Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Roles of Water Molecules in Trapping Carbon Dioxide Molecules inside the Interlayer Space of Graphene Oxides

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S1 Dependence of total energy of $C_{64}O_4(OH)_{16} \cdot 4H_2O$ on *k*-point meshes

k point mesh	Total energy (Hartree)
2 × 2	-4253.75783049
4 × 4	-4253.75777580
6 × 6	-4253.75777579
8 × 8	-4253.75777403
10× 10	-4253.75777962

The 10 × 10 k point mesh was used to optimise large super cell of graphene oxides models with and without carbon dioxide.

S2 Cartesian coordinates of optimised geometries in Figure 2. Tv corresponds to translation vectors in the unit cell.

(a)(i) Water dimer at the PBE/6-31G** level of theory

O	-3.04112800	0.54811900	0.00000000
H	-2.08580400	0.78331000	0.00000000
H	-3.51218100	1.39838200	0.00000000
H	0.17727000	0.52284800	0.77386200
O	-0.20830500	0.97089300	0.00000000
H	0.17727000	0.52284700	-0.77386200

(a)(ii) Water dimer at the B97D/6-31G** level of theory

O	-3.06490800	0.54723300	0.00000000
H	-2.11778800	0.77512500	0.00000000
H	-3.51891900	1.39795700	0.00000000
H	0.19446200	0.52407700	0.76581400
O	-0.18018800	0.97792900	0.00000000
H	0.19446200	0.52407700	-0.76581400

(b)(i) Water binding into a single graphene oxide layer at the PBE/6-31G** level of theory

C	3.09089194	0.51947045	-4.91797320
C	0.61103686	0.47859931	-5.31830765
C	1.87515360	2.68774472	-5.28883284
C	4.35681547	-0.22567816	-5.29185495
C	-0.65406469	2.68887742	-5.31112259
C	3.09313452	1.98474408	-5.31707989
C	1.82757369	-0.22438562	-5.30908230
C	0.60671416	1.94374223	-4.91780205
O	0.51528659	1.91585868	-3.43927005
O	3.01378160	0.54613547	-3.44125259
H	1.32315434	1.42957166	-3.12017927
H	3.86220401	0.96704610	-3.13265984
H	1.32572741	-0.46948099	-1.06085406
O	0.97853481	-0.83612093	-1.89285685
H	1.79434248	-0.94193360	-2.42912023
Tv	4.96361209	0.00000000	0.00000000
Tv	-2.48098605	4.31873788	0.00000000

(b) (ii) Water binding into a single graphene oxide layer at the B97D/6-31G** level of theory

C	3.04011797	0.43381990	-4.97873033
C	0.55516550	0.39136568	-5.38000355

C	1.82269433	2.60738788	-5.35058622
C	4.31032482	-0.31350374	-5.35435181
C	-0.71505921	2.60862585	-5.37333409
C	3.04179744	1.90399345	-5.37988495
C	1.77260362	-0.31225435	-5.37072332
C	0.54985845	1.86120019	-4.97721974
O	0.45372447	1.83643931	-3.49618327
O	2.96495174	0.46034610	-3.50035200
H	1.24814295	1.35416345	-3.16454095
H	3.80543014	0.87658287	-3.18875026
H	1.45994130	-0.41170889	-0.83611215
O	1.02336544	-0.81761831	-1.59929954
H	1.76348526	-0.96037529	-2.21589874
Tv	4.97401082	0.00000000	0.00000000
Tv	-2.48707042	4.32731695	0.00000000

(c)(i) Carbon dioxide binding into a single graphene oxide layer at the PBE/6-31G** level of theory

C	2.72069238	0.56809100	-5.05129295
C	0.24184255	0.52489495	-5.45177672
C	1.50462852	2.73767614	-5.42600607
C	3.98601052	-0.17910897	-5.42667092
C	-1.02343879	2.73788471	-5.43418352
C	2.72307262	2.03372224	-5.45173502
C	1.45805752	-0.17920982	-5.43342424
C	0.23895160	1.99068949	-5.05154124
O	0.17166235	1.95304848	-3.57040238
O	2.65932797	0.60673440	-3.57073998
H	1.02038432	1.51823442	-3.28531576
H	3.51401932	1.03551826	-3.29272274
C	1.38198534	-0.89400958	-1.33110662
O	0.36660516	-0.84199967	-1.93341834
O	2.37635305	-0.94640520	-0.69997921
Tv	4.96287212	0.00000000	0.00000000
Tv	-2.48143079	4.32259525	0.00000000

(c)(ii) Carbon dioxide binding into a single graphene oxide layer at the B97D/6-31G** level of theory

C	2.70393617	0.38927376	-5.30523060
C	0.21971592	0.34480031	-5.70740676
C	1.48752643	2.56334954	-5.68279594
C	3.97436168	-0.35913284	-5.68173436
C	-1.04955552	2.56338224	-5.69156600
C	2.70719412	1.85945326	-5.70814645
C	1.43729251	-0.35940104	-5.69163047
C	0.21726716	1.81471541	-5.30565260
O	0.15071000	1.78133002	-3.82235119
O	2.63434196	0.42395915	-3.82187753
H	0.98385558	1.33438888	-3.53568997
H	3.46581490	0.87267630	-3.53409693
C	1.25241266	-1.15246514	-1.00307550
O	0.27386415	-1.09383799	-1.65535381
O	2.21991875	-1.21269679	-0.33685805
Tv	4.97434517	0.00000000	0.00000000
Tv	-2.48664870	4.32911893	0.00000000

S3 Cartesian coordinates of optimised geometries in Figure 3. Tv corresponds to translation vectors in the unit cell. The optimised structures were obtained at the PBE/6-31G** level of theory.

(a) $C_{16}(OH)_2$,

C	1.31759366	-2.27921132	-0.07067845
C	-1.16433991	-2.25927037	-0.08005978
C	0.06157314	-0.09975531	-0.06483370

C	2.55448364	-2.97889942	-0.04709428
C	-2.38565012	-0.10051508	-0.07470569
C	2.70655983	-0.03258224	-5.06596163
C	0.22070801	-0.05298860	-5.07499852
C	1.48554096	2.12592237	-5.07122200
C	3.95194132	-0.75107965	-5.08794315
C	-1.03473392	2.12670720	-5.08181290
C	2.70957375	1.40593980	-5.09255649
C	1.45783651	-0.75219428	-5.09891540
C	0.22332812	1.40034330	-4.70127268
C	1.31987156	-0.82608531	-0.44501345
C	-1.16130687	-0.82059115	-0.05412216
C	0.08110919	-2.97764026	-0.05721576
O	0.17672061	1.44942966	-3.20325369
O	1.26394231	-0.78554615	-1.94332663
H	1.84617164	-1.50369404	-2.32318772
H	0.66302123	0.66522260	-2.81853563
Tv	4.96751715	0.00000000	0.00000000
Tv	-2.47688850	4.29787024	0.00000000

(b) $C_{16}(OH)_4$

C	1.30130671	-2.59717992	0.52393813
C	-1.18295976	-2.55263784	0.12896198
C	0.03479579	-0.38354462	0.52172227
C	2.51829071	-3.30029077	0.51176897
C	-2.40129614	-0.38497528	0.49703684
C	2.53583779	-0.46261698	-5.24319485
C	0.05553918	-0.50764137	-5.63720727
C	1.31659716	1.70466699	-5.61041589
C	3.80059811	-1.21165933	-5.61363448
C	-1.21137329	1.70627844	-5.63532444
C	2.53571696	1.00208991	-5.64739584
C	1.27237313	-1.21058103	-5.62418705
C	0.04826318	0.95849997	-5.23950156
C	1.29460604	-1.13147127	0.12697066
C	-1.18219741	-1.08766467	0.53352980
C	0.08236771	-3.30139847	0.49864574
O	-0.05468224	0.93641744	-3.76072373
O	2.47487864	-0.41193693	-3.76537821
O	-1.24966703	-2.50387962	-1.34886692
O	1.19423722	-1.15535244	-1.35211375
H	2.01401188	-1.60610638	-1.69226570
H	-0.42005024	-2.02166759	-1.62144361
H	0.76604087	0.49114946	-3.41675743
H	3.30531718	0.07340126	-3.49823918
Tv	4.96422510	0.00000000	0.00000000
Tv	-2.48269824	4.32258368	0.00000000

(c) $C_{16}(OH)_6$

C	1.05718966	-2.29541102	1.37503180
C	-1.43481782	-2.32582004	0.85940027
C	-0.18609115	-0.06703673	1.35884238
C	2.32689657	-3.02117377	1.38727895
C	-2.70061149	-0.06536894	0.98877249
C	2.59775426	-1.64299502	-5.65150195
C	0.08334400	-1.67248660	-6.03302341
C	1.34386983	0.53833928	-6.01469238
C	3.88712788	-2.37827957	-6.04140088
C	-1.22972530	0.54545771	-6.04500570
C	2.57268608	-0.16238295	-6.01962554
O	2.58180467	-1.71742605	-4.17572859
H	0.66326349	-2.02760143	-3.12162861
C	1.31223323	-2.37324061	-6.03270509
O	0.41590753	-2.82377014	-2.60240891
H	-0.78902853	-2.28075056	-1.07033074

C	0.05567538	-0.19485229	-5.65068404
O	-0.01623958	-0.25465543	-4.17073191
H	-0.01414857	0.69020340	-3.85973827
C	1.01707705	-0.84573920	0.88484556
O	0.74209126	-1.03758972	-0.53217540
H	3.33538703	-1.14648048	-3.86461504
C	-1.41863058	-0.79856825	0.97742152
O	-1.93816847	-0.21918791	-0.23653005
H	-1.49615935	1.53305333	-1.86315750
C	-0.14770024	-2.95790909	1.33183992
O	-1.54440162	-2.68128765	-0.55764181
H	-4.20927540	-0.11736841	-0.90622481
Tv	5.02576143	0.00000000	0.00000000
Tv	-2.55337727	4.33012935	0.00000000

