	254.7	1.1	2.2	270.1	0.3	3.1	251.2	0.6	1.4	251.1	0.6	1.4
279.4	0.5	0.1	261.9	0.1	1.0	278.2	0.7	1.1	254.8	0.8	4.9	254.7	0.7	4.5
280.7	0.4	4.4	263.0	0.4	0.5	280.2	2.9	0.5	263.2	0.4	1.2	260.3	0.9	0.6
290.1	1.0	0.6	268.1	1.4	2.0	281.0	0.3	2.6	264.8	0.5	2.3	264.1	0.6	1.3
298.3	0.9	2.2	272.3	0.6	4.8	288.9	2.7	1.9	267.5	2.9	4.2	266.4	1.4	4.4
362.3	2.9	0.2	343.9	2.1	0.1	309.1	2.1	2.3	277.1	3.2	1.5	268.4	2.6	1.8
373.8	24.3	2.0	346.0	8.5	0.8	353.9	4.2	0.4	329.6	5.5	0.8	329.5	5.4	0.8
374.1	7.8	1.0	354.8	29.7	4.7	366.4	9.2	1.1	339.2	2.6	0.9	339.2	2.5	0.9
385.8	11.7	1.7	358.5	10.7	7.5	372.5	19.7	2.3	348.2	25.0	4.8	348.2	24.9	4.8
386.9	0.7	3.0	365.5	0.9	3.4	381.7	14.5	4.0	353.4	14.0	8.6	353.4	14.1	8.5
400.5	0.1	0.3	370.9	14.9	2.2	400.7	0.7	0.1	383.0	0.1	0.6	383.0	0.1	0.6
403.7	0.6	0.5	382.8	1.0	0.3	407.4	0.2	0.6	384.2	0.3	0.3	384.2	0.3	0.3
404.6	0.2	1.3	383.8	0.2	0.9	408.6	0.5	0.3	385.2	0.1	0.2	385.2	0.1	0.2
405.5	0.1	0.5	384.6	0.1	0.6	409.3	0.1	0.2	388.4	0.6	1.2	388.4	0.6	1.1
412.6	0.6	0.1	385.5	0.9	0.6	413.0	0.5	0.4	388.9	0.7	0.8	388.8	0.7	0.8
416.5	8.8	0.9	389.0	0.1	0.2	418.4	0.6	0.1	390.8	0.1	0.4	390.8	0.1	0.4
417.8	5.3	0.5	389.8	0.8	0.3	419.4	0.3	0.4	392.2	0.0	1.7	392.1	0.0	1.7
421.1	6.4	0.5	392.0	0.1	0.3	420.5	0.9	0.5	393.4	0.4	1.0	393.3	0.4	1.0
427.5	5.9	0.7	395.4	0.1	0.3	440.7	6.2	1.1	409.4	1.1	13.9	409.3	1.1	13.9
441.2	0.9	0.2	403.6	1.3	1.7	443.7	10.8	1.1	411.8	16.9	3.0	411.8	17.1	3.0
443.7	8.5	0.7	416.8	13.8	2.1	451.7	3.0	1.4	421.2	8.2	3.5	421.1	8.0	3.4
450.6	14.6	1.7	419.7	26.8	0.5	453.5	10.0	1.9	425.3	12.8	11.1	425.2	12.6	10.8
452.9	8.7	1.7	422.2	9.5	1.3	456.9	10.6	0.4	426.5	13.1	8.0	426.3	12.4	8.5
455.3	26.3	0.9	424.8	7.0	0.3	465.1	11.0	1.6	436.3	14.9	4.7	436.2	17.5	4.9
456.0	5.5	0.4	426.1	27.6	4.3	470.4	16.8	0.6	438.8	10.8	1.9	438.6	12.4	1.9
464.9	0.2	4.5	436.2	8.3	1.0	483.7	19.9	1.4	454.2	16.0	6.2	444.3	9.9	1.4
465.9	14.1	1.9	439.7	1.0	5.4	493.1	33.6	0.3	462.8	13.0	1.5	454.1	15.3	6.1
474.8	14.6	0.2	442.0	18.0	1.6	494.6	27.8	0.9	466.4	36.3	0.1	466.3	36.4	0.1

479.1	34.8	5.4	449.0	20.8	12.0	498.0	27.3	0.8	468.6	21.4	2.4	468.4	20.2	2.4
489.2	1.1	2.2	452.1	3.6	4.3	501.6	29.7	0.9	472.6	36.8	0.7	472.5	39.3	0.7
492.6	5.0	0.1	462.3	1.0	5.4	507.3	50.9	0.6	477.0	48.3	4.0	476.9	50.0	4.4
499.5	66.9	0.2	468.5	0.9	2.2	515.9	11.3	0.5	484.9	10.1	1.2	478.3	2.1	3.3
502.1	49.0	0.7	472.1	70.8	0.4	517.4	2.0	1.9	488.4	14.4	3.0	485.0	11.3	1.3
505.1	10.7	1.6	474.5	50.7	0.5	523.1	32.9	1.1	492.0	17.5	1.4	491.7	22.5	0.7
510.7	28.2	1.2	481.3	38.5	4.8	528.7	15.0	5.7	501.9	93.7	2.2	501.8	95.4	2.2
523.9	10.5	0.4	493.1	3.1	0.0	534.7	75.3	1.0	510.9	7.4	15.7	510.8	7.4	15.7
528.4	62.6	0.2	497.6	62.7	0.8	541.3	18.9	1.0	523.2	0.6	7.1	523.0	0.6	6.9
538.7	139.4	1.6	504.9	139.7	1.9	546.8	6.3	6.0	527.6	1.7	8.8	527.3	1.7	9.0
540.2	4.5	8.2	510.6	8.3	9.0	606.0	11.5	1.7	561.3	2.1	10.7	560.7	2.0	10.4
559.3	11.9	15.8	528.7	8.4	29.4	608.6	34.7	0.4	566.8	22.0	3.1	566.0	22.7	3.0
619.8	90.9	0.6	584.3	62.6	0.4	611.7	19.7	9.0	578.5	14.3	9.2	571.6	11.3	9.4
628.3	31.3	2.0	602.3	4.9	0.9	629.8	0.8	3.1	602.2	0.1	4.1	602.2	0.1	3.9
628.8	1.1	1.5	602.7	7.4	1.7	630.4	1.9	4.8	602.4	3.4	0.3	602.3	4.9	0.6
629.5	2.8	2.3	603.1	0.2	2.9	630.6	1.1	1.3	603.1	2.0	5.8	603.0	1.9	5.9
629.6	0.2	2.8	603.4	2.1	9.6	631.8	1.2	5.9	603.3	1.0	2.6	603.3	1.3	2.5
630.0	0.2	2.7	603.7	0.1	1.1	632.4	0.4	5.9	603.6	0.1	1.7	603.5	0.1	1.4
630.6	0.5	10.5	604.1	0.4	5.9	632.7	1.4	4.9	603.9	0.4	7.8	603.9	0.4	8.0
631.0	2.1	5.7	604.6	0.1	10.9	633.5	0.9	6.1	604.5	0.5	12.3	604.4	0.4	12.3
631.2	4.7	9.7	604.9	1.7	8.9	634.4	0.2	7.7	604.6	1.1	9.7	604.6	1.2	9.7
641.8	301.4	3.9	623.6	246.7	5.3	679.5	75.3	4.4	642.4	44.0	4.0	620.1	46.0	2.8
700.2	52.5	3.1	666.6	67.6	1.2	693.9	14.5	6.7	649.8	41.1	4.8	649.7	40.8	4.7
705.9	20.1	0.3	668.6	1.8	12.8	702.4	40.8	1.8	667.9	57.3	8.7	667.8	57.3	8.9
706.7	6.7	6.3	669.1	35.9	1.7	704.1	47.6	0.3	668.9	8.3	1.7	668.9	7.2	1.7
706.9	56.1	0.7	669.8	14.6	5.3	706.9	23.9	2.4	670.7	23.8	1.8	670.7	24.0	1.8
708.7	11.4	10.1	671.3	25.8	3.0	707.6	38.3	7.0	671.5	35.3	1.1	671.5	35.4	1.1
710.9	63.3	0.4	672.1	52.1	0.3	709.5	14.7	0.4	672.8	23.0	2.2	672.8	23.4	2.2
712.9	2.7	0.5	672.6	71.7	0.6	710.2	21.4	0.5	673.5	3.7	1.7	673.5	3.5	1.7
713.2	56.5	0.8	674.3	2.0	1.3	713.0	9.9	1.4	674.1	6.5	4.5	674.1	6.5	4.5

714.5	31.5	4.4	676.1	27.1	1.2	713.8	19.6	2.0	675.3	17.6	3.3	675.3	17.5	3.3
715.3	8.1	2.2	677.0	8.6	3.6	715.7	12.6	1.2	676.3	73.9	1.2	676.2	70.5	1.3
717.4	33.8	5.2	677.7	14.3	1.0	718.9	7.8	2.8	677.8	6.2	1.2	677.8	7.2	1.2
722.1	2.9	0.8	678.0	23.8	2.2	719.3	34.8	1.9	678.1	4.4	1.1	678.1	4.6	1.1
724.7	5.9	4.0	681.4	3.5	1.1	723.1	13.1	2.7	680.1	15.9	3.8	680.1	16.3	3.8
727.3	2.3	1.2	683.1	2.2	3.3	724.5	7.4	2.3	682.0	7.9	4.2	682.0	7.9	4.2
728.6	2.3	0.6	685.8	1.8	3.0	728.2	1.3	3.0	686.0	11.2	11.3	686.0	11.2	11.5
731.4	11.2	1.0	687.5	6.4	2.1	729.5	6.6	0.9	688.4	7.5	3.1	688.3	6.6	3.2
747.1	101.9	0.5	697.7	84.6	2.7	742.8	137.0	0.4	692.0	85.2	1.2	692.0	85.0	1.2
752.3	68.4	0.2	702.1	48.9	7.6	746.7	44.4	1.8	701.2	60.4	10.8	701.2	60.5	10.7
756.4	11.5	1.0	713.0	30.9	1.3	755.2	45.2	1.1	710.2	41.8	7.9	710.2	41.1	8.7
757.2	76.7	0.5	714.4	32.8	1.8	755.9	48.2	0.8	711.9	7.5	4.8	711.9	7.5	4.8
762.1	15.9	0.2	714.5	79.3	0.6	759.2	17.7	0.6	713.8	57.5	2.1	713.8	57.4	1.9
763.1	34.6	0.9	716.2	8.6	1.0	761.1	64.2	0.6	715.5	47.6	0.1	715.5	47.7	0.1
764.1	9.3	1.7	718.0	12.9	3.9	766.4	14.1	0.8	718.0	10.7	2.1	718.0	10.4	2.0
769.1	15.4	0.5	720.0	4.7	1.7	767.6	18.9	0.3	718.7	8.3	1.9	718.7	8.1	2.0
771.7	5.6	1.0	721.9	11.0	1.2	775.1	4.4	1.0	723.5	11.2	0.7	723.5	10.9	0.7
774.9	34.5	6.2	723.0	15.6	1.5	777.2	27.3	3.9	724.6	5.0	6.1	724.5	6.2	7.4
808.1	13.3	2.1	741.3	13.9	2.5	800.4	140.5	1.8	745.2	19.7	3.9	730.9	6.8	18.1
814.1	174.4	4.5	748.2	114.6	7.9	811.1	39.3	2.2	750.7	101.6	4.1	745.2	19.6	3.9
816.5	189.0	2.3	773.7	245.7	3.5	819.5	123.3	0.7	759.6	91.7	6.7	750.7	101.4	4.2
822.7	54.8	2.4	781.1	56.1	6.4	829.9	60.3	3.7	774.1	7.0	17.4	759.6	91.5	7.5
854.5	3.5	2.0	798.6	1.8	1.3	850.4	2.0	0.6	778.1	136.0	10.3	777.6	134.8	3.6
857.5	1.1	0.3	802.0	1.1	0.7	861.0	1.4	0.5	798.3	2.4	0.4	798.3	2.4	0.4
860.9	2.2	1.3	803.6	1.7	0.9	862.1	1.4	0.8	800.9	0.9	1.9	800.9	1.0	2.0
866.7	0.3	0.7	808.2	4.0	0.7	862.9	2.4	0.7	805.9	0.7	0.6	805.9	0.8	0.6
870.1	1.1	0.6	808.8	1.4	0.6	869.1	2.1	0.8	809.6	1.9	0.9	809.5	1.9	0.9
872.3	4.5	0.4	814.9	2.0	0.6	875.7	2.2	1.0	813.4	2.1	1.2	813.4	2.1	1.5
874.0	4.8	0.6	817.3	2.4	1.4	877.5	2.6	1.1	815.5	2.7	0.3	815.4	2.6	0.3
889.6	1.2	0.8	819.8	4.7	1.1	888.5	2.5	1.1	817.4	0.0	0.6	817.4	0.0	0.6

