Supporting Information for:

Unlocking the Facet-Dependent Ligand Exchange on Rutile TiO_2 of a Rhenium Bipyridyl Catalyst for CO_2 Reduction

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Section 1: TiO_2 (100) crystal preparation and ReC0A attachment procedure.

The crystals were submerged in a mixture of 3:1 ratio of H_2SO_4:H_2O_2 for 20 min and then sonicated for 45 min. Afterwards, they were rinsed with Milli-Q water (18 MΩ*cm) and placed in 1M NaOH for 10 min. After rinsing with Milli-Q water once again, the crystals were put into a 1M HCl solution under UV light for 5 min. The crystals were then rinsed with Milli-Q water and acetone, dried with air, and immersed in 1 mM ReC0A in acetonitrile (MeCN) overnight. The VSFG spectra of the Rhenium complex were measured at multiple occasions by cleaning and re-soaking the same crystal in the sample solution; the reproducibility of distinguishing results – the redshift of the high frequency mode, relative spectral intensities, and orientation dependence – indicates that the overall crystal structure of the TiO_2 substrate is not disrupted during our experiment. The most distinguishing feature of our SFG spectrum is the substantial redshift of the high frequency carbonyl mode of the Rhenium complex. Such a drastic change in CO vibrational frequency must be associated with the change in molecular property, and cannot be explained by minor surface reconstruction. We would also note that the strong agreement between the computational and experimental results suggest that major surface reconstruction does not occur. The molecular orientation used to compute the theoretical spectrum was generated by optimizing the catalyst on a bare TiO_2 (100) crystal surface (structure shown in Figure 8c of the manuscript). The spectrum computed for this structure matches both the experimentally measured spectral shape and the rotational anisotropy measurements, which implies that any surface restructuring that occurs does not have a significant effect on the catalyst orientation.

Section 2: Experimental VSFG procedure. All SFG experiments were performed using a 7W, 1-kHz, 60-fs Ti:sapphire 800-nm laser. Approximately 2W are directed, by use of a beamsplitter, to an optical parametric amplifier (OPA), not used in this experiment. The remaining 5W are split, with 4W directed to an IR OPA and 1W to a home-built 4f stretcher, which gives us a ~7 cm^{-1} (FWHM) 800-nm beam. A schematic of the SFG setup is shown in Figure S1. The IR and 800-nm beams are focused by the

same off-axis parabolic mirror to the sample. A translation stage on the 800-nm path enables proper temporal overlap between IR and visible beams. The 800-nm beam polarization is controlled by a half-wave plate; the IR polarization and intensity are controlled by a half-wave plate and polarizer, used in combination. We control the polarization of the SFG light by using a half-wave plate and polarizing beam splitter. By changing the relative polarization of the input and output beams, the VSFG spectra can be collected with different polarization combinations including PPP, SSP, SPS and PSS; where the polarization of the SFG, visible and IR beams are written from left to right. The VSFG signal is detected using liquid nitrogen cooled CCD detector operating at a temperature of -120 ºC. The Acton SpectraPro-300i spectrometer utilizes a 1200 grooves/mm, 750-nm blaze grating. The spectrometer is a 300 mm fl, f/4 model and the camera uses a 1340x100 pixel sensor.

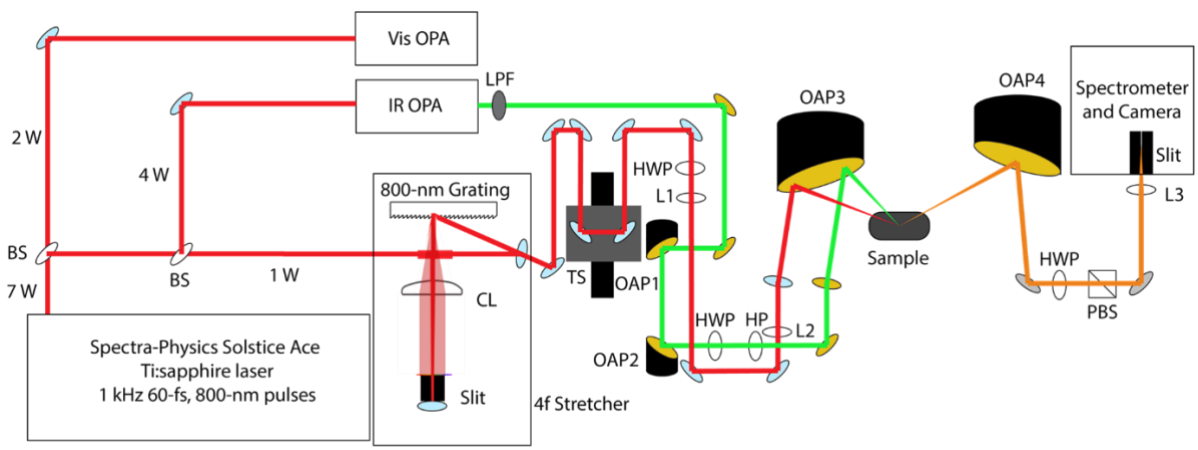

Figure S1. A schematic of the VSFG experimental setup. BS: Beamsplitter. CL: 40 cm cylindrical lens. TS: Translation stage. HWP: Half-wave plate. L1: 100 cm lens. L2: -5 cm lens. L3: 4 cm lens. LPF: Edmund Optics 2.4 µm longpass filter. HP: CaF_2 holographic wire grid polarizer. OAP1: 8 inch 90° off-axis parabolic mirror. OAP2: 4 inch 90° off-axis parabolic mirror. OAP3: 4 inch 60° off-axis parabolic mirror. OAP4: 4 inch 60° off-axis parabolic mirror. PBS: Polarizing beam-splitter.

Section 3: Fitted amplitudes of experimental VSFG.

Table S1: The resonant amplitude ($A_{q,eff}$), non-resonant amplitude ($A_{NR,eff}$), and phase (δ) as a function of in-plane rotational angle, as extracted from the global fitting procedure for all eighteen spectra using Equation 1 in the main text. The frequency (ω_q) and the linewidth (Γ_q) of each mode is kept constant during global fitting. The extracted frequencies are: 1924 cm^{-1} ($A'(2)$), 1945 cm^{-1}(A''), and 2020 cm^{-1} ($A'(1)$); with bandwidths of 52 cm^{-1}, 35 cm^{-1} and 17 cm^{-1}, respectively.

	Amplitudes ($A_{q,eff}$) extracted from global fitting	δ

In-plane angle of rotation	$A_{A'(2),eff}$	$A_{A'',eff}$	$A_{A'(1),eff}$	$A_{NR,eff}$	
0	48.1542	-41.2064	2.92279	-0.0432919	25.5327
20	44.5063	-32.3259	2.90063	-0.0633668	24.2724
40	49.3023	-31.0447	3.22257	-0.113779	24.0295
60	51.7294	-27.3404	3.73744	-0.174897	23.9132
80	50.535	-23.519	4.26023	-0.207894	23.8653
90	50.5149	-23.5603	5.18691	-0.223515	23.8116
100	51.216	-24.3502	5.20599	-0.223099	23.8263
120	53.2934	-26.1694	4.39956	-0.220823	23.9437
140	50.6032	-26.7149	3.31992	-0.165935	23.9955
160	46.9418	-29.0001	2.68102	-0.107034	24.1254
180	43.6834	-34.6949	1.7687	-0.0524381	25.3932
200	47.4616	-36.9341	2.34847	-0.0590933	24.887
220	50.0791	-34.7359	2.23034	-0.0820443	24.4828
240	48.5455	-25.3388	3.11134	-0.167337	24.0289
260	49.2667	-22.9715	4.05114	-0.210998	23.9835
280	49.6056	-22.6735	4.3878	-0.220472	23.9598
300	46.3945	-21.2658	3.65284	-0.187805	23.9512
320	51.1536	-30.8445	3.03825	-0.131849	24.0343
340	48.1657	-36.6043	2.41456	-0.0548318	24.8603
360	43.4905	-36.2717	2.59213	-0.0365376	25.5464

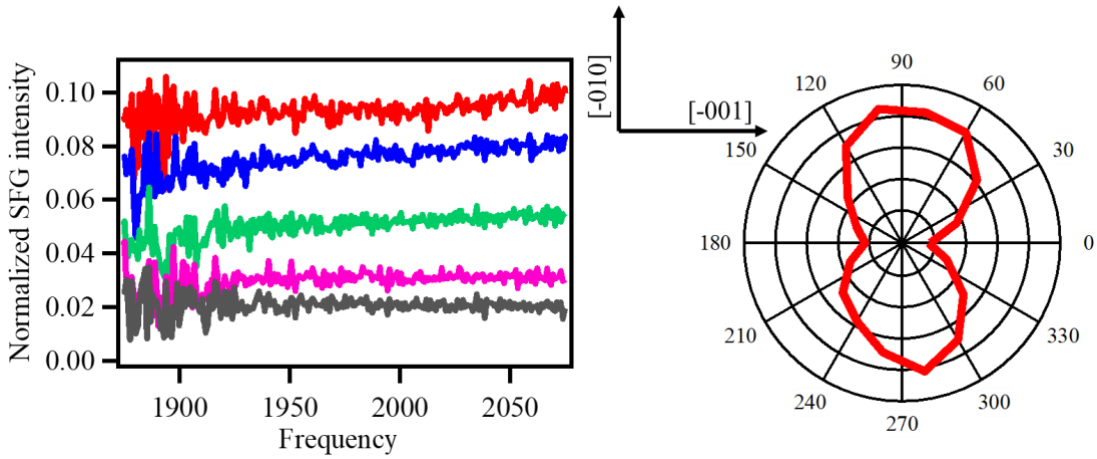

Figure S2. (left) Non-resonant PPP VSFG response from the TiO_2 (100) crystal without any Rhenium molecules attached to it, shown for five consecutive 20° rotation of the TiO_2 crystal. (b) Polar plot of the azimuthal dependence of the non-resonant amplitude as a function of rotational angle. The in-plane crystal axes are also shown.

Section S4. Periodic calculations of TiO_2 (100) and small cluster optimization.

The rutile TiO_2 crystal geometry was calculated with periodic DFT as implemented in the Vienna Ab Initio Simulation Program (VASP) version 5.4[1-4] using the Perdew-Burke-Ernzerhof (PBE)

functional[5] and the projector-augmented wave (PAW) method[6, 7] with Ti 3s and 3p electrons treated explicitly. A plane wave cutoff of 500 eV was used with a convergence criterion of 10^{-6} eV for the electronic energy and 0.01 eV/Å for the geometric optimization. Bulk optimization of atomic positions and lattice vectors was performed with a 13 × 13 × 13 γ-centered k-point grid and Gaussian smearing (σ= 0.1 eV). The optimized positions and lattice vectors were used to generate a 4 × 4 × 2 TiO_2 slab (note that each of the two TiO_2 units in the vertical direction contains two layers of Ti atoms). The bottom layer (two layers of Ti atoms) was frozen to maintain the bulk structure, while the top layer was relaxed. A 3 × 3 × 1 k-point grid was used for the slab optimizations with a 20 Å vacuum spacer to prevent interactions between the surface and its periodic image. The optimized slab model was used to build a cluster model for spectroscopic simulations.

A 3 × 3 × 1 TiO_2 cluster was used to model the surface in subsequent calculations. To ensure neutrality, the open valences of unsaturated oxides were capped with hydrogen atoms at positions mimicking the Ti framework. Oxides at the surface were left uncapped to accurately simulate the interfacial crystalline environment (Figure S3). All hydrogen atom caps were allowed to relax while TiO_2 atoms remained frozen. Due to cases where proximity of the carboxylate groups to the hydrogen caps impacted the binding configuration, the positions of surface-facing hydrogens were rotated to avoid non-physical edge effects.

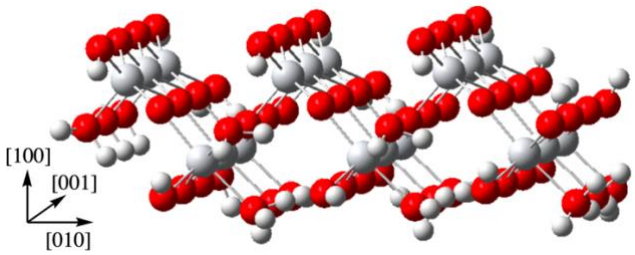

Figure S3. Molecular model of the 3 × 3 ×1 TiO_2 (100) cluster. Hydrogen caps were added to mimic the position of missing Ti atoms, and the number of caps was chosen to ensure neutrality.

Normal mode frequencies were scaled by 0.949 in accordance with reported scaling factors for the ωb97xd/6-31G(d) model chemistry.[8] Polarizability derivatives were printed from Raman calculations using the "iop(7/33=1)" keyword in Gaussian 16 Revision C.01.[9] All optimizations were done using Gaussian 16 Revision C.01 with its default optimization criteria and integration grid.

Section S5. ReOH configuration 5 VSFG spectrum from free molecule.

Due to near degeneracy with a spurious electronic state, the DFT-computed Raman activities for the carbonyl stretching modes of ReOH **5**, ReOH **8**, and ReC0A dimer Cl:CO on TiO_2 (100) diverge, reaching magnitudes over 10^6 $Å^4$/amu. The typical values for the carbonyl stretches are between 10-100 $Å^4$/amu. The Gaussian 16 software uses analytic derivatives of the polarizability to evaluate Raman activities, which in the sum over states approach has an electronic energy difference term in the denominator that can cause this divergence.[10] Raman calculations were attempted with an alternate functional (B3LYP) and several different cluster models. None of these attempts managed to avoid the diverging Raman activity issue. We hypothesize that the flat-lying binding orientation of the complex causes interaction between the bipyridyl aromatic system and the TiO_2 (100) surface which lead to the spurious vibronic coupling in these binding orientations. Our solution was to calculate Raman activities of an unbound ReOH molecule that is oriented identically to the bound molecule in cartesian space.

For ReOH **5**, this method is important because configuration **5** produces a spectrum that reproduces experiment. To preserve the effects of binding on the minimum energy geometry of the ReOH **5** molecule, the bipyridyl N-C-C-N dihedral, which was slightly twisted in the bound structure of **5**, was frozen. All other bond lengths, angles, and dihedrals were allowed to relax at the wB97XD/6-31G(d) level with the LANL2DZ ECP on Re (Figure S4). We validated the free molecule approximation by comparing the VSFG signal and anisotropy of the free and bound molecule in a system whose bound spectrum could be computed, **3b**. The results are shown below in Figure S5. The VSFG line shape of the free molecule shows agreement with the values of the bound spectrum, showing only an amplitude decrease on the order of 10%.

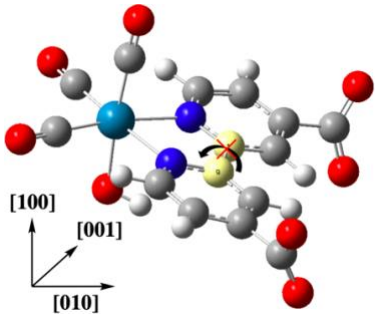

Figure S4. Free molecule approach to calculating Raman activities. The highlighted bond is the axis about which the dihedral rotation was frozen. The molecule retains its orientation with respect to the crystal axes.

The free molecule anisotropy also shows qualitative agreement with that of the bound molecule, reproducing the intensity ratios along the [010] axis and displaying matching lobe shapes.

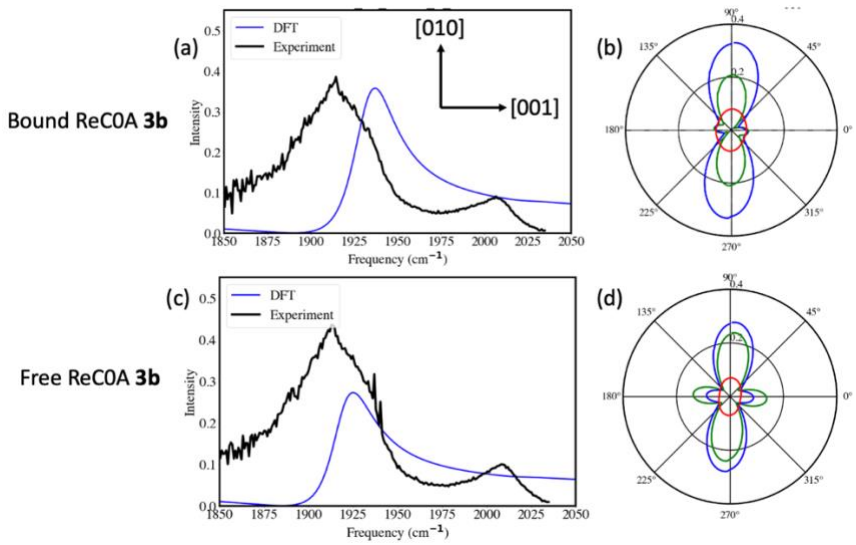

Figure S5. Validation of the free molecule approach to computing VSFG intensities. (a) VSFG line shape and (b) anisotropy for **3b** from Raman calculations including the surface explicitly. (c) VSFG line shape and (b) anisotropy for the free molecule **3b** oriented exactly similar to the bound complex.

Section S6. Refractive indices for theoretical VSFG spectra generation.

The effective second-order susceptibility for PPP fields, $\chi^{(2)}_{q,eff,ppp}$, is dependent on the refractive indices of the medium, bulk material, and interface through Fresnel factors.[11, 12] Both PPP and SSP polarization combinations were measured experimentally. The PPP signal was strong, but the SSP signal was too weak to measure accurately and not conducive to comparison with the calculations; therefore, the strong PPP signal was utilized and the SSP analysis omitted. The PPP signal was computed as given in Equation 2 of Ge et al,[13] including the appropriate contributions from the ZZZ, XXZ, XZX, and ZXX components of the second order susceptibility.

The indices of refraction, *n*, were determined to be 1.000275 (Vis), 1.000273 (IR), and 1.000276 (SFG) for air and 2.52 (Vis), 2.45 (IR), and 2.56 (SFG) for undoped rutile TiO_2. The resulting interfacial refractive indices were calculated as 1.62 (Vis), 1.59 (IR), and 1.64 (SFG) using the method reported by Zhuang *et al.*[14] Input parameters of *n* for air, TiO_2, and the interface were obtained by averaging of *n* over the three fields. These refractive indices were employed to model 5% Nb doped rutile TiO_2. Samples of rutile TiO_2 with up to 6% Nb-doping showed less than a 10% increase in refractive index for wavelengths

in the visible region.[15] In the DFT-based simulations, values of *n* were varied within 10% of the undoped refractive indices with negligible effect on the calculated VSFG spectral features.

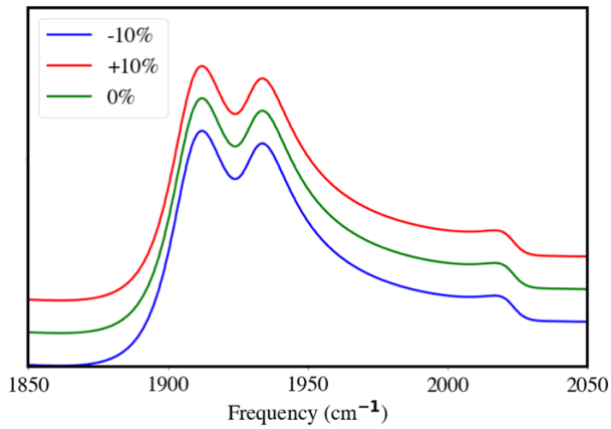

Figure S6. VSFG spectrum of ReOH **6** for for small changes in refractive index. Changing the refractive indices within 10% of the values for undoped rutile TiO_2(100) gave rise to negligible changes to the VSFG spectral features. The y-coordinates were shifted for clarity, as the -10%, 0, and +10% spectra completely overlap. This result supports the conclusion that refractive indices of the undoped material can be used for the 5%-Nb doped sample.

Section S7. Parameters for theoretical calculation of VSFG spectra.

Parameter	Value
Visible beam wavelength	800 nm
Visible beam angle	65º
Infrared beam wavelength	5000 nm
Infrared beam angle	59º
n_{Air}	1.000275 (Vis), 1.000273 (IR), and 1.000276 (SFG)
n_{TiO2}	2.52 (Vis), 2.45 (IR), and 2.56 (SFG)
$n_{interface}$	1.62 (Vis), 1.59 (IR), and 1.64 (SFG)
Peak width (Γ)	11.5 cm^{-1} [A'(2)], 11.5 cm^{-1} [A''], 11.5 cm^{-1} [A'(1)]
Normal mode frequency scaling factor	0.949
Resonant amplitude scaling factor, *k*	1.8

Section S8. Theoretical simulation of VSFG rotational anisotropy. Azimuthal dependence of the PPP intensity was computed by applying the ZYZ Euler rotation matrix, Equation S1, to the hyperpolarizability elements, Equation S2.

$$R_{ia}R_{jb}R_{kc} = Z_{\phi}Z_{\theta}Z_{\psi} = \begin{pmatrix} -\sin\phi\cos\theta\sin\psi + \cos\phi\cos\psi & -\sin\phi\cos\theta\cos\psi - \cos\phi\sin\psi & \sin\phi\sin\theta \\ \cos\phi\cos\theta\cos\psi + \sin\phi\cos\psi & \cos\phi\cos\theta\cos\psi - \sin\phi\sin\psi & -\cos\phi\sin\theta \\ \sin\theta\sin\psi & \sin\theta\cos\psi & \cos\theta \end{pmatrix} \quad \text{(S1)}$$

$$\chi_{ijk}^{(2)} = N_s \sum_{abc} R_{ia}R_{jb}R_{kc}\beta_{abc} \quad \text{(S2)}$$

where N_s in Equation S2 is the molecule number density and the rotation matrices transform hyperpolarizability elements from the molecular (*a*,*b*,*c*) to the laboratory coordinate frame (*i*,*j*,*k*) = (*x*,*y*,*z*) through the Euler angles (θ,ψ,φ). The ZXZ rotation matrix formalism is used for all rotations.

Rotation about the azimuthal angle in the laboratory frame, φ, must be achieved in terms of molecular coordinates for calculation of the azimuthal dependence. Notice that for θ = 0, the molecular *c* axis aligns with the *z* axis, making the Euler angles ψ and φ equivalent, as shown in Figure S7. The molecular c axis for the computations was defined as the surface normal (θ = 0) to yield correspondence with the laboratory frame. Thus, manipulation of the molecular azimuthal angle, ψ, produces the same effect as varying φ in the laboratory frame. The ψ angle was scanned from 0 to 360 degrees in 5-degree increments to compare with experimental measurement of two-fold azimuthal anisotropy.

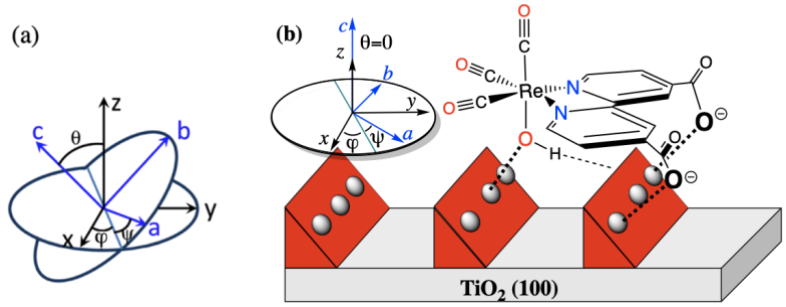

Figure S7. (a) Relationship between laboratory (x, y, z) and molecular (a, b, c) coordinates through the Euler angles, $\theta, \psi, and\ \phi$. (b) Enforced alignment of molecular *c* axis with the surface normal enables correspondence between azimuthal simulations and measurements.

Section S9. Geometry visualizations, dipole derivative vectors, VSFG spectra and anisotropy plots for calculated binding orientations.

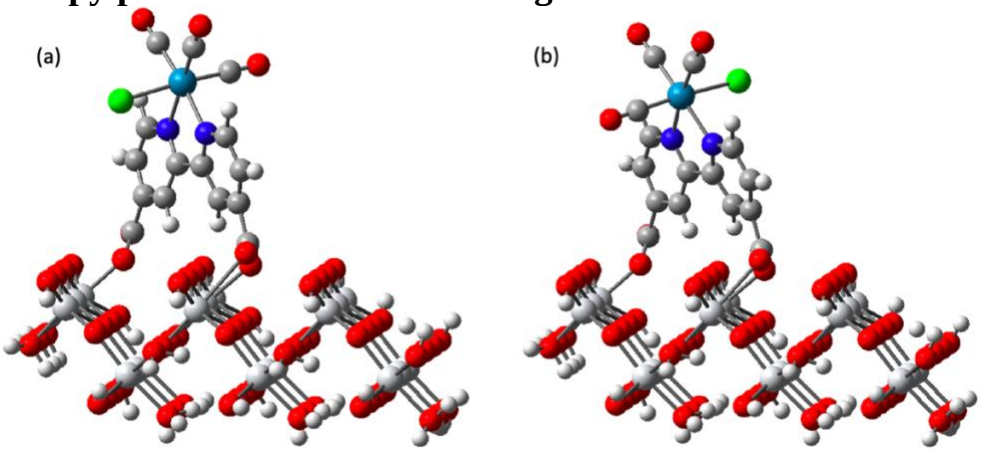

Figure S8. DFT-optimized geometry of ReC0A binding configurations (a) **1a** and (b) **1b**.

