Electronic Supplementary Information for

Porous Nanographene Formation on γ-Alumina Nanoparticles *via* Transition-Metal-Free Methane Activation

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S1. Materials and Methods

S1.1 Sample

Methane (CH_4) was purchased from Sumitomo Seika Chemicals Co.,Ltd. with Pure grade (>99.0%) and SEG grade (>99.99%). Deuterated methane (CD_4, 99%-*d*) was purchased from Cambridge Isotope Laboratories, Inc. (DLM-144-PK, Lot: l-23094/E10089963). High purity γ-alumina nanoparticles (ANPs, TH 80/170; γ-Al_2O_3, particle size: ~10 nm, specific surface area: 158 $m^2\ g^{-1}$) were donated from Sasol Limited. with Na (equivalent to Na_2O) = 20 ppm and Fe (equivalent to Fe_2O_3) = 50–100 ppm. All the chemicals were used as received unless otherwise noted.

S1.2 Reaction Kinetics

Thermogravimetry was conducted on a thermogravimeter (Netzsch, STA 2500 *Regulus*) under a steady flow of He with various concentration of CH_4 at the total flow rate of 100 mL min^{-1}. The standard reactor volume was 50 mL. To suppress air contamination during the analysis, the thermogravimeter was surrounded by a chamber filled with Ar gas supplied at a flow rate of 1 L min^{-1}. Typically, 32 mg of γ-ANPs was used for the kinetic analysis of CH_4-CVD. The samples were loaded on the reactor of the thermogravimeter, and first heated from room temperature to a specified temperature (1128 – 1173 K) at 10 K min^{-1} under a steady flow of He. This was followed by the constant-temperature heating at the specified temperature for 30 min under a steady flow of He. After the pretreatment, CH_4 was introduced to the reactor with a specified partial pressure to initiate CH_4-CVD. The rate of CH_4-CVD for the kinetic analysis of the first-layer deposition was determined at an inflection point. Formation of nanoporous graphene was confirmed by x-ray diffraction and Raman spectroscopy (Figure S1).

S1.3 Characterization of γ-Al_2O_3 Nanoparticles

High resolution annular dark-field scanning transmission electron microscopy (ADF-STEM) images were captured using JEM-ARM200-F (JEOL Ltd, Japan) at an accelerating voltage of 200kV.

In situ infrared (IR) spectra of the Al_2O_3 nanoparticles (ca. 18.0 mg) at the specified temperature were recorded on a Nicolet 6700 FT-IR spectrometer (ThermoScientific) with a diffuse reflectance infrared Fourier transform (DRIFT) method under a steady flow of Ar at 30 mL min^{-1}. The intensity was reported as the Kubelka-Munk function.[S1] The temperature of the sample during the *in-situ* IR measurements was monitored by using an infrared thermometer (Keyence, FT-H40K) to ensure the temperature. We performed 120 scans.

Temperature programmed desorption (TPD) was measured on a gas chromatogram (GC, Varian 490-GC, GL Science). Approximately 1 g of γ-ANP was gently packed in a quartz reactor tube with stacked height of 3~4 cm using quartz wool (4-9 μm, Toso Company, Ltd.). The reactor tube was heated at the rate of 10 K min^{-1} under a steady flow of He (200 mL min^{-1}), and the evolved H_2O was analyzed by GC. The sampling interval was approximately 2.5 min.

TPD of H_2O was immediately followed by TPD of NH_3 with the same configuration of experiment. All the processes are under a steady flow at a total flow rate of 200 mL min^{-1}. After cooling to r.t. under He, a mixture of 1.0% of NH_3 and 99% of He was introduced to the quartz reactor tube for 30 min. Then, the reactor tube was subjected to a steady flow of 100% He for 60 min to remove off the gas-phase NH_3. The reactor tube was then heated at the rate of 5 K min^{-1} under a steady flow of He, and the desorbed NH_3 was analyzed by GC.

Magic-angle-spinning (MAS) ^{27}Al nuclear magnetic resonance (NMR) of solid samples were recorded on a JEOL ECA800 (208 MHz) spectrometer. Samples were spun at 25 kHz. The data acquisition employed short radiofrequency pulses (18º flip angle) with relaxation delays of 10 s. The chemical shifts have been reported in δ ppm units with reference to an external standard of a 1 M aqueous solution of aluminium nitrate ($Al(NO_3)_3$, 0.00 ppm).

S1.4 Quantum Chemistry Calculations

Density functional theory (DFT) calculations on γ-Al_2O_3 surfaces with methane were performed by using the "Vienna *ab initio* simulation package" (VASP, version 6.1.1).[S2] We performed geometry optimization of local minima (EQs) and transition states (TSs) with the Perdew–Burke–Ernzerhof (PBE) generalized-gradient approximation (GGA) for the exchange and correlation terms,[S3] together with the Grimme's-D3 dispersion correction.[S4] A plane-wave basis set was employed within the framework of the projector augmented wave method.[S5,S6] The plane-wave cutoff was 450 eV. K-point mesh ware sampled by the (3×3×1) Monkhorst-Pack *k*-point sampling scheme. We used the threshold of self-consistent field energy calculation of 1.0×10^{-6} eV $atom^{-1}$.

The surface of γ-Al_2O_3 was modeled using a supercell approach with periodic boundary conditions. To generate the surface models, we first optimized the internal coordinates and cell parameters of the bulk structure of γ-Al_2O_3. As a starting point, we used the coordinates of γ-Al_2O_3 ($P2_1/m$ space group).[S9] The optimized lattice parameters of γ-Al_2O_3 were found to be a = 5.538 Å, b = 8.347 Å, c = 8.024 Å, β = 90.60 deg and $\alpha = \gamma$ = 90.00 deg, in good agreement with previous DFT calculations using the dual-range local meta-GGA ML-11 functional and the meta non-separable gradient approximation MN12-L functionals.[S7] Starting from the optimized structure, we constructed a partially hydrated γ-Al_2O_3 (100) surface with an oxygen vacancy as a surface slab containing 96 atoms (corresponding to 4 atomic layers) with a thickness of 12 Å and a vacuum of 15 Å. The initial surface hydration was 7.1 μmol m^{-2}. During the structural optimization for γ-Al_2O_3, the all atoms were relaxed. The structure of the triclinic surface unit cell was a = 8.071 Å, b = 8.404 Å, c = 26.383 Å, and $\alpha = \beta = \gamma$ = 90.00 deg.

TSs for the elementary reactions were located by using the climbing image nudged elastic band (CI-NEB) method.[S8,S9] The convergence of forces for the geometry optimizations of both EQs and TSs were set to be 0.03 eV $Å^{-1}$. All optimized structures are collected in S3 according to the POSCAR format for VASP.

The VASPKIT was used to deal with the charge density and the spin density.[S10]Atomistic models of alumina surfaces were constructed according to the results of ADF-STEM, TPD, and IR analysis of γ-ANPs. Previous DFT calculations suggest that (100) and (110) surfaces are the most stable surface of γ-Al_2O_3,[S11] and indeed the high-resolution ADF-STEM of γ-ANPs (Figure 2) shows the presence of {100} surfaces. Significant desorption of water upon heating [S11,S12] was confirmed by TPD (Figure 3b), while isolated hydroxyl groups at around 3701 cm^{-1} were confirmed by IR (Figure 3a) to remain even after annealing at 900 ºC for 30

min. Indeed, introduction of hydroxyl groups on surface models gave both thermodynamically and kinetically favored process in CH_4 activation on surfaces of γ-Al_2O_3.[S12,13]

S2. Supplementary Figures, Tables, and Discussions

S2.1 Characterization of Nano-Porous Graphene (**NPG**)

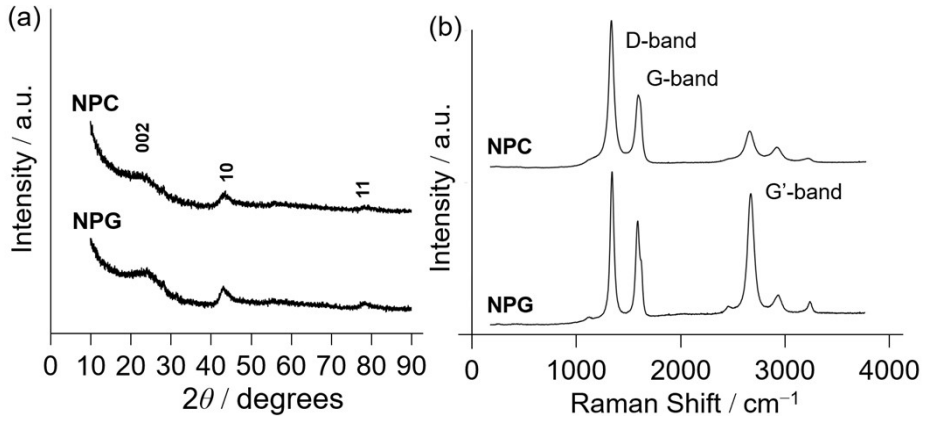

Figure S1. (a) XRD patterns and (b) Raman spectra of nano-porous carbon (**NPC**) and nano-porous graphene (**NPG**).

NPG was prepared and characterized by N_2 physisorption, XRD, and Raman spectroscopy. The specific surface area of **NPC** was determined by N_2 physisorption and the subsequent BET analysis to be 2.3×10^3 m^2 g^{-1}, while **NPG** gave 1.8×10^3 m^2 g^{-1}. These values are well approaching to an ideal value for 2-dimensional graphene (2627 m^2 g^{-1}). Single-layered deposition by CH_4-CVD with a specified reaction time was also confirmed by TEM.[S14] Both XRD and Raman showed single-walled nature of **NPG**: The suppressed 002 peaks at $2\theta = 22^\circ$ for carbons indicates the fewer stacking of graphene layer, while sharp peaks for 10 at $2\theta = 43^\circ$ indicates the successful growth of hexagons (nanographene) developed in a 2D plane.[S14] Raman spectra of **NPG** showed an intensified and red-shifted G'-band, supporting the growth of single-walled graphene structures[S14-S16] in **NPG** after annealing.