935.6	0.0	3.1	871.5	0.1	6.8	928.9	0.2	4.2	822.1	2.9	0.4	822.1	3.1	0.4
937.4	0.2	0.6	876.3	0.4	5.0	941.5	0.2	4.5	871.1	0.4	4.7	871.1	0.4	4.7
940.1	0.4	1.7	878.9	0.3	3.8	945.0	0.1	0.6	873.8	0.4	9.7	873.8	0.4	9.6
948.1	0.6	1.2	879.5	0.0	1.0	950.1	0.7	0.4	880.1	0.2	8.0	880.1	0.2	8.0
951.6	1.1	1.1	887.6	0.2	1.2	952.4	0.4	2.0	884.4	0.4	1.2	884.4	0.4	1.2
955.4	1.0	0.8	889.2	1.0	2.1	955.4	0.4	2.6	888.4	0.4	2.3	888.3	0.4	2.4
959.0	0.5	0.3	892.5	0.6	1.7	963.8	2.8	16.2	892.4	0.1	5.3	892.4	0.1	5.5
980.8	0.9	6.5	895.9	0.3	1.8	964.6	0.1	1.1	898.8	0.8	1.4	898.8	0.8	1.4
987.6	0.6	0.6	921.8	0.4	1.8	969.3	0.3	10.1	901.0	0.1	0.8	901.0	0.1	0.8
993.3	0.0	0.5	925.5	0.1	1.4	985.3	0.6	1.6	922.8	0.9	0.5	922.8	0.9	0.5
995.9	1.2	0.5	927.2	0.9	1.4	994.2	0.5	1.1	924.4	0.4	4.4	924.4	0.4	4.4
1000.0	0.1	0.8	931.3	0.2	2.0	995.4	1.7	4.2	928.0	0.2	0.5	928.0	0.2	0.5
1001.8	0.2	0.2	931.5	2.2	0.2	998.6	0.9	2.6	929.8	0.7	1.5	929.8	0.7	1.5
1002.9	0.4	2.3	935.8	0.2	3.0	1004.0	2.4	0.7	934.8	1.7	2.8	934.8	1.7	2.9
1003.9	1.3	0.6	937.3	0.3	5.8	1005.9	1.2	1.8	935.3	1.5	0.3	935.3	1.5	0.3
1009.9	0.3	0.9	939.8	0.3	0.2	1008.6	0.4	0.1	939.5	0.1	1.0	939.5	0.1	1.0
1011.4	0.1	0.7	945.6	0.1	0.1	1010.5	0.2	3.4	941.4	0.6	2.0	941.4	0.6	2.0
1016.6	0.2	4.4	948.3	0.1	0.2	1013.4	2.0	4.1	947.3	0.2	0.1	947.3	0.2	0.1
1017.0	0.3	7.2	949.3	0.0	0.4	1014.1	0.7	11.4	947.5	0.2	0.3	947.5	0.2	0.3
1017.5	0.9	27.2	951.2	0.1	0.6	1014.6	0.2	1.7	949.0	0.2	0.7	949.0	0.2	0.7
1017.8	0.4	7.0	951.5	0.2	0.4	1014.7	0.3	0.3	950.1	0.1	0.3	950.1	0.1	0.3
1018.2	0.2	14.7	953.6	0.1	1.7	1016.0	0.4	0.3	951.5	0.9	0.7	951.5	0.9	0.8
1018.8	1.4	22.8	954.9	0.1	3.6	1018.5	0.7	19.1	954.6	0.3	0.4	954.6	0.3	0.4
1019.2	0.1	33.1	958.0	0.1	0.2	1019.1	1.4	19.9	959.8	0.9	9.2	959.8	0.9	9.2
1019.5	2.2	22.7	976.8	1.0	23.3	1019.2	2.4	41.7	962.9	1.6	10.6	962.9	1.6	10.6
1020.2	0.8	37.8	977.3	0.2	27.1	1019.3	0.4	17.1	977.5	1.5	21.9	977.5	1.6	21.9
1020.7	0.1	5.3	977.5	2.0	23.9	1020.7	1.0	43.7	977.7	1.5	28.1	977.7	1.6	28.1
1022.1	0.8	35.9	978.0	1.6	33.1	1021.4	0.1	30.0	977.9	1.7	28.0	977.9	1.7	28.0
1024.6	0.7	2.2	978.2	0.3	37.0	1022.9	1.9	22.9	978.3	0.8	24.5	978.3	0.8	24.5
1026.9	2.9	5.7	978.5	1.5	43.5	1024.4	1.3	10.1	978.5	1.7	59.9	978.5	1.7	59.9

1030.0	0.4	2.8	978.8	0.8	38.6	1031.2	1.9	9.5	978.8	1.1	66.8	978.8	1.1	66.8
1031.5	0.6	0.4	979.8	0.4	96.7	1043.4	0.9	12.9	979.7	0.5	69.7	979.7	0.5	69.7
1059.8	1.0	6.5	1014.8	0.4	5.3	1057.6	3.9	14.7	983.9	0.9	30.1	983.9	0.9	30.3
1060.8	0.5	7.7	1015.2	0.8	10.8	1060.6	4.3	9.3	1014.9	1.2	18.4	1014.9	1.2	18.4
1061.2	2.8	28.8	1016.4	3.4	52.7	1060.7	0.9	21.7	1015.7	1.3	44.5	1015.7	1.3	44.4
1061.8	4.1	54.7	1016.4	2.0	88.5	1062.3	2.3	45.6	1016.3	3.3	54.5	1016.3	3.3	54.5
1062.0	2.5	33.4	1016.6	2.5	59.8	1062.5	3.0	85.3	1016.6	3.9	136.5	1016.6	3.9	136.9
1062.3	1.8	68.4	1016.6	2.7	35.0	1062.6	3.3	86.8	1016.7	2.8	31.5	1016.7	2.8	31.2
1063.2	2.7	77.0	1017.4	4.1	133.5	1063.1	3.9	27.7	1017.0	2.7	55.9	1017.0	2.7	55.6
1064.9	1.3	55.9	1017.7	4.0	132.3	1063.7	2.0	36.4	1017.2	5.1	144.9	1017.2	5.1	145.4
1103.2	0.2	1.4	1051.0	0.1	1.1	1065.3	0.9	17.2	1017.4	3.2	100.8	1017.4	3.2	100.6
1109.1	0.7	3.8	1054.8	0.3	5.7	1099.5	1.7	2.4	1042.8	0.4	6.4	1042.8	0.4	6.4
1120.9	0.3	0.2	1070.0	0.2	6.5	1115.6	0.5	2.5	1057.5	1.0	5.5	1057.5	1.1	5.5
1122.5	0.9	0.6	1070.6	7.3	1.2	1122.1	2.9	0.4	1070.7	12.2	3.4	1070.7	12.2	3.4
1123.6	6.2	1.4	1074.9	2.4	0.4	1123.8	1.5	1.8	1071.0	0.1	5.0	1071.0	0.1	5.0
1124.6	1.3	1.4	1075.2	13.5	3.9	1123.9	3.6	0.2	1072.8	3.6	2.6	1072.8	3.6	2.6
1125.5	0.6	1.1	1076.1	21.2	6.9	1126.4	1.8	0.6	1074.6	4.2	3.3	1074.6	4.2	3.3
1128.9	3.6	1.9	1076.2	6.7	3.4	1126.4	3.1	1.8	1075.7	2.4	6.7	1075.7	2.4	6.7
1133.9	1.1	2.0	1077.5	1.9	6.8	1128.0	1.9	1.0	1076.2	7.2	7.0	1076.2	7.2	7.0
1137.9	4.7	1.2	1078.4	5.0	6.9	1137.0	5.4	0.7	1076.4	14.3	10.8	1076.4	14.3	10.8
1145.3	11.9	2.7	1079.0	15.1	21.7	1138.4	15.2	13.0	1078.0	24.9	14.5	1078.0	24.9	14.4
1146.4	11.1	7.5	1079.9	31.5	11.1	1140.4	43.1	3.9	1078.7	9.0	9.2	1078.7	9.1	9.2
1147.0	47.4	12.1	1080.7	39.7	17.5	1145.0	40.3	23.3	1079.8	19.6	70.2	1079.8	19.6	70.2
1147.4	18.8	27.0	1081.3	23.5	35.3	1145.7	18.6	30.6	1080.1	22.7	52.2	1080.1	22.7	52.3
1148.2	86.3	11.7	1081.5	11.0	15.6	1146.6	19.9	30.6	1081.0	35.8	35.3	1081.0	35.8	35.3
1148.5	5.9	30.5	1082.3	31.9	40.5	1146.9	34.9	57.5	1082.1	21.8	8.3	1082.1	21.8	8.3
1149.1	36.7	45.5	1082.5	12.5	93.1	1147.9	34.0	21.4	1082.6	7.8	129.0	1082.6	7.8	129.0
1150.8	30.4	29.7	1083.6	9.2	24.7	1150.2	41.1	11.9	1086.0	41.9	13.9	1086.0	41.9	13.9
1184.8	4.5	1.1	1120.5	13.7	0.4	1157.3	2.2	7.2	1087.9	1.6	20.7	1087.9	1.6	20.7
1185.8	18.5	1.8	1124.0	33.2	0.2	1185.2	1.5	3.6	1119.5	16.9	0.2	1119.5	16.9	0.2