(d) $C_{32}(OH)_2$

C	0.90579046	-3.19895957	0.19556554
C	-1.56597455	-3.19082067	-0.31875934
C	-0.34051736	-1.04262228	0.19376839
C	2.14555692	-3.90689088	0.25748065
C	-2.79702357	-1.03852706	0.08531342
C	3.29133107	1.97109927	-5.04307416
C	0.81225069	1.96364943	-4.96799173
C	2.04464153	4.11397729	-5.01734052
C	4.52594813	1.25528189	-5.01932631
C	-0.43262710	4.11750843	-4.96549370
C	3.28670362	3.39883550	-5.01896587
C	2.05253043	1.25466675	-5.02917402
C	0.81446066	3.40187735	-4.98468600
C	0.90588988	-1.76046003	0.21593587
C	-1.56752385	-1.73792849	0.08175049
C	-0.30814205	-3.91651025	0.08232246
O	-1.62242313	-3.21768682	-1.78553951
H	-0.77116894	-2.83953858	-2.13660710
C	5.86406904	-3.19203142	0.14797642
C	3.38467924	-3.19069839	0.27000471
C	4.62078182	-1.04174835	0.14843005
C	7.07889479	-3.91842017	0.07464430
C	2.13828754	-1.04818276	0.24438110
C	8.24073467	1.97045911	-4.49391462
C	5.76828489	1.97015184	-4.93738929
C	7.00905285	4.12181694	-4.87612174
C	9.50081233	1.24666371	-4.86724490
C	4.52531844	4.11926671	-4.93624815
C	8.24044600	3.42284691	-4.86673699
C	6.98492720	1.24368942	-4.86865912
C	5.75946226	3.39849614	-4.88935833
C	5.85548221	-1.76208527	0.09816066
C	3.38168877	-1.76314222	0.24218871
C	4.62044970	-3.90570036	0.24208243
O	8.21046756	1.92237047	-2.96558697
H	8.73965270	2.68285200	-2.64828917
Tv	9.90429842	0.00000000	0.00000000
Tv	-2.48150863	4.29208284	0.00000000

(e) $C_{32}(OH)_4$

C	0.84062297	-3.08169216	0.21795392
C	-1.62598882	-3.06564496	-0.35928657
C	-0.40379537	-0.92589035	0.23558296
C	2.08817307	-3.79087192	0.28777957
C	-2.84284481	-0.90615821	-0.01228691
C	3.31638061	1.71966187	-5.00948766
C	0.84061350	1.69386961	-4.95373239
C	2.09778046	3.88538234	-4.94518901
C	4.55612862	0.99888620	-5.00887567

C	-0.42434507	3.88063035	-4.95862806
C	3.30828647	3.15703708	-5.01044680
C	2.07667723	0.99910281	-5.01407852
C	0.83828791	3.15406604	-4.56838285
C	0.84070104	-1.64487302	0.27474597
C	-1.63139726	-1.61395944	0.07536909
C	-0.36702427	-3.80293333	0.03645891
O	0.75806953	3.18997816	-3.08397175
O	-1.69577151	-3.02382556	-1.83548388
H	-0.81137410	-2.73729727	-2.19300382
H	1.63252074	2.88714237	-2.71005083
C	5.79156148	-3.10969105	0.09411965
C	3.31918625	-3.08029406	0.27799449
C	4.52615755	-0.92044423	0.06207377
C	7.00154869	-3.81852995	0.01324989
C	2.07191069	-0.93333784	0.30293594
C	8.27150974	1.72531486	-4.55577268
C	5.80489332	1.72312915	-5.00360132
C	7.03515829	3.87879794	-4.99546968
C	9.53533576	0.99673765	-4.94058973
C	4.55696547	3.88174809	-4.99835710
C	8.27262178	3.18366403	-4.94666796
C	7.01379783	0.99390211	-4.93756098
C	5.79697990	3.15993610	-4.99103041
C	5.77740695	-1.66130025	-0.35311518
C	3.31970026	-1.64303068	0.23545544
C	4.56361729	-3.79889498	0.25024103
O	8.23282455	1.70069036	-3.06777803
O	5.68700321	-1.72281044	-1.82798756
H	6.50401905	-2.20638514	-2.12104092
H	9.03909107	2.21416990	-2.78772747
Tv	9.89646110	0.00000000	0.00000000
Tv	-2.48520346	4.30015054	0.00000000

(f) $C_{32}(OH)_6$

C	1.27509848	-2.55013560	0.39409271
C	-1.19859700	-2.51436379	-0.02276380
C	0.01109734	-0.35851430	0.42341991
C	2.52016254	-3.24416966	0.45459028
C	-2.42861230	-0.35620185	0.37123080
C	2.52424784	-0.38749553	-5.49496524
C	0.03592166	-0.41047501	-5.45741583
C	1.29041961	1.77474716	-5.46358024
C	3.76575855	-1.11985507	-5.49900595
C	-1.22842023	1.78132409	-5.48749476
C	2.51262902	1.05568626	-5.49191860
C	1.28078909	-1.10442954	-5.51851235
C	0.03119608	1.05187628	-5.10300864
C	1.27026468	-1.08821481	0.03884325
C	-1.20207060	-1.05437390	0.40093891
C	0.06664577	-3.25841538	0.35350410
O	-0.07685545	1.09880851	-3.55407868
O	-1.23420815	-2.44384285	-1.48934577
O	1.16205269	-1.04350762	-1.51153283
H	1.88338096	-1.60280173	-1.88475361
H	-0.41997944	-1.92601102	-1.73930664
H	0.64466484	0.54151682	-3.17779461
C	6.24611008	-2.55997506	0.39062157
C	3.76350416	-2.52748021	0.43047780
C	4.97589114	-0.35611501	0.37541180
C	7.46040538	-3.26745591	0.33714960
C	2.52943149	-0.36539447	0.39881947
C	7.49163428	-0.37427591	-5.03836401
C	5.00684082	-0.41990922	-5.45250879
C	6.26108560	1.78374362	-5.43141532

C	8.75642892	-1.11840266	-5.41592455
C	3.73684774	1.78401410	-5.43732973
C	7.48744520	1.08546316	-5.46203796
C	6.22123314	-1.12726466	-5.39839861
C	4.99611495	1.03889410	-5.05519727
C	6.23561729	-1.10117951	-0.00529502
C	3.75169056	-1.08439518	0.42732531
C	5.00485923	-3.26005455	0.43511576
O	4.87308073	0.99166309	-3.60289682
O	7.45909645	-0.30443415	-3.57143411
O	6.11487168	-1.14806597	-1.45840637
H	6.92708565	-1.58344241	-1.82828001
H	5.68432337	0.55711492	-3.23038480
H	8.27414339	0.21381017	-3.32450272
Tv	9.92916673	0.00000000	0.00000000
Tv	-2.48804277	4.31131523	0.00000000

S4 Cartesian coordinates of optimized geometries in Figure 4. Tv corresponds to translation vectors in the unit cell. The optimised structures were obtained at the PBE/6-31G level of theory.**

$C_{64}O_4(OH)_{16}$•$4H_2O$

C	1.03999507	-2.31835347	1.40403407
C	-1.45193557	-2.34871944	0.88795628
C	-0.20277640	-0.08972099	1.38885978
C	2.30993485	-3.04404226	1.41709301
C	-2.71728444	-0.08829176	1.01829109
C	2.55651582	-1.63723099	-5.62996127
C	0.04206250	-1.66695903	-6.01200952
C	1.30277626	0.54410189	-5.99179185
C	3.84560513	-2.37271060	-6.02002185
C	-1.27067011	0.55105502	-6.02371570
C	2.53157862	-0.15656734	-5.99784488
O	2.53989713	-1.71048449	-4.15474096
H	0.63018424	-2.02994372	-3.09518926
C	1.27094807	-2.36759489	-6.01187034
O	0.40512550	-2.82736316	-2.56772192
H	-0.80819816	-2.30610304	-1.04477342
C	0.01428049	-0.18959803	-5.62868338
O	-0.05976456	-0.25304169	-4.14892564
H	-0.07190056	0.68999655	-3.83356469
C	1.00047609	-0.86827046	0.91491675
O	0.72429715	-1.05783127	-0.50207104
H	3.29375409	-1.13972286	-3.84372248
C	-1.43536595	-0.82135065	1.00617980
O	-1.95480109	-0.24201789	-0.20728833
H	-1.50230061	1.55928969	-1.82943897
C	-0.16481466	-2.98091994	1.36009464
O	-1.56325934	-2.70431281	-0.52953480
H	-4.23034476	-0.13597586	-0.87418630
C	6.06575390	-2.31842975	1.40360954
C	3.57381118	-2.34880769	0.88755873
C	4.82295459	-0.08982030	1.38836519
C	7.33566109	-3.04414636	1.41689542
C	2.30850021	-0.08837000	1.01794163
C	7.58226151	-1.63736751	-5.63073979
C	5.06781247	-1.66702434	-6.01248708
C	6.32863897	0.54406730	-5.99254614
C	8.87147307	-2.37271797	-6.02046615
C	3.75507603	0.55097166	-6.02426426
C	7.55745021	-0.15658462	-5.99815717
O	7.56529722	-1.71108167	-4.15542004

H	5.65591941	-2.03108930	-3.09606209
C	6.29669703	-2.36768248	-6.01273589
O	5.43012317	-2.82808796	-2.56827493
H	4.21708711	-2.30685323	-1.04556968
C	5.04013926	-0.18963363	-5.62946369
O	4.96644525	-0.25276751	-4.14962527
H	4.95460274	0.69047913	-3.83478673
C	6.02632454	-0.86829069	0.91465941
O	5.75048593	-1.05771381	-0.50241462
H	8.31911715	-1.14046876	-3.84404154
C	3.59041430	-0.82144106	1.00558833
O	3.07073489	-0.24222707	-0.20781034
H	3.52319159	1.55824530	-1.83029249
C	4.86098047	-2.98098833	1.35955720
O	3.46211208	-2.70464373	-0.52987113
H	0.79476444	-0.13612621	-0.87399643
C	-1.51267028	2.01214743	1.40314921
C	-4.00457741	1.98172556	0.88724652
C	-2.75550338	4.24053136	1.38853894
C	-0.24273907	1.28649581	1.41644210
C	-5.26996187	4.24211744	1.01780626
C	0.00388169	2.69341986	-5.63088816
C	-2.51062726	2.66331496	-6.01280328
C	-1.24991476	4.87457244	-5.99320275
C	1.29290871	1.95753986	-6.02016861
C	-3.82337037	4.88154364	-6.02503065
C	-0.02109947	4.17389193	-5.99962675
O	-0.01237484	2.62155506	-4.15570893
H	-1.91834004	2.29950924	-3.09718981
C	-1.28173253	1.96267260	-6.01194007
O	-2.14261053	1.50267009	-2.56847087
H	-3.36024918	2.02458890	-1.04494685
C	-2.53836033	4.14085042	-5.63018115
O	-2.61209007	4.07809958	-4.15033809
H	-2.62137675	5.02152409	-3.83576716
C	-1.55222753	3.46220354	0.91413281
O	-1.82837407	3.27291966	-0.50293010
H	0.74180886	3.19229395	-3.84537760
C	-3.98805095	3.50906043	1.00552295
O	-4.50743207	4.08878422	-0.20783732
H	-4.05769637	5.88599052	-1.83051108
C	-2.71752719	1.34961834	1.35968764
O	-4.11550294	1.62609883	-0.53034552
H	-6.78302456	4.19493327	-0.87477249
C	3.51309050	2.01207417	1.40274868
C	1.02117536	1.98163531	0.88684198
C	2.27021967	4.24043105	1.38802534
C	4.78298710	1.28638974	1.41626951
C	-0.24418116	4.24203718	1.01742879
C	5.02962745	2.69328532	-5.63168968
C	2.51512075	2.66324864	-6.01329084
C	3.77594697	4.87454084	-5.99396706
C	6.31877967	1.95752947	-6.02062290
C	1.20237370	4.88145930	-6.02555221
C	5.00477120	4.17387763	-5.99996704
O	5.01302735	2.62096584	-4.15642500
H	3.10712522	2.29854188	-3.09804445
C	3.74401649	1.96258600	-6.01283162
O	2.88251817	1.50200421	-2.56901759
H	1.66513399	2.02372865	-1.04573578
C	2.48750444	4.14081081	-5.63096244
O	2.41415371	4.07834973	-4.15103862
H	2.40535145	5.02196852	-3.83696259
C	3.47362487	3.46218933	0.91389447
O	3.19782269	3.27305311	-0.50326366