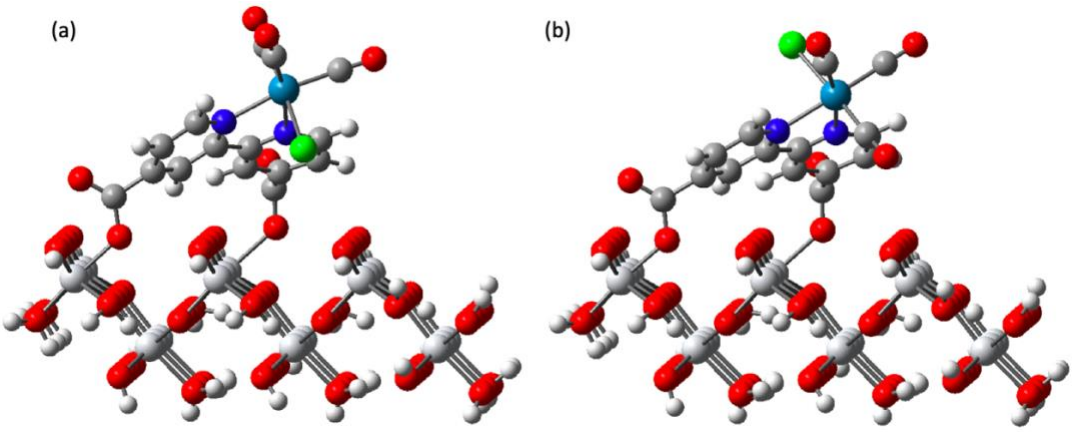

Figure S9. DFT-optimized geometry of ReC0A binding configurations (a) **2a** and (b) **2b**.

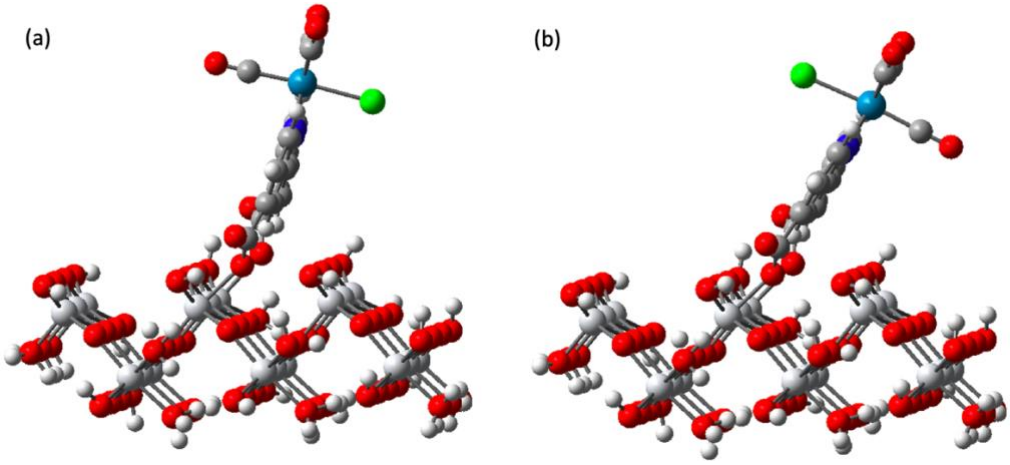

Figure S10. DFT-optimized geometry of ReC0A binding configurations (a) **3a** and (b) **3b**.

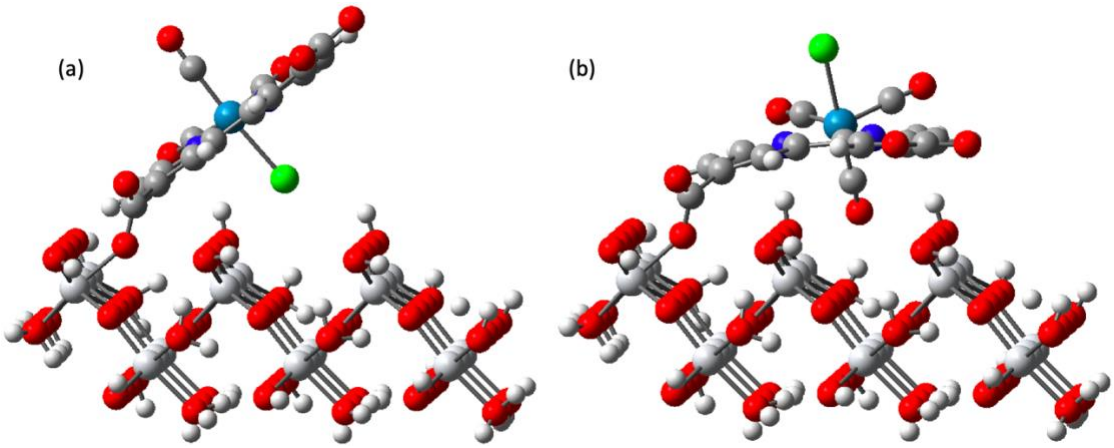

Figure S11. DFT-optimized geometry of ReC0A binding configurations (a) **4a** and (b) **4b**.

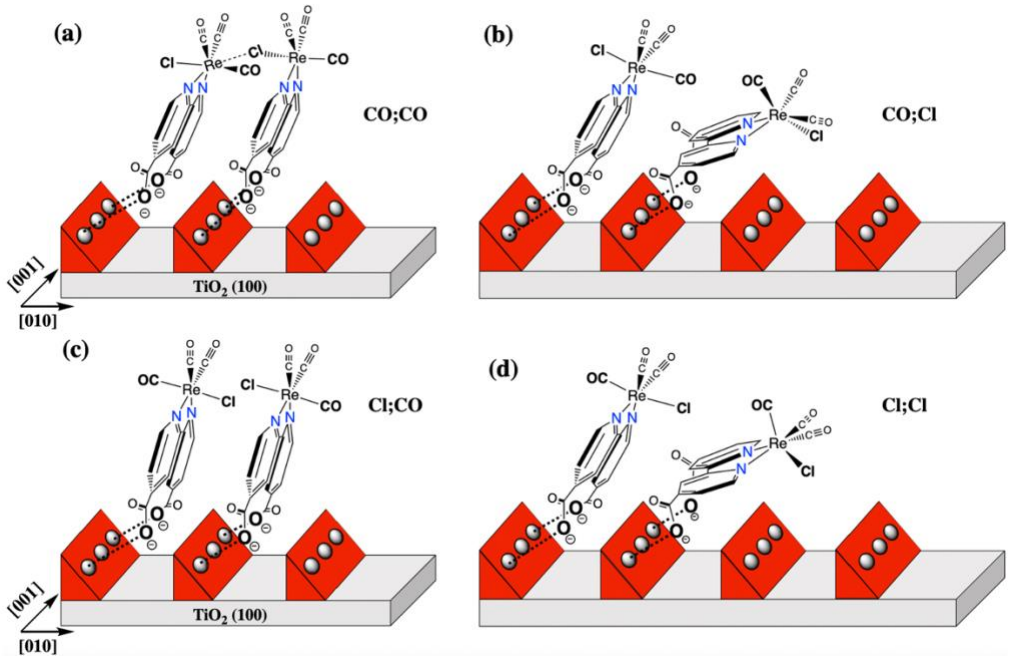

Figure S12. Opitimized ReC0A dimers on TiO_2 (100) surface. The nomenclature shows which axial ligand points toward the surface on the ReC0A molecules from left to right. As shown in the cartoons of (b) and (c), the TiO_2 cluster model was extended to avoid nonphysical edge effects as repulsion of the ReC0A molecules caused dramatic tilting.

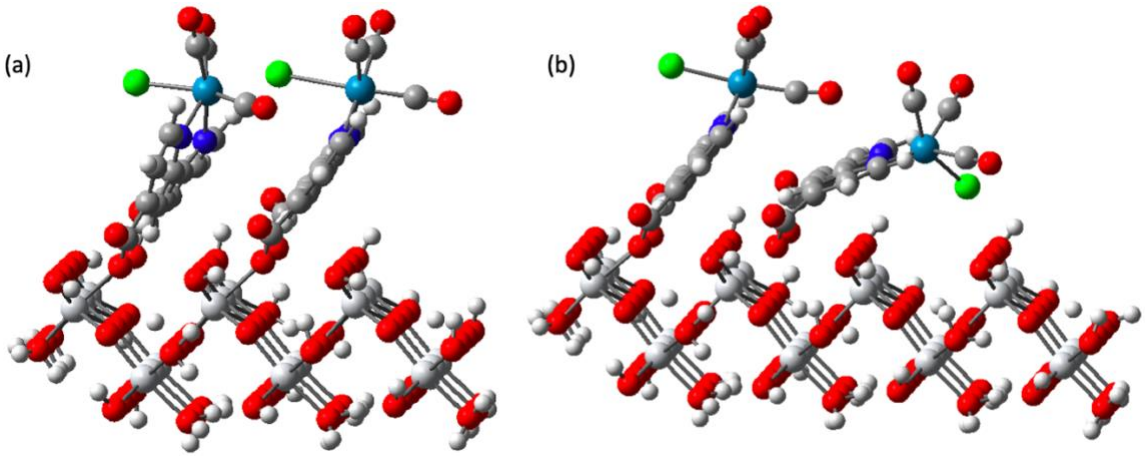

Figure S13. DFT-optimized geometry of ReC0A dimeric configurations with axial (a) CO and CO (b) CO and Cl pointing toward the surface.

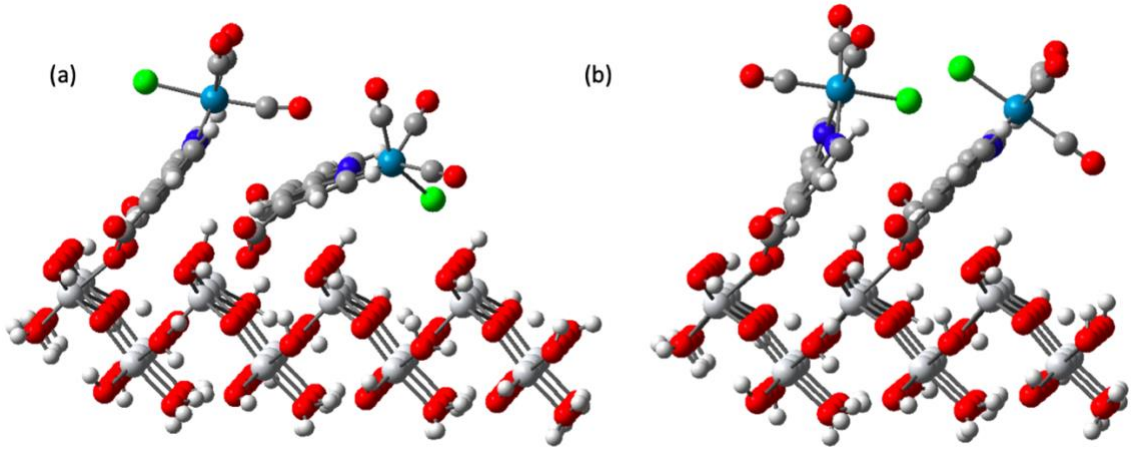

Figure S14. DFT-optimized geometry of ReC0A dimeric configurations with axial (a) CO and CO (b) CO and Cl pointing toward the surface.

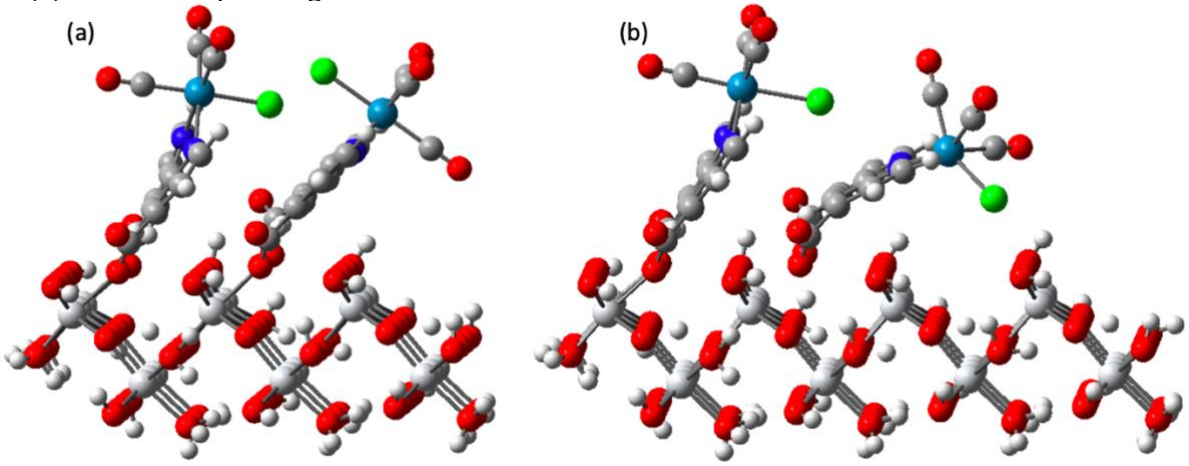

Figure S15. DFT-optimized geometry of ReC0A dimeric configurations with axial (a) Cl and CO (b) Cl and Cl pointing toward the surface.

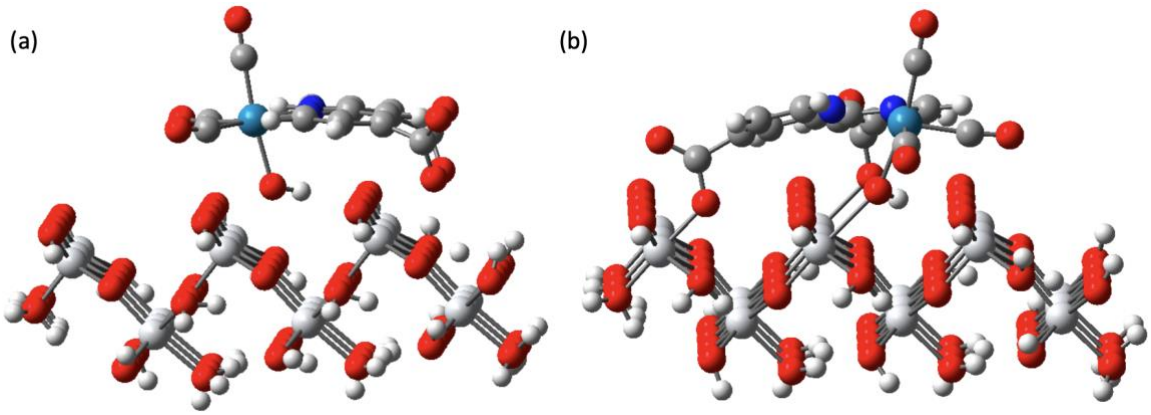

Figure S16. DFT-optimized geometry of ReOH configurations (a) **5** and (b) **6.**

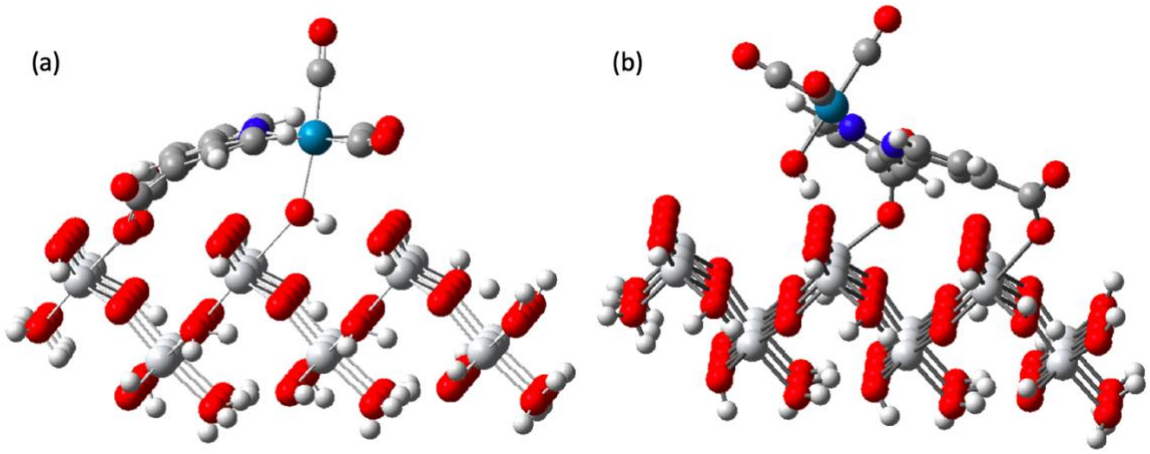

Figure S17. DFT-optimized geometry of ReOH configurations (a) **7** and (b) **8.**

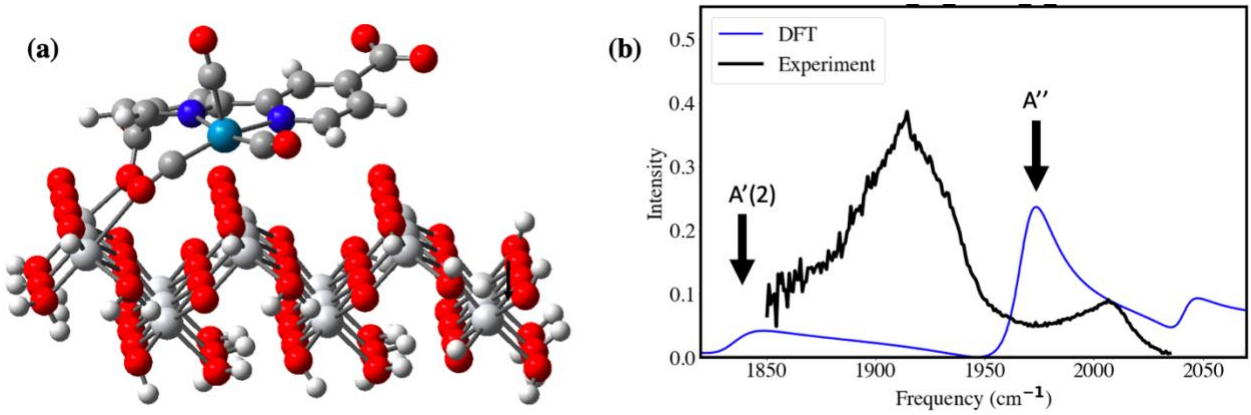

Figure S18. (a) Rhenium complex with CO-Ti (IV) interaction. (b) Comparison of DFT (blue) and experimental SFG (black) spectra shows a large splitting of the lower frequency A'(2) and A'' modes due to the equatorial CO-Ti interaction, contradicting the closely spaced frequencies measured by experimental SFG.

VSFG Spectra

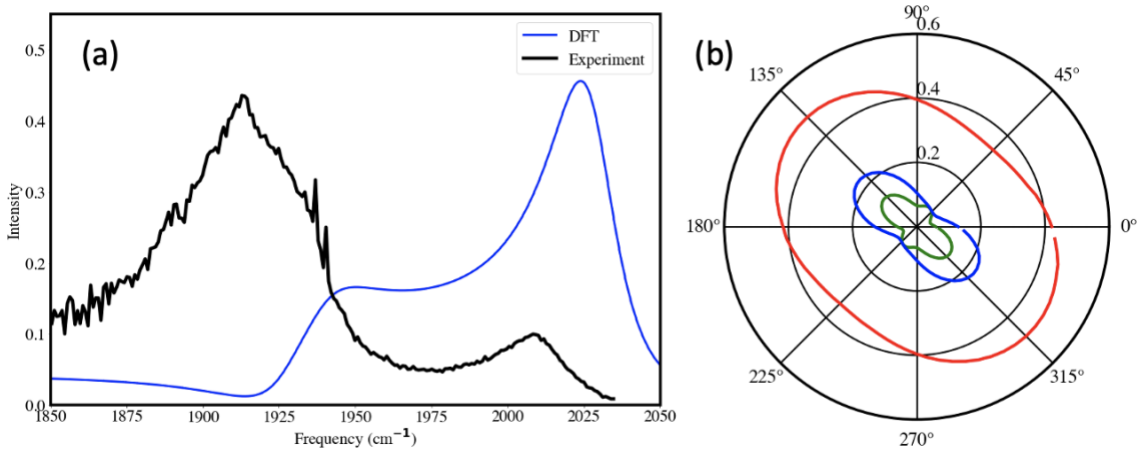

Figure S19. (a) VSFG spectra and (b) anisotropy plots for **1a**.

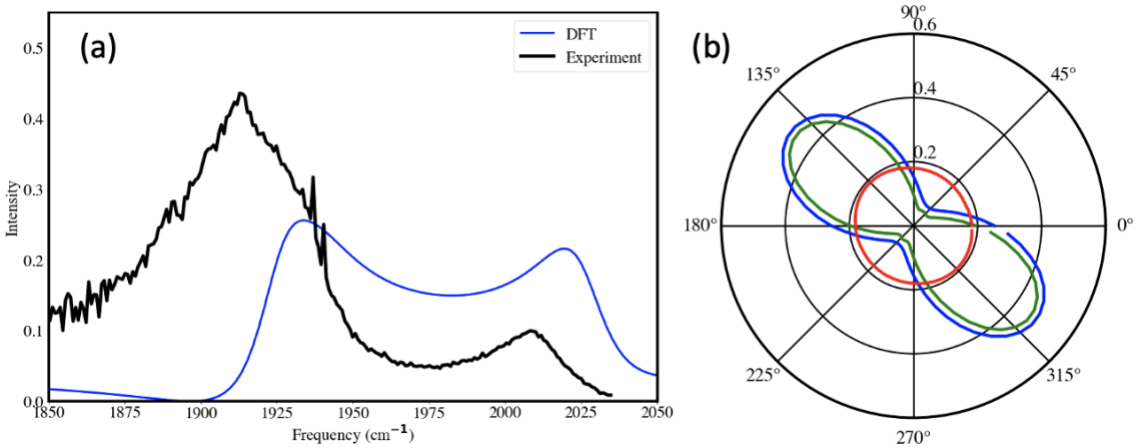

Figure S20. (a) VSFG spectra and (b) anisotropy plots for **1b**.

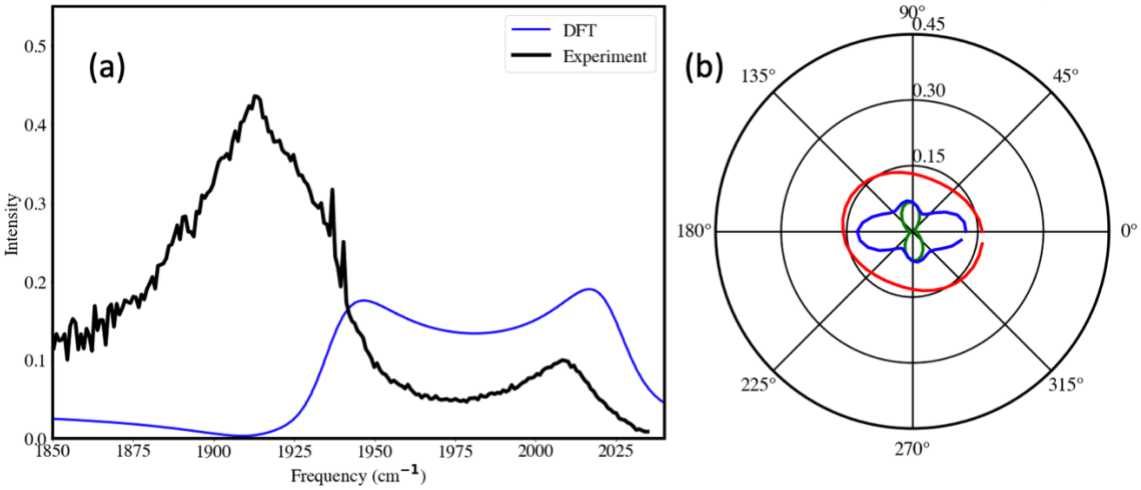

Figure S21. (a) VSFG spectra and (b) anisotropy plots for **2a**.

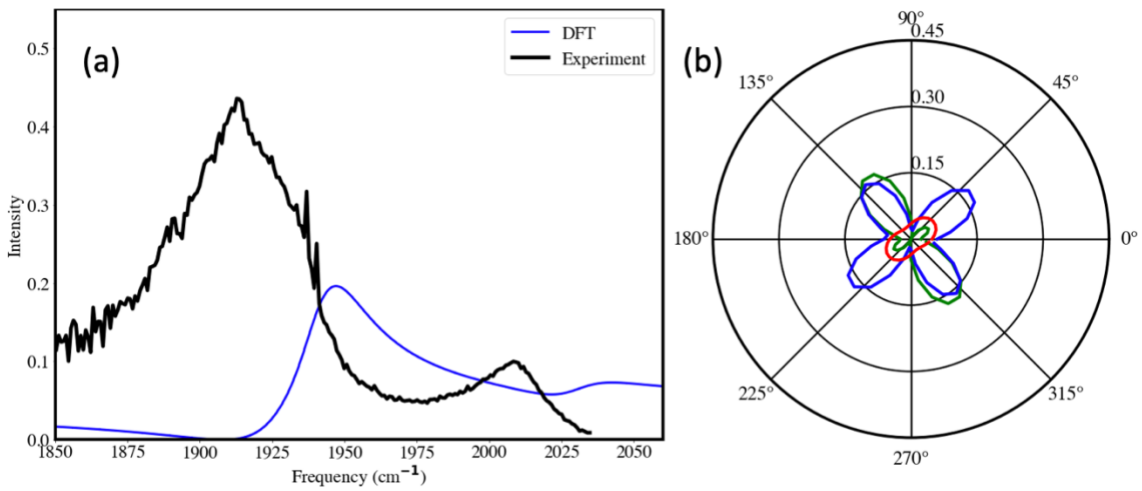

Figure S22. (a) VSFG spectra and (b) anisotropy plots **2b**.

