Supporting Information for

The carbon chain growth during onset CVD graphene formation on γ-Al_2O_3 is promoted by unsaturated CH_2 ends

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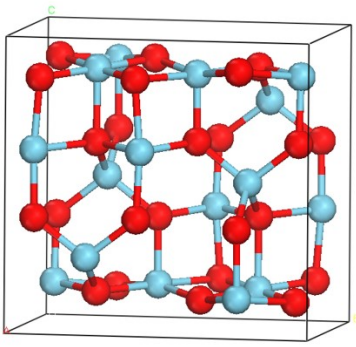
S1. Supplementary Figures



Crystallographic structure of bulk γ-alumina

Space group	P21/m	experimental value
a (Å)	5.538	5.587
b (Å)	8.347	8.413
c (Å)	8.024	8.068
β (°)	90.603	90.59
Atom	Position	(x, y, z)

Figure S1. The bulk cell of γ-Al_2O_3 (red and blue sphere represent the O anions and Al cations respectively).

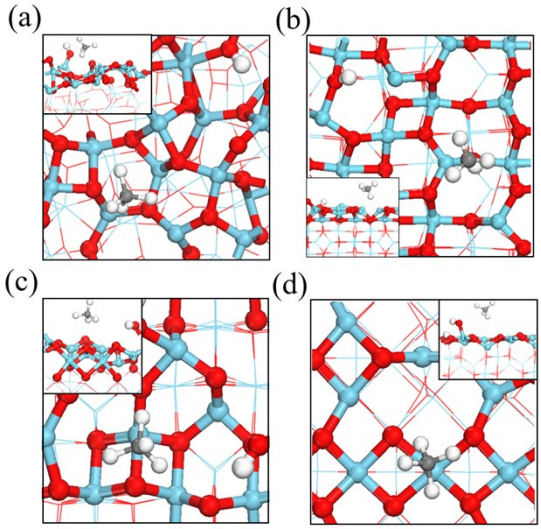


Figure S2. Top views of CH_4* adsorption models on **(a)** γ-Al_2O_3(111); **(b)** γ-Al_2O_3(110); **(c)** γ-Al_2O_3(100); **(d)** γ-Al_2O_3(001). The insets represent the corresponding side views. (Red, blue, grey, and white spheres represent the O, Al, C and H atoms, respectively).

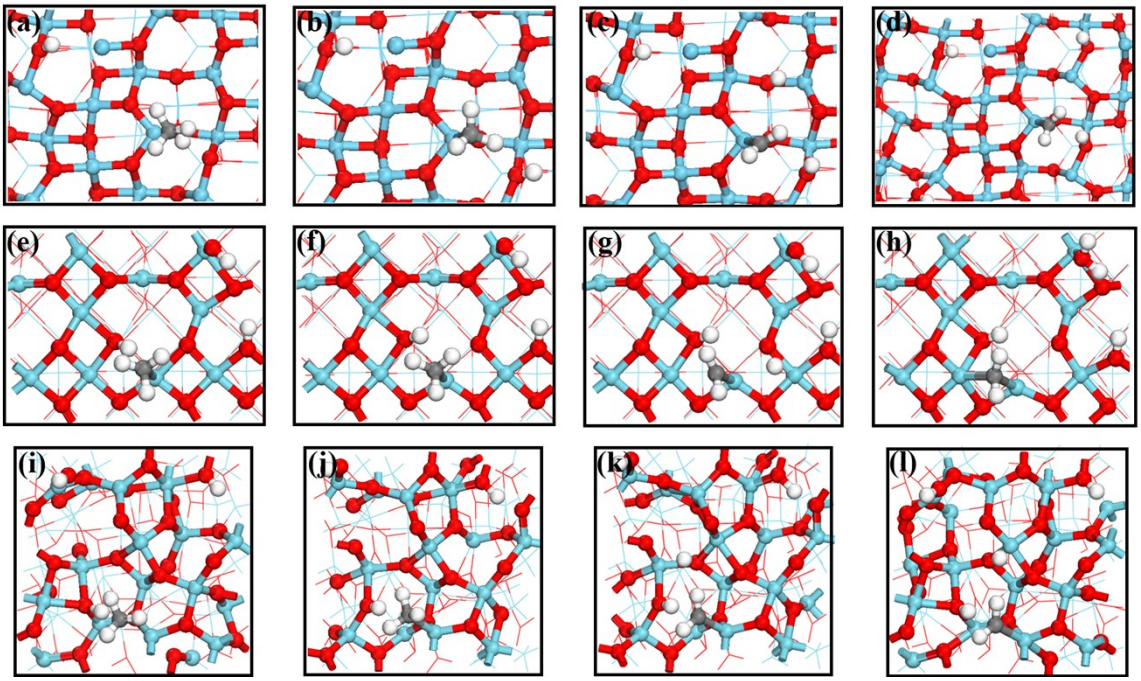


Figure S3. The structures include intermediates and translation states of the first two steps of the CH_4 dehydrogenation on γ-Al_2O_3 (110): **(a)** TS1; **(b)** CH_3; **(c)**TS2; **(d)** CH_2; γ-Al_2O_3 (001): **(e)** TS1; **(f)** CH_3; **(g)** TS2; **(h)** CH_2; and γ-Al_2O_3 (111): **(i)** TS1; **(j)** CH_3; **(k)**TS2; **(l)** CH_2. (Red, blue, grey, and white spheres represent the O, Al, C and H atoms, respectively).

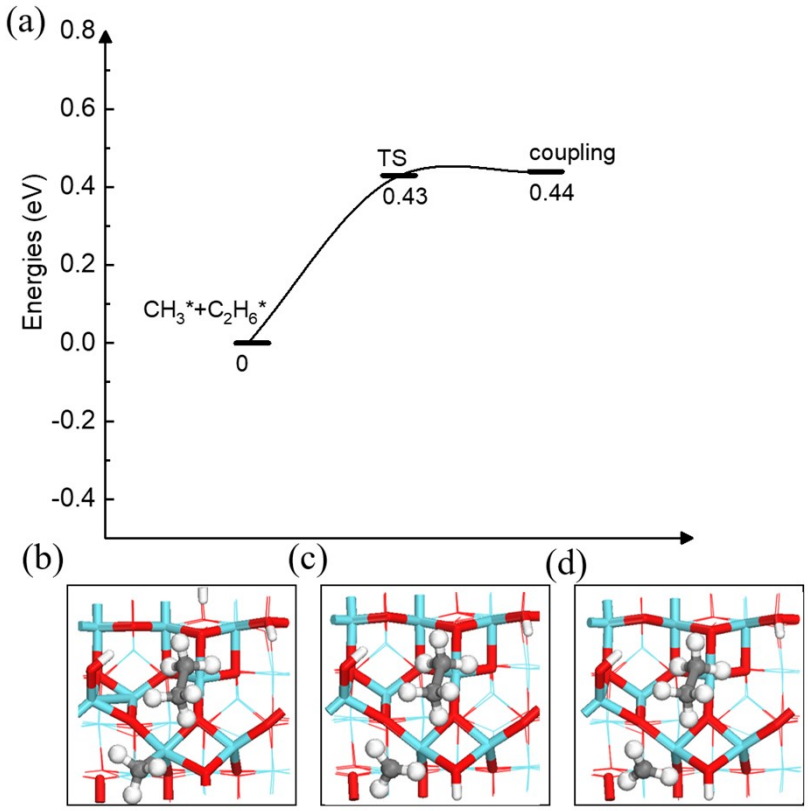


Figure S4. The energy diagram **(a)** for the C_2H_6* coupling with CH_3* reaction and corresponding structures **(b)** initial state; **(c)** translation state; **(d)** final state. (Red and blue sphere represent the O anions and Al cations respectively)

