Supporting Information for:

Surface-Induced Anisotropic Binding of a Rhenium CO_2-Reduction Catalyst on Rutile TiO_2 (110) Surfaces

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Section 1. AFM image of TiO_2 (110) single crystal surface.

After the cleaning procedure, the morphology of the TiO_2 (110) single crystal surface was examined by the AFM measurement in air at room temperature. As shown in the Figure S1, the AFM image of TiO_2 (110) surface exhibits smooth wide terraces with steps. In order to precisely determine the direction of crystal axes of TiO_2 (110), the crystals were also examined by X-ray crystallography. In the SFG measurements, the single crystals were mounted on a rotation stage. The error of the rotation angle (the angle between the [-110] axis and the plane of the incident fields) for the TiO_2 crystals is less than 1°.

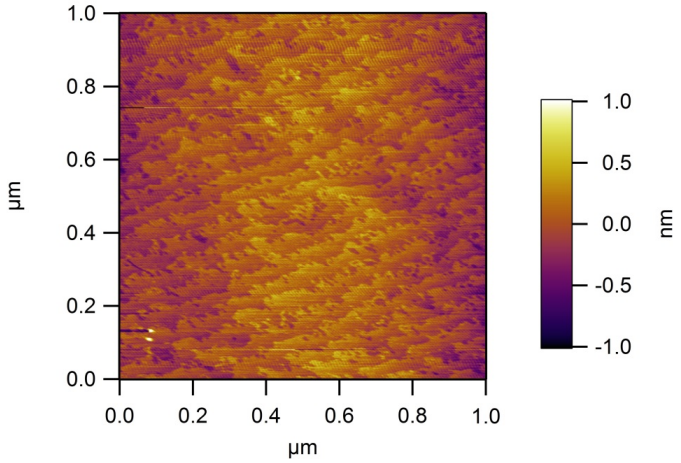


Figure S1. AFM image of clean TiO_2 (110) single crystal surface observed in air at room temperature.

Section 2. FTIR and SFG spectra of ReC0A samples with different immersion time.

TiO_2 nanoporous thin film was prepared on sapphire substrate. Firstly, the TiO_2 colloid was Prepared by diluting a solution of 20 nm-sized paste (Dyesol, 90-T) in terpineol (1:3, v/v). Then, the TiO_2 colloid layer with thickness of 40 μm was coated on the sapphire substrate. After that, the TiO_2 colloid thin film was calcinated at 500 ^{o}C in air for 2 hours to generate a TiO_2 nanoporous thin film with thickness of about 200 nm. The nanoporous TiO_2 thin film was immersed into the 1 mM ReC0A/ethanol solution with different immersion time. After washed by ethanol to remove nonadsorbed ReC0A molecules, the sample was measured by FTIR. The procedure used to prepare ReC0A/TiO_2 (001) samples has been described in the main text.

Figure S2a shows the IR spectra of ReC0A adsorbed on TiO_2 thin film with 5 hours of immersion time in solutions of different concentrations. For the sample prepared by 0.01 mM ReC0A/ethanol solution, three bands can be observed: an in-phase symmetric a′(1) stretch at ~2036 cm^{-1} with a shoulder at 2043 cm^{-1}, an anti-symmetric a″ stretch at ~1932 cm^{-1}, and an out-of-phase symmetric a′(2) stretch at ~1915 cm^{-1}. The peak area increases at higher solution concentration, indicating the coverage of the ReC0A increases. Especially for the sample prepared with 1 mM ReC0A/ethanol solution, two peaks at 2038 cm^{-1} and 2046 cm^{-1} can be clearly observed. To further examine the coverage dependence of the C=O stretches, we prepared the samples by using 1 mM ReC0A/ethanol solution with different immersion times. As can be seen in Figure S3a, when the immersion time increase to 10 hours, the peak at 2050 cm^{-1} dominates the a′(1) stretch. In addition, the frequencies of a″ and a′(2) stretches shift to ~1938 cm^{-1} and 1917 cm^{-1}, respectively. When the immersion time further increased to 20 hours and 40 hours, no apparent changes of both peak position and intensity were observed, indicating the coverage of ReC0A has been saturated on the TiO_2 thin film surface. The peak shift with increase of surface coverage of ReC0A has been reported by Zanni and coworkers, which is attributed to the dye aggregation on the surface.[1-2] According to their reports, ReC0A dimers or trimers can be formed on the TiO_2 surface especially for the full-coverage samples.

As described in the main text, we have prepared the ReC0A/TiO_2 single crystal samples by immersing the crystal into 1 mM ReC0A/ethanol (saturated) solution longer than 20 hours. Therefore, full-coverage ReC0A monolayer could be formed on the surface of TiO_2 single crystal. To examine the effect of surface coverage on molecular orientation, ReC0A/TiO_2 (001) samples with different surface coverage were prepared and measured by SFG spectroscopy. As shown in Figure S2b, SFG spectra of ReC0A/TiO_2 (001) show that the peak intensity of a′ stretch increases as the concentration increases (surface coverage also increases as shown in Figure S2a). In addition, a weak band around 1920 cm^{-1} appears as the concentration increased to 0.1 mM. This weak band was observed for the samples prepared by increasing the immersion time in 1 mM solution (Figure S3b). The change of this weak band may be due to the orientation change of ReC0A molecules. In the case of submonolayer (e.g. 5 hours immersion time in 0.01 mM solution), ReC0A molecules may tend to be perpendicular to the TiO_2 surface. When the surface coverage increases, they may tend to be tilted and lead to the appearance of the a′(2) band. For the samples prepared by using 1 mM solution, it is noted that there is no significant

change of amplitude ratio between low and high frequency modes, indicating no apparent change of molecular orientation. It is also noted that there is significant nonresonant signal from the TiO_2 single crystal contributing to the SFG signal. This strong interference makes a quantitative analysis of the weak band unreliable. On the other hand, for the ReC0A/TiO_2 (110) sample, the peak intensity (amplitude) of the low frequency mode is larger and shows significant dependence on the azimuthal orientation of the TiO_2 (110) surface.

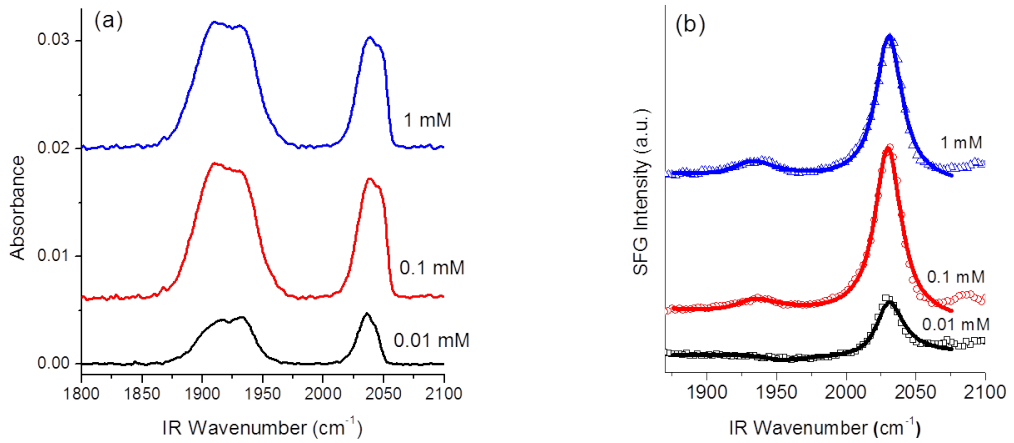


Figure S2. (a) FTIR spectra of ReC0A adsorbed on TiO_2 nanoporous thin film with 5 hours of immersion time using 0.01, 0.1, and 1 mM ReC0A/ethanol solutions. (b) SFG spectra of ReC0A monolayer adsorbed on TiO_2 (001) surface with 5 hours of immersion time using 0.01, 0.1, and 1 mM ReC0A/ethanol solutions. Solid curves are fitting results according to equation (1). The immersion time for each sample is given in the figure. The spectra are offset for clarity.

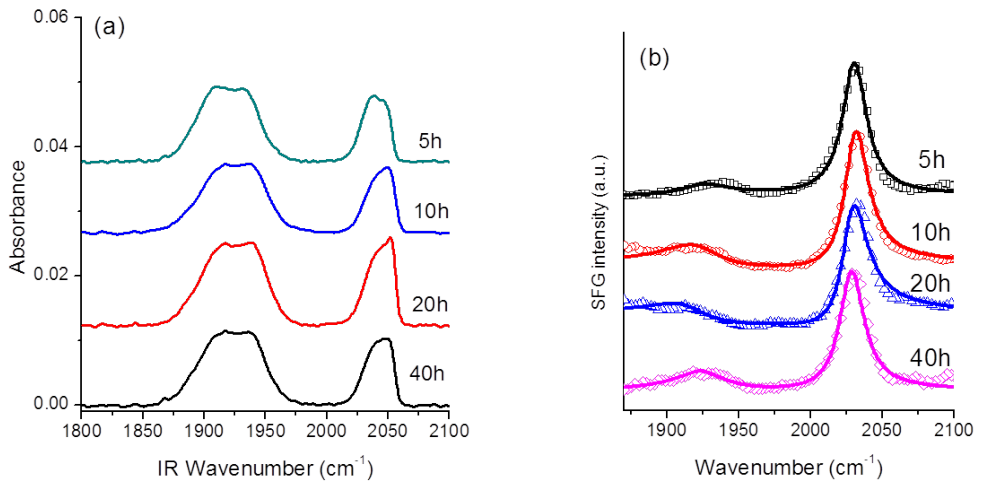


Figure S3. (a) FTIR spectra of ReC0A adsorbed on TiO_2 nanoporous thin film with different immersion time using 1 mM ReC0A/ethanol solution. The spectra are offset for clarity. (b) SFG spectra of ReC0A monolayer adsorbed on TiO_2 (001) surface with different immersion time. Solid curves are fitting results according to equation (1). The peak intensity of a′(1) stretch in in (b) have been normalized. The immersion time for each sample is given in the figure.

Section 3. Fitted amplitude values.

Figure S4 shows the azimuthal dependence of fitted amplitude values with standard deviations based on PPP-polarized SFG spectra of different samples. The spectra were fitted by using equation (1) in main text. The average fitted amplitude values were also shown in Figure 4. The amplitude of the a′(1) mode at $\gamma = 90^{o}$ for ReC0A/TiO_2 (110) system is normalized to one with all other data points for each mode scaled accordingly. The fitted frequencies for a'(1) and a'(2) modes are 2040 cm^{-1} and 1917 cm^{-1}, respectively, while their damping coefficients are 11.5 cm^{-1} and 26.9 cm^{-1}, respectively. The nonresonant signal is much weaker than resonant signal, so the phase δ which could not be precisely obtained was set to zero in the fitting process.

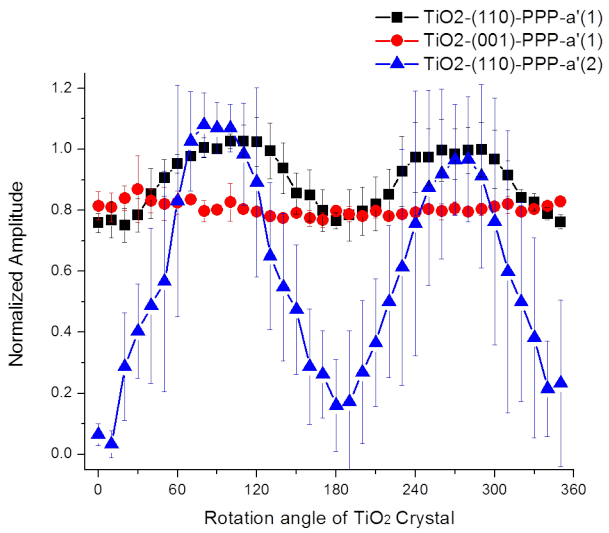


Figure S4. Azimuthal dependence of fitted amplitude values with standard deviations based on PPP-polarized SFG spectra. The fitted amplitude values are also given in Figure 4.

Section 4. Dipole derivatives and displacement vectors for the monomer, theoretical SFG spectra, electronic energies, orientation angles, for all orientations of the dimer on TiO_2 along with dipole derivatives and displacement vectors for all stretches for when both CO groups face the surface.

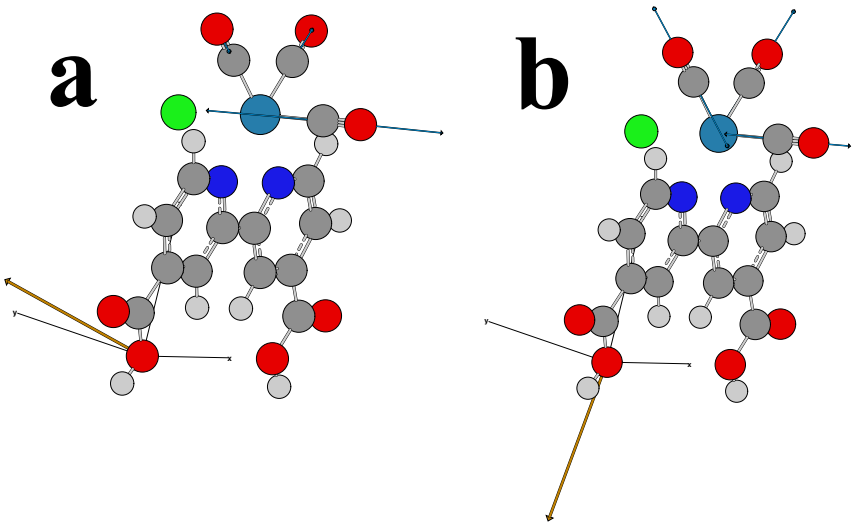


Figure S5. Dipole derivative centered in the middle of the coordinate system (gold arrow) and displacement vectors (blue arrows) for the a′(2) mode at 1920 cm^{-1} (panel a) and for the a′(1)

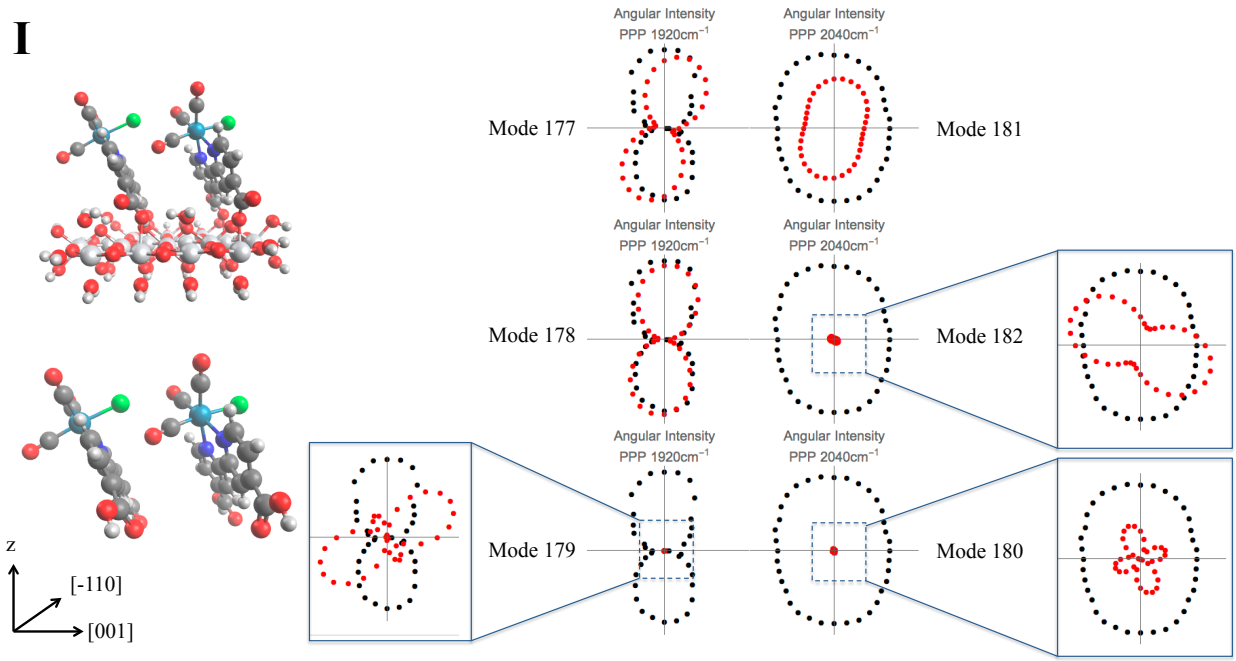
mode at 2040 cm^{-1} (panel b) stretches. The atoms are colored as follows: with green = Cl, silver = Ti, cerulean = Re, white = H, red = O, gray = C, and blue = N.