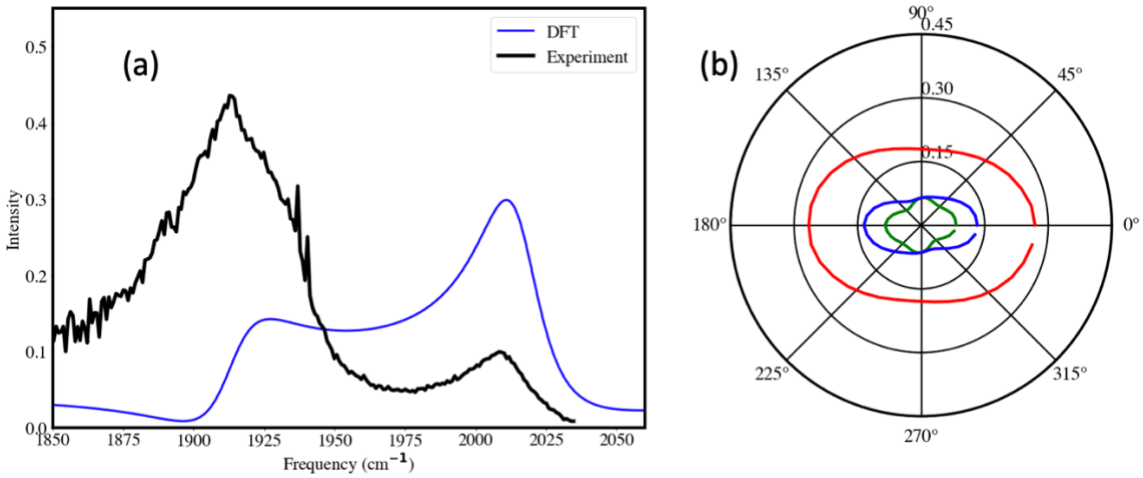

Figure S23. (a) VSFG spectra and (b) anisotropy plots for **3a.**

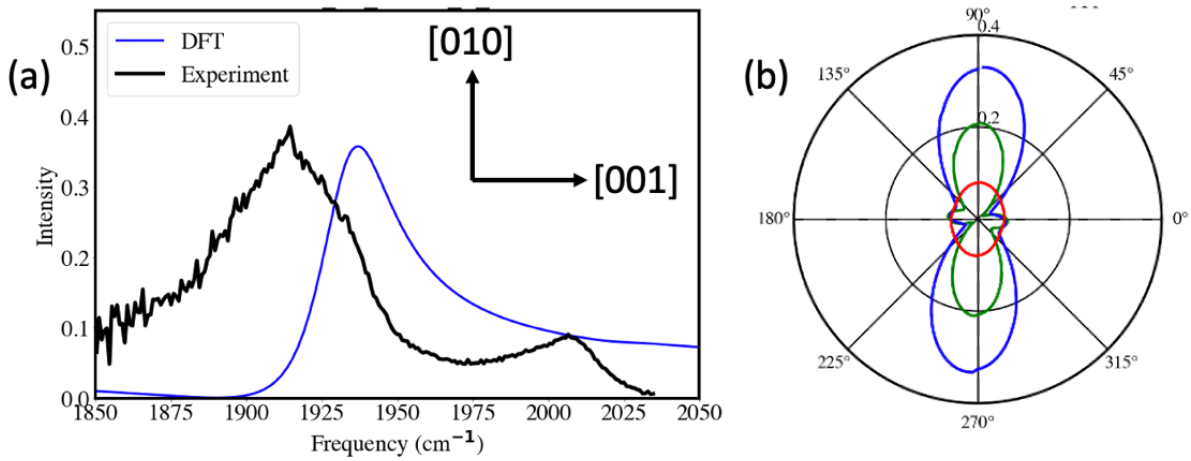

Figure S24. (a) VSFG spectra and (b) anisotropy plots for **3b.**

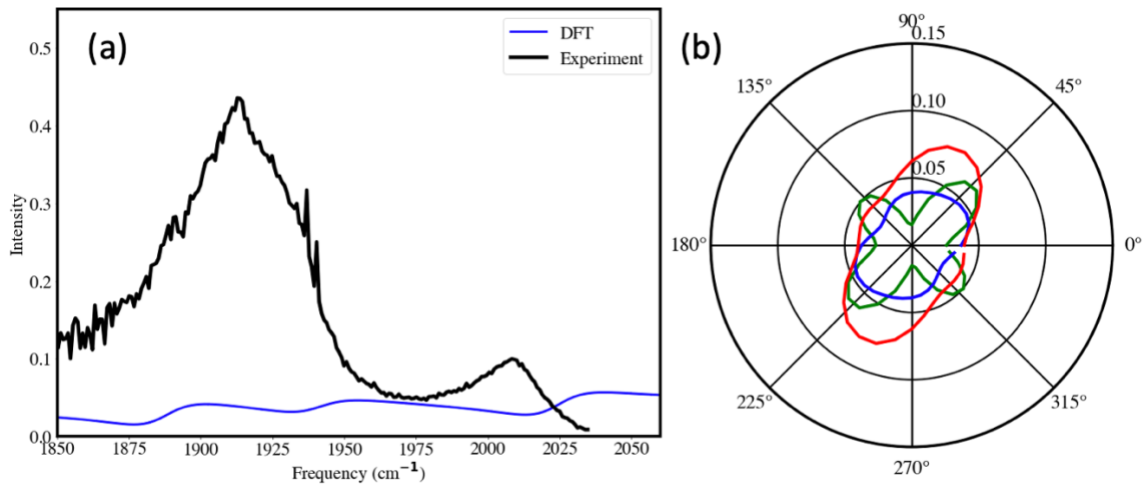

Figure S25. (a) VSFG spectra and (b) anisotropy plots for **4a.**

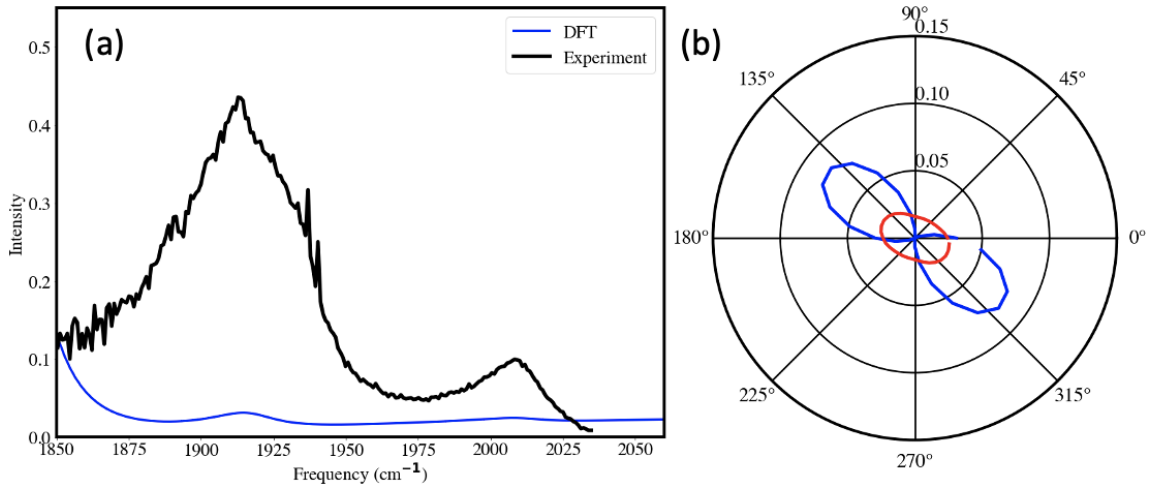

Figure S26. (a) VSFG spectra and (b) anisotropy plots for **4b.**

ReC0A dimers.

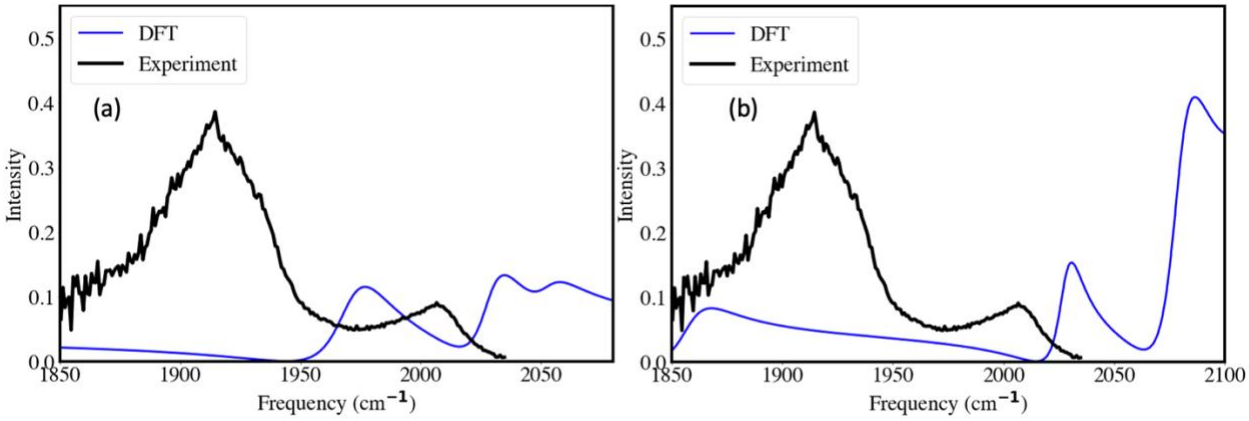

Figure S27. VSFG spectra for ReC0A dimers (a) **CO:CO** and (b) **CO;Cl**. Due to the large deviations in these spectra from experiments, the anisotropy information was not necessary to conclusively rule out these dimers.

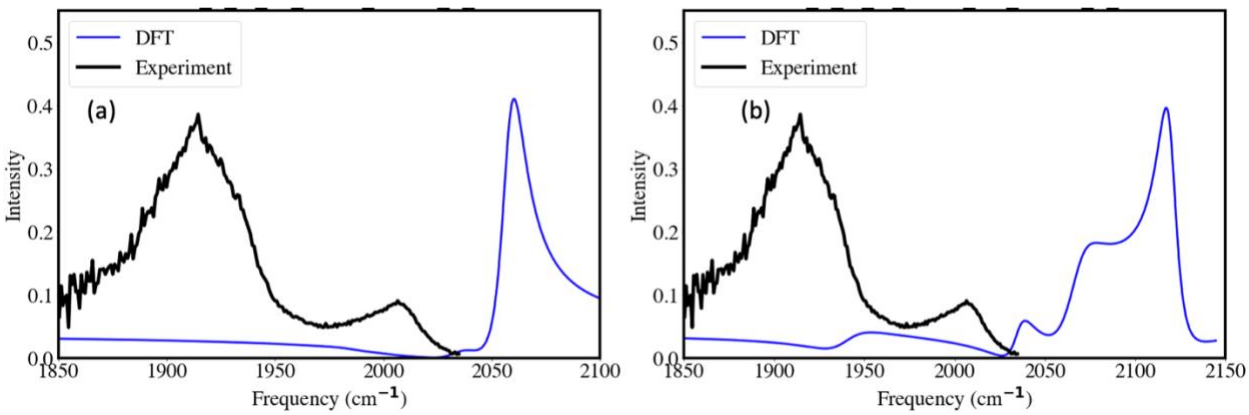

Figure S28. VSFG spectra for ReC0A dimers (a) **Cl:CO** and (b) **Cl;Cl**. Due to exploding Raman activites, plot (a) was constructed with a scaling factor of 0.0015. Despite scaling issues, the high frequency A'(1) mode clearly dominates the SFG spectra of both dimers due to their upright orientation.

ReOH monomers

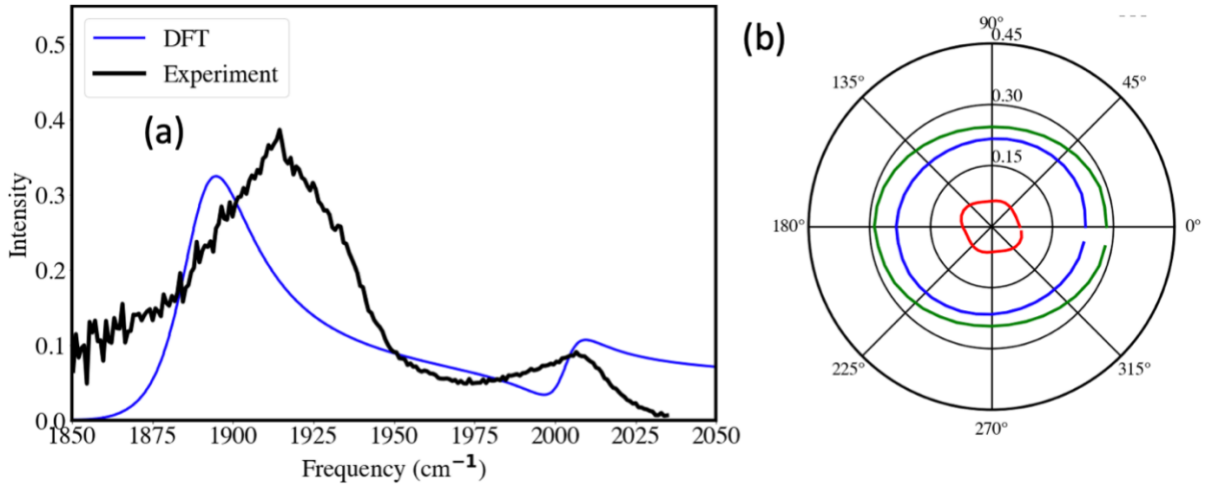

Figure S29. (a) VSFG spectra and (b) anisotropy plot for ReOH **6.** For clarity, the scaling factor *k*=1.2 was used for this plot.

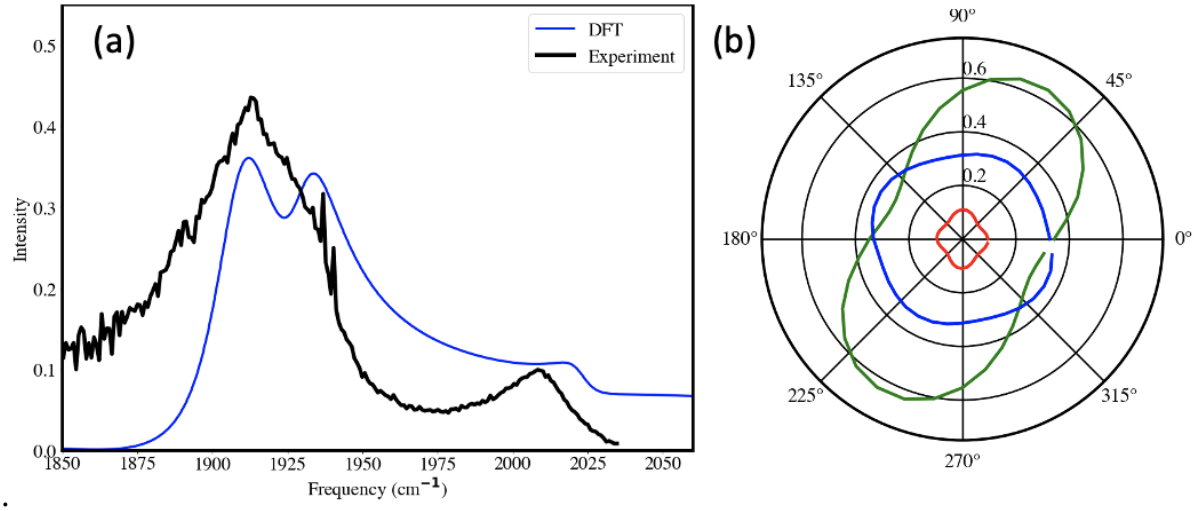

Figure S30. (a) VSFG spectra and (b) anisotropy plots for ReOH **7.**

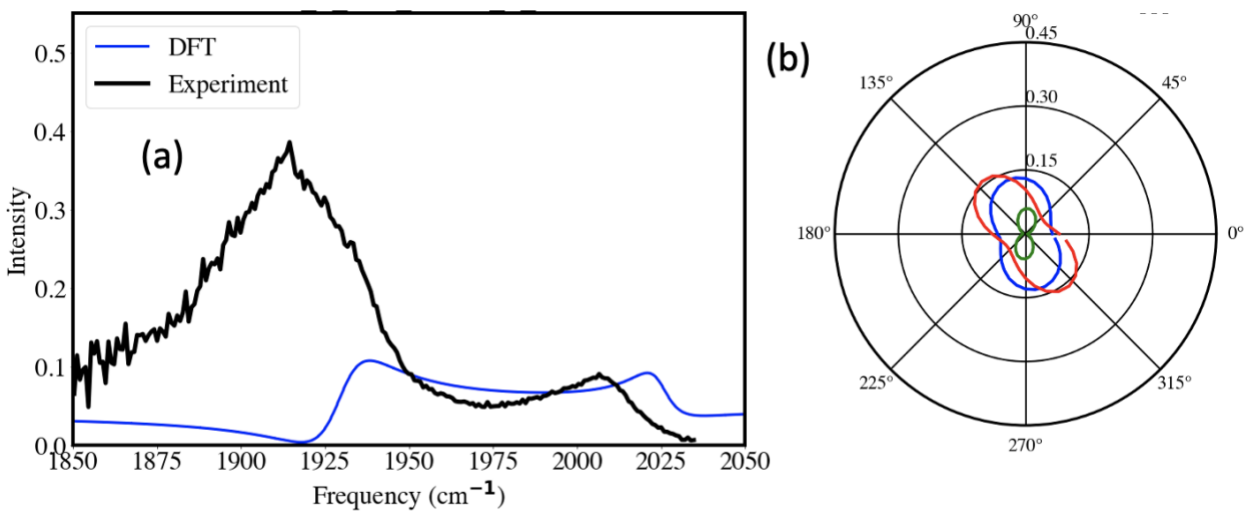

Figure S31. (a) VSFG spectra and (b) anisotropy plots for ReOH **8.** Due to exploding Raman activities, the free molecule approximation was used as discussed in Section 9.

Section S10. Binding orientations for Raman calculations of differentially substituted Rhenium bipyridyl molecules on TiO_2 (100).

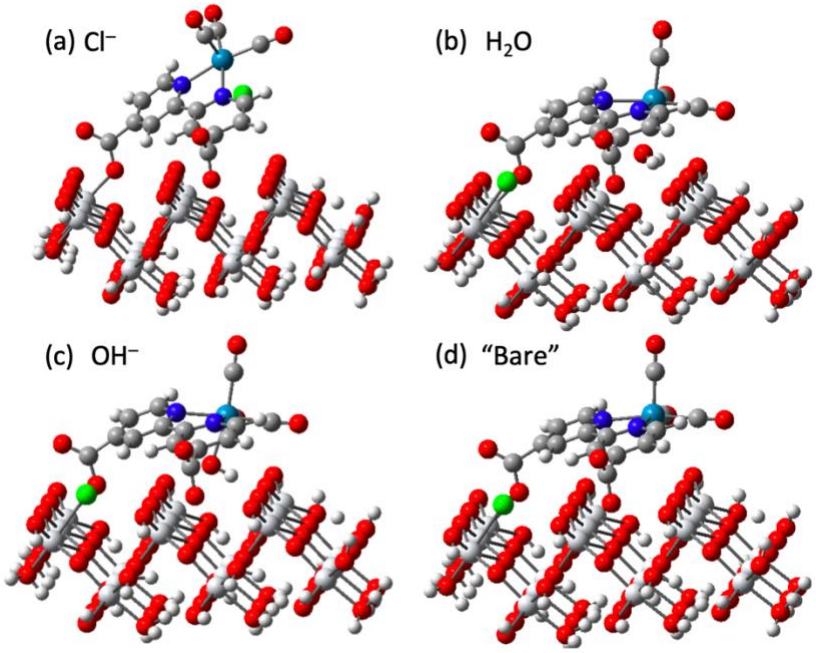

Figure S32. Analogous bidentate binding orientations for Raman calculations (not orientation specific) to determine the vibrational red shift for the carbonyl stretching modes. For ligand exchanged configurations, chloride was still included as a surface ligand in each simulation to maintain consistency in atomistic details across these calculations.

Section S11. References

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Section S12. Coordinates of optimized geometries.

Coordinates of ReC0A monomer 1a.

O	11.60942000	1.48394000	4.13357000
O	11.60942000	4.45183000	4.13357000
O	11.60942000	7.41972000	4.13357000
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O	16.25319000	4.45183000	4.13357000
O	16.25319000	7.41972000	4.13357000
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Coordinates of ReC0A monomer 1b.

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Ti	7.80430000	2.96791000	7.82303000
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H	2.62029100	11.30687500	8.52453900
H	7.29482600	11.26288200	8.41179200
H	7.33960300	0.67897600	8.28331500
H	8.44004600	11.09632200	6.60247700
H	9.60385500	10.06241000	6.36632000
H	4.98380300	10.08413600	6.34889600
H	3.78384900	11.01175400	6.50624900
H	13.71220900	11.11627600	7.68430400
H	11.96090100	11.24133600	8.36942600
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H	16.12825900	0.39877200	7.31745700
H	16.33454400	8.47399700	7.20521000
H	9.78360300	9.26185800	3.92023900
H	2.37768100	8.86253300	5.58942800
H	1.18408300	9.53022900	6.43559100
H	2.45853100	5.93033400	5.62517100
H	1.23831800	5.25053600	6.41129900
H	2.50156700	2.87113700	5.65366000
H	1.32663000	2.19766200	6.47555100
H	14.16117900	-0.76352000	5.20951100
H	13.83610600	9.77775700	5.05460000
H	7.53035900	0.26272700	6.37368200
H	6.54861200	-0.84679200	5.96775400
H	11.02350100	-0.86180700	5.97565300
H	12.12675500	0.17418800	6.13605900
H	16.92046600	1.05920800	4.71488800
H	15.95427800	0.78179700	3.52823800
H	17.00398600	4.51111100	4.75814900
H	16.26907400	3.53128500	3.80250600
H	16.21655200	6.53540700	3.72195100
H	15.98405900	8.06867700	3.46409500
H	12.22278600	6.62455700	4.19962600
H	12.30374300	8.13769000	4.29998800

H	12.54271100	4.13682100	4.35125800
H	11.35984600	4.03634000	3.29550600
H	12.35772800	2.14059500	4.34003500
H	12.19260500	0.67157500	4.11608900
H	7.55370800	6.61289000	4.15445300
H	7.66630000	8.13550600	4.28067800
H	7.88629600	4.12256800	4.34414700
H	6.68644500	4.01347700	3.31338900
H	7.75514700	2.06748100	4.33924200
H	7.42691500	0.63798700	3.93525300
H	4.74507800	-0.84525300	5.11993600
H	4.92500400	9.11652400	3.76716600
H	14.58819800	9.96011700	6.89676300
C	6.45736600	7.54055800	12.62331700
C	6.10306000	8.14956800	11.42376200
C	5.19586100	9.19101200	11.42416300
C	4.65186200	9.59048200	12.64663800
C	4.97573200	8.86963800	13.78704100
H	6.51405700	7.80932100	10.48052900
H	3.96148200	10.42476400	12.70265600
H	4.52741200	9.10029100	14.74690100
C	7.45863100	6.46399500	12.64713800
C	8.23778500	6.21955900	11.53577000
N	7.52544300	5.69406900	13.75164900
C	8.98611700	5.05473200	11.44335600
H	8.22010900	6.87017600	10.67445900
C	8.33480600	4.62168000	13.71074400
C	9.03558700	4.23761700	12.56923700
H	8.37920300	4.03342200	14.62057800
H	9.58866800	3.30483600	12.54892400
C	4.82435500	9.85709700	10.11777100
O	4.62462000	8.99129000	9.14888100
O	4.70599300	11.06842800	10.06814400
C	9.41497800	4.70163000	10.01372700
O	9.47897400	3.49985800	9.72794800
O	9.43500400	5.71941600	9.24846400
Re	6.28382400	6.43150800	15.44087800
N	5.84733600	7.84781100	13.78186200
C	5.23282800	7.31172600	16.76785100
C	6.87275800	5.15767600	16.73878600
O	4.58237200	7.86966100	17.55297600
O	7.24307600	4.37846700	17.51388000
Cl	8.22654400	7.94727900	15.90596000
C	4.81786200	5.32130500	14.94672000
O	3.91201400	4.65186500	14.65595200

Coordinates of ReC0A monomer 2a.

