Supporting Information

CO_2 Adsorption on $Ti_3O_6^-$: A Novel Carbonate Binding Motif

Sreekanta Debnath,[a,b] Xiaowei Song,[b] Matias R. Fagiani,[a,b] Marissa L. Weichman,[c,†] Min Gao,[d,e] Satoshi Maeda,[e,f] Tetsuya Taketsugu,[e,f,g] Wieland Schöllkopf,[b] Andrey Lyalin,[g,*] Daniel M. Neumark,[c,h,*] Knut R. Asmis[a,*]

[a] *Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig, Linnéstrasse 2, D-04103 Leipzig, Germany*

[b] *Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany*

[c] *Department of Chemistry, University of California, Berkeley, California 94720, United States*

[d] *Institute for Catalysis, Hokkaido University, Sapporo 001-0021, Japan*

[e] *Department of Chemistry, Faculty of Science, Hokkaido University, Sapporo 060-0810, Japan*

[f] *Institute for Chemical Reaction Design and Discovery (WPI-ICReDD), Hokkaido University, Sapporo 001-0021, Japan*

[g] *Global Research Center for Environment and Energy based on Nanomaterials Science (GREEN), National Institute for Material Science (NIMS), Tsukuba 305-0044, Japan.*

[h] *Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, United States*

[†] *Current affiliation: JILA, National Institute of Standards and Technology, Boulder, Colorado 80305, USA*

[*] *knut.asmis@uni-leipzig.de, dneumark@berkeley.edu, lyalin.andrey@nims.go.jp*

S1. Quadrupole mass spectra

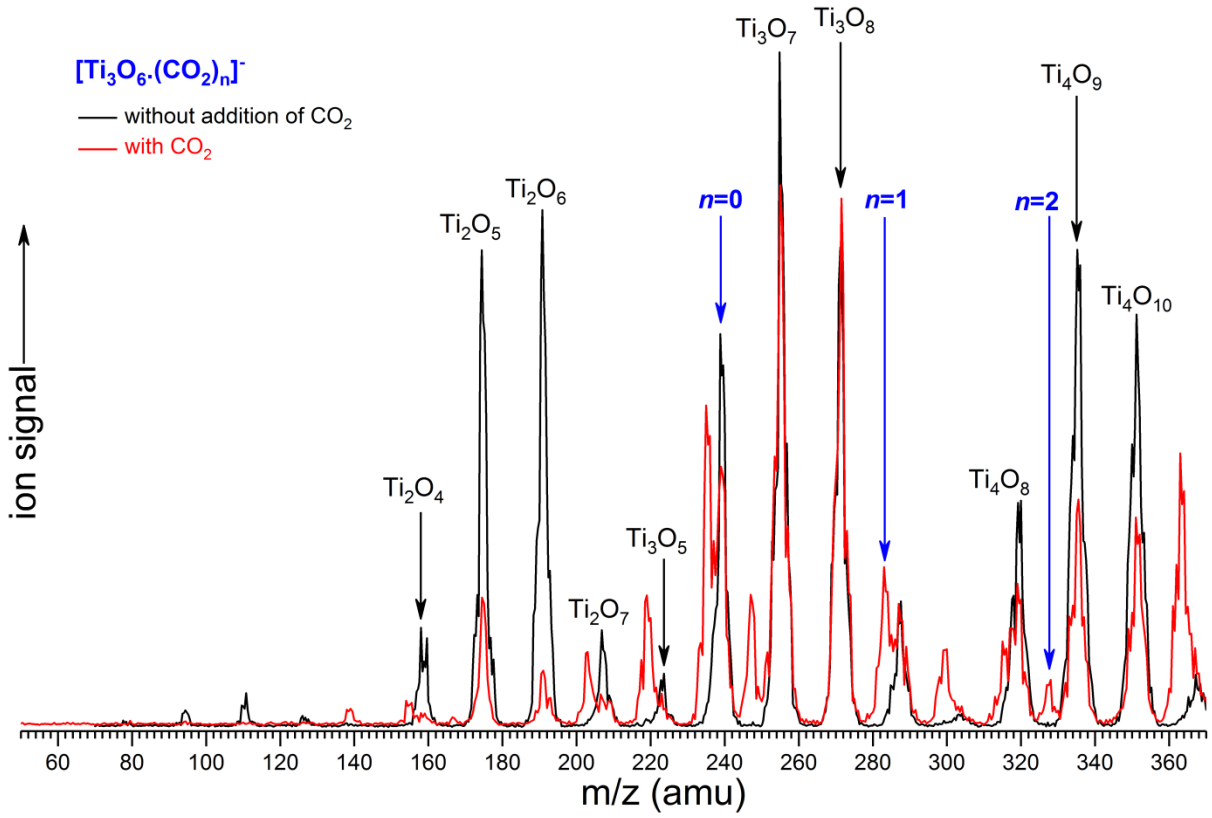

Fig.S1: Quadrupole mass spectrum of the ions produced by pulsed laser vaporization of a pure Ti metal rod and quenching in a gas pulse of 0.75 % O_2 seeded in He. Pure CO_2 was added from a second gas channel to the source block to get CO_2 reaction product.