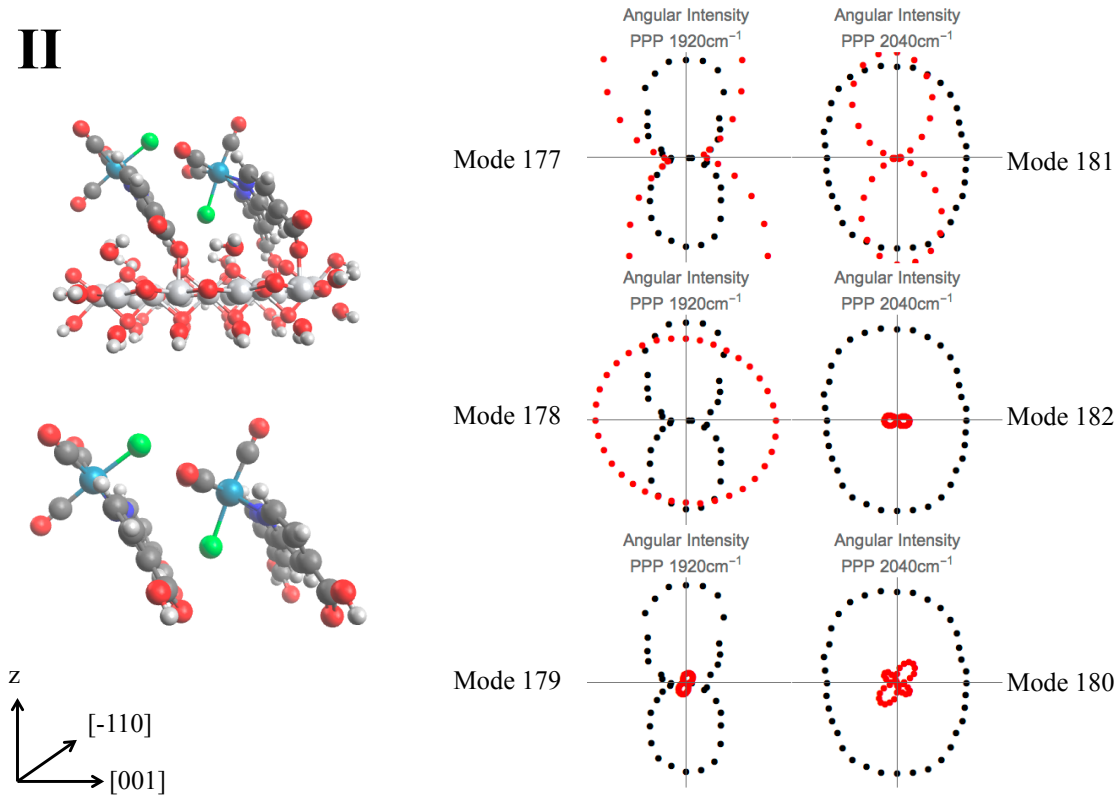
Table S1. Computed theoretical tilt angles (θ, negative when Cl faces the surface) and electronic (SCF) energies for fully relaxed ReC0A dimer molecules (ΔE_1) on the cluster of TiO_2, that geometry in the gas-phase with a neutralizing proton added (ΔG_2), and approximately placed on the cluster of TiO_2 for orientation I (ΔE_3) for each possible orientation of the axial ligands.

Label for Figure S6	**Outer Ligand Facing Down**	**Inner Ligand Facing Down**	**ΔE_1 (kcal/mol)**	**ΔG_2 (kcal/mol)**	**ΔE_3 (kcal/mol)**	**Outer θ**	**Inner θ**
I	CO	CO	8.47	4.95	-28.50	26°	18°
II	CO	Cl	4.36	11.32	14.72	32°	-37°
III	Cl	CO	2.52	8.56	5.38	-29°	18°
IV	Cl	Cl	0	0.00	0	-19°	-23°

Table S2. Theoretical scaled (0.98) frequencies and mode assignment for the carbonyl stretching region of Structure I in Figure S6

Mode	**Frequency (cm^{-1})**	**Name**	**Mode Assignment**
177	1917.66	a′(2)	Uncoupled out of phase of one monomer
178	1925.18	a′(2)	Uncoupled out of phase of the other monomer
179	1943.62	a″	Antisymmetrically coupled antisymmetric
180	1948.29	a″	Symmetrically coupled antisymmetric
181	2023.48	a′(1)	Antisymmetrically coupled symmetric
182	2024.97	a′(1)	Symmetrically coupled symmetric


I
Angular Intensity
PPP 1920cm^{-1}
Angular Intensity
PPP 2040cm^{-1}
Mode 177
Mode 181
Mode 178
Mode 182
Mode 179
Mode 180
z
[-110]
[001]


II
Angular Intensity
PPP 1920cm^{-1}
Angular Intensity
PPP 2040cm^{-1}
Mode 177
Mode 181
Mode 178
Mode 182
Mode 179
Mode 180
z
[-110]
[001]

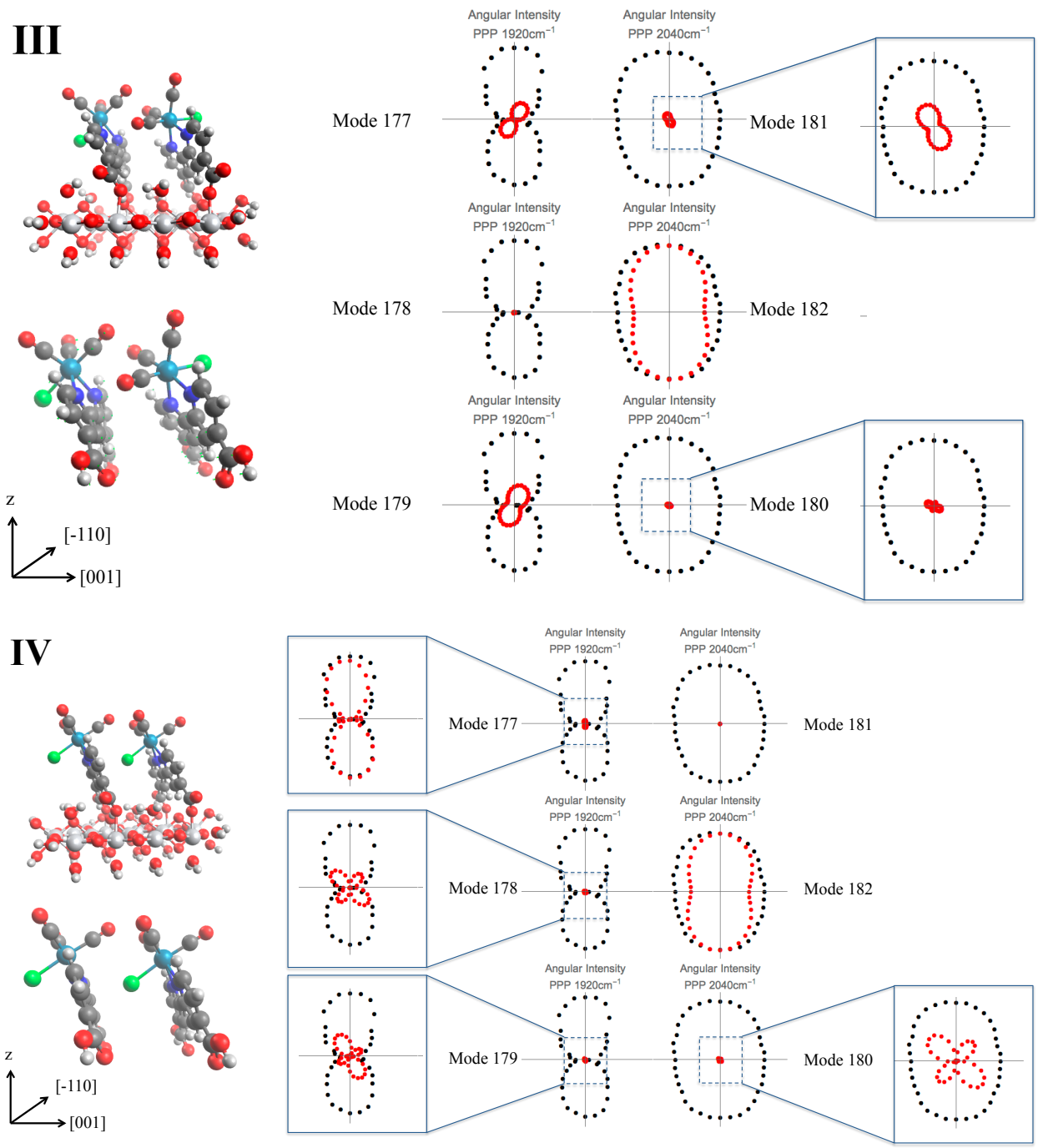


Figure S6. For each possible orientation of the axial ligands relative to the surface (I-IV), as listed in Table S2, the geometry of the molecule, adsorbed and in the gas-phase, the SFG spectra around all γ angles for all stretches with possible matches to the 1920 cm^{-1} (a′(2)) and 2040 cm^{-1}. The vertical axis in the SFG spectra indicate the (001) direction while the horizontal axes indicate the [-110] direction. The red dots indicate the theoretical spectra while the black dots indicate the experimental spectra. Two consecutive dots are separated by 10° in the style of

Figure 2b. Blue insets are included on spectra that would be too small to see when normalized. The atoms are colored as follows: with green = Cl, silver = Ti, cerulean = Re, white = H, red = O, gray = C, and blue = N.

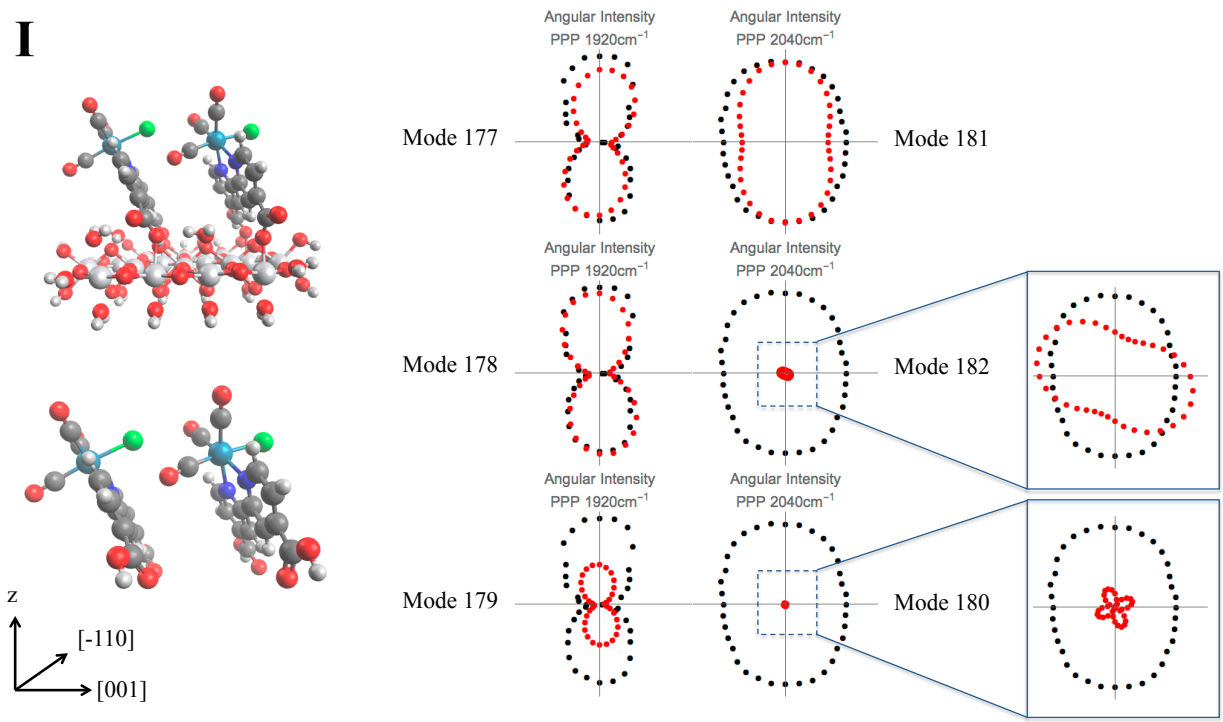


Figure S7. Panel I of Figure S5 with an additional tilt of θ of 4° for the whole dimer.