O	11.60942000	1.48394000	4.13357000
O	11.60942000	4.45183000	4.13357000
O	11.60942000	7.41972000	4.13357000
O	16.25319000	1.48394000	4.13357000
O	16.25319000	4.45183000	4.13357000
O	16.25319000	7.41972000	4.13357000
O	6.96566000	1.48394000	4.13357000
O	6.96566000	4.45183000	4.13357000
O	6.96566000	7.41972000	4.13357000
O	13.92680000	0.00000000	4.66430000
O	13.92680000	2.96789000	4.66430000
O	13.92680000	5.93578000	4.66430000
O	13.92680000	8.90366000	4.66430000
O	4.63927000	0.00000000	4.66430000
O	4.63927000	2.96789000	4.66430000
O	4.63927000	5.93578000	4.66430000
O	4.63927000	8.90366000	4.66430000
O	9.28303000	0.00000000	4.66430000
O	9.28303000	2.96789000	4.66430000
O	9.28303000	5.93578000	4.66430000
O	9.28303000	8.90366000	4.66430000
O	1.93144000	2.96789000	6.47971000
O	1.93144000	5.93578000	6.47971000
O	1.93144000	8.90366000	6.47971000
O	11.21897000	0.00000000	6.47971000
O	11.21897000	2.96789000	6.47971000
O	11.21897000	5.93578000	6.47971000
O	11.21897000	8.90366000	6.47971000
O	15.86274000	0.00000000	6.47971000
O	15.86274000	2.96789000	6.47971000
O	15.86274000	5.93578000	6.47971000
O	15.86274000	8.90366000	6.47971000
O	6.57521000	0.00000000	6.47971000
O	6.57521000	2.96789000	6.47971000
O	6.57521000	5.93578000	6.47971000
O	6.57521000	8.90366000	6.47971000
O	13.64470000	1.48394000	7.05216000
O	13.64470000	10.38760000	7.05216000
O	13.64470000	4.45183000	7.05216000
O	13.64470000	7.41972000	7.05216000
O	4.35717000	1.48394000	7.05216000
O	4.35717000	10.38760000	7.05216000
O	4.35717000	4.45183000	7.05216000
O	4.35717000	7.41972000	7.05216000
O	9.00094000	1.48394000	7.05216000

O	9.00094000	10.38760000	7.05216000
O	9.00094000	4.45183000	7.05216000
O	9.00094000	7.41972000	7.05216000
O	11.96008000	1.48394000	8.82195000
O	11.96008000	10.38760000	8.82195000
O	11.96008000	4.45183000	8.82195000
O	11.96008000	7.41972000	8.82195000
O	2.67255000	1.48394000	8.82195000
O	2.67255000	10.38760000	8.82195000
O	2.67255000	4.45183000	8.82195000
O	2.67255000	7.41972000	8.82195000
O	7.31635000	1.48395300	8.82186600
O	7.31627500	10.38762000	8.82201200
O	7.31631000	4.45183000	8.82195000
O	7.31631000	7.41972000	8.82195000
Ti	10.17496000	1.48394000	5.55848000
Ti	10.17496000	4.45183000	5.55848000
Ti	10.17496000	7.41972000	5.55848000
Ti	14.81872000	1.48394000	5.55848000
Ti	14.81872000	4.45183000	5.55848000
Ti	14.81872000	7.41972000	5.55848000
Ti	5.53119000	1.48394000	5.55848000
Ti	5.53119000	4.45183000	5.55848000
Ti	5.53119000	7.41972000	5.55848000
Ti	12.44806000	2.96789000	7.82300000
Ti	12.44806000	5.93578000	7.82300000
Ti	12.44806000	8.90366000	7.82300000
Ti	3.16053000	2.96789000	7.82300000
Ti	3.16053000	5.93578000	7.82300000
Ti	3.16053000	8.90366000	7.82300000
Ti	7.80430000	2.96791000	7.82303000
Ti	7.80430000	5.93578000	7.82300000
Ti	7.80430000	8.90367200	7.82298200
H	3.24777500	0.74192500	8.56773600
H	3.03049100	11.28431300	8.75843400
H	7.19879400	10.31109400	9.77865500
H	8.07881300	0.90953400	8.98697000
H	9.82249600	9.99070100	6.62016400
H	9.33408000	10.99049300	7.73419200
H	5.20160100	10.53126900	7.54777600
H	4.73269800	10.07258400	6.17123500
H	13.71220900	11.11627600	7.68430400
H	11.67471100	10.23025000	9.73159200
H	12.72306100	0.89172300	8.71601200
H	9.75853800	-0.83745800	4.62855500
H	16.12825900	0.39877200	7.31745700

H	16.33454400	8.47399700	7.20521000
H	9.78360300	9.26185800	3.92023900
H	2.37768100	8.86253300	5.58942800
H	1.18408300	9.53022900	6.43559100
H	2.45853100	5.93033400	5.62517100
H	1.23831800	5.25053600	6.41129900
H	2.50156700	2.87113700	5.65366000
H	1.32663000	2.19766200	6.47555100
H	14.16117900	-0.76352000	5.20951100
H	13.83610600	9.77775700	5.05460000
H	6.68301700	0.31528100	7.41862000
H	7.51708400	-0.03537500	6.17724600
H	12.19659500	0.28138800	6.48769800
H	11.00104000	0.18184500	7.42414100
H	16.92046600	1.05920800	4.71488800
H	15.95427800	0.78179700	3.52823800
H	17.00398600	4.51111100	4.75814900
H	16.26907400	3.53128500	3.80250600
H	16.21655200	6.53540700	3.72195100
H	15.98405900	8.06867700	3.46409500
H	12.22278600	6.62455700	4.19962600
H	12.30374300	8.13769000	4.29998800
H	12.54271100	4.13682100	4.35125800
H	11.35984600	4.03634000	3.29550600
H	12.35772800	2.14059500	4.34003500
H	12.19260500	0.67157500	4.11608900
H	7.55370800	6.61289000	4.15445300
H	7.66630000	8.13550600	4.28067800
H	7.88629600	4.12256800	4.34414700
H	6.68644500	4.01347700	3.31338900
H	7.75514700	2.06748100	4.33924200
H	7.42691500	0.63798700	3.93525300
H	4.74507800	-0.84525300	5.11993600
H	4.92500400	9.11652400	3.76716600
H	14.58819800	9.96011700	6.89676300
C	8.85144600	5.23569800	11.97932500
C	8.79910200	6.43883900	11.26682500
C	9.95752700	7.20270100	11.10372900
C	11.14747300	6.67745800	11.60762200
C	11.12834800	5.48906400	12.30730100
H	7.86591800	6.79281700	10.84470100
H	12.07425900	7.21354300	11.45659500
H	12.03480800	5.06628600	12.72276900
C	7.70386900	4.30386900	12.15705300
C	6.55484200	4.34108200	11.36933900
N	7.89943300	3.30926700	13.04957700

C	5.64440200	3.29008800	11.42404800
H	6.41920400	5.13411100	10.65049600
C	6.98251900	2.33914300	13.16015800
C	5.85393000	2.28924400	12.36876800
H	7.19382000	1.56678900	13.88945400
H	5.15025400	1.47079900	12.46754600
C	10.02881900	8.61066500	10.49238100
O	9.33508200	8.91032900	9.48686700
O	10.81639400	9.37553300	11.08835200
C	4.41633400	3.18308900	10.53954100
O	4.66015600	3.14685300	9.27308600
O	3.32891100	3.11455100	11.10571300
Re	9.84275000	3.19605800	14.05261000
N	9.99999800	4.80384700	12.53958200
C	11.67374700	3.15937300	14.62120000
C	9.46170100	1.77047600	15.26133900
O	12.78646500	3.15419300	14.94486800
O	9.19112100	0.90255200	15.98592100
O	9.12565100	5.26075400	16.20456500
C	9.39988100	4.48377700	15.38041700
Cl	10.29943500	1.57152600	12.21326400

Coordinates of ReC0A monomer 2b.

O	11.60942000	1.48394000	4.13357000
O	11.60942000	4.45183000	4.13357000
O	11.60942000	7.41972000	4.13357000
O	16.25319000	1.48394000	4.13357000
O	16.25319000	4.45183000	4.13357000
O	16.25319000	7.41972000	4.13357000
O	6.96566000	1.48394000	4.13357000
O	6.96566000	4.45183000	4.13357000
O	6.96566000	7.41972000	4.13357000
O	13.92680000	0.00000000	4.66430000
O	13.92680000	2.96789000	4.66430000
O	13.92680000	5.93578000	4.66430000
O	13.92680000	8.90366000	4.66430000
O	4.63927000	0.00000000	4.66430000
O	4.63927000	2.96789000	4.66430000
O	4.63927000	5.93578000	4.66430000
O	4.63927000	8.90366000	4.66430000
O	9.28303000	0.00000000	4.66430000
O	9.28303000	2.96789000	4.66430000
O	9.28303000	5.93578000	4.66430000
O	9.28303000	8.90366000	4.66430000
O	1.93144000	2.96789000	6.47971000
O	1.93144000	5.93578000	6.47971000

O	1.93144000	8.90366000	6.47971000
O	11.21897000	0.00000000	6.47971000
O	11.21897000	2.96789000	6.47971000
O	11.21897000	5.93578000	6.47971000
O	11.21897000	8.90366000	6.47971000
O	15.86274000	0.00000000	6.47971000
O	15.86274000	2.96789000	6.47971000
O	15.86274000	5.93578000	6.47971000
O	15.86274000	8.90366000	6.47971000
O	6.57521000	0.00000000	6.47971000
O	6.57521000	2.96789000	6.47971000
O	6.57521000	5.93578000	6.47971000
O	6.57521000	8.90366000	6.47971000
O	13.64470000	1.48394000	7.05216000
O	13.64470000	10.38760000	7.05216000
O	13.64470000	4.45183000	7.05216000
O	13.64470000	7.41972000	7.05216000
O	4.35717000	1.48394000	7.05216000
O	4.35717000	10.38760000	7.05216000
O	4.35717000	4.45183000	7.05216000
O	4.35717000	7.41972000	7.05216000
O	9.00094000	1.48394000	7.05216000
O	9.00094000	10.38760000	7.05216000
O	9.00094000	4.45183000	7.05216000
O	9.00094000	7.41972000	7.05216000
O	11.96008000	1.48394000	8.82195000
O	11.96008000	10.38760000	8.82195000
O	11.96008000	4.45183000	8.82195000
O	11.96008000	7.41972000	8.82195000
O	2.67255000	1.48394000	8.82195000
O	2.67255000	10.38760000	8.82195000
O	2.67255000	4.45183000	8.82195000
O	2.67255000	7.41972000	8.82195000
O	7.31635000	1.48395300	8.82186600
O	7.31627500	10.38762000	8.82201200
O	7.31631000	4.45183000	8.82195000
O	7.31631000	7.41972000	8.82195000
Ti	10.17496000	1.48394000	5.55848000
Ti	10.17496000	4.45183000	5.55848000
Ti	10.17496000	7.41972000	5.55848000
Ti	14.81872000	1.48394000	5.55848000
Ti	14.81872000	4.45183000	5.55848000
Ti	14.81872000	7.41972000	5.55848000
Ti	5.53119000	1.48394000	5.55848000
Ti	5.53119000	4.45183000	5.55848000
Ti	5.53119000	7.41972000	5.55848000

Ti	12.44806000	2.96789000	7.82300000
Ti	12.44806000	5.93578000	7.82300000
Ti	12.44806000	8.90366000	7.82300000
Ti	3.16053000	2.96789000	7.82300000
Ti	3.16053000	5.93578000	7.82300000
Ti	3.16053000	8.90366000	7.82300000
Ti	7.80430000	2.96791000	7.82303000
Ti	7.80430000	5.93578000	7.82300000
Ti	7.80430000	8.90367200	7.82298200
H	3.24777500	0.74192500	8.56773600
H	3.03049100	11.28431300	8.75843400
H	8.07872400	10.96204800	8.98717000
H	8.07881300	0.90953400	8.98697000
H	9.82249600	9.99070100	6.62016400
H	9.33408000	10.99049300	7.73419200
H	5.20160100	10.53126900	7.54777600
H	4.73269800	10.07258400	6.17123500
H	13.71220900	11.11627600	7.68430400
H	12.72306100	10.97981800	8.71601400
H	12.72306100	0.89172300	8.71601200
H	9.75853800	-0.83745800	4.62855500
H	16.12825900	0.39877200	7.31745700
H	16.33454400	8.47399700	7.20521000
H	9.78360300	9.26185800	3.92023900
H	2.37768100	8.86253300	5.58942800
H	1.18408300	9.53022900	6.43559100
H	2.45853100	5.93033400	5.62517100
H	1.23831800	5.25053600	6.41129900
H	2.50156700	2.87113700	5.65366000
H	1.32663000	2.19766200	6.47555100
H	14.16117900	-0.76352000	5.20951100
H	13.83610600	9.77775700	5.05460000
H	6.68301700	0.31528100	7.41862000
H	7.51708400	-0.03537500	6.17724600
H	12.19659500	0.28138800	6.48769800
H	11.00104000	0.18184500	7.42414100
H	16.92046600	1.05920800	4.71488800
H	15.95427800	0.78179700	3.52823800
H	17.00398600	4.51111100	4.75814900
H	16.26907400	3.53128500	3.80250600
H	16.21655200	6.53540700	3.72195100
H	15.98405900	8.06867700	3.46409500
H	12.22278600	6.62455700	4.19962600
H	12.30374300	8.13769000	4.29998800
H	12.54271100	4.13682100	4.35125800
H	11.35984600	4.03634000	3.29550600

H	12.35772800	2.14059500	4.34003500
H	12.19260500	0.67157500	4.11608900
H	7.55370800	6.61289000	4.15445300
H	7.66630000	8.13550600	4.28067800
H	7.88629600	4.12256800	4.34414700
H	6.68644500	4.01347700	3.31338900
H	7.75514700	2.06748100	4.33924200
H	7.42691500	0.63798700	3.93525300
H	4.74507800	-0.84525300	5.11993600
H	4.92500400	9.11652400	3.76716600
H	14.58819800	9.96011700	6.89676300
C	8.77599200	5.66004300	12.09123500
C	8.57593300	6.82978700	11.36674800
C	9.58662900	7.79081100	11.27662300
C	10.77483100	7.53570000	11.95541600
C	10.89630000	6.36944300	12.68932800
H	7.65277200	6.99339100	10.82901400
H	11.60270400	8.23267800	11.90153700
H	11.80397600	6.14578000	13.23760300
C	7.81249700	4.52519400	12.10489100
C	6.62727800	4.50430100	11.36988900
N	8.21259700	3.44172500	12.80460700
C	5.87452800	3.33464100	11.28521100
H	6.32306400	5.38088400	10.81476900
C	7.46631400	2.33031200	12.76449400
C	6.30997700	2.23150900	12.01521600
H	7.82867200	1.49561700	13.35328400
H	5.75390100	1.30104500	11.99609000
C	9.41658200	9.08098300	10.47624000
O	9.43513400	8.93096400	9.20996200
O	9.30372800	10.13612500	11.10037100
C	4.57750600	3.21984300	10.49341400
O	4.72053800	3.12800900	9.21473400
O	3.53443400	3.20182500	11.13851200
Re	10.00938100	3.66775900	14.05488000
N	9.92580100	5.44911400	12.76887000
C	11.51721600	4.16627100	15.11639700
C	9.77528100	2.11522600	15.13839700
O	12.43124900	4.49852800	15.75086600
O	9.59941900	1.16102000	15.77937000
Cl	8.44951300	5.00395300	15.52672400
C	11.13641700	2.69588900	12.85414100
O	11.83674000	2.08017200	12.16750700

Coordinates of ReC0A monomer 3a.

O	11.60942000	1.48394000	4.13357000

O	11.60942000	4.45183000	4.13357000
O	11.60942000	7.41972000	4.13357000
O	16.25319000	1.48394000	4.13357000
O	16.25319000	4.45183000	4.13357000
O	16.25319000	7.41972000	4.13357000
O	6.96566000	1.48394000	4.13357000
O	6.96566000	4.45183000	4.13357000
O	6.96566000	7.41972000	4.13357000
O	13.92680000	0.00000000	4.66430000
O	13.92680000	2.96789000	4.66430000
O	13.92680000	5.93578000	4.66430000
O	13.92680000	8.90366000	4.66430000
O	4.63927000	0.00000000	4.66430000
O	4.63927000	2.96789000	4.66430000
O	4.63927000	5.93578000	4.66430000
O	4.63927000	8.90366000	4.66430000
O	9.28303000	0.00000000	4.66430000
O	9.28303000	2.96789000	4.66430000
O	9.28303000	5.93578000	4.66430000
O	9.28303000	8.90366000	4.66430000
O	1.93144000	2.96789000	6.47971000
O	1.93144000	5.93578000	6.47971000
O	1.93144000	8.90366000	6.47971000
O	11.21897000	0.00000000	6.47971000
O	11.21897000	2.96789000	6.47971000
O	11.21897000	5.93578000	6.47971000
O	11.21897000	8.90366000	6.47971000
O	15.86274000	0.00000000	6.47971000
O	15.86274000	2.96789000	6.47971000
O	15.86274000	5.93578000	6.47971000
O	15.86274000	8.90366000	6.47971000
O	6.57521000	0.00000000	6.47971000
O	6.57521000	2.96789000	6.47971000
O	6.57521000	5.93578000	6.47971000
O	6.57521000	8.90366000	6.47971000
O	13.64470000	1.48394000	7.05216000
O	13.64470000	10.38760000	7.05216000
O	13.64470000	4.45183000	7.05216000
O	13.64470000	7.41972000	7.05216000
O	4.35717000	1.48394000	7.05216000
O	4.35717000	10.38760000	7.05216000
O	4.35717000	4.45183000	7.05216000
O	4.35717000	7.41972000	7.05216000
O	9.00094000	1.48394000	7.05216000
O	9.00094000	10.38760000	7.05216000
O	9.00094000	4.45183000	7.05216000

O	9.00094000	7.41972000	7.05216000
O	11.96008000	1.48394000	8.82195000
O	11.96008000	10.38760000	8.82195000
O	11.96008000	4.45183000	8.82195000
O	11.96008000	7.41972000	8.82195000
O	2.67255000	1.48394000	8.82195000
O	2.67255000	10.38760000	8.82195000
O	2.67255000	4.45183000	8.82195000
O	2.67255000	7.41972000	8.82195000
O	7.31635000	1.48395300	8.82186600
O	7.31627500	10.38762000	8.82201200
O	7.31631000	4.45183000	8.82195000
O	7.31631000	7.41972000	8.82195000
Ti	10.17496000	1.48394000	5.55848000
Ti	10.17496000	4.45183000	5.55848000
Ti	10.17496000	7.41972000	5.55848000
Ti	14.81872000	1.48394000	5.55848000
Ti	14.81872000	4.45183000	5.55848000
Ti	14.81872000	7.41972000	5.55848000
Ti	5.53119000	1.48394000	5.55848000
Ti	5.53119000	4.45183000	5.55848000
Ti	5.53119000	7.41972000	5.55848000
Ti	12.44806000	2.96789000	7.82300000
Ti	12.44806000	5.93578000	7.82300000
Ti	12.44806000	8.90366000	7.82300000
Ti	3.16053000	2.96789000	7.82300000
Ti	3.16053000	5.93578000	7.82300000
Ti	3.16053000	8.90366000	7.82300000
Ti	7.80430000	2.96791000	7.82303000
Ti	7.80430000	5.93578000	7.82300000
Ti	7.80430000	8.90367200	7.82298200
H	3.25125000	0.72957300	8.61600500
H	3.19118900	11.20538200	8.87717500
H	7.51751600	10.57143800	9.74748300
H	8.02933800	0.85109300	8.99351100
H	9.78428300	9.94313200	6.60464900
H	9.40526400	10.95860800	7.72361200
H	5.28471000	9.97728700	6.85783900
H	4.17437700	10.85249200	6.21888000
H	13.65714600	11.27484800	7.41625900
H	12.44623000	10.82206500	9.52981200
H	12.71582500	0.88078800	8.71202800
H	9.81010400	-0.78221800	4.46468500
H	15.91572000	0.28976000	7.39800700
H	16.05192300	8.47482100	7.32772400
H	9.88759400	9.62719900	4.45572000

H	2.41908300	8.80736200	5.61065000
H	1.24988900	9.60045600	6.42342000
H	2.39998000	5.83255200	5.59899100
H	1.00935600	5.62922300	6.42492700
H	2.51842600	2.96560000	5.65048700
H	1.39510500	2.15253400	6.39873300
H	14.07708000	-0.72261300	5.28720000
H	14.37720900	9.74280600	4.79546700
H	7.19472200	0.41777800	7.14183900
H	7.18325000	-0.48421200	5.88972200
H	12.20927400	0.29077000	6.51197600
H	10.99039900	0.25303800	7.41562000
H	16.78092700	0.81302000	4.62041300
H	15.90007900	1.01591200	3.36161000
H	16.69960800	3.68792400	4.60315600
H	15.78567500	4.01976900	3.39715600
H	16.49484800	6.47348400	4.05242400
H	15.80469300	7.68324700	3.31561900
H	12.42868400	6.83677700	4.35238500
H	11.96487600	8.22494200	3.73139600
H	12.48710500	3.96265700	4.27996100
H	11.38176600	4.44849800	3.19843000
H	12.52319700	1.85168700	4.37410300
H	11.76281700	0.75280400	3.52312400
H	7.72189200	6.79756500	4.33596900
H	7.46335200	8.27416400	4.20487400
H	7.90898800	4.73975500	4.28178900
H	6.81816700	4.21324500	3.21075400
H	7.73705100	2.11172800	4.33185100
H	7.42429500	0.64916300	3.91028000
H	4.17242400	-0.57870700	5.28162100
H	4.74177400	8.97486600	3.70412600
H	14.56750700	9.98985700	6.81044500
C	10.80969500	4.97659500	12.44298900
C	10.40830700	4.27639400	11.31658400
C	10.37066700	2.88816900	11.33860600
C	10.82893200	2.23882400	12.47873800
C	11.24312200	2.99758900	13.56212200
H	10.08388900	4.76536900	10.40947500
H	10.82409700	1.15544600	12.51811600
H	11.59162200	2.53225400	14.47734300
C	10.73130700	6.44922000	12.51769100
C	10.33987900	7.23479900	11.43467200
N	10.97858800	6.99094600	13.72945200
C	10.11900300	8.59123300	11.61985700
H	10.17857000	6.82078700	10.44792800

C	10.85495900	8.31923700	13.88059300
C	10.40299800	9.14320900	12.86802700
H	11.09500200	8.70717800	14.86397600
H	10.23162400	10.19971400	13.03830200
C	9.69922500	2.15726400	10.17858400
O	9.40938900	2.94600100	9.23094500
O	9.44946800	0.95130300	10.31537700
C	9.42779700	9.41794400	10.53977900
O	9.39923600	8.89633400	9.39614100
O	8.90392100	10.48525300	10.93409100
Re	11.47124300	5.59644100	15.36353400
N	11.19821400	4.33922700	13.57104900
C	11.98829500	4.21792200	16.58202600
C	9.64060000	5.38664800	15.84007300
C	11.71812400	6.88806700	16.74624000
O	12.29667900	3.36680000	17.31153800
O	8.52839800	5.26330300	16.16366300
O	11.85612400	7.69310600	17.57590800
Cl	13.84236300	5.89808900	14.61025600

Coordinates of ReC0A monomer 3b.