1186.3	0.8	2.0	1144.9	0.0	0.5	1187.3	8.1	3.4	1129.3	26.8	0.8	1129.3	26.8	0.8
1186.7	0.5	2.1	1145.1	0.2	0.8	1187.6	18.7	2.3	1144.6	0.9	1.5	1144.6	0.9	1.5
1188.4	6.8	3.2	1145.6	0.2	1.2	1188.6	1.1	3.2	1145.1	0.2	1.5	1145.1	0.2	1.5
1188.5	0.7	4.8	1145.8	0.8	3.1	1190.5	1.7	3.0	1145.5	0.3	2.5	1145.5	0.3	2.5
1189.8	4.5	3.6	1145.9	0.5	5.8	1192.0	9.5	2.9	1145.7	0.1	3.3	1145.7	0.1	3.3
1190.1	0.5	3.1	1146.3	0.2	6.0	1192.9	0.5	3.2	1145.9	0.7	2.8	1145.9	0.7	2.8
1192.6	13.3	1.4	1146.6	0.0	1.8	1193.0	0.9	2.0	1146.2	0.2	5.7	1146.2	0.2	5.7
1195.1	33.8	0.4	1147.0	0.3	1.2	1194.7	3.1	2.8	1146.5	0.2	3.1	1146.5	0.2	3.1
1226.4	1.7	2.9	1174.3	2.1	2.1	1209.3	37.2	2.2	1146.6	0.1	0.8	1146.6	0.1	0.8
1228.5	13.0	8.7	1175.4	4.7	7.1	1224.4	7.1	4.6	1174.7	9.1	7.5	1174.7	9.1	7.5
1228.8	1.4	0.9	1175.8	11.2	5.0	1228.3	2.7	2.0	1176.3	3.3	7.4	1176.2	3.3	7.4
1230.9	6.8	4.1	1176.5	3.5	0.7	1230.0	9.5	2.8	1177.3	6.7	2.8	1177.3	6.7	2.8
1232.3	3.8	1.0	1177.7	14.5	3.1	1230.1	9.5	3.2	1178.1	3.2	3.8	1178.1	3.2	3.8
1233.1	6.9	1.9	1178.2	0.3	3.8	1233.1	9.3	4.1	1178.2	8.8	3.0	1178.2	8.8	2.9
1238.5	0.4	5.4	1179.0	5.6	3.7	1235.0	3.6	5.4	1180.1	6.9	7.1	1180.1	6.9	7.1
1241.0	1.0	6.2	1180.7	0.5	8.0	1237.0	5.0	10.7	1181.6	16.6	2.4	1181.6	16.6	2.4
1330.2	0.9	0.2	1292.1	0.6	1.9	1238.7	10.4	3.9	1183.5	6.1	5.8	1183.5	6.1	5.8
1330.5	2.2	0.6	1292.4	7.6	2.4	1328.4	2.2	1.3	1289.9	5.2	0.9	1289.9	5.2	0.9
1331.5	4.3	0.2	1293.6	5.6	0.6	1329.4	1.6	0.7	1291.7	3.8	1.5	1291.7	3.8	1.5
1331.8	5.6	2.6	1294.1	5.9	3.8	1330.9	2.5	1.5	1293.0	5.0	1.8	1293.0	5.0	1.8
1338.1	3.0	0.7	1297.7	3.9	0.6	1331.7	3.1	1.3	1294.7	5.4	3.0	1294.7	5.5	3.0
1340.2	0.3	1.1	1298.4	0.9	0.9	1337.3	0.7	0.7	1300.0	4.4	1.0	1300.0	4.4	1.0
1340.5	6.4	2.4	1299.2	10.7	0.4	1337.7	5.8	1.4	1303.9	2.5	1.1	1303.9	2.5	1.1
1342.4	3.7	1.9	1299.6	0.6	2.4	1341.4	2.3	1.4	1304.6	0.7	1.6	1304.6	0.7	1.6
1367.7	2.5	1.5	1342.4	0.1	0.6	1343.5	2.2	3.0	1309.4	1.7	2.3	1309.4	1.8	2.3
1370.2	0.3	3.2	1342.8	0.5	0.6	1365.0	2.0	1.6	1341.9	1.3	2.5	1341.9	1.3	2.5
1371.5	0.4	0.6	1343.3	3.4	0.3	1368.6	2.1	0.6	1342.4	2.7	1.3	1342.4	2.7	1.3
1372.0	0.6	5.2	1343.5	0.8	2.7	1369.4	1.9	0.5	1342.6	1.4	4.5	1342.6	1.4	4.5
1373.0	1.6	1.8	1346.0	1.2	1.3	1370.9	2.2	4.4	1343.2	2.0	3.1	1343.2	2.0	3.1
1374.9	1.4	4.3	1346.4	0.1	0.7	1372.9	3.2	0.7	1345.4	0.9	3.4	1345.4	0.9	3.4

1377.0	3.2	1.7	1347.2	6.2	4.2	1378.8	0.3	1.6	1345.8	0.1	1.0	1345.8	0.1	1.0
1378.3	3.3	1.0	1347.5	0.5	6.3	1380.4	1.8	1.3	1346.2	4.8	2.7	1346.2	4.8	2.7
1419.2	15.3	1.8	1355.7	9.1	2.1	1383.2	3.4	2.8	1346.9	4.4	4.3	1346.9	4.4	4.3
1426.4	16.9	2.0	1366.6	10.7	1.9	1415.0	14.6	5.0	1356.9	9.1	5.1	1356.9	9.1	5.1
1482.0	4.6	1.1	1416.3	2.1	1.5	1429.3	16.2	3.3	1366.2	10.6	4.3	1366.2	10.6	4.2
1482.6	17.0	1.5	1417.0	10.9	1.3	1482.0	12.9	0.5	1415.7	8.8	0.5	1415.7	8.8	0.5
1483.3	30.0	0.9	1417.6	42.9	1.8	1483.3	9.0	0.8	1415.9	10.5	2.7	1415.9	10.5	2.7
1483.8	30.7	3.3	1418.1	26.6	4.5	1483.6	16.2	0.4	1416.2	19.2	0.7	1416.2	19.2	0.7
1486.2	19.2	2.0	1419.8	5.2	4.0	1484.4	30.5	2.2	1417.3	28.3	2.3	1417.3	28.3	2.3
1486.4	18.3	1.7	1420.3	26.1	2.3	1485.8	32.7	3.0	1419.4	31.5	2.9	1419.4	31.5	2.9
1488.0	33.6	1.9	1420.6	18.0	2.7	1487.7	21.1	3.2	1420.0	14.6	7.6	1420.0	14.6	7.6
1488.3	4.2	4.9	1421.5	13.9	11.3	1489.7	14.0	3.3	1420.8	9.8	3.2	1420.8	9.8	3.2
1538.1	5.3	1.3	1465.7	7.7	2.5	1490.7	26.7	3.8	1421.8	23.9	14.3	1421.8	23.9	14.3
1539.2	6.1	1.1	1466.8	1.4	0.6	1534.9	9.5	1.8	1465.0	10.1	0.5	1465.0	10.1	0.5
1540.3	0.4	0.9	1467.1	1.2	1.0	1537.3	6.9	0.7	1466.1	8.1	3.6	1466.1	8.1	3.6
1540.8	9.9	1.3	1467.2	8.6	3.7	1538.5	7.5	1.5	1466.5	8.2	4.4	1466.5	8.2	4.4
1541.1	12.0	1.0	1467.4	7.5	1.7	1540.0	12.7	0.5	1466.6	9.5	2.7	1466.6	9.5	2.7
1541.6	9.0	1.1	1467.7	14.4	1.0	1540.1	5.3	2.0	1467.7	7.8	0.5	1467.7	7.8	0.5
1542.8	7.0	0.4	1467.9	13.1	1.9	1540.6	6.8	0.5	1468.1	6.2	0.8	1468.1	6.2	0.8
1545.3	8.5	1.5	1468.4	13.3	2.3	1540.9	10.6	0.6	1468.5	5.4	1.6	1468.5	5.4	1.6
1660.8	0.7	4.6	1573.3	0.3	2.6	1544.2	13.4	1.2	1469.6	20.8	1.7	1469.6	20.8	1.7
1661.1	2.0	2.5	1573.7	0.4	1.5	1660.1	0.5	8.0	1572.1	0.8	1.3	1572.1	0.8	1.3
1662.0	1.7	10.7	1574.3	3.6	9.1	1660.5	3.7	2.4	1572.4	2.1	12.1	1572.4	2.1	12.1
1663.4	0.7	8.8	1574.7	2.8	28.2	1661.1	4.2	3.7	1572.8	6.8	1.3	1572.8	6.8	1.3
1663.8	4.7	6.7	1576.0	3.9	5.3	1662.5	13.6	9.0	1573.1	6.7	8.8	1573.1	6.7	8.8
1664.7	1.6	2.3	1576.6	8.2	12.3	1662.8	0.8	11.5	1574.4	7.9	21.1	1574.4	7.9	21.1
1665.3	12.0	15.3	1576.8	2.0	2.9	1664.2	2.6	7.5	1575.4	0.6	7.0	1575.4	0.6	7.0
1666.1	3.7	14.2	1577.3	7.3	24.5	1664.3	3.8	10.9	1575.4	3.5	6.1	1575.4	3.5	6.1
1681.9	0.5	13.2	1587.2	0.1	19.4	1665.3	5.1	14.7	1575.8	2.5	27.8	1575.8	2.5	27.8
1683.1	0.1	48.0	1587.9	0.1	12.2	1681.3	0.3	12.3	1587.0	0.3	25.7	1587.0	0.3	25.7