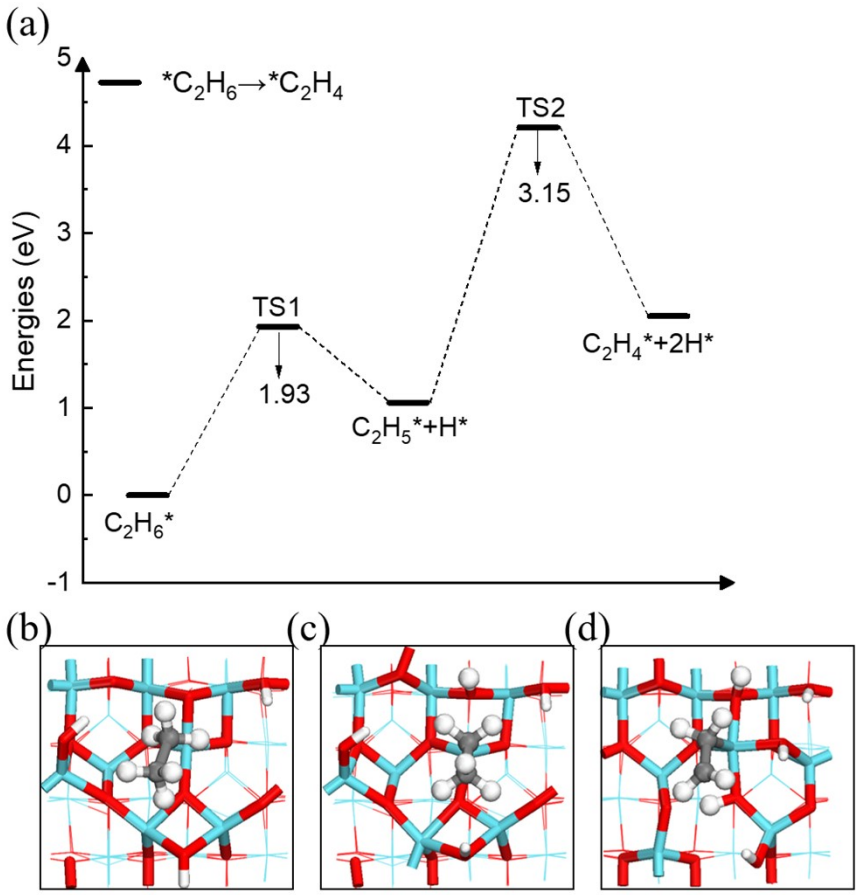


Figure S5. (a) The energy diagram of C_2H_6 dehydrogenation process. The structures of **(b)** C_2H_6*, **(c)** C_2H_5*+H*, and **(d)** C_2H_4*+2H* (Red and blue sphere represent the O anions and Al cations respectively)

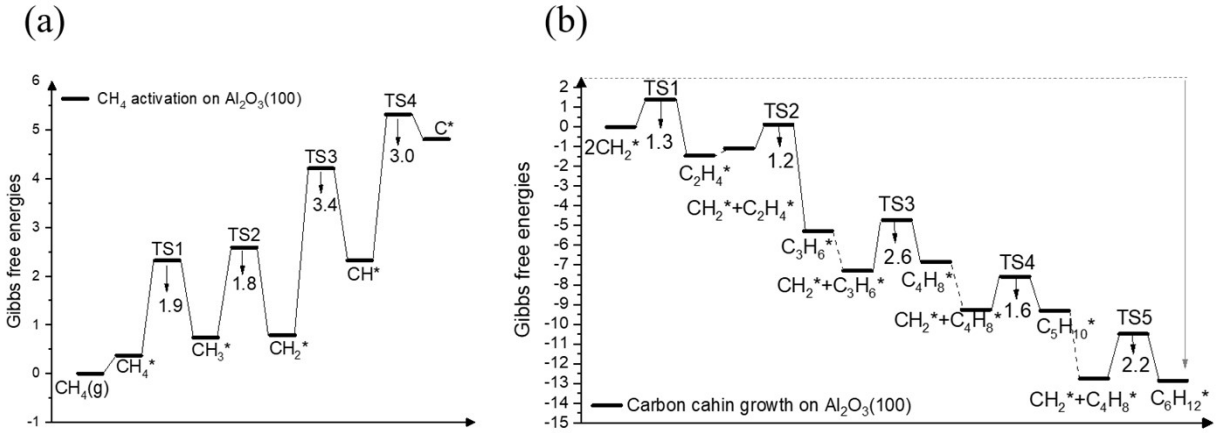


Figure S6. The Gibbs energy profile of the **(a)** complete CH_4* dehydrogenation and **(b)** formation of C_nH_{2n}* (n = 2-6) species via CH_2* coupling on the γ-Al_2O_3 (100) surface computed by performing frequency analysis for the intermediates and transition states at the experimental temperature of 1000K.

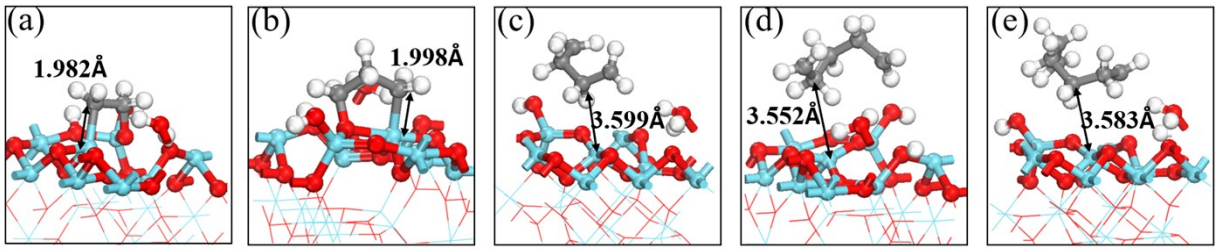


Figure S7. Structures and bond length between carbon end near surface and center sites of **(a)** C_2H_4*, **(b)** C_3H_6*, **(c)** C_4H_8*, **(d)** C_5H_{10}*, **(e)** C_6H_{12}* on the γ-Al_2O_3(100) surface. (Red and blue sphere represent the O anions and Al cations respectively)