S2.2 Reductive treatment of ANP by H_2 before CH_4-CVD

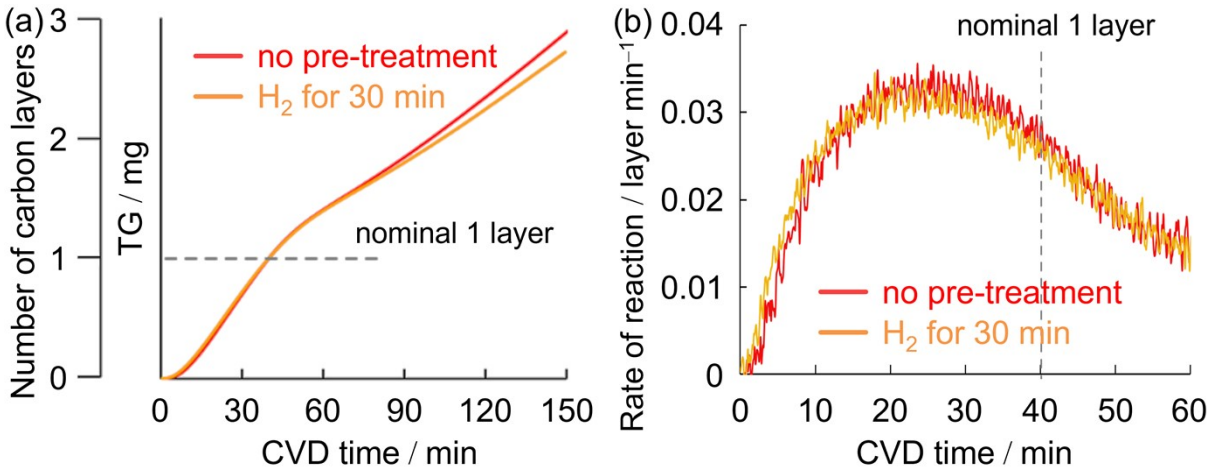

Figure S2. Kinetic analysis of CH_4-CVD for porous nanographene with or without pre-treatment of H_2 gas before CH_4-CVD. For the control experiment, He was introduced instead of H_2 for the same period. (a) Weight changes during CH_4-CVD at 900°C as monitored by TG. CH_4 was introduced to the reactor at 0 min. (b) The rate of reaction for CH_4-CVD.

S2.3 Surface Characterization by STEM

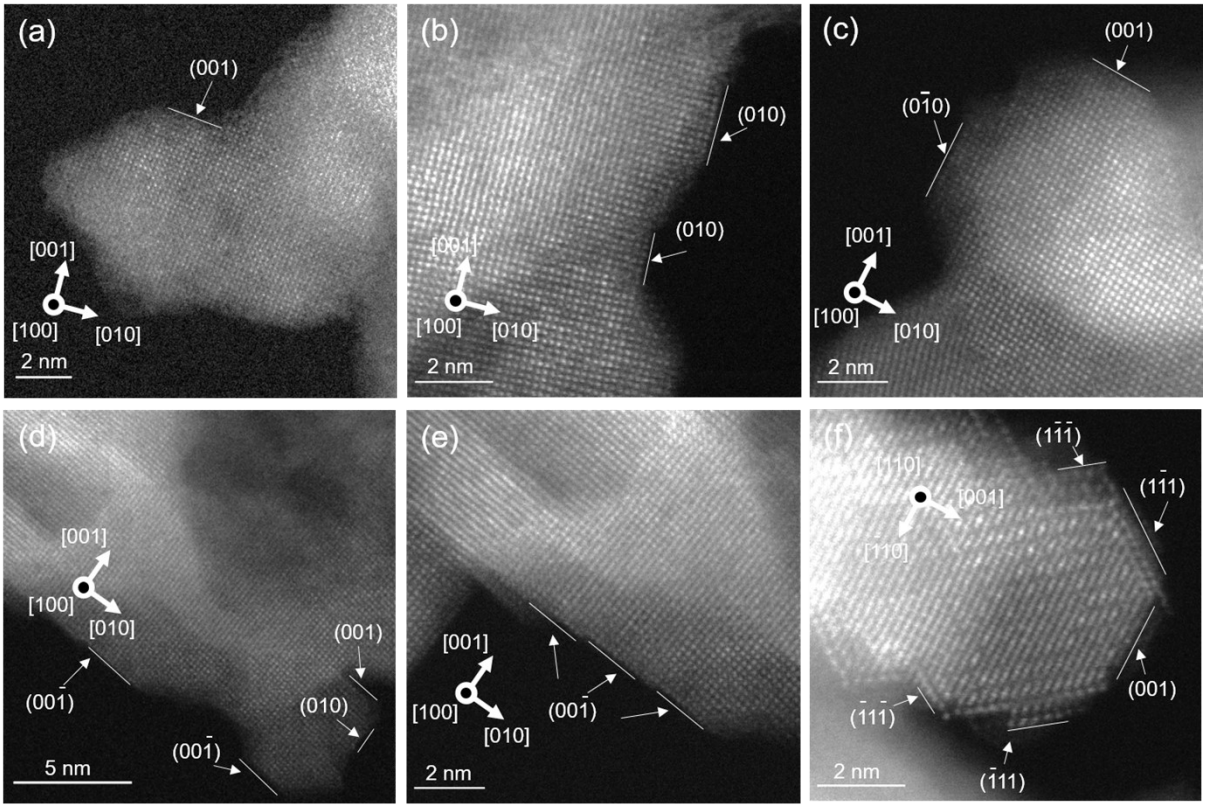

Figure S3. High resolution STEM-ADF image of γ-ANPs. (a–e) [100] orientation, and (f) [110] orientation.

S2.4 Stability of Surface OH groups toward Surface Activation

In order to analyze the stability of the OH groups on the γ-ANP surface for the surface activation, we performed the *in-situ* IR experiments under a steady flow of CD_4. We find that almost all protons are labile in the presence of CD_4 at temperatures higher than 600 ºC (Figures S4, S5) while the structure of bulk region remained almost unchanged during the CH_4-CVD according to the ^{27}Al NMR spectra (Figure S9). The D-H exchange between CD_4 and isolated OH groups occurred on the γ-ANP surface above 600 ºC, and the OH stretching band at ν_{OH} = 3701 cm^{-1} depressed with time constants of 1.2 min and the OD stretching band at ν_{OD} = 2730 cm^{-1} evolved as shown in Figure S4.

This isotope shift can be quantitively rationalized by the change of the reduced mass μ by the H-D exchange. The vibration frequency ν of the OH stretching mode is described in eq. (S1) under the harmonic approximation,

$$\nu = \frac{1}{2\pi}\sqrt{\frac{k_f}{\mu}} = \frac{1}{2\pi}\sqrt{\frac{k_f}{\frac{m_O m_H}{m_O + m_H}}}, \qquad \text{(S1)}$$

where m_O = 16 amu, and m_H = 1 amu are the masses of oxygen and hydrogen atoms, respectively. The effect of isotope exchange on the vibrational force constant k_f is negligible and the frequency of the deuterated system ν_{OD} can be written as the rate between reduced mass of OD group μ_{OD} and that of OH $\mu_{OH,}$, and the frequency of the original system ν_{OH} = 3701 cm^{-1},

$$\nu_{OD} = \frac{\sqrt{\mu_{OD}}}{\sqrt{\mu_{OH}}}\nu_{OH} = \frac{\sqrt{\frac{m_O m_D}{m_O + m_D}}}{\sqrt{\frac{m_O m_H}{m_O + m_H}}}\nu_{OH}, \qquad \text{(S2)}$$

where m_D = 2 amu is the mass of deuterium. Resultant ν_{OD} is calculated to be 2693 cm^{-1}, which qualitatively agrees with the experimental value (2730 cm^{-1}).

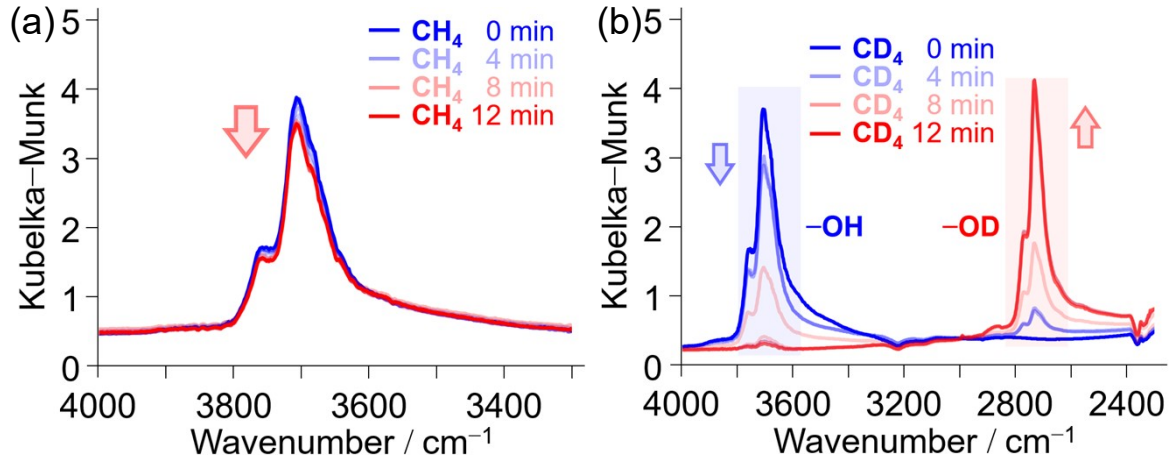

Figure S4. Temporal profiles of the OH stretching bands in IR spectra of ANPs at 900 ºC (a) in the presence of CH_4 (2 mL min^{-1}) and (b) in the presence of CD_4 (2 mL min^{-1}). Depletion at 2350 cm^{-1} is due to CO_2.