1683.2	0.3	11.2	1588.3	0.4	38.7	1681.5	1.3	48.8	1587.1	0.5	45.0	1587.1	0.5	45.0
1683.4	0.1	47.8	1588.5	1.0	49.0	1682.5	0.1	11.0	1587.6	0.4	15.2	1587.6	0.4	15.2
1684.4	1.3	41.2	1588.7	0.6	48.3	1682.8	0.1	45.1	1588.1	0.6	29.2	1588.1	0.6	29.2
1684.5	0.5	39.6	1588.9	1.5	28.9	1682.9	0.4	32.3	1588.3	0.8	62.8	1588.3	0.8	62.8
1685.0	4.4	18.4	1589.3	1.3	41.5	1683.6	0.2	56.3	1588.4	1.1	79.9	1588.4	1.1	79.9
1685.8	0.4	48.1	1589.4	1.5	65.0	1684.0	0.1	44.2	1588.6	0.1	66.6	1588.6	0.1	66.6
1786.5	367.4	53.1	1674.2	261.6	25.6	1684.9	1.2	24.5	1588.9	0.7	27.7	1588.9	0.7	27.7
2063.1	247.0	17.3	1923.6	158.9	8.9	2063.9	221.1	15.6	1935.4	194.3	18.0	1935.4	194.2	18.0
2093.9	912.7	60.6	1947.1	726.8	44.2	2098.0	929.1	77.0	1964.8	714.3	47.8	1964.8	714.1	47.8
3115.0	4.5	89.2	3000.0	5.3	104.2	3124.5	2.9	76.9	3007.6	3.2	108.9	3007.6	3.2	108.9
3124.7	3.8	83.1	3001.1	4.1	108.1	3130.2	3.1	76.5	3010.4	3.9	110.6	3010.4	3.9	110.6
3191.7	1.8	40.9	3074.9	2.5	44.4	3197.8	1.3	47.6	3081.0	1.5	49.3	3081.0	1.5	49.3
3200.2	1.8	40.1	3076.0	2.3	49.6	3204.9	0.9	49.4	3082.9	1.5	53.9	3082.9	1.5	53.9
3221.6	0.6	17.2	3092.9	35.8	104.0	3218.4	3.5	12.2	3098.5	85.0	68.2	3098.5	85.0	68.2
3224.5	0.2	17.3	3110.4	1.1	13.3	3218.8	6.5	16.5	3110.8	1.2	17.8	3110.8	1.2	17.8
3225.9	0.9	12.9	3110.7	0.6	14.0	3222.7	34.9	35.7	3111.4	4.8	23.4	3111.4	4.8	23.4
3226.6	9.8	41.8	3112.3	0.2	32.7	3222.9	8.4	44.9	3112.4	2.3	28.4	3112.4	2.3	28.4
3226.7	3.5	18.3	3113.6	0.3	38.0	3226.7	4.2	47.8	3114.4	3.1	39.0	3114.4	3.1	39.0
3229.8	0.3	31.4	3118.0	0.9	28.8	3229.2	0.5	59.9	3116.9	0.2	33.6	3116.9	0.2	33.6
3232.1	2.9	52.0	3118.3	1.0	42.7	3230.0	0.1	47.7	3117.2	2.5	19.8	3117.2	2.5	19.8
3233.2	1.5	13.9	3118.5	0.0	18.7	3230.1	2.0	14.8	3117.8	39.4	109.7	3117.8	39.4	109.7
3233.3	1.1	40.0	3118.9	1.4	47.7	3230.7	4.9	46.8	3118.7	1.7	38.6	3118.7	1.7	38.6
3234.7	1.4	32.2	3121.0	1.3	32.8	3232.0	4.5	15.1	3119.0	0.5	21.2	3119.0	0.5	21.2
3234.7	4.2	39.8	3121.7	2.3	54.7	3232.3	2.6	58.1	3121.1	0.6	43.7	3121.1	0.6	43.6
3235.1	3.4	98.3	3122.0	4.7	93.0	3233.5	17.0	57.5	3121.3	2.3	63.3	3121.3	2.3	63.3
3235.6	3.2	58.7	3123.7	2.6	84.1	3237.4	1.4	68.1	3123.3	9.3	39.5	3123.3	9.3	39.5
3238.1	3.2	87.7	3126.5	3.1	81.1	3238.3	1.1	63.0	3124.8	2.4	65.9	3124.8	2.4	65.9
3242.0	2.4	77.7	3127.0	2.1	59.5	3240.1	5.7	68.6	3126.4	18.1	107.3	3126.4	18.1	107.3
3243.2	4.2	101.4	3127.4	5.3	146.9	3240.8	57.5	50.6	3126.5	7.7	98.7	3126.5	7.7	98.7
3244.0	2.0	73.4	3130.4	3.0	102.8	3241.2	19.1	121.3	3127.1	2.9	74.1	3127.1	2.9	74.1

3245.9	11.9	47.8	3133.0	2.2	23.5	3241.8	6.0	77.2	3128.1	4.9	118.9	3128.1	4.9	118.9
3246.2	8.4	51.6	3133.3	9.7	58.0	3244.6	7.5	77.0	3132.6	6.0	41.0	3132.6	6.0	41.0
3247.3	3.1	29.8	3133.7	24.6	146.2	3246.3	11.0	93.6	3133.0	12.3	88.9	3133.0	12.3	88.9
3247.9	19.5	104.3	3134.3	15.5	138.6	3247.3	14.3	17.0	3133.7	1.5	46.1	3133.7	1.5	46.0
3248.4	14.6	98.5	3135.3	10.4	39.7	3248.6	9.1	61.0	3133.8	15.1	88.8	3133.8	15.1	88.9
3249.7	10.6	45.7	3135.8	14.4	65.6	3248.8	12.6	83.1	3135.3	14.3	85.1	3135.3	14.3	85.1
3253.3	7.1	24.3	3136.2	14.4	66.6	3249.1	21.9	67.9	3135.5	9.5	86.0	3135.5	9.5	86.0
3253.7	21.1	68.8	3141.4	16.4	91.6	3249.3	11.0	101.2	3136.4	21.2	66.4	3136.4	21.2	66.4
3254.7	18.7	87.4	3141.7	12.7	23.2	3250.2	3.7	128.8	3137.4	14.9	82.1	3137.4	14.9	82.1
3256.3	7.1	44.4	3142.7	14.8	233.7	3254.3	20.3	213.4	3140.4	34.5	222.4	3140.4	34.5	222.4
3256.4	10.8	189.1	3143.2	6.5	124.4	3256.2	4.3	22.7	3142.6	3.5	48.4	3142.6	3.5	48.4
3258.8	18.4	257.1	3143.8	26.5	413.4	3257.0	38.3	209.4	3143.0	50.6	586.5	3143.0	50.6	586.5
3258.9	1.7	27.1	3144.5	20.0	341.9	3257.2	9.6	102.8	3143.6	3.9	126.0	3143.6	3.9	126.0
3259.5	28.5	457.2	3144.9	11.3	216.6	3257.8	53.5	201.7	3144.1	20.6	367.3	3144.1	20.6	367.3
3259.8	13.3	357.6	3145.3	13.9	246.4	3258.2	11.1	101.7	3145.7	12.8	221.5	3145.7	12.8	221.5
3259.9	9.9	73.1	3147.8	16.8	245.7	3260.6	19.1	288.6	3146.0	8.6	180.8	3146.0	8.6	180.8
3262.3	15.9	302.6	3148.0	21.5	521.8	3261.5	15.8	275.5	3146.4	18.8	364.5	3146.4	18.8	364.5
3265.0	14.7	318.6	3152.2	5.9	164.0	3263.9	11.8	60.1	3149.2	23.9	311.7	3149.2	23.9	311.7
3265.7	7.5	268.6	3152.4	6.8	180.3	3264.0	8.8	270.9	3153.2	6.3	152.3	3153.2	6.3	152.3
3276.8	31.4	27.7	3162.5	16.9	71.7	3264.4	12.3	261.3	3153.4	5.3	138.2	3153.4	5.3	138.2
3279.7	12.6	111.4	3167.8	3.4	12.5	3264.5	8.0	326.5	3153.8	7.9	139.5	3153.8	7.9	139.5
3290.0	6.4	43.8	3168.7	26.2	78.6	3281.9	8.2	107.3	3156.2	2.4	107.7	3156.2	2.4	107.7
3296.9	5.1	95.7	3174.2	8.8	82.0	3286.4	10.7	59.8	3168.1	7.5	60.3	3168.1	7.5	60.3

Optimized Cartesian x, y, z coordinates in Å



IR	0.539286	1.462371	-0.540548
IR	0.908459	-1.280886	-0.736535
IR	-1.871027	-0.187471	-0.388962
IR	-0.109704	-0.030562	1.618463
C	-0.637765	-1.561595	2.639579
C	1.435286	0.423592	2.484871
O	2.416215	0.682992	3.057815
O	-0.879254	-2.501638	3.264082
C	2.096184	0.286270	-0.959875
C	1.070407	-1.823372	-2.513396
C	0.600406	2.030305	-2.352086
O	1.129080	-2.129501	-3.626264
O	0.630408	2.310418	-3.471004
O	3.241132	0.446636	-1.315002
P	1.622029	3.332920	0.358527
P	2.608212	-2.639335	0.086559
P	-4.080118	-0.558418	0.238291
C	-4.211317	-1.377035	1.864616
H	-3.767078	-0.733051	2.624606
H	-5.248226	-1.583955	2.132935
H	-3.640286	-2.306118	1.814874
C	0.867595	3.924514	1.911657
H	1.339066	4.851033	2.243818
H	-0.187271	4.106973	1.701246
H	0.937040	3.158254	2.682400
C	3.891013	-1.719254	0.998278
H	4.702529	-2.389939	1.287627
H	4.273544	-0.945217	0.331930
H	3.464786	-1.233034	1.875042
C	-1.317166	1.236486	2.841114
H	-1.344039	2.179372	2.288929
H	-2.319272	0.802134	2.806069
C	-0.911992	1.442701	4.293377
H	0.074805	1.905645	4.385213
H	-1.627401	2.096303	4.807083
H	-0.878440	0.495302	4.838688
O	-2.294364	1.688695	-0.392440
O	-1.284367	2.563711	-0.261087
O	-1.811452	-2.115007	-0.366808

O	-0.625668	-2.732911	-0.327198
C	3.608439	-3.499039	-1.177554
C	3.844779	-4.875011	-1.165414
C	4.177114	-2.704768	-2.182689
C	4.636945	-5.455916	-2.157732
H	3.415269	-5.500192	-0.390264
C	4.971681	-3.287657	-3.165441
H	3.998307	-1.632016	-2.196828
C	5.200662	-4.665225	-3.157605
H	4.812005	-6.526393	-2.146888
H	5.405287	-2.666671	-3.941634
H	5.813979	-5.119306	-3.928886
C	2.026079	-3.933007	1.222708
C	2.491552	-4.028360	2.537490
C	1.058925	-4.838434	0.767439
C	2.007134	-5.025847	3.384330
H	3.229173	-3.329969	2.915513
C	0.581803	-5.836782	1.612073
H	0.659975	-4.750759	-0.237264
C	1.056277	-5.933050	2.921801
H	2.373092	-5.091135	4.403366
H	-0.170231	-6.529544	1.251846
H	0.678315	-6.707557	3.581262
C	3.397359	3.168093	0.702821
C	3.916967	3.221596	1.998822
C	4.263631	2.956381	-0.376626
C	5.285597	3.063779	2.214600
H	3.264096	3.373813	2.850502
C	5.629802	2.806300	-0.161374
H	3.870331	2.893636	-1.384546
C	6.144158	2.856588	1.135674
H	5.678510	3.099563	3.224908
H	6.290385	2.634867	-1.004235
H	7.208578	2.729522	1.303907
C	1.509437	4.852413	-0.662807
C	0.303272	5.122390	-1.322050
C	2.550330	5.783982	-0.726193
C	0.148327	6.306049	-2.039777
H	-0.517863	4.412459	-1.270279
C	2.393596	6.965224	-1.451077
H	3.489793	5.590829	-0.219832
C	1.192251	7.228944	-2.108885
H	-0.789128	6.503864	-2.548298

H	3.209061	7.678808	-1.500050
H	1.071476	8.148161	-2.672474
C	-5.125101	0.930107	0.360373
C	-6.143209	1.188758	-0.561925
C	-4.830501	1.884719	1.341774
C	-6.874079	2.373948	-0.486981
H	-6.369464	0.471952	-1.343715
C	-5.565488	3.063216	1.419598
H	-4.008636	1.725346	2.031616
C	-6.591251	3.310891	0.505708
H	-7.661025	2.566368	-1.208007
H	-5.326703	3.797299	2.181325
H	-7.158131	4.234162	0.561322
C	-4.990223	-1.658420	-0.898916
C	-6.222646	-2.221685	-0.544782
C	-4.464508	-1.909238	-2.170032
C	-6.916244	-3.024189	-1.447882
H	-6.659153	-2.025230	0.429485
C	-5.159718	-2.709073	-3.076262
H	-3.504651	-1.488094	-2.453218
C	-6.384710	-3.268419	-2.716459
H	-7.870415	-3.456424	-1.165049
H	-4.738631	-2.898675	-4.057939
H	-6.925763	-3.894078	-3.418974

Ir4(CO)5[P(CH3)(C6H5)2]3(O2)2(C2H5)(H)