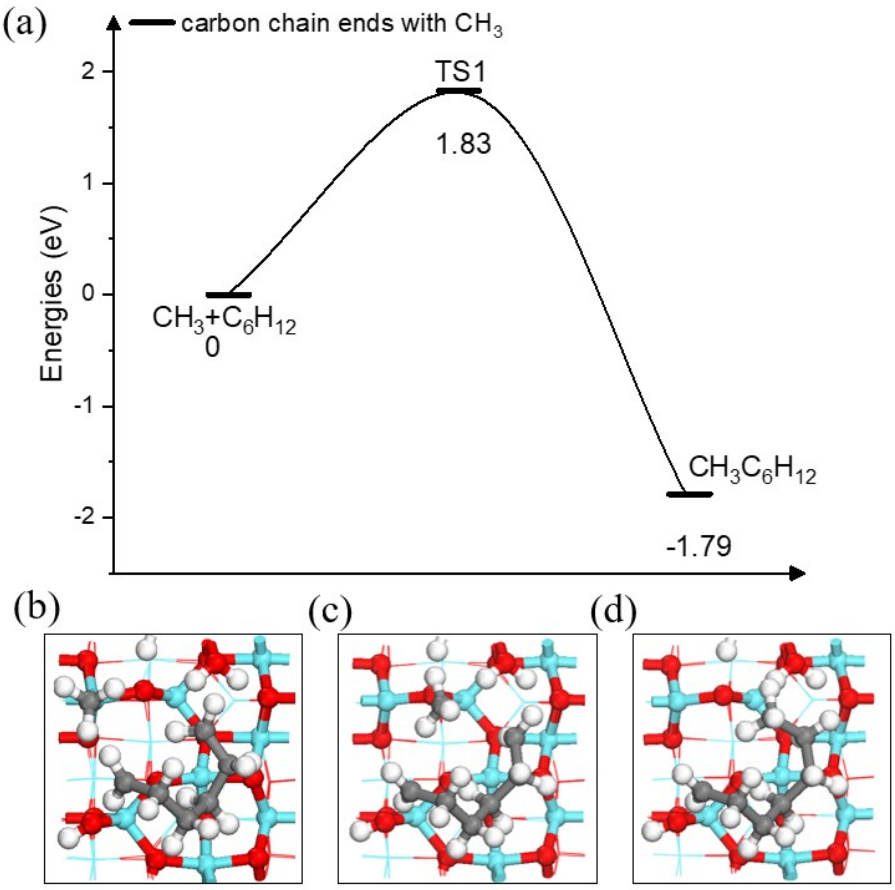


Figure S8. The **(a)** energy profiles for C_6H_{12}* chain ends with CH_3* and corresponding structures **(b)** C_6H_{12}*+CH_3*; **(c)** TS; **(d)** $CH_3C_6H_{12}$* on the γ-Al_2O_3(100) surface. (Red and blue sphere represent the O anions and Al cations respectively)

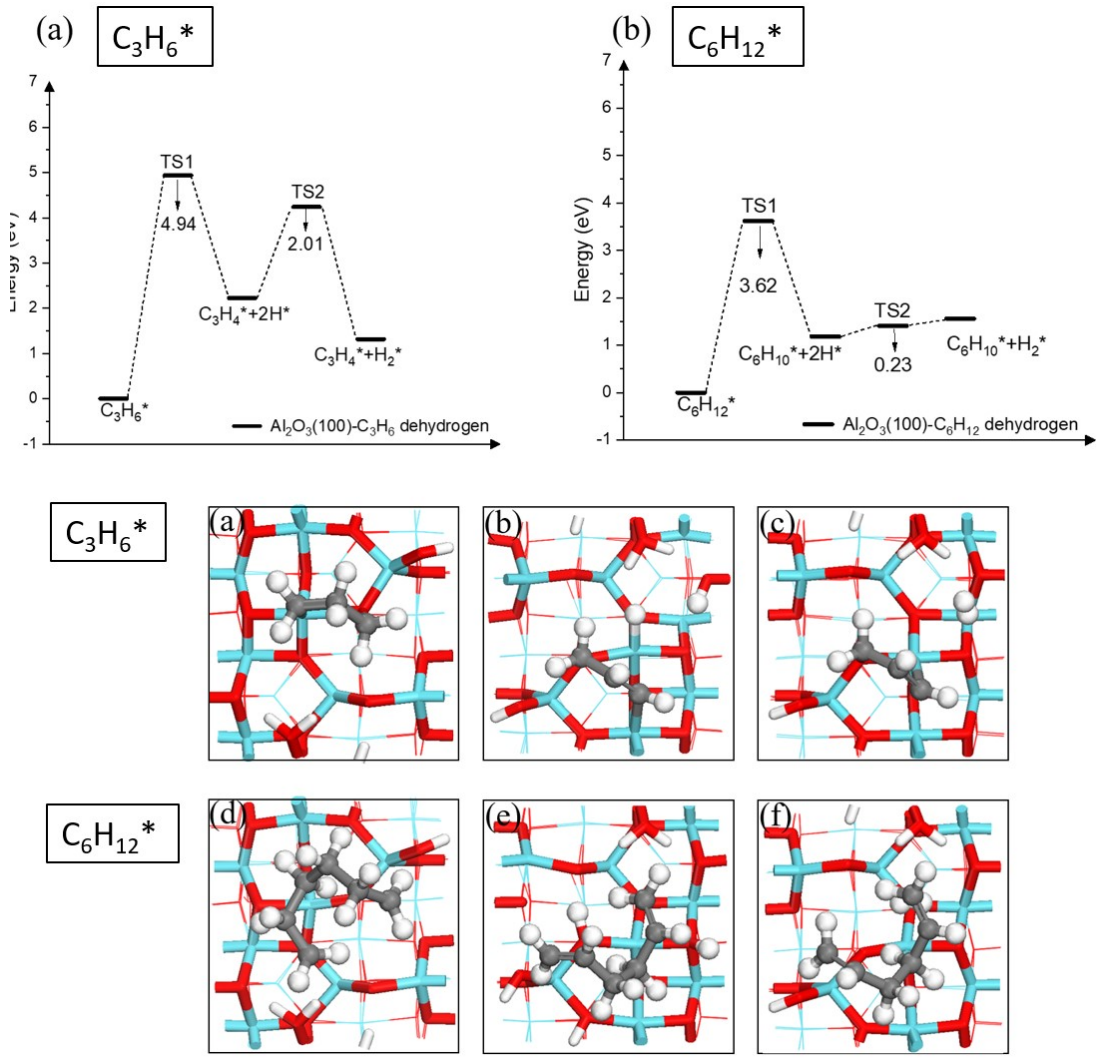


Figure S9. Upper panel: The energy profiles for the dehydrogenation of **(a)** C_3H_6* and **(b)** C_6H_{12}* on γ-Al_2O_3 (100) via a **concerted** pathway. **Lower panel:** Structures of the intermediates during the dehydrogenation of C_3H_6* on γ-Al_2O_3 (100): **(a)** C_3H_6*; **(b)** C_3H_4*+2H*; **(c)** C_3H_4*+H_2*. Structures during the dehydrogenation of C_6H_{12}* on γ-Al_2O_3 (100): **(d)** C_6H_{12}*; **(e)** C_6H_{10}*+2H*; **(f)** C_6H_{10}*+H_2* (Red and blue sphere represent the O anions and Al cations respectively).