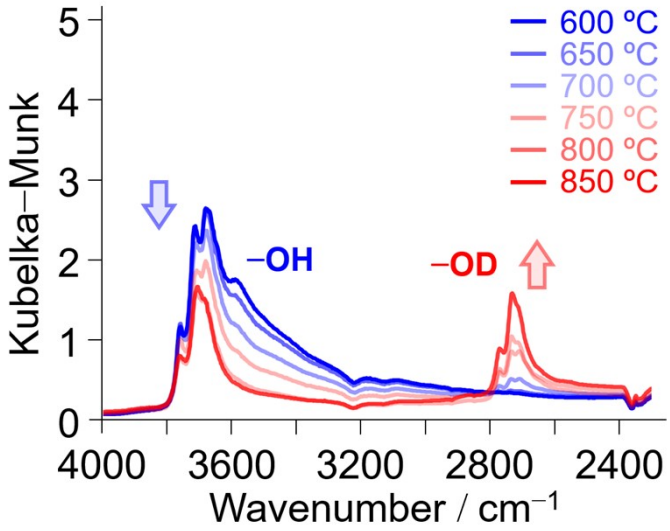

Figure S5. Time-course of IR spectra of γ-ANPs in the presence of CD_4 at the elevation rate of 16.7 K min^{-1} from 600 ºC to 850 ºC. Depletion at 2350 cm^{-1} is due to CO_2.

S2.5 Stability of Oxygen Vacancy Sites and Reactivity of CH_4 on Them

Table S1. Summary of H_2O/NH_3 TPD[a] and CH_4-CVD.

Conditions for pre-activation[b]	Evolved gas		Rate of reactions[d]
	H_2O[c]	NH_3	
700 ºC for 30 min	1.1 mmol g^{-1}	33 μmol g^{-1}	---
900 ºC for 30 min	1.4 mmol g^{-1}	19 μmol g^{-1}	4.8×10^{-9} mol s^{-1}
1000 ºC for 30 min	1.5 mmol g^{-1}	21 μmol g^{-1}	3.6×10^{-9} mol s^{-1}

[a] The details are shown in the section S1.3; [b] under a steady flow of He; [c] The amount of water desorbed at the temperatures higher than 300 ºC; [d] The rate for the first-layer deposition under the standard CH_4-CVD condition at 900 ºC with a steady flow of CH_4 (20 mL min^{-1}).

S2.6 Density Functional Chemical Calculations

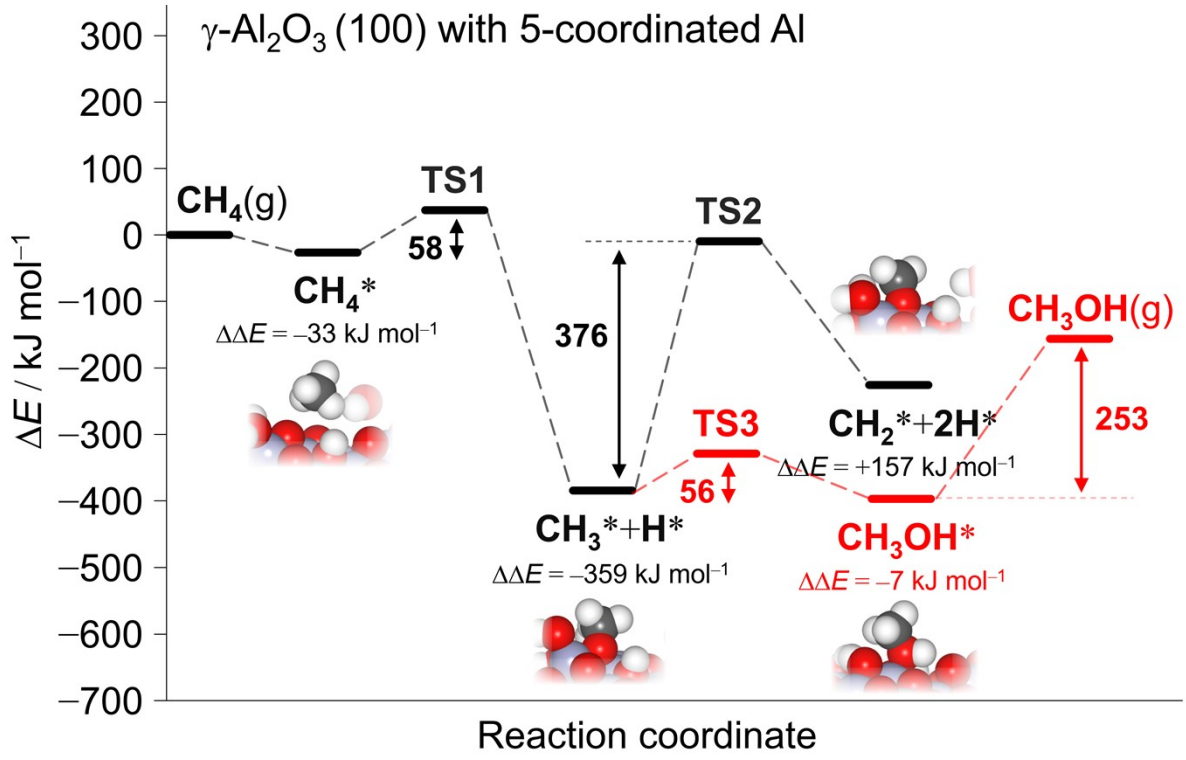

Figure S6. Black line: Energy profile for the formation of a CH_4 σ complex and the subsequent C–H bond cleavage on a γ-Al_2O_3 (100) surface. Red line: Conversion of CH_4 to CH_3OH on a γ-Al_2O_3 (100) surface. The reactive site is a 5-coordinated-Al.

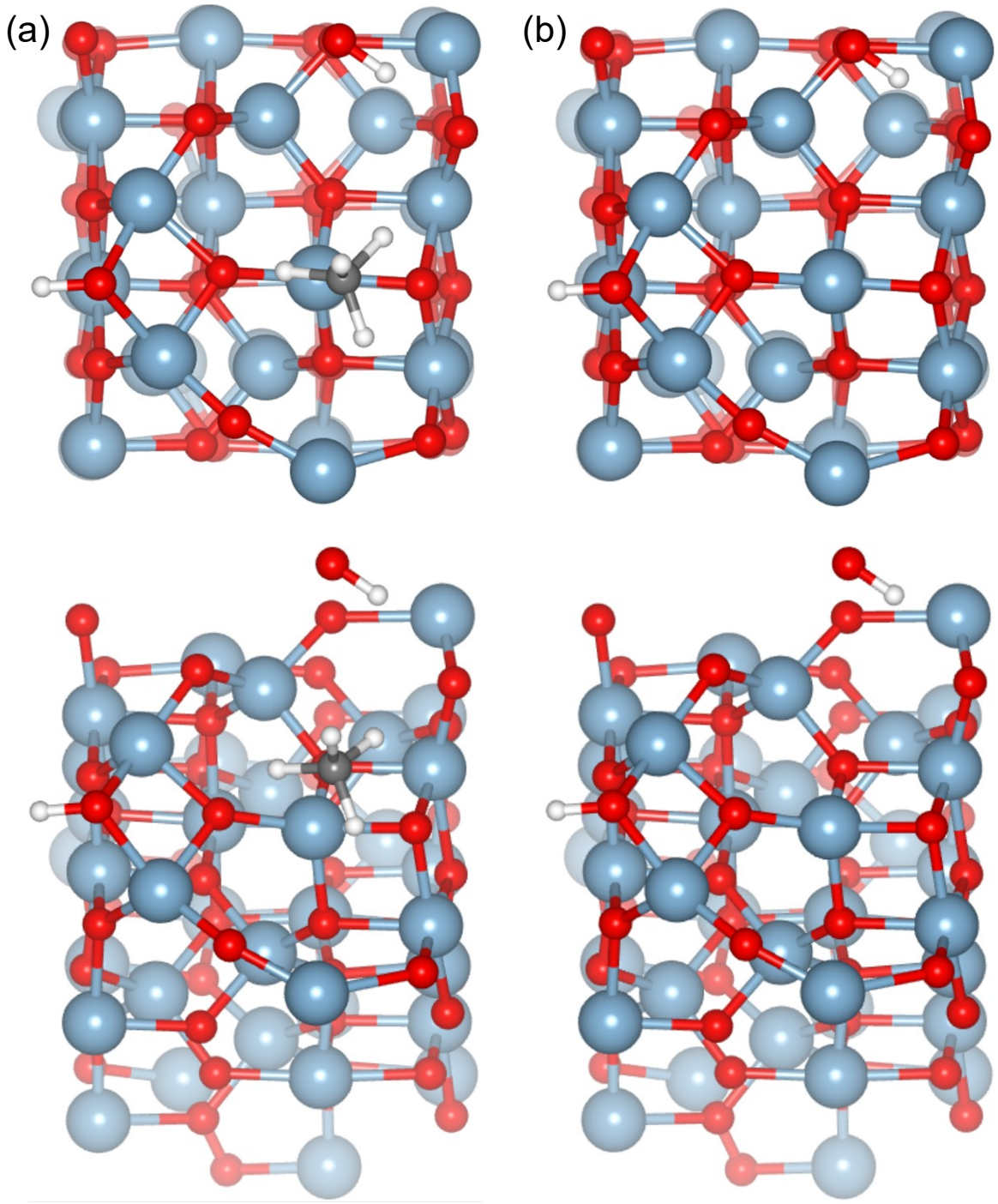

Figure S7. (a) Geometry of a γ-Al_2O_3 (100) surface with an adsorbed CH_4 and (b) the same geometry without CH_4 for clarity. Red: oxygen, Blue; aluminum, gray: carbon, and white: hydrogen atoms. The reactive site is tetrahedrally-coordinated (4-coordinated) Al center, and the coordinate is the same for CH_4* in Figure 4a of the manuscript. The coordinates are shown in Section S3.