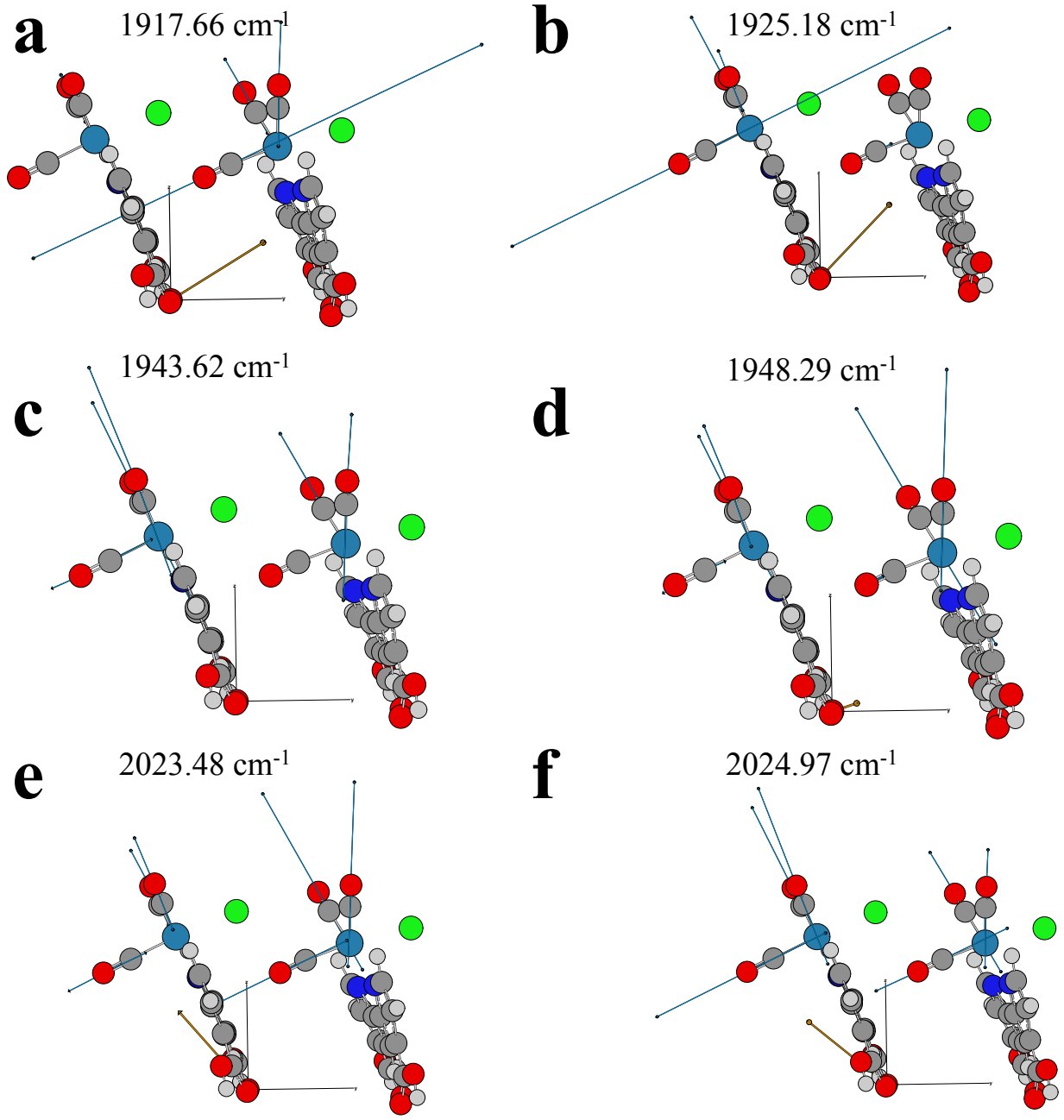


Figure S8. Dipole derivative centered in the middle of the coordinate system (gold arrow), displacement vectors (blue arrows), and theoretically scaled frequency for the mostly uncoupled a′(2) modes (panels a and b), for the antisymmetrically and symmetrically coupled a″ modes (panels c and d respectively), and for the antisymmetrically and symmetrically coupled a′(1) mode (panels e and f respectively) stretches in the dimer with both CO's facing the surface. The atoms are colored as follows: with green = Cl, silver = Ti, cerulean = Re, white = H, red = O, gray = C, and blue = N.

Section 5. References.

1. Laaser, J. E.; Christianson, J. R.; Oudenhoven, T. A.; Joo, Y.; Gopalan, P.; Schmidt, J. R.; Zanni, M. T., Dye Self-Association Identified by Intermolecular Couplings between Vibrational Modes as Revealed by Infrared Spectroscopy, and Implications for Electron Injection. *J. Phys. Chem. C* **2014**, *118*, 5854-5861.

2. Oudenhoven, T. A.; Joo, Y.; Laaser, J. E.; Gopalan, P.; Zanni, M. T., Dye Aggregation Identified by Vibrational Coupling Using 2d Ir Spectroscopy. *J. Chem. Phys.* **2015**, *142*, 212449.

Section 6. Theoretical coordinates.

Below are the xyz theoretical coordinates for the molecules used in this study with the number of atoms in the first line, followed by the name and electronic (SCF) energy in Hartrees, and the Cartesian coordinates.

34
Gas-phase ReC0A complex SCF Energy: -1751.59618665

O	0.00000000	0.00000000	0.00000000
O	6.08445000	0.00000000	0.00000000
C	5.71586926	0.00000000	4.74207913
N	4.37313624	0.01342891	4.67285319
H	7.60506469	-0.02071442	3.71702818
C	5.92711915	-0.00795817	2.36137952
H	4.06433948	0.01341384	1.31189792
C	6.52697070	-0.01283355	3.62048928
C	4.53873414	0.00637129	2.28213723
H	2.02011048	0.01342012	1.31189763
C	3.78018068	0.01743804	3.45324376
H	6.14219388	0.00560016	5.73589828
C	1.54571614	0.00636587	2.28213599
C	2.30426868	0.01743189	3.45324331
C	0.15733115	-0.00797736	2.36137853
N	1.71131324	0.01341143	4.67285265
C	-0.44252130	-0.01286610	3.62048830
C	0.36858026	-0.00003198	4.74207892
H	-1.52061432	-0.02075903	3.71702667
Re	3.04222308	0.19652168	6.42793545
C	4.41212172	0.50420547	7.77806207
H	-0.05774412	0.00555874	5.73589707
O	5.24843491	0.69264180	8.54595138
C	1.67231872	0.50418073	7.77806082
C	3.04223929	-1.70500148	6.80905438
O	3.04224840	-2.83994221	7.03089601
O	0.83600691	0.69261054	8.54595360
Cl	3.04220447	2.63120384	5.79156852
C	-0.71326038	-0.01697119	1.14797806

C	6.79771063	-0.01695215	1.14797891
O	8.00198868	-0.03803356	1.17748443
O	-1.91753833	-0.03806837	1.17748310
H	-0.62584072	-0.00232507	-0.74106762
H	6.71029128	-0.00232355	-0.74106707

151
Monomer on TiO2 along [-110] axis SCF Energy: -6847.17502927

O	8.72051	2.20690	3.72340
O	15.20600	2.20790	3.72500
O	8.67490	5.16251	3.73040
O	8.68679	11.09027	3.73350
O	8.79934	8.11976	3.73780
O	15.17380	5.17200	3.73820
O	15.19159	11.07960	3.74050
O	15.29700	8.12161	3.75030
O	11.97249	8.12670	4.28020
O	18.44317	8.11730	4.28139
O	11.99179	5.13730	4.28080
O	12.01990	14.03890	4.28430
O	18.53823	2.19630	4.28680
O	12.04820	2.19240	4.28630
O	18.45710	11.06954	4.28674
O	11.96240	11.07530	4.29080
O	18.46999	5.15079	4.28861
Ti	8.76740	2.18410	5.56810
Ti	15.27060	2.17310	5.57250
Ti	8.71619	5.14020	5.56790
O	16.53370	0.71830	5.58910
O	10.04660	0.73180	5.59631
Ti	8.70405	11.06670	5.58943
Ti	15.20300	5.13739	5.58383
Ti	15.19191	11.06120	5.59741
Ti	15.28260	8.10407	5.61444
Ti	8.75976	8.09906	5.62343
Ti	11.99980	6.54795	5.65490
Ti	11.98538	9.66935	5.68290
O	13.93760	6.70949	5.68810
O	7.45696	12.63287	5.67791
Ti	18.49752	9.61831	5.71548
O	13.94500	12.62450	5.68641
O	7.46172	6.68865	5.69020
O	10.02427	3.72446	5.69151
O	16.50110	3.73060	5.74209
O	10.01644	9.65573	5.77819
Ti	12.01520	0.70570	5.74530

Ti	18.48382	6.60858	5.74222
Ti	18.49353	3.66520	5.74877
O	10.02515	6.56555	5.74191
O	13.94750	9.54049	5.77380
Ti	11.99431	3.63330	5.75810
Ti	11.98171	12.58060	5.76050
O	7.48582	9.55211	5.78310
O	16.47960	12.50060	5.77110
O	9.99145	12.51615	5.77630
O	7.49703	3.62025	5.83840
O	13.97750	3.61080	5.79401
O	16.48141	6.57303	5.83840
O	16.48181	9.64395	5.85808
O	7.52340	0.71350	5.93429
O	14.01330	0.70860	5.93310
O	12.11610	5.15041	6.88021
O	18.61312	11.06378	6.89122
O	12.10941	11.07729	6.88980
O	18.61352	5.15532	6.89612
O	18.33670	2.18750	6.90190
O	11.85970	14.03780	6.90830
O	18.66754	8.18035	6.96214
O	11.85590	2.18440	6.91330
O	11.89634	8.07090	7.02392
H	10.98590	8.03827	7.36211
H	13.71895	5.10990	7.60417
H	7.73903	5.43996	7.93601
H	13.65910	10.98836	7.57783
H	8.05183	10.55367	8.15446
O	9.10055	7.93112	7.75070
O	14.71328	5.24665	7.64359
O	14.66466	11.02730	7.72799
O	8.66425	5.23455	7.72993
O	8.48797	11.30436	7.69612
O	15.24968	8.01502	7.68870
H	18.02172	8.30163	7.77374
H	14.82725	6.18610	7.89465
H	9.36852	11.47474	8.06898
H	9.14302	6.07570	7.90603
H	14.79543	11.89427	8.13831
C	8.53042	8.46843	8.77786
C	15.88405	8.38320	8.73387
O	17.10652	8.57115	8.84397
O	7.42371	9.00489	8.80123
H	13.19136	8.33892	8.96327
H	11.24793	8.24753	9.05600

C	10.73828	8.41039	9.99147
C	9.35706	8.49082	10.04483
C	13.67638	8.47837	9.92691
C	15.06009	8.53984	9.98163
C	11.48317	8.60094	11.14579
C	12.95693	8.62234	11.11172
C	8.75499	8.72166	11.27998
H	7.67874	8.81976	11.35729
C	15.68566	8.74019	11.20853
H	16.76508	8.79840	11.27101
N	10.89859	8.80414	12.34037
C	9.55897	8.85097	12.40044
N	13.56454	8.81362	12.29889
C	14.90225	8.87090	12.34109
Cl	12.24342	11.52357	13.01437
H	9.13290	9.02477	13.38090
H	15.34332	9.03472	13.31643
Re	12.25213	9.22433	14.01729
C	12.25817	7.41927	14.63227
C	10.91750	9.70618	15.30217
C	13.61983	9.70495	15.26806
O	12.26060	6.32095	15.00732
O	10.07993	9.99638	16.04593
O	14.47612	9.99449	15.99064
H	7.86147	-0.15838	6.15141
O	20.45829	3.57252	5.97559
H	21.00615	3.21420	5.27340
O	11.92449	-0.64106	7.19389
H	11.71311	-1.49976	6.82034
O	12.16897	-0.75430	4.41671
O	20.45947	6.65405	5.86792
H	20.99138	6.65682	5.06877
O	20.47569	9.58140	5.78891
H	20.98715	10.20522	5.26846
H	16.02291	11.08435	3.26039
H	14.36014	11.08438	3.26066
H	16.13207	8.12602	3.27676
H	14.46935	8.12619	3.26391
H	15.99749	5.18124	3.24520
H	14.33493	5.18075	3.27149
H	16.02011	2.21748	3.21634
H	14.35835	2.21639	3.27442
H	9.51350	11.09643	3.24569
H	7.85081	11.09644	3.26144
H	9.64056	8.12487	3.27535
H	7.97815	8.12500	3.24052

H	9.49529	5.16852	3.23188
H	7.83294	5.16812	3.26924
H	9.53942	2.21309	3.22246
H	7.87718	2.21257	3.26472
H	7.80904	13.52460	5.72824
H	12.74184	14.33530	7.14264
H	17.41996	12.30879	5.74795
H	19.53629	11.26804	7.05735
H	19.21197	1.87661	7.14450
H	17.47618	0.90087	5.58702
H	17.71736	1.84346	3.93562
H	17.61638	11.39969	3.96148
H	11.19749	14.38693	3.93200
H	13.03512	-1.06049	4.13808
H	20.86305	3.88590	6.78771
H	20.88538	6.67336	6.72808
H	20.92340	8.93958	6.34500
H	6.57624	0.86534	5.89649
H	6.50751	12.49144	5.66991
H	16.17674	13.40501	5.88024
H	11.37737	-1.15599	4.05117

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Monomer on TiO2 along (001) axis SCF Energy: -6847.13712738

O	-2.74399	5.95108	-2.94383
O	-6.09421	0.66617	-1.23871
O	-0.38493	4.29746	-3.60573
O	4.28938	0.89574	-4.91635
O	1.88769	2.50440	-4.22294
O	-3.73333	-1.00265	-1.89315
O	0.92135	-4.39780	-3.19835
O	-1.46452	-2.78988	-2.50459
O	0.43307	-0.03490	-2.88155
O	-2.91785	-5.30183	-1.17839
O	-1.93656	1.66019	-2.21192
O	5.07707	-3.45656	-4.17845
O	-7.63924	-1.99029	0.16679
O	-4.28861	3.30004	-1.53783
O	-0.59279	-7.00215	-1.82549
O	2.76945	-1.71310	-3.52919
O	-5.27109	-3.62535	-0.50568
Ti	-2.17502	6.09674	-1.19435
Ti	-5.54295	0.80454	0.52072
Ti	0.18494	4.44674	-1.86458