IR	0.070671	1.246295	0.020999
IR	-0.875028	-1.152779	0.186074
IR	1.798389	-0.847456	-0.582813
IR	-0.136486	-0.149929	-2.427317
C	-1.364182	0.420480	-3.736698
C	1.532617	0.195207	-3.277193
O	2.458961	0.547153	-3.873765
O	-2.091867	0.772835	-4.563064
C	-1.603120	0.443498	-1.040319
C	-0.807459	-1.326693	2.032753
C	0.043112	1.562339	1.875326
O	-0.810414	-1.464499	3.184896
O	-0.057779	1.813906	2.999479
O	-2.727952	0.897959	-1.185015
P	-0.692617	3.389580	-0.507781
P	-3.050428	-2.043196	-0.002467

P	3.071279	-1.584524	1.244484
C	2.480451	-3.175344	1.900162
H	3.060137	-3.472388	2.775994
H	1.417865	-3.105596	2.135791
H	2.594988	-3.911611	1.104782
C	-1.191266	3.652387	-2.239983
H	-2.072136	3.032744	-2.413578
H	-1.430054	4.702115	-2.421464
H	-0.395226	3.318083	-2.905492
C	-3.623500	-2.201633	-1.722487
H	-2.962461	-2.912433	-2.220318
H	-4.653192	-2.561414	-1.765923
H	-3.531706	-1.233341	-2.215260
C	-0.329308	-2.091633	-3.352971
H	-0.635871	-2.718770	-2.516161
H	-1.131364	-2.084479	-4.094583
C	0.942119	-2.658571	-3.967685
H	1.745974	-2.689336	-3.229012
H	0.765279	-3.687318	-4.305017
H	1.277121	-2.079666	-4.833217
O	2.701422	0.848190	-0.564635
O	1.933494	1.943874	-0.366375
H	2.987504	-1.354669	-1.509206
O	-0.124710	-2.943338	-0.323778
O	1.192277	-2.726946	-0.697299
C	4.861945	-1.867790	1.014826
C	5.310942	-2.433585	-0.182593
C	5.778950	-1.607140	2.039075
C	6.659430	-2.736689	-0.354820
H	4.606307	-2.624515	-0.985802
C	7.129691	-1.903093	1.861644
H	5.446066	-1.161941	2.970662
C	7.572422	-2.469278	0.665897
H	6.998651	-3.171705	-1.288519
H	7.836780	-1.688191	2.655637
H	8.624578	-2.694065	0.527219
C	2.974292	-0.387460	2.611301
C	2.391332	-0.709106	3.839215
C	3.469374	0.907228	2.400387
C	2.311906	0.248737	4.849823
H	1.981689	-1.696674	4.016708
C	3.391560	1.858539	3.411283
H	3.897441	1.174848	1.440751

C	2.813987	1.531065	4.639507
H	1.844976	-0.005076	5.794832
H	3.765327	2.860516	3.232037
H	2.740681	2.277918	5.422478
C	-3.335580	-3.698718	0.716678
C	-4.648994	-4.166052	0.865258
C	-2.266422	-4.510421	1.104049
C	-4.889556	-5.428545	1.398338
H	-5.488089	-3.536343	0.584424
C	-2.511912	-5.775543	1.639468
H	-1.245911	-4.168570	0.968181
C	-3.818106	-6.236229	1.788791
H	-5.908675	-5.780873	1.515684
H	-1.677867	-6.401621	1.937226
H	-4.004178	-7.219046	2.208819
C	-4.292769	-1.026052	0.861151
C	-5.162501	-0.172389	0.180018
C	-4.340431	-1.085364	2.259582
C	-6.089736	0.591555	0.888002
H	-5.108569	-0.078597	-0.897324
C	-5.262734	-0.319279	2.965618
H	-3.667511	-1.741614	2.802860
C	-6.146469	0.515925	2.278704
H	-6.757973	1.255139	0.350564
H	-5.295271	-0.377951	4.047993
H	-6.871040	1.109141	2.827104
C	-2.125476	3.978569	0.452757
C	-2.429389	5.345811	0.480756
C	-2.945116	3.074142	1.132058
C	-3.532975	5.804937	1.193767
H	-1.793033	6.057222	-0.037088
C	-4.049033	3.536948	1.846436
H	-2.736862	2.010523	1.093227
C	-4.343048	4.898352	1.881628
H	-3.756958	6.865967	1.218704
H	-4.675891	2.825287	2.371484
H	-5.200486	5.256007	2.442148
C	0.621207	4.600469	-0.173251
C	1.522579	4.970356	-1.174081
C	0.831431	5.040346	1.139554
C	2.606126	5.794450	-0.873493
H	1.399618	4.605429	-2.187735
C	1.912458	5.863705	1.438125

H	0.149632	4.742140	1.929909
C	2.801818	6.244568	0.430901
H	3.303298	6.073746	-1.655657
H	2.063896	6.206066	2.456161
H	3.646505	6.883799	0.664672

Ir₄(CO)₅[P(CH₃)(C₆H₅)₂]₃(O₂)₂

IR	0.210524	1.281026	-0.934981
IR	1.090525	-1.310955	-0.507388
IR	-1.756786	-0.996529	-0.283900
IR	-0.159478	0.099013	1.497739
C	-0.476501	-1.144763	2.892391
C	1.266194	0.901062	2.340693
O	2.202309	1.316633	2.885570
O	-0.631789	-1.918626	3.738560
C	1.994515	0.513734	-0.798071
C	1.510186	-1.803121	-2.207580
C	0.545393	1.745420	-2.757585
O	1.754476	-2.066438	-3.309298
O	0.788654	2.021479	-3.850165
O	3.147067	0.825574	-0.951235
P	0.264209	3.410269	-0.057127
P	2.973659	-2.366914	0.455384
P	-3.857783	-1.435827	0.661915
C	-3.798086	-2.740419	1.927629
H	-3.199711	-2.368340	2.759475
H	-4.797871	-2.993241	2.285078
H	-3.295512	-3.616295	1.514819
C	-1.179098	3.725640	1.023350
H	-1.289770	4.787823	1.250105
H	-2.057258	3.373540	0.478462
H	-1.076112	3.143505	1.942051
C	2.617051	-2.746407	2.203999
H	1.727558	-3.378730	2.212322
H	3.458837	-3.265659	2.665671
H	2.390623	-1.829961	2.749499
O	-1.883550	1.634728	-1.329456
O	-2.573283	0.521202	-0.991354
O	0.048973	-3.066210	0.138237
O	-1.297781	-2.743400	0.135310
C	3.421105	-3.998337	-0.230356
C	4.706818	-4.526255	-0.056767

C	2.438093	-4.765877	-0.864233
C	5.010996	-5.800203	-0.530942
H	5.476481	-3.940870	0.435847
C	2.746778	-6.041135	-1.334630
H	1.428146	-4.379703	-0.967693
C	4.031168	-6.559000	-1.174114
H	6.010632	-6.200260	-0.399638
H	1.980628	-6.628964	-1.828090
H	4.269036	-7.549570	-1.547306
C	4.507095	-1.400788	0.447105
C	4.843915	-0.585586	1.529018
C	5.275186	-1.348606	-0.721330
C	5.948461	0.261341	1.451969
H	4.244339	-0.582796	2.432304
C	6.382343	-0.511490	-0.793975
H	5.000435	-1.950479	-1.581985
C	6.720535	0.297640	0.292603
H	6.195915	0.897789	2.294433
H	6.969367	-0.473805	-1.704889
H	7.578125	0.959242	0.230675
C	1.720801	3.891141	0.916803
C	1.618806	4.566992	2.137022
C	2.984816	3.568728	0.410837
C	2.768444	4.912518	2.845599
H	0.649327	4.820869	2.550850
C	4.131371	3.916973	1.119652
H	3.078832	3.009791	-0.513373
C	4.026559	4.588628	2.337852
H	2.680666	5.428051	3.795828
H	5.103690	3.645406	0.723498
H	4.920243	4.853283	2.893187
C	0.086752	4.751641	-1.290878
C	-0.954711	4.645866	-2.222779
C	0.933931	5.861512	-1.324823
C	-1.144456	5.644212	-3.173770
H	-1.609481	3.777746	-2.214231
C	0.744691	6.856750	-2.284791
H	1.745539	5.950847	-0.610975
C	-0.293358	6.751102	-3.208940
H	-1.948281	5.553129	-3.896184
H	1.412544	7.711212	-2.311399
H	-0.435429	7.522925	-3.958014
C	-4.636064	-0.013434	1.498077

C	-5.990992	-0.070224	1.846727
C	-3.886632	1.117190	1.833616
C	-6.584789	0.986450	2.532141
H	-6.589739	-0.933135	1.569942
C	-4.482125	2.174719	2.517584
H	-2.843922	1.185217	1.540910
C	-5.829165	2.111235	2.870308
H	-7.635449	0.935443	2.796491
H	-3.894135	3.052046	2.765462
H	-6.293247	2.937695	3.397881
C	-5.094527	-1.968795	-0.559789
C	-5.585793	-3.276045	-0.606809
C	-5.499602	-1.039485	-1.528623
C	-6.492438	-3.646806	-1.600583
H	-5.267777	-4.013780	0.121805
C	-6.406520	-1.412411	-2.515146
H	-5.096209	-0.031385	-1.512232
C	-6.906954	-2.716341	-2.551891
H	-6.872611	-4.662145	-1.631459
H	-6.717636	-0.688980	-3.260585
H	-7.612279	-3.006537	-3.323122

Ir₄(CO)₅P(CH₃)₂(O₂)₂(C₂H₅)

IR	-0.915680	-1.074216	-0.902363
IR	0.476225	1.464493	-0.640592
IR	1.653506	-0.716640	0.539639
IR	-0.855731	0.138534	1.469082
C	-0.083565	1.231129	2.832463
C	-2.658064	0.456741	1.793821
O	-3.781435	0.708413	1.975375
O	0.341991	1.932525	3.646304
C	-1.221160	0.758456	-1.532586
C	1.268159	1.822021	-2.283878
C	-0.455796	-1.699080	-2.644721
O	1.741136	2.006844	-3.327612
O	-0.141776	-2.013867	-3.712322
O	-2.058439	1.336103	-2.198098
P	-3.042081	-1.866227	-0.958246
P	-0.497492	3.546210	-0.514431
P	3.798983	-1.475728	-0.137751
C	3.843086	-3.072859	-1.017864
H	3.216734	-3.002070	-1.908576

H	4.863219	-3.339700	-1.304358
H	3.422387	-3.844520	-0.371680
C	5.059809	-1.647904	1.176462
H	4.743310	-2.416359	1.883580
H	6.035126	-1.914316	0.760972
H	5.136045	-0.698133	1.708694
C	4.550371	-0.283499	-1.298028
H	3.926158	-0.215313	-2.190215
H	4.567546	0.696611	-0.818365
H	5.564775	-0.579121	-1.577735
C	-4.349987	-0.624231	-1.188587
H	-4.077486	0.009877	-2.033706
H	-5.310831	-1.112948	-1.365536
H	-4.415861	0.002929	-0.300286
C	-3.358941	-3.061966	-2.303947
H	-4.375292	-3.458532	-2.243694
H	-3.219996	-2.566579	-3.266240
H	-2.642614	-3.881802	-2.227915
C	-3.524290	-2.808256	0.527474
H	-4.504129	-3.271931	0.390690
H	-2.772900	-3.578554	0.710822
H	-3.549399	-2.138824	1.386789
C	0.510712	4.698868	0.467769
H	1.488537	4.811516	-0.002034
H	0.018263	5.670913	0.545697
H	0.664836	4.272384	1.459729
C	-2.138687	3.588814	0.274995
H	-2.555183	4.598529	0.233949
H	-2.795196	2.896754	-0.253190
H	-2.044206	3.269461	1.313093
C	-0.770497	4.372367	-2.112720
H	-1.275290	5.330482	-1.970909
H	0.186699	4.535016	-2.610115
H	-1.386073	3.711239	-2.725082
C	-0.871143	-1.548527	2.776291
H	-1.216529	-2.376572	2.156026
H	0.185243	-1.721888	2.998539
C	-1.671801	-1.447596	4.063827
H	-2.741200	-1.318113	3.873694
H	-1.551104	-2.363537	4.654706
H	-1.341978	-0.609669	4.684126
O	1.066510	-2.571158	0.422977
O	-0.164672	-2.888494	0.016011