S2. Experimental spectra compared to computed spectra for all the isomers

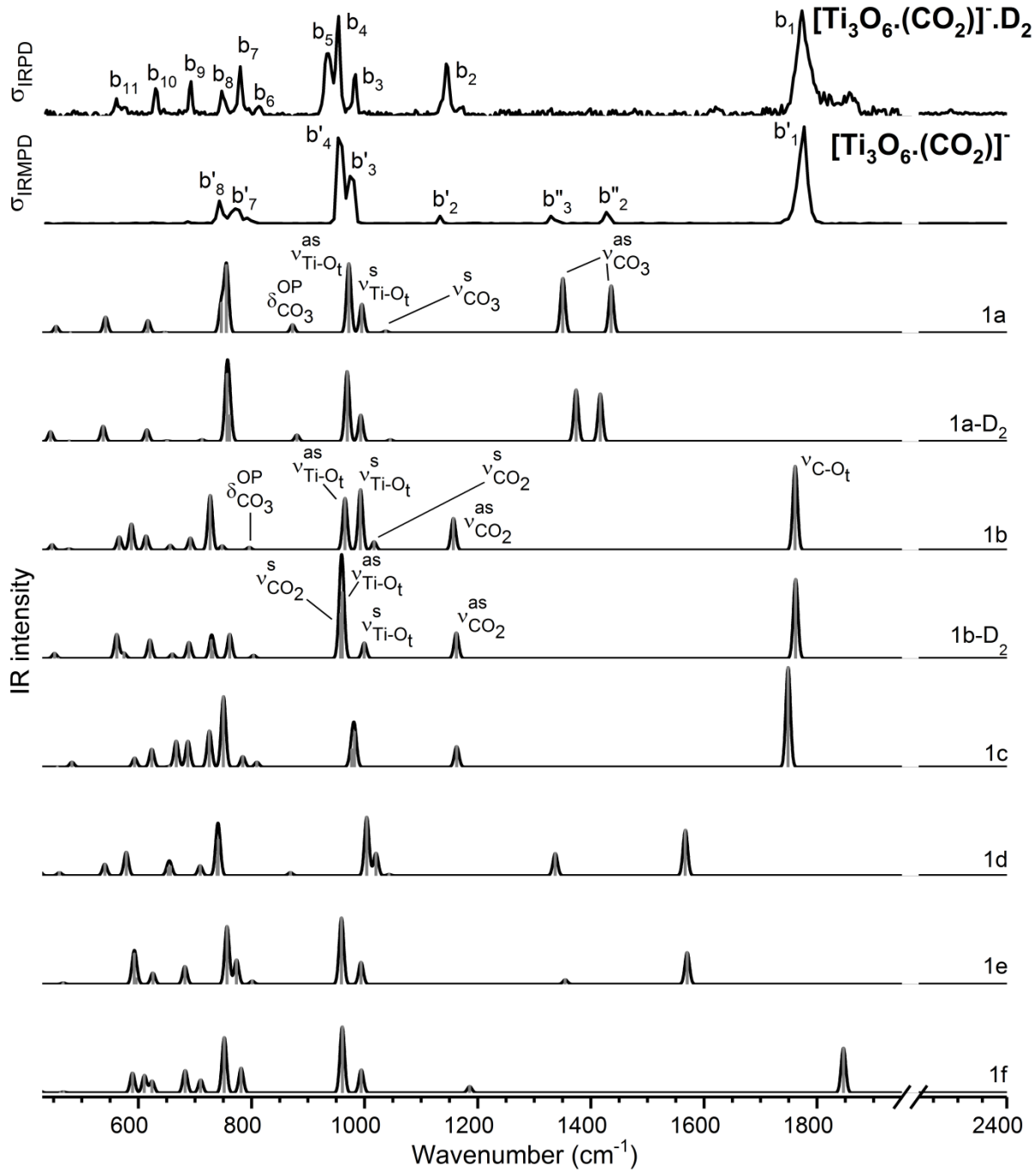

Fig.S2: Experimental IRPD spectra of D_2 tagged $[Ti_3O_6.(CO_2)]^-$ (D_2 loss – top trace, CO_2 loss – second trace from the top) compared with calculated harmonic spectrum (using Gaussian convolution, FWHM=10) of different possible isomers for the species, using ωB97XD/aug-cc-pVTZ level of theory and numbers in parenthesis indicates relative energy of the isomers. A scaling factor of 0.96 is used for the whole region.