Table S2. Calculated Bader charges *q* (in units of |*e*|) of adsorbed **CH_4*** and **CH_3*** species on a γ-Al_2O_3 (100) surface associated with the $CH_4 \rightarrow CH_3 + H$ elementary step. The value in brackets indicates the formal oxidation state corresponding to the Bader charge.

Property	**Initial State**	**Transition State (TS1)**	**Final State**
q(CH_4*)	–0.005	---	---
q(CH_3*)	---	–0.65	–0.61
q(C)	–0.16	–0.77	–0.71
q(H3*des)	+0.071	+0.66	+0.66
q(Al7)	+2.43 (+3)	+2.35 (+3)	+2.35 (+3)
q(O23)	–1.58 (–2)	–1.49 (–2)	–1.59 (–2)

Table S3. Calculated Bader charges *q* (in units of |*e*|) of adsorbed **CH_3*** and **CH_2*** species on a γ-Al_2O_3 (100) surface associated with the $CH_3 \rightarrow CH_2 + H$ elementary step. The value in brackets indicates the formal oxidation state corresponding to the Bader charge.

Property	**Initial State**	**Transition State (TS2)**	**Final State**
q(CH_3*)	–0.61	---	---
q(CH_2*)	---	–0.71	–0.71
q(C)	–0.71	–0.89	–0.80
q(H5*des)	+0.06	+0.64	+0.67
q(Al7)	+2.35 (+3)	+2.35 (+3)	+2.38 (+3)
q(O45)	–1.63 (–2)	–1.50 (–2)	–1.57 (–2)

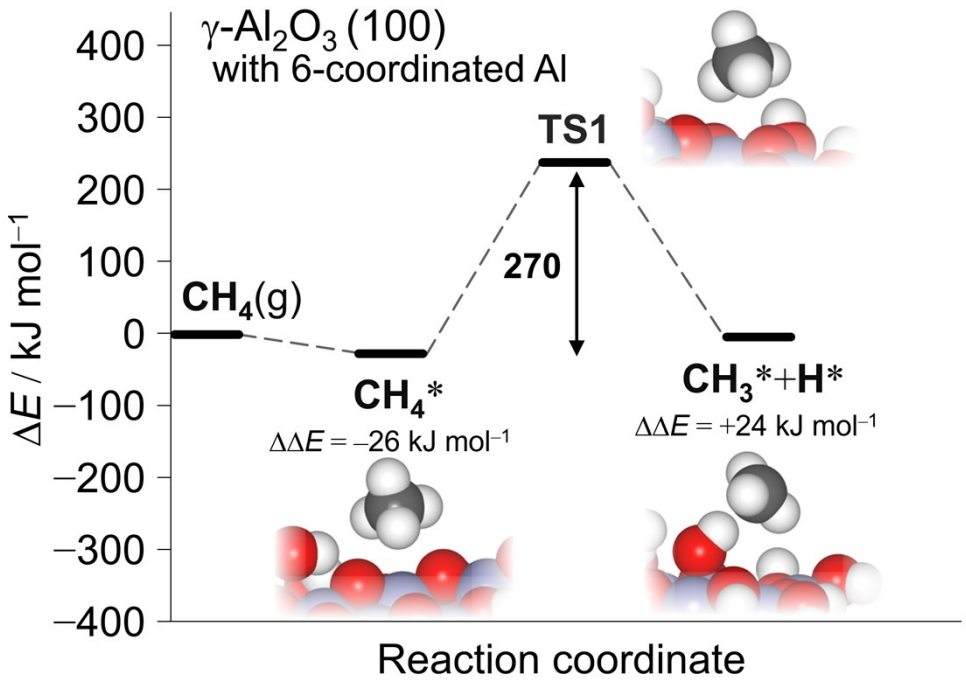

Figure S8. Energy profile for the formation of a CH_4 σ complex and the subsequent C–H bond cleavage on a γ-Al_2O_3 (100) surface with no oxygen defect. The reactive site is an octahedrally-coordinated (6-coordinated) Al center, and the clouded surface gives radical mechanism rather than the Lewis acid-base mechanism for the bond cleavage reaction.

S2.7 MAS ^{27}Al NMR

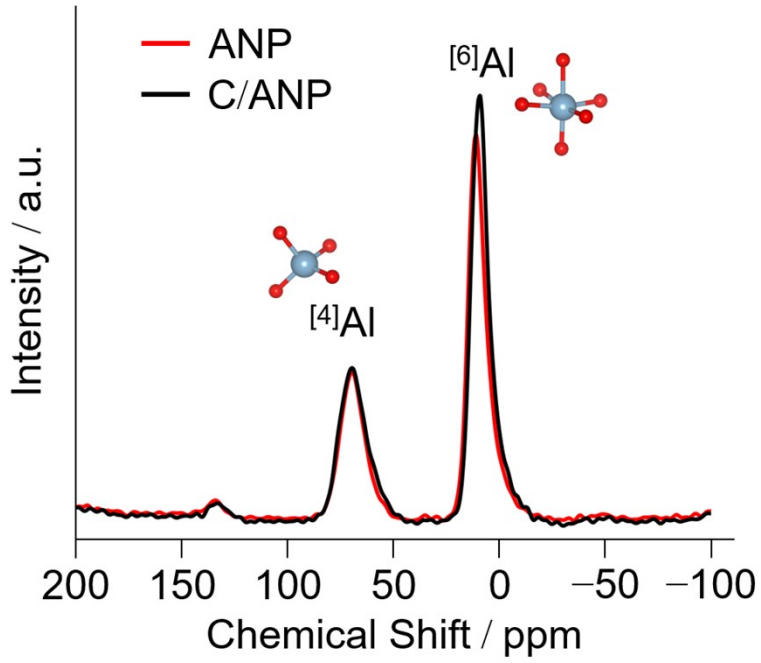

Figure S9. Normalized MAS ^{27}Al NMR of γ-ANPs before and after CH_4-CVD. Relative intensity of the peak for octahedrally coordinated Al-center ($^{[6]}$Al) in the up-field (δ = 9 ppm)[S17] was enhanced as compared with that for tetrahedrally coordinated Al-center ($^{[4]}$Al) in the down-field (δ = 68 ppm)[S17] after CH_4-CVD.

S2.8 Structural Analysis of ANPs by XRD

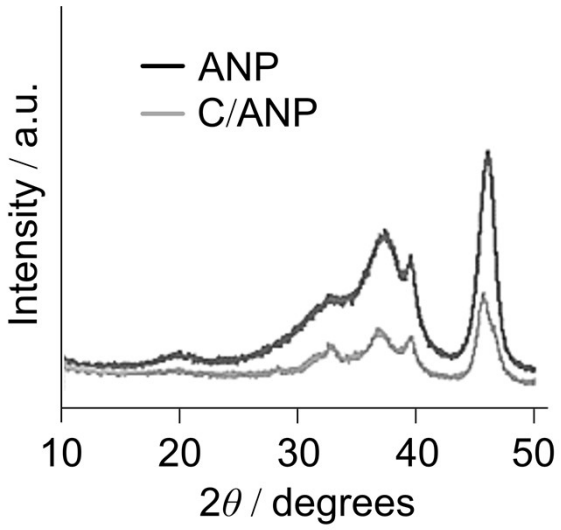

Figure S10. XRD of γ-ANPs before (ANP) and after CH_4-CVD (C/ANP).

S2.9 Crystal Structure Dependency on CH_4-CVD

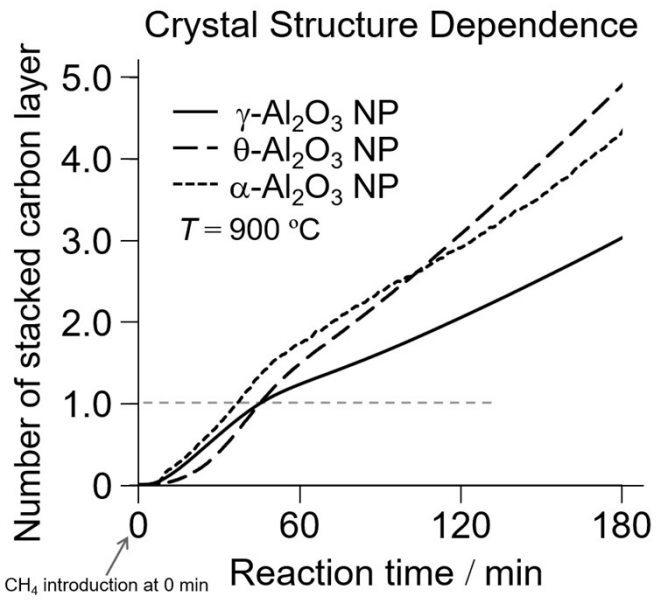

Figure S11. Time-course of weight changes during CH_4-CVD on various crystal structures of Al_2O_3 at 900 ºC as monitored by TG.

Curvature reflecting the difference in the rates of CH_4-CVD reactions was recognized at nearly single-layered deposition of carbon (Figs. 1a and 1b), but there was exception at higher partial pressure of CH_4 or at lower temperatures showing the curvature at the number of carbon layers > 1. We also noticed such exceptions for θ-ANP and α-ANP (Fig. S11). This could indicate that a mixture growth on the Al_2O_3 nanoparticles (first layer) and on carbon layer (second layer) was significant under these conditions. Thus, lower partial pressure of CH_4 and higher reaction temperatures as well as the use of γ-ANP would be important for single-layered carbon deposition.