O	2.502113	0.876836	1.113186
O	1.932744	2.062166	0.753729

Ir4(CO)5P(CH3)2(O2)2(C2H5) H

IR	-1.181116	-0.969129	-0.894298
IR	0.261762	1.353989	-0.726397
IR	1.927499	-0.562671	0.208259
IR	-0.673437	0.216597	1.528003
C	0.188555	1.457364	2.694870
C	-2.413255	0.170866	2.118371
O	-3.525194	0.272089	2.452935
O	0.638235	2.255123	3.401604
C	-1.783081	0.824281	-1.137894
C	0.688061	1.469359	-2.551355
C	-1.194786	-1.442456	-2.726199
O	0.897756	1.490859	-3.692668
O	-1.214878	-1.683792	-3.857593
O	-2.734303	1.503269	-1.435556
P	-3.033975	-2.240646	-0.412498
P	-0.652846	3.512383	-0.383897
P	4.039186	-1.475439	-0.133167
C	4.227675	-3.228722	0.313628
H	3.445960	-3.800820	-0.186658
H	5.212982	-3.600582	0.023861
H	4.092637	-3.338286	1.390339
C	5.369849	-0.591054	0.737082
H	5.264414	-0.756717	1.810130
H	6.350965	-0.936719	0.404730
H	5.259863	0.476709	0.543032
C	4.489342	-1.387004	-1.897240
H	3.752627	-1.944388	-2.477655
H	4.460871	-0.343679	-2.215165
H	5.485615	-1.801008	-2.071089
C	-4.596973	-1.305445	-0.419883
H	-4.686309	-0.788367	-1.376433
H	-5.450482	-1.971594	-0.271221
H	-4.574888	-0.553134	0.367658
C	-3.346398	-3.588519	-1.609156
H	-4.219808	-4.177766	-1.319046
H	-3.510390	-3.164076	-2.600892
H	-2.466640	-4.233460	-1.649518
C	-3.028280	-3.148806	1.171063

H	-3.910609	-3.788102	1.254734
H	-2.124272	-3.759625	1.208275
H	-3.006234	-2.444910	2.002166
C	0.582581	4.686236	0.265246
H	1.429722	4.738608	-0.419478
H	0.135193	5.676348	0.382466
H	0.952205	4.324669	1.225331
C	-2.053292	3.701030	0.773609
H	-2.424795	4.729097	0.758058
H	-2.849515	3.019510	0.476185
H	-1.720867	3.449458	1.781124
C	-1.261453	4.310917	-1.906784
H	-1.661549	5.305899	-1.695993
H	-0.441223	4.390123	-2.622195
H	-2.043437	3.678608	-2.328332
C	-0.303979	-1.439312	2.815310
H	-0.528616	-2.322530	2.214465
H	0.778510	-1.400009	2.960169
C	-0.990411	-1.511317	4.172076
H	-2.073353	-1.635791	4.082301
H	-0.609783	-2.365634	4.744115
H	-0.809600	-0.609199	4.762844
O	1.302065	-2.325469	-0.031307
O	0.057541	-2.676517	-0.392416
O	2.764622	1.124699	0.441618
O	2.008546	2.169559	0.032775
H	2.432690	-0.886749	1.654865

Ir₄(CO)₅P(CH₃)₂(O₂)₂

IR	-0.976037	-1.352555	-0.539944
IR	-0.655657	1.411748	-0.625098
IR	1.811500	-0.152397	-0.628508
IR	0.253663	-0.052192	1.508239
C	1.211443	1.251191	2.505103
C	-1.193308	-0.162255	2.620791
O	-2.120143	-0.208035	3.324562
O	1.713547	2.097533	3.114412
C	-2.226675	0.138575	-0.342183
C	-1.112055	1.762259	-2.348995
C	-1.650521	-1.810846	-2.259324
O	-1.393488	1.950583	-3.458729
O	-2.081650	-2.054859	-3.303108

O	-3.405159	0.333721	-0.134448
P	-2.062061	-3.034253	0.586090
P	-1.836160	3.264072	0.142683
P	4.094537	-0.401744	-0.136022
C	4.657092	-2.114051	0.119214
H	4.415068	-2.702612	-0.766300
H	5.731334	-2.149335	0.314077
H	4.112603	-2.541067	0.962418
C	4.565249	0.493274	1.379691
H	4.038440	0.056746	2.229551
H	5.643467	0.444404	1.549688
H	4.251234	1.533053	1.275840
C	5.201654	0.286489	-1.413236
H	5.063418	-0.259750	-2.347505
H	4.928105	1.330343	-1.576537
H	6.248172	0.223505	-1.105386
C	-3.690049	-2.618534	1.283708
H	-4.315994	-2.206833	0.490895
H	-4.160747	-3.502081	1.721610
H	-3.570314	-1.846152	2.043198
C	-2.386579	-4.506371	-0.446436
H	-2.820695	-5.318240	0.142179
H	-3.071189	-4.237086	-1.252446
H	-1.443139	-4.833770	-0.887327
C	-1.107687	-3.733008	1.977705
H	-1.573233	-4.643455	2.363874
H	-0.102313	-3.951295	1.612594
H	-1.036007	-2.990171	2.772650
C	-2.290508	3.091473	1.898348
H	-1.385654	2.954186	2.491553
H	-2.828571	3.976348	2.246745
H	-2.922120	2.208404	2.004935
C	-3.418514	3.587183	-0.694280
H	-3.950007	4.414813	-0.219174
H	-3.232935	3.826742	-1.742543
H	-4.012168	2.672804	-0.638475
C	-0.895905	4.819095	0.047066
H	-1.445985	5.641033	0.511280
H	0.064764	4.673411	0.543269
H	-0.697043	5.049993	-1.000491
O	0.648502	-2.723957	-0.845503
O	1.790286	-1.998566	-0.880301
O	1.131585	2.564609	-0.522339

O 2.187492 1.669420 -0.622737

Ir₄(CO)₆(OO)₂(H)(PMe₃)₃

IR -0.858765 -1.259007 -0.747618
IR -0.255971 1.474054 -0.637055
IR 1.933687 -0.273395 0.149998
IR -0.489958 0.015998 1.643170
C 0.198485 1.537843 2.599772
C -2.314411 0.102883 2.065817
O -3.446305 0.128138 2.324759
O 0.569539 2.466523 3.178647
C -1.882706 0.380080 -1.075079
C 0.164450 1.846655 -2.424975
C -0.754416 -1.705239 -2.565605
O 0.403411 2.013027 -3.546458
O -0.691966 -1.926564 -3.700395
O -3.009059 0.674277 -1.415766
P -2.548425 -2.761400 -0.325692
P -1.537183 3.382581 -0.334570
P 4.157800 -0.611306 -0.357577
C 4.781086 -2.298999 -0.072962
H 4.189095 -3.001533 -0.659526
H 5.836333 -2.372561 -0.345726
H 4.651412 -2.549200 0.980784
C 5.304383 0.467299 0.560571
H 5.254604 0.215180 1.620762
H 6.328406 0.345964 0.200152
H 4.983104 1.502482 0.438831
C 4.539557 -0.272244 -2.112183
H 3.929850 -0.921711 -2.742127
H 4.280387 0.764859 -2.331216
H 5.598229 -0.440023 -2.326389
C -4.231215 -2.077798 -0.419487
H -4.366028 -1.592587 -1.386455
H -4.972294 -2.868569 -0.279658
H -4.351566 -1.315367 0.350385
C -2.580521 -4.184475 -1.470590
H -3.360396 -4.896249 -1.189755
H -2.761476 -3.830999 -2.486794
H -1.607306 -4.677579 -1.441736
C -2.472598 -3.571508 1.307134
H -3.229947 -4.355723 1.382620
H -1.479411 -4.002391 1.442426

H	-2.638259	-2.828430	2.087194
C	-0.572983	4.818255	0.240767
H	0.209490	5.039538	-0.486261
H	-1.218503	5.690333	0.370031
H	-0.090333	4.569144	1.186966
C	-2.893407	3.235907	0.872351
H	-3.488492	4.152366	0.894643
H	-3.522745	2.394358	0.580223
H	-2.476360	3.044438	1.861201
C	-2.388051	3.958287	-1.839294
H	-3.014058	4.828211	-1.626966
H	-1.650943	4.216309	-2.601163
H	-3.005145	3.135316	-2.204650
O	1.780600	-2.283738	0.000363
O	0.594591	-2.824392	-0.210699
O	2.459469	1.666243	0.280074
O	1.494199	2.551581	0.101177
H	2.441113	-0.476027	1.607405
C	0.001155	-1.585675	2.585311
O	0.310902	-2.535644	3.164411

Ir₄(CO)₆(OO)₂(H)(PMePh₂)₃

IR	-0.552455	1.100465	-0.328854
IR	1.466072	-0.637784	-0.234869
IR	-1.123803	-1.550498	0.823951
C	1.718892	1.574281	2.465591
C	-1.185059	0.930175	3.063511
O	-2.111239	1.326993	3.626501
O	2.567366	2.323938	2.723106
C	1.468469	1.366649	-0.524883
C	1.567813	-1.156272	-2.039389
C	-0.926039	1.132505	-2.177855
O	1.584225	-1.440708	-3.161938
O	-1.052459	1.173889	-3.325352
O	2.207166	2.272840	-0.732650
P	-0.985370	3.392196	0.061994
P	3.778950	-0.815341	0.260115
P	-2.184333	-2.997500	-0.803012
C	-1.030975	-4.284517	-1.378611
H	-1.474572	-4.887202	-2.173153
H	-0.103538	-3.817984	-1.715257
H	-0.792632	-4.914643	-0.521388
C	0.190729	4.228552	1.174459