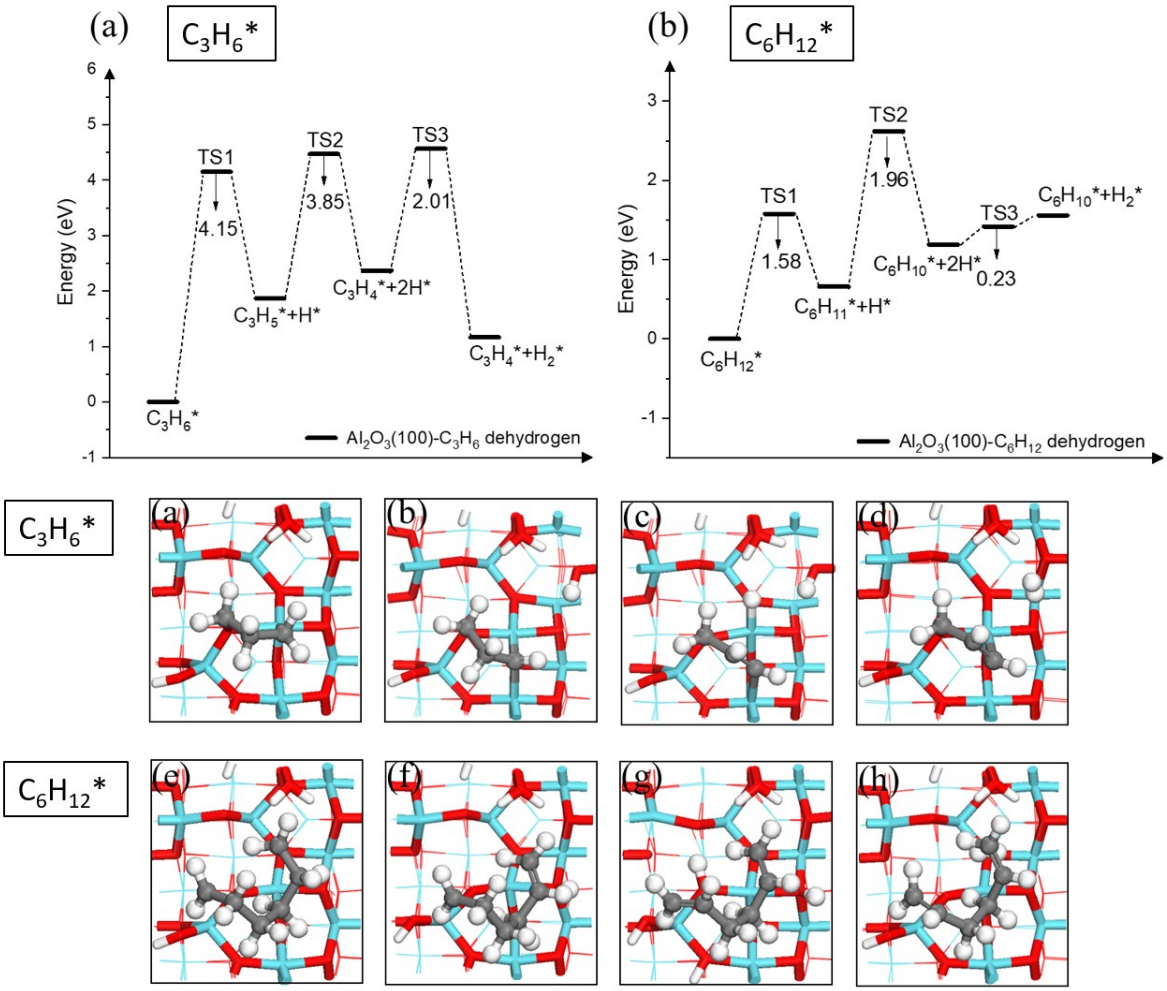


Figure S10. Upper panel: The energy profiles for the dehydrogenation of **(a)** C_3H_6* and **(b)** C_6H_{12}* on γ-Al_2O_3 (100) via a **stepwise** pathway. **Lower panel:** Structures of the intermediates during the dehydrogenation of C_3H_6* on γ-Al_2O_3 (100): **(a)** C_3H_6*; **(b)** C_3H_5*+H*; **(c)** C_3H_4*+2H*; **(d)** C_3H_4*+H_2*. Structures during the dehydrogenation of C_6H_{12}* on γ-Al_2O_3 (100): **(e)** C_6H_{12}*; **(f)** C_6H_{11}*+H*; **(g)** C_6H_{10}*+2H*; **(h)** C_6H_{10}*+H_2* (Red and blue sphere represent the O anions and Al cations respectively).

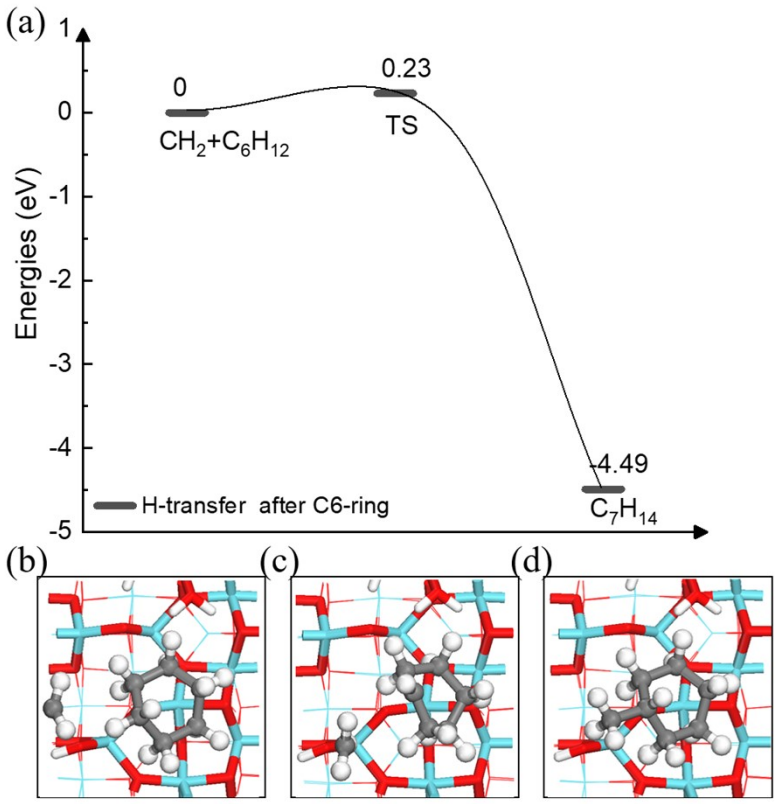


Figure S11. Energy diagram **(a)** for further H behaviour after carbon ring formation and corresponding structures **(b)** CH_2*+C_6H_{12}* ring; **(c)** TS; **(d)** $CH_2C_6H_{12}$*. (Red and blue sphere represent the O anions and Al cations respectively).

References

S1 G. Paglia, C. E. Buckley, A. L. Rohl, R. D. Hart, K. Winter, A. J. Studer, B. A. Hunter and J. V. Hanna, *Chemistry of Materials*, 2004, **16**, 220-236.

S2. J. Gu, J. Wang and J. Leszczynski, *ACS Omega*, 2018, **3**, 1881-1888.

S2. Optimized Structures from VASP Calculations

Coordinates: CH_4* adsorption on the γ-Al_2O_3 (111) surface in Figure S2.

cell_length_a		10.112600		
cell_length_b		9.829600		
cell_length_c		27.073799		
cell_angle_alpha		90.000000		
cell_angle_beta		90.000000		
cell_angle_gamma		90.000000		
cell_volume		2691.211970		
space_group_name_H-M_alt		'P 1'		
space_group_IT_number		1		
O1	1.0	0.819257	0.371908	0.089444
O2	1.0	0.018866	0.664535	0.254293
O3	1.0	0.247982	0.918766	0.410950
O4	1.0	0.256150	0.287974	0.066855
O5	1.0	0.417984	0.490382	0.197551
O6	1.0	0.648964	0.698980	0.393103
O7	1.0	0.510751	0.170797	0.054205
O8	1.0	0.690956	0.468741	0.197851
O9	1.0	0.882188	0.657524	0.348402
O10	1.0	0.031475	0.394091	0.047973
O11	1.0	0.234296	0.653838	0.205509
O12	1.0	0.444275	0.853149	0.362310
O13	1.0	0.062191	0.844296	0.045342
O14	1.0	0.255163	0.131917	0.203636
O15	1.0	0.476393	0.234819	0.357440
O16	1.0	0.632052	0.657766	0.007201
O17	1.0	0.682432	0.965955	0.230601
O18	1.0	0.947710	0.120050	0.332579
O19	1.0	0.278992	0.838751	0.094445
O20	1.0	0.449446	0.032651	0.252297
O21	1.0	0.733193	0.202116	0.418223
O22	1.0	0.016504	0.134210	0.229462
O23	1.0	0.816621	0.923384	0.086748
O24	1.0	0.097018	0.519382	0.396076
O25	1.0	0.666423	0.246776	0.145589
O26	1.0	0.863794	0.446051	0.270107
O27	1.0	-0.001652	0.775980	0.435845
O28	1.0	0.113521	0.593951	0.113528
O29	1.0	0.349496	0.820219	0.276053
O30	1.0	0.549099	0.990652	0.427082
O31	1.0	0.722533	0.294184	0.995741
O32	1.0	0.903016	0.588554	0.162489
O33	1.0	0.129342	0.804355	0.325466
O34	1.0	0.250618	0.041111	0.018704
O35	1.0	0.427240	0.250322	0.157915
O36	1.0	0.633461	0.477137	0.314429
O37	1.0	0.306843	0.609032	0.036583
O38	1.0	0.386880	0.855144	0.179233
O39	1.0	0.657349	0.036466	0.337789
O40	1.0	0.807942	0.845083	0.995227
O41	1.0	0.860213	0.073619	0.160965
O42	1.0	0.067098	0.350516	0.312745
O43	1.0	0.114343	0.070985	0.116820
O44	1.0	0.330629	0.308070	0.273145
O45	1.0	0.601661	0.441870	0.417682
O46	1.0	0.744914	0.788737	0.158743
O47	1.0	0.017405	0.186361	0.424501
O48	1.0	0.905377	0.920798	0.282566