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S3. Appendix: Optimized Structures and Energies in Quantum Chemistry Calculations

S3.1 Optimized Structures and Energies for Figure 4

Coordinate for a γ-Al_2O_3 (100) surface with CH_4 σ-complex with a surface proton density of 7.1 μmol m^{-2} at a 4-coordinated Al site.
Spin Multiplicity $<S^2>$: 0.006
Absolute Energy: –719.479682 eV.

cell_length_a	8.07075
cell_length_b	8.40443
cell_length_c	26.38316
cell_angle_alpha	90
cell_angle_beta	90
cell_angle_gamma	90
symmetry_space_group_name_H-M	'P 1'
symmetry_Int_Tables_number	1

H1	1.0	0.012525	0.411272	0.458504	H
H2	1.0	0.389156	0.758581	0.967927	H
H3	1.0	0.698026	0.308049	0.531916	H
H4	1.0	0.739746	0.514269	0.518631	H
H5	1.0	0.530180	0.443189	0.520374	H
H6	1.0	0.646493	0.458356	0.577451	H
H7	1.0	0.865656	0.323823	0.970992	H
H8	1.0	0.746757	0.853057	0.493596	H
C1	1.0	0.654231	0.430645	0.536903	C
O1	1.0	0.110810	0.590287	0.157363	O
O2	1.0	0.126991	0.579497	0.367156	O
O3	1.0	0.616791	0.907808	0.048522	O
O4	1.0	0.618926	0.917007	0.260722	O
O5	1.0	0.844216	0.414243	0.993966	O
O6	1.0	0.863210	0.412263	0.207681	O
O7	1.0	0.830444	0.416952	0.419161	O
O8	1.0	0.368215	0.102009	0.097134	O
O9	1.0	0.363299	0.085661	0.312928	O
O10	1.0	0.910452	0.097248	0.108539	O
O11	1.0	0.901999	0.110408	0.320372	O
O12	1.0	0.418851	0.425306	0.999761	O
O13	1.0	0.396402	0.420826	0.210593	O
O14	1.0	0.401961	0.441531	0.423833	O
O15	1.0	0.159017	0.913791	0.060543	O
O16	1.0	0.152386	0.907277	0.268392	O
O17	1.0	0.644021	0.580040	0.158151	O
O18	1.0	0.638591	0.601353	0.369087	O
O19	1.0	0.907293	0.404002	0.107473	O
O20	1.0	0.908008	0.411988	0.322313	O
O21	1.0	0.421249	0.085696	0.000782	O
O22	1.0	0.396766	0.084955	0.212754	O
O23	1.0	0.426853	0.132654	0.444146	O
O24	1.0	0.156904	0.597636	0.059375	O
O25	1.0	0.156913	0.596491	0.269328	O
O26	1.0	0.643976	0.920901	0.159718	O
O27	1.0	0.646395	0.916486	0.382605	O
O28	1.0	0.112524	0.911602	0.158270	O
O29	1.0	0.103110	0.923428	0.366921	O
O30	1.0	0.617146	0.603980	0.047211	O
O31	1.0	0.618472	0.589456	0.258414	O
O32	1.0	0.845170	0.118494	0.998522	O
O33	1.0	0.863477	0.090727	0.207279	O
O34	1.0	0.845781	0.093978	0.425296	O

O35	1.0	0.366314	0.408812	0.095626	O
O36	1.0	0.369713	0.412090	0.310746	O
O37	1.0	0.137828	0.253004	0.157850	O
O38	1.0	0.142084	0.251362	0.371803	O
O39	1.0	0.638516	0.258524	0.057742	O
O40	1.0	0.647124	0.253117	0.260716	O
O41	1.0	0.891289	0.752840	0.109178	O
O42	1.0	0.894881	0.740346	0.320221	O
O43	1.0	0.330572	0.756593	0.000109	O
O44	1.0	0.363575	0.752308	0.213126	O
O45	1.0	0.354565	0.755493	0.425107	O
O46	1.0	0.900661	0.757970	0.999763	O
O47	1.0	0.894859	0.750823	0.210337	O
O48	1.0	0.914227	0.730620	0.424643	O
O49	1.0	0.383665	0.753497	0.104142	O
O50	1.0	0.382431	0.755530	0.315846	O
O51	1.0	0.122889	0.256524	0.053850	O
O52	1.0	0.114393	0.256781	0.266551	O
O53	1.0	0.645985	0.251255	0.163526	O
O54	1.0	0.633320	0.260363	0.366448	O
O55	1.0	0.135368	0.417876	0.462171	O
O56	1.0	0.648143	0.919690	0.495631	O
Al1	1.0	0.394203	0.925716	0.056171	Al
Al2	1.0	0.388366	0.925054	0.268298	Al
Al3	1.0	0.137549	0.424010	0.111684	Al
Al4	1.0	0.141246	0.417788	0.321118	Al
Al5	1.0	0.637737	0.429274	0.013999	Al
Al6	1.0	0.622752	0.427441	0.213397	Al
Al7	1.0	0.608664	0.430060	0.405948	Al
Al8	1.0	0.870145	0.920810	0.162533	Al
Al9	1.0	0.887620	0.909823	0.392393	Al
Al10	1.0	0.643600	0.080089	0.013552	Al
Al11	1.0	0.625514	0.075905	0.214252	Al
Al12	1.0	0.616620	0.031576	0.440742	Al
Al13	1.0	0.869725	0.582574	0.161939	Al
Al14	1.0	0.870383	0.590931	0.376095	Al
Al15	1.0	0.392237	0.586595	0.055100	Al
Al16	1.0	0.392264	0.581774	0.269067	Al
Al17	1.0	0.141404	0.079642	0.113867	Al
Al18	1.0	0.132394	0.082742	0.323974	Al
Al19	1.0	0.896764	0.243816	0.053385	Al
Al20	1.0	0.880726	0.261485	0.272586	Al
Al21	1.0	0.506431	0.257764	0.115979	Al
Al22	1.0	0.502352	0.244985	0.315937	Al
Al23	1.0	0.883448	0.251325	0.161685	Al
Al24	1.0	0.864478	0.244070	0.377086	Al
Al25	1.0	0.102397	0.758243	0.015780	Al
Al26	1.0	0.130648	0.750868	0.221422	Al
Al27	1.0	0.233455	0.589466	0.428129	Al
Al28	1.0	0.514930	0.750651	0.164319	Al
Al29	1.0	0.500458	0.764329	0.377473	Al
Al30	1.0	0.139321	0.752232	0.113593	Al
Al31	1.0	0.130852	0.757320	0.325584	Al
Al32	1.0	0.769038	0.756627	0.052245	Al
Al33	1.0	0.753830	0.752164	0.270819	Al
Al34	1.0	0.325129	0.255271	0.029516	Al
Al35	1.0	0.266034	0.253710	0.218426	Al
Al36	1.0	0.275653	0.267166	0.429342	Al

Coordinate for a calculated transition state of the initial CH_4 activation on a γ-Al_2O_3 (100) surface (**TS1**) in Figure 4.
Spin Multiplicity $<S^2>$: 0.023
Absolute Energy: –718.02755056 eV.

cell_length_a	8.07075
cell_length_b	8.40443
cell_length_c	26.38316
cell_angle_alpha	90
cell_angle_beta	90
cell_angle_gamma	90
symmetry_space_group_name_H-M	'P 1'
symmetry_Int_Tables_number	1

H1	1.0	0.999497	0.303556	0.474501	H
H2	1.0	0.391601	0.760793	0.967337	H
H3	1.0	0.464363	0.203673	0.481020	H
H4	1.0	0.712861	0.509912	0.506832	H
H5	1.0	0.497569	0.470945	0.516232	H
H6	1.0	0.648007	0.314327	0.518546	H
H7	1.0	0.867957	0.324562	0.970619	H
H8	1.0	0.748970	0.925398	0.510760	H
C1	1.0	0.612045	0.425223	0.498948	C
O1	1.0	0.113042	0.593115	0.156824	O
O2	1.0	0.126718	0.578692	0.361392	O
O3	1.0	0.619109	0.909381	0.048429	O
O4	1.0	0.622889	0.918380	0.260880	O
O5	1.0	0.846619	0.415135	0.993565	O
O6	1.0	0.865476	0.413679	0.207422	O
O7	1.0	0.851724	0.406386	0.417653	O
O8	1.0	0.370901	0.103750	0.097220	O
O9	1.0	0.368545	0.085289	0.314086	O
O10	1.0	0.913061	0.098563	0.108779	O
O11	1.0	0.901088	0.108167	0.319443	O
O12	1.0	0.421397	0.426836	0.999488	O
O13	1.0	0.399752	0.422687	0.209564	O
O14	1.0	0.349399	0.459011	0.423588	O
O15	1.0	0.161162	0.915648	0.060206	O
O16	1.0	0.155682	0.907326	0.267459	O
O17	1.0	0.646804	0.582088	0.158380	O
O18	1.0	0.638885	0.589620	0.379247	O
O19	1.0	0.909879	0.405488	0.107293	O
O20	1.0	0.906185	0.410968	0.319885	O
O21	1.0	0.423676	0.087517	0.000850	O
O22	1.0	0.399038	0.085276	0.213286	O
O23	1.0	0.433242	0.151370	0.448863	O
O24	1.0	0.158967	0.599496	0.058812	O
O25	1.0	0.158247	0.598853	0.266641	O
O26	1.0	0.646398	0.923337	0.159765	O
O27	1.0	0.656598	0.900214	0.386540	O
O28	1.0	0.115218	0.912400	0.158116	O
O29	1.0	0.107945	0.917818	0.364187	O
O30	1.0	0.619791	0.605317	0.047068	O
O31	1.0	0.621889	0.589424	0.259167	O
O32	1.0	0.848004	0.119304	0.998647	O
O33	1.0	0.865736	0.093410	0.207568	O
O34	1.0	0.860184	0.080717	0.423242	O
O35	1.0	0.368541	0.410650	0.095187	O
O36	1.0	0.371357	0.410520	0.309106	O
O37	1.0	0.140856	0.254879	0.157817	O
O38	1.0	0.141113	0.247560	0.369739	O
O39	1.0	0.641399	0.260330	0.057827	O
O40	1.0	0.647898	0.254125	0.262151	O
O41	1.0	0.893263	0.754927	0.109062	O
O42	1.0	0.886538	0.741288	0.323430	O
O43	1.0	0.333227	0.758422	0.999492	O
O44	1.0	0.368685	0.754016	0.212698	O