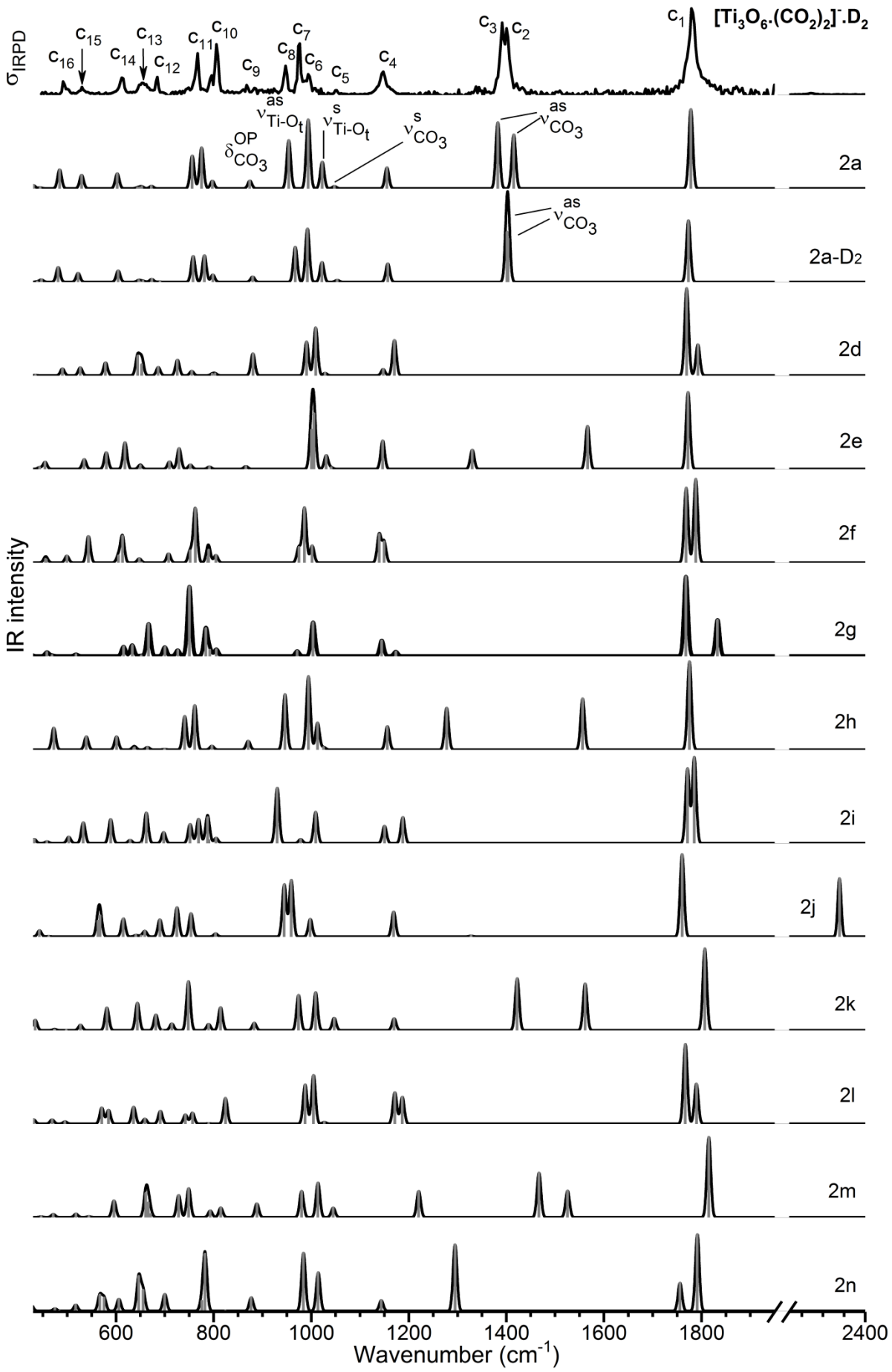
σIRPD
[Ti3O6.(CO2)2]-.D2
c1
c2
c3
c4
c5
c6
c7
c8
c9
c10
c11
c12
c13
c14
c15
c16
as
νTi-Ot
s
νTi-Ot
δOP CO3
s
νCO3
as
νCO3
2a
as
νCO3
2a-D2
2d
2e
2f
2g
2h
2i
2j
2k
2l
2m
2n
IR intensity
600
800
1000
1200
1400
1600
1800
2400
Wavenumber (cm-1)

Fig.S3: Experimental IRPD spectra of D_2 tagged $[Ti_3O_6.(CO_2)_2]^-$ (top trace) compared with calculated harmonic spectrum (using Gaussian convolution, FWHM=10) of different possible isomers for the species, using ωB97XD/aug-cc-pVTZ level of theory and numbers in parenthesis indicates relative energy of the isomers. A scaling factor of 0.96 is used for the whole region.

S3. Additional possible isomers, spin densities and NBO charges

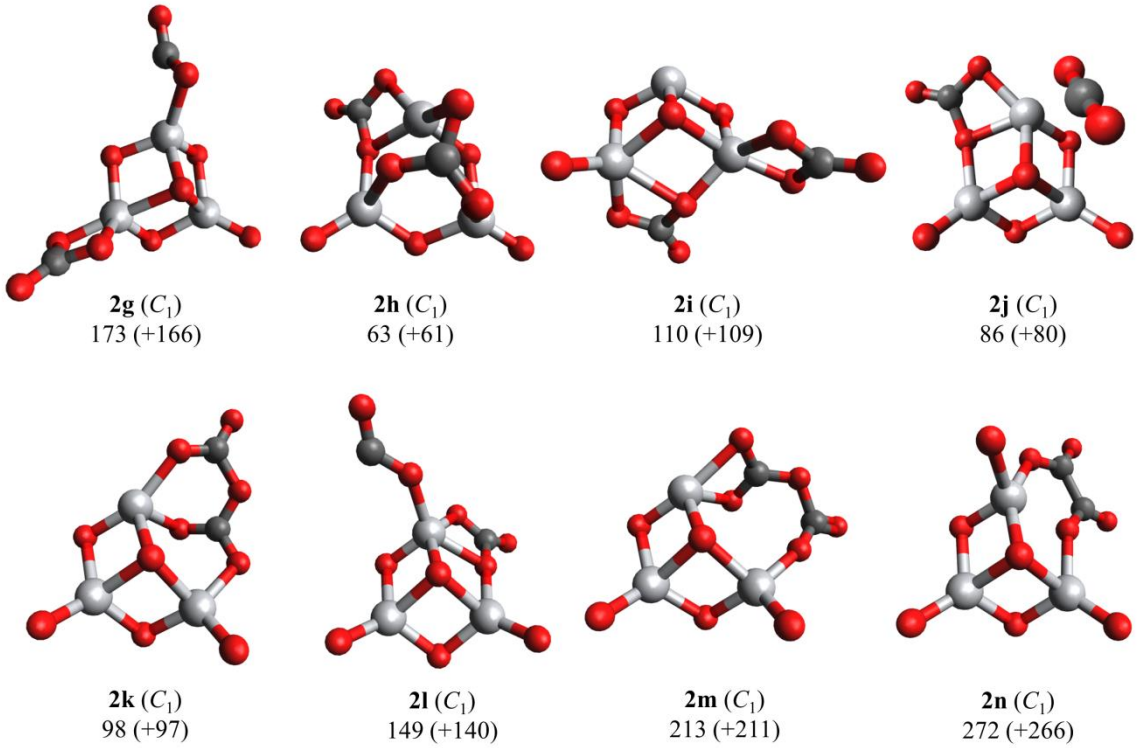

Fig.S4: ωB97X-D/aug-cc-pVTZ minimum-energy structures, symmetry (in parentheses) and relative CCSD(T) single-point energy (in $kJ \cdot mol^{-1}$) of energetically low-lying $[Ti_3O_6 (CO_2)_{,2}]^-$ isomers (2a-2f in main manuscript). The ZPE-corrected energies are given in parentheses. The isomers are labelled with ***n*x**, where *n* is the number of CO_2 molecules adsorbed and x = g, h, i,… indicates the energetic ordering. Atoms in grey represent Ti, dark grey C, and red O. .