O49	1.0	0.401289	0.320163	0.988908
O50	1.0	0.484915	0.670474	0.122460
O51	1.0	0.656944	0.789661	0.306305
O52	1.0	0.015837	0.297567	0.141734
O53	1.0	0.228099	0.558084	0.295268
O54	1.0	0.432439	0.721393	0.458853
O55	1.0	0.563866	0.991304	0.132170
O56	1.0	0.770524	0.216944	0.276530
O57	1.0	0.855781	0.514578	0.450621
O58	1.0	0.869470	0.510693	0.980853
O59	1.0	0.015000	0.825938	0.154877
O60	1.0	0.222550	0.060657	0.318060
O61	1.0	0.953615	0.142598	0.037927
O62	1.0	0.129259	0.416148	0.218040
O63	1.0	0.406030	0.540192	0.373967
O64	1.0	0.506136	0.456783	0.057786
O65	1.0	0.570329	0.703433	0.221152
O66	1.0	0.816329	0.935135	0.398533
O67	1.0	0.875685	0.643125	0.069663
O68	1.0	0.135030	0.911433	0.234294
O69	1.0	0.239712	0.321506	0.375628
O70	1.0	0.511349	0.833591	0.051992
O71	1.0	0.558967	0.290535	0.237912
O72	1.0	0.875482	0.365063	0.370093
O73	1.0	0.166963	0.933282	0.510193
O74	1.0	0.560651	0.941856	0.953501
Al1	1.0	0.182719	0.704565	0.068916
Al2	1.0	0.305762	0.958123	0.224179
Al3	1.0	0.592610	0.128491	0.389662
Al4	1.0	0.622508	0.846588	0.001426
Al5	1.0	0.715637	0.966361	0.165550
Al6	1.0	0.900123	0.290995	0.310459
Al7	1.0	0.179468	0.965496	0.069431
Al8	1.0	0.416232	0.195191	0.226515
Al9	1.0	0.522261	0.408669	0.359347
Al10	1.0	0.055758	0.033644	0.284755
Al11	1.0	0.876418	0.774601	0.115798
Al12	1.0	0.058477	0.329434	0.386714
Al13	1.0	0.568649	0.320331	0.018998
Al14	1.0	0.723567	0.639094	0.190576
Al15	1.0	0.962202	0.768679	0.307189
Al16	1.0	0.085172	0.236248	0.079355
Al17	1.0	0.290475	0.465413	0.240934
Al18	1.0	0.518456	0.609602	0.422376
Al19	1.0	0.837752	0.244092	0.136433
Al20	1.0	0.033392	0.483404	0.269491
Al21	1.0	0.122843	0.882074	0.452717
Al22	1.0	0.333100	0.432042	0.038209
Al23	1.0	0.418471	0.670596	0.184942
Al24	1.0	0.631148	0.874314	0.369350
Al25	1.0	0.533319	0.161082	0.118437
Al26	1.0	0.699021	0.378897	0.258644
Al27	1.0	0.953451	0.615743	0.412852
Al28	1.0	0.871831	0.326835	0.026200
Al29	1.0	0.068811	0.658453	0.175993
Al30	1.0	0.284018	0.894319	0.340115
Al31	1.0	0.451235	0.854644	0.114999
Al32	1.0	0.761791	0.037569	0.283558
Al33	1.0	0.771288	0.383199	0.422808
Al34	1.0	0.807873	0.660077	0.010311

Al35	1.0	0.025954	0.997820	0.176182
Al36	1.0	0.306421	0.217733	0.329200
Al37	1.0	0.349857	0.176602	0.025554
Al38	1.0	0.550914	0.371297	0.178914
Al39	1.0	0.707901	0.635389	0.334738
Al40	1.0	0.955909	0.495213	0.100750
Al41	1.0	0.195044	0.733717	0.265167
Al42	1.0	0.415025	0.875519	0.428115
Al43	1.0	0.910657	0.956810	0.035066
Al44	1.0	0.118445	0.247359	0.195999
Al45	1.0	0.240286	0.501089	0.359468
Al46	1.0	0.501091	0.642811	0.055719
Al47	1.0	0.545320	0.860492	0.256602
Al48	1.0	0.882685	0.107376	0.395867
H1	1.0	0.870359	0.868230	0.417605
H2	1.0	0.125096	0.903008	0.540340
H3	1.0	0.808788	0.477272	0.955545
H4	1.0	0.465380	0.945606	0.949755
H5	1.0	0.319328	0.243297	0.519734
H6	1.0	0.485666	0.280777	0.501274
H7	1.0	0.360935	0.242692	0.455820
H8	1.0	0.355284	0.399682	0.488716
C1	1.0	0.381059	0.291394	0.491451

Coordinates of CH_4* adsorbed on the γ-Al_2O_3 (110) surface in Figure S2.

cell_length_a		16.049000		
cell_length_b		11.076900		
cell_length_c		24.804501		
cell_angle_alpha		90.000000		
cell_angle_beta		90.000000		
cell_angle_gamma		90.000000		
cell_volume		4409.574405		
space_group_name_H-M_alt		'P 1'		
space_group_IT_number		1		
O1	1.0	0.435578	0.189526	0.118153
O2	1.0	0.042305	0.305995	0.277913
O3	1.0	0.043206	0.306161	0.174324
O4	1.0	0.437983	0.188407	0.341705
O5	1.0	0.179624	0.440593	0.341802
O6	1.0	0.297707	0.042371	0.168496
O7	1.0	0.297034	0.040976	0.285385
O8	1.0	0.183196	0.443590	0.114198
O9	1.0	0.064137	0.065748	0.174203
O10	1.0	0.416571	0.411991	0.344346
O11	1.0	0.422636	0.415619	0.115715
O12	1.0	0.062212	0.065736	0.278277
O13	1.0	0.305664	0.307463	0.285654
O14	1.0	0.175562	0.177150	0.114216
O15	1.0	0.172865	0.179687	0.340945
O16	1.0	0.306551	0.311209	0.171788
O17	1.0	0.428018	0.181883	0.228600
O18	1.0	0.065898	0.327268	0.055880
O19	1.0	0.050353	0.331398	0.397720
O20	1.0	0.171047	0.439625	0.227059
O21	1.0	0.318636	0.043769	0.058829
O22	1.0	0.320757	0.041788	0.393818
O23	1.0	0.038383	0.073593	0.059541
O24	1.0	0.034476	0.080077	0.391752
O25	1.0	0.432667	0.421556	0.229814