O	-7.33862	0.60943	1.19127
O	-3.97320	5.88816	-0.50922
Ti	4.87678	1.06703	-3.16393
Ti	-3.16425	-0.83572	-0.14483
Ti	1.52278	-4.21535	-1.45088
Ti	-0.85328	-2.59554	-0.75408
Ti	2.51655	2.72306	-2.45820
Ti	-0.37188	0.97368	-1.23297
Ti	2.10901	-0.79838	-1.90365
O	-1.23467	-0.69468	-0.72843
O	6.78690	1.19505	-3.75635
Ti	-1.28559	-6.07235	-0.15109
O	3.43025	-4.08591	-2.04200
O	2.09611	4.59399	-2.42325
O	-1.56770	4.20263	-1.09043
O	-4.89315	-1.07371	0.65728
O	3.14726	0.82265	-2.32852
Ti	-4.96176	4.31285	0.15366
Ti	-3.64613	-4.33624	0.53917
Ti	-5.97217	-2.65910	1.20154
O	0.69140	2.58063	-1.67393
O	1.02330	-2.31495	-1.27442
Ti	-2.63565	2.65565	-0.49007
Ti	4.43473	-2.45417	-2.47847
O	4.37482	2.94435	-2.96569
O	2.05062	-6.07239	-1.26909
O	5.41763	-0.79414	-2.97222
O	-0.29534	6.33498	-1.59325
O	-3.66639	1.05592	0.06963
O	-2.60728	-2.67539	0.11110
O	-0.17665	-4.43135	-0.55231
O	-2.57172	7.98587	-0.85067
O	-5.92981	2.70050	0.85429
O	-1.12919	1.79213	0.25855
O	0.18504	-6.88480	0.66228
O	3.55619	-1.59335	-1.05066
O	-4.47776	-3.50338	1.97936
O	-6.67559	-1.57890	2.57128
O	6.02839	-3.08241	-1.75646
O	-2.08334	-5.28290	1.47596
O	-3.32514	3.70459	0.88007
O	1.31110	0.26755	-0.31925
H	1.88943	0.82400	0.21146
H	1.52154	3.87108	0.31869
H	5.48318	1.35730	-0.38083
O	-2.22372	-0.61329	1.65524

O	0.62902	4.27293	0.29616
O	5.85605	1.01729	-1.21570
O	2.18594	-4.16120	0.38646
H	-1.50281	-4.83189	2.10471
H	5.83302	0.04003	-1.15396
H	0.01703	3.53166	0.52329
C	-1.93252	0.34184	2.47011
C	3.42853	-4.16530	0.78389
O	4.24648	-5.05329	0.62994
O	-2.71008	0.94524	3.20518
H	1.77162	-2.22033	1.31127
H	0.25019	-1.20808	2.05502
C	0.51744	-0.24112	2.45476
C	-0.47607	0.68950	2.66614
C	2.72015	-2.02032	1.78056
C	3.75279	-2.91481	1.56673
C	1.83929	0.07473	2.75325
C	2.93215	-0.87704	2.51512
C	-0.11277	1.94129	3.17067
H	-0.87202	2.69720	3.33528
C	5.00652	-2.61010	2.07676
H	5.84809	-3.27032	1.90363
N	2.18649	1.26958	3.26448
C	1.21707	2.19036	3.44935
N	4.15049	-0.56890	3.00915
C	5.16333	-1.41996	2.77760
Cl	4.96757	2.16209	1.60547
H	1.53955	3.14329	3.85259
H	6.12795	-1.12580	3.17418
Re	4.28049	1.39984	3.96866
C	3.77070	0.76118	5.67883
C	4.19911	3.21596	4.58453
C	6.13175	1.30086	4.45873
O	3.45740	0.36366	6.72101
O	4.11705	4.31576	4.93270
O	7.24902	1.20980	4.74165
H	-3.36276	8.22947	-0.36434
O	-6.98555	-4.18600	1.95124
H	-7.78419	-4.49237	1.51544
O	-5.49806	5.29162	1.78913
H	-6.19046	5.92068	1.57359
O	-6.63396	4.90004	-0.72915
O	-4.58928	-5.96039	1.16603
H	-5.12668	-6.46945	0.55475
O	-2.31292	-7.65621	0.44588
H	-2.25729	-8.47813	-0.04704

H	0.33685	-5.12230	-3.43196
H	1.19619	-3.76740	-3.86854
H	-2.04949	-3.51672	-2.73081
H	-1.19438	-2.16319	-3.17973
H	-4.31503	-1.72476	-2.14172
H	-3.44755	-0.36736	-2.55370
H	-6.67591	-0.04976	-1.50457
H	-5.79877	1.31027	-1.88636
H	3.70536	0.17344	-5.15855
H	4.56987	1.52964	-5.58059
H	1.30375	1.77321	-4.43729
H	2.15147	3.12443	-4.90678
H	-0.96928	3.57936	-3.85963
H	-0.09822	4.93760	-4.26117
H	-3.32828	5.23388	-3.20043
H	-2.45568	6.59251	-3.59733
H	7.32556	0.40255	-3.81468
H	5.88502	-3.94973	-1.37075
H	1.40561	-6.73099	-1.00130
H	-0.07576	-7.73853	1.01545
H	-7.29295	-2.09170	3.09807
H	-7.68223	-0.26319	1.39638
H	-7.60994	-1.15206	-0.30023
H	-0.00540	-6.53620	-2.42505
H	5.66008	-3.01824	-4.80261
H	-7.41559	4.34371	-0.69521
H	-6.67826	-4.61994	2.75053
H	-4.50916	-6.23882	2.08128
H	-2.86669	-7.60222	1.22821
H	-1.97492	8.66724	-1.16873
H	7.16326	2.04891	-3.98188
H	2.95733	-6.33304	-1.44693
H	-6.66309	5.74108	-1.19111
O	-5.18869	0.70965	2.59133
H	-5.63642	-0.09396	2.91561
H	-4.24151	0.72926	2.88376
O	3.10014	3.26063	-0.39702
H	3.59845	4.08012	-0.55140
H	3.65178	2.73233	0.23912

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Dimer on TiO2 along [-110] axis; outer CO, inner CO facing surface;SCF Energy: -8598.85901413

O	8.72050	2.20690	3.72340
O	15.20600	2.20790	3.72500
O	8.67490	5.16250	3.73040

O	8.68670	11.09030	3.73350
O	8.79930	8.11970	3.73780
O	15.17380	5.17200	3.73820
O	15.19160	11.07960	3.74050
O	15.29700	8.12160	3.75030
O	11.97250	8.12670	4.28020
O	18.44320	8.11730	4.28140
O	11.99180	5.13730	4.28080
O	12.01990	14.03890	4.28430
O	18.53820	2.19630	4.28680
O	12.04820	2.19240	4.28630
O	18.45710	11.06950	4.28670
O	11.96240	11.07530	4.29080
O	18.47000	5.15080	4.28860
Ti	8.76740	2.18410	5.56810
Ti	15.27060	2.17310	5.57250
Ti	8.71620	5.14020	5.56790
O	16.53370	0.71830	5.58910
O	10.04660	0.73180	5.59630
Ti	8.70430	11.06660	5.58950
Ti	15.20300	5.13740	5.58380
Ti	15.19190	11.06120	5.59740
Ti	15.28260	8.10410	5.61450
Ti	8.75980	8.09910	5.62340
Ti	11.99980	6.54790	5.65490
Ti	11.98540	9.66940	5.68290
O	13.93760	6.70950	5.68810
O	7.45700	12.63290	5.67790
Ti	18.49740	9.61860	5.71550
O	13.94500	12.62450	5.68640
O	7.46180	6.68870	5.69020
O	10.02420	3.72440	5.69150
O	16.50110	3.73060	5.74210
O	10.01640	9.65570	5.77820
Ti	12.01520	0.70570	5.74530
Ti	18.48400	6.60830	5.74220
Ti	18.49350	3.66520	5.74880
O	10.02510	6.56560	5.74190
O	13.94750	9.54050	5.77380
Ti	11.99430	3.63330	5.75810
Ti	11.98170	12.58060	5.76050
O	7.48580	9.55210	5.78310
O	16.47960	12.50060	5.77110
O	9.99140	12.51620	5.77630
O	7.49710	3.62020	5.83840
O	13.97750	3.61080	5.79400

O	16.48140	6.57300	5.83840
O	16.48180	9.64400	5.85810
O	7.52340	0.71350	5.93430
O	14.01330	0.70860	5.93310
O	12.11610	5.15040	6.88020
O	18.61310	11.06380	6.89120
O	12.10940	11.07730	6.88980
O	18.61350	5.15530	6.89610
O	18.33670	2.18750	6.90190
O	11.85970	14.03780	6.90830
O	18.43720	8.11280	6.90340
O	11.85590	2.18440	6.91330
O	11.92296	8.06470	7.03128
H	11.01657	7.99181	7.38190
H	13.65856	5.13472	7.55323
H	7.76702	5.10495	7.98914
H	13.62999	11.01102	7.54623
H	7.96844	10.59051	8.14184
O	9.10577	7.96484	7.77201
O	14.67038	5.23827	7.63270
O	14.64174	11.05961	7.71537
O	8.68931	5.23687	7.72297
O	8.44831	11.32450	7.70437
O	15.25150	8.03032	7.76288
H	17.64664	8.37152	8.02668
H	14.80099	6.16124	7.92447
H	9.32525	11.44572	8.10198
H	8.91687	6.17156	7.92649
H	14.75487	11.95088	8.07691
C	8.48910	8.57303	8.73352
C	15.82817	8.52449	8.75607
O	17.09544	8.65846	8.88054
O	7.31758	8.94476	8.72493
H	13.17280	8.54606	8.95988
H	11.22556	8.57862	9.00452
C	10.71416	8.94298	9.87939
C	9.33157	8.94631	9.93789
C	13.65023	8.94414	9.85262
C	15.03274	8.98440	9.92329
C	11.44629	9.45310	10.93990
C	12.91782	9.47174	10.91421
C	8.72553	9.42733	11.09617
H	7.64560	9.44166	11.18258
C	15.65429	9.51604	11.05127
H	16.73308	9.54926	11.13517
N	10.85863	9.96097	12.03744

C	9.52206	9.91371	12.12126
N	13.51909	10.03865	11.97811
C	14.85665	10.03557	12.05433
Cl	12.40296	8.65171	14.53479
H	9.08849	10.30377	13.03381
H	15.28520	10.47493	12.94626
Re	12.20042	10.91048	13.50672
C	12.09239	12.58508	12.59860
C	10.86159	11.44648	14.76828
C	13.56068	11.58206	14.67197
O	12.04141	13.60290	12.04224
O	10.02432	11.74433	15.50757
O	14.41796	11.96746	15.34770
O	8.91667	2.13036	7.49831
O	15.32845	2.21189	7.68110
H	17.52176	2.62029	8.21329
C	8.22279	2.01509	8.57014
C	15.71123	2.73254	8.73009
O	16.97383	2.91646	9.00387
O	7.05048	1.66539	8.66585
H	13.01136	2.38379	8.81321
H	10.87749	2.45373	8.68687
C	10.40784	2.60293	9.65763
C	9.03829	2.38542	9.78702
C	13.40890	2.89759	9.68837
C	14.77035	3.15964	9.79637
C	11.11859	3.03884	10.76653
C	12.57358	3.31047	10.73307
C	8.43374	2.55963	11.02288
H	7.37360	2.36919	11.14490
C	15.26256	3.84074	10.90938
H	16.31796	4.05678	11.01437
N	10.51160	3.28093	11.95017
C	9.20608	3.01659	12.07861
N	13.05988	3.96552	11.80680
C	14.37044	4.23229	11.88599
Cl	12.50304	2.02332	14.12537
H	8.77681	3.20236	13.05548
H	14.69909	4.75945	12.77253
Re	11.68780	4.31343	13.48306
C	11.01816	5.95383	12.79198
C	10.38696	4.32493	14.88747
C	12.94742	5.15138	14.66652
O	10.54287	6.88973	12.29445
O	9.57545	4.29869	15.71192
O	13.76569	5.59595	15.34990

H	7.86147	-0.15838	6.15141
O	20.45829	3.57252	5.97558
H	21.00615	3.21420	5.27340
O	11.92449	-0.64106	7.19389
H	11.71311	-1.49976	6.82034
O	12.16897	-0.75430	4.41671
O	20.45947	6.65401	5.86794
H	20.99138	6.65688	5.06877
O	20.47569	9.58141	5.78892
H	20.98715	10.20518	5.26842
H	16.02291	11.08436	3.26039
H	14.36014	11.08436	3.26066
H	16.13207	8.12604	3.27676
H	14.46935	8.12617	3.26391
H	15.99749	5.18124	3.24520
H	14.33493	5.18075	3.27149
H	16.02011	2.21748	3.21634
H	14.35835	2.21639	3.27442
H	9.51350	11.09653	3.24568
H	7.85080	11.09633	3.26144
H	9.64055	8.12475	3.27534
H	7.97815	8.12513	3.24052
H	9.49529	5.16855	3.23188
H	7.83294	5.16810	3.26924
H	9.53942	2.21309	3.22246
H	7.87718	2.21257	3.26472
H	7.80904	13.52460	5.72823
H	12.74184	14.33530	7.14264
H	17.41996	12.30879	5.74795
H	19.53629	11.26804	7.05735
H	19.21197	1.87661	7.14450
H	17.47618	0.90087	5.58702
H	17.71736	1.84346	3.93562
H	17.61638	11.39972	3.96151
H	11.19749	14.38693	3.93200
H	13.03512	-1.06049	4.13808
H	20.86305	3.88590	6.78771
H	20.88538	6.67330	6.72808
H	20.92340	8.93961	6.34503
H	6.57624	0.86534	5.89649
H	6.50751	12.49144	5.66992
H	16.22058	-0.18914	5.59945
H	16.17674	13.40501	5.88024
H	11.37737	-1.15599	4.05117

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Dimer in gas-phase; outer CO, inner CO facing surface;SCF Energy: -3502.764674

O	15.25150	8.03030	7.76290
O	9.10580	7.96480	7.77200
H	17.64660	8.37150	8.02670
C	8.48910	8.57300	8.73350
C	15.82820	8.52450	8.75610
O	17.09540	8.65850	8.88050
O	7.31760	8.94480	8.72490
H	13.17280	8.54610	8.95990
H	11.22560	8.57860	9.00450
C	10.71420	8.94300	9.87940
C	9.33160	8.94630	9.93790
C	13.65020	8.94410	9.85260
C	15.03270	8.98440	9.92330
C	11.44630	9.45310	10.93990
C	12.91780	9.47170	10.91420
C	8.72550	9.42730	11.09620
H	7.64560	9.44170	11.18260
C	15.65430	9.51600	11.05130
H	16.73310	9.54930	11.13520
N	10.85860	9.96100	12.03740
C	9.52210	9.91370	12.12130
N	13.51910	10.03870	11.97810
C	14.85670	10.03560	12.05430
Cl	12.40300	8.65170	14.53480
H	9.08850	10.30380	13.03380
H	15.28520	10.47490	12.94630
Re	12.20040	10.91050	13.50670
C	12.09240	12.58510	12.59860
C	10.86160	11.44650	14.76830
C	13.56070	11.58210	14.67200
O	12.04140	13.60290	12.04220
O	10.02430	11.74430	15.50760
O	14.41800	11.96750	15.34770
O	8.91670	2.13040	7.49830
O	15.32850	2.21190	7.68110
H	17.52180	2.62030	8.21330
C	8.22280	2.01510	8.57010
C	15.71120	2.73250	8.73010
O	16.97380	2.91650	9.00390
O	7.05050	1.66540	8.66590
H	13.01140	2.38380	8.81320
H	10.87750	2.45370	8.68690
C	10.40780	2.60290	9.65760
C	9.03830	2.38540	9.78700
C	13.40890	2.89760	9.68840