O	11.60942000	1.48394000	4.13357000
O	11.60942000	4.45183000	4.13357000
O	11.60942000	7.41972000	4.13357000
O	16.25319000	1.48394000	4.13357000
O	16.25319000	4.45183000	4.13357000
O	16.25319000	7.41972000	4.13357000
O	6.96566000	1.48394000	4.13357000
O	6.96566000	4.45183000	4.13357000
O	6.96566000	7.41972000	4.13357000
O	13.92680000	0.00000000	4.66430000
O	13.92680000	2.96789000	4.66430000
O	13.92680000	5.93578000	4.66430000
O	13.92680000	8.90366000	4.66430000
O	4.63927000	0.00000000	4.66430000
O	4.63927000	2.96789000	4.66430000
O	4.63927000	5.93578000	4.66430000
O	4.63927000	8.90366000	4.66430000
O	9.28303000	0.00000000	4.66430000
O	9.28303000	2.96789000	4.66430000
O	9.28303000	5.93578000	4.66430000
O	9.28303000	8.90366000	4.66430000
O	1.93144000	2.96789000	6.47971000
O	1.93144000	5.93578000	6.47971000
O	1.93144000	8.90366000	6.47971000
O	11.21897000	0.00000000	6.47971000

O	11.21897000	2.96789000	6.47971000
O	11.21897000	5.93578000	6.47971000
O	11.21897000	8.90366000	6.47971000
O	15.86274000	0.00000000	6.47971000
O	15.86274000	2.96789000	6.47971000
O	15.86274000	5.93578000	6.47971000
O	15.86274000	8.90366000	6.47971000
O	6.57521000	0.00000000	6.47971000
O	6.57521000	2.96789000	6.47971000
O	6.57521000	5.93578000	6.47971000
O	6.57521000	8.90366000	6.47971000
O	13.64470000	1.48394000	7.05216000
O	13.64470000	10.38760000	7.05216000
O	13.64470000	4.45183000	7.05216000
O	13.64470000	7.41972000	7.05216000
O	4.35717000	1.48394000	7.05216000
O	4.35717000	10.38760000	7.05216000
O	4.35717000	4.45183000	7.05216000
O	4.35717000	7.41972000	7.05216000
O	9.00094000	1.48394000	7.05216000
O	9.00094000	10.38760000	7.05216000
O	9.00094000	4.45183000	7.05216000
O	9.00094000	7.41972000	7.05216000
O	11.96008000	1.48394000	8.82195000
O	11.96008000	10.38760000	8.82195000
O	11.96008000	4.45183000	8.82195000
O	11.96008000	7.41972000	8.82195000
O	2.67255000	1.48394000	8.82195000
O	2.67255000	10.38760000	8.82195000
O	2.67255000	4.45183000	8.82195000
O	2.67255000	7.41972000	8.82195000
O	7.31635000	1.48395300	8.82186600
O	7.31627500	10.38762000	8.82201200
O	7.31631000	4.45183000	8.82195000
O	7.31631000	7.41972000	8.82195000
Ti	10.17496000	1.48394000	5.55848000
Ti	10.17496000	4.45183000	5.55848000
Ti	10.17496000	7.41972000	5.55848000
Ti	14.81872000	1.48394000	5.55848000
Ti	14.81872000	4.45183000	5.55848000
Ti	14.81872000	7.41972000	5.55848000
Ti	5.53119000	1.48394000	5.55848000
Ti	5.53119000	4.45183000	5.55848000
Ti	5.53119000	7.41972000	5.55848000
Ti	12.44806000	2.96789000	7.82300000
Ti	12.44806000	5.93578000	7.82300000

Ti	12.44806000	8.90366000	7.82300000
Ti	3.16053000	2.96789000	7.82300000
Ti	3.16053000	5.93578000	7.82300000
Ti	3.16053000	8.90366000	7.82300000
Ti	7.80430000	2.96791000	7.82303000
Ti	7.80430000	5.93578000	7.82300000
Ti	7.80430000	8.90367200	7.82298200
H	3.25125000	0.72957300	8.61600500
H	3.19118900	11.20538200	8.87717500
H	7.51751600	10.57143800	9.74748300
H	8.02933800	0.85109300	8.99351100
H	9.78428300	9.94313200	6.60464900
H	9.40526400	10.95860800	7.72361200
H	5.28471000	9.97728700	6.85783900
H	4.17437700	10.85249200	6.21888000
H	13.65714600	11.27484800	7.41625900
H	12.44623000	10.82206500	9.52981200
H	12.71582500	0.88078800	8.71202800
H	9.81010400	-0.78221800	4.46468500
H	15.91572000	0.28976000	7.39800700
H	16.05192300	8.47482100	7.32772400
H	9.88759400	9.62719900	4.45572000
H	2.41908300	8.80736200	5.61065000
H	1.24988900	9.60045600	6.42342000
H	2.39998000	5.83255200	5.59899100
H	1.00935600	5.62922300	6.42492700
H	2.51842600	2.96560000	5.65048700
H	1.39510500	2.15253400	6.39873300
H	14.07708000	-0.72261300	5.28720000
H	14.37720900	9.74280600	4.79546700
H	7.19472200	0.41777800	7.14183900
H	7.18325000	-0.48421200	5.88972200
H	12.20927400	0.29077000	6.51197600
H	10.99039900	0.25303800	7.41562000
H	16.78092700	0.81302000	4.62041300
H	15.90007900	1.01591200	3.36161000
H	16.69960800	3.68792400	4.60315600
H	15.78567500	4.01976900	3.39715600
H	16.49484800	6.47348400	4.05242400
H	15.80469300	7.68324700	3.31561900
H	12.42868400	6.83677700	4.35238500
H	11.96487600	8.22494200	3.73139600
H	12.48710500	3.96265700	4.27996100
H	11.38176600	4.44849800	3.19843000
H	12.52319700	1.85168700	4.37410300
H	11.76281700	0.75280400	3.52312400

H	7.72189200	6.79756500	4.33596900
H	7.46335200	8.27416400	4.20487400
H	7.90898800	4.73975500	4.28178900
H	6.81816700	4.21324500	3.21075400
H	7.73705100	2.11172800	4.33185100
H	7.42429500	0.64916300	3.91028000
H	4.17242400	-0.57870700	5.28162100
H	4.74177400	8.97486600	3.70412600
H	14.56750700	9.98985700	6.81044500
C	11.10885200	5.00801700	12.22002800
C	10.45634200	4.29168400	11.23233600
C	10.47743700	2.90446100	11.24584100
C	11.17022300	2.27034500	12.26879200
C	11.81597600	3.04587800	13.22060600
H	9.92899100	4.77251700	10.42265700
H	11.20289700	1.18772400	12.31135100
H	12.37154400	2.59331000	14.03389800
C	11.06879700	6.48192400	12.26930700
C	10.42172100	7.24241100	11.30132700
N	11.67156800	7.06040900	13.32858500
C	10.31425300	8.61449600	11.46097500
H	9.99323500	6.79662700	10.41553000
C	11.59039900	8.39219800	13.47095200
C	10.90032900	9.19721900	12.58174100
H	12.08157100	8.80409000	14.34499000
H	10.80276000	10.26313400	12.75429100
C	9.71066500	2.16677300	10.15703200
O	9.39326500	2.94844500	9.20618600
O	9.45137700	0.96614800	10.30852700
C	9.48833000	9.41839000	10.47129500
O	9.39491300	8.89670600	9.32517800
O	8.95889400	10.46483300	10.90128600
Re	12.69332400	5.69924900	14.73205900
N	11.78831200	4.38733000	13.20872500
C	13.39737600	4.32986300	15.86333800
C	13.27134600	7.02027100	15.98236600
O	13.81022100	3.47939500	16.53807600
O	13.60599200	7.84896400	16.72638800
C	14.33488400	5.82385400	13.77023800
O	15.34163800	5.91132800	13.19894300
Cl	10.43226900	5.55873100	15.84058100

Coordinates of ReC0A monomer 4a.

O	11.60942000	1.48394000	4.13357000
O	11.60942000	4.45183000	4.13357000
O	11.60942000	7.41972000	4.13357000

O	16.25319000	1.48394000	4.13357000
O	16.25319000	4.45183000	4.13357000
O	16.25319000	7.41972000	4.13357000
O	6.96566000	1.48394000	4.13357000
O	6.96566000	4.45183000	4.13357000
O	6.96566000	7.41972000	4.13357000
O	13.92680000	0.00000000	4.66430000
O	13.92680000	2.96789000	4.66430000
O	13.92680000	5.93578000	4.66430000
O	13.92680000	8.90366000	4.66430000
O	4.63927000	0.00000000	4.66430000
O	4.63927000	2.96789000	4.66430000
O	4.63927000	5.93578000	4.66430000
O	4.63927000	8.90366000	4.66430000
O	9.28303000	0.00000000	4.66430000
O	9.28303000	2.96789000	4.66430000
O	9.28303000	5.93578000	4.66430000
O	9.28303000	8.90366000	4.66430000
O	1.93144000	2.96789000	6.47971000
O	1.93144000	5.93578000	6.47971000
O	1.93144000	8.90366000	6.47971000
O	11.21897000	0.00000000	6.47971000
O	11.21886400	2.96778900	6.47980700
O	11.21897100	5.93577900	6.47970900
O	11.21897000	8.90366000	6.47971000
O	15.86274000	0.00000000	6.47971000
O	15.86274000	2.96789000	6.47971000
O	15.86274000	5.93578000	6.47971000
O	15.86274000	8.90366000	6.47971000
O	6.57521000	0.00000000	6.47971000
O	6.57499700	2.96776800	6.47990500
O	6.57513700	5.93583100	6.47977700
O	6.57516500	8.90366000	6.47975100
O	13.64486800	1.48434700	7.05163800
O	13.64470000	10.38760000	7.05216000
O	13.64454200	4.45186300	7.05200900
O	13.64471200	7.41969200	7.05212400
O	4.35717000	1.48394000	7.05216000
O	4.35717000	10.38760000	7.05216000
O	4.35717000	4.45183000	7.05216000
O	4.35717000	7.41972000	7.05216000
O	9.00100000	1.48409700	7.05195000
O	9.00088400	10.38760000	7.05207200
O	9.00085900	4.45191600	7.05199500
O	9.00101900	7.41973900	7.05231900
O	11.96023900	1.48394000	8.82202800

O	11.96008000	10.38760000	8.82195000
O	11.96003300	4.45104200	8.82378900
O	11.96008800	7.41972000	8.82195400
O	2.67255000	1.48394000	8.82195000
O	2.67255000	10.38760000	8.82195000
O	2.67255000	4.45183000	8.82195000
O	2.67255000	7.41972000	8.82195000
O	7.31666600	1.48395300	8.82202000
O	7.31640000	10.38762000	8.82207300
O	7.31698600	4.45298200	8.82119500
O	7.31629800	7.41967200	8.82201600
Ti	10.17496000	1.48394000	5.55848000
Ti	10.17495700	4.45182900	5.55847800
Ti	10.17487500	7.41975400	5.55841300
Ti	14.81872000	1.48394000	5.55848000
Ti	14.81872000	4.45183000	5.55848000
Ti	14.81872000	7.41972000	5.55848000
Ti	5.53119000	1.48394000	5.55848000
Ti	5.53119000	4.45183000	5.55848000
Ti	5.53119000	7.41972000	5.55848000
Ti	12.44774900	2.96791700	7.82280800
Ti	12.44783900	5.93575700	7.82285800
Ti	12.44807900	8.90366000	7.82300900
Ti	3.16053000	2.96789000	7.82300000
Ti	3.16053000	5.93578000	7.82300000
Ti	3.16053000	8.90366000	7.82300000
Ti	7.80407500	2.96746300	7.82344000
Ti	7.80442300	5.93537200	7.82210000
Ti	7.80419000	8.90367200	7.82303400
H	3.24777500	0.74192500	8.56773600
H	3.03049100	11.28431300	8.75843400
H	7.19879400	10.31109400	9.77865500
H	8.07881300	0.90953400	8.98697000
H	9.82249600	9.99070100	6.62016400
H	9.33408000	10.99049300	7.73419200
H	5.20160100	10.53126900	7.54777600
H	4.73269800	10.07258400	6.17123500
H	13.71220900	11.11627600	7.68430400
H	11.67471100	10.23025000	9.73159200
H	12.72306100	0.89172300	8.71601200
H	9.75853800	-0.83745800	4.62855500
H	16.12825900	0.39877200	7.31745700
H	16.33454400	8.47399700	7.20521000
H	9.78360300	9.26185800	3.92023900
H	2.37768100	8.86253300	5.58942800
H	1.18408300	9.53022900	6.43559100

H	2.45853100	5.93033400	5.62517100
H	1.23831800	5.25053600	6.41129900
H	2.50156700	2.87113700	5.65366000
H	1.32663000	2.19766200	6.47555100
H	14.16117900	-0.76352000	5.20951100
H	13.83610600	9.77775700	5.05460000
H	6.68301700	0.31528100	7.41862000
H	7.51708400	-0.03537500	6.17724600
H	12.19659500	0.28138800	6.48769800
H	11.00104000	0.18184500	7.42414100
H	16.92046600	1.05920800	4.71488800
H	15.95427800	0.78179700	3.52823800
H	17.00398600	4.51111100	4.75814900
H	16.26907400	3.53128500	3.80250600
H	16.21655200	6.53540700	3.72195100
H	15.98405900	8.06867700	3.46409500
H	12.22278600	6.62455700	4.19962600
H	12.30374300	8.13769000	4.29998800
H	12.54271100	4.13682100	4.35125800
H	11.35984600	4.03634000	3.29550600
H	12.35772800	2.14059500	4.34003500
H	12.19260500	0.67157500	4.11608900
H	7.55370800	6.61289000	4.15445300
H	7.66630000	8.13550600	4.28067800
H	7.88629600	4.12256800	4.34414700
H	6.68644500	4.01347700	3.31338900
H	7.75514700	2.06748100	4.33924200
H	7.42691500	0.63798700	3.93525300
H	4.74507800	-0.84525300	5.11993600
H	4.92500400	9.11652400	3.76716600
H	14.58819800	9.96011700	6.89676300
C	8.45454400	5.55723000	13.14675700
C	9.07853700	4.44283400	13.68973400
C	10.13534100	4.59551800	14.58472200
C	10.57180600	5.88898200	14.85128200
C	9.91302000	6.96188900	14.27803200
H	8.76058600	3.42788300	13.47736500
H	11.40621700	6.02252300	15.53093900
H	10.21429900	7.98431500	14.47722200
C	7.28078400	5.47431200	12.24735100
C	6.73788500	4.26798200	11.79699500
N	6.72876000	6.66254900	11.91455700
C	5.60893200	4.27621900	10.98731000
H	7.20493300	3.32396100	12.04917000
C	5.61348300	6.66838300	11.17396300
C	5.02482100	5.51184700	10.71751300

H	5.18876400	7.63932300	10.95018800
H	4.08958300	5.55688600	10.17728200
C	10.75675300	3.36592700	15.31485900
O	11.65680100	3.66104300	16.12491700
O	10.24080000	2.27565000	15.00359100
C	4.98611300	3.00958300	10.39736800
O	4.81242000	2.03232100	11.10414800
O	4.70025800	3.16276700	9.14648900
Re	7.58745400	8.48615500	12.80076200
N	8.85225500	6.81361600	13.46893200
C	8.51848000	9.94242000	13.63887100
C	6.44616200	8.27940000	14.30876300
C	6.36829100	9.70881600	12.01899500
O	9.08742500	10.81133500	14.15064600
O	5.74758700	8.17701900	15.23127100
O	5.59798400	10.41259700	11.48847300
Cl	9.24835700	8.72402100	10.88787600

Coordinates of ReC0A monomer 4b.

O	11.60942000	1.48394000	4.13357000
O	11.60942000	4.45183000	4.13357000
O	11.60942000	7.41972000	4.13357000
O	16.25319000	1.48394000	4.13357000
O	16.25319000	4.45183000	4.13357000
O	16.25319000	7.41972000	4.13357000
O	6.96566000	1.48394000	4.13357000
O	6.96566000	4.45183000	4.13357000
O	6.96566000	7.41972000	4.13357000
O	13.92680000	0.00000000	4.66430000
O	13.92680000	2.96789000	4.66430000
O	13.92680000	5.93578000	4.66430000
O	13.92680000	8.90366000	4.66430000
O	4.63927000	0.00000000	4.66430000
O	4.63927000	2.96789000	4.66430000
O	4.63927000	5.93578000	4.66430000
O	4.63927000	8.90366000	4.66430000
O	9.28303000	0.00000000	4.66430000
O	9.28303000	2.96789000	4.66430000
O	9.28303000	5.93578000	4.66430000
O	9.28303000	8.90366000	4.66430000
O	1.93144000	2.96789000	6.47971000
O	1.93144000	5.93578000	6.47971000
O	1.93144000	8.90366000	6.47971000
O	11.21897000	0.00000000	6.47971000
O	11.21886400	2.96778900	6.47980700
O	11.21897100	5.93577900	6.47970900

O	11.21897000	8.90366000	6.47971000
O	15.86274000	0.00000000	6.47971000
O	15.86274000	2.96789000	6.47971000
O	15.86274000	5.93578000	6.47971000
O	15.86274000	8.90366000	6.47971000
O	6.57521000	0.00000000	6.47971000
O	6.57499700	2.96776800	6.47990500
O	6.57513700	5.93583100	6.47977700
O	6.57516500	8.90366000	6.47975100
O	13.64486800	1.48434700	7.05163800
O	13.64470000	10.38760000	7.05216000
O	13.64454200	4.45186300	7.05200900
O	13.64471200	7.41969200	7.05212400
O	4.35717000	1.48394000	7.05216000
O	4.35717000	10.38760000	7.05216000
O	4.35717000	4.45183000	7.05216000
O	4.35717000	7.41972000	7.05216000
O	9.00100000	1.48409700	7.05195000
O	9.00088400	10.38760000	7.05207200
O	9.00085900	4.45191600	7.05199500
O	9.00101900	7.41973900	7.05231900
O	11.96023900	1.48394000	8.82202800
O	11.96008000	10.38760000	8.82195000
O	11.96003300	4.45104200	8.82378900
O	11.96008800	7.41972000	8.82195400
O	2.67255000	1.48394000	8.82195000
O	2.67255000	10.38760000	8.82195000
O	2.67255000	4.45183000	8.82195000
O	2.67255000	7.41972000	8.82195000
O	7.31666600	1.48395300	8.82202000
O	7.31640000	10.38762000	8.82207300
O	7.31698600	4.45298200	8.82119500
O	7.31629800	7.41967200	8.82201600
Ti	10.17496000	1.48394000	5.55848000
Ti	10.17495700	4.45182900	5.55847800
Ti	10.17487500	7.41975400	5.55841300
Ti	14.81872000	1.48394000	5.55848000
Ti	14.81872000	4.45183000	5.55848000
Ti	14.81872000	7.41972000	5.55848000
Ti	5.53119000	1.48394000	5.55848000
Ti	5.53119000	4.45183000	5.55848000
Ti	5.53119000	7.41972000	5.55848000
Ti	12.44774900	2.96791700	7.82280800
Ti	12.44783900	5.93575700	7.82285800
Ti	12.44807900	8.90366000	7.82300900
Ti	3.16053000	2.96789000	7.82300000

Ti	3.16053000	5.93578000	7.82300000
Ti	3.16053000	8.90366000	7.82300000
Ti	7.80407500	2.96746300	7.82344000
Ti	7.80442300	5.93537200	7.82210000
Ti	7.80419000	8.90367200	7.82303400
H	3.24777500	0.74192500	8.56773600
H	3.03049100	11.28431300	8.75843400
H	7.19879400	10.31109400	9.77865500
H	8.07881300	0.90953400	8.98697000
H	9.82249600	9.99070100	6.62016400
H	9.33408000	10.99049300	7.73419200
H	5.20160100	10.53126900	7.54777600
H	4.73269800	10.07258400	6.17123500
H	13.71220900	11.11627600	7.68430400
H	11.67471100	10.23025000	9.73159200
H	12.72306100	0.89172300	8.71601200
H	9.75853800	-0.83745800	4.62855500
H	16.12825900	0.39877200	7.31745700
H	16.33454400	8.47399700	7.20521000
H	9.78360300	9.26185800	3.92023900
H	2.37768100	8.86253300	5.58942800
H	1.18408300	9.53022900	6.43559100
H	2.45853100	5.93033400	5.62517100
H	1.23831800	5.25053600	6.41129900
H	2.50156700	2.87113700	5.65366000
H	1.32663000	2.19766200	6.47555100
H	14.16117900	-0.76352000	5.20951100
H	13.83610600	9.77775700	5.05460000
H	6.68301700	0.31528100	7.41862000
H	7.51708400	-0.03537500	6.17724600
H	12.19659500	0.28138800	6.48769800
H	11.00104000	0.18184500	7.42414100
H	16.92046600	1.05920800	4.71488800
H	15.95427800	0.78179700	3.52823800
H	17.00398600	4.51111100	4.75814900
H	16.26907400	3.53128500	3.80250600
H	16.21655200	6.53540700	3.72195100
H	15.98405900	8.06867700	3.46409500
H	12.22278600	6.62455700	4.19962600
H	12.30374300	8.13769000	4.29998800
H	12.54271100	4.13682100	4.35125800
H	11.35984600	4.03634000	3.29550600
H	12.35772800	2.14059500	4.34003500
H	12.19260500	0.67157500	4.11608900
H	7.55370800	6.61289000	4.15445300
H	7.66630000	8.13550600	4.28067800

H	7.88629600	4.12256800	4.34414700
H	6.68644500	4.01347700	3.31338900
H	7.75514700	2.06748100	4.33924200
H	7.42691500	0.63798700	3.93525300
H	4.74507800	-0.84525300	5.11993600
H	4.92500400	9.11652400	3.76716600
H	14.58819800	9.96011700	6.89676300
C	9.39701200	4.35296300	11.88114100
C	9.97135800	3.09233800	11.88418200
C	11.35485900	2.94634400	11.93502400
C	12.11752400	4.10828700	11.95395500
C	11.48679500	5.34200600	11.96782000
H	9.38845600	2.17875100	11.85628100
H	13.19832000	4.02458700	11.95192600
H	12.05405200	6.26573800	11.98098000
C	7.94616300	4.57300100	11.72770300
C	7.05434600	3.53138600	11.47020000
N	7.54365400	5.86000500	11.70527700
C	5.76983700	3.82435100	11.04819300
H	7.39734900	2.50544200	11.44416900
C	6.25798900	6.13258700	11.43195200
C	5.35253000	5.15663500	11.07476200
H	5.98178300	7.17970900	11.44756900
H	4.34455200	5.42853600	10.77571100
C	11.99472700	1.52970900	11.99652000
O	13.24085800	1.53172300	12.01062700
O	11.16653900	0.59719300	12.05329600
C	4.92337100	2.76071800	10.36867000
O	4.61086400	1.72427500	10.92578700
O	4.66290100	3.14602600	9.15724700
Re	9.06106300	7.36567500	12.21469300
N	10.15206900	5.47691100	11.95290800
C	10.51283300	8.43098000	12.89019400
C	7.85204800	8.82034900	12.44292500
O	11.39168800	9.06953300	13.28877600
O	7.08642400	9.70007600	12.48235200
Cl	8.61853800	6.52343200	14.54783700
C	9.38371100	8.11826800	10.52122500
O	9.53510900	8.78813000	9.56412300

Coordinates of ReC0A dimer CO;CO.

O	11.60942000	1.48394000	4.13357000
O	11.60942000	4.45183000	4.13357000
O	11.60942000	7.41972000	4.13357000
O	16.25319000	1.48394000	4.13357000
O	16.25319000	4.45183000	4.13357000

O	16.25319000	7.41972000	4.13357000
O	6.96566000	1.48394000	4.13357000
O	6.96566000	4.45183000	4.13357000
O	6.96566000	7.41972000	4.13357000
O	13.92680000	0.00000000	4.66430000
O	13.92680000	2.96789000	4.66430000
O	13.92680000	5.93578000	4.66430000
O	13.92680000	8.90366000	4.66430000
O	4.63927000	0.00000000	4.66430000
O	4.63927000	2.96789000	4.66430000
O	4.63927000	5.93578000	4.66430000
O	4.63927000	8.90366000	4.66430000
O	9.28303000	0.00000000	4.66430000
O	9.28303000	2.96789000	4.66430000
O	9.28303000	5.93578000	4.66430000
O	9.28303000	8.90366000	4.66430000
O	1.93145900	2.96773400	6.47969200
O	1.93144100	5.93578000	6.47970900
O	1.93145400	8.90375100	6.47969700
O	11.21897000	0.00000000	6.47971000
O	11.21897000	2.96789000	6.47971000
O	11.21897000	5.93578000	6.47971000
O	11.21897000	8.90366000	6.47971000
O	15.86274000	0.00000000	6.47971000
O	15.86274000	2.96789000	6.47971000
O	15.86274000	5.93578000	6.47971000
O	15.86274000	8.90366000	6.47971000
O	6.57521000	0.00000000	6.47971000
O	6.57520900	2.96789100	6.47971100
O	6.57520900	5.93578000	6.47971100
O	6.57521000	8.90366100	6.47971000
O	13.64470000	1.48394000	7.05216000
O	13.64470000	10.38760000	7.05216000
O	13.64470000	4.45183000	7.05216000
O	13.64470000	7.41972000	7.05216000
O	4.35713600	1.48392300	7.05213900
O	4.35715300	10.38761700	7.05216700
O	4.35719700	4.45181700	7.05217600
O	4.35718500	7.41972700	7.05217000
O	9.00094100	1.48394100	7.05216000
O	9.00093900	10.38760100	7.05216000
O	9.00094500	4.45182800	7.05216400
O	9.00093600	7.41972000	7.05215500
O	11.96008000	1.48394000	8.82195000
O	11.96008000	10.38760000	8.82195000
O	11.96008000	4.45183000	8.82195000

O	11.96008000	7.41972000	8.82195000
O	2.67255200	1.48394000	8.82195100
O	2.67255500	10.38759600	8.82195900
O	2.67255100	4.45182700	8.82195500
O	2.67255000	7.41972100	8.82195200
O	7.31635200	1.48395600	8.82187200
O	7.31628900	10.38762700	8.82200900
O	7.31631100	4.45182900	8.82195100
O	7.31630900	7.41971900	8.82194800
Ti	10.17495900	1.48394000	5.55847900
Ti	10.17495800	4.45183100	5.55847800
Ti	10.17496100	7.41972100	5.55848100
Ti	14.81872000	1.48394000	5.55848000
Ti	14.81872000	4.45183000	5.55848000
Ti	14.81872000	7.41972000	5.55848000
Ti	5.53120500	1.48394600	5.55849200
Ti	5.53117900	4.45183400	5.55847100
Ti	5.53118400	7.41971800	5.55847500
Ti	12.44806000	2.96789000	7.82300000
Ti	12.44806000	5.93578000	7.82300000
Ti	12.44806000	8.90366000	7.82300000
Ti	3.16052200	2.96805900	7.82301400
Ti	3.16054800	5.93578000	7.82301000
Ti	3.16050800	8.90356400	7.82299200
Ti	7.80429500	2.96790500	7.82301500
Ti	7.80430700	5.93578000	7.82300500
Ti	7.80429600	8.90366700	7.82298600
H	3.25124300	0.72957000	8.61599700
H	3.19118400	11.20538600	8.87716700
H	7.51750600	10.57143200	9.74748600
H	8.02933700	0.85109000	8.99350600
H	9.78428300	9.94313200	6.60464900
H	9.40526500	10.95860700	7.72361200
H	5.28471200	9.97728800	6.85784400
H	4.17438600	10.85248000	6.21887100
H	13.65714600	11.27484800	7.41625900
H	12.44623000	10.82206500	9.52981200
H	12.71582500	0.88078800	8.71202800
H	9.81010400	-0.78221800	4.46468500
H	15.91572000	0.28976000	7.39800700
H	16.05192300	8.47482100	7.32772400
H	9.88759400	9.62719900	4.45572000
H	2.41908200	8.80734400	5.61065100
H	1.24988400	9.60045100	6.42342500
H	2.39998000	5.83255200	5.59899100
H	1.00935600	5.62922300	6.42492700