O45	1.0	0.349534	0.776355	0.424455	O
O46	1.0	0.902932	0.759458	0.999535	O
O47	1.0	0.897402	0.753153	0.210552	O
O48	1.0	0.964270	0.713645	0.425268	O
O49	1.0	0.385732	0.755260	0.103694	O
O50	1.0	0.389613	0.752501	0.315629	O
O51	1.0	0.125258	0.257644	0.053872	O
O52	1.0	0.116790	0.254067	0.266009	O
O53	1.0	0.648053	0.252371	0.163919	O
O54	1.0	0.624181	0.254044	0.374885	O
O55	1.0	0.117701	0.298000	0.481721	O
O56	1.0	0.644366	0.970071	0.499747	O
Al1	1.0	0.396595	0.927902	0.055970	Al
Al2	1.0	0.393809	0.925308	0.269246	Al
Al3	1.0	0.140103	0.425627	0.111445	Al
Al4	1.0	0.143285	0.412341	0.319894	Al
Al5	1.0	0.640387	0.430767	0.013662	Al
Al6	1.0	0.625883	0.428248	0.213944	Al
Al7	1.0	0.600066	0.427930	0.423068	Al
Al8	1.0	0.871843	0.923062	0.162576	Al
Al9	1.0	0.900949	0.894152	0.391853	Al
Al10	1.0	0.646109	0.081643	0.013449	Al
Al11	1.0	0.626771	0.077917	0.214738	Al
Al12	1.0	0.636791	0.039557	0.437749	Al
Al13	1.0	0.871849	0.584469	0.162040	Al
Al14	1.0	0.871069	0.572901	0.376016	Al
Al15	1.0	0.394550	0.588439	0.054525	Al
Al16	1.0	0.394471	0.581973	0.268389	Al
Al17	1.0	0.144107	0.081770	0.113767	Al
Al18	1.0	0.134109	0.080999	0.322633	Al
Al19	1.0	0.898979	0.245267	0.053265	Al
Al20	1.0	0.881748	0.258503	0.271649	Al
Al21	1.0	0.509082	0.260270	0.116128	Al
Al22	1.0	0.506438	0.248153	0.319780	Al
Al23	1.0	0.886093	0.253226	0.161517	Al
Al24	1.0	0.865835	0.239222	0.376911	Al
Al25	1.0	0.105029	0.760190	0.014987	Al
Al26	1.0	0.136600	0.753706	0.218841	Al
Al27	1.0	0.198504	0.632965	0.423595	Al
Al28	1.0	0.517792	0.752739	0.163589	Al
Al29	1.0	0.501539	0.754008	0.379385	Al
Al30	1.0	0.140113	0.754163	0.112582	Al
Al31	1.0	0.129084	0.754056	0.321303	Al
Al32	1.0	0.771397	0.758233	0.051973	Al
Al33	1.0	0.755889	0.753181	0.270756	Al
Al34	1.0	0.327714	0.257262	0.029553	Al
Al35	1.0	0.270742	0.255243	0.218564	Al
Al36	1.0	0.248800	0.273813	0.430931	Al

Coordinate for a γ-Al_2O_3 (100) surface with CH_3* and H* in Figure 4.
Spin Multiplicity $<S^2>$: 0.007
Absolute Energy: –719.813245 eV.

cell_length_a	8.07075
cell_length_b	8.40443
cell_length_c	26.38316
cell_angle_alpha	90
cell_angle_beta	90
cell_angle_gamma	90
symmetry_space_group_name_H-M	'P 1'
symmetry_Int_Tables_number	1

H1	1.0	-0.004326	0.114684	0.471138	H
H2	1.0	0.396313	0.760229	0.967201	H
H3	1.0	0.340699	0.011573	0.438921	H
H4	1.0	0.678107	0.493944	0.515064	H
H5	1.0	0.461261	0.470217	0.501968	H
H6	1.0	0.590864	0.299604	0.511193	H
H7	1.0	0.875143	0.330013	0.970016	H
H8	1.0	0.726134	0.985651	0.505465	H
C1	1.0	0.584738	0.420596	0.495413	C
O1	1.0	0.116963	0.595673	0.156889	O
O2	1.0	0.127031	0.583898	0.361491	O
O3	1.0	0.623370	0.909859	0.047825	O
O4	1.0	0.625803	0.922371	0.260012	O
O5	1.0	0.852515	0.415672	0.994563	O
O6	1.0	0.868931	0.416026	0.207254	O
O7	1.0	0.872482	0.411024	0.415214	O
O8	1.0	0.374490	0.104932	0.096133	O
O9	1.0	0.371849	0.091680	0.312306	O
O10	1.0	0.916527	0.101232	0.108425	O
O11	1.0	0.904701	0.110176	0.316610	O
O12	1.0	0.424901	0.427211	0.999764	O
O13	1.0	0.402877	0.426410	0.212065	O
O14	1.0	0.229187	0.452750	0.450958	O
O15	1.0	0.164972	0.916449	0.059688	O
O16	1.0	0.160988	0.910541	0.266955	O
O17	1.0	0.650472	0.585679	0.158917	O
O18	1.0	0.641266	0.585107	0.379536	O
O19	1.0	0.913705	0.408118	0.107082	O
O20	1.0	0.907356	0.415113	0.318240	O
O21	1.0	0.427888	0.087161	0.999961	O
O22	1.0	0.402894	0.088393	0.211796	O
O23	1.0	0.391491	0.112797	0.427314	O
O24	1.0	0.163568	0.600402	0.058958	O
O25	1.0	0.163165	0.601261	0.266954	O
O26	1.0	0.650657	0.927176	0.159254	O
O27	1.0	0.650978	0.901542	0.382163	O
O28	1.0	0.118821	0.915450	0.157633	O
O29	1.0	0.108897	0.922304	0.363544	O
O30	1.0	0.624352	0.605315	0.047140	O
O31	1.0	0.626151	0.593090	0.259677	O
O32	1.0	0.853148	0.119133	0.998216	O
O33	1.0	0.869034	0.097899	0.207070	O
O34	1.0	0.857302	0.083186	0.418245	O
O35	1.0	0.373406	0.412702	0.096046	O
O36	1.0	0.376920	0.417662	0.313114	O
O37	1.0	0.145244	0.257361	0.157382	O
O38	1.0	0.132699	0.251776	0.368848	O
O39	1.0	0.645768	0.260115	0.057344	O
O40	1.0	0.650207	0.258155	0.262771	O
O41	1.0	0.897041	0.756852	0.108850	O
O42	1.0	0.888893	0.747190	0.322234	O
O43	1.0	0.337813	0.758303	0.999452	O
O44	1.0	0.372714	0.757188	0.212478	O

O45	1.0	0.343279	0.758062	0.423731	O
O46	1.0	0.907298	0.758639	0.999254	O
O47	1.0	0.901589	0.756533	0.210252	O
O48	1.0	0.949849	0.721497	0.422927	O
O49	1.0	0.390133	0.757377	0.103506	O
O50	1.0	0.391773	0.755765	0.315568	O
O51	1.0	0.129501	0.259032	0.053685	O
O52	1.0	0.122325	0.260175	0.265663	O
O53	1.0	0.650225	0.257051	0.163843	O
O54	1.0	0.627870	0.252732	0.378451	O
O55	1.0	0.110388	0.136214	0.481041	O
O56	1.0	0.622031	0.019165	0.490685	O
Al1	1.0	0.400716	0.928118	0.055188	Al
Al2	1.0	0.398005	0.928747	0.268527	Al
Al3	1.0	0.144332	0.428055	0.111255	Al
Al4	1.0	0.147228	0.417449	0.320148	Al
Al5	1.0	0.644240	0.431057	0.013445	Al
Al6	1.0	0.628937	0.432042	0.214289	Al
Al7	1.0	0.653507	0.427700	0.425303	Al
Al8	1.0	0.875919	0.926438	0.162111	Al
Al9	1.0	0.892324	0.897468	0.387192	Al
Al10	1.0	0.650870	0.081580	0.012481	Al
Al11	1.0	0.629915	0.082712	0.214452	Al
Al12	1.0	0.621760	0.065672	0.426422	Al
Al13	1.0	0.875714	0.587463	0.161850	Al
Al14	1.0	0.877923	0.578601	0.371540	Al
Al15	1.0	0.399266	0.588814	0.054929	Al
Al16	1.0	0.398834	0.583147	0.269081	Al
Al17	1.0	0.147847	0.084120	0.113173	Al
Al18	1.0	0.138861	0.084000	0.321493	Al
Al19	1.0	0.903063	0.246714	0.052460	Al
Al20	1.0	0.886181	0.262611	0.269675	Al
Al21	1.0	0.513448	0.259784	0.115332	Al
Al22	1.0	0.509749	0.252317	0.321821	Al
Al23	1.0	0.888794	0.256622	0.160708	Al
Al24	1.0	0.889578	0.242327	0.374261	Al
Al25	1.0	0.109491	0.760092	0.014665	Al
Al26	1.0	0.141156	0.755348	0.218921	Al
Al27	1.0	0.168364	0.636762	0.428145	Al
Al28	1.0	0.521579	0.756624	0.163369	Al
Al29	1.0	0.500764	0.749241	0.380059	Al
Al30	1.0	0.144067	0.756419	0.112403	Al
Al31	1.0	0.140586	0.758313	0.321915	Al
Al32	1.0	0.775638	0.758745	0.051649	Al
Al33	1.0	0.758913	0.758292	0.269582	Al
Al34	1.0	0.331225	0.256146	0.028750	Al
Al35	1.0	0.274456	0.257429	0.217978	Al
Al36	1.0	0.216650	0.253043	0.437741	Al