C	14.77040	3.15960	9.79640
C	11.11860	3.03880	10.76650
C	12.57360	3.31050	10.73310
C	8.43370	2.55960	11.02290
H	7.37360	2.36920	11.14490
C	15.26260	3.84070	10.90940
H	16.31800	4.05680	11.01440
N	10.51160	3.28090	11.95020
C	9.20610	3.01660	12.07860
N	13.05990	3.96550	11.80680
C	14.37040	4.23230	11.88600
Cl	12.50300	2.02330	14.12540
H	8.77680	3.20240	13.05550
H	14.69910	4.75950	12.77250
Re	11.68780	4.31340	13.48310
C	11.01820	5.95380	12.79200
C	10.38700	4.32490	14.88750
C	12.94740	5.15140	14.66650
O	10.54290	6.88970	12.29440
O	9.57550	4.29870	15.71190
O	13.76570	5.59600	15.34990
H	6.69966	1.47921	7.79192
H	6.91506	8.71487	7.88425

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Dimer on TiO2 along [-110] axis; outer CO, inner Cl facing surface; SCF Energy: -8598.86555334

O	8.72050	2.20690	3.72340
O	15.20600	2.20790	3.72500
O	8.67490	5.16250	3.73040
O	8.68670	11.09030	3.73350
O	8.79930	8.11970	3.73780
O	15.17380	5.17200	3.73820
O	15.19160	11.07960	3.74050
O	15.29700	8.12160	3.75030
O	11.97250	8.12670	4.28020
O	18.44320	8.11730	4.28140
O	11.99180	5.13730	4.28080
O	12.01990	14.03890	4.28430
O	18.53820	2.19630	4.28680
O	12.04820	2.19240	4.28630
O	18.45710	11.06950	4.28670
O	11.96240	11.07530	4.29080
O	18.47000	5.15080	4.28860
Ti	8.76740	2.18410	5.56810

Ti	15.27060	2.17310	5.57250
Ti	8.71620	5.14020	5.56790
O	16.53370	0.71830	5.58910
O	10.04660	0.73180	5.59630
Ti	8.70430	11.06660	5.58950
Ti	15.20300	5.13740	5.58380
Ti	15.19190	11.06120	5.59740
Ti	15.28260	8.10410	5.61450
Ti	8.75980	8.09910	5.62340
Ti	11.99980	6.54790	5.65490
Ti	11.98540	9.66940	5.68290
O	13.93760	6.70950	5.68810
O	7.45700	12.63290	5.67790
Ti	18.49740	9.61860	5.71550
O	13.94500	12.62450	5.68640
O	7.46180	6.68870	5.69020
O	10.02420	3.72440	5.69150
O	16.50110	3.73060	5.74210
O	10.01640	9.65570	5.77820
Ti	12.01520	0.70570	5.74530
Ti	18.48400	6.60830	5.74220
Ti	18.49350	3.66520	5.74880
O	10.02510	6.56560	5.74190
O	13.94750	9.54050	5.77380
Ti	11.99430	3.63330	5.75810
Ti	11.98170	12.58060	5.76050
O	7.48580	9.55210	5.78310
O	16.47960	12.50060	5.77110
O	9.99140	12.51620	5.77630
O	7.49710	3.62020	5.83840
O	13.97750	3.61080	5.79400
O	16.48140	6.57300	5.83840
O	16.48180	9.64400	5.85810
O	7.52340	0.71350	5.93430
O	14.01330	0.70860	5.93310
O	12.11610	5.15040	6.88020
O	18.61310	11.06380	6.89120
O	12.10940	11.07730	6.88980
O	18.61350	5.15530	6.89610
O	18.33670	2.18750	6.90190
O	11.85970	14.03780	6.90830
O	18.43720	8.11280	6.90340
O	11.85590	2.18440	6.91330
O	11.93154	8.06785	7.00580
H	11.05968	7.95459	7.42622
H	13.66540	5.12645	7.58671

H	7.69515	5.33975	7.93263
H	13.63410	11.03729	7.53509
H	7.89226	10.61944	8.12148
O	9.12067	8.00395	7.76950
O	14.67656	5.22438	7.64000
O	14.64678	11.09206	7.69934
O	8.64035	5.27793	7.72322
O	8.39137	11.34716	7.69839
O	15.25212	8.06176	7.77083
H	17.62402	8.35263	8.07646
H	14.79764	6.13312	7.97676
H	9.25207	11.45905	8.13226
H	9.01516	6.16259	7.93239
H	14.75628	11.98824	8.04998
C	8.48872	8.64978	8.69631
C	15.81380	8.56169	8.76801
O	17.08940	8.64327	8.91899
O	7.28357	8.89432	8.71310
H	13.17490	8.82111	8.84802
H	11.23147	8.81739	8.90861
C	10.71603	9.27647	9.73091
C	9.33567	9.24566	9.80776
C	13.64413	9.20440	9.74846
C	15.01726	9.10858	9.89363
C	11.44631	9.90597	10.72749
C	12.91472	9.83461	10.75365
C	8.72683	9.86960	10.89629
H	7.64828	9.85841	10.99855
C	15.62540	9.59960	11.04763
H	16.69403	9.51649	11.19928
N	10.85457	10.55117	11.74885
C	9.51722	10.51589	11.83454
N	13.51085	10.37718	11.83159
C	14.83343	10.23121	11.99010
Cl	11.97540	9.62868	14.59418
H	9.08201	11.01933	12.68861
H	15.25403	10.64851	12.89612
Re	12.21449	11.62427	13.11440
C	12.42368	13.08063	11.90192
C	10.89217	12.57436	14.12139
C	13.58023	12.32850	14.25194
O	12.58129	13.96223	11.16264
O	10.06559	13.12779	14.71202
O	14.43793	12.72242	14.92307
O	8.91681	2.08241	7.50920
O	15.36147	2.17946	7.66031

H	17.56858	2.41955	8.22283
C	8.19822	2.39360	8.52806
C	15.76791	2.55656	8.75777
O	17.03437	2.61156	9.06227
O	6.98483	2.27535	8.64785
H	13.04434	2.47630	8.74528
H	10.89613	2.37486	8.74498
C	10.43005	2.89122	9.58208
C	9.04078	2.96678	9.64488
C	13.46596	2.92066	9.64804
C	14.84288	2.98995	9.83041
C	11.17155	3.55183	10.54978
C	12.65188	3.51960	10.61322
C	8.43725	3.64416	10.69473
H	7.35643	3.68579	10.76734
C	15.37804	3.55995	10.98462
H	16.44688	3.60310	11.14723
N	10.57897	4.29467	11.51348
C	9.24378	4.31655	11.59610
N	13.18685	4.16180	11.67424
C	14.50795	4.14081	11.88105
Cl	12.19262	6.51777	10.16874
H	8.82602	4.91886	12.39446
H	14.86219	4.65432	12.76661
Re	11.89709	5.70063	12.54050
C	11.71720	4.91885	14.26284
C	10.53811	6.99449	12.95014
C	13.31664	6.84577	13.14194
O	11.61450	4.42759	15.31007
O	9.62956	7.68356	13.13240
O	14.26576	7.44279	13.42585
H	7.86147	-0.15838	6.15141
O	20.45829	3.57252	5.97558
H	21.00615	3.21420	5.27340
O	11.92449	-0.64106	7.19389
H	11.71311	-1.49976	6.82034
O	12.16897	-0.75430	4.41671
O	20.45947	6.65401	5.86794
H	20.99138	6.65688	5.06877
O	20.47569	9.58141	5.78892
H	20.98715	10.20518	5.26842
H	16.02291	11.08436	3.26039
H	14.36014	11.08436	3.26066
H	16.13207	8.12604	3.27676
H	14.46935	8.12617	3.26391
H	15.99749	5.18124	3.24520

H	14.33493	5.18075	3.27149
H	16.02011	2.21748	3.21634
H	14.35835	2.21639	3.27442
H	9.51350	11.09653	3.24568
H	7.85080	11.09633	3.26144
H	9.64055	8.12475	3.27534
H	7.97815	8.12513	3.24052
H	9.49529	5.16855	3.23188
H	7.83294	5.16810	3.26924
H	9.53942	2.21309	3.22246
H	7.87718	2.21257	3.26472
H	7.80904	13.52460	5.72823
H	12.74184	14.33530	7.14264
H	17.41996	12.30879	5.74795
H	19.53629	11.26804	7.05735
H	19.21197	1.87661	7.14450
H	17.47618	0.90087	5.58702
H	17.71736	1.84346	3.93562
H	17.61638	11.39972	3.96151
H	11.19749	14.38693	3.93200
H	13.03512	-1.06049	4.13808
H	20.86305	3.88590	6.78771
H	20.88538	6.67330	6.72808
H	20.92340	8.93961	6.34503
H	6.57624	0.86534	5.89649
H	6.50751	12.49144	5.66992
H	16.22058	-0.18914	5.59945
H	16.17674	13.40501	5.88024
H	11.37737	-1.15599	4.05117

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Dimer in gas-phase; outer CO, inner Cl facing surface;SCF Energy: -3502.754532

O	15.25210	8.06180	7.77080
O	9.12070	8.00390	7.76950
H	17.62400	8.35260	8.07650
C	8.48870	8.64980	8.69630
C	15.81380	8.56170	8.76800
O	17.08940	8.64330	8.91900
O	7.28360	8.89430	8.71310
H	13.17490	8.82110	8.84800
H	11.23150	8.81740	8.90860
C	10.71600	9.27650	9.73090
C	9.33570	9.24570	9.80780
C	13.64410	9.20440	9.74850
C	15.01730	9.10860	9.89360
C	11.44630	9.90600	10.72750

C	12.91470	9.83460	10.75370
C	8.72680	9.86960	10.89630
H	7.64830	9.85840	10.99850
C	15.62540	9.59960	11.04760
H	16.69400	9.51650	11.19930
N	10.85460	10.55120	11.74880
C	9.51720	10.51590	11.83450
N	13.51080	10.37720	11.83160
C	14.83340	10.23120	11.99010
Cl	11.97540	9.62870	14.59420
H	9.08200	11.01930	12.68860
H	15.25400	10.64850	12.89610
Re	12.21450	11.62430	13.11440
C	12.42370	13.08060	11.90190
C	10.89220	12.57440	14.12140
C	13.58020	12.32850	14.25190
O	12.58130	13.96220	11.16260
O	10.06560	13.12780	14.71200
O	14.43790	12.72240	14.92310
O	8.91680	2.08240	7.50920
O	15.36150	2.17950	7.66030
H	17.56860	2.41960	8.22280
C	8.19820	2.39360	8.52810
C	15.76790	2.55660	8.75780
O	17.03440	2.61160	9.06230
O	6.98480	2.27530	8.64790
H	13.04430	2.47630	8.74530
H	10.89610	2.37490	8.74500
C	10.43000	2.89120	9.58210
C	9.04080	2.96680	9.64490
C	13.46600	2.92070	9.64800
C	14.84290	2.98990	9.83040
C	11.17150	3.55180	10.54980
C	12.65190	3.51960	10.61320
C	8.43730	3.64420	10.69470
H	7.35640	3.68580	10.76730
C	15.37800	3.56000	10.98460
H	16.44690	3.60310	11.14720
N	10.57900	4.29470	11.51350
C	9.24380	4.31660	11.59610
N	13.18680	4.16180	11.67420
C	14.50790	4.14080	11.88110
Cl	12.19260	6.51780	10.16870
H	8.82600	4.91890	12.39450
H	14.86220	4.65430	12.76660
Re	11.89710	5.70060	12.54050

C	11.71720	4.91880	14.26280
C	10.53810	6.99450	12.95010
C	13.31660	6.84580	13.14190
O	11.61450	4.42760	15.31010
O	9.62960	7.68360	13.13240
O	14.26580	7.44280	13.42590
H	6.61873	1.90137	7.84306
H	6.87226	8.53048	7.92568

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Dimer on TiO2 along [-110] axis; outer Cl, inner CO facing surface; SCF Energy: -8598.868494

O	-3.82399	-4.10462	4.92440
O	-6.49090	-1.37583	-0.31980
O	-2.32151	-1.62628	5.50581
O	0.64103	3.39141	6.59445
O	-0.88790	0.92484	5.94980
O	-4.98499	1.11336	0.24882
O	-2.03564	6.11675	1.32929
O	-3.55108	3.65601	0.68977
O	-1.77686	2.08781	3.08264
O	-4.44322	4.80177	-2.15138
O	-3.27961	-0.43270	2.51202
O	1.16399	7.10696	4.13904
O	-7.43983	-0.16803	-3.32985
O	-4.77164	-2.90158	1.91692
O	-2.96824	7.30285	-1.61780
O	-0.28976	4.57402	3.63200
O	-5.93258	2.30161	-2.72751
Ti	-2.44914	-4.70944	3.85218
Ti	-5.12728	-1.98412	-1.41046
Ti	-0.94965	-2.23057	4.44206
O	-6.36209	-2.68866	-2.71071
O	-3.68054	-5.40878	2.53263
Ti	2.03601	2.76989	5.53930
Ti	-3.60818	0.49092	-0.81191
Ti	-0.63021	5.49214	0.28863
Ti	-2.13360	3.02357	-0.34302
Ti	0.55468	0.27220	4.92492
Ti	-1.53044	0.31299	1.99991
Ti	0.05817	2.93791	2.57513
O	-2.22162	1.25400	0.44460
O	3.40006	3.54092	6.78901
Ti	-2.62193	5.62390	-2.71755
O	0.73264	6.26060	1.53711
O	0.43421	-1.48871	5.67532