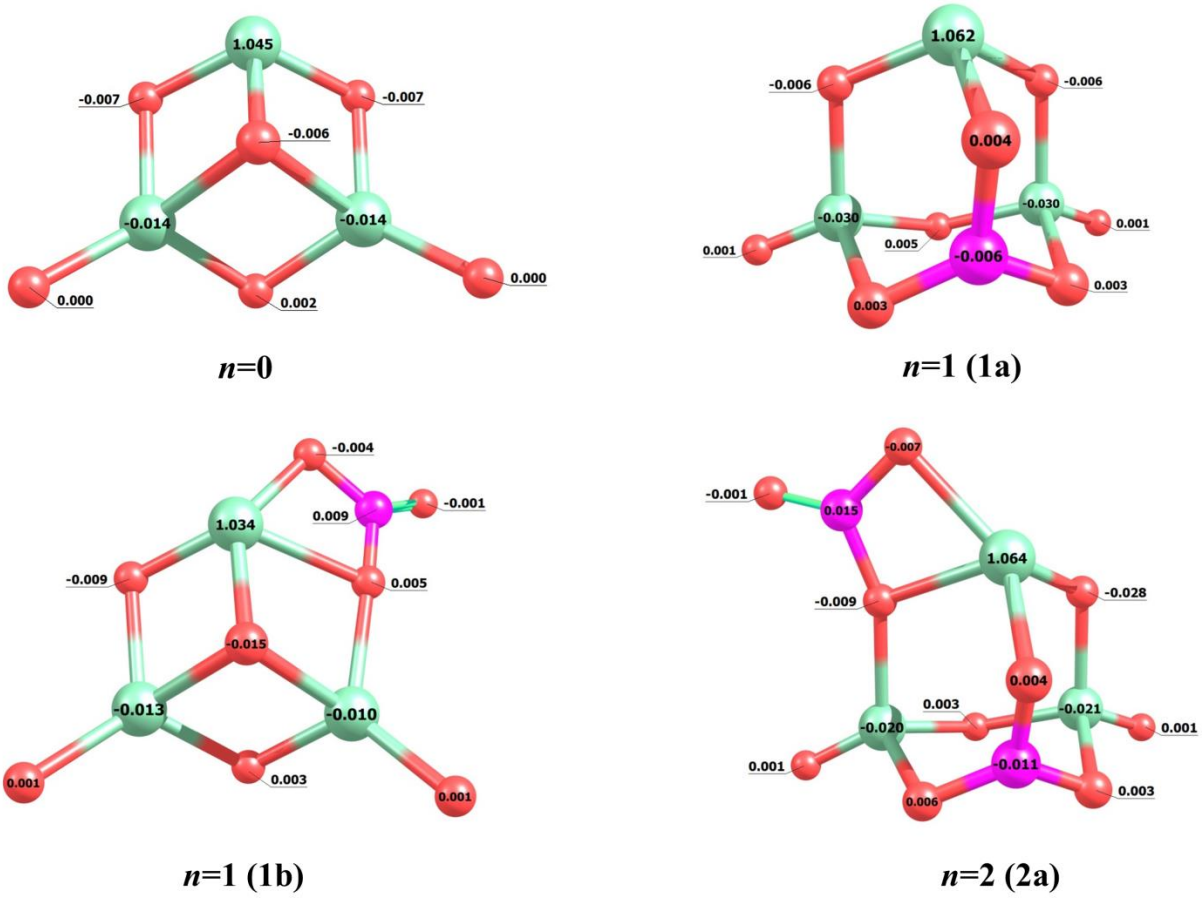

Fig.S5: Spin density plot of $[Ti_3O_6.(CO_2)_{n=0\text{-}2}]^-$ clusters. (Colour code : sky blue: Ti, orange red: O, pink: C)