O26	1.0	0.310052	0.299853	0.060233
O27	1.0	0.303860	0.294009	0.398466
O28	1.0	0.177585	0.177293	0.227298
O29	1.0	0.176797	0.063637	0.440917
O30	1.0	0.674751	0.048355	0.012382
O31	1.0	0.946869	0.205104	0.110087
O32	1.0	0.541884	0.298097	0.281224
O33	1.0	0.542942	0.303333	0.175419
O34	1.0	0.941012	0.209972	0.340573
O35	1.0	0.683120	0.440601	0.342563
O36	1.0	0.795225	0.044186	0.169712
O37	1.0	0.797511	0.046875	0.283110
O38	1.0	0.679902	0.438283	0.120128
O39	1.0	0.561898	0.063024	0.175380
O40	1.0	0.917150	0.425603	0.338153
O41	1.0	0.911585	0.414630	0.108958
O42	1.0	0.564240	0.062903	0.280493
O43	1.0	0.807133	0.319758	0.282750
O44	1.0	0.668000	0.171912	0.113400
O45	1.0	0.672520	0.178432	0.341063
O46	1.0	0.805966	0.314932	0.167002
O47	1.0	0.925849	0.190431	0.225241
O48	1.0	0.544714	0.308179	0.065730
O49	1.0	0.545922	0.303778	0.396901
O50	1.0	0.672617	0.435784	0.229996
O51	1.0	0.822635	0.062791	0.061646
O52	1.0	0.825950	0.060711	0.391463
O53	1.0	0.528817	0.060384	0.064359
O54	1.0	0.535388	0.057176	0.391337
O55	1.0	0.932005	0.430746	0.224593
O56	1.0	0.770081	0.307776	0.047088
O57	1.0	0.809312	0.310257	0.397385
O58	1.0	0.677003	0.176135	0.226770
O59	1.0	0.441393	0.698264	0.113000
O60	1.0	0.042834	0.805179	0.278714
O61	1.0	0.041619	0.804170	0.174629
O62	1.0	0.446178	0.693295	0.341942
O63	1.0	0.180849	0.946103	0.341002
O64	1.0	0.299281	0.545169	0.169589
O65	1.0	0.296399	0.541425	0.286212
O66	1.0	0.180701	0.940759	0.113120
O67	1.0	0.062561	0.569004	0.173377
O68	1.0	0.414500	0.904865	0.344545
O69	1.0	0.413085	0.911109	0.112486
O70	1.0	0.061104	0.565526	0.278271
O71	1.0	0.306577	0.804641	0.286408
O72	1.0	0.173342	0.679683	0.113294
O73	1.0	0.171744	0.677535	0.340337
O74	1.0	0.306790	0.807524	0.172041
O75	1.0	0.427910	0.680621	0.227845
O76	1.0	0.045178	0.818629	0.059643
O77	1.0	0.048623	0.830160	0.395559
O78	1.0	0.171976	0.937358	0.227155
O79	1.0	0.323991	0.544256	0.061280
O80	1.0	0.320609	0.548799	0.394292
O81	1.0	0.032278	0.569802	0.062303
O82	1.0	0.033428	0.579298	0.392233
O83	1.0	0.433738	0.922701	0.228006
O84	1.0	0.303048	0.791364	0.057028
O85	1.0	0.270093	0.799439	0.404743

O86	1.0	0.177079	0.676828	0.227447
O87	1.0	0.933489	0.699251	0.112753
O88	1.0	0.542921	0.798655	0.278948
O89	1.0	0.541979	0.797281	0.174391
O90	1.0	0.937136	0.706001	0.340609
O91	1.0	0.686378	0.945073	0.340106
O92	1.0	0.795802	0.563557	0.168808
O93	1.0	0.795636	0.560663	0.286008
O94	1.0	0.682604	0.942059	0.112100
O95	1.0	0.561025	0.545504	0.175433
O96	1.0	0.919089	0.928325	0.335965
O97	1.0	0.917997	0.928484	0.115259
O98	1.0	0.561426	0.559077	0.280232
O99	1.0	0.804690	0.803169	0.285842
O100	1.0	0.672015	0.676873	0.118906
O101	1.0	0.674335	0.675017	0.336265
O102	1.0	0.804372	0.803941	0.167179
O103	1.0	0.926032	0.690779	0.226893
O104	1.0	0.550957	0.817748	0.053398
O105	1.0	0.563397	0.811354	0.396517
O106	1.0	0.670688	0.935753	0.226804
O107	1.0	0.815527	0.559111	0.065759
O108	1.0	0.820779	0.563837	0.387395
O109	1.0	0.537179	0.560930	0.068065
O110	1.0	0.536959	0.562286	0.393521
O111	1.0	0.930920	0.927723	0.226047
O112	1.0	0.809891	0.809469	0.062339
O113	1.0	0.811978	0.812128	0.390610
O114	1.0	0.672607	0.673774	0.227250
Al1	1.0	0.290889	0.417296	0.343529
Al2	1.0	0.183882	0.059155	0.167820
Al3	1.0	0.182645	0.061443	0.286344
Al4	1.0	0.293491	0.420160	0.113533
Al5	1.0	0.417925	0.300995	0.172946
Al6	1.0	0.065050	0.218402	0.344212
Al7	1.0	0.067124	0.210606	0.109409
Al8	1.0	0.417961	0.299371	0.285867
Al9	1.0	0.054545	0.438411	0.225315
Al10	1.0	0.421554	0.053419	0.082717
Al11	1.0	0.426250	0.046590	0.374414
Al12	1.0	0.239690	0.311075	0.228367
Al13	1.0	0.249821	0.167082	0.062044
Al14	1.0	0.245936	0.157790	0.394216
Al15	1.0	0.054735	0.183923	0.226196
Al16	1.0	0.427085	0.300917	0.056500
Al17	1.0	0.421188	0.298516	0.401227
Al18	1.0	0.122984	0.472824	0.053489
Al19	1.0	0.115538	0.469529	0.401332
Al20	1.0	0.359258	0.048723	0.227278
Al21	1.0	0.798382	0.935447	0.341636
Al22	1.0	0.680431	0.556683	0.171406
Al23	1.0	0.678458	0.554096	0.285506
Al24	1.0	0.796593	0.934546	0.111045
Al25	1.0	0.924173	0.809690	0.169891
Al26	1.0	0.565108	0.697808	0.342868
Al27	1.0	0.564800	0.706612	0.104996
Al28	1.0	0.924801	0.810451	0.282200
Al29	1.0	0.552433	0.928675	0.227925
Al30	1.0	0.925985	0.555242	0.078592
Al31	1.0	0.929846	0.562658	0.373044