O	-2.10191	-2.91831	3.05285
O	-4.72534	-0.20477	-2.21089
O	0.93419	2.06665	4.11126
Ti	-4.39007	-4.65156	0.85293
Ti	-4.10180	3.06339	-3.28018
Ti	-5.57281	0.57595	-3.83763
O	-0.64268	-0.53139	3.55113
O	-0.74436	3.62451	0.91403
Ti	-2.90734	-2.18839	1.40589
Ti	1.57499	5.37318	3.07493
O	1.92737	0.91278	6.13534
O	-0.30775	7.19436	-0.58242
O	2.37380	4.47618	4.66333
O	-1.00223	-4.11781	4.99464
O	-3.70736	-1.38482	-0.22172
O	-3.22217	2.15947	-1.72131
O	-1.67125	4.75064	-1.16280
O	-2.39390	-6.59671	4.38047
O	-5.06776	-3.87007	-0.86684
O	-1.34372	-1.22208	0.96227
O	-1.05091	6.50924	-3.19951
O	1.63093	3.78493	2.06206
O	-4.00272	1.51038	-4.29890
O	-5.36887	-1.11814	-4.62902
O	3.22858	6.17781	2.80294
O	-2.44530	3.93527	-3.61167
O	-2.69500	-3.85105	0.60381
O	0.30820	1.11635	1.57084
H	0.94848	0.60521	2.09644
H	-1.49305	-0.81160	-0.62647
H	1.25556	-3.46988	3.84955
H	1.47819	4.12703	0.40480
H	4.04119	1.25438	4.56994
O	1.97499	-0.42382	3.43318
O	-1.78328	-0.31557	-1.47527
O	1.18022	4.51109	-0.48984
O	0.75444	-2.87046	3.27670
O	3.87317	2.22029	4.59001
O	-0.56946	2.20127	-1.53728
H	-1.16134	3.37379	-3.58771
H	-1.15675	0.43180	-1.53374
H	3.86252	2.59015	3.69201
H	1.28995	-2.05065	3.17785
H	1.89316	5.12353	-0.72367
C	3.26669	-0.45453	3.47322
C	0.12987	2.30552	-2.56566

O	-0.19544	2.94430	-3.62637
O	3.96233	-0.54666	4.48281
H	1.42679	1.28368	-0.47728
H	2.19423	-0.05322	0.94642
C	3.27257	-0.00957	0.97521
C	3.96917	-0.26006	2.14550
C	1.98274	1.16645	-1.40661
C	1.44572	1.61536	-2.60281
C	3.97678	0.30914	-0.17500
C	3.28455	0.67228	-1.41946
C	5.36109	-0.23155	2.10312
H	5.93378	-0.42539	3.00210
C	2.17135	1.47283	-3.78520
H	1.76819	1.80423	-4.73414
N	5.31994	0.31556	-0.22059
C	5.99539	0.04237	0.90267
N	4.01912	0.60951	-2.54505
C	3.45210	0.95227	-3.71069
Cl	5.55544	3.08107	-1.77494
H	7.07556	0.05427	0.82335
H	4.07317	0.84938	-4.59161
Re	6.20917	0.67867	-2.19634
C	6.66370	-1.15942	-2.42421
C	7.99208	1.04276	-1.61230
C	6.72212	1.05128	-4.00308
O	6.99518	-2.26302	-2.54925
O	9.05562	1.27206	-1.22119
O	6.98801	1.27962	-5.10568
O	-1.05033	-5.32280	2.64111
O	-3.53784	-2.60339	-2.65820
H	-3.81505	-1.48525	-4.63513
C	-0.03650	-6.09711	2.52584
C	-2.62084	-2.26796	-3.41063
O	-2.82850	-1.67540	-4.55243
O	0.32569	-6.97801	3.29974
H	-1.63410	-3.83053	-1.42146
H	-0.79554	-4.51749	0.47921
C	0.20117	-4.92493	0.31791
C	0.74122	-5.79455	1.26093
C	-0.86111	-3.37915	-2.04173
C	-1.19676	-2.54239	-3.09684
C	0.97159	-4.57254	-0.77972
C	0.49450	-3.62637	-1.80845
C	2.00564	-6.32537	1.04496
H	2.43135	-7.02521	1.75521
C	-0.19545	-1.91896	-3.84083

H	-0.43702	-1.24055	-4.64922
N	2.23169	-5.03030	-0.95127
C	2.72041	-5.91301	-0.07037
N	1.45824	-3.04900	-2.55200
C	1.11804	-2.18819	-3.52241
Cl	2.26994	-5.46629	-4.16873
H	3.72513	-6.26997	-0.26395
H	1.93402	-1.73636	-4.07206
Re	3.43519	-4.00225	-2.49148
C	4.25074	-3.05554	-1.06516
C	4.95902	-5.17057	-2.56086
C	4.21610	-2.88395	-3.82756
O	4.76697	-2.58078	-0.13715
O	5.84923	-5.90378	-2.59837
O	4.60473	-2.15309	-4.64032
H	-2.80367	-7.26314	3.82412
O	-6.25486	1.24977	-5.57003
H	-7.19451	1.40755	-5.68732
O	-3.92271	-6.30402	-0.13261
H	-4.54985	-6.99670	0.08758
O	-6.19588	-5.38588	1.19968
O	-4.79602	3.89191	-4.93910
H	-5.62234	4.38029	-4.92230
O	-3.39864	6.40065	-4.36490
H	-3.69366	7.31417	-4.37200
H	-2.74113	6.62801	0.92619
H	-2.05672	5.92838	2.27040
H	-4.25331	4.16641	0.27987
H	-3.57884	3.47122	1.63139
H	-5.69493	1.62944	-0.14011
H	-4.99102	0.92094	1.18931
H	-7.20868	-0.85834	-0.69221
H	-6.48117	-1.57741	0.61870
H	-0.06774	3.90455	6.19957
H	0.62834	3.19969	7.53502
H	-1.58387	1.43474	5.52886
H	-0.92617	0.74709	6.89244
H	-3.03588	-1.11247	5.12205
H	-2.32362	-1.82449	6.44513
H	-4.53950	-3.59055	4.54324
H	-3.82360	-4.30419	5.86348
H	3.73956	4.42672	6.64174
H	3.19295	6.72369	2.01405
H	-0.80826	7.43533	-1.36537
H	-1.20204	7.01587	-4.00081
H	-5.69970	-1.09244	-5.52985

H	-6.66015	-2.13706	-3.43770
H	-7.54611	-0.69659	-2.53554
H	-2.70489	7.33513	-0.69519
H	1.40806	7.17090	5.06529
H	-6.91773	-5.18904	0.59819
H	-5.64589	1.41868	-6.29268
H	-4.30628	3.80524	-5.76023
H	-3.48019	5.86374	-5.15653
H	-1.95700	-6.85436	5.19556
H	3.71392	3.02443	7.53489
H	-6.67922	-3.59131	-2.63174
H	0.35241	7.79609	-0.23070
H	-6.34958	-5.93874	1.96930

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Dimer in gas-phase; outer Cl, inner CO facing surface;SCF Energy: -3502.75892

O	0.00000	0.00000	0.00000
O	6.16873	0.12555	0.04962
H	-2.39029	-0.35767	0.29615
C	6.75185	-0.50341	1.01679
C	-0.58761	-0.26874	1.06776
O	-1.84520	-0.47152	1.19551
O	7.90046	-0.94197	1.01276
H	2.06623	-0.39922	1.23375
H	4.08645	0.11392	1.47564
C	4.54146	-0.46919	2.26217
C	5.88544	-0.80057	2.22307
C	1.58929	-0.42438	2.21266
C	0.21024	-0.33729	2.31983
C	3.76977	-0.90217	3.32868
C	2.32151	-0.65629	3.37415
C	6.41925	-1.51639	3.29201
H	7.46788	-1.78865	3.29092
C	-0.39167	-0.38412	3.57698
H	-1.46604	-0.30550	3.68774
N	4.28957	-1.57430	4.36988
C	5.59571	-1.86801	4.34866
N	1.73728	-0.78482	4.57935
C	0.41362	-0.59760	4.68281
Cl	2.00153	-3.78176	4.47628
H	5.97638	-2.40716	5.20754
H	-0.00262	-0.67574	5.67930
Re	2.90533	-2.00080	6.02156
C	3.65469	-0.63091	7.11655
C	3.97559	-3.30177	6.92400
C	1.49785	-2.27448	7.29063

O	4.13865	0.16018	7.81182
O	4.64386	-4.09518	7.43438
O	0.61894	-2.41863	8.02907
O	6.25069	5.93393	-0.14021
O	-0.20006	5.75433	0.00458
H	-2.37747	5.27263	0.51665
C	6.89324	6.10142	0.95510
C	-0.56622	5.13429	1.00507
O	-1.82207	4.92516	1.28281
O	8.03104	6.53881	1.09725
H	2.09687	5.63495	1.17468
H	4.27129	5.48150	0.98431
C	4.72050	5.35379	1.96782
C	6.06541	5.66434	2.14671
C	1.73127	4.96686	1.95304
C	0.39361	4.60031	2.00262
C	4.00551	4.85023	3.04376
C	2.58609	4.45749	2.93438
C	6.63176	5.51606	3.40541
H	7.67079	5.77838	3.56982
C	-0.04739	3.69210	2.96462
H	-1.08085	3.37174	3.00188
N	4.57651	4.63479	4.24976
C	5.85479	4.99244	4.42877
N	2.14840	3.60714	3.88326
C	0.86804	3.20841	3.87410
Cl	2.15150	5.51998	6.21928
H	6.26062	4.82329	5.41925
H	0.57752	2.50660	4.64560
Re	3.40785	3.41389	5.67139
C	4.52409	1.96404	5.17362
C	4.46000	3.65218	7.26133
C	2.19258	2.29457	6.62837
O	5.30178	1.14784	4.88680
O	5.09770	3.83391	8.20566
O	1.39683	1.61408	7.12779
H	8.31452	-0.74690	0.16890
H	8.40154	6.75220	0.23772

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Dimer on TiO2 along [-110] axis; outer Cl, inner Cl facing surface; SCF Energy: -8598.872509

O	8.72050	2.20690	3.72340
O	15.20600	2.20790	3.72500
O	8.67490	5.16250	3.73040
O	8.68670	11.09030	3.73350

O	8.79930	8.11970	3.73780
O	15.17380	5.17200	3.73820
O	15.19160	11.07960	3.74050
O	15.29700	8.12160	3.75030
O	11.97250	8.12670	4.28020
O	18.44320	8.11730	4.28140
O	11.99180	5.13730	4.28080
O	12.01990	14.03890	4.28430
O	18.53820	2.19630	4.28680
O	12.04820	2.19240	4.28630
O	18.45710	11.06950	4.28670
O	11.96240	11.07530	4.29080
O	18.47000	5.15080	4.28860
Ti	8.76740	2.18410	5.56810
Ti	15.27060	2.17310	5.57250
Ti	8.71620	5.14020	5.56790
O	16.53370	0.71830	5.58910
O	10.04660	0.73180	5.59630
Ti	8.70430	11.06660	5.58950
Ti	15.20300	5.13740	5.58380
Ti	15.19190	11.06120	5.59740
Ti	15.28260	8.10410	5.61450
Ti	8.75980	8.09910	5.62340
Ti	11.99980	6.54790	5.65490
Ti	11.98540	9.66940	5.68290
O	13.93760	6.70950	5.68810
O	7.45700	12.63290	5.67790
Ti	18.49740	9.61860	5.71550
O	13.94500	12.62450	5.68640
O	7.46180	6.68870	5.69020
O	10.02420	3.72440	5.69150
O	16.50110	3.73060	5.74210
O	10.01640	9.65570	5.77820
Ti	12.01520	0.70570	5.74530
Ti	18.48400	6.60830	5.74220
Ti	18.49350	3.66520	5.74880
O	10.02510	6.56560	5.74190
O	13.94750	9.54050	5.77380
Ti	11.99430	3.63330	5.75810
Ti	11.98170	12.58060	5.76050
O	7.48580	9.55210	5.78310
O	16.47960	12.50060	5.77110
O	9.99140	12.51620	5.77630
O	7.49710	3.62020	5.83840
O	13.97750	3.61080	5.79400
O	16.48140	6.57300	5.83840

O	16.48180	9.64400	5.85810
O	7.52340	0.71350	5.93430
O	14.01330	0.70860	5.93310
O	12.11610	5.15040	6.88020
O	18.61310	11.06380	6.89120
O	12.10940	11.07730	6.88980
O	18.61350	5.15530	6.89610
O	18.33670	2.18750	6.90190
O	11.85970	14.03780	6.90830
O	18.43720	8.11280	6.90340
O	11.85590	2.18440	6.91330
O	11.92236	8.05971	7.02250
H	11.02511	7.97689	7.39307
H	13.66232	5.12883	7.56581
H	7.69925	5.17878	7.94374
H	13.63985	11.00690	7.56057
H	7.97940	10.60372	8.15870
O	9.09298	7.96596	7.75624
O	14.67287	5.22473	7.64385
O	14.65108	11.03897	7.71716
O	8.64020	5.25539	7.71854
O	8.45410	11.32800	7.70181
O	15.24163	8.02921	7.75586
H	17.61504	8.40044	8.04112
H	14.80143	6.14538	7.94493
H	9.31851	11.48987	8.11332
H	8.90807	6.18132	7.91903
H	14.78002	11.90288	8.13584
C	8.47521	8.56789	8.72325
C	15.80227	8.51282	8.76324
O	17.06946	8.67966	8.88500
O	7.30640	8.94749	8.71257
H	13.14686	8.64644	8.92095
H	11.20652	8.68322	8.96376
C	10.69125	8.94344	9.87196
C	9.31133	8.89595	9.94119
C	13.62418	8.92772	9.85627
C	15.00427	8.89726	9.95262
C	11.42067	9.34190	10.98089
C	12.89260	9.33102	10.97136
C	8.69806	9.25920	11.13931
H	7.61821	9.24770	11.22761
C	15.62412	9.25333	11.14966
H	16.70168	9.23660	11.25216
N	10.82804	9.70895	12.12859
C	9.49044	9.65661	12.20341

N	13.49052	9.69138	12.12058
C	14.82606	9.64534	12.20750
Cl	12.22804	12.50238	12.20457
H	9.05470	9.95804	13.14813
H	15.25394	9.94395	13.15631
Re	12.16972	10.47158	13.68737
C	12.13690	8.85635	14.70714
C	10.82689	11.24253	14.81413
C	13.53402	11.19059	14.81743
O	12.12109	7.90537	15.36897
O	9.98748	11.70276	15.46420
O	14.39382	11.61378	15.46878
O	8.92255	2.10274	7.52099
O	15.32863	2.20241	7.67426
H	17.54895	2.51463	8.20432
C	8.20585	2.47513	8.51909
C	15.74550	2.59073	8.76361
O	17.01320	2.72499	9.03621
O	6.98209	2.48922	8.59579
H	13.01988	2.58713	8.75777
H	10.91013	2.48088	8.73349
C	10.43737	2.85106	9.64222
C	9.04740	2.91177	9.69936
C	13.45172	2.87083	9.71871
C	14.83127	2.90462	9.89029
C	11.16671	3.27700	10.74549
C	12.64586	3.23112	10.80485
C	8.43272	3.39847	10.84382
H	7.35138	3.45016	10.89916
C	15.37627	3.25404	11.12439
H	16.44696	3.28676	11.27741
N	10.56204	3.75548	11.85736
C	9.22570	3.81818	11.89716
N	13.18514	3.57897	11.99264
C	14.51463	3.57810	12.14964
Cl	12.18282	6.42807	11.96920
H	8.79330	4.21779	12.80638
H	14.88445	3.86804	13.12485
Re	11.84494	4.45611	13.48427
C	11.60646	2.85958	14.48953
C	10.49810	5.36467	14.50635
C	13.19428	5.06852	14.70173
O	11.46389	1.87923	15.09605
O	9.64296	5.90111	15.06877
O	14.06301	5.39869	15.39127
H	7.86147	-0.15838	6.15141