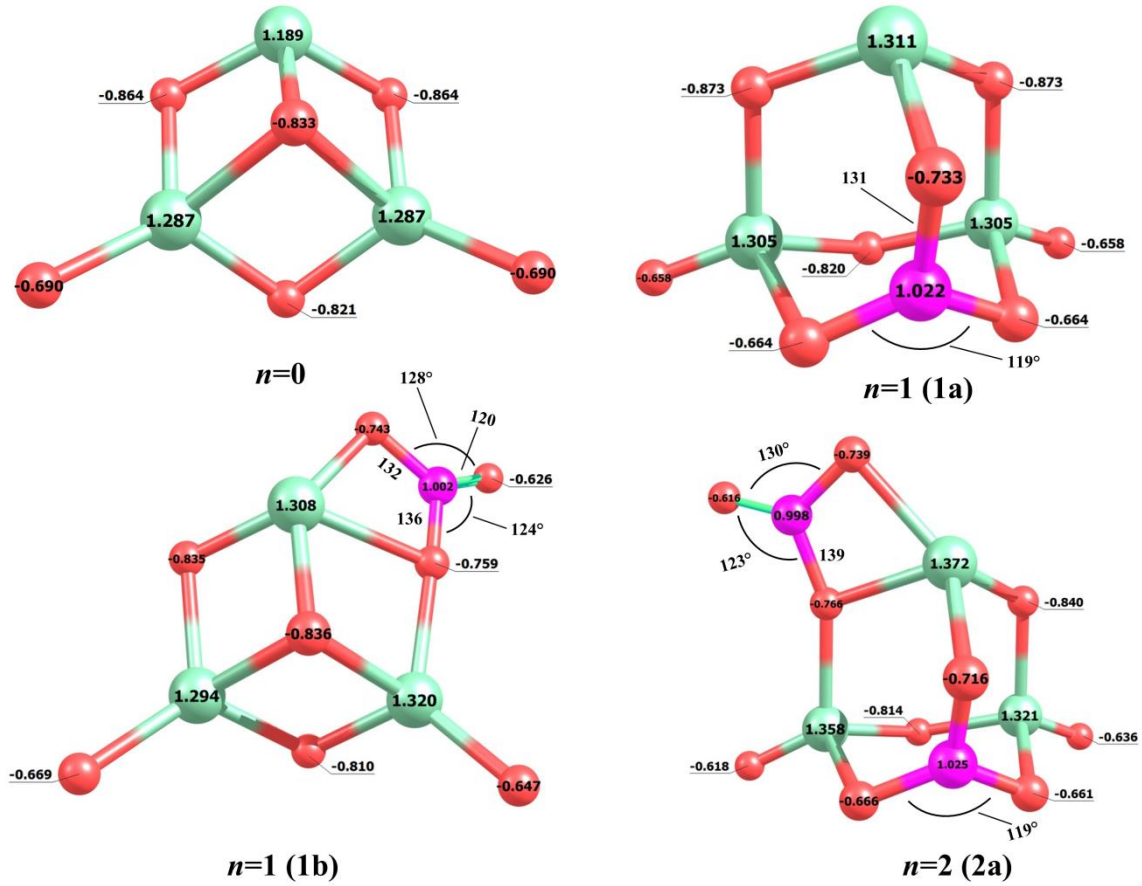

Fig.S6: NBO charges on the C and O atoms of the adsorbed CO_2 on $Ti_3O_6^-$ cluster forming $[Ti_3O_6.(CO_2)_{n=0-2}]^-$ clusters. Bond lengths (in pm) and bond angles (in degrees) are also shown. (Colour code : sky blue: Ti, orange red: O, pink: C)

Table.S1: Spin densities and NBO charges on different atoms of $[Ti_3O_6.(CO_2)_{n=0-2}]^-$ clusters. Ti atom of the Ti^{3+} center is named as Ti_a and then anticlockwise other Ti atoms named as b, c. For bidentate bridged CO_3^-, free C-O oxygen named as O_a and then same naming as Ti atoms, and for the tridentate CO_3^- the oxygen connected to the Ti^{3+} centre named as O_a and then followed same naming as above. All the calculations are performed with ωB97XD/aug-cc-pVTZ level of theory.

Isomer	**Spin densities**			**NBO charges**				
	Ti_a	**Ti_b**	**Ti_c**	**C**	**O_a**	**O_b**	**O_c**	**CO_3^-**
Ti_3O_6	1.044	-0.013	-0.013			n.a		
1a	1.064	-0.030	-0.030	1.022	-0.733	-0.664	-0.664	-1.039
1b	1.034	-0.012	-0.011	1.002	-0.626	-0.743	-0.759	-1.126
2a	1.062	-0.019	-0.023	1.025	-0.716	-0.666	-0.661	-1.018
				0.998	-0.616	-0.766	-0.739	-1.123

S4. Isomer energies

Table.S2: ωB97XD/aug-cc-pVTZ relative electronic energies ΔE_{DFT} and ZPE-corrected relative energies $\Delta E_{0,DFT}$ of the **neutral** analogues of $[Ti_3O_6 (CO_2)_{n=1,2}]^-$. CCSD(T)/def2-TZVP relative electronic energies $\Delta E_{CCSD(T)}$ at the DFT minimum-energy geometry and ZPE-corrected relative electronic energies $\Delta E_{0,CCSD(T)/DFT}$ using the DFT ZPE-correction are also shown. All energies are given in kJ/mol

isomer	**label (Dixon et.al)**	ΔE_{DFT}[a]	$\Delta E_{0,DFT}$[b]	$\Delta E_{CCSD(T)}$[a]	$\Delta E_{0,CCSD(T)/DFT}$[b]
n=1					
1a	n.a	19.6	18.3	**0.0**	**0.0**
1b	3-4 Bc	28.4	25.2	8.9	7.0
1d	3-4 Ba	**0.0**	**0.0**	11.0	12.3

[a] Absolute energies: -3188.90843 a.u (**1a**, DFT), -3182.69384 a.u (**1a**, CCSD(T)),

-3188.90509 a.u (**1b**, DFT), -3182.69046 a.u (**1b**, CCSD(T)),

-3188.91590 a.u (**1d**, DFT), -3182.68965 a.u (**1d**, CCSD(T)),

[b] ZPE determined from ωB97XD/aug-cc-pVTZ harmonic vibrational frequencies.

Table.S3: ωB97XD/aug-cc-pVTZ relative electronic energies ΔE_{DFT} and ZPE-corrected relative energies $\Delta E_{0,DFT}$ of the lowest-energy minimum-energy isomers of $[Ti_3O_6 (CO_2)_2]^-$. CCSD(T)/def2-TZVP relative electronic energies $\Delta E_{CCSD(T)}$ at the DFT minimum-energy geometry and ZPE-corrected relative electronic energies $\Delta E_{0,CCSD(T)/DFT}$ using the DFT ZPE-correction are also shown. All energies are given in kJ/mol.

isomer	ΔE_{DFT}[a]	$\Delta E_{0,DFT}$[b]	$\Delta E_{CCSD(T)}$[a]	$\Delta E_{0,CCSD(T)/DFT}$[b]
n=2				
2a	**0.0**	**0.0**	**0.0**	**0.0**
2b	18.5	17.8	14.9	14.2
2c	24.5	24.2	41.8	41.6
2d	32.5	30.6	27.4	25.4
2e	39.2	38.8	75.4	75.1
2f	41.4	40.1	47.5	46.2
2g	48.1	41.1	173.2	166.2
2h	47.9	46.5	62.8	61.4
2i	67.4	66.3	110.4	109.3
2j	82.0	77.0	85.6	80.5
2k	93.6	92.9	98.1	97.5
2l	105.0	95.7	149.4	140.1
2m	119.2	118.0	212.6	211.4
2n	213.0	206.6	272.0	265.6

S5. Cartesian atomic coordinates of all calculated isomers

Table S4: Optimized Cartesian coordinates (Å) of the low-lying $[Ti_3O_6.(CO_2)_n]^-$ isomers (n=1,2) calculated with ωB97XD/aug-cc-pVTZ.