Al32	1.0	0.737505	0.805971	0.226412
Al33	1.0	0.780366	0.686631	0.105593
Al34	1.0	0.782230	0.689686	0.347839
Al35	1.0	0.549219	0.676726	0.226225
Al36	1.0	0.927430	0.818643	0.055070
Al37	1.0	0.928833	0.822926	0.399291
Al38	1.0	0.608389	0.952079	0.058732
Al39	1.0	0.616481	0.949845	0.394388
Al40	1.0	0.861782	0.558225	0.226668
Al41	1.0	0.795931	0.424803	0.343220
Al42	1.0	0.681200	0.057090	0.167919
Al43	1.0	0.683100	0.060882	0.285490
Al44	1.0	0.788881	0.416767	0.106260
Al45	1.0	0.921628	0.308396	0.166209
Al46	1.0	0.559066	0.187522	0.343893
Al47	1.0	0.555737	0.182265	0.112776
Al48	1.0	0.921876	0.311039	0.281445
Al49	1.0	0.551317	0.427995	0.231742
Al50	1.0	0.931182	0.066714	0.078275
Al51	1.0	0.931877	0.066749	0.369179
Al52	1.0	0.742116	0.307748	0.225283
Al53	1.0	0.734185	0.156579	0.057422
Al54	1.0	0.751567	0.176603	0.390720
Al55	1.0	0.552274	0.179279	0.228128
Al56	1.0	0.956021	0.317780	0.040986
Al57	1.0	0.932188	0.321762	0.399226
Al58	1.0	0.574231	0.433986	0.104611
Al59	1.0	0.597689	0.436074	0.384489
Al60	1.0	0.861819	0.057699	0.225611
Al61	1.0	0.290965	0.911700	0.343520
Al62	1.0	0.184618	0.562866	0.167038
Al63	1.0	0.181272	0.558900	0.287545
Al64	1.0	0.290039	0.907820	0.111898
Al65	1.0	0.419766	0.801201	0.170792
Al66	1.0	0.063572	0.708829	0.344619
Al67	1.0	0.062291	0.697493	0.110446
Al68	1.0	0.420378	0.799218	0.286496
Al69	1.0	0.055658	0.937910	0.226305
Al70	1.0	0.426932	0.558184	0.082149
Al71	1.0	0.425616	0.557916	0.375211
Al72	1.0	0.240920	0.808251	0.228946
Al73	1.0	0.240075	0.652395	0.053624
Al74	1.0	0.229693	0.641644	0.402333
Al75	1.0	0.056296	0.683773	0.226905
Al76	1.0	0.419496	0.802578	0.052899
Al77	1.0	0.451085	0.805271	0.411586
Al78	1.0	0.107881	0.950609	0.060367
Al79	1.0	0.110287	0.964399	0.394174
Al80	1.0	0.359070	0.549369	0.228640
H1	1.0	0.140275	0.106158	0.465877
H2	1.0	0.309453	0.817019	0.434522
H3	1.0	0.715165	0.005115	0.990182
H4	1.0	0.819287	0.315095	0.021612
H5	1.0	0.610510	0.390681	0.516374
H6	1.0	0.635538	0.545346	0.500640
H7	1.0	0.714141	0.447304	0.527560
H8	1.0	0.681067	0.423561	0.461436
C1	1.0	0.658768	0.452427	0.501730

Coordinates of CH_4* adsorbed on the γ-Al_2O_3 (100) surface in Figure S2.

cell_length_a		8.070750		
cell_length_b		8.404430		
cell_length_c		26.383160		
cell_angle_alpha		90.000000		
cell_angle_beta		90.000000		
cell_angle_gamma		90.000000		
cell_volume		1789.571263		
space_group_name_H-M_alt		'P 1'		
space_group_IT_number		1		
H1	1.0	0.011995	0.411980	0.458362
H2	1.0	0.388516	0.757855	0.967723
H3	1.0	0.701996	0.310403	0.531470
H4	1.0	0.739848	0.517488	0.518411
H5	1.0	0.531436	0.443476	0.521332
H6	1.0	0.651554	0.458819	0.577695
H7	1.0	0.864255	0.321243	0.970611
H8	1.0	0.749368	0.868595	0.498552
C1	1.0	0.656831	0.432299	0.537025
O1	1.0	0.110355	0.590023	0.157307
O2	1.0	0.127574	0.579320	0.367007
O3	1.0	0.616367	0.906845	0.048312
O4	1.0	0.618793	0.916997	0.260781
O5	1.0	0.842993	0.412690	0.993249
O6	1.0	0.862823	0.412072	0.207481
O7	1.0	0.830288	0.416327	0.419013
O8	1.0	0.367782	0.101448	0.096769
O9	1.0	0.363075	0.085601	0.313034
O10	1.0	0.909850	0.096841	0.108340
O11	1.0	0.901975	0.110546	0.320052
O12	1.0	0.418243	0.424242	0.999535
O13	1.0	0.396020	0.420990	0.210599
O14	1.0	0.401479	0.440688	0.423466
O15	1.0	0.158528	0.913090	0.060366
O16	1.0	0.152330	0.907300	0.268427
O17	1.0	0.643793	0.580283	0.158147
O18	1.0	0.638861	0.601021	0.369084
O19	1.0	0.906940	0.403539	0.107200
O20	1.0	0.907963	0.412418	0.322125
O21	1.0	0.421012	0.084471	0.000490
O22	1.0	0.396501	0.084787	0.212795
O23	1.0	0.425799	0.132068	0.443652
O24	1.0	0.156529	0.596839	0.059345
O25	1.0	0.156970	0.596681	0.269381
O26	1.0	0.643594	0.920681	0.159702
O27	1.0	0.647280	0.915096	0.384065
O28	1.0	0.112204	0.911557	0.158119
O29	1.0	0.103082	0.923220	0.366950
O30	1.0	0.616698	0.602830	0.047033
O31	1.0	0.618404	0.589566	0.258341
O32	1.0	0.845029	0.117150	0.998252
O33	1.0	0.863178	0.090741	0.207056
O34	1.0	0.847355	0.094149	0.425274
O35	1.0	0.366119	0.408225	0.095512
O36	1.0	0.369909	0.411785	0.310746
O37	1.0	0.137682	0.252628	0.157589
O38	1.0	0.140569	0.251312	0.371687
O39	1.0	0.638326	0.257541	0.057404
O40	1.0	0.647067	0.253191	0.260571

O41	1.0	0.890991	0.752512	0.109077
O42	1.0	0.894782	0.740319	0.320262
O43	1.0	0.330025	0.755498	-0.000068
O44	1.0	0.363326	0.752439	0.213206
O45	1.0	0.355803	0.754586	0.425805
O46	1.0	0.900105	0.756489	0.999731
O47	1.0	0.894823	0.750912	0.210329
O48	1.0	0.916333	0.729148	0.424727
O49	1.0	0.383126	0.753032	0.104044
O50	1.0	0.382787	0.755529	0.316090
O51	1.0	0.122474	0.255618	0.053593
O52	1.0	0.114414	0.257124	0.266400
O53	1.0	0.645264	0.251118	0.163344
O54	1.0	0.633729	0.259415	0.366352
O55	1.0	0.134978	0.417864	0.462110
O56	1.0	0.649978	0.933993	0.498296
Al1	1.0	0.393827	0.924909	0.055948
Al2	1.0	0.388279	0.925025	0.268401
Al3	1.0	0.137210	0.423706	0.111502
Al4	1.0	0.141260	0.417668	0.320981
Al5	1.0	0.637077	0.428391	0.013607
Al6	1.0	0.622266	0.427525	0.213232
Al7	1.0	0.608572	0.429243	0.405775
Al8	1.0	0.869882	0.920728	0.162404
Al9	1.0	0.888687	0.909175	0.393135
Al10	1.0	0.643419	0.078865	0.013214
Al11	1.0	0.625276	0.075739	0.214196
Al12	1.0	0.617303	0.033912	0.441223
Al13	1.0	0.869510	0.582630	0.161945
Al14	1.0	0.870450	0.590419	0.375990
Al15	1.0	0.391889	0.585678	0.054972
Al16	1.0	0.392415	0.581705	0.269190
Al17	1.0	0.140791	0.079366	0.113529
Al18	1.0	0.131958	0.082379	0.323834
Al19	1.0	0.896264	0.242999	0.053073
Al20	1.0	0.880673	0.261988	0.272415
Al21	1.0	0.506331	0.256924	0.115619
Al22	1.0	0.502555	0.244628	0.315852
Al23	1.0	0.882906	0.251160	0.161435
Al24	1.0	0.865463	0.243667	0.376900
Al25	1.0	0.101850	0.757194	0.015675
Al26	1.0	0.130473	0.750847	0.221439
Al27	1.0	0.233448	0.589176	0.428065
Al28	1.0	0.514249	0.750595	0.164254
Al29	1.0	0.500707	0.763878	0.377911
Al30	1.0	0.138870	0.751935	0.113515
Al31	1.0	0.130781	0.757184	0.325564
Al32	1.0	0.768441	0.755528	0.052162
Al33	1.0	0.753796	0.752181	0.270864
Al34	1.0	0.324773	0.254093	0.029223
Al35	1.0	0.265788	0.253636	0.218239
Al36	1.0	0.274648	0.266707	0.429159