H	5.76726792	3.19143595	-3.84573133
C	1.03773037	3.50897000	1.00490548
O	0.51809398	4.08855803	-0.20838934
H	0.96764452	5.88462127	-1.83133875
C	2.30826689	1.34955797	1.35917018
O	0.90990249	1.62574687	-0.53069575
H	-1.75793229	4.19475291	-0.87461665
Tv	10.05158362	0.00000000	0.00000000
Tv	-5.10551341	8.66074421	0.00000000

S5 Cartesian coordinates of optimized geometries in Figure 5. Tv corresponds to translation vectors in the unit cell. The optimised structures were obtained at the PBE/6-31G level of theory.**

(i) $C_{64}O_4(OH)_{16}$

C	1.26177383	-2.69579356	0.98340288
C	-1.22580899	-2.72228070	0.48490598
C	0.01707706	-0.46571548	0.94842669
C	2.53212895	-3.42129508	0.97427981
C	-2.50365072	-0.46512178	0.59464859
C	2.34655415	-0.69060821	-4.83952989
C	-0.17062241	-0.71835791	-5.22156804
C	1.08875707	1.49211743	-5.19776597
C	3.63550283	-1.42494239	-5.23322630
C	-1.48641244	1.50017988	-5.22617680
C	2.31881785	0.79138744	-5.20142044
O	2.35054001	-0.77064615	-3.36471598
C	1.05856787	-1.41869800	-5.21423915
H	-0.46552905	-2.54911836	-1.29989280
C	-0.20072866	0.75904925	-4.83443034
O	-0.27316414	0.68271091	-3.35641484
H	-0.24991347	1.61650326	-3.01450760
C	1.21647661	-1.24995794	0.47601703
O	0.95724618	-1.47791724	-0.94746549
H	3.18380330	-0.30538055	-3.07692590
C	-1.21973371	-1.19818026	0.59794812
O	-1.73992070	-0.61736146	-0.61918866
C	0.05577112	-3.35982396	0.96422327
O	-1.24273075	-3.05539240	-0.93945418
H	-3.98498805	-0.59733169	-1.39757520
C	6.29071234	-2.69579665	0.98322314
C	3.80306856	-2.72235921	0.48511181
C	5.04602710	-0.46572648	0.94807132
C	7.56105872	-3.42131204	0.97393731
C	2.52527105	-0.46518008	0.59479948
C	7.37547111	-0.69063250	-4.83931305
C	4.85829141	-0.71836230	-5.22152724
C	6.11764392	1.49208527	-5.19747435
C	8.66439562	-1.42496018	-5.23307584
C	3.54250057	1.50017788	-5.22617702
C	7.34770565	0.79136665	-5.20116882
O	7.37959475	-0.77084552	-3.36448313
C	6.08748342	-1.41869528	-5.21409589
H	4.56285055	-2.54930793	-1.30004192
C	4.82812764	0.75900278	-4.83427495
O	4.75535158	0.68247352	-3.35626349
H	4.77903473	1.61612302	-3.01405182
C	6.24540043	-1.24997549	0.47570650
O	5.98626725	-1.47829366	-0.94776397
H	8.21309020	-0.30606788	-3.07667216
C	3.80918094	-1.19825225	0.59791620
O	3.28879393	-0.61761735	-0.61917970

C	5.08473026	-3.35985122	0.96427292
O	3.78596505	-3.05576039	-0.93923150
H	1.04338876	-0.59660989	-1.39673389
C	-1.29516439	1.63457943	0.98400336
C	-3.78272667	1.60821248	0.48546070
C	-2.53985340	3.86489019	0.94901743
C	-0.02481041	0.90907276	0.97452650
C	-5.06060969	3.86538180	0.59523650
C	-0.21036693	3.63981783	-4.83881048
C	-2.72754941	3.61221108	-5.22083226
C	-1.46817998	5.82256689	-5.19716521
C	1.07857696	2.90564121	-5.23286827
C	-4.04334811	5.83062096	-5.22558194
C	-0.23811465	5.12185145	-5.20048692
O	-0.20639779	3.55927420	-3.36400464
C	-1.49836094	2.91187472	-5.21387433
H	-3.02229452	1.78171013	-1.29914348
C	-2.75766920	5.08959264	-4.83359106
O	-2.83013492	5.01327619	-3.35561829
H	-2.80691001	5.94700828	-3.01360662
C	-1.34046718	3.08051356	0.47682225
O	-1.59973063	2.85264558	-0.94666636
H	0.62678855	4.02449762	-3.07595463
C	-3.77666832	3.13233563	0.59867993
O	-4.29688456	3.71287383	-0.61855857
C	-2.50113624	0.97050024	0.96447215
O	-3.79956986	1.27536271	-0.93895738
H	-6.54194974	3.73332468	-1.39662260
C	3.73377312	1.63457742	0.98382269
C	1.24614913	1.60813380	0.48565841
C	2.48909597	3.86487936	0.94865098
C	5.00412020	0.90905518	0.97418999
C	-0.03168800	3.86532317	0.59539037
C	4.81855086	3.63979401	-4.83858853
C	2.30136417	3.61220682	-5.22078340
C	3.56070775	5.82253542	-5.19687047
C	6.10746984	2.90562374	-5.23272079
C	0.98556512	5.83061762	-5.22558834
C	4.79077198	5.12183110	-5.20023025
O	4.82266375	3.55907535	-3.36376551
C	3.53055432	2.91187857	-5.21372291
H	2.00608917	1.78148859	-1.29930300
C	2.27118597	5.08954890	-4.83343339
O	2.19837526	5.01305635	-3.35546318
H	2.22203104	5.94665147	-3.01316459
C	3.68845683	3.08049787	0.47650388
O	3.42929987	2.85226009	-0.94697161
H	5.65609282	4.02379897	-3.07570365
C	1.25224657	3.13226351	0.59863995
O	0.73182208	3.71261995	-0.61855162
C	2.52782109	0.97047369	0.96451477
O	1.22911514	1.27499082	-0.93873845
H	-1.51359017	3.73406647	-1.39575647
Tv	10.05778989	0.00000000	0.00000000
Tv	-5.11387627	8.66101031	0.00000000

(ii) $C_{64}O_4(OH)_{16} \cdot H_2O$

C	0.09630824	-1.86682098	1.30748241
C	-2.39383357	-1.89559306	0.78014273
C	-1.14895753	0.36181100	1.23499109
C	1.36650358	-2.59190065	1.29016692
C	-3.66779843	0.36367967	0.87245288
C	4.17167897	-2.39924781	-5.09983328
C	1.64701907	-2.42656026	-5.43898796
C	2.90703166	-0.21697107	-5.45039685

C	5.45873122	-3.12964416	-5.52253400
C	0.33238624	-0.20832609	-5.44356145
C	4.13734237	-0.91852114	-5.46356004
O	4.21185204	-2.47398040	-3.61361940
C	2.87500879	-3.12794363	-5.44435836
H	-1.70595867	-1.75504861	-1.06004569
C	1.62361108	-0.94721038	-5.06362769
O	1.58088514	-1.00306900	-3.58512977
H	1.60969899	-0.05621856	-3.28700626
C	0.05509277	-0.42715805	0.77678785
O	-0.19487263	-0.71822986	-0.62853501
H	5.04671529	-1.98312379	-3.35706290
C	-2.38378383	-0.36932278	0.87473080
O	-2.90555351	0.20587569	-0.34592426
H	-1.38907921	1.60994879	-1.65339939
C	-1.11076944	-2.52819319	1.27445954
O	-2.45699090	-2.24835723	-0.63815732
H	-5.23087924	0.32683283	-1.02547519
C	5.12391094	-1.85904161	1.26575365
C	2.63153889	-1.89149750	0.77424186
C	3.88346168	0.36303097	1.24833781
C	6.39489410	-2.58225832	1.29235188
C	1.36187340	0.36531967	0.89957609
C	9.19365898	-2.40136780	-5.05204888
C	6.68225686	-2.42539755	-5.48335376
C	7.93940072	-0.21502152	-5.42677767
C	10.48412839	-3.13450146	-5.44415249
C	5.36008817	-0.21071007	-5.50127049
C	9.16843147	-0.91746968	-5.41374990
O	9.18958271	-2.49297513	-3.56990048
C	7.91089761	-3.12611479	-5.45271573
H	3.30024191	-1.71286258	-1.07190505
C	6.64384492	-0.95124687	-5.09268339
O	6.55578552	-1.02805597	-3.61664722
H	6.50287572	-0.07829642	-3.32078034
C	5.07912199	-0.41597610	0.75910814
O	4.79828364	-0.60156695	-0.66814999
H	10.01062716	-2.00950220	-3.28050094
C	2.64473972	-0.36714490	0.88877102
O	2.12099937	0.23136530	-0.31847925
C	3.91688309	-2.52150944	1.24914145
O	2.57218159	-2.23488361	-0.64733952
H	-0.22908172	0.12474521	-1.15213885
C	-2.45989627	2.46303098	1.27881959
C	-4.95002872	2.43883796	0.76855945
C	-3.70193847	4.69359217	1.25888530
C	-1.18885479	1.73613399	1.29282687
C	-6.22124751	4.69638025	0.91501514
C	1.61075366	1.93558712	-5.08551053
C	-0.90987869	1.91038513	-5.43978066
C	0.36288757	4.11790046	-5.50931278
C	2.89689350	1.19642894	-5.47686644
C	-2.22189730	4.12115639	-5.45062176
C	1.59104118	3.41373700	-5.47422010
O	1.61490309	1.86720308	-3.59690497
H	-0.56616363	1.65301854	-2.91078335
C	0.31945932	1.20460631	-5.44322895
O	-1.23123233	1.07567084	-2.46567582
H	-4.31215317	2.64204288	-1.09361145
C	-0.91800702	3.40098702	-5.09251054
O	-0.89124509	3.43264298	-3.62535649
H	-0.84956582	4.39892903	-3.37558906
C	-2.50073926	3.91336422	0.78839236
O	-2.75765874	3.71481847	-0.64420625
H	2.43477095	2.36476533	-3.31458788