H	1.192100	4.086087	0.766441
H	-0.032032	5.295661	1.232955
H	0.153482	3.773269	2.163494
C	4.145129	-1.191030	2.004398
H	3.627805	-2.123009	2.236403
H	5.218925	-1.311758	2.160133
H	3.746054	-0.408634	2.649068
O	-2.650947	-0.464396	0.712185
O	-2.532594	0.784468	0.202909
H	-1.875740	-2.334619	1.965559
O	1.447212	-2.595182	0.476571
O	0.199593	-2.888513	0.953529
C	-3.694188	-3.922080	-0.355441
C	-3.961294	-4.213623	0.984191
C	-4.562528	-4.392098	-1.349414
C	-5.080365	-4.971254	1.328710
H	-3.299766	-3.838566	1.758211
C	-5.680749	-5.146746	-1.004074
H	-4.374574	-4.158068	-2.392676
C	-5.941190	-5.438421	0.336783
H	-5.282165	-5.187647	2.372022
H	-6.351996	-5.502732	-1.778218
H	-6.815464	-6.021805	0.605620
C	-2.681745	-2.066633	-2.284261
C	-2.040870	-2.224689	-3.515863
C	-3.723398	-1.136331	-2.162542
C	-2.452927	-1.481570	-4.621443
H	-1.216152	-2.919979	-3.626010
C	-4.132187	-0.397873	-3.268127
H	-4.207844	-0.986626	-1.203682
C	-3.501860	-0.572254	-4.501520
H	-1.946427	-1.605990	-5.571942
H	-4.935820	0.322983	-3.165044
H	-3.814948	0.011388	-5.360232
C	4.682086	-2.150979	-0.611587
C	6.067006	-2.060826	-0.801433
C	4.006413	-3.303531	-1.024600
C	6.763535	-3.102171	-1.410486
H	6.604379	-1.171663	-0.488019
C	4.707092	-4.345676	-1.630545
H	2.939417	-3.398864	-0.852029
C	6.083628	-4.247391	-1.828304
H	7.834520	-3.018017	-1.560293

H	4.175416	-5.236587	-1.946668
H	6.624754	-5.058590	-2.303856
C	4.735460	0.671325	-0.155518
C	5.200197	1.554321	0.818760
C	4.926730	0.975540	-1.509226
C	5.857690	2.727400	0.445076
H	5.043652	1.350015	1.871637
C	5.591051	2.137652	-1.880662
H	4.553871	0.300717	-2.274290
C	6.056264	3.019788	-0.901937
H	6.207692	3.413178	1.208630
H	5.738022	2.362682	-2.931280
H	6.566382	3.932391	-1.190820
C	-0.932888	4.483626	-1.408779
C	-1.825063	5.551225	-1.557363
C	0.071402	4.292724	-2.364244
C	-1.722617	6.406492	-2.653400
H	-2.606646	5.715624	-0.823875
C	0.176801	5.153116	-3.454728
H	0.781115	3.480194	-2.255541
C	-0.722146	6.209427	-3.604982
H	-2.425145	7.225806	-2.762553
H	0.958173	4.994499	-4.189832
H	-0.643624	6.874943	-4.458136
C	-2.631105	3.698006	0.767897
C	-2.810385	4.242662	2.039957
C	-3.752265	3.332078	0.011960
C	-4.095422	4.430008	2.549825
H	-1.958033	4.518873	2.649930
C	-5.032357	3.527467	0.516353
H	-3.621839	2.884983	-0.968206
C	-5.207089	4.076347	1.788985
H	-4.224600	4.847548	3.542168
H	-5.894599	3.237782	-0.074056
H	-6.205707	4.218614	2.187882
IR	0.362484	0.270981	2.147892
C	0.939168	-1.160508	3.274823
O	1.279100	-2.026766	3.958236

C1 BP86

IR	0.165303	1.397433	-0.288239
IR	-0.149755	-1.382657	-0.339097
C	0.227878	1.963706	-2.126981

C	-0.161427	-1.815899	-2.217101
O	0.243521	2.131135	-3.294852
O	-0.149882	-1.877633	-3.396168
I	0.398315	3.727623	1.300671
I	-0.477213	-3.917225	0.888170
P	2.539397	1.277005	-0.355144
P	2.178968	-1.800258	-0.239850
P	-2.172055	1.810205	-0.318085
P	-2.516393	-1.256626	-0.368135
C	3.107027	-0.378726	-0.991058
H	4.196797	-0.502971	-0.880212
H	2.846810	-0.386613	-2.061986
C	-3.063123	0.370455	-1.085512
H	-2.736740	0.347408	-2.137396
H	-4.158097	0.495120	-1.047392
C	-2.669250	3.216374	-1.415197
C	-2.599087	4.529387	-0.893774
C	-3.064153	3.034059	-2.758109
C	-2.923405	5.632197	-1.701325
H	-2.273344	4.688097	0.138062
C	-3.392200	4.140401	-3.563478
H	-3.118259	2.035856	-3.200414
C	-3.323555	5.443067	-3.038077
H	-2.859185	6.641701	-1.283985
H	-3.696798	3.981123	-4.602294
H	-3.577005	6.303369	-3.665205
C	-3.145648	2.161266	1.213020
C	-4.488968	2.585574	1.081280
C	-2.583337	2.013872	2.496452
C	-5.261399	2.855324	2.222659
H	-4.929011	2.730541	0.089447
C	-3.361339	2.289014	3.636163
H	-1.545811	1.694413	2.610365
C	-4.696292	2.709822	3.505002
H	-6.298454	3.186881	2.111596
H	-2.915908	2.176523	4.629014
H	-5.294931	2.927267	4.395261
C	-3.505350	-1.414618	1.182859
C	-4.917182	-1.369098	1.101589
C	-2.886313	-1.599005	2.434911

C	-5.698823	-1.504583	2.260086
H	-5.413849	-1.251512	0.133016
C	-3.674378	-1.739667	3.592215
H	-1.797983	-1.635953	2.508771
C	-5.076858	-1.694082	3.510149
H	-6.790128	-1.469334	2.186990
H	-3.185278	-1.886888	4.559634
H	-5.685334	-1.806381	4.413054
C	-3.351177	-2.468326	-1.490083
C	-3.756805	-3.717225	-0.966668
C	-3.536498	-2.208720	-2.865659
C	-4.351503	-4.677635	-1.802930
H	-3.597514	-3.942151	0.090652
C	-4.136494	-3.169637	-3.699286
H	-3.210195	-1.264954	-3.311137
C	-4.547606	-4.406673	-3.170118
H	-4.655936	-5.641594	-1.384236
H	-4.275257	-2.952250	-4.762631
H	-5.012265	-5.155085	-3.819427
C	3.322403	2.430877	-1.578100
C	4.204468	1.990038	-2.589434
C	3.039850	3.812058	-1.470315
C	4.788320	2.910680	-3.480415
H	4.449326	0.930961	-2.700298
C	3.627969	4.728084	-2.357970
H	2.353021	4.166946	-0.693023
C	4.503324	4.282654	-3.367213
H	5.464668	2.551820	-4.262450
H	3.395295	5.793085	-2.263026
H	4.956067	4.997915	-4.060859
C	3.569586	1.543198	1.156467
C	4.940798	1.856687	1.012978
C	3.013884	1.409713	2.445220
C	5.750608	2.022444	2.149232
H	5.375622	1.993791	0.018106
C	3.830692	1.575434	3.578224
H	1.952077	1.188003	2.570574
C	5.196079	1.881498	3.436041
H	6.809423	2.273017	2.030161
H	3.392069	1.471083	4.574972

H	5.824614	2.017385	4.321881
C	2.762621	-3.222674	-1.268810
C	2.948622	-4.483386	-0.658099
C	2.960715	-3.098663	-2.661716
C	3.342360	-5.592850	-1.426223
H	2.775741	-4.601121	0.414305
C	3.359039	-4.209303	-3.426848
H	2.792711	-2.147045	-3.173925
C	3.552986	-5.459718	-2.811170
H	3.477048	-6.564048	-0.940552
H	3.508826	-4.097503	-4.504940
H	3.859451	-6.324414	-3.407864
C	3.044088	-2.093336	1.365448
C	4.451979	-2.238889	1.369325
C	2.331807	-2.211281	2.574942
C	5.136632	-2.490561	2.568750
H	5.020388	-2.179324	0.435444
C	3.021556	-2.469895	3.774080
H	1.245718	-2.107401	2.581839
C	4.420224	-2.608669	3.776449
H	6.225409	-2.599435	2.560649
H	2.458432	-2.562673	4.707453
H	4.952607	-2.809189	4.711539
C	-0.010388	-0.029559	1.231457
O	-0.019510	-0.045936	2.456647

C1 wB97xD

IR	-0.005207	-1.387833	-0.277814
IR	-0.002145	1.374436	-0.385191
C	-0.031566	-2.046971	-2.083097
C	-0.037675	1.705561	-2.279454
O	-0.063396	-2.327512	-3.205476
O	-0.063680	1.726496	-3.438831
I	0.043435	-3.646479	1.365619
I	0.019182	3.982944	0.630212
P	-2.361713	-1.519191	-0.353329
P	-2.346559	1.507001	-0.264255
P	2.347539	-1.525182	-0.360338
P	2.346736	1.494384	-0.351679
C	-3.065748	0.020358	-1.059194

H	-4.157705	0.014883	-1.051115
H	-2.711958	0.058938	-2.091298
C	3.044748	-0.013814	-1.132412
H	2.668753	0.006130	-2.156452
H	4.136589	-0.025878	-1.151466
C	2.945135	-2.864976	-1.451668
C	3.057635	-4.155182	-0.919398
C	3.217136	-2.659183	-2.806465
C	3.442078	-5.217877	-1.731437
H	2.836069	-4.330408	0.127353
C	3.603196	-3.724642	-3.618760
H	3.121407	-1.676896	-3.254604
C	3.716968	-5.006036	-3.083177
H	3.522311	-6.212413	-1.306888
H	3.807362	-3.552004	-4.669645
H	4.014426	-5.835405	-3.715916
C	3.383704	-1.730864	1.126310
C	4.741056	-2.036677	0.963816
C	2.867150	-1.526288	2.405199
C	5.575083	-2.134803	2.072461
H	5.149411	-2.213010	-0.026528
C	3.707766	-1.618814	3.513409
H	1.818553	-1.296594	2.546226
C	5.057050	-1.923545	3.351891
H	6.624167	-2.375721	1.939418
H	3.299825	-1.451067	4.503593
H	5.705840	-1.996344	4.218475
C	3.219919	1.636021	1.242887
C	4.612158	1.480263	1.282695
C	2.527969	1.924937	2.418579
C	5.298670	1.600234	2.484586
H	5.170097	1.271501	0.375557
C	3.219428	2.055896	3.621997
H	1.453704	2.044769	2.402711
C	4.600753	1.891314	3.659303
H	6.373944	1.462911	2.507873
H	2.670809	2.278764	4.530031
H	5.135667	1.984969	4.598479
C	3.087748	2.826387	-1.358570
C	3.549919	3.993186	-0.742941

C	3.136201	2.722086	-2.752618
C	4.065913	5.034022	-1.511811
H	3.497356	4.096729	0.334512
C	3.655081	3.761883	-3.519866
H	2.758510	1.841145	-3.260598
C	4.123004	4.920619	-2.900262
H	4.415684	5.937236	-1.024315
H	3.687095	3.668837	-4.599793
H	4.523071	5.733016	-3.497451
C	-2.988182	-2.797878	-1.504007
C	-3.675524	-2.490321	-2.681293
C	-2.740736	-4.139872	-1.188602
C	-4.102623	-3.506805	-3.536051
H	-3.887657	-1.463943	-2.955040
C	-3.168504	-5.151859	-2.041660
H	-2.199806	-4.390213	-0.281308
C	-3.849172	-4.839212	-3.219762
H	-4.629800	-3.254041	-4.449558
H	-2.963997	-6.186259	-1.788686
H	-4.177052	-5.628826	-3.887274
C	-3.366437	-1.795272	1.142398
C	-4.709550	-2.163808	1.000348
C	-2.835519	-1.575865	2.413829
C	-5.519447	-2.300823	2.123632
H	-5.124605	-2.356659	0.015798
C	-3.650876	-1.711435	3.535689
H	-1.794714	-1.304114	2.538174
C	-4.989194	-2.072428	3.394777
H	-6.558428	-2.590169	2.008302
H	-3.233020	-1.533667	4.519930
H	-5.618575	-2.179081	4.272137
C	-3.122803	2.862346	-1.212301
C	-3.569503	4.008971	-0.549232
C	-3.217874	2.795895	-2.606301
C	-4.115851	5.067952	-1.270738
H	-3.481146	4.083005	0.528329
C	-3.767579	3.853891	-3.326102
H	-2.853418	1.931803	-3.151510
C	-4.219237	4.992542	-2.659121
H	-4.452564	5.955684	-0.746972