Coordinate for a calculated transition state of PT from CH_3* on a γ-Al_2O_3 (100) surface (**TS2**) in Figure 4.
Spin Multiplicity $<S^2>$: 0.9998
Absolute Energy: –718.93307207 eV.

cell_length_a	8.07075
cell_length_b	8.40443
cell_length_c	26.38316
cell_angle_alpha	90
cell_angle_beta	90
cell_angle_gamma	90
symmetry_space_group_name_H-M	'P 1'
symmetry_Int_Tables_number	1

H1	1.0	0.000663	0.098484	0.472939	H
H2	1.0	0.396912	0.756187	0.967692	H
H3	1.0	0.355404	0.042160	0.458310	H
H4	1.0	0.569990	0.537756	0.513039	H
H5	1.0	0.406994	0.617345	0.449918	H
H6	1.0	0.485566	0.339893	0.503906	H
H7	1.0	0.915912	0.381922	0.973496	H
H8	1.0	0.729544	1.008597	0.508057	H
C1	1.0	0.547045	0.441050	0.486035	C
O1	1.0	0.120565	0.598794	0.158752	O
O2	1.0	0.125383	0.581729	0.361714	O
O3	1.0	0.628490	0.910692	0.045091	O
O4	1.0	0.628314	0.922044	0.261775	O
O5	1.0	0.874987	0.422266	0.005803	O
O6	1.0	0.870680	0.413376	0.209338	O
O7	1.0	0.872812	0.411366	0.414755	O
O8	1.0	0.380443	0.104325	0.096707	O
O9	1.0	0.375803	0.086628	0.314925	O
O10	1.0	0.918223	0.100509	0.111144	O
O11	1.0	0.910629	0.104167	0.318073	O
O12	1.0	0.406694	0.425967	0.003096	O
O13	1.0	0.405188	0.424012	0.215668	O
O14	1.0	0.208745	0.448376	0.456177	O
O15	1.0	0.168280	0.915592	0.060751	O
O16	1.0	0.163321	0.907638	0.267751	O
O17	1.0	0.652457	0.584320	0.160713	O
O18	1.0	0.644802	0.582467	0.376281	O
O19	1.0	0.918301	0.410038	0.111017	O
O20	1.0	0.910240	0.408566	0.318695	O
O21	1.0	0.424616	0.080839	0.999729	O
O22	1.0	0.404279	0.085175	0.214548	O
O23	1.0	0.394740	0.118196	0.432529	O
O24	1.0	0.165748	0.600441	0.060988	O
O25	1.0	0.164625	0.599654	0.267849	O
O26	1.0	0.652603	0.925691	0.160927	O
O27	1.0	0.646141	0.899344	0.384869	O
O28	1.0	0.121897	0.913822	0.158363	O
O29	1.0	0.117397	0.914956	0.365218	O
O30	1.0	0.625061	0.598315	0.042565	O
O31	1.0	0.629387	0.590772	0.261505	O
O32	1.0	0.866567	0.111268	0.001625	O
O33	1.0	0.870635	0.097596	0.209123	O
O34	1.0	0.859022	0.081272	0.417596	O
O35	1.0	0.379013	0.419829	0.101983	O
O36	1.0	0.379486	0.418772	0.315762	O
O37	1.0	0.148336	0.255353	0.159299	O
O38	1.0	0.135903	0.249948	0.370361	O
O39	1.0	0.651295	0.261489	0.056814	O
O40	1.0	0.652681	0.255029	0.264359	O
O41	1.0	0.895484	0.755261	0.108235	O
O42	1.0	0.889032	0.749246	0.321978	O
O43	1.0	0.338254	0.757043	0.999788	O
O44	1.0	0.377545	0.754988	0.214036	O

O45	1.0	0.360350	0.706795	0.428420	O
O46	1.0	0.914182	0.756822	0.997505	O
O47	1.0	0.903685	0.755934	0.210312	O
O48	1.0	0.942266	0.720401	0.422287	O
O49	1.0	0.395821	0.757383	0.103689	O
O50	1.0	0.390590	0.753704	0.317220	O
O51	1.0	0.132650	0.255642	0.058170	O
O52	1.0	0.128094	0.255528	0.267359	O
O53	1.0	0.648411	0.255405	0.164884	O
O54	1.0	0.626325	0.250001	0.378802	O
O55	1.0	0.115258	0.122495	0.481851	O
O56	1.0	0.625826	0.038580	0.492180	O
Al1	1.0	0.407330	0.927410	0.054332	Al
Al2	1.0	0.400547	0.928424	0.267938	Al
Al3	1.0	0.151125	0.427717	0.112534	Al
Al4	1.0	0.150887	0.415117	0.319086	Al
Al5	1.0	0.644007	0.422818	0.003990	Al
Al6	1.0	0.632371	0.430670	0.214493	Al
Al7	1.0	0.654230	0.425111	0.421487	Al
Al8	1.0	0.878422	0.926549	0.160137	Al
Al9	1.0	0.893716	0.897774	0.384698	Al
Al10	1.0	0.656572	0.087745	0.008909	Al
Al11	1.0	0.631617	0.080199	0.214026	Al
Al12	1.0	0.624890	0.068868	0.426530	Al
Al13	1.0	0.878168	0.584467	0.160145	Al
Al14	1.0	0.876298	0.575699	0.367880	Al
Al15	1.0	0.403561	0.581084	0.055172	Al
Al16	1.0	0.401712	0.580068	0.268545	Al
Al17	1.0	0.151911	0.085074	0.112396	Al
Al18	1.0	0.145278	0.079746	0.322243	Al
Al19	1.0	0.902135	0.249431	0.052301	Al
Al20	1.0	0.888997	0.253901	0.268415	Al
Al21	1.0	0.521372	0.262485	0.112660	Al
Al22	1.0	0.511387	0.250749	0.320644	Al
Al23	1.0	0.891545	0.255763	0.161640	Al
Al24	1.0	0.895630	0.240816	0.373692	Al
Al25	1.0	0.113617	0.758940	0.015237	Al
Al26	1.0	0.143116	0.753350	0.217142	Al
Al27	1.0	0.143115	0.622243	0.428438	Al
Al28	1.0	0.522675	0.755080	0.162397	Al
Al29	1.0	0.505705	0.744315	0.376432	Al
Al30	1.0	0.147830	0.756266	0.112153	Al
Al31	1.0	0.141062	0.755724	0.320408	Al
Al32	1.0	0.775731	0.753500	0.048283	Al
Al33	1.0	0.762506	0.757479	0.267077	Al
Al34	1.0	0.324584	0.247461	0.026250	Al
Al35	1.0	0.275808	0.254662	0.217260	Al
Al36	1.0	0.209086	0.249486	0.438825	Al

Coordinate for a γ-Al_2O_3 (100) surface with CH_2* and 2H* in Figure 4.
Spin Multiplicity <S^2>: 1.000
Absolute Energy: –719.36810744 eV.

cell_length_a	8.07075
cell_length_b	8.40443
cell_length_c	26.38316
cell_angle_alpha	90
cell_angle_beta	90
cell_angle_gamma	90
symmetry_space_group_name_H-M	'P 1'
symmetry_Int_Tables_number	1

H1	1.0	0.079779	0.095029	0.474032	H
H2	1.0	0.397238	0.758259	0.968677	H
H3	1.0	0.357707	0.157557	0.472574	H
H4	1.0	0.603288	0.320753	0.514956	H
H5	1.0	0.427236	0.808728	0.454746	H
H6	1.0	0.419664	0.409670	0.489593	H
H7	1.0	0.916659	0.369523	0.973787	H
H8	1.0	0.684742	0.826576	0.482903	H
C1	1.0	0.531145	0.340427	0.480117	C
O1	1.0	0.121353	0.600596	0.159491	O
O2	1.0	0.123568	0.593266	0.363603	O
O3	1.0	0.626054	0.915197	0.039483	O
O4	1.0	0.627913	0.922997	0.262659	O
O5	1.0	0.880715	0.415935	0.005880	O
O6	1.0	0.870565	0.411351	0.211296	O
O7	1.0	0.879607	0.409240	0.419945	O
O8	1.0	0.384737	0.090903	0.103519	O
O9	1.0	0.376251	0.087098	0.318723	O
O10	1.0	0.920717	0.099535	0.113344	O
O11	1.0	0.910493	0.099070	0.320589	O
O12	1.0	0.395071	0.429703	0.001965	O
O13	1.0	0.404050	0.422950	0.218525	O
O14	1.0	0.178255	0.519761	0.462814	O
O15	1.0	0.166705	0.914035	0.062202	O
O16	1.0	0.163582	0.911087	0.268103	O
O17	1.0	0.653450	0.586146	0.163009	O
O18	1.0	0.646876	0.591286	0.383010	O
O19	1.0	0.920165	0.411699	0.112884	O
O20	1.0	0.903819	0.411520	0.321816	O
O21	1.0	0.402242	0.079584	0.000606	O
O22	1.0	0.403408	0.088154	0.218131	O
O23	1.0	0.476024	0.181952	0.460761	O
O24	1.0	0.165534	0.600134	0.061994	O
O25	1.0	0.162087	0.600224	0.268844	O
O26	1.0	0.653096	0.925128	0.162403	O
O27	1.0	0.648280	0.916291	0.376687	O
O28	1.0	0.122031	0.911006	0.159463	O
O29	1.0	0.118320	0.917499	0.365632	O
O30	1.0	0.625623	0.593553	0.039312	O
O31	1.0	0.629333	0.587967	0.263685	O
O32	1.0	0.879793	0.099433	0.004726	O
O33	1.0	0.870219	0.099378	0.210961	O
O34	1.0	0.859060	0.086542	0.420877	O
O35	1.0	0.383189	0.423625	0.104382	O
O36	1.0	0.377777	0.423218	0.318619	O
O37	1.0	0.147189	0.255793	0.160798	O
O38	1.0	0.124604	0.265577	0.373730	O
O39	1.0	0.658713	0.259204	0.058293	O
O40	1.0	0.653322	0.254561	0.265591	O
O41	1.0	0.889930	0.755689	0.107561	O
O42	1.0	0.886862	0.753173	0.320384	O
O43	1.0	0.336950	0.756031	1.000531	O
O44	1.0	0.378588	0.754679	0.214870	O