C	-4.93862021	3.96382481	0.89619205
O	-5.46844014	4.55284415	-0.31164489
C	-3.66432691	1.79935784	1.23146052
O	-5.02286446	2.10915614	-0.65614439
H	-7.77477806	4.66451430	-0.96904108
C	2.57730270	2.46357257	1.30811167
C	0.09375368	2.44603476	0.84977404
C	1.33018498	4.70317814	1.30318368
C	3.84550528	1.73847659	1.28096239
C	-1.19262215	4.69778337	0.91749370
C	6.62611233	1.91891255	-5.06130552
C	4.11951650	1.90407903	-5.47071021
C	5.38776338	4.11269992	-5.41148084
C	7.92613356	1.19947581	-5.45037821
C	2.81424944	4.12285293	-5.47261209
C	6.61593667	3.40893114	-5.40231994
O	6.54243770	1.78616830	-3.59414654
C	5.34672135	1.20220975	-5.48971715
H	0.85380039	2.68848159	-0.93499573
C	4.09393988	3.37921131	-5.06959643
O	4.01055881	3.31149125	-3.59026575
H	4.04540674	4.25887152	-3.28752790
C	2.52616790	3.91474022	0.81694698
O	2.24988469	3.73210734	-0.61512372
H	7.48079207	1.73222607	-3.23383810
C	0.09260333	3.96984860	0.95782272
O	-0.41289527	4.52649166	-0.28265835
C	1.37317141	1.79484771	1.30737644
O	0.11197642	2.13113280	-0.56769242
H	-2.69807354	4.63467593	-1.02025426
Tv	10.05848697	0.00000000	0.00000000
Tv	-5.10815416	8.66124735	0.00000000

(iii) $C_{64}O_4(OH)_{16} \cdot 2\ H_2O$

C	1.06437755	-2.32678608	1.27088556
C	-1.41630595	-2.35618261	0.73363599
C	-0.17440173	-0.09864302	1.19739440
C	2.33517800	-3.05129425	1.30119982
C	-2.69485283	-0.09563172	0.87186267
C	2.59555877	-1.53835190	-5.38624795
C	0.08170343	-1.56333112	-5.77176708
C	1.34187617	0.64671901	-5.75466667
C	3.88615398	-2.26807815	-5.78474126
C	-1.23287558	0.65500051	-5.80154677
C	2.57065273	-0.05551972	-5.74981724
O	2.57316901	-1.62987592	-3.90958372
C	1.30952107	-2.26471373	-5.77042379
H	-0.65231977	-2.18665018	-1.05715774
C	0.05140909	-0.08459770	-5.39671055
O	-0.02299430	-0.12782807	-3.91677794
H	-0.07658081	0.82471056	-3.64094911
C	1.02980018	-0.88597915	0.74713106
O	0.78504250	-1.11595995	-0.68020810
H	3.37737549	-1.13593692	-3.60125182
C	-1.41152322	-0.82966294	0.84772498
O	-1.95218632	-0.25821819	-0.36500880
H	-1.63195409	1.34017636	-1.88941460
C	-0.14086757	-2.99031899	1.23078499
O	-1.43270182	-2.69044954	-0.69967416
H	-4.26698229	-0.11428624	-0.98973227
C	6.09839476	-2.32784615	1.24525945
C	3.59720411	-2.35614862	0.76506061
C	4.84780837	-0.09781942	1.27589189
C	7.36822300	-3.05355579	1.22463868
C	2.33405750	-0.09810556	0.87224950

C	7.62438180	-1.53205109	-5.40557433
C	5.10842887	-1.56183898	-5.77365960
C	6.36957219	0.64816089	-5.76505634
C	8.91522775	-2.26973844	-5.78644343
C	3.79314793	0.65353921	-5.78019379
C	7.59857339	-0.05208515	-5.77661373
O	7.61162842	-1.59264651	-3.92599072
H	5.72730882	-1.98274534	-3.01007463
C	6.33812097	-2.26302972	-5.78282520
O	5.35225319	-2.81626828	-2.64763116
H	4.21385873	-2.30634691	-1.17456332
C	5.08220344	-0.08363929	-5.39278672
O	5.01761525	-0.12598415	-3.90987848
H	5.07976501	0.82716313	-3.62023589
C	6.04834960	-0.87149488	0.77979290
O	5.75539791	-1.04495053	-0.63153395
H	8.35681258	-1.00200008	-3.62785759
C	3.61635256	-0.82913650	0.88169122
O	3.11639029	-0.24164837	-0.33645536
C	4.89279197	-2.98976712	1.21813468
O	3.47070813	-2.70870496	-0.64352862
H	0.91406912	-0.22846716	-1.10019597
C	-1.48536682	2.00226340	1.24581490
C	-3.98638000	1.97413063	0.76488711
C	-2.73603467	4.23234562	1.27671910
C	-0.21551655	1.27657773	1.22518614
C	-5.24971520	4.23212430	0.87237274
C	0.04077546	2.79850069	-5.40606030
C	-2.47528441	2.76816634	-5.77385389
C	-1.21417887	4.97838145	-5.76636806
C	1.33147060	2.06030968	-5.78614987
C	-3.79057112	4.98368656	-5.78099933
C	0.01485808	4.27813073	-5.77833637
O	0.02841931	2.74020050	-3.92677363
H	-1.85729939	2.35173790	-3.01450172
C	-1.24555520	2.06700536	-5.78252248
O	-2.22460719	1.51655114	-2.64772735
H	-3.36888209	2.02502603	-1.17391401
C	-2.50140730	4.24660477	-5.39372121
O	-2.56559614	4.20481366	-3.91078312
H	-2.50186990	5.15803841	-3.62136775
C	-1.53545640	3.45867010	0.78059718
O	-1.82860095	3.28538958	-0.63073731
H	0.77399040	3.33087299	-3.62967883
C	-3.96740327	3.50115051	0.88190940
O	-4.46700632	4.08899741	-0.33621210
C	-2.69101972	1.34038572	1.21821997
O	-4.11224415	1.62200438	-0.64397964
H	-6.66827673	4.10130962	-1.10071639
C	3.53598050	2.00312366	1.27037059
C	1.05520775	1.97368326	0.73378692
C	2.29715621	4.23129178	1.19689529
C	4.80675138	1.27860413	1.30044780
C	-0.22332627	4.23425527	0.87209459
C	5.06715147	2.79173419	-5.38654822
C	2.55325877	2.76658419	-5.77194515
C	3.81347768	4.97668544	-5.75600074
C	6.35770443	2.06177690	-5.78446124
C	1.23867064	4.98506429	-5.80268710
C	5.04227377	4.27444410	-5.75089827
O	5.04509221	2.70103302	-3.90982770
C	3.78105859	2.06516128	-5.77017383
H	1.81899011	2.14221405	-1.05750159
C	2.52309634	4.24550398	-5.39785068
O	2.44960659	4.20353919	-3.91775941

H	2.40278171	5.15691810	-3.64301850
C	3.50144296	3.44400076	0.74674004
O	3.25697031	3.21401872	-0.68061259
H	5.84939181	3.19514809	-3.60203791
C	1.06006211	3.50021933	0.84753901
O	0.51885555	4.07115957	-0.36514396
H	0.83225379	5.65510111	-1.89207427
C	2.33074684	1.33955119	1.23055409
O	1.03842167	1.63912561	-0.69952548
H	-1.79615862	4.21622144	-0.98876463
Tv	10.05522572	0.00000000	0.00000000
Tv	-5.11239253	8.66004439	0.00000000

(iv) $C_{64}O_4(OH)_{16} \cdot 3\ H_2O$

C	1.05389431	-2.32792668	1.36080521
C	-1.43576835	-2.35676700	0.82727813
C	-0.18794653	-0.09835526	1.33861917
C	2.32479479	-3.05270750	1.38567948
C	-2.70008899	-0.09529767	0.97511392
C	2.54694578	-1.60660557	-5.57510615
C	0.03085415	-1.63801129	-5.94977681
C	1.29050236	0.57415048	-5.94034559
C	3.83421013	-2.34243277	-5.96594205
C	-1.28252601	0.58160821	-5.97353832
C	2.51955281	-0.12709784	-5.94713458
O	2.54554883	-1.66990944	-4.09451138
H	0.62304301	-2.01775882	-3.07888581
C	1.25956510	-2.33899708	-5.94431438
O	0.40318614	-2.82623224	-2.56667567
H	-0.79891333	-2.34658423	-1.11721563
C	0.00196304	-0.15852112	-5.57621754
O	-0.07262763	-0.21478408	-4.09261437
H	-0.15963432	0.72790783	-3.78746696
C	1.02147139	-0.87347134	0.88436740
O	0.75898470	-1.04972061	-0.53815765
H	3.34969173	-1.15790767	-3.80704839
C	-1.41838698	-0.82951470	0.95024085
O	-1.94541447	-0.24516202	-0.25642549
H	-1.51756073	1.56240261	-1.84574734
C	-0.14979423	-2.99066114	1.29789640
O	-1.55745130	-2.71957106	-0.58509002
H	-4.25162680	-0.12982268	-0.89491571
C	6.08715780	-2.32551545	1.36940138
C	3.59207284	-2.35452421	0.86599547
C	4.84420090	-0.09598816	1.37067985
C	7.35805996	-3.05102472	1.36825739
C	2.32884127	-0.09434981	1.00868740
C	7.57097580	-1.60527178	-5.57975779
C	5.05626891	-1.63555624	-5.95563469
C	6.31788236	0.57483663	-5.94602718
C	8.86144580	-2.34399305	-5.95885904
C	3.74254983	0.58161680	-5.97497295
C	7.54680201	-0.12589337	-5.95267735
O	7.54943450	-1.66527985	-4.10470895
H	5.66976115	-2.01203970	-3.09964243
C	6.28563932	-2.33643258	-5.96038940
O	5.43139660	-2.81455926	-2.58479847
H	4.23733632	-2.30169617	-1.06555107
C	5.02919349	-0.15648996	-5.58046695
O	4.95857828	-0.19616610	-4.09464965
H	5.02664950	0.75763254	-3.80458592
C	6.04368373	-0.87381989	0.88328472
O	5.75474419	-1.05776329	-0.53015965
H	8.30658210	-1.09768697	-3.79669315
C	3.60999611	-0.82813835	0.99065290