H	2.51842600	2.96562900	5.65048700
H	1.39509400	2.15254000	6.39874300
H	14.07708000	-0.72261300	5.28720000
H	14.37720900	9.74280600	4.79546700
H	7.19472200	0.41777800	7.14183900
H	7.18325000	-0.48421200	5.88972200
H	12.20927400	0.29077000	6.51197600
H	10.99039900	0.25303800	7.41562000
H	16.78092700	0.81302000	4.62041300
H	15.90007900	1.01591200	3.36161000
H	16.69960800	3.68792400	4.60315600
H	15.78567500	4.01976900	3.39715600
H	16.49484800	6.47348400	4.05242400
H	15.80469300	7.68324700	3.31561900
H	12.42868400	6.83677700	4.35238500
H	11.96487600	8.22494200	3.73139600
H	12.48710500	3.96265700	4.27996100
H	11.38176600	4.44849800	3.19843000
H	12.52319700	1.85168700	4.37410300
H	11.76281700	0.75280400	3.52312400
H	7.72189200	6.79756500	4.33596900
H	7.46335200	8.27416400	4.20487400
H	7.90898800	4.73975500	4.28178900
H	6.81816700	4.21324500	3.21075400
H	7.73705100	2.11172800	4.33185100
H	7.42429500	0.64916300	3.91028000
H	4.17242400	-0.57870700	5.28162100
H	4.74177400	8.97486600	3.70412600
H	14.56750700	9.98985700	6.81044500
C	6.32790700	5.11319400	12.14999700
C	5.82717100	4.35002100	11.11801900
C	5.64822800	2.98487600	11.28235500
C	5.96375500	2.40760500	12.51052400
C	6.44936400	3.21087600	13.51615700
H	5.60602200	4.77172600	10.14918900
H	5.82070700	1.34293700	12.65297200
H	6.70150400	2.81025900	14.49091500
C	6.50020800	6.56258400	12.04747700
C	5.86132000	7.31616000	11.07541900
N	7.26115800	7.12897300	13.01378300
C	5.94942800	8.70234600	11.10422000
H	5.25678900	6.85051700	10.31171600
C	7.43493600	8.46334200	12.97775800
C	6.77970800	9.27656100	12.06465900
H	8.10791600	8.88137000	13.71879000
H	6.92573900	10.34871200	12.09616900

C	4.98145000	2.19519000	10.16241700
O	4.69601400	2.97741800	9.19408000
O	4.74144300	1.01177800	10.36187000
C	5.10135300	9.54543700	10.14321500
O	4.72925200	8.87535400	9.11134300
O	4.83014000	10.69538500	10.46534300
Re	7.47918300	5.85365700	14.77235600
N	6.64495900	4.54107100	13.34277700
C	7.26090900	4.74794100	16.34292800
C	7.28717400	7.45489900	16.04709400
O	7.07911300	4.09348100	17.26867400
O	7.18723300	8.33627000	16.75629800
C	8.86453100	4.47166600	14.37074500
O	9.53568100	3.55499700	14.32912800
Cl	5.09622500	6.38773000	15.03037700
C	11.25472800	5.19561600	12.13339900
C	10.57806500	4.44921200	11.18800300
C	10.63573000	3.05796600	11.23201200
C	11.44631800	2.46150300	12.19052400
C	12.08846400	3.26248400	13.11889800
H	10.01200600	4.89361400	10.38056400
H	11.53513600	1.38166400	12.21749400
H	12.69269500	2.83942000	13.91399500
C	11.26999400	6.66772600	12.13433900
C	10.56288900	7.41674200	11.21502900
N	12.00633300	7.25904600	13.10865200
C	10.55861900	8.79969400	11.32176200
H	9.99979700	6.97122800	10.40672800
C	12.04978200	8.60350900	13.17082400
C	11.32150200	9.40500500	12.31479600
H	12.66462600	9.02253900	13.95927700
H	11.31855900	10.48433600	12.41851300
C	9.76663500	2.26625600	10.25039200
O	9.42876400	2.98471500	9.27439000
O	9.47804900	1.10381200	10.55926400
C	9.65505900	9.57548200	10.38271000
O	9.42624800	8.94996000	9.32244900
O	9.21522100	10.66347500	10.80567200
Re	12.53858700	5.94158700	14.73198500
N	11.95970900	4.60312600	13.13113200
C	12.56619400	4.60552000	16.11622300
C	12.90918500	7.31203900	16.03490000
O	12.53803000	3.78773300	16.93443000
O	13.13878500	8.14896100	16.80068400
C	14.38258900	5.70127000	14.45504900
O	15.51498900	5.55997300	14.27386800

Cl	9.78236900	6.81882200	15.21568900

Coordinates of ReC0A dimer CO;Cl.

Ti	10.17409900	4.45158300	5.55769100
O	9.00009400	4.45156200	7.05135700
O	11.60856200	4.45158100	4.13278400
Ti	7.80344900	5.93553100	7.82217900
Ti	7.80340800	2.96765100	7.82225100
O	11.21811200	2.96764100	6.47892400
O	11.21811200	5.93553100	6.47892400
O	9.28217200	5.93553100	4.66351400
O	9.28217200	2.96764100	4.66351400
H	12.48624700	3.96240800	4.27917500
H	11.38090800	4.44824900	3.19764400
O	6.57436600	5.93553100	6.47891100
O	9.00011100	7.41951000	7.05134400
O	7.31541600	7.41947000	8.82114400
O	7.31544100	4.45157600	8.82116600
O	6.57434400	2.96762200	6.47893100
O	7.31545900	1.48369500	8.82104900
O	9.00014700	1.48372300	7.05141200
Ti	10.17408300	1.48368400	5.55767900
Ti	12.44720200	2.96764100	7.82221400
Ti	10.17409700	7.41946900	5.55768900
Ti	12.44720200	5.93553100	7.82221400
Ti	5.53026100	7.41945500	5.55767600
Ti	5.53013700	4.45165400	5.55755700
Ti	7.80342400	8.90342400	7.82215600
Ti	5.53038300	1.48370500	5.55771200
H	8.02849800	0.85088300	8.99279200
O	11.60856200	1.48369100	4.13278400
O	11.21811200	-0.00024900	6.47892400
O	9.28217200	-0.00024900	4.66351400
O	13.64384200	4.45158100	7.05137400
O	11.95922200	1.48369100	8.82116400
O	11.95922200	4.45158100	8.82116400
O	13.64384200	1.48369100	7.05137400
O	9.28217200	8.90341100	4.66351400
O	11.60856200	7.41947100	4.13278400
O	11.21811200	8.90341100	6.47892400
O	13.64384200	7.41947100	7.05137400
O	11.95922200	7.41947100	8.82116400
O	4.35682100	7.41991100	7.05131900
O	6.96480200	7.41947100	4.13278400
O	4.63841200	5.93553100	4.66351400
O	4.63841200	8.90341100	4.66351400

O	6.57437200	8.90344600	6.47890500
O	4.35688500	4.45128700	7.05169700
O	6.96480200	4.45158100	4.13278400
O	4.63841200	2.96764100	4.66351400
O	9.00008800	10.38737500	7.05142800
O	7.31544700	10.38733900	8.82128900
O	6.96480200	1.48369100	4.13278400
O	6.57435200	-0.00024900	6.47892400
O	4.35651000	1.48400300	7.05108200
O	4.63841200	-0.00024900	4.66351400
H	12.52233900	1.85143800	4.37331700
H	11.76195900	0.75255500	3.52233800
H	10.98954100	0.25278900	7.41483400
H	9.80924600	-0.78246700	4.46389900
Ti	14.81786200	4.45158100	5.55769400
H	12.71496700	0.88053900	8.71124200
Ti	14.81786200	1.48369100	5.55769400
H	9.88673600	9.62695000	4.45493400
H	11.96401800	8.22469300	3.73061000
Ti	12.44720200	8.90341100	7.82221400
Ti	14.81786200	7.41947100	5.55769400
Ti	3.16023600	8.90078400	7.82088800
Ti	3.15977400	5.93553100	7.82230700
H	7.72103400	6.79731600	4.33518300
H	7.46249400	8.27391500	4.20408800
H	4.74091600	8.97461700	3.70334000
Ti	3.15862300	2.96944600	7.82237700
H	7.90813000	4.73950600	4.28100300
H	6.81730900	4.21299600	3.20996800
H	9.78339800	9.94288100	6.60381700
H	9.40445600	10.95832000	7.72282900
H	7.51661900	10.57116800	9.74671000
H	7.73619300	2.11147900	4.33106500
H	7.42343700	0.64891400	3.90949400
H	7.19386400	0.41752900	7.14105300
H	7.18239200	-0.48446100	5.88893600
H	4.17156600	-0.57895600	5.28083500
O	16.25233200	4.45158100	4.13278400
O	15.86188200	2.96764100	6.47892400
O	15.86188200	5.93553100	6.47892400
O	13.92594200	5.93553100	4.66351400
O	13.92594200	2.96764100	4.66351400
O	16.25233200	1.48369100	4.13278400
O	15.86188200	-0.00024900	6.47892400
O	13.92594200	-0.00024900	4.66351400
O	11.95922200	10.38735100	8.82116400

O	13.64384200	10.38735100	7.05137400
O	16.25233200	7.41947100	4.13278400
O	13.92594200	8.90341100	4.66351400
O	15.86188200	8.90341100	6.47892400
O	1.93013200	8.90491500	6.47932400
O	2.67138700	10.38708500	8.82141000
O	2.67159100	7.41981300	8.82162100
O	4.35621400	10.38722500	7.05097900
O	1.93061700	5.93553100	6.47889200
O	2.67166400	4.45122200	8.82168400
O	1.93134300	2.96615200	6.47822300
O	2.67118800	1.48383600	8.82113400
H	17.13002000	3.96240700	4.27917600
H	16.02467800	4.44825000	3.19764100
Ti	17.09173200	2.96764100	7.82285400
Ti	17.09173200	5.93553100	7.82285400
H	17.16610800	1.85143200	4.37331200
H	16.40572300	0.75255200	3.52233300
H	16.79388500	0.22903900	6.49887700
H	15.53965300	-0.10839200	7.37674000
H	14.07622200	-0.72286200	5.28641400
H	12.44537200	10.82181600	9.52902600
H	13.65628800	11.27459900	7.41547300
H	17.07245600	6.83677400	4.35238500
H	16.60779000	8.22469500	3.73060700
H	14.37635100	9.74255700	4.79468100
Ti	17.09173200	8.90341100	7.82285400
H	2.41828100	8.80786100	5.60981200
H	1.24876600	9.59996800	6.42288500
H	3.19034400	11.20512300	8.87641000
H	4.17362500	10.85210600	6.21799500
H	2.39912200	5.83230300	5.59820500
H	1.00849800	5.62897400	6.42414100
H	2.51756900	2.96526900	5.64970200
H	1.39404400	2.15240000	6.39813500
H	3.25060000	0.72941800	8.61545800
O	18.28462200	4.45158100	7.05211400
O	16.60316200	1.48369100	8.82221400
O	16.60316200	4.45158100	8.82221400
O	18.28462200	1.48369100	7.05211400
O	18.28462200	7.41947100	7.05211400
O	16.60316200	7.41947100	8.82221400
O	18.28462200	10.38735100	7.05211400
O	16.60316200	10.38735100	8.82221400
Ti	19.46326200	4.45158100	5.55497400
H	17.29007300	0.80694000	8.75183000

Ti	19.46326200	1.48369100	5.55497400
Ti	19.46326200	7.41947100	5.55497400
H	19.20832800	9.99088000	6.80967700
H	18.29672800	11.27438800	7.41673700
H	17.08954500	10.82238600	9.52956900
O	20.89609200	4.45158100	4.13278400
O	18.57330200	5.93553100	4.66786400
O	18.57330200	2.96764100	4.66786400
O	20.50617200	2.96764100	6.48185400
O	20.50617200	5.93553100	6.48185400
O	20.89609200	1.48369100	4.13278400
O	18.57330200	-0.00024900	4.66786400
O	20.50617200	-0.00024900	6.48185400
O	20.89609200	7.41947100	4.13278400
O	18.57330200	8.90341100	4.66786400
O	20.50617200	8.90341100	6.48185400
H	21.34171100	3.68693700	4.60191700
H	20.42851300	4.02049800	3.39584200
H	21.42310200	0.81194900	4.61928400
H	20.54290000	1.01657600	3.36030900
H	18.91713300	-0.73413200	5.20137100
H	20.75785400	0.36755500	7.33935700
H	21.13701700	6.47310900	4.05096100
H	20.44812200	7.68402500	3.31487600
H	19.02436800	9.74188600	4.80102800
H	21.34305200	8.55626200	6.79921600
H	12.42868400	6.83677700	4.35238500
H	5.28478500	9.97734700	6.85807000
H	12.20927400	0.29077000	6.51197600
H	14.56750700	9.98985700	6.81044500
C	6.54599000	5.24484100	12.06634900
C	5.84512400	4.49369600	11.13929300
C	5.91944800	3.10909500	11.15315400
C	6.74374100	2.50981000	12.09905100
C	7.41069600	3.31556700	13.00948000
H	5.24233400	4.95219500	10.37094100
H	6.85862300	1.43281300	12.11408700
H	8.04223000	2.88771300	13.78051100
C	6.51879800	6.71926800	12.06513900
C	5.81367800	7.44652800	11.11491300
N	7.23865600	7.33352700	13.03031600
C	5.81780500	8.83224200	11.15115400
H	5.27320500	6.95723300	10.32012100
C	7.25479600	8.67595800	13.05811800
C	6.55317300	9.45703700	12.15355700
H	7.84952800	9.12838000	13.84284300

H	6.59730200	10.53746700	12.21108700
C	5.07438900	2.31047600	10.16492400
O	4.70208200	3.04766500	9.17940800
O	4.81373100	1.14269500	10.42115700
C	5.03819800	9.63001500	10.11488600
O	4.71367900	8.91383600	9.08717800
O	4.78114200	10.80825800	10.33172400
Re	7.93826400	5.99483700	14.64938100
N	7.30534700	4.65630200	13.01823400
C	8.16689900	4.64001000	15.98723500
C	8.19644500	7.36164600	15.97119600
O	8.29152600	3.80686500	16.78043600
O	8.34653800	8.20611100	16.74914700
C	9.80576300	5.94475400	14.39661800
O	10.98080400	5.88340100	14.40641700
Cl	5.47877500	5.99514500	15.19497200
C	11.56422300	5.06403800	11.69303000
C	10.51979200	4.29240300	11.25489000
C	10.68961400	2.91368800	11.13675000
C	11.86392300	2.31958300	11.61443400
C	12.87022900	3.12640600	12.05937100
H	9.60686600	4.73193900	10.87209400
H	11.98709000	1.24646300	11.54728200
H	13.82148300	2.72382400	12.38464500
C	11.55134100	6.52227500	11.72444500
C	10.52103600	7.28244200	11.21921500
N	12.68528100	7.08789100	12.20991200
C	10.62650000	8.66902400	11.24155500
H	9.67024100	6.83488900	10.72010900
C	12.75789700	8.43139900	12.28500900
C	11.73464100	9.24619800	11.85320100
H	13.68014000	8.85125100	12.66734500
H	11.81338700	10.32482100	11.92830200
C	9.71875100	2.14528600	10.25760900
O	9.42522700	2.91190900	9.30351100
O	9.44035900	0.97552500	10.52082700
C	9.63225600	9.48517900	10.43614000
O	9.42570400	8.91336900	9.33836500
O	9.20445800	10.54522100	10.91350700
Re	14.28053400	5.73856500	12.56989600
N	12.75498200	4.49107300	12.05659600
C	15.80772800	4.44765900	12.40187500
C	15.01483900	7.05807300	13.83905700
O	16.67281500	3.72016600	12.28887400
O	15.37129100	7.83051500	14.59956700
C	13.94751000	4.84350100	14.28589000

O	13.79154500	4.30662000	15.28042500
Cl	15.68766000	7.02510000	11.19889600

Coordinates of ReC0A dimer Cl;CO.

O	11.60942000	1.48394000	4.13357000
O	11.60942000	4.45183000	4.13357000
O	11.60942000	7.41972000	4.13357000
O	16.25319000	1.48394000	4.13357000
O	16.25319000	4.45183000	4.13357000
O	16.25319000	7.41972000	4.13357000
O	6.96566000	1.48394000	4.13357000
O	6.96566000	4.45183000	4.13357000
O	6.96566000	7.41972000	4.13357000
O	13.92680000	0.00000000	4.66430000
O	13.92680000	2.96789000	4.66430000
O	13.92680000	5.93578000	4.66430000
O	13.92680000	8.90366000	4.66430000
O	4.63927000	0.00000000	4.66430000
O	4.63927000	2.96789000	4.66430000
O	4.63927000	5.93578000	4.66430000
O	4.63927000	8.90366000	4.66430000
O	9.28303000	0.00000000	4.66430000
O	9.28303000	2.96789000	4.66430000
O	9.28303000	5.93578000	4.66430000
O	9.28303000	8.90366000	4.66430000
O	1.93137800	2.96806700	6.47976700
O	1.93144900	5.93578000	6.47970200
O	1.93139700	8.90430500	6.47975000
O	11.21897000	0.00000000	6.47971000
O	11.21897000	2.96789000	6.47971000
O	11.21897000	5.93578000	6.47971000
O	11.21897000	8.90366000	6.47971000
O	15.86274000	0.00000000	6.47971000
O	15.86274000	2.96789000	6.47971000
O	15.86274000	5.93578000	6.47971000
O	15.86274000	8.90366000	6.47971000
O	6.57521000	0.00000000	6.47971000
O	6.57521200	2.96788600	6.47970900
O	6.57521100	5.93578000	6.47970900
O	6.57520900	8.90365500	6.47971100
O	13.64470000	1.48394000	7.05216000
O	13.64470000	10.38760000	7.05216000
O	13.64470000	4.45183000	7.05216000
O	13.64470000	7.41972000	7.05216000
O	4.35721400	1.48396000	7.05219000
O	4.35693300	10.38780500	7.05218700

O	4.35708400	4.45186900	7.05210100
O	4.35728900	7.41977300	7.05224300
O	9.00094700	1.48394100	7.05216800
O	9.00094100	10.38759400	7.05215100
O	9.00093600	4.45183100	7.05215500
O	9.00095200	7.41972200	7.05217400
O	11.96008000	1.48394000	8.82195000
O	11.96008000	10.38760000	8.82195000
O	11.96008000	4.45183000	8.82195000
O	11.96008000	7.41972000	8.82195000
O	2.67250000	1.48392900	8.82190900
O	2.67254300	10.38759400	8.82195600
O	2.67250800	4.45184000	8.82191400
O	2.67256400	7.41974000	8.82198700
O	7.31634900	1.48394700	8.82185700
O	7.31625000	10.38760500	8.82202200
O	7.31631300	4.45183100	8.82195000
O	7.31630900	7.41972200	8.82195200
Ti	10.17495800	1.48393900	5.55847800
Ti	10.17496300	4.45182900	5.55848200
Ti	10.17495500	7.41971800	5.55847600
Ti	14.81872000	1.48394000	5.55848000
Ti	14.81872000	4.45183000	5.55848000
Ti	14.81872000	7.41972000	5.55848000
Ti	5.53116900	1.48393200	5.55846300
Ti	5.53122900	4.45181400	5.55851100
Ti	5.53114500	7.41970200	5.55844500
Ti	12.44806000	2.96789000	7.82300000
Ti	12.44806000	5.93578000	7.82300000
Ti	12.44806000	8.90366000	7.82300000
Ti	3.16063000	2.96776100	7.82301900
Ti	3.16055700	5.93578000	7.82301800
Ti	3.16061700	8.90294200	7.82286300
Ti	7.80428400	2.96792200	7.82303100
Ti	7.80430600	5.93578000	7.82300500
Ti	7.80428800	8.90369700	7.82294600
H	3.25128700	0.72959000	8.61604800
H	3.19116700	11.20539900	8.87714000
H	7.51753700	10.57145000	9.74747600
H	8.02934100	0.85110000	8.99352300
H	9.78428700	9.94313200	6.60465600
H	9.40525900	10.95861200	7.72361200
H	5.28474200	9.97731300	6.85793900
H	4.17448900	10.85234800	6.21877500
H	13.65714600	11.27484800	7.41625900
H	12.44623000	10.82206500	9.52981200

H	12.71582500	0.88078800	8.71202800
H	9.81010400	-0.78221800	4.46468500
H	15.91572000	0.28976000	7.39800700
H	16.05192300	8.47482100	7.32772400
H	9.88759400	9.62719900	4.45572000
H	2.41907300	8.80723600	5.61065900
H	1.24987700	9.60044500	6.42343100
H	2.39998000	5.83255200	5.59899100
H	1.00935600	5.62922300	6.42492700
H	2.51842600	2.96554500	5.65048700
H	1.39512900	2.15252000	6.39871100
H	14.07708000	-0.72261300	5.28720000
H	14.37720900	9.74280600	4.79546700
H	7.19472200	0.41777800	7.14183900
H	7.18325000	-0.48421200	5.88972200
H	12.20927400	0.29077000	6.51197600
H	10.99039900	0.25303800	7.41562000
H	16.78092700	0.81302000	4.62041300
H	15.90007900	1.01591200	3.36161000
H	16.69960800	3.68792400	4.60315600
H	15.78567500	4.01976900	3.39715600
H	16.49484800	6.47348400	4.05242400
H	15.80469300	7.68324700	3.31561900
H	12.42868400	6.83677700	4.35238500
H	11.96487600	8.22494200	3.73139600
H	12.48710500	3.96265700	4.27996100
H	11.38176600	4.44849800	3.19843000
H	12.52319700	1.85168700	4.37410300
H	11.76281700	0.75280400	3.52312400
H	7.72189200	6.79756500	4.33596900
H	7.46335200	8.27416400	4.20487400
H	7.90898800	4.73975500	4.28178900
H	6.81816700	4.21324500	3.21075400
H	7.73705100	2.11172800	4.33185100
H	7.42429500	0.64916300	3.91028000
H	4.17242400	-0.57870700	5.28162100
H	4.74177400	8.97486600	3.70412600
H	14.56750700	9.98985700	6.81044500
C	6.46712200	5.32274500	12.08520800
C	5.83478600	4.55778200	11.12664500
C	6.00075900	3.17708400	11.10677200
C	6.90312200	2.61940900	12.00622500
C	7.49740900	3.44077700	12.95500900
H	5.18668700	4.99522800	10.38165000
H	7.13040300	1.56092000	11.96162400
H	8.17351500	3.03554000	13.70046800

C	6.30653700	6.78441400	12.15256200
C	5.78088400	7.52141300	11.10098900
N	6.71324400	7.38308000	13.29463800
C	5.67296900	8.89881600	11.21005600
H	5.49122600	7.05522400	10.17203700
C	6.64531500	8.72413500	13.38648000
C	6.13485200	9.51237400	12.37120700
H	7.01217500	9.15758200	14.30963600
H	6.09423100	10.59023700	12.46803900
C	5.11697900	2.35109900	10.17031700
O	4.71384400	3.06300100	9.18532300
O	4.84007200	1.20614900	10.50139800
C	5.00537900	9.69484600	10.09918500
O	4.71652800	8.95330100	9.08559100
O	4.76536300	10.88301900	10.28391700
Re	7.36810800	6.00847100	14.87306600
N	7.25142800	4.76219000	13.04184800
C	7.95896900	4.59141400	16.05651900
C	7.33355200	7.23838400	16.34867200
O	8.30968100	3.73325400	16.74302300
O	7.29904000	7.98981100	17.22715200
C	11.45103500	4.99007600	11.93643900
C	10.60379900	4.25842200	11.13648900
C	10.63836200	2.87060300	11.18371600
C	11.51422700	2.25376400	12.06587700
C	12.33985500	3.04464800	12.84476800
H	9.93269600	4.70898200	10.41918600
H	11.55965400	1.17178300	12.11081800
H	13.05079500	2.60545400	13.53521500
C	11.47281700	6.45444400	11.92099000
C	10.61230800	7.20878500	11.14796300
N	12.35417600	7.04599900	12.77256500
C	10.58182500	8.58983900	11.29717800
H	9.94161900	6.75749000	10.43017100
C	12.37598400	8.40135500	12.86131900
C	11.48186200	9.19174100	12.18373200
H	13.11324300	8.82328600	13.53288500
H	11.46376800	10.26593000	12.32789800
C	9.73771200	2.12969500	10.20459000
O	9.41309600	2.90368400	9.26610800
O	9.44069000	0.95371900	10.45039600
C	9.57700600	9.38154500	10.48026000
O	9.43801600	8.90613900	9.33315100
O	9.02599300	10.34154600	11.05071400
Re	13.40163200	5.75073200	14.05678800
N	12.31495000	4.38909600	12.78931800

C	14.33016600	4.32111800	15.06026100
C	14.15144900	7.14025400	15.17765600
O	14.87129200	3.47269600	15.61228800
O	14.57816000	7.98506500	15.83672800
Cl	9.61932000	6.85232500	14.38151200
C	5.52389600	5.57560300	15.20172400
O	4.41833900	5.33461500	15.41719600
Cl	11.51626900	5.53641500	15.49335500
C	14.96225200	5.83074500	12.86146400
O	15.87112900	5.89064700	12.17105800

Coordinates of ReC0A dimer Cl;Cl.