Coordinates of CH_4* adsorbed on the γ-Al_2O_3 (001) surface in Figure S2.

cell_length_a	11.076900
cell_length_b	8.346800
cell_length_c	26.206800
cell_angle_alpha	90.000000
cell_angle_beta	90.000000

cell_angle_gamma 90.000000
cell_volume 2422.993327
space_group_name_H-M_alt 'P 1'
space_group_IT_number 1

O1	1.0	0.197385	0.403294	0.121937
O2	1.0	0.203463	0.394172	0.430501
O3	1.0	0.308883	0.902940	0.184585
O4	1.0	0.308845	0.592514	0.184394
O5	1.0	0.197954	0.090600	0.121867
O6	1.0	0.203928	0.090638	0.430269
O7	1.0	0.448244	0.082092	0.270446
O8	1.0	0.056539	0.597191	0.026875
O9	1.0	0.045917	0.572461	0.340170
O10	1.0	0.056279	0.896614	0.026744
O11	1.0	0.048177	0.903293	0.343229
O12	1.0	0.448559	0.418511	0.270172
O13	1.0	0.072532	0.591392	0.196025
O14	1.0	0.430855	0.085588	0.109248
O15	1.0	0.439357	0.099896	0.415889
O16	1.0	0.430610	0.409476	0.109388
O17	1.0	0.435371	0.405229	0.416292
O18	1.0	0.071915	0.905025	0.196994
O19	1.0	0.305317	0.901875	0.039729
O20	1.0	0.312169	0.919743	0.345250
O21	1.0	0.184349	0.417198	0.263877
O22	1.0	0.181865	0.078525	0.265084
O23	1.0	0.305378	0.592545	0.039956
O24	1.0	0.312132	0.575644	0.345220
O25	1.0	0.199460	0.747784	0.112985
O26	1.0	0.174190	0.738943	0.420711
O27	1.0	0.312595	0.247388	0.190775
O28	1.0	0.443970	0.748974	0.262382
O29	1.0	0.079707	0.246722	0.042174
O30	1.0	0.059470	0.251361	0.348589
O31	1.0	0.073651	0.244351	0.188364
O32	1.0	0.437801	0.747586	0.118126
O33	1.0	0.398686	0.748849	0.425208
O34	1.0	0.323910	0.247462	0.035712
O35	1.0	0.320387	0.248555	0.344164
O36	1.0	0.181233	0.747178	0.266253
O37	1.0	0.701140	0.401631	0.117885
O38	1.0	0.704553	0.405646	0.428426
O39	1.0	0.807867	0.905015	0.183338
O40	1.0	0.807893	0.590411	0.183348
O41	1.0	0.700375	0.092338	0.117499
O42	1.0	0.693383	0.110586	0.428589
O43	1.0	0.945227	0.075786	0.274027
O44	1.0	0.525267	0.596238	0.026960
O45	1.0	0.548931	0.586363	0.341678
O46	1.0	0.525897	0.899353	0.027637
O47	1.0	0.548148	0.916054	0.340923
O48	1.0	0.947952	0.412881	0.266908
O49	1.0	0.573935	0.591234	0.196673
O50	1.0	0.940449	0.091386	0.109535
O51	1.0	0.939837	0.097677	0.416101
O52	1.0	0.940803	0.401568	0.109772
O53	1.0	0.952024	0.375363	0.436880
O54	1.0	0.573742	0.906022	0.196518
O55	1.0	0.834886	0.917142	0.041316
O56	1.0	0.813976	0.909568	0.354451

O57	1.0	0.684353	0.415224	0.263246
O58	1.0	0.685432	0.079866	0.264138
O59	1.0	0.835247	0.576334	0.041571
O60	1.0	0.809412	0.569400	0.342594
O61	1.0	0.693803	0.747143	0.113040
O62	1.0	0.667150	0.752187	0.420802
O63	1.0	0.810797	0.244475	0.190699
O64	1.0	0.941959	0.747453	0.262244
O65	1.0	0.548655	0.248020	0.041025
O66	1.0	0.560338	0.253587	0.346305
O67	1.0	0.573089	0.247648	0.184329
O68	1.0	0.926625	0.747479	0.116189
O69	1.0	0.910821	0.681562	0.426302
O70	1.0	0.860949	0.246973	0.031499
O71	1.0	0.822990	0.251769	0.346675
O72	1.0	0.683478	0.750461	0.266668
O73	1.0	0.359662	0.760837	0.943739
O74	1.0	0.815916	0.920266	0.491672
Al1	1.0	0.438763	0.080682	0.038191
Al2	1.0	0.434604	0.074146	0.340912
Al3	1.0	0.066046	0.574404	0.269985
Al4	1.0	0.064842	0.918936	0.272791
Al5	1.0	0.438260	0.414750	0.038444
Al6	1.0	0.435117	0.425242	0.340205
Al7	1.0	0.312889	0.577056	0.112370
Al8	1.0	0.288385	0.578805	0.413500
Al9	1.0	0.195140	0.074940	0.196076
Al10	1.0	0.194847	0.419172	0.195232
Al11	1.0	0.312922	0.918274	0.112280
Al12	1.0	0.280421	0.904088	0.412313
Al13	1.0	0.442612	0.747390	0.191113
Al14	1.0	0.066641	0.245840	0.117636
Al15	1.0	0.077750	0.234948	0.418861
Al16	1.0	0.407973	0.748633	0.005825
Al17	1.0	0.313471	0.747501	0.304899
Al18	1.0	0.186734	0.249543	0.305026
Al19	1.0	0.187667	0.748221	0.189055
Al20	1.0	0.315348	0.247203	0.113888
Al21	1.0	0.318552	0.245783	0.417553
Al22	1.0	0.446542	0.249804	0.229909
Al23	1.0	0.172797	0.747268	0.042402
Al24	1.0	0.035770	0.732546	0.385547
Al25	1.0	0.957292	0.068164	0.038185
Al26	1.0	0.933240	0.063268	0.345337
Al27	1.0	0.568141	0.574810	0.271449
Al28	1.0	0.566133	0.923874	0.271306
Al29	1.0	0.957710	0.425347	0.038446
Al30	1.0	0.931071	0.418673	0.334074
Al31	1.0	0.813722	0.573823	0.110850
Al32	1.0	0.766941	0.593102	0.408312
Al33	1.0	0.695761	0.078138	0.194130
Al34	1.0	0.697760	0.416083	0.194001
Al35	1.0	0.812888	0.920368	0.110587
Al36	1.0	0.773560	0.919574	0.427277
Al37	1.0	0.942406	0.748316	0.188674
Al38	1.0	0.570703	0.246989	0.111157
Al39	1.0	0.572407	0.253962	0.416290
Al40	1.0	0.936217	0.746864	0.041050
Al41	1.0	0.814077	0.753605	0.307115
Al42	1.0	0.689885	0.248784	0.304960

Al43	1.0	0.690243	0.747907	0.191394
Al44	1.0	0.819071	0.246675	0.103179
Al45	1.0	0.817726	0.247219	0.422060
Al46	1.0	0.942345	0.237535	0.230153
Al47	1.0	0.567945	0.747416	0.072896
Al48	1.0	0.532732	0.753837	0.384777
H1	1.0	0.955066	0.494613	0.443280
H2	1.0	0.168741	0.246710	0.032412
H3	1.0	0.396374	0.710091	0.914529
H4	1.0	0.879558	0.845403	0.500141
H5	1.0	0.528618	0.370960	0.516064
H6	1.0	0.477320	0.287824	0.574853
H7	1.0	0.565803	0.165761	0.532787
H8	1.0	0.634607	0.329955	0.565450
C1	1.0	0.551490	0.287836	0.547121