H	-3.836191	3.790552	-4.406479
H	-4.643272	5.819046	-3.219227
C	-3.172369	1.605369	1.358296
C	-4.557046	1.404179	1.441636
C	-2.451580	1.903538	2.514118
C	-5.206537	1.484643	2.666866
H	-5.139133	1.188262	0.551804
C	-3.106201	1.992530	3.742028
H	-1.383330	2.062360	2.462776
C	-4.479177	1.780359	3.822550
H	-6.275336	1.311848	2.723733
H	-2.535234	2.221440	4.634689
H	-4.985300	1.841833	4.780127
C	0.013112	0.067493	1.212818
O	0.026635	0.096943	2.418500

C2 BP86

IR	-1.323918	0.377907	-0.284085
IR	1.342953	-0.316010	-0.274946
C	-1.559014	0.599389	-2.115953
C	1.730989	-0.494590	-2.085092
O	-1.611602	0.727499	-3.291479
O	1.936735	-0.588069	-3.244447
I	-3.915131	0.944482	0.751993
I	3.959218	-1.069072	0.580805
P	-0.914125	2.711719	-0.004457
P	2.130142	1.940127	-0.244238
P	-2.106596	-1.884463	-0.442062
P	0.838460	-2.663110	-0.191100
C	0.798034	3.191422	-0.574598
H	1.093232	4.173750	-0.174747
H	0.700927	3.275863	-1.668518
C	-0.770480	-3.020152	-1.044695
H	-0.602112	-2.777815	-2.105341
H	-1.061833	-4.080229	-0.965789
C	-3.430694	-2.121332	-1.713339
C	-4.787875	-2.032129	-1.325717
C	-3.120871	-2.310440	-3.078104
C	-5.809025	-2.155169	-2.283389
H	-5.044549	-1.853462	-0.278928

C	-4.144705	-2.432346	-4.034965
H	-2.083669	-2.351328	-3.422058
C	-5.492740	-2.359142	-3.639942
H	-6.854188	-2.083800	-1.967402
H	-3.886003	-2.578330	-5.087971
H	-6.289877	-2.454671	-4.383663
C	-2.771069	-2.762627	1.037358
C	-3.409939	-4.012338	0.856549
C	-2.636895	-2.223265	2.333795
C	-3.919481	-4.711911	1.963105
H	-3.533313	-4.434091	-0.146251
C	-3.151120	-2.930725	3.435900
H	-2.112306	-1.272682	2.470053
C	-3.794311	-4.168375	3.256840
H	-4.419367	-5.674223	1.814860
H	-3.046187	-2.508093	4.439667
H	-4.195964	-4.710036	4.119212
C	0.719445	-3.522958	1.434047
C	0.440045	-4.910101	1.465339
C	0.935176	-2.822227	2.638749
C	0.380931	-5.589842	2.692363
H	0.290649	-5.469964	0.536516
C	0.884644	-3.514208	3.863024
H	1.106348	-1.741016	2.603084
C	0.611100	-4.892712	3.895537
H	0.163757	-6.662259	2.709798
H	1.054420	-2.967989	4.795985
H	0.572104	-5.424824	4.851402
C	1.990122	-3.750125	-1.151713
C	3.029071	-4.436391	-0.482934
C	1.882432	-3.873462	-2.554517
C	3.922732	-5.248476	-1.202112
H	3.140747	-4.336626	0.598849
C	2.779791	-4.683765	-3.272822
H	1.112677	-3.333534	-3.112574
C	3.800829	-5.377402	-2.598162
H	4.721979	-5.772502	-0.669371
H	2.682396	-4.766561	-4.359450
H	4.499281	-6.008035	-3.156818
C	-1.890215	3.871667	-1.073094

C	-1.466619	5.218350	-1.194919
C	-3.037034	3.453464	-1.778013
C	-2.171644	6.121145	-2.008910
H	-0.594108	5.579606	-0.642378
C	-3.740050	4.357913	-2.595867
H	-3.400423	2.429050	-1.666499
C	-3.311338	5.691413	-2.716166
H	-1.832077	7.158473	-2.088187
H	-4.627677	4.014395	-3.135331
H	-3.860433	6.392700	-3.352204
C	-1.099940	3.387771	1.697242
C	-2.048350	4.397583	1.976669
C	-0.328121	2.839620	2.746259
C	-2.191416	4.885705	3.287371
H	-2.683520	4.796522	1.182756
C	-0.474549	3.339014	4.051370
H	0.357188	2.010312	2.552957
C	-1.399647	4.362831	4.327020
H	-2.929207	5.666647	3.495924
H	0.130567	2.914740	4.858377
H	-1.513345	4.742692	5.347484
C	3.360063	2.322631	-1.571766
C	4.741174	2.231082	-1.285172
C	2.950691	2.604988	-2.893919
C	5.691207	2.450900	-2.297549
H	5.072679	1.976251	-0.275731
C	3.903497	2.827451	-3.903841
H	1.890697	2.636380	-3.163951
C	5.277064	2.756512	-3.607575
H	6.757011	2.375513	-2.061717
H	3.570099	3.046638	-4.922597
H	6.018389	2.928019	-4.394098
C	2.939152	2.616270	1.277884
C	3.441446	3.938286	1.228946
C	3.056211	1.875781	2.471429
C	4.050840	4.512035	2.357627
H	3.385028	4.519524	0.302545
C	3.669320	2.453539	3.598530
H	2.662995	0.859294	2.520236
C	4.166596	3.768207	3.547719

H	4.439216	5.533701	2.304899
H	3.759674	1.868438	4.518755
H	4.643231	4.211782	4.427547
O	-0.750132	0.090044	1.659872
O	0.743942	0.034568	1.657387

C2 wB97xD

IR	-1.194536	0.649064	-0.263589
IR	1.221014	-0.609149	-0.304099
C	-1.377556	0.946056	-2.084140
C	1.486028	-0.851903	-2.124776
O	-1.396421	1.101143	-3.234277
O	1.600785	-0.982435	-3.270746
I	-3.502939	1.752454	0.885291
I	3.588256	-1.912288	0.457266
P	-0.255752	2.815418	-0.030095
P	2.475529	1.400024	-0.270126
P	-2.448215	-1.357469	-0.480252
P	0.180195	-2.750748	-0.190343
C	1.461933	2.866065	-0.689299
H	1.977399	3.786354	-0.415006
H	1.326821	2.857562	-1.772640
C	-1.400502	-2.716047	-1.116681
H	-1.126400	-2.457374	-2.140384
H	-1.920281	-3.675921	-1.122915
C	-3.766965	-1.219573	-1.738536
C	-5.049319	-0.813554	-1.349746
C	-3.498563	-1.417534	-3.096281
C	-6.044521	-0.623031	-2.304161
H	-5.268667	-0.637133	-0.303390
C	-4.495585	-1.226805	-4.051063
H	-2.509739	-1.704593	-3.436467
C	-5.772324	-0.830232	-3.656778
H	-7.032197	-0.304941	-1.989132
H	-4.271536	-1.382143	-5.100532
H	-6.548711	-0.679380	-4.399137
C	-3.272615	-2.117720	0.953608
C	-4.189431	-3.153813	0.733857
C	-2.946769	-1.734700	2.256153
C	-4.786268	-3.798837	1.812115

H	-4.452700	-3.449776	-0.277215
C	-3.547249	-2.387326	3.331373
H	-2.208307	-0.955371	2.418692
C	-4.465600	-3.412515	3.115317
H	-5.502331	-4.594566	1.637453
H	-3.288256	-2.093561	4.342316
H	-4.929833	-3.913094	3.958665
C	-0.225994	-3.465685	1.431917
C	-1.002560	-4.631208	1.489275
C	0.257798	-2.892040	2.608279
C	-1.295831	-5.216069	2.714543
H	-1.377284	-5.093320	0.581405
C	-0.029244	-3.491703	3.834834
H	0.810058	-1.960164	2.556950
C	-0.802378	-4.647605	3.892075
H	-1.908115	-6.110023	2.753328
H	0.345824	-3.041897	4.747403
H	-1.028514	-5.105734	4.849250
C	1.063634	-4.108557	-1.039601
C	1.799361	-5.035702	-0.294953
C	1.057946	-4.204172	-2.434824
C	2.505181	-6.049988	-0.936612
H	1.831733	-4.962132	0.785597
C	1.765077	-5.218839	-3.076000
H	0.516704	-3.488614	-3.044220
C	2.489618	-6.145721	-2.327622
H	3.077414	-6.758134	-0.347639
H	1.753870	-5.280721	-4.158577
H	3.042649	-6.934506	-2.826262
C	-0.987833	4.134369	-1.078637
C	-0.276735	5.330327	-1.265785
C	-2.224851	3.985089	-1.708399
C	-0.788118	6.345916	-2.067612
H	0.674548	5.490678	-0.769571
C	-2.736185	5.000699	-2.515891
H	-2.811828	3.088822	-1.554932
C	-2.022130	6.181308	-2.700079
H	-0.227068	7.265168	-2.195861
H	-3.698637	4.863316	-2.995689
H	-2.421701	6.970511	-3.328030

C	-0.184816	3.521835	1.644087
C	-0.738070	4.773904	1.932493
C	0.413321	2.771357	2.661610
C	-0.650032	5.292627	3.222379
H	-1.252426	5.340984	1.166195
C	0.511056	3.303799	3.943810
H	0.767803	1.766506	2.463624
C	-0.013653	4.564059	4.227445
H	-1.086423	6.261020	3.441709
H	0.987950	2.721715	4.724902
H	0.058898	4.972559	5.230165
C	3.793922	1.461740	-1.533857
C	5.117958	1.184476	-1.178673
C	3.477962	1.681674	-2.878815
C	6.112731	1.153089	-2.152960
H	5.371109	0.980990	-0.144764
C	4.473837	1.651410	-3.851650
H	2.453625	1.856105	-3.192494
C	5.795393	1.390758	-3.489949
H	7.135410	0.933399	-1.867151
H	4.216014	1.821484	-4.891024
H	6.571075	1.363567	-4.247569
C	3.323658	1.911983	1.266832
C	4.005641	3.136277	1.262531
C	3.300708	1.146467	2.433774
C	4.639881	3.598071	2.411158
H	4.066242	3.729487	0.354878
C	3.940754	1.608795	3.582158
H	2.764377	0.208125	2.457824
C	4.604729	2.833343	3.578384
H	5.161578	4.548510	2.394559
H	3.912927	1.007576	4.484201
H	5.095177	3.191812	4.477166
O	-0.663114	0.181288	1.655148
O	0.743271	-0.155174	1.629024

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