O	3.09256609	-0.23786144	-0.21556107
C	4.88093698	-2.98720247	1.33437835
O	3.48247969	-2.70444456	-0.55277714
H	0.85933420	-0.13189578	-0.90673928
C	-1.49572039	2.00402999	1.36381778
C	-3.98902741	1.97262922	0.85055805
C	-2.74404086	4.23211681	1.35420689
C	-0.22655539	1.27760721	1.36874312
C	-5.25684337	4.23189606	0.95301627
C	-0.00656713	2.72516026	-5.58060042
C	-2.52341068	2.69362624	-5.95439233
C	-1.26353318	4.90466734	-5.93986512
C	1.28105414	1.98759538	-5.97070361
C	-3.83770943	4.90955168	-5.95125179
C	-0.03424376	4.20511857	-5.95209866
O	-0.00881862	2.66403805	-4.10499473
H	-1.92458838	2.32965154	-3.10046162
C	-1.29371046	1.99347187	-5.95588629
O	-2.13895399	1.51038803	-2.60091119
H	-3.35599535	2.01195238	-1.07970396
C	-2.54960270	4.16965963	-5.56732986
O	-2.61257603	4.10274370	-4.08866265
H	-2.62952695	5.04524968	-3.77500864
C	-1.53709021	3.45578385	0.88494528
O	-1.80573843	3.27089531	-0.53430431
H	0.75689289	3.23524874	-3.81400559
C	-3.97367637	3.50038538	0.96088102
O	-4.48248393	4.07505979	-0.26133620
H	-4.05128645	5.86891511	-1.83763238
C	-2.69988762	1.34143361	1.32153567
O	-4.10505550	1.61261364	-0.55940063
H	-6.76993197	4.13735465	-0.96047223
C	3.53365374	2.00657762	1.37728462
C	1.04558333	1.97577278	0.88087657
C	2.29286578	4.23376968	1.34223611
C	4.80271716	1.28067339	1.38962592
C	-0.22798713	4.23528706	0.99558169
C	5.01500300	2.71750521	-5.56389631
C	2.50277374	2.69401073	-5.95969691
C	3.76344893	4.90342363	-5.92442930
C	6.30673356	1.98864946	-5.96283646
C	1.18956423	4.91262546	-5.97639707
C	4.99204965	4.20186746	-5.92036747
O	4.98081485	2.61360184	-4.09201746
C	3.73060176	1.99296900	-5.96031580
H	1.79808820	2.16158179	-0.91487477
C	2.47191362	4.17053328	-5.57106016
O	2.38956485	4.10624082	-4.09719686
H	2.34867283	5.04930523	-3.78939074
C	3.48853773	3.44721620	0.85657249
O	3.21756913	3.22683260	-0.56595991
H	5.71809250	3.18883751	-3.75894982
C	1.05420212	3.50240735	0.99174845
O	0.53083737	4.07395362	-0.22914508
H	0.96696546	5.88316802	-1.84703144
C	2.32782151	1.34258349	1.36288426
O	1.01979236	1.65062417	-0.55784386
H	-1.73517446	4.19357786	-0.90378961
Tv	10.05288508	0.00000000	0.00000000
Tv	-5.10775347	8.66062696	0.00000000

S6 Cartesian coordinates of optimized geometries in Figure 7. Tv corresponds to translation vectors in the unit cell. The optimised structures were obtained at the

PBE/6-31G** level of theory.

(i) $CO_2@C_{64}O_4(OH)_{16}$

C	0.55255649	-2.06723430	1.94124864
C	-1.93808630	-2.09434108	1.46124494
C	-0.69347774	0.16112747	1.94100747
C	1.82236474	-2.79142628	1.94079080
C	-3.21199744	0.16184212	1.57869044
C	2.89134916	-2.48540960	-6.43267278
C	0.37466676	-2.51001987	-6.80874204
C	1.63322229	-0.30212322	-6.79794103
C	4.17998829	-3.21817959	-6.83155086
C	-0.94294759	-0.29489564	-6.83110960
C	2.86232753	-1.00337215	-6.79782005
O	2.89659317	-2.56239008	-4.95219134
C	1.60333476	-3.21114136	-6.80875060
H	-1.21241044	-1.89594157	-0.33817891
C	0.34342421	-1.03139652	-6.43257625
O	0.27591960	-1.06573581	-4.95224003
H	0.27935977	-0.10581622	-4.68159863
C	0.50409283	-0.61799976	1.45120727
O	0.22950679	-0.80286878	0.02272773
H	3.72160396	-2.07134603	-4.68213018
C	-1.92964658	-0.56957475	1.58020887
O	-2.44598370	0.01394816	0.36356161
C	-0.65248066	-2.73154207	1.92725498
O	-1.97431802	-2.41721784	0.03134723
H	-4.69683051	0.06390791	-0.36873269
C	5.57974405	-2.06847231	1.96631072
C	3.09419116	-2.09597552	1.45114327
C	4.33307422	0.16086158	1.92123247
C	6.85051999	-2.79323861	1.96160711
C	1.81435167	0.16164243	1.56092979
C	7.91803211	-2.48580766	-6.43641936
C	5.40204474	-2.51140940	-6.81596501
C	6.66044128	-0.30274749	-6.80126513
C	9.20803620	-3.21738125	-6.83146036
C	4.08525912	-0.29477918	-6.82613873
C	7.88953640	-1.00383960	-6.80183615
O	7.92038470	-2.56459754	-4.95659551
C	6.63070418	-3.21242129	-6.81405145
H	3.85557739	-1.92234042	-0.33736371
C	5.37209205	-1.03383730	-6.43475303
O	5.30845041	-1.08565480	-4.95681973
H	5.32998244	-0.13547227	-4.66146697
C	5.53693216	-0.62359712	1.46032261
O	5.28444893	-0.83952769	0.03491215
H	8.73789601	-2.06390518	-4.68368889
C	3.09850316	-0.57098152	1.56133494
O	2.57540777	0.00366110	0.34339132
C	4.37386949	-2.73095593	1.94095290
O	3.07652300	-2.42632396	0.02244960
H	0.26763110	0.12384288	-0.33753282
C	-2.00731020	2.26155166	1.96181260
C	-4.49268836	2.23409170	1.45196891
C	-3.25288122	4.49077481	1.92730122
C	-0.73660211	1.53663837	1.96560792
C	-5.77076305	4.49075685	1.56627165
C	0.33059076	1.84343269	-6.43490806
C	-2.18434966	1.81806939	-6.81434951
C	-0.92494062	4.02631584	-6.80283753
C	1.62164132	1.11137834	-6.82601563
C	-3.50046728	4.03495416	-6.83150377
C	0.30407238	3.32503891	-6.80173689

O	0.31833780	1.76186794	-4.95703471
C	-0.95580427	1.11688318	-6.81600609
H	-3.74400893	2.41898453	-0.33912419
C	-2.21432354	3.29667544	-6.43696893
O	-2.28143669	3.25920689	-4.95743237
H	-2.26375636	4.21764681	-4.68408353
C	-2.05033285	3.70793187	1.46086583
O	-2.30957724	3.51219987	0.03111025
H	1.12576297	2.26336243	-4.66211710
C	-4.48764020	3.75871034	1.56655873
O	-5.00820799	4.33712252	0.34950410
C	-3.21274252	1.59839556	1.93780937
O	-4.51347133	1.90402362	0.02386990
H	-7.30155681	4.44862458	-0.33867344
C	3.02107442	2.26041459	1.93877841
C	0.52846867	2.23448754	1.45944592
C	1.77648477	4.48923327	1.93735884
C	4.29105730	1.53608515	1.93883043
C	-0.74238457	4.49090461	1.57954580
C	5.36014492	1.84459889	-6.43683016
C	2.84370701	1.81821121	-6.80994158
C	4.10303259	4.02699160	-6.80617351
C	6.64902057	1.11069338	-6.83078446
C	1.52689803	4.03369082	-6.83083942
C	5.33204136	3.32583288	-6.80585899
O	5.36282056	1.77046668	-4.95732937
C	4.07254943	1.11699773	-6.81003085
H	1.20884433	2.43189301	-0.37071082
C	2.81447097	3.29741373	-6.43706272
O	2.75091507	3.26253822	-4.95751645
H	2.76395137	4.22136912	-4.68474000
C	2.97491453	3.71053482	1.45150749
O	2.70232018	3.52387795	0.02332357
H	6.18298623	2.26724312	-4.68478611
C	0.53969601	3.75906002	1.57812057
O	0.02219977	4.34377959	0.36290745
C	1.81607300	1.59711985	1.92029252
O	0.47070356	1.90707738	0.03399591
H	-2.25009351	4.43405661	-0.33696964
C	3.17449717	1.01333514	-2.44177128
O	4.19876962	0.42850005	-2.44922772
O	2.14049112	1.58071641	-2.45042945
Tv	10.05515026	0.00000000	0.00000000
Tv	-5.11638335	8.65789892	0.00000000

(ii) $CO_2@C_{64}O_4(OH)_{16} \cdot H_2O$

C	0.44113096	-2.27481738	1.81280331
C	-2.05178468	-2.30364994	1.34061262
C	-0.80449513	-0.04719083	1.81385661
C	1.70990876	-3.00060238	1.81194026
C	-3.32346006	-0.04669082	1.45478724
C	3.27004824	-1.87617764	-6.01048194
C	0.74957550	-1.90021703	-6.37052356
C	2.00690488	0.30841945	-6.35755071
C	4.55419037	-2.60710492	-6.43051227
C	-0.56718333	0.31529893	-6.40770895
C	3.23675047	-0.39269186	-6.36643641
O	3.29329027	-1.95751839	-4.52832920
C	1.97761861	-2.60171214	-6.37155563
H	-1.35068488	-2.10338759	-0.47136566
C	0.71540000	-0.42022570	-5.99563151
O	0.63226968	-0.46152085	-4.51542871
H	0.54775641	0.48591468	-4.22597850
C	0.39096295	-0.82636273	1.31791236
O	0.11063269	-1.02097153	-0.10734195

H	4.12781553	-1.47804454	-4.26296979
C	-2.04142848	-0.77813900	1.45612975
O	-2.55687484	-0.19486798	0.23916743
H	-1.36709683	1.95500685	-1.66605199
C	-0.76342013	-2.93980084	1.80091366
O	-2.10062965	-2.63064853	-0.08669269
H	-4.78699329	-0.17695581	-0.50873187
C	5.46706465	-2.27705137	1.85368547
C	2.98262078	-2.30541577	1.32478031
C	4.22049581	-0.04806897	1.79242310
C	6.73806134	-3.00199905	1.85049882
C	1.70074566	-0.04710429	1.42736590
C	8.28910039	-1.87640484	-6.01660920
C	5.77718149	-1.90231826	-6.42280998
C	7.03666730	0.30755747	-6.38790666
C	9.58322137	-2.60902299	-6.39479498
C	4.46020124	0.31537947	-6.39712637
C	8.26509620	-0.39426033	-6.38445959
O	8.26999350	-1.95744884	-4.53887854
C	7.00614932	-2.60304192	-6.41246462
H	3.74200536	-2.13535673	-0.46589525
C	5.75134289	-0.42889743	-6.02603321
O	5.70871719	-0.51239645	-4.55623672
H	5.76173632	0.42682432	-4.23242372
C	5.42584812	-0.83499741	1.33868996
O	5.17939936	-1.06785355	-0.08239911
H	9.05939073	-1.42561647	-4.24368066
C	2.98591228	-0.78017106	1.43115267
O	2.46364638	-0.20826604	0.21227315
C	4.26080455	-2.93867138	1.82194233
O	2.96569302	-2.64061285	-0.10241126
H	0.12873355	-0.10459093	-0.49089639
C	-2.11811886	2.05439363	1.83680760
C	-4.60286988	2.02537452	1.32097741
C	-3.36356879	4.28217607	1.79718557
C	-0.84754451	1.32832466	1.84356933
C	-5.88112734	4.28255987	1.44313012
C	0.70156983	2.46074532	-6.02794354
C	-1.80998643	2.42913166	-6.38790530
C	-0.54903980	4.63812635	-6.40538695
C	1.99610818	1.72154350	-6.39266209
C	-3.12502440	4.64442781	-6.38760214
C	0.68019981	3.93710445	-6.41074427
O	0.66999956	2.41125100	-4.55079534
H	-1.15442048	2.26905393	-3.16198233
C	-0.58151687	1.72726654	-6.40185023
O	-1.57882787	1.62248538	-2.56147877
H	-3.87059234	2.18802611	-0.49501383
C	-1.83213948	3.90915641	-6.01471237
O	-1.87584766	3.88607313	-4.53269153
H	-1.86447204	4.84899120	-4.26997228
C	-2.15899283	3.50064441	1.33577092
O	-2.41611645	3.30638292	-0.09991183
H	1.48287844	2.90327113	-4.25322084
C	-4.59787899	3.54972709	1.43580511
O	-5.12340460	4.12839340	0.22238498
C	-3.32336901	1.39107032	1.80851861
O	-4.63205364	1.68608308	-0.10247136
H	-7.41675293	4.24307245	-0.45717548
C	2.90948443	2.05079346	1.81423306
C	0.41590680	2.02809920	1.33742115
C	1.66587153	4.28117679	1.82610895
C	4.17988950	1.32707110	1.81268433
C	-0.85272438	4.28435032	1.45913302
C	5.73577347	2.44883421	-5.98814851