O	20.45829	3.57252	5.97558
H	21.00615	3.21420	5.27340
O	11.92449	-0.64106	7.19389
H	11.71311	-1.49976	6.82034
O	12.16897	-0.75430	4.41671
O	20.45947	6.65401	5.86794
H	20.99138	6.65688	5.06877
O	20.47569	9.58141	5.78892
H	20.98715	10.20518	5.26842
H	16.02291	11.08436	3.26039
H	14.36014	11.08436	3.26066
H	16.13207	8.12604	3.27676
H	14.46935	8.12617	3.26391
H	15.99749	5.18124	3.24520
H	14.33493	5.18075	3.27149
H	16.02011	2.21748	3.21634
H	14.35835	2.21639	3.27442
H	9.51350	11.09653	3.24568
H	7.85080	11.09633	3.26144
H	9.64055	8.12475	3.27534
H	7.97815	8.12513	3.24052
H	9.49529	5.16855	3.23188
H	7.83294	5.16810	3.26924
H	9.53942	2.21309	3.22246
H	7.87718	2.21257	3.26472
H	7.80904	13.52460	5.72823
H	12.74184	14.33530	7.14264
H	17.41996	12.30879	5.74795
H	19.53629	11.26804	7.05735
H	19.21197	1.87661	7.14450
H	17.47618	0.90087	5.58702
H	17.71736	1.84346	3.93562
H	17.61638	11.39972	3.96151
H	11.19749	14.38693	3.93200
H	13.03512	-1.06049	4.13808
H	20.86305	3.88590	6.78771
H	20.88538	6.67330	6.72808
H	20.92340	8.93961	6.34503
H	6.57624	0.86534	5.89649
H	6.50751	12.49144	5.66992
H	16.22058	-0.18914	5.59945
H	16.17674	13.40501	5.88024
H	11.37737	-1.15599	4.05117

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Dimer in gas-phase; outer Cl, inner Cl facing surface;SCF Energy: -3502.772565

O	15.24160	8.02920	7.75590
O	9.09300	7.96600	7.75620
H	17.61500	8.40040	8.04110
C	8.47520	8.56790	8.72330
C	15.80230	8.51280	8.76320
O	17.06950	8.67970	8.88500
O	7.30640	8.94750	8.71260
H	13.14690	8.64640	8.92090
H	11.20650	8.68320	8.96380
C	10.69130	8.94340	9.87200
C	9.31130	8.89590	9.94120
C	13.62420	8.92770	9.85630
C	15.00430	8.89730	9.95260
C	11.42070	9.34190	10.98090
C	12.89260	9.33100	10.97140
C	8.69810	9.25920	11.13930
H	7.61820	9.24770	11.22760
C	15.62410	9.25330	11.14970
H	16.70170	9.23660	11.25220
N	10.82800	9.70890	12.12860
C	9.49040	9.65660	12.20340
N	13.49050	9.69140	12.12060
C	14.82610	9.64530	12.20750
Cl	12.22800	12.50240	12.20460
H	9.05470	9.95800	13.14810
H	15.25390	9.94390	13.15630
Re	12.16970	10.47160	13.68740
C	12.13690	8.85640	14.70710
C	10.82690	11.24250	14.81410
C	13.53400	11.19060	14.81740
O	12.12110	7.90540	15.36900
O	9.98750	11.70280	15.46420
O	14.39380	11.61380	15.46880
O	8.92250	2.10270	7.52100
O	15.32860	2.20240	7.67430
H	17.54900	2.51460	8.20430
C	8.20580	2.47510	8.51910
C	15.74550	2.59070	8.76360
O	17.01320	2.72500	9.03620
O	6.98210	2.48920	8.59580
H	13.01990	2.58710	8.75780
H	10.91010	2.48090	8.73350
C	10.43740	2.85110	9.64220
C	9.04740	2.91180	9.69940
C	13.45170	2.87080	9.71870
C	14.83130	2.90460	9.89030

C	11.16670	3.27700	10.74550
C	12.64590	3.23110	10.80490
C	8.43270	3.39850	10.84380
H	7.35140	3.45020	10.89920
C	15.37630	3.25400	11.12440
H	16.44700	3.28680	11.27740
N	10.56200	3.75550	11.85740
C	9.22570	3.81820	11.89720
N	13.18510	3.57900	11.99260
C	14.51460	3.57810	12.14960
Cl	12.18280	6.42810	11.96920
H	8.79330	4.21780	12.80640
H	14.88440	3.86800	13.12490
Re	11.84490	4.45610	13.48430
C	11.60650	2.85960	14.48950
C	10.49810	5.36470	14.50630
C	13.19430	5.06850	14.70170
O	11.46390	1.87920	15.09600
O	9.64300	5.90110	15.06880
O	14.06300	5.39870	15.39130
H	6.60615	2.16989	7.77221
H	6.90703	8.72998	7.86715

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Dimer on TiO2 along [-110] axis; outer CO, inner Cl facing surface on cluster of outer CO and inner CO; SCF Energy: -8598.79014831

O	8.72050	2.20690	3.72340
O	15.20600	2.20790	3.72500
O	8.67490	5.16250	3.73040
O	8.68670	11.09030	3.73350
O	8.79930	8.11970	3.73780
O	15.17380	5.17200	3.73820
O	15.19160	11.07960	3.74050
O	15.29700	8.12160	3.75030
O	11.97250	8.12670	4.28020
O	18.44320	8.11730	4.28140
O	11.99180	5.13730	4.28080
O	12.01990	14.03890	4.28430
O	18.53820	2.19630	4.28680
O	12.04820	2.19240	4.28630
O	18.45710	11.06950	4.28670
O	11.96240	11.07530	4.29080
O	18.47000	5.15080	4.28860
Ti	8.76740	2.18410	5.56810
Ti	15.27060	2.17310	5.57250

Ti	8.71620	5.14020	5.56790
O	16.53370	0.71830	5.58910
O	10.04660	0.73180	5.59630
Ti	8.70430	11.06660	5.58950
Ti	15.20300	5.13740	5.58380
Ti	15.19190	11.06120	5.59740
Ti	15.28260	8.10410	5.61450
Ti	8.75980	8.09910	5.62340
Ti	11.99980	6.54790	5.65490
Ti	11.98540	9.66940	5.68290
O	13.93760	6.70950	5.68810
O	7.45700	12.63290	5.67790
Ti	18.49740	9.61860	5.71550
O	13.94500	12.62450	5.68640
O	7.46180	6.68870	5.69020
O	10.02420	3.72440	5.69150
O	16.50110	3.73060	5.74210
O	10.01640	9.65570	5.77820
Ti	12.01520	0.70570	5.74530
Ti	18.48400	6.60830	5.74220
Ti	18.49350	3.66520	5.74880
O	10.02510	6.56560	5.74190
O	13.94750	9.54050	5.77380
Ti	11.99430	3.63330	5.75810
Ti	11.98170	12.58060	5.76050
O	7.48580	9.55210	5.78310
O	16.47960	12.50060	5.77110
O	9.99140	12.51620	5.77630
O	7.49710	3.62020	5.83840
O	13.97750	3.61080	5.79400
O	16.48140	6.57300	5.83840
O	16.48180	9.64400	5.85810
O	7.52340	0.71350	5.93430
O	14.01330	0.70860	5.93310
O	12.11610	5.15040	6.88020
O	18.61310	11.06380	6.89120
O	12.10940	11.07730	6.88980
O	18.61350	5.15530	6.89610
O	18.33670	2.18750	6.90190
O	11.85970	14.03780	6.90830
O	18.43720	8.11280	6.90340
O	11.85590	2.18440	6.91330
O	11.92300	8.06470	7.03130
H	11.01660	7.99180	7.38190
H	13.65860	5.13470	7.55320
H	7.76700	5.10490	7.98910

H	13.63000	11.01100	7.54620
H	7.96840	10.59050	8.14180
O	9.10580	7.96480	7.77200
O	14.67040	5.23830	7.63270
O	14.64170	11.05960	7.71540
O	8.68930	5.23690	7.72300
O	8.44830	11.32450	7.70440
O	15.25150	8.03030	7.76290
H	17.64660	8.37150	8.02670
H	14.80100	6.16120	7.92450
H	9.32530	11.44570	8.10200
H	8.91690	6.17160	7.92650
H	14.75490	11.95090	8.07690
C	8.48910	8.57300	8.73350
C	15.82820	8.52450	8.75610
O	17.09540	8.65850	8.88050
O	7.31760	8.94480	8.72490
O	8.91670	2.13040	7.49830
O	15.32850	2.21190	7.68110
H	17.52180	2.62030	8.21330
C	8.22280	2.01510	8.57010
C	15.71120	2.73250	8.73010
O	16.97380	2.91650	9.00390
O	7.05050	1.66540	8.66590
H	7.86150	-0.15840	6.15140
O	20.45830	3.57250	5.97560
H	21.00620	3.21420	5.27340
O	11.92450	-0.64110	7.19390
H	11.71310	-1.49980	6.82030
O	12.16900	-0.75430	4.41670
O	20.45950	6.65400	5.86790
H	20.99140	6.65690	5.06880
O	20.47570	9.58140	5.78890
H	20.98710	10.20520	5.26840
H	16.02290	11.08440	3.26040
H	14.36010	11.08440	3.26070
H	16.13210	8.12600	3.27680
H	14.46940	8.12620	3.26390
H	15.99750	5.18120	3.24520
H	14.33490	5.18070	3.27150
H	16.02010	2.21750	3.21630
H	14.35830	2.21640	3.27440
H	9.51350	11.09650	3.24570
H	7.85080	11.09630	3.26140
H	9.64050	8.12480	3.27530
H	7.97820	8.12510	3.24050

H	9.49530	5.16850	3.23190
H	7.83290	5.16810	3.26920
H	9.53940	2.21310	3.22250
H	7.87720	2.21260	3.26470
H	7.80900	13.52460	5.72820
H	12.74180	14.33530	7.14260
H	17.42000	12.30880	5.74800
H	19.53630	11.26800	7.05730
H	19.21200	1.87660	7.14450
H	17.47620	0.90090	5.58700
H	17.71740	1.84350	3.93560
H	17.61640	11.39970	3.96150
H	11.19750	14.38690	3.93200
H	13.03510	-1.06050	4.13810
H	20.86310	3.88590	6.78770
H	20.88540	6.67330	6.72810
H	20.92340	8.93960	6.34500
H	6.57620	0.86530	5.89650
H	6.50750	12.49140	5.66990
H	16.22060	-0.18910	5.59950
H	16.17670	13.40500	5.88020
H	11.37740	-1.15600	4.05120
H	13.11108	8.76090	8.86500
H	11.17202	8.68230	8.98488
C	10.66473	9.11922	9.82420
C	9.28963	9.03516	9.94309
C	13.59260	9.15976	9.75214
C	14.97227	9.11650	9.85490
C	11.40053	9.77390	10.80031
C	12.87070	9.75898	10.78141
C	8.69088	9.63251	11.05192
H	7.61724	9.57959	11.18696
C	15.59616	9.62770	10.99157
H	16.67130	9.58539	11.11027
N	10.81608	10.39336	11.84153
C	9.48428	10.30644	11.96789
N	13.47829	10.32146	11.84257
C	14.80976	10.22606	11.96009
Cl	12.05813	9.50770	14.64803
H	9.05646	10.79063	12.83670
H	15.24160	10.65701	12.85433
Re	12.17502	11.51463	13.16886
C	12.29092	12.98087	11.95582
C	10.84871	12.41070	14.21919
C	13.54691	12.26806	14.26668
O	12.39185	13.86968	11.21526

O	10.01998	12.93045	14.83675
O	14.40902	12.69301	14.91281
H	13.22095	2.41604	8.74334
H	11.07923	2.23209	8.80825
C	10.61953	2.72803	9.66106
C	9.23103	2.74998	9.76651
C	13.65276	2.87413	9.63435
C	15.03093	2.99579	9.77488
C	11.36444	3.41429	10.60806
C	12.84623	3.43890	10.62612
C	8.63444	3.40110	10.83669
H	7.55547	3.40091	10.94241
C	15.57888	3.58322	10.91426
H	16.64982	3.66701	11.04431
N	10.77368	4.13149	11.59208
C	9.44178	4.10181	11.71548
N	13.38836	4.09860	11.67261
C	14.71501	4.12793	11.83901
Cl	12.25882	6.41830	10.20671
H	9.02584	4.68564	12.52844
H	15.07632	4.65251	12.71513
Re	12.06772	5.58453	12.58345
C	11.97081	4.79218	14.30760
C	10.67326	6.82419	13.03904
C	13.45999	6.78201	13.14538
O	11.91918	4.29483	15.35576
O	9.74500	7.47739	13.25148
O	14.39384	7.41438	13.40243

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Dimer on TiO2 along [-110] axis; outer Cl, inner Cl facing surface on cluster of outer CO and inner CO; SCF Energy: -8598.81360301

O	8.72050	2.20690	3.72340
O	15.20600	2.20790	3.72500
O	8.67490	5.16250	3.73040
O	8.68670	11.09030	3.73350
O	8.79930	8.11970	3.73780
O	15.17380	5.17200	3.73820
O	15.19160	11.07960	3.74050
O	15.29700	8.12160	3.75030
O	11.97250	8.12670	4.28020
O	18.44320	8.11730	4.28140
O	11.99180	5.13730	4.28080
O	12.01990	14.03890	4.28430
O	18.53820	2.19630	4.28680
O	12.04820	2.19240	4.28630