Ti	10.17409800	4.45158300	5.55769100
O	9.00009200	4.45156400	7.05135800
O	11.60856200	4.45158100	4.13278400
Ti	7.80344600	5.93553100	7.82218100
Ti	7.80339500	2.96766900	7.82226500
O	11.21811200	2.96764100	6.47892400
O	11.21811200	5.93553100	6.47892400
O	9.28217200	5.93553100	4.66351400
O	9.28217200	2.96764100	4.66351400
H	12.48624700	3.96240800	4.27917500
H	11.38090800	4.44824900	3.19764400
O	6.57436300	5.93553100	6.47891400
O	9.00011200	7.41950900	7.05134700
O	7.31541900	7.41947000	8.82114600
O	7.31544300	4.45157500	8.82116900
O	6.57435800	2.96760500	6.47891800
O	7.31547000	1.48369700	8.82105800
O	9.00013700	1.48372000	7.05140200
Ti	10.17408900	1.48368600	5.55768400
Ti	12.44720200	2.96764100	7.82221400
Ti	10.17409500	7.41946800	5.55768800
Ti	12.44720200	5.93553100	7.82221400
Ti	5.53028400	7.41945200	5.55765600
Ti	5.53014400	4.45165600	5.55754600
Ti	7.80343700	8.90341400	7.82214700
Ti	5.53037200	1.48370700	5.55772600
H	8.02849500	0.85087600	8.99278000
O	11.60856200	1.48369100	4.13278400
O	11.21811200	-0.00024900	6.47892400
O	9.28217200	-0.00024900	4.66351400
O	13.64384200	4.45158100	7.05137400
O	11.95922200	1.48369100	8.82116400
O	11.95922200	4.45158100	8.82116400
O	13.64384200	1.48369100	7.05137400

O	9.28217200	8.90341100	4.66351400
O	11.60856200	7.41947100	4.13278400
O	11.21811200	8.90341100	6.47892400
O	13.64384200	7.41947100	7.05137400
O	11.95922200	7.41947100	8.82116400
O	4.35682900	7.41991600	7.05132100
O	6.96480200	7.41947100	4.13278400
O	4.63841200	5.93553100	4.66351400
O	4.63841200	8.90341100	4.66351400
O	6.57434000	8.90346000	6.47893500
O	4.35689900	4.45128100	7.05170800
O	6.96480200	4.45158100	4.13278400
O	4.63841200	2.96764100	4.66351400
O	9.00008700	10.38737200	7.05142100
O	7.31543100	10.38733200	8.82129100
O	6.96480200	1.48369100	4.13278400
O	6.57435200	-0.00024900	6.47892400
O	4.35650500	1.48399600	7.05108700
O	4.63841200	-0.00024900	4.66351400
H	12.52233900	1.85143800	4.37331700
H	11.76195900	0.75255500	3.52233800
H	10.98954100	0.25278900	7.41483400
H	9.80924600	-0.78246700	4.46389900
Ti	14.81786200	4.45158100	5.55769400
H	12.71496700	0.88053900	8.71124200
Ti	14.81786200	1.48369100	5.55769400
H	9.88673600	9.62695000	4.45493400
H	11.96401800	8.22469300	3.73061000
Ti	12.44720200	8.90341100	7.82221400
Ti	14.81786200	7.41947100	5.55769400
Ti	3.16027300	8.90083700	7.82084500
Ti	3.15978100	5.93553100	7.82230900
H	7.72103400	6.79731600	4.33518300
H	7.46249400	8.27391500	4.20408800
H	4.74091600	8.97461700	3.70334000
Ti	3.15865800	2.96940700	7.82232700
H	7.90813000	4.73950600	4.28100300
H	6.81730900	4.21299600	3.20996800
H	9.78340100	9.94288100	6.60382200
H	9.40445600	10.95832000	7.72282900
H	7.51663400	10.57117600	9.74670500
H	7.73619300	2.11147900	4.33106500
H	7.42343700	0.64891400	3.90949400
H	7.19386400	0.41752900	7.14105300
H	7.18239200	-0.48446100	5.88893600
H	4.17156600	-0.57895600	5.28083500

O	16.25233200	4.45158100	4.13278400
O	15.86188200	2.96764100	6.47892400
O	15.86188200	5.93553100	6.47892400
O	13.92594200	5.93553100	4.66351400
O	13.92594200	2.96764100	4.66351400
O	16.25233200	1.48369100	4.13278400
O	15.86188200	-0.00024900	6.47892400
O	13.92594200	-0.00024900	4.66351400
O	11.95922200	10.38735100	8.82116400
O	13.64384200	10.38735100	7.05137400
O	16.25233200	7.41947100	4.13278400
O	13.92594200	8.90341100	4.66351400
O	15.86188200	8.90341100	6.47892400
O	1.93002400	8.90490000	6.47943500
O	2.67136800	10.38707800	8.82141100
O	2.67159100	7.41980400	8.82160900
O	4.35620800	10.38722800	7.05097600
O	1.93062900	5.93553100	6.47888100
O	2.67165900	4.45122500	8.82167600
O	1.93125900	2.96614900	6.47830600
O	2.67117500	1.48384700	8.82114400
H	17.13002000	3.96240700	4.27917600
H	16.02467800	4.44825000	3.19764100
Ti	17.09173200	2.96764100	7.82285400
Ti	17.09173200	5.93553100	7.82285400
H	17.16610800	1.85143200	4.37331200
H	16.40572300	0.75255200	3.52233300
H	16.79388500	0.22903900	6.49887700
H	15.53965300	-0.10839200	7.37674000
H	14.07622200	-0.72286200	5.28641400
H	12.44537200	10.82181600	9.52902600
H	13.65628800	11.27459900	7.41547300
H	17.07245600	6.83677400	4.35238500
H	16.60779000	8.22469500	3.73060700
H	14.37635100	9.74255700	4.79468100
Ti	17.09173200	8.90341100	7.82285400
H	2.41827500	8.80778000	5.60981800
H	1.24883700	9.60003100	6.42281200
H	3.19035000	11.20511900	8.87641900
H	4.17362500	10.85210600	6.21799500
H	2.39912200	5.83230300	5.59820500
H	1.00849800	5.62897400	6.42414100
H	2.51756800	2.96532100	5.64970100
H	1.39409600	2.15237100	6.39808500
H	3.25060100	0.72941800	8.61546000
O	18.28462200	4.45158100	7.05211400

O	16.60316200	1.48369100	8.82221400
O	16.60316200	4.45158100	8.82221400
O	18.28462200	1.48369100	7.05211400
O	18.28462200	7.41947100	7.05211400
O	16.60316200	7.41947100	8.82221400
O	18.28462200	10.38735100	7.05211400
O	16.60316200	10.38735100	8.82221400
Ti	19.46326200	4.45158100	5.55497400
H	17.29007300	0.80694000	8.75183000
Ti	19.46326200	1.48369100	5.55497400
Ti	19.46326200	7.41947100	5.55497400
H	19.20832800	9.99088000	6.80967700
H	18.29672800	11.27438800	7.41673700
H	17.08954500	10.82238600	9.52956900
O	20.89609200	4.45158100	4.13278400
O	18.57330200	5.93553100	4.66786400
O	18.57330200	2.96764100	4.66786400
O	20.50617200	2.96764100	6.48185400
O	20.50617200	5.93553100	6.48185400
O	20.89609200	1.48369100	4.13278400
O	18.57330200	-0.00024900	4.66786400
O	20.50617200	-0.00024900	6.48185400
O	20.89609200	7.41947100	4.13278400
O	18.57330200	8.90341100	4.66786400
O	20.50617200	8.90341100	6.48185400
H	21.34171100	3.68693700	4.60191700
H	20.42851300	4.02049800	3.39584200
H	21.42310200	0.81194900	4.61928400
H	20.54290000	1.01657600	3.36030900
H	18.91713300	-0.73413200	5.20137100
H	20.75785400	0.36755500	7.33935700
H	21.13701700	6.47310900	4.05096100
H	20.44812200	7.68402500	3.31487600
H	19.02436800	9.74188600	4.80102800
H	21.34305200	8.55626200	6.79921600
H	12.42868400	6.83677700	4.35238500
H	5.28478800	9.97735000	6.85808100
H	12.20927400	0.29077000	6.51197600
H	14.56750700	9.98985700	6.81044500
C	6.50752900	5.27729300	12.10016800
C	5.85021500	4.52373800	11.14410900
C	5.94857700	3.13844300	11.14814100
C	6.78281500	2.55109400	12.09273500
C	7.40402200	3.36107900	13.03534900
H	5.24926400	4.97748900	10.37089400
H	6.93265200	1.47815700	12.09151200

H	8.03274000	2.93969200	13.81224700
C	6.43514100	6.75166900	12.12439600
C	5.81106700	7.47758100	11.11794100
N	7.01834100	7.36561900	13.17865300
C	5.77311900	8.86255700	11.17857800
H	5.36912300	6.99183500	10.26251400
C	7.02015900	8.70787500	13.21649700
C	6.40616800	9.48837900	12.24840400
H	7.52423200	9.15588400	14.06489600
H	6.42469000	10.56906900	12.31661000
C	5.09254200	2.33190000	10.17147700
O	4.70821400	3.05945600	9.18482700
O	4.82486300	1.17106800	10.45113200
C	5.03113300	9.65383400	10.10979100
O	4.71589700	8.92560500	9.08909800
O	4.77893000	10.83668200	10.30979400
Re	7.59348700	6.00706100	14.84867400
N	7.24445500	4.69499600	13.07603900
C	8.09160200	4.64588000	16.09754100
C	7.81580500	7.33326300	16.20556700
O	8.39712800	3.80493900	16.83400200
O	7.94484900	8.16026300	17.00877600
C	11.53333800	5.02695900	11.74478700
C	10.51318700	4.26569500	11.22874900
C	10.66763000	2.88659900	11.14852100
C	11.79968000	2.30366900	11.70616800
C	12.78822600	3.12134300	12.20964000
H	9.63820500	4.71089800	10.77313900
H	11.93575800	1.23071000	11.65228700
H	13.72447200	2.70626000	12.56180000
C	11.52733200	6.48455800	11.71935600
C	10.52895400	7.25026100	11.16144100
N	12.65429800	7.07416700	12.22101600
C	10.61820200	8.63156200	11.20756100
H	9.69259900	6.79857800	10.64396400
C	12.69836800	8.43647100	12.34614800
C	11.69351600	9.23047100	11.87768900
H	13.58388900	8.84731500	12.81480200
H	11.73452300	10.30826900	11.98332900
C	9.72584200	2.13240400	10.22202200
O	9.41670500	2.91114400	9.27860800
O	9.45183700	0.95116900	10.44877900
C	9.60839800	9.44586400	10.43042200
O	9.43320700	8.92062100	9.30585800
O	9.13320800	10.46112700	10.95884800
Re	14.21324800	5.84378600	12.68452100

N	12.67566000	4.46697000	12.21562000
C	15.05492900	4.43928600	13.80353100
C	15.65274400	7.21921500	12.68190200
O	15.47838900	3.62544400	14.48043500
O	16.46764900	8.01633900	12.65588200
C	13.79822900	6.52056800	14.48748500
O	13.60512200	6.93549300	15.53175600
Cl	15.67117600	4.78222400	11.17563100
Cl	10.08846500	6.28967900	14.33418300
C	5.76301900	5.80676700	15.30610800
O	4.64832200	5.68867600	15.60847200

Coordinates of ReC0A monomer 5.

O	11.60829600	-1.48541300	4.14918400
O	11.60829400	-4.45329800	4.14918400
O	11.60829400	-7.42118800	4.14918400
O	16.25206400	-1.48540800	4.14918400
O	16.25206400	-4.45329800	4.14918400
O	16.25206400	-7.42118800	4.14918400
O	6.96453400	-1.48540800	4.14918400
O	6.96453400	-4.45329800	4.14918400
O	6.96453400	-7.42118800	4.14918400
O	13.92567400	-0.00146800	4.67991300
O	13.92567400	-2.96935800	4.67991300
O	13.92567400	-5.93724800	4.67991300
O	13.92567400	-8.90512800	4.67991300
O	4.63814400	-0.00146800	4.67991300
O	4.63814400	-2.96935800	4.67991300
O	4.63814400	-5.93724800	4.67991300
O	4.63814400	-8.90512800	4.67991300
O	9.28190400	-0.00146800	4.67991300
O	9.28190400	-2.96935800	4.67991300
O	9.28190400	-5.93724800	4.67991300
O	9.28190400	-8.90512800	4.67991300
O	1.93037400	-2.96943000	6.49526800
O	1.93032500	-5.93723300	6.49531400
O	1.93032500	-8.90515600	6.49531300
O	11.21784400	-0.00146800	6.49532400
O	11.21784400	-2.96935800	6.49532400
O	11.21784400	-5.93724800	6.49532400
O	11.21784400	-8.90512800	6.49532400
O	15.86161400	-0.00146800	6.49532400
O	15.86161400	-2.96935800	6.49532400
O	15.86161400	-5.93724800	6.49532400
O	15.86161400	-8.90512800	6.49532400
O	6.57408400	-0.00146800	6.49532400

O	6.57401000	-2.96942800	6.49539100
O	6.57410200	-5.93724800	6.49530800
O	6.57402500	-8.90554200	6.49537800
O	13.64357400	-1.48540800	7.06777400
O	13.64357400	-10.38906800	7.06777400
O	13.64357400	-4.45329800	7.06777400
O	13.64357400	-7.42118800	7.06777400
O	4.35599700	-1.48529000	7.06792700
O	4.35600200	-10.38912300	7.06781200
O	4.35613600	-4.45326500	7.06784400
O	4.35610200	-7.42097700	7.06747300
O	8.99978600	-1.48539900	7.06774700
O	8.99994000	-10.38896700	7.06777500
O	8.99968100	-4.45366400	7.06827400
O	8.99971700	-7.42112800	7.06773900
O	11.95895400	-1.48540800	8.83756300
O	11.95895400	-10.38906800	8.83756300
O	11.95895400	-4.45329800	8.83756300
O	11.95895400	-7.42118800	8.83756300
O	2.67129600	-1.48543300	8.83753800
O	2.67162700	-10.38909500	8.83762400
O	2.67209800	-4.45264900	8.83793400
O	2.67140600	-7.42121100	8.83758900
O	7.31338200	-1.48673300	8.83646700
O	7.31487400	-10.38903200	8.83757400
O	7.31513400	-4.45329800	8.83753900
O	7.31523900	-7.42119600	8.83760100
Ti	10.17383400	-1.48540800	5.57409400
Ti	10.17383400	-4.45329800	5.57409400
Ti	10.17388200	-7.42120700	5.57413200
Ti	14.81759400	-1.48540800	5.57409400
Ti	14.81759400	-4.45329800	5.57409400
Ti	14.81759400	-7.42118800	5.57409400
Ti	5.53006200	-1.48540700	5.57409200
Ti	5.53002100	-4.45331500	5.57406000
Ti	5.53009100	-7.42119100	5.57409200
Ti	12.44693400	-2.96935800	7.83861400
Ti	12.44693300	-5.93724800	7.83861200
Ti	12.44693400	-8.90512800	7.83861400
Ti	3.15946000	-2.96958300	7.83828200
Ti	3.15884100	-5.93768400	7.83898700
Ti	3.15954000	-8.90502000	7.83865000
Ti	7.80465100	-2.96850900	7.83808100
Ti	7.80292800	-5.93724800	7.83847900
Ti	7.80308200	-8.90495600	7.83845000
H	2.72203200	-0.70119000	8.26438500

H	2.61902000	-11.30832200	8.54011400
H	7.29380900	-11.26436600	8.42743500
H	7.33908000	-0.67982000	8.29989500
H	8.43892200	-11.09777100	6.61805800
H	9.60275500	-10.06387100	6.38196000
H	4.98269700	-10.08559800	6.36452900
H	3.78272900	-11.01320000	6.52183100
H	13.71108300	-11.11774400	7.69991800
H	11.95977500	-11.24280400	8.38503900
H	12.09303500	-0.75193200	8.21457100
H	9.75741200	0.83599000	4.64416900
H	16.12713300	-0.40024000	7.33307000
H	16.33341800	-8.47546500	7.22082300
H	9.78247700	-9.26332600	3.93585300
H	2.37655500	-8.86400100	5.60504200
H	1.18295700	-9.53169700	6.45120500
H	2.45740500	-5.93180200	5.64078500
H	1.23719200	-5.25200400	6.42691300
H	2.50044100	-2.87260500	5.66927400
H	1.32550400	-2.19913000	6.49116500
H	14.16005300	0.76205200	5.22512400
H	13.83498000	-9.77922500	5.07021400
H	7.52923300	-0.26419500	6.38929600
H	6.54748600	0.84532400	5.98336800
H	11.02237500	0.86033900	5.99126700
H	12.12562900	-0.17565600	6.15167300
H	16.91934000	-1.06067600	4.73050200
H	15.95315200	-0.78326500	3.54385100
H	17.00286000	-4.51257900	4.77376300
H	16.26794800	-3.53275300	3.81812000
H	16.21542600	-6.53687500	3.73756500
H	15.98293300	-8.07014500	3.47970900
H	12.22166000	-6.62602500	4.21524000
H	12.30261700	-8.13915800	4.31560200
H	12.54158500	-4.13828900	4.36687200
H	11.35872000	-4.03780800	3.31112000
H	12.35660200	-2.14206300	4.35564900
H	12.19147900	-0.67304300	4.13170300
H	7.55258200	-6.61435800	4.17006600
H	7.66517400	-8.13697400	4.29629200
H	7.88517000	-4.12403600	4.35976100
H	6.68531900	-4.01494500	3.32900200
H	7.75402100	-2.06894900	4.35485600
H	7.42578900	-0.63945500	3.95086700
H	4.74395200	0.84378500	5.13554900
H	4.92387800	-9.11799200	3.78278000

H	14.58819800	-9.96011700	6.89676300
C	9.51206800	-3.34925100	11.78397600
C	9.85982200	-2.04026200	12.08154700
C	11.19907600	-1.68916700	12.22764400
C	12.14566900	-2.68406000	12.00900600
C	11.73262000	-3.97282100	11.70684900
H	9.12366100	-1.25866100	12.23159100
H	13.19697400	-2.43158300	12.08725600
H	12.44662900	-4.76761700	11.52968600
C	8.11214800	-3.79073100	11.63934600
C	7.07550800	-2.89019800	11.41220400
N	7.89641200	-5.11986300	11.61726900
C	5.83240600	-3.38485000	11.06633300
H	7.27620500	-1.83212000	11.31262900
C	6.64960800	-5.58606800	11.45761600
C	5.59110300	-4.75370400	11.16892700
H	6.54141900	-6.66398700	11.46301100
H	4.62103800	-5.16712700	10.91166800
C	11.59388800	-0.25397200	12.67775400
O	12.80778500	-0.10232600	12.91876300
O	10.63491200	0.54202300	12.76825500
C	4.87026000	-2.48813300	10.33231800
O	4.52744300	-1.40145500	10.75253400
O	4.54941700	-3.08072300	9.21229000
Re	9.66622500	-6.38837600	11.49826300
N	10.44035400	-4.31822800	11.62564700
C	11.37709900	-7.27401300	11.46584200
C	9.74615200	-6.53790600	13.38514700
C	8.80045500	-8.08696600	11.44227700
O	12.40789900	-7.78156800	11.62110500
O	9.76464700	-6.63868100	14.54810800
O	8.26029900	-9.11751900	11.48660300
O	9.39880100	-6.01699100	9.34513000
H	10.07544800	-6.58534200	8.95157900

Coordinates of ReC0A monomer 6.

O	11.60942000	-1.48394000	4.13357000
O	11.60942000	-4.45183000	4.13357000
O	11.60942000	-7.41972000	4.13357000
O	16.25319000	-1.48394000	4.13357000
O	16.25319000	-4.45183000	4.13357000
O	16.25319000	-7.41972000	4.13357000
O	6.96566000	-1.48394000	4.13357000
O	6.96566000	-4.45183000	4.13357000
O	6.96566000	-7.41972000	4.13357000
O	13.92680000	0.00000000	4.66430000

O	13.92680000	-2.96789000	4.66430000
O	13.92680000	-5.93578000	4.66430000
O	13.92680000	-8.90366000	4.66430000
O	4.63927000	0.00000000	4.66430000
O	4.63927000	-2.96789000	4.66430000
O	4.63927000	-5.93578000	4.66430000
O	4.63927000	-8.90366000	4.66430000
O	9.28303000	0.00000000	4.66430000
O	9.28303000	-2.96789000	4.66430000
O	9.28303000	-5.93578000	4.66430000
O	9.28303000	-8.90366000	4.66430000
O	1.93144100	-2.96789000	6.47971000
O	1.93143800	-5.93578000	6.47971200
O	1.93143000	-8.90365000	6.47971900
O	11.21897000	0.00000000	6.47971000
O	11.21897000	-2.96789000	6.47971000
O	11.21896700	-5.93578000	6.47971300
O	11.21897000	-8.90365000	6.47971000
O	15.86274000	0.00000000	6.47971000
O	15.86274000	-2.96789000	6.47971000
O	15.86274000	-5.93578000	6.47971000
O	15.86274000	-8.90366000	6.47971000
O	6.57521000	0.00000000	6.47971000
O	6.57520400	-2.96788000	6.47971500
O	6.57520900	-5.93578000	6.47971100
O	6.57521000	-8.90366000	6.47971000
O	13.64470000	-1.48394000	7.05216000
O	13.64504800	-10.38740000	7.05231800
O	13.64469300	-4.45183000	7.05214900
O	13.64475900	-7.41976000	7.05217900
O	4.35717000	-1.48394000	7.05216000
O	4.35716800	-10.38760000	7.05214900
O	4.35715800	-4.45183000	7.05214800
O	4.35718600	-7.41972000	7.05218000
O	9.00093700	-1.48393000	7.05216600
O	9.00094000	-10.38760000	7.05216100
O	9.00093400	-4.45183000	7.05215200
O	9.00094200	-7.41972000	7.05216300
O	11.96008000	-1.48394000	8.82195000
O	11.96045300	-10.38761000	8.82212100
O	11.96005300	-4.45183000	8.82193700
O	11.96012700	-7.41972000	8.82197300
O	2.67255000	-1.48394000	8.82195000
O	2.67262800	-10.38761000	8.82197500
O	2.67256300	-4.45183000	8.82195700
O	2.67254700	-7.41972000	8.82195200

O	7.31634500	-1.48395000	8.82186500
O	7.31628200	-10.38762000	8.82201500
O	7.31630100	-4.45183000	8.82194900
O	7.31632100	-7.41972000	8.82195500
Ti	10.17495700	-1.48394000	5.55847800
Ti	10.17496400	-4.45183000	5.55848300
Ti	10.17496500	-7.41972000	5.55847600
Ti	14.81872000	-1.48394000	5.55848000
Ti	14.81872000	-4.45183000	5.55848000
Ti	14.81870200	-7.41971000	5.55846600
Ti	5.53119000	-1.48394000	5.55848000
Ti	5.53119400	-4.45183000	5.55848300
Ti	5.53118100	-7.41972000	5.55847300
Ti	12.44806000	-2.96789000	7.82300000
Ti	12.44813400	-5.93578000	7.82303500
Ti	12.44754100	-8.90370000	7.82269000
Ti	3.16053200	-2.96789000	7.82300300
Ti	3.16051100	-5.93578000	7.82299300
Ti	3.16058200	-8.90368000	7.82297900
Ti	7.80436000	-2.96794000	7.82303800
Ti	7.80428000	-5.93578000	7.82298600
Ti	7.80429100	-8.90367000	7.82297700
H	2.72309300	-0.69973000	8.24875200
H	2.62023000	-11.30687000	8.52452200
H	7.29482600	-11.26288000	8.41179200
H	7.33959800	-0.67898000	8.28331400
H	8.44004600	-11.09632000	6.60247700
H	9.60385500	-10.06241000	6.36632000
H	4.98380400	-10.08414000	6.34889700
H	3.78384700	-11.01176000	6.50625800
H	13.71200400	-11.11639000	7.68419800
H	11.96068200	-11.24130000	8.36936600
H	12.09416100	-0.75046000	8.19895700
H	9.75853800	0.83746000	4.62855500
H	16.12825900	-0.39877000	7.31745700
H	16.33454400	-8.47400000	7.20521000
H	9.78360300	-9.26186000	3.92023900
H	2.37768100	-8.86253000	5.58942800
H	1.18408300	-9.53023000	6.43559100
H	2.45853100	-5.93033000	5.62517100
H	1.23831800	-5.25054000	6.41129900
H	2.50156700	-2.87114000	5.65366000
H	1.32663000	-2.19766000	6.47555100
H	14.16117900	0.76352000	5.20951100
H	13.83610600	-9.77776000	5.05460000
H	7.53035900	-0.26273000	6.37368200

H	6.54861200	0.84679000	5.96775400
H	11.02350100	0.86181000	5.97565300
H	12.12675500	-0.17419000	6.13605900
H	16.92046600	-1.05921000	4.71488800
H	15.95427800	-0.78180000	3.52823800
H	17.00398600	-4.51111000	4.75814900
H	16.26907400	-3.53129000	3.80250600
H	16.21655200	-6.53541000	3.72195100
H	15.98405900	-8.06868000	3.46409500
H	12.22278600	-6.62456000	4.19962600
H	12.30374300	-8.13769000	4.29998800
H	12.54271100	-4.13682000	4.35125800
H	11.35984600	-4.03634000	3.29550600
H	12.35772800	-2.14060000	4.34003500
H	12.19260500	-0.67158000	4.11608900
H	7.55370800	-6.61289000	4.15445300
H	7.66630000	-8.13551000	4.28067800
H	7.88629600	-4.12257000	4.34414700
H	6.68644500	-4.01348000	3.31338900
H	7.75514700	-2.06748000	4.33924200
H	7.42691500	-0.63799000	3.93525300
H	4.74507800	0.84525000	5.11993600
H	4.92500400	-9.11652000	3.76716600
H	14.58822700	-9.96015000	6.89686200
C	7.74900700	-7.89928100	11.61649000
C	6.40963500	-7.74249800	11.27877100
C	5.60292700	-8.86611600	11.23339200
C	6.07235900	-10.08249500	11.71626800
C	7.40868700	-10.16755800	12.02752200
H	6.04823500	-6.79274000	10.90896100
H	5.44229000	-10.96467300	11.72155300
H	7.87624400	-11.10630700	12.30131000
C	8.75233700	-6.81080700	11.54133300
C	8.43527000	-5.48736500	11.27628500
N	10.03537800	-7.20835900	11.68897000
C	9.45569500	-4.54858700	11.08897100
H	7.40792000	-5.18170000	11.12679700
C	11.00945300	-6.29158900	11.60942200
C	10.76526500	-4.96333400	11.31925500
H	12.02110200	-6.66162500	11.72379600
H	11.59186200	-4.27910600	11.18272400
C	4.30430200	-8.85520100	10.49473300
O	4.53178300	-8.86427100	9.20495000
O	3.22456800	-8.87685400	11.05953000
C	9.15532700	-3.13780700	10.58808500
O	9.34637600	-3.02626000	9.33543700

O	8.79344600	-2.31158900	11.42191300
Re	10.34432500	-9.35279300	11.48943100
N	8.22977600	-9.12073000	11.90541300
C	10.36898000	-11.20266600	11.01770300
C	12.22978700	-9.26703100	11.16635500
O	10.35938600	-12.32677600	10.71377000
O	13.38644600	-9.18831000	11.08128800
C	10.73693500	-9.71551700	13.30693100
O	10.94364100	-9.95196500	14.43408100
O	9.53175300	-8.85085600	9.49503400
H	10.11743000	-8.15016800	9.16989100

Coordinates of ReC0A monomer 7.