C	3.21857338	2.42786699	-6.37482249
C	4.47997591	4.63574039	-6.36146968
C	7.02342427	1.72141636	-6.39882334
C	1.90432544	4.64420276	-6.42669251
C	5.70842097	3.93345104	-6.34863886
O	5.72279954	2.34040799	-4.51172330
C	4.44738634	1.72687747	-6.37412584
H	1.10279600	2.21033730	-0.49795355
C	3.18577657	3.90842193	-6.00853456
O	3.10055049	3.87985938	-4.52888558
H	3.12363523	4.84116519	-4.26284363
C	2.86314460	3.50362640	1.33462105
O	2.58428573	3.32000246	-0.09010652
H	6.56464398	2.76169865	-4.19550323
C	0.42912603	3.55251180	1.46030656
O	-0.08333829	4.13992607	0.24396133
C	1.70435775	1.38747948	1.78974012
O	0.35168283	1.70380926	-0.09182266
H	-2.37244028	4.23134249	-0.46548469
C	3.13405136	0.91607335	-2.37029221
O	4.12428682	0.27871999	-2.39671414
O	2.13706976	1.54365265	-2.36656774
Tv	10.05414460	0.00000000	0.00000000
Tv	-5.11458400	8.65856796	0.00000000

(iii) $CO_2@C_{64}O_4(OH)_{16} \cdot 2\ H_2O$

C	0.43847343	-2.24836359	1.72889931
C	-2.05402358	-2.27420486	1.26444741
C	-0.80621613	-0.01953269	1.74137897
C	1.70720015	-2.97335585	1.72794017
C	-3.32538362	-0.01851458	1.38264219
C	3.31803729	-1.89465028	-5.87483091
C	0.79729259	-1.91604999	-6.24631348
C	2.05659020	0.29230320	-6.23034560
C	4.60176489	-2.62182897	-6.30209902
C	-0.51760637	0.29994898	-6.30506754
C	3.28647961	-0.40980116	-6.22629972
O	3.32950551	-1.99983949	-4.39467843
C	2.02531383	-2.61701776	-6.24622797
H	-1.34111880	-2.08097750	-0.54762229
C	0.76185267	-0.43446518	-5.87871660
O	0.66752142	-0.47024384	-4.39825003
H	0.58352934	0.47891892	-4.11312791
C	0.38681792	-0.79845513	1.23831441
O	0.10080051	-0.99149627	-0.18573624
H	4.18855500	-1.59607807	-4.09791850
C	-2.04341030	-0.74939851	1.38357776
O	-2.55868505	-0.16472608	0.16628879
H	-1.38685897	1.90926178	-1.66159194
C	-0.76600223	-2.91402363	1.71662781
O	-2.10215467	-2.59755988	-0.16682133
H	-4.80323526	-0.14439034	-0.58570709
C	5.46436820	-2.24968747	1.77681074
C	2.98095216	-2.27967606	1.23876814
C	4.21692694	-0.02150485	1.70927286
C	6.73593749	-2.97421389	1.77196262
C	1.69783273	-0.02079829	1.34549775
C	8.33685214	-1.88734753	-5.89823664
C	5.82491773	-1.91754988	-6.29707622
C	7.08583635	0.29265056	-6.28837593
C	9.63037073	-2.62506607	-6.26640889
C	4.50887024	0.29858899	-6.26490534
C	8.31420823	-0.40919708	-6.28149238
O	8.32419987	-1.95149434	-4.41687711
H	6.51917529	-2.18867464	-3.14834533

C	7.05444409	-2.61834168	-6.28675714
O	6.13283200	-2.86162361	-2.54878982
H	3.73308269	-2.13547407	-0.57058489
C	5.80543572	-0.44265826	-5.90839768
O	5.78900680	-0.51368258	-4.43757807
H	5.83476737	0.43032251	-4.12221737
C	5.42460496	-0.80767162	1.26328006
O	5.18243106	-1.03998452	-0.16284459
H	9.11546063	-1.41459876	-4.13064098
C	2.98360409	-0.75491391	1.34652660
O	2.45804900	-0.18407152	0.13000479
C	4.25797799	-2.91162365	1.74000519
O	2.95762364	-2.62243336	-0.18562184
H	0.11574409	-0.07625943	-0.57281009
C	-2.12026674	2.08192915	1.76695382
C	-4.60350875	2.05218858	1.24238647
C	-3.36657494	4.30956789	1.71428803
C	-0.84953615	1.35581032	1.77430331
C	-5.88422329	4.30949911	1.35375426
C	0.74650454	2.44550654	-5.91908050
C	-1.76172167	2.41401911	-6.28839030
C	-0.50012279	4.62346060	-6.28653597
C	2.04508258	1.70550846	-6.27217648
C	-3.07670021	4.62938028	-6.26529630
C	0.72912037	3.92290485	-6.29560383
O	0.69056307	2.39307637	-4.44703866
H	-1.14007008	2.19218153	-3.15310629
C	-0.53300347	1.71182648	-6.30577732
O	-1.56706964	1.54571884	-2.55184141
H	-3.86785503	2.20973724	-0.57342939
C	-1.78297286	3.89109132	-5.90058100
O	-1.82450588	3.84978811	-4.42154814
H	-1.77167084	4.80598601	-4.13879471
C	-2.16104814	3.52628867	1.25920372
O	-2.41504590	3.32337868	-0.17493974
H	1.46776028	2.92569032	-4.12496490
C	-4.60039296	3.57666204	1.35224207
O	-5.12443238	4.15237356	0.13624249
C	-3.32592477	1.41898587	1.73710771
O	-4.62871221	1.70874663	-0.17836573
H	-7.44699446	4.24517983	-0.57381116
C	2.90765379	2.07877609	1.73004896
C	0.41250922	2.05508669	1.26251319
C	1.66473967	4.30918675	1.74167053
C	4.17697866	1.35389530	1.72898737
C	-0.85479270	4.31099201	1.38127231
C	5.78634370	2.43256984	-5.87301768
C	3.26726893	2.41178151	-6.25405850
C	4.52707085	4.62025778	-6.22672393
C	7.07152073	1.70674118	-6.29740673
C	1.95382657	4.62902624	-6.30113151
C	5.75630526	3.91858291	-6.22441063
O	5.78663316	2.31787361	-4.39673478
C	4.49570039	1.71046331	-6.25066278
H	1.08127702	2.23496368	-0.58198517
C	3.23220209	3.89068917	-5.87795135
O	3.13501970	3.83557571	-4.40168928
H	3.09988746	4.78170729	-4.09935540
C	2.85952838	3.53148759	1.24480960
O	2.57436421	3.33615301	-0.17482523
H	6.63011764	2.74209870	-4.08665629
C	0.42699102	3.57978306	1.38251175
O	-0.08676929	4.16565972	0.16538351
H	1.14762110	6.18430081	-1.65961498
C	1.70299777	1.41407819	1.70842192

O	0.33754435	1.72827167	-0.16190297
H	-2.36171204	4.24353826	-0.55138995
C	3.14484637	0.91215160	-2.37069448
O	4.16377574	0.32293077	-2.41034728
O	2.11983849	1.49038553	-2.35296382
Tv	10.05393964	0.00000000	0.00000000
Tv	-5.11304105	8.65854979	0.00000000

(iv) $CO_2@C_{64}O_4(OH)_{16} \cdot 3\ H_2O$

C	0.87884809	-2.29740919	1.61295466
C	-1.61077488	-2.32228660	1.10375425
C	-0.36701483	-0.06988066	1.63065484
C	2.15065366	-3.01901989	1.62047209
C	-2.87836391	-0.06397517	1.25249769
C	2.70962195	-1.85442719	-5.94524641
C	0.18977094	-1.87831486	-6.31096565
C	1.44824909	0.33040181	-6.28425776
C	3.99147931	-2.58800082	-6.36474003
C	-1.12262663	0.33824307	-6.34561794
C	2.67733903	-0.37146189	-6.30217903
O	2.72477097	-1.94205821	-4.46165732
H	0.68991806	-2.02893005	-3.13892089
C	1.41800558	-2.57963369	-6.31149773
O	0.47375630	-2.74525252	-2.50523486
H	-0.95211009	-2.22270079	-0.79673673
C	0.15645436	-0.40001498	-5.92845543
O	0.05985066	-0.45757904	-4.44538796
H	-0.03089167	0.48038917	-4.12443870
C	0.83368074	-0.84236656	1.14362366
O	0.55363866	-1.02008428	-0.28175613
H	3.58531946	-1.52764458	-4.18451483
C	-1.59761792	-0.79754772	1.23842050
O	-2.11231562	-0.20059998	0.03134582
H	-1.34903365	1.73442921	-1.73337622
C	-0.32509645	-2.96117179	1.56701512
O	-1.70356030	-2.66610983	-0.31953720
H	-4.38300814	-0.14667535	-0.68643121
C	5.90928270	-2.29315804	1.63659320
C	3.42086124	-2.32269217	1.11526505
C	4.66328972	-0.06550343	1.59837533
C	7.18132318	-3.01839957	1.63473866
C	2.14218730	-0.06530124	1.25687183
C	7.72586167	-1.85171897	-5.97045536
C	5.21471301	-1.88375354	-6.38349491
C	6.47938029	0.33028066	-6.36549991
C	9.02114366	-2.58630629	-6.33767576
C	3.90019130	0.33652609	-6.35399627
C	7.70795469	-0.37120159	-6.34302238
O	7.69506551	-1.92730136	-4.49266517
H	5.93119861	-2.12154166	-3.18087268
C	6.44461613	-2.58323320	-6.36795023
O	5.65013554	-2.80620461	-2.53733866
H	4.12984943	-2.21292337	-0.75089152
C	5.19588125	-0.40784646	-6.00235776
O	5.17055662	-0.48896173	-4.52890521
H	5.26744269	0.44462793	-4.20000128
C	5.86839554	-0.84677218	1.13497904
O	5.60638995	-1.05531443	-0.28612752
H	8.48529585	-1.40934446	-4.17812158
C	3.42824759	-0.79773969	1.23351942
O	2.89102712	-0.21781504	0.03024874
C	3.20366797	1.07620126	-2.48094871
C	4.70244412	-2.95377429	1.60455968
O	3.36362606	-2.66965061	-0.31141191
H	0.58194617	-0.09720700	-0.64904817