Isomer		x	y	z
1a	Ti	0.656893	-0.412899	1.592554
	Ti	-1.942848	0.040596	0.000000
	Ti	0.656893	-0.412899	-1.592554
	O	1.401944	-0.867598	-2.964180
	O	1.339432	-1.066624	-0.000000
	O	-1.257310	-0.672020	1.477161
	O	1.401944	-0.867598	2.964180
	O	-1.257310	-0.672020	-1.477161
	O	0.656893	1.569963	-1.116053
	C	0.047059	1.706780	0.000000
	O	-1.247861	1.885156	0.000000
	O	0.656893	1.569963	1.116053
1a-D2	Ti	0.718989	-0.418080	1.593425
	Ti	-1.924554	-0.016013	-0.000000
	Ti	0.718989	-0.418080	-1.593425
	O	1.467674	-0.869631	-2.965628
	O	1.393085	-1.080312	0.000000
	O	-1.196166	-0.673997	1.482950
	O	1.467674	-0.869631	2.965628
	O	-1.196166	-0.673997	-1.482950
	O	0.718989	1.552701	-1.115609
	C	0.101200	1.692596	-0.000000
	O	-1.182670	1.872413	-0.000000
	O	0.718989	1.552701	1.115609
	D	-3.532073	1.391555	-0.000000
	D	-3.901702	0.718676	-0.000000
1b	Ti	1.926826	-0.500417	-0.299269
	Ti	-0.606592	-1.268923	0.552455
	Ti	0.030153	1.583162	0.030137
	O	3.505320	-0.752946	0.021334
	O	0.712622	-1.997597	-0.410413
	O	1.361585	1.093658	-1.136124
	O	0.639434	0.067323	1.139497
	O	-1.646418	0.500683	-0.097076
	O	0.072679	3.091645	0.630682
	C	-2.761399	-0.250167	-0.306470
	O	-3.786253	0.189915	-0.744438
	O	-2.501483	-1.493066	0.047253
1b-D2	Ti	1.982218	-0.395049	-0.264622
	Ti	-0.607473	-1.312037	0.307194
	Ti	0.025407	1.568160	0.069267
	O	3.534460	-0.716705	0.128893

	O	0.738074	-1.843155	-0.706431
	O	1.495896	1.256171	-1.001266
	O	0.625138	0.034703	1.130454
	O	-1.519482	0.388925	-0.469123
	O	-0.115256	3.019194	0.788849
	C	-2.770015	-0.171337	-0.308646
	O	-3.780558	0.405821	-0.595176
	O	-2.622610	-1.376179	0.181803
	D	-0.757532	-2.868723	1.683684
	D	-0.271021	-2.397091	2.043717
1c	Ti	-1.770986	-0.982807	-0.081115
	Ti	-1.287389	1.640100	0.321034
	Ti	0.919320	0.058022	-0.303703
	O	-2.650518	-2.254809	0.427895
	O	-2.612711	0.711815	-0.458906
	O	-0.133604	-1.178224	-1.045570
	O	-0.671681	0.119096	1.152836
	O	0.280598	1.765616	-0.618638
	O	2.198132	-0.348614	1.090321
	C	3.206867	-0.317311	0.216285
	O	2.695671	-0.054529	-0.998629
	O	4.371366	-0.489483	0.463885
1d	Ti	0.354865	0.107221	1.589660
	Ti	-1.847590	0.690606	-0.000000
	Ti	0.354865	0.107221	-1.589660
	O	-1.531060	-0.134776	1.578155
	O	0.917248	-1.917732	1.142569
	O	0.917248	0.803919	2.930699
	O	-1.531060	-0.134776	-1.578155
	O	0.917248	0.803919	-2.930699
	O	0.917248	-1.917732	-1.142569
	C	1.239103	-1.477370	0.000000
	O	1.743480	-0.251093	0.000000
	O	-0.150560	1.367417	-0.000000
1e	Ti	1.222410	-1.399769	-0.043028
	Ti	1.222410	1.399769	-0.043028
	Ti	-1.200514	0.000000	-0.175592
	O	0.267256	0.000000	1.029654
	O	2.284185	-0.000000	-0.658064
	O	1.894844	2.729813	0.620773
	O	1.894844	-2.729813	0.620773
	O	-0.527698	-1.439028	-0.917989
	O	-0.527698	1.439028	-0.917989
	C	-3.562425	0.000000	0.453117
	O	-3.321163	0.000000	-0.762395
	O	-2.714594	0.000000	1.364929
1f	Ti	0.997345	0.788764	1.403082
	Ti	-0.600454	-1.024079	0.000000
	Ti	0.997345	0.788764	-1.403082
	O	0.997345	1.730171	-2.734645