O	18.45710	11.06950	4.28670
O	11.96240	11.07530	4.29080
O	18.47000	5.15080	4.28860
Ti	8.76740	2.18410	5.56810
Ti	15.27060	2.17310	5.57250
Ti	8.71620	5.14020	5.56790
O	16.53370	0.71830	5.58910
O	10.04660	0.73180	5.59630
Ti	8.70430	11.06660	5.58950
Ti	15.20300	5.13740	5.58380
Ti	15.19190	11.06120	5.59740
Ti	15.28260	8.10410	5.61450
Ti	8.75980	8.09910	5.62340
Ti	11.99980	6.54790	5.65490
Ti	11.98540	9.66940	5.68290
O	13.93760	6.70950	5.68810
O	7.45700	12.63290	5.67790
Ti	18.49740	9.61860	5.71550
O	13.94500	12.62450	5.68640
O	7.46180	6.68870	5.69020
O	10.02420	3.72440	5.69150
O	16.50110	3.73060	5.74210
O	10.01640	9.65570	5.77820
Ti	12.01520	0.70570	5.74530
Ti	18.48400	6.60830	5.74220
Ti	18.49350	3.66520	5.74880
O	10.02510	6.56560	5.74190
O	13.94750	9.54050	5.77380
Ti	11.99430	3.63330	5.75810
Ti	11.98170	12.58060	5.76050
O	7.48580	9.55210	5.78310
O	16.47960	12.50060	5.77110
O	9.99140	12.51620	5.77630
O	7.49710	3.62020	5.83840
O	13.97750	3.61080	5.79400
O	16.48140	6.57300	5.83840
O	16.48180	9.64400	5.85810
O	7.52340	0.71350	5.93430
O	14.01330	0.70860	5.93310
O	12.11610	5.15040	6.88020
O	18.61310	11.06380	6.89120
O	12.10940	11.07730	6.88980
O	18.61350	5.15530	6.89610
O	18.33670	2.18750	6.90190
O	11.85970	14.03780	6.90830
O	18.43720	8.11280	6.90340

O	11.85590	2.18440	6.91330
O	11.92300	8.06470	7.03130
H	11.01660	7.99180	7.38190
H	13.65860	5.13470	7.55320
H	7.76700	5.10490	7.98910
H	13.63000	11.01100	7.54620
H	7.96840	10.59050	8.14180
O	9.10580	7.96480	7.77200
O	14.67040	5.23830	7.63270
O	14.64170	11.05960	7.71540
O	8.68930	5.23690	7.72300
O	8.44830	11.32450	7.70440
O	15.25150	8.03030	7.76290
H	17.64660	8.37150	8.02670
H	14.80100	6.16120	7.92450
H	9.32530	11.44570	8.10200
H	8.91690	6.17160	7.92650
H	14.75490	11.95090	8.07690
C	8.48910	8.57300	8.73350
C	15.82820	8.52450	8.75610
O	17.09540	8.65850	8.88050
O	7.31760	8.94480	8.72490
O	8.91670	2.13040	7.49830
O	15.32850	2.21190	7.68110
H	17.52180	2.62030	8.21330
C	8.22280	2.01510	8.57010
C	15.71120	2.73250	8.73010
O	16.97380	2.91650	9.00390
O	7.05050	1.66540	8.66590
H	7.86150	-0.15840	6.15140
O	20.45830	3.57250	5.97560
H	21.00620	3.21420	5.27340
O	11.92450	-0.64110	7.19390
H	11.71310	-1.49980	6.82030
O	12.16900	-0.75430	4.41670
O	20.45950	6.65400	5.86790
H	20.99140	6.65690	5.06880
O	20.47570	9.58140	5.78890
H	20.98710	10.20520	5.26840
H	16.02290	11.08440	3.26040
H	14.36010	11.08440	3.26070
H	16.13210	8.12600	3.27680
H	14.46940	8.12620	3.26390
H	15.99750	5.18120	3.24520
H	14.33490	5.18070	3.27150
H	16.02010	2.21750	3.21630

H	14.35830	2.21640	3.27440
H	9.51350	11.09650	3.24570
H	7.85080	11.09630	3.26140
H	9.64050	8.12480	3.27530
H	7.97820	8.12510	3.24050
H	9.49530	5.16850	3.23190
H	7.83290	5.16810	3.26920
H	9.53940	2.21310	3.22250
H	7.87720	2.21260	3.26470
H	7.80900	13.52460	5.72820
H	12.74180	14.33530	7.14260
H	17.42000	12.30880	5.74800
H	19.53630	11.26800	7.05730
H	19.21200	1.87660	7.14450
H	17.47620	0.90090	5.58700
H	17.71740	1.84350	3.93560
H	17.61640	11.39970	3.96150
H	11.19750	14.38690	3.93200
H	13.03510	-1.06050	4.13810
H	20.86310	3.88590	6.78770
H	20.88540	6.67330	6.72810
H	20.92340	8.93960	6.34500
H	6.57620	0.86530	5.89650
H	6.50750	12.49140	5.66990
H	16.22060	-0.18910	5.59950
H	16.17670	13.40500	5.88020
H	11.37740	-1.15600	4.05120
H	13.15381	8.63260	9.01502
H	11.21658	8.69090	9.12505
C	10.73577	8.93845	10.05537
C	9.35844	8.90547	10.17081
C	13.66603	8.88924	9.93897
C	15.04813	8.84097	9.98735
C	11.50726	9.30581	11.14640
C	12.97774	9.27813	11.08630
C	8.79081	9.25130	11.39622
H	7.71447	9.25046	11.52119
C	15.71257	9.16531	11.16941
H	16.79275	9.13409	11.23460
N	10.95844	9.65614	12.32082
C	9.62362	9.61775	12.44031
N	13.61872	9.60809	12.22134
C	14.95584	9.54483	12.26153
Cl	12.39426	12.43117	12.40468
H	9.22400	9.90483	13.40520
H	15.41926	9.81906	13.20091

Re	12.36158	10.37136	13.84771
C	12.34371	8.73618	14.83545
C	11.06737	11.13456	15.03491
C	13.77218	11.05138	14.94450
O	12.33880	7.77213	15.47836
O	10.25624	11.59115	15.72243
O	14.65874	11.45126	15.57441
H	12.94728	2.57976	8.73527
H	10.83673	2.49842	8.78109
C	10.39976	2.85544	9.71266
C	9.01335	2.93099	9.81861
C	13.41493	2.83880	9.68631
C	14.79988	2.85318	9.81122
C	11.17129	3.25030	10.79864
C	12.65098	3.18614	10.80644
C	8.44390	3.40130	10.99288
H	7.36582	3.46433	11.08629
C	15.39074	3.17103	11.03268
H	16.46634	3.18835	11.14957
N	10.61063	3.71297	11.93993
C	9.27732	3.79026	12.02670
N	13.23445	3.50351	11.98170
C	14.56841	3.48407	12.09305
Cl	12.26684	6.36386	12.04959
H	8.88099	4.17619	12.95797
H	14.97466	3.74973	13.06072
Re	11.95655	4.36540	13.53564
C	11.73296	2.75159	14.51630
C	10.65648	5.26844	14.62111
C	13.35394	4.93724	14.71814
O	11.59909	1.76073	15.10760
O	9.82761	5.80308	15.22316
O	14.24955	5.24326	15.38406

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Dimer on TiO2 along [-110] axis; outer Cl, inner CO facing surface on cluster of outer CO and inner CO; SCF Energy: -8598.80503405

O	8.72050	2.20690	3.72340
O	15.20600	2.20790	3.72500
O	8.67490	5.16250	3.73040
O	8.68670	11.09030	3.73350
O	8.79930	8.11970	3.73780
O	15.17380	5.17200	3.73820
O	15.19160	11.07960	3.74050
O	15.29700	8.12160	3.75030
O	11.97250	8.12670	4.28020

O	18.44320	8.11730	4.28140
O	11.99180	5.13730	4.28080
O	12.01990	14.03890	4.28430
O	18.53820	2.19630	4.28680
O	12.04820	2.19240	4.28630
O	18.45710	11.06950	4.28670
O	11.96240	11.07530	4.29080
O	18.47000	5.15080	4.28860
Ti	8.76740	2.18410	5.56810
Ti	15.27060	2.17310	5.57250
Ti	8.71620	5.14020	5.56790
O	16.53370	0.71830	5.58910
O	10.04660	0.73180	5.59630
Ti	8.70430	11.06660	5.58950
Ti	15.20300	5.13740	5.58380
Ti	15.19190	11.06120	5.59740
Ti	15.28260	8.10410	5.61450
Ti	8.75980	8.09910	5.62340
Ti	11.99980	6.54790	5.65490
Ti	11.98540	9.66940	5.68290
O	13.93760	6.70950	5.68810
O	7.45700	12.63290	5.67790
Ti	18.49740	9.61860	5.71550
O	13.94500	12.62450	5.68640
O	7.46180	6.68870	5.69020
O	10.02420	3.72440	5.69150
O	16.50110	3.73060	5.74210
O	10.01640	9.65570	5.77820
Ti	12.01520	0.70570	5.74530
Ti	18.48400	6.60830	5.74220
Ti	18.49350	3.66520	5.74880
O	10.02510	6.56560	5.74190
O	13.94750	9.54050	5.77380
Ti	11.99430	3.63330	5.75810
Ti	11.98170	12.58060	5.76050
O	7.48580	9.55210	5.78310
O	16.47960	12.50060	5.77110
O	9.99140	12.51620	5.77630
O	7.49710	3.62020	5.83840
O	13.97750	3.61080	5.79400
O	16.48140	6.57300	5.83840
O	16.48180	9.64400	5.85810
O	7.52340	0.71350	5.93430
O	14.01330	0.70860	5.93310
O	12.11610	5.15040	6.88020
O	18.61310	11.06380	6.89120

O	12.10940	11.07730	6.88980
O	18.61350	5.15530	6.89610
O	18.33670	2.18750	6.90190
O	11.85970	14.03780	6.90830
O	18.43720	8.11280	6.90340
O	11.85590	2.18440	6.91330
O	11.92300	8.06470	7.03130
H	11.01660	7.99180	7.38190
H	13.65860	5.13470	7.55320
H	7.76700	5.10490	7.98910
H	13.63000	11.01100	7.54620
H	7.96840	10.59050	8.14180
O	9.10580	7.96480	7.77200
O	14.67040	5.23830	7.63270
O	14.64170	11.05960	7.71540
O	8.68930	5.23690	7.72300
O	8.44830	11.32450	7.70440
O	15.25150	8.03030	7.76290
H	17.64660	8.37150	8.02670
H	14.80100	6.16120	7.92450
H	9.32530	11.44570	8.10200
H	8.91690	6.17160	7.92650
H	14.75490	11.95090	8.07690
C	8.48910	8.57300	8.73350
C	15.82820	8.52450	8.75610
O	17.09540	8.65850	8.88050
O	7.31760	8.94480	8.72490
O	8.91670	2.13040	7.49830
O	15.32850	2.21190	7.68110
H	17.52180	2.62030	8.21330
C	8.22280	2.01510	8.57010
C	15.71120	2.73250	8.73010
O	16.97380	2.91650	9.00390
O	7.05050	1.66540	8.66590
H	7.86150	-0.15840	6.15140
O	20.45830	3.57250	5.97560
H	21.00620	3.21420	5.27340
O	11.92450	-0.64110	7.19390
H	11.71310	-1.49980	6.82030
O	12.16900	-0.75430	4.41670
O	20.45950	6.65400	5.86790
H	20.99140	6.65690	5.06880
O	20.47570	9.58140	5.78890
H	20.98710	10.20520	5.26840
H	16.02290	11.08440	3.26040
H	14.36010	11.08440	3.26070

H	16.13210	8.12600	3.27680
H	14.46940	8.12620	3.26390
H	15.99750	5.18120	3.24520
H	14.33490	5.18070	3.27150
H	16.02010	2.21750	3.21630
H	14.35830	2.21640	3.27440
H	9.51350	11.09650	3.24570
H	7.85080	11.09630	3.26140
H	9.64050	8.12480	3.27530
H	7.97820	8.12510	3.24050
H	9.49530	5.16850	3.23190
H	7.83290	5.16810	3.26920
H	9.53940	2.21310	3.22250
H	7.87720	2.21260	3.26470
H	7.80900	13.52460	5.72820
H	12.74180	14.33530	7.14260
H	17.42000	12.30880	5.74800
H	19.53630	11.26800	7.05730
H	19.21200	1.87660	7.14450
H	17.47620	0.90090	5.58700
H	17.71740	1.84350	3.93560
H	17.61640	11.39970	3.96150
H	11.19750	14.38690	3.93200
H	13.03510	-1.06050	4.13810
H	20.86310	3.88590	6.78770
H	20.88540	6.67330	6.72810
H	20.92340	8.93960	6.34500
H	6.57620	0.86530	5.89650
H	6.50750	12.49140	5.66990
H	16.22060	-0.18910	5.59950
H	16.17670	13.40500	5.88020
H	11.37740	-1.15600	4.05120
H	13.20373	8.53093	8.93962
H	11.16154	8.13467	9.21448
C	10.75549	8.73671	10.01345
C	9.43274	9.14636	10.00128
C	13.69862	8.51993	9.90984
C	15.07190	8.35153	9.99123
C	11.57003	9.11488	11.06888
C	13.00198	8.78443	11.08616
C	8.96083	9.88311	11.08501
H	7.93009	10.21617	11.10504
C	15.69774	8.35253	11.23751
H	16.76746	8.21034	11.32810
N	11.10905	9.80742	12.12430
C	9.82217	10.17711	12.12906

N	13.61403	8.86845	12.28142
C	14.92610	8.60336	12.35937
Cl	13.52396	11.87647	12.20528
H	9.48904	10.73032	12.99868
H	15.36382	8.64865	13.34866
Re	12.54499	10.13840	13.75360
C	11.73626	8.80545	14.85193
C	11.56895	11.49202	14.68496
C	13.98839	10.31868	14.99880
O	11.21922	8.03815	15.55005
O	10.95746	12.31878	15.21326
O	14.88720	10.40501	15.72215
H	12.81872	2.50957	8.83663
H	10.65398	2.79138	8.68704
C	10.23056	2.93683	9.67949
C	8.87316	2.70389	9.88055
C	13.23657	3.14857	9.61311
C	14.59408	3.43593	9.64101
C	10.99280	3.38867	10.74591
C	12.43061	3.69873	10.61358
C	8.33889	2.87439	11.15042
H	7.28937	2.67184	11.33179
C	15.10452	4.30868	10.60149
H	16.15547	4.56779	10.62227
N	10.45690	3.62693	11.96366
C	9.16324	3.34308	12.16329
N	12.93413	4.51403	11.56058
C	14.23527	4.83735	11.53103
Cl	12.86048	2.58502	13.88210
H	8.78567	3.52729	13.16222
H	14.58005	5.51445	12.30227
Re	11.72010	4.76546	13.37273
C	10.68203	6.28218	12.90608
C	10.68419	4.57565	14.97977
C	13.01563	5.80377	14.31564
O	9.94849	7.14481	12.63950
O	10.05382	4.42354	15.93420
O	13.85861	6.43237	14.80548