C	-1.67581632	2.03522564	1.66091425
C	-4.15634549	2.00593030	1.12435257
C	-2.92091269	4.26492077	1.60253417
C	-0.40798584	1.30609118	1.67633632
C	-5.43699091	4.26146177	1.21910501
C	0.14566632	2.48325374	-5.95103035
C	-2.36514458	2.45112502	-6.33853914
C	-1.10778625	4.65877772	-6.32266847
C	1.43747862	1.74336810	-6.32501020
C	-3.68120334	4.66780080	-6.33349788
C	0.12157903	3.95898176	-6.33605813
O	0.11503730	2.43219608	-4.48008328
H	-1.62447266	2.21745907	-3.16383799
C	-1.13635700	1.75002358	-6.33482941
O	-1.84086506	1.48955272	-2.54313179
H	-3.44482130	2.12334235	-0.73026718
C	-2.39461802	3.92697117	-5.94659528
O	-2.46820084	3.86910376	-4.46585359
H	-2.49402408	4.81680637	-4.16064220
C	-1.71421803	3.48054556	1.15191187
O	-1.96881230	3.27416405	-0.27596798
H	0.91160997	2.94781500	-4.17450939
C	-4.15251791	3.53097152	1.23018766
O	-4.66827767	4.09827282	0.00575422
H	-4.04741875	6.10137928	-1.74686459
C	-2.87939043	1.37136816	1.61801145
O	-4.19911442	1.65365953	-0.28817597
H	-6.96336886	4.19708063	-0.68766651
C	3.35319350	2.03452571	1.61956633
C	0.85421871	2.00739788	1.16740383
C	2.11333663	4.26533168	1.61761220
C	4.62285673	1.30998886	1.62115391
C	-0.40867730	4.26643326	1.26598848
C	5.17735824	2.47267708	-5.96139988
C	2.65930300	2.44967697	-6.32524124
C	3.92037592	4.65989708	-6.30932749
C	6.46626108	1.74457374	-6.37058624
C	1.34614314	4.66547501	-6.36556809
C	5.14913374	3.95846777	-6.31089250
O	5.17389866	2.36678280	-4.48919337
C	3.88768634	1.74835697	-6.33776865
H	1.46613741	2.23601111	-0.69021963
C	2.62818549	3.92992994	-5.95001835
O	2.54485025	3.87943947	-4.47727906
H	2.51827650	4.82504444	-4.16944573
C	3.30569999	3.48123521	1.11990479
O	3.01832251	3.28211673	-0.30251289
H	5.94818038	2.90678955	-4.17389294
C	0.87213629	3.53422055	1.27398260
O	0.35808803	4.10770325	0.04970465
H	1.06502489	6.07459314	-1.74137897
C	2.14746574	1.37099332	1.61248414
O	0.76796901	1.68014059	-0.25904489
H	-1.90040050	4.18833333	-0.66303112
O	2.10794893	1.46643479	-2.67820469
O	4.28586437	0.65570659	-2.29987625
Tv	10.05261481	0.00000000	0.00000000
Tv	-5.10977345	8.65955652	0.00000000

S7 Cartesian coordinates of transition states (TS) for CO_2 migration within graphene oxide models in Figure 10. Tv corresponds to translation vectors in the unit cell. *T* represents degree of CO_2 migration from the original position.

(i) TS in $CO_2@C_{64}O_4(OH)_{16}$. (T = 3.2 Å)

C	0.55255600	-2.06723400	1.94124900
C	-1.93808600	-2.09434100	1.46124500
C	-0.69347800	0.16112700	1.94100700
C	1.82236500	-2.79142600	1.94079100
C	-3.21199700	0.16184200	1.57869000
C	2.89134900	-2.48541000	-6.43267300
C	0.37466700	-2.51002000	-6.80874200
C	1.63322200	-0.30212300	-6.79794100
C	4.17998800	-3.21818000	-6.83155100
C	-0.94294800	-0.29489600	-6.83111000
C	2.86232800	-1.00337200	-6.79782000
O	2.89659300	-2.56239000	-4.95219100
C	1.60333500	-3.21114100	-6.80875100
H	-1.21241000	-1.89594200	-0.33817900
C	0.34342400	-1.03139700	-6.43257600
O	0.27592000	-1.06573600	-4.95224000
H	0.27936000	-0.10581600	-4.68159900
C	0.50409300	-0.61800000	1.45120700
O	0.22950700	-0.80286900	0.02272800
H	3.72160400	-2.07134600	-4.68213000
C	-1.92964700	-0.56957500	1.58020900
O	-2.44598400	0.01394800	0.36356200
C	-0.65248100	-2.73154200	1.92725500
O	-1.97431800	-2.41721800	0.03134700
H	-4.69683100	0.06390800	-0.36873300
C	5.57974400	-2.06847200	1.96631100
C	3.09419100	-2.09597600	1.45114300
C	4.33307400	0.16086200	1.92123200
C	6.85052000	-2.79323900	1.96160700
C	1.81435200	0.16164200	1.56093000
C	7.91803200	-2.48580800	-6.43641900
C	5.40204500	-2.51140900	-6.81596500
C	6.66044100	-0.30274700	-6.80126500
C	9.20803600	-3.21738100	-6.83146000
C	4.08525900	-0.29477900	-6.82613900
C	7.88953600	-1.00384000	-6.80183600
O	7.92038500	-2.56459800	-4.95659600
C	6.63070400	-3.21242100	-6.81405100
H	3.85557700	-1.92234000	-0.33736400
C	5.37209200	-1.03383700	-6.43475300
O	5.30845000	-1.08565500	-4.95682000
H	5.32998200	-0.13547200	-4.66146700
C	5.53693200	-0.62359700	1.46032300
O	5.28444900	-0.83952800	0.03491200
H	8.73789600	-2.06390500	-4.68368900
C	3.09850300	-0.57098200	1.56133500
O	2.57540800	0.00366100	0.34339100
C	4.37386900	-2.73095600	1.94095300
O	3.07652300	-2.42632400	0.02245000
H	0.26763100	0.12384300	-0.33753300
C	-2.00731000	2.26155200	1.96181300
C	-4.49268800	2.23409200	1.45196900
C	-3.25288100	4.49077500	1.92730100
C	-0.73660200	1.53663800	1.96560800
C	-5.77076300	4.49075700	1.56627200
C	0.33059100	1.84343300	-6.43490800
C	-2.18435000	1.81806900	-6.81435000
C	-0.92494100	4.02631600	-6.80283800
C	1.62164100	1.11137800	-6.82601600
C	-3.50046700	4.03495400	-6.83150400
C	0.30407200	3.32503900	-6.80173700
O	0.31833800	1.76186800	-4.95703500
C	-0.95580400	1.11688300	-6.81600600
H	-3.74400900	2.41898500	-0.33912400

C	-2.21432400	3.29667500	-6.43696900
O	-2.28143700	3.25920700	-4.95743200
H	-2.26375600	4.21764700	-4.68408400
C	-2.05033300	3.70793200	1.46086600
O	-2.30957700	3.51220000	0.03111000
H	1.12576300	2.26336200	-4.66211700
C	-4.48764000	3.75871000	1.56655900
O	-5.00820800	4.33712300	0.34950400
C	-3.21274300	1.59839600	1.93780900
O	-4.51347100	1.90402400	0.02387000
H	-7.30155700	4.44862500	-0.33867300
C	3.02107400	2.26041500	1.93877800
C	0.52846900	2.23448800	1.45944600
C	1.77648500	4.48923300	1.93735900
C	4.29105700	1.53608500	1.93883000
C	-0.74238500	4.49090500	1.57954600
C	5.36014500	1.84459900	-6.43683000
C	2.84370700	1.81821100	-6.80994200
C	4.10303300	4.02699200	-6.80617400
C	6.64902100	1.11069300	-6.83078400
C	1.52689800	4.03369100	-6.83083900
C	5.33204100	3.32583300	-6.80585900
O	5.36282100	1.77046700	-4.95732900
C	4.07254900	1.11699800	-6.81003100
H	1.20884400	2.43189300	-0.37071100
C	2.81447100	3.29741400	-6.43706300
O	2.75091500	3.26253800	-4.95751600
H	2.76395100	4.22136900	-4.68474000
C	2.97491500	3.71053500	1.45150700
O	2.70232000	3.52387800	0.02332400
H	6.18298600	2.26724300	-4.68478600
C	0.53969600	3.75906000	1.57812100
O	0.02220000	4.34378000	0.36290700
C	1.81607300	1.59712000	1.92029300
O	0.47070400	1.90707700	0.03399600
H	-2.25009400	4.43405700	-0.33697000
C	1.63531400	-1.79207400	-2.46621000
O	0.60128700	-1.22468100	-2.47486800
O	2.66934100	-2.35946600	-2.45755100
Tv	10.05515000	0.00000000	0.00000000
Tv	-5.11638300	8.65789900	0.00000000

(ii) TS in $CO_2@C_{64}O_4(OH)_{16} \bullet H_2O$. ($T$ = 2.6 Å)

C	0.44113100	-2.27481700	1.81280300
C	-2.05178500	-2.30365000	1.34061300
C	-0.80449500	-0.04719100	1.81385700
C	1.70990900	-3.00060200	1.81194000
C	-3.32346000	-0.04669100	1.45478700
C	3.27004800	-1.87617800	-6.01048200
C	0.74957600	-1.90021700	-6.37052400
C	2.00690500	0.30841900	-6.35755100
C	4.55419000	-2.60710500	-6.43051200
C	-0.56718300	0.31529900	-6.40770900
C	3.23675000	-0.39269200	-6.36643600
O	3.29329000	-1.95751800	-4.52832900
C	1.97761900	-2.60171200	-6.37155600
H	-1.35068500	-2.10338800	-0.47136600
C	0.71540000	-0.42022600	-5.99563200
O	0.63227000	-0.46152100	-4.51542900
H	0.54775600	0.48591500	-4.22597900
C	0.39096300	-0.82636300	1.31791200
O	0.11063300	-1.02097200	-0.10734200
H	4.12781600	-1.47804500	-4.26297000
C	-2.04142800	-0.77813900	1.45613000
O	-2.55687500	-0.19486800	0.23916700