O	11.60942000	1.48394000	4.13357000
O	11.60942000	4.45183000	4.13357000
O	11.60942000	7.41972000	4.13357000
O	16.25319000	1.48394000	4.13357000
O	16.25319000	4.45183000	4.13357000
O	16.25319000	7.41972000	4.13357000
O	6.96566000	1.48394000	4.13357000
O	6.96566000	4.45183000	4.13357000
O	6.96566000	7.41972000	4.13357000
O	13.92680000	0.00000000	4.66430000
O	13.92680000	2.96789000	4.66430000
O	13.92680000	5.93578000	4.66430000
O	13.92680000	8.90366000	4.66430000
O	4.63927000	0.00000000	4.66430000
O	4.63927000	2.96789000	4.66430000
O	4.63927000	5.93578000	4.66430000
O	4.63927000	8.90366000	4.66430000
O	9.28303000	0.00000000	4.66430000
O	9.28303000	2.96789000	4.66430000
O	9.28303000	5.93578000	4.66430000
O	9.28303000	8.90366000	4.66430000
O	1.93144300	2.96786800	6.47970700
O	1.93142900	5.93578000	6.47972000
O	1.93145000	8.90368800	6.47970100
O	11.21897000	0.00000000	6.47971000
O	11.21897000	2.96789000	6.47971000
O	11.21897000	5.93578000	6.47971000
O	11.21897000	8.90366000	6.47971000
O	15.86274000	0.00000000	6.47971000
O	15.86274000	2.96789000	6.47971000
O	15.86274000	5.93578000	6.47971000
O	15.86274000	8.90366000	6.47971000
O	6.57521000	0.00000000	6.47971000

O	6.57521000	2.96789000	6.47971000
O	6.57521000	5.93578000	6.47971000
O	6.57521000	8.90366000	6.47971000
O	13.64470000	1.48394000	7.05216000
O	13.64470000	10.38760000	7.05216000
O	13.64470000	4.45183000	7.05216000
O	13.64470000	7.41972000	7.05216000
O	4.35729400	1.48399300	7.05224900
O	4.35712400	10.38765500	7.05219300
O	4.35714200	4.45183600	7.05212800
O	4.35715200	7.41971600	7.05214000
O	9.00094000	1.48394000	7.05216000
O	9.00094000	10.38760000	7.05216000
O	9.00094000	4.45183000	7.05216000
O	9.00094000	7.41972000	7.05216000
O	11.96008000	1.48394000	8.82195000
O	11.96008000	10.38760000	8.82195000
O	11.96008000	4.45183000	8.82195000
O	11.96008000	7.41972000	8.82195000
O	2.67240700	1.48397500	8.82193200
O	2.67276000	10.38762700	8.82201300
O	2.67257400	4.45180600	8.82199800
O	2.67252900	7.41974300	8.82197400
O	7.31635000	1.48395300	8.82186600
O	7.31627500	10.38762000	8.82201200
O	7.31631000	4.45183000	8.82195000
O	7.31631000	7.41972000	8.82195000
Ti	10.17496000	1.48394000	5.55848000
Ti	10.17496000	4.45183000	5.55848000
Ti	10.17496000	7.41972000	5.55848000
Ti	14.81872000	1.48394000	5.55848000
Ti	14.81872000	4.45183000	5.55848000
Ti	14.81872000	7.41972000	5.55848000
Ti	5.53112800	1.48391500	5.55843100
Ti	5.53121300	4.45182100	5.55849800
Ti	5.53120300	7.41972500	5.55849100
Ti	12.44806000	2.96789000	7.82300000
Ti	12.44805900	5.93578000	7.82299900
Ti	12.44806000	8.90366000	7.82300000
Ti	3.16047300	2.96791300	7.82290400
Ti	3.16051100	5.93578000	7.82297400
Ti	3.16053900	8.90355200	7.82297800
Ti	7.80430000	2.96791000	7.82303000
Ti	7.80430000	5.93578000	7.82300000
Ti	7.80430000	8.90367200	7.82298200
H	2.72320200	0.69971600	8.24878300

H	2.62014600	11.30685400	8.52450000
H	7.29482600	11.26288200	8.41179200
H	7.33960300	0.67897600	8.28331500
H	8.44004600	11.09632200	6.60247700
H	9.60385500	10.06241000	6.36632000
H	4.98382300	10.08413000	6.34891600
H	3.78385500	11.01173200	6.50621700
H	13.71220900	11.11627600	7.68430400
H	11.96090100	11.24133600	8.36942600
H	12.09416100	0.75046400	8.19895700
H	9.75853800	-0.83745800	4.62855500
H	16.12825900	0.39877200	7.31745700
H	16.33454400	8.47399700	7.20521000
H	9.78360300	9.26185800	3.92023900
H	2.37768100	8.86253300	5.58942800
H	1.18408300	9.53022900	6.43559100
H	2.45853100	5.93033400	5.62517100
H	1.23831800	5.25053600	6.41129900
H	2.50156700	2.87113700	5.65366000
H	1.32663000	2.19766200	6.47555100
H	14.16117900	-0.76352000	5.20951100
H	13.83610600	9.77775700	5.05460000
H	7.53035900	0.26272700	6.37368200
H	6.54861200	-0.84679200	5.96775400
H	11.02350100	-0.86180700	5.97565300
H	12.12675500	0.17418800	6.13605900
H	16.92046600	1.05920800	4.71488800
H	15.95427800	0.78179700	3.52823800
H	17.00398600	4.51111100	4.75814900
H	16.26907400	3.53128500	3.80250600
H	16.21655200	6.53540700	3.72195100
H	15.98405900	8.06867700	3.46409500
H	12.22278600	6.62455700	4.19962600
H	12.30374300	8.13769000	4.29998800
H	12.54271100	4.13682100	4.35125800
H	11.35984600	4.03634000	3.29550600
H	12.35772800	2.14059500	4.34003500
H	12.19260500	0.67157500	4.11608900
H	7.55370800	6.61289000	4.15445300
H	7.66630000	8.13550600	4.28067800
H	7.88629600	4.12256800	4.34414700
H	6.68644500	4.01347700	3.31338900
H	7.75514700	2.06748100	4.33924200
H	7.42691500	0.63798700	3.93525300
H	4.74507800	-0.84525300	5.11993600
H	4.92500400	9.11652400	3.76716600

H	14.58819800	9.96011700	6.89676300
C	6.95456300	6.74491800	11.49200400
C	5.85023400	7.49530900	11.09665600
C	5.96491500	8.87154300	10.99167000
C	7.12557000	9.48033100	11.46186100
C	8.19569000	8.67384500	11.80128500
H	4.96134400	7.01091300	10.71372100
H	7.24509700	10.55316700	11.39572100
H	9.16738700	9.09228400	12.03815000
C	6.96896100	5.26794000	11.49304600
C	5.86007200	4.50416700	11.16454800
N	8.16943400	4.69460100	11.70472400
C	5.98950400	3.12876400	11.04518000
H	4.93478700	4.96853500	10.84755000
C	8.25924100	3.35938300	11.72698000
C	7.18458900	2.53723800	11.43545800
H	9.24835800	2.95290100	11.90417400
H	7.31865000	1.46767700	11.34794900
C	5.01001500	9.66452500	10.12974500
O	4.62448300	8.93571000	9.11279700
O	4.72902900	10.82783400	10.36928800
C	4.95642300	2.33612200	10.27134100
O	4.56721600	3.04135600	9.25559100
O	4.63283600	1.21177600	10.62209300
Re	9.90509900	6.02833500	11.62342000
N	8.13189300	7.33728400	11.75172600
C	11.22999900	7.43106100	11.53955000
C	11.28866100	4.66716000	11.50441700
O	11.92830100	8.34573400	11.64801900
O	12.03271700	3.79697500	11.62054400
O	10.21375000	6.01270400	14.66463100
C	10.11987000	6.01434400	13.49223600
O	9.39543300	6.03842100	9.47780500
H	10.12268800	6.54371100	9.08360300

Coordinates of ReC0A monomer 8.

O	11.60829400	1.48540800	-4.14918400
O	11.60829400	4.45329800	-4.14918400
O	11.60829400	7.42118800	-4.14918400
O	16.25206400	1.48540800	-4.14918400
O	16.25206400	4.45329800	-4.14918400
O	16.25206400	7.42118800	-4.14918400
O	6.96453400	1.48540800	-4.14918400
O	6.96453400	4.45329800	-4.14918400
O	6.96453400	7.42118800	-4.14918400
O	13.92567400	0.00146800	-4.67991300

O	13.92567400	2.96935800	-4.67991300
O	13.92567400	5.93724800	-4.67991300
O	13.92567300	8.90512900	-4.67991200
O	4.63814400	0.00146800	-4.67991300
O	4.63814400	2.96935800	-4.67991300
O	4.63814400	5.93724800	-4.67991300
O	4.63814400	8.90512800	-4.67991300
O	9.28190400	0.00146800	-4.67991300
O	9.28190400	2.96935800	-4.67991300
O	9.28190400	5.93724800	-4.67991300
O	9.28190400	8.90512800	-4.67991300
O	1.93031700	2.96933600	-6.49532100
O	1.93030300	5.93724800	-6.49533400
O	1.93032400	8.90515600	-6.49531400
O	11.21784400	0.00146800	-6.49532400
O	11.21784400	2.96935800	-6.49532400
O	11.21784400	5.93724800	-6.49532400
O	11.21784400	8.90512800	-6.49532400
O	15.86161400	0.00146800	-6.49532400
O	15.86161400	2.96935800	-6.49532400
O	15.86161400	5.93724800	-6.49532400
O	15.86161400	8.90512800	-6.49532400
O	6.57408400	0.00146800	-6.49532400
O	6.57408200	2.96936000	-6.49532600
O	6.57400700	5.93719800	-6.49539500
O	6.57399000	8.90520700	-6.49541000
O	13.64357400	1.48540800	-7.06777400
O	13.64357400	10.38906800	-7.06777400
O	13.64357400	4.45329800	-7.06777400
O	13.64357400	7.42118800	-7.06777400
O	4.35616800	1.48546100	-7.06786300
O	4.35599800	10.38912300	-7.06780600
O	4.35601600	4.45330400	-7.06774200
O	4.35602600	7.42118400	-7.06775400
O	8.99983500	1.48541600	-7.06779100
O	8.99981400	10.38907000	-7.06777700
O	8.99968500	4.45309400	-7.06794800
O	8.99980800	7.42121700	-7.06772000
O	11.95895400	1.48540800	-8.83756300
O	11.95895400	10.38906800	-8.83756300
O	11.95895400	4.45329800	-8.83756300
O	11.95895400	7.42118800	-8.83756300
O	2.67128100	1.48544300	-8.83754600
O	2.67163400	10.38909500	-8.83762700
O	2.67144800	4.45327400	-8.83761100
O	2.67140300	7.42121100	-8.83758700

O	7.31523800	1.48542200	-8.83748900
O	7.31477000	10.38903900	-8.83751200
O	7.31517400	4.45329600	-8.83756000
O	7.31521100	7.42129200	-8.83769100
Ti	10.17382400	1.48540400	-5.57408600
Ti	10.17382600	4.45330100	-5.57408800
Ti	10.17385300	7.42119500	-5.57410900
Ti	14.81759400	1.48540800	-5.57409400
Ti	14.81759400	4.45329800	-5.57409400
Ti	14.81759400	7.42118800	-5.57409400
Ti	5.53000200	1.48538300	-5.57404500
Ti	5.53008700	4.45328900	-5.57411200
Ti	5.53012900	7.42118600	-5.57405800
Ti	12.44693400	2.96935800	-7.83861400
Ti	12.44693300	5.93724800	-7.83861200
Ti	12.44693400	8.90512800	-7.83861400
Ti	3.15934700	2.96938100	-7.83851800
Ti	3.15938500	5.93724800	-7.83858800
Ti	3.15941300	8.90502000	-7.83859200
Ti	7.80314300	2.96936100	-7.83859200
Ti	7.80349100	5.93758100	-7.83829300
Ti	7.80329900	8.90485000	-7.83864300
H	2.72207600	0.70118400	-8.26439700
H	2.61902000	11.30832200	-8.54011400
H	7.29390700	11.26438100	-8.42746200
H	7.33846800	0.68044500	-8.29892700
H	8.43891800	11.09780500	-6.61811600
H	9.60270500	10.06388500	-6.38191000
H	4.98269700	10.08559800	-6.36452900
H	3.78272900	11.01320000	-6.52183100
H	13.71108300	11.11774400	-7.69991800
H	11.95977500	11.24280400	-8.38503900
H	12.09303500	0.75193200	-8.21457100
H	9.75741200	-0.83599000	-4.64416900
H	16.12713300	0.40024000	-7.33307000
H	16.33341800	8.47546500	-7.22082300
H	9.78247700	9.26332600	-3.93585300
H	2.37655500	8.86400100	-5.60504200
H	1.18295700	9.53169700	-6.45120500
H	2.45740500	5.93180200	-5.64078500
H	1.23719200	5.25200400	-6.42691300
H	2.50044100	2.87260500	-5.66927400
H	1.32550400	2.19913000	-6.49116500
H	14.16005300	-0.76205200	-5.22512400
H	13.83498000	9.77922500	-5.07021400
H	7.52923300	0.26419500	-6.38929600

H	6.54748600	-0.84532400	-5.98336800
H	11.02237500	-0.86033900	-5.99126700
H	12.12562900	0.17565600	-6.15167300
H	16.91934000	1.06067600	-4.73050200
H	15.95315200	0.78326500	-3.54385100
H	17.00286000	4.51257900	-4.77376300
H	16.26794800	3.53275300	-3.81812000
H	16.21542600	6.53687500	-3.73756500
H	15.98293300	8.07014500	-3.47970900
H	12.22166000	6.62602500	-4.21524000
H	12.30261700	8.13915800	-4.31560200
H	12.54158500	4.13828900	-4.36687200
H	11.35872000	4.03780800	-3.31112000
H	12.35660200	2.14206300	-4.35564900
H	12.19147900	0.67304300	-4.13170300
H	7.55258200	6.61435800	-4.17006600
H	7.66517400	8.13697400	-4.29629200
H	7.88517000	4.12403600	-4.35976100
H	6.68531900	4.01494500	-3.32900200
H	7.75402100	2.06894900	-4.35485600
H	7.42578900	0.63945500	-3.95086700
H	4.74395200	-0.84378500	-5.13554900
H	4.92387800	9.11799200	-3.78278000
H	14.58819800	9.96011700	-6.89676300
C	10.13666100	8.05774000	-11.65985400
C	11.48738500	8.10608000	-11.32028100
C	12.17371900	9.32200600	-11.31665500
C	11.46892100	10.43857400	-11.77114700
C	10.14280000	10.32310700	-12.13242700
H	11.99838000	7.20836300	-11.00821200
H	11.97089400	11.39755100	-11.82355700
H	9.57824400	11.17961300	-12.48589500
C	9.33034600	6.81182300	-11.61421400
C	9.75169500	5.63990700	-10.98178200
N	8.12884800	6.88686800	-12.23272400
C	8.96037800	4.49124100	-11.06200200
H	10.68357300	5.60131400	-10.42404200
C	7.35577800	5.78817000	-12.28025300
C	7.74562300	4.58169800	-11.74730500
H	6.39786800	5.90296200	-12.77471800
H	7.10019900	3.71390900	-11.82285700
C	13.63191700	9.52060800	-10.82877800
O	14.32235900	10.21764100	-11.58741400
O	13.95185600	9.00492100	-9.72148300
C	9.37090000	3.12783000	-10.49797700
O	9.62423700	2.28870000	-11.35711400

O	9.38399300	3.01887200	-9.23281800
Re	7.50815000	8.82019400	-13.06349200
N	9.46837700	9.16067200	-12.07626300
C	7.20174600	10.61545400	-13.67120900
C	8.45994500	8.41678500	-14.71149700
C	5.85293800	8.27505400	-13.84318500
O	7.05114900	11.71074900	-14.03074800
O	9.01321100	8.19245700	-15.70532000
O	4.85141600	7.91675600	-14.31165400
O	6.48945200	9.14739600	-11.31431600
H	7.00689300	9.59115100	-10.62617900

Coordinates of Ti-CO interaction complex.

O	11.60829400	1.48540800	-4.14918400
O	11.60829400	4.45329800	-4.14918400
O	11.60829400	7.42118800	-4.14918400
O	16.25206400	1.48540800	-4.14918400
O	16.25206400	4.45329800	-4.14918400
O	16.25206400	7.42118800	-4.14918400
O	6.96453400	1.48540800	-4.14918400
O	6.96453400	4.45329800	-4.14918400
O	6.96453400	7.42118800	-4.14918400
O	13.92567400	0.00146800	-4.67991300
O	13.92567400	2.96935800	-4.67991300
O	13.92567400	5.93724800	-4.67991300
O	13.92567400	8.90512800	-4.67991300
O	4.63814400	0.00146800	-4.67991300
O	4.63814400	2.96935800	-4.67991300
O	4.63814400	5.93724800	-4.67991300
O	4.63814400	8.90512800	-4.67991300
O	9.28190400	0.00146800	-4.67991300
O	9.28190400	2.96935800	-4.67991300
O	9.28190400	5.93724800	-4.67991300
O	9.28190400	8.90512800	-4.67991300
O	1.93031200	2.96937200	-6.49532500
O	1.93030900	5.93724800	-6.49532900
O	1.93032500	8.90515600	-6.49531300
O	11.21784400	0.00146800	-6.49532400
O	11.21784400	2.96935800	-6.49532400
O	11.21784400	5.93724800	-6.49532400
O	11.21784400	8.90512800	-6.49532400
O	15.86161400	0.00146800	-6.49532400
O	15.86161400	2.96935800	-6.49532400
O	15.86161400	5.93724800	-6.49532400
O	15.86161400	8.90512800	-6.49532400
O	6.57408400	0.00146800	-6.49532400

O	6.57408400	2.96935800	-6.49532400
O	6.57410200	5.93724800	-6.49530800
O	6.57402500	8.90554200	-6.49537800
O	13.64357400	1.48540800	-7.06777400
O	13.64357400	10.38906800	-7.06777400
O	13.64357400	4.45329800	-7.06777400
O	13.64357400	7.42118800	-7.06777400
O	4.35604900	1.48541500	-7.06776600
O	4.35600200	10.38912300	-7.06781200
O	4.35611300	4.45326700	-7.06782200
O	4.35601700	7.42118400	-7.06773900
O	8.99981400	1.48540800	-7.06777400
O	8.99994000	10.38896700	-7.06777500
O	8.99983500	4.45329800	-7.06780600
O	8.99971700	7.42112800	-7.06773900
O	11.95895400	1.48540800	-8.83756300
O	11.95895400	10.38906800	-8.83756300
O	11.95895400	4.45329800	-8.83756300
O	11.95895400	7.42118800	-8.83756300
O	2.67132000	1.48543300	-8.83755000
O	2.67162700	10.38909500	-8.83762400
O	2.67143100	4.45327900	-8.83759600
O	2.67138000	7.42121100	-8.83757600
O	7.31522400	1.48542100	-8.83748000
O	7.31487400	10.38903200	-8.83757400
O	7.31518700	4.45329800	-8.83756500
O	7.31523900	7.42119600	-8.83760100
Ti	10.17383400	1.48540800	-5.57409400
Ti	10.17383400	4.45329800	-5.57409400
Ti	10.17388200	7.42120700	-5.57413200
Ti	14.81759400	1.48540800	-5.57409400
Ti	14.81759400	4.45329800	-5.57409400
Ti	14.81759400	7.42118800	-5.57409400
Ti	5.53006200	1.48540700	-5.57409200
Ti	5.53002100	4.45331500	-5.57406000
Ti	5.53009100	7.42119100	-5.57409200
Ti	12.44693400	2.96935800	-7.83861400
Ti	12.44693300	5.93724800	-7.83861200
Ti	12.44693400	8.90512800	-7.83861400
Ti	3.15948600	2.96935000	-7.83864100
Ti	3.15941400	5.93724800	-7.83861800
Ti	3.15941500	8.90502000	-7.83858900
Ti	7.80317400	2.96937800	-7.83864400
Ti	7.80318900	5.93724800	-7.83860800
Ti	7.80308200	8.90495600	-7.83845000
H	2.72203200	0.70119000	-8.26438500

H	2.61902000	11.30832200	-8.54011400
H	7.29380900	11.26436600	-8.42743500
H	7.33847700	0.68044400	-8.29892900
H	8.43892200	11.09777100	-6.61805800
H	9.60275500	10.06387100	-6.38196000
H	4.98269700	10.08559800	-6.36452900
H	3.78272900	11.01320000	-6.52183100
H	13.71108300	11.11774400	-7.69991800
H	11.95977500	11.24280400	-8.38503900
H	12.09303500	0.75193200	-8.21457100
H	9.75741200	-0.83599000	-4.64416900
H	16.12713300	0.40024000	-7.33307000
H	16.33341800	8.47546500	-7.22082300
H	9.78247700	9.26332600	-3.93585300
H	2.37655500	8.86400100	-5.60504200
H	1.18295700	9.53169700	-6.45120500
H	2.45740500	5.93180200	-5.64078500
H	1.23719200	5.25200400	-6.42691300
H	2.50044100	2.87260500	-5.66927400
H	1.32550400	2.19913000	-6.49116500
H	14.16005300	-0.76205200	-5.22512400
H	13.83498000	9.77922500	-5.07021400
H	7.52923300	0.26419500	-6.38929600
H	6.54748600	-0.84532400	-5.98336800
H	11.02237500	-0.86033900	-5.99126700
H	12.12562900	0.17565600	-6.15167300
H	16.91934000	1.06067600	-4.73050200
H	15.95315200	0.78326500	-3.54385100
H	17.00286000	4.51257900	-4.77376300
H	16.26794800	3.53275300	-3.81812000
H	16.21542600	6.53687500	-3.73756500
H	15.98293300	8.07014500	-3.47970900
H	12.22166000	6.62602500	-4.21524000
H	12.30261700	8.13915800	-4.31560200
H	12.54158500	4.13828900	-4.36687200
H	11.35872000	4.03780800	-3.31112000
H	12.35660200	2.14206300	-4.35564900
H	12.19147900	0.67304300	-4.13170300
H	7.55258200	6.61435800	-4.17006600
H	7.66517400	8.13697400	-4.29629200
H	7.88517000	4.12403600	-4.35976100
H	6.68531900	4.01494500	-3.32900200
H	7.75402100	2.06894900	-4.35485600
H	7.42578900	0.63945500	-3.95086700
H	4.74395200	-0.84378500	-5.13554900
H	4.92387800	9.11799200	-3.78278000

H	14.58819800	9.96011700	-6.89676300
C	8.58654200	5.30779900	-11.67760300
C	9.55246400	4.39484200	-12.04906400
C	10.89336600	4.78240200	-12.11144800
C	11.21260900	6.07080800	-11.69941200
C	10.20150900	6.95071300	-11.35427800
H	9.32269800	3.37448300	-12.34016200
H	12.25293900	6.37242000	-11.67584500
H	10.42716100	7.96599000	-11.05068700
C	7.15397600	4.97903100	-11.59124600
C	6.67929500	3.67280200	-11.44648200
N	6.32058700	6.02964800	-11.48997600
C	5.34129800	3.49667800	-11.15972800
H	7.37401500	2.84614400	-11.34880300
C	4.98652500	5.82599500	-11.46411600
C	4.45713900	4.57469200	-11.31815700
H	4.36265300	6.71220700	-11.48921500
H	3.39237100	4.44689300	-11.16589000
C	11.95755700	3.82027800	-12.72155600
O	13.10534900	4.29501900	-12.75154300
O	11.47204300	2.74886200	-13.13165100
C	4.85744600	2.35995100	-10.28389800
O	4.74321000	1.20102900	-10.60076900
O	4.62436100	2.96127900	-9.14574500
Re	7.21399100	7.94898700	-11.14196400
N	8.89937800	6.60269300	-11.38347200
C	8.28938600	9.57744200	-11.09989300
C	6.84697600	8.38265600	-12.94809500
C	5.66711400	8.75555600	-10.42324700
O	8.93786300	10.51704200	-11.25079100
O	6.58915800	8.64168100	-14.04601600
O	4.75121500	9.07702500	-9.75720500