	O	2.173963	1.121648	-0.000000
	O	-0.447813	0.860776	-0.000000
	O	0.401827	-1.074817	1.444461
	O	0.401827	-1.074817	-1.444461
	O	0.997345	1.730171	2.734645
	C	-2.912387	-1.472840	0.000000
	O	-2.091859	-2.429624	0.000000
	O	-4.082494	-1.280863	0.000000
2a	Ti	0.363085	1.738179	-0.022090
	Ti	0.679669	-1.592185	0.216930
	Ti	-2.038259	-0.291691	-0.636957
	O	0.864441	3.263336	-0.169311
	O	1.588076	0.170100	-0.290857
	O	-1.104460	1.277859	-1.011040
	O	-1.983229	-0.176801	1.381653
	O	-0.741712	-1.723288	-0.818168
	O	-3.485185	-0.486900	-1.336924
	C	2.783677	-0.475292	-0.556209
	O	3.769378	0.098071	-0.914594
	O	2.595142	-1.751204	-0.332469
	C	-0.768433	-0.017974	1.757783
	O	-0.242042	1.153832	1.796971
	O	-0.034205	-1.054388	2.009382
2a-D2	Ti	0.292832	1.799661	0.039423
	Ti	0.741453	-1.589325	0.147932
	Ti	-2.029582	-0.288403	-0.662467
	O	0.753152	3.342105	-0.062627
	O	1.557653	0.271879	-0.243090
	O	-1.146432	1.318735	-0.985263
	O	-1.992258	-0.233145	1.351106
	O	-0.684690	-1.675028	-0.876466
	O	-3.467004	-0.509522	-1.375928
	C	2.762369	-0.297273	-0.596101
	O	3.710061	0.339746	-0.952172
	O	2.644049	-1.595488	-0.454404
	C	-0.784720	-0.044060	1.746802
	O	-0.310175	1.148863	1.830736
	O	-0.018610	-1.055326	1.966142
	D	1.054047	-3.636305	0.692777
	D	0.610626	-3.420754	1.271200
2b	Ti	-1.402867	-0.169791	0.338281
	Ti	1.039363	-1.256387	-0.576252
	Ti	0.858378	1.594262	0.005765
	O	-3.113749	-0.488674	1.107297
	O	-0.425302	-1.730638	0.416063
	O	-0.593232	1.232807	1.138679
	O	0.073669	0.244075	-1.142431
	O	2.326667	0.277612	0.198689
	O	1.062571	3.096607	-0.554106
	C	3.340889	-0.633824	0.279534
	O	4.430424	-0.376005	0.697554

	O	2.889886	-1.790086	-0.164663
	C	-3.735318	-0.254444	-0.062745
	O	-2.797730	0.056225	-0.965350
	O	-4.918283	-0.317954	-0.255755
2c	Ti	-1.464895	-0.030387	-0.279266
	Ti	-0.001343	2.168161	0.451412
	Ti	1.466075	-0.028286	-0.277947
	O	-3.055806	-0.774488	-1.004815
	O	-1.551335	1.801306	-0.456206
	O	0.001541	-0.690756	-1.147614
	O	-0.000448	0.493100	1.116324
	O	1.550353	1.803742	-0.454173
	O	3.057553	-0.771116	-1.003734
	C	-3.420491	-1.283086	0.187672
	O	-2.464221	-0.966090	1.068205
	O	-4.423272	-1.901416	0.411804
	C	3.420440	-1.283312	0.187743
	O	4.422122	-1.903635	0.411253
	O	2.463999	-0.966943	1.068349
2d	Ti	-1.534432	-1.349231	0.065669
	Ti	0.083113	1.172001	0.485455
	Ti	1.266889	-1.412798	-0.313338
	O	-2.583501	-2.306994	0.841123
	O	-1.896696	0.525806	-0.347516
	O	-0.269187	-2.145068	-1.037105
	O	0.042811	-0.642225	1.065796
	O	1.620196	0.539341	-0.714393
	O	2.425027	-2.423874	0.180295
	C	-2.239024	1.838433	-0.393539
	O	-3.289564	2.240417	-0.800353
	O	-1.224571	2.554157	0.060148
	C	2.504142	1.429410	-0.075397
	O	1.837900	2.046582	0.857943
	O	3.645931	1.533554	-0.408148
2e	Ti	-0.346440	1.485635	-0.490685
	Ti	-0.764220	-1.494355	-0.414672
	Ti	1.918058	-0.699877	-0.040013
	O	-0.704786	2.681719	-1.493627
	O	-1.876453	0.300465	-0.059177
	O	1.703169	1.454734	0.003421
	O	0.338720	-0.210083	-1.264163
	O	0.719725	-2.112814	0.384549
	O	3.288651	-1.218180	-0.706485
	C	-2.919064	-0.449992	0.398065
	O	-3.945504	0.015060	0.799504
	O	-2.583590	-1.721840	0.306270
	C	1.285722	1.251039	1.246209
	O	1.872861	0.324666	1.868662
	O	0.191869	1.834129	1.527608
2f	Ti	1.034812	-0.125925	0.196037
	Ti	-1.726445	0.728934	-0.690407