H	-1.36709700	1.95500700	-1.66605200
C	-0.76342000	-2.93980100	1.80091400
O	-2.10063000	-2.63064900	-0.08669300
H	-4.78699300	-0.17695600	-0.50873200
C	5.46706500	-2.27705100	1.85368500
C	2.98262100	-2.30541600	1.32478000
C	4.22049600	-0.04806900	1.79242300
C	6.73806100	-3.00199900	1.85049900
C	1.70074600	-0.04710400	1.42736600
C	8.28910000	-1.87640500	-6.01660900
C	5.77718100	-1.90231800	-6.42281000
C	7.03666700	0.30755700	-6.38790700
C	9.58322100	-2.60902300	-6.39479500
C	4.46020100	0.31537900	-6.39712600
C	8.26509600	-0.39426000	-6.38446000
O	8.26999400	-1.95744900	-4.53887900
C	7.00614900	-2.60304200	-6.41246500
H	3.74200500	-2.13535700	-0.46589500
C	5.75134300	-0.42889700	-6.02603300
O	5.70871700	-0.51239600	-4.55623700
H	5.76173600	0.42682400	-4.23242400
C	5.42584800	-0.83499700	1.33869000
O	5.17939900	-1.06785400	-0.08239900
H	9.05939100	-1.42561600	-4.24368100
C	2.98591200	-0.78017100	1.43115300
O	2.46364600	-0.20826600	0.21227300
C	4.26080500	-2.93867100	1.82194200
O	2.96569300	-2.64061300	-0.10241100
H	0.12873400	-0.10459100	-0.49089600
C	-2.11811900	2.05439400	1.83680800
C	-4.60287000	2.02537500	1.32097700
C	-3.36356900	4.28217600	1.79718600
C	-0.84754500	1.32832500	1.84356900
C	-5.88112700	4.28256000	1.44313000
C	0.70157000	2.46074500	-6.02794400
C	-1.80998600	2.42913200	-6.38790500
C	-0.54904000	4.63812600	-6.40538700
C	1.99610800	1.72154400	-6.39266200
C	-3.12502400	4.64442800	-6.38760200
C	0.68020000	3.93710400	-6.41074400
O	0.67000000	2.41125100	-4.55079500
H	-1.15442000	2.26905400	-3.16198200
C	-0.58151700	1.72726700	-6.40185000
O	-1.57882800	1.62248500	-2.56147900
H	-3.87059200	2.18802600	-0.49501400
C	-1.83213900	3.90915600	-6.01471200
O	-1.87584800	3.88607300	-4.53269200
H	-1.86447200	4.84899100	-4.26997200
C	-2.15899300	3.50064400	1.33577100
O	-2.41611600	3.30638300	-0.09991200
H	1.48287800	2.90327100	-4.25322100
C	-4.59787900	3.54972700	1.43580500
O	-5.12340500	4.12839300	0.22238500
C	-3.32336900	1.39107000	1.80851900
O	-4.63205400	1.68608300	-0.10247100
H	-7.41675300	4.24307200	-0.45717500
C	2.90948400	2.05079300	1.81423300
C	0.41590700	2.02809900	1.33742100
C	1.66587200	4.28117700	1.82610900
C	4.17989000	1.32707100	1.81268400
C	-0.85272400	4.28435000	1.45913300
C	5.73577300	2.44883400	-5.98814900
C	3.21857300	2.42786700	-6.37482200
C	4.47997600	4.63574000	-6.36147000
C	7.02342400	1.72141600	-6.39882300

C	1.90432500	4.64420300	-6.42669300
C	5.70842100	3.93345100	-6.34863900
O	5.72280000	2.34040800	-4.51172300
C	4.44738600	1.72687700	-6.37412600
H	1.10279600	2.21033700	-0.49795400
C	3.18577700	3.90842200	-6.00853500
O	3.10055000	3.87985900	-4.52888600
H	3.12363500	4.84116500	-4.26284400
C	2.86314500	3.50362600	1.33462100
O	2.58428600	3.32000200	-0.09010700
H	6.56464400	2.76169900	-4.19550300
C	0.42912600	3.55251200	1.46030700
O	-0.08333800	4.13992600	0.24396100
C	1.70435800	1.38747900	1.78974000
O	0.35168300	1.70380900	-0.09182300
H	-2.37244000	4.23134200	-0.46548500
C	1.72752100	-1.27058000	-2.35543900
O	2.71775600	-1.90793300	-2.38186100
O	0.73053900	-0.64300000	-2.35171400
Tv	10.05414500	0.00000000	0.00000000
Tv	-5.11458400	8.65856800	0.00000000

(iii) TS in $CO_2@C_{64}O_4(OH)_{16} \cdot 2H_2O$. ($T$ = 2.6 Å)

C	0.43847300	-2.24836400	1.72889900
C	-2.05402400	-2.27420500	1.26444700
C	-0.80621600	-0.01953300	1.74137900
C	1.70720000	-2.97335600	1.72794000
C	-3.32538400	-0.01851500	1.38264200
C	3.31803700	-1.89465000	-5.87483100
C	0.79729300	-1.91605000	-6.24631300
C	2.05659000	0.29230300	-6.23034600
C	4.60176500	-2.62182900	-6.30209900
C	-0.51760600	0.29994900	-6.30506800
C	3.28648000	-0.40980100	-6.22630000
O	3.32950600	-1.99983900	-4.39467800
C	2.02531400	-2.61701800	-6.24622800
H	-1.34111900	-2.08097800	-0.54762200
C	0.76185300	-0.43446500	-5.87871700
O	0.66752100	-0.47024400	-4.39825000
H	0.58352900	0.47891900	-4.11312800
C	0.38681800	-0.79845500	1.23831400
O	0.10080100	-0.99149600	-0.18573600
H	4.18855500	-1.59607800	-4.09791900
C	-2.04341000	-0.74939900	1.38357800
O	-2.55868500	-0.16472600	0.16628900
H	-1.38685900	1.90926200	-1.66159200
C	-0.76600200	-2.91402400	1.71662800
O	-2.10215500	-2.59756000	-0.16682100
H	-4.80323500	-0.14439000	-0.58570700
C	5.46436800	-2.24968700	1.77681100
C	2.98095200	-2.27967600	1.23876800
C	4.21692700	-0.02150500	1.70927300
C	6.73593700	-2.97421400	1.77196300
C	1.69783300	-0.02079800	1.34549800
C	8.33685200	-1.88734800	-5.89823700
C	5.82491800	-1.91755000	-6.29707600
C	7.08583600	0.29265100	-6.28837600
C	9.63037100	-2.62506600	-6.26640900
C	4.50887000	0.29858900	-6.26490500
C	8.31420800	-0.40919700	-6.28149200
O	8.32420000	-1.95149400	-4.41687700
H	6.51917500	-2.18867500	-3.14834500
C	7.05444400	-2.61834200	-6.28675700
O	6.13283200	-2.86162400	-2.54879000
H	3.73308300	-2.13547400	-0.57058500

C	5.80543600	-0.44265800	-5.90839800
O	5.78900700	-0.51368300	-4.43757800
H	5.83476700	0.43032300	-4.12221700
C	5.42460500	-0.80767200	1.26328000
O	5.18243100	-1.03998500	-0.16284500
H	9.11546100	-1.41459900	-4.13064100
C	2.98360400	-0.75491400	1.34652700
O	2.45804900	-0.18407200	0.13000500
C	4.25797800	-2.91162400	1.74000500
O	2.95762400	-2.62243300	-0.18562200
H	0.11574400	-0.07625900	-0.57281000
C	-2.12026700	2.08192900	1.76695400
C	-4.60350900	2.05218900	1.24238600
C	-3.36657500	4.30956800	1.71428800
C	-0.84953600	1.35581000	1.77430300
C	-5.88422300	4.30949900	1.35375400
C	0.74650500	2.44550700	-5.91908100
C	-1.76172200	2.41401900	-6.28839000
C	-0.50012300	4.62346100	-6.28653600
C	2.04508300	1.70550800	-6.27217600
C	-3.07670000	4.62938000	-6.26529600
C	0.72912000	3.92290500	-6.29560400
O	0.69056300	2.39307600	-4.44703900
H	-1.14007000	2.19218200	-3.15310600
C	-0.53300300	1.71182600	-6.30577700
O	-1.56707000	1.54571900	-2.55184100
H	-3.86785500	2.20973700	-0.57342900
C	-1.78297300	3.89109100	-5.90058100
O	-1.82450600	3.84978800	-4.42154800
H	-1.77167100	4.80598600	-4.13879500
C	-2.16104800	3.52628900	1.25920400
O	-2.41504600	3.32337900	-0.17494000
H	1.46776000	2.92569000	-4.12496500
C	-4.60039300	3.57666200	1.35224200
O	-5.12443200	4.15237400	0.13624200
C	-3.32592500	1.41898600	1.73710800
O	-4.62871200	1.70874700	-0.17836600
H	-7.44699400	4.24518000	-0.57381100
C	2.90765400	2.07877600	1.73004900
C	0.41250900	2.05508700	1.26251300
C	1.66474000	4.30918700	1.74167100
C	4.17697900	1.35389500	1.72898700
C	-0.85479300	4.31099200	1.38127200
C	5.78634400	2.43257000	-5.87301800
C	3.26726900	2.41178200	-6.25405800
C	4.52707100	4.62025800	-6.22672400
C	7.07152100	1.70674100	-6.29740700
C	1.95382700	4.62902600	-6.30113200
C	5.75630500	3.91858300	-6.22441100
O	5.78663300	2.31787400	-4.39673500
C	4.49570000	1.71046300	-6.25066300
H	1.08127700	2.23496400	-0.58198500
C	3.23220200	3.89068900	-5.87795100
O	3.13502000	3.83557600	-4.40168900
H	3.09988700	4.78170700	-4.09935500
C	2.85952800	3.53148800	1.24481000
O	2.57436400	3.33615300	-0.17482500
H	6.63011800	2.74209900	-4.08665600
C	0.42699100	3.57978300	1.38251200
O	-0.08676900	4.16566000	0.16538400
H	1.14762100	6.18430100	-1.65961500
C	1.70299800	1.41407800	1.70842200
O	0.33754400	1.72827200	-0.16190300
H	-2.36171200	4.24353800	-0.55139000
C	1.85019700	-1.34244700	-2.34483600

O	2.86912700	-1.93166800	-2.38448800
O	0.82518900	-0.76421300	-2.32710500
Tv	10.05394000	0.00000000	0.00000000
Tv	-5.11304100	8.65855000	0.00000000

S8. Complete lists in Ref. 58.

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J.Gaussian 09, Gaussian, Inc.: Wallingford, CT, **2009**.