	Ti	-1.296042	-1.795105	0.329125
	O	2.786413	0.379794	0.764577
	O	0.080629	1.586586	0.069783
	O	0.298453	-1.245484	1.316678
	O	-0.465875	-0.657169	-1.050519
	O	-2.675122	-0.487172	0.239195
	O	-1.648185	-3.350444	0.030624
	C	-0.579899	2.775998	0.256416
	O	-0.074369	3.741829	0.740874
	O	-1.808197	2.628739	-0.191886
	C	3.354023	-0.277848	-0.257127
	O	2.364531	-0.836716	-0.973417
	O	4.527234	-0.355312	-0.490948
2g	Ti	1.339208	-0.209513	-0.348335
	Ti	-1.472095	-0.357518	-0.014001
	Ti	-0.311707	2.126530	-0.007138
	O	2.919605	-1.056004	-0.962786
	O	-0.155744	-1.134588	-0.966222
	O	1.271892	1.497878	-0.855820
	O	-0.193717	0.445905	1.024970
	O	-1.869721	1.202981	-0.717292
	O	-0.422075	3.581167	0.701572
	C	-3.362184	-1.813103	0.027142
	O	-2.831965	-1.354418	1.087423
	O	-4.265983	-2.519498	-0.271562
	C	3.342964	-1.286243	0.296898
	O	4.360904	-1.841252	0.602867
	O	2.423852	-0.786284	1.129871
2h	Ti	0.419048	1.655328	0.282597
	Ti	0.700604	-1.299576	0.028871
	Ti	-2.065528	0.023962	-0.697882
	O	0.804353	3.038305	1.019517
	O	1.791206	0.407301	-0.451770
	O	-1.146155	1.661572	-0.634005
	O	-0.042130	0.054156	1.488345
	O	-0.683002	-1.244574	-1.101053
	O	-3.406209	-0.009739	-1.599413
	C	2.938731	-0.346488	-0.629742
	O	3.989187	0.136787	-0.935630
	O	2.633487	-1.598550	-0.405625
	C	-1.014859	-0.873320	1.564298
	O	-0.576059	-2.045681	1.678905
	O	-2.206424	-0.528932	1.302450
2i	Ti	1.909295	0.083380	0.631582
	Ti	0.684422	-1.999391	-0.697046
	Ti	-1.143036	0.010279	-0.167634
	O	2.760056	0.001214	1.994244
	O	2.304594	-1.298037	-0.682337
	O	0.165869	1.373590	0.113267
	O	0.218038	-1.109665	0.834082
	O	-0.739008	-1.078040	-1.528209

	O	-2.818461	0.829240	-0.531892
	C	-3.419280	0.179052	0.480304
	O	-2.485525	-0.576225	1.072084
	O	-4.575111	0.257719	0.786925
	C	1.061301	2.245365	-0.507915
	O	2.261916	1.821972	-0.274265
	O	0.686742	3.200683	-1.122172
2j	Ti	-1.725432	-0.761587	-0.787115
	Ti	0.455350	0.988063	-0.674422
	Ti	0.463694	-1.592881	0.738784
	O	-3.357641	-0.708536	-0.722307
	O	-0.750942	0.507880	-1.893094
	O	-0.777599	-2.333859	-0.405101
	O	-0.647550	0.028545	0.704377
	O	1.830734	-0.514426	-0.276762
	O	0.736984	-2.322565	2.165310
	C	2.886744	0.379603	-0.351895
	O	4.024134	0.046794	-0.169016
	O	2.406599	1.557552	-0.642050
	C	-1.244536	2.583433	1.271892
	O	-0.469641	2.785805	0.417544
	O	-2.009167	2.488149	2.118671
2k	Ti	-2.199166	-0.891126	0.144154
	Ti	0.546372	-1.364903	-0.114911
	Ti	-0.938882	1.641496	-0.073828
	O	-3.539569	-1.432815	-0.602320
	O	-0.837801	-2.202594	0.612962
	O	-2.237580	0.808817	0.926093
	O	-0.695876	-0.097909	-0.954474
	O	2.869012	0.922219	0.113810
	O	-1.510181	2.837146	-0.999919
	C	3.383951	-0.358349	-0.328671
	O	4.573164	-0.454903	-0.333250
	O	2.483283	-1.172795	-0.723145
	C	1.664523	0.980725	0.678595
	O	1.220778	-0.030030	1.290914
	O	1.015524	2.046046	0.529497
2l	Ti	0.776065	-1.804895	-0.667733
	Ti	-0.980681	0.347278	-0.173527
	Ti	1.927430	0.348128	0.726696
	O	0.721669	-3.421758	-0.600114
	O	-0.685319	-0.729634	-1.477167
	O	2.414747	-0.935869	-0.503344
	O	0.225051	-0.663325	0.894478
	O	0.683161	1.692303	-0.035581
	O	2.887600	0.581246	2.007745
	C	-0.054129	2.662327	-0.651147
	O	0.363829	3.746982	-0.924387
	O	-1.246051	2.156962	-0.863226
	C	-3.648943	-0.783694	0.587941
	O	-4.655074	-0.846151	1.215444

	O	-2.670048	0.061361	0.648608
2m	Ti	2.352138	-0.006008	-0.403880
	Ti	0.311703	-1.741441	0.297889
	Ti	0.056875	1.598629	0.235898
	O	3.881156	0.224078	0.092745
	O	1.777539	-1.854033	-0.684234
	O	1.403432	1.466421	-1.025516
	O	0.831376	-0.075972	0.981880
	O	0.243463	2.858088	1.227401
	O	-1.285067	-1.345518	-0.908513
	C	-2.970864	0.709201	-0.402261
	O	-1.856136	1.261782	-0.154822
	O	-3.937798	1.113460	-0.971031
	C	-2.029590	-1.390816	0.122742
	O	-3.087046	-0.601788	0.204792
	O	-1.702547	-2.126052	1.089692
2n	Ti	2.142691	-0.591390	-0.613044
	Ti	-0.431145	-1.188493	0.401449
	Ti	0.761356	1.668743	0.322861
	O	3.628681	-1.228473	-0.489639
	O	0.575883	-1.726900	-0.911907
	O	1.944880	1.231167	-1.008229
	O	1.060469	-0.144404	1.021252
	O	-1.071737	0.828039	0.007147
	O	1.069092	2.974247	1.227933
	C	-2.332079	1.007741	-0.379838
	O	-2.805924	2.055617	-0.695551
	O	-2.306115	-1.345037	-0.064298
	C	-3.096663	-0.352045	-0.370182
	O	-4.266078	-0.413094	-0.624531
	O	-0.558078	-2.417302	1.794355