O45	1.0	0.360321	0.770179	0.424507	O
O46	1.0	0.917166	0.751242	0.995804	O
O47	1.0	0.904146	0.755899	0.210164	O
O48	1.0	0.929007	0.743496	0.419779	O
O49	1.0	0.399276	0.756265	0.103390	O
O50	1.0	0.389177	0.754057	0.316716	O
O51	1.0	0.135567	0.255375	0.060405	O
O52	1.0	0.127168	0.256458	0.270445	O
O53	1.0	0.644221	0.255980	0.165449	O
O54	1.0	0.637476	0.255373	0.375665	O
O55	1.0	0.153410	0.185340	0.479809	O
O56	1.0	0.596360	0.904684	0.479278	O
Al1	1.0	0.408178	0.934694	0.053845	Al
Al2	1.0	0.400732	0.930643	0.267648	Al
Al3	1.0	0.155411	0.427125	0.111603	Al
Al4	1.0	0.148791	0.423542	0.319581	Al
Al5	1.0	0.643209	0.409991	0.000243	Al
Al6	1.0	0.632123	0.430459	0.213680	Al
Al7	1.0	0.651572	0.419574	0.420742	Al
Al8	1.0	0.878671	0.925491	0.157790	Al
Al9	1.0	0.887641	0.915107	0.375289	Al
Al10	1.0	0.661471	0.097459	0.000751	Al
Al11	1.0	0.631218	0.080496	0.213066	Al
Al12	1.0	0.639194	0.047698	0.430433	Al
Al13	1.0	0.878810	0.585425	0.157592	Al
Al14	1.0	0.878338	0.588647	0.368872	Al
Al15	1.0	0.405746	0.578288	0.054253	Al
Al16	1.0	0.401535	0.580929	0.267802	Al
Al17	1.0	0.157388	0.084697	0.112202	Al
Al18	1.0	0.149922	0.087425	0.323640	Al
Al19	1.0	0.898938	0.244944	0.052523	Al
Al20	1.0	0.887232	0.253727	0.266480	Al
Al21	1.0	0.519482	0.257911	0.110234	Al
Al22	1.0	0.510186	0.253916	0.319183	Al
Al23	1.0	0.891926	0.256169	0.161806	Al
Al24	1.0	0.878552	0.243499	0.370784	Al
Al25	1.0	0.114313	0.759396	0.015223	Al
Al26	1.0	0.142446	0.755189	0.214890	Al
Al27	1.0	0.147274	0.686564	0.425673	Al
Al28	1.0	0.521598	0.755444	0.161020	Al
Al29	1.0	0.510662	0.755810	0.372960	Al
Al30	1.0	0.152382	0.755995	0.111672	Al
Al31	1.0	0.140528	0.760338	0.318041	Al
Al32	1.0	0.770914	0.755334	0.044189	Al
Al33	1.0	0.760781	0.756533	0.263898	Al
Al34	1.0	0.295973	0.251953	0.013661	Al
Al35	1.0	0.272525	0.255636	0.217071	Al
Al36	1.0	0.098190	0.345192	0.439948	Al

S3.2 Optimized Structures and Energies for Figure S6

Coordinate for a γ-Al_2O_3 (100) surface with CH_4 σ-complex at a 5-coordinated Al site.
Absolute Energy: −731.75658299 eV.

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	0.917929	0.402544	0.444165	H
H2	1.0	0.430293	0.072259	0.963119	H
H3	1.0	0.698900	0.423558	0.558535	H
H4	1.0	0.730352	0.582663	0.514720	H
H5	1.0	0.525923	0.532422	0.535311	H
H6	1.0	0.666923	0.627423	0.578229	H
H7	1.0	0.122325	0.404754	0.500383	H
H8	1.0	0.381135	0.753554	0.962556	H
H9	1.0	0.828333	0.320928	0.952131	H
H10	1.0	0.683783	0.834203	0.495196	H
C1	1.0	0.655790	0.541785	0.547048	C
O1	1.0	0.604802	0.267201	0.465222	O
O2	1.0	0.109730	0.590496	0.154556	O
O3	1.0	0.118468	0.569548	0.362387	O
O4	1.0	0.623466	0.914940	0.035307	O
O5	1.0	0.615635	0.912945	0.257862	O
O6	1.0	0.768406	0.421576	0.956204	O
O7	1.0	0.857361	0.407709	0.206065	O
O8	1.0	0.844424	0.403586	0.414270	O
O9	1.0	0.374276	0.112646	0.087387	O
O10	1.0	0.358715	0.080144	0.311606	O
O11	1.0	0.904955	0.088489	0.108383	O
O12	1.0	0.896492	0.099626	0.314347	O
O13	1.0	0.396195	0.414241	-0.002523	O
O14	1.0	0.390985	0.419350	0.208524	O
O15	1.0	0.372114	0.429061	0.412812	O
O16	1.0	0.159240	0.915713	0.058801	O
O17	1.0	0.150357	0.899657	0.266537	O
O18	1.0	0.639829	0.575840	0.154991	O
O19	1.0	0.635591	0.585039	0.377484	O
O20	1.0	0.903535	0.402527	0.108172	O
O21	1.0	0.899693	0.403782	0.318544	O
O22	1.0	0.354199	0.072712	-0.007826	O
O23	1.0	0.390596	0.077464	0.210980	O
O24	1.0	0.394823	0.104127	0.438144	O
O25	1.0	0.146444	0.602103	0.055203	O
O26	1.0	0.153712	0.593196	0.266492	O
O27	1.0	0.639858	0.915177	0.156130	O
O28	1.0	0.652038	0.905160	0.391172	O
O29	1.0	0.111136	0.908170	0.155449	O
O30	1.0	0.095962	0.913099	0.364212	O
O31	1.0	0.608673	0.597327	0.037566	O
O32	1.0	0.615430	0.583986	0.256325	O
O33	1.0	0.882552	0.131634	-0.004844	O
O34	1.0	0.856913	0.086509	0.205219	O
O35	1.0	0.864681	0.089454	0.423095	O
O36	1.0	0.361784	0.415886	0.094312	O
O37	1.0	0.363630	0.403622	0.307228	O
O38	1.0	0.136280	0.246876	0.156200	O
O39	1.0	0.125258	0.242344	0.367612	O

O40	1.0	0.653850	0.276956	0.052860	O
O41	1.0	0.639738	0.247904	0.257526	O
O42	1.0	0.884933	0.748002	0.106051	O
O43	1.0	0.884514	0.729793	0.317959	O
O44	1.0	0.322869	0.751616	-0.005031	O
O45	1.0	0.361172	0.748195	0.210311	O
O46	1.0	0.347875	0.743636	0.426894	O
O47	1.0	0.890003	0.788142	-0.001557	O
O48	1.0	0.891849	0.746854	0.207378	O
O49	1.0	0.933763	0.707033	0.423979	O
O50	1.0	0.387970	0.755409	0.098207	O
O51	1.0	0.385257	0.748502	0.315627	O
O52	1.0	0.109821	0.258259	0.056550	O
O53	1.0	0.109794	0.250978	0.263153	O
O54	1.0	0.638194	0.246269	0.159947	O
O55	1.0	0.635417	0.252517	0.363681	O
O56	1.0	0.123261	0.405014	0.463552	O
O57	1.0	0.654476	0.945339	0.499832	O
Al1	1.0	0.404301	0.930189	0.048975	Al
Al2	1.0	0.387492	0.918819	0.267365	Al
Al3	1.0	0.134695	0.419214	0.110633	Al
Al4	1.0	0.135111	0.409157	0.316515	Al
Al5	1.0	0.620626	0.417023	0.002354	Al
Al6	1.0	0.616051	0.422591	0.210667	Al
Al7	1.0	0.592059	0.402196	0.412065	Al
Al8	1.0	0.866548	0.917168	0.159876	Al
Al9	1.0	0.892460	0.895831	0.397868	Al
Al10	1.0	0.759752	-0.029019	-0.019659	Al
Al11	1.0	0.617312	0.071677	0.210614	Al
Al12	1.0	0.624204	0.059495	0.443816	Al
Al13	1.0	0.866364	0.576373	0.159069	Al
Al14	1.0	0.863482	0.581133	0.371262	Al
Al15	1.0	0.383929	0.581840	0.049298	Al
Al16	1.0	0.389975	0.576565	0.267520	Al
Al17	1.0	0.141190	0.078655	0.110946	Al
Al18	1.0	0.125043	0.071328	0.319852	Al
Al19	1.0	0.878344	0.225629	0.054976	Al
Al20	1.0	0.874268	0.254232	0.268168	Al
Al21	1.0	0.519161	0.270225	0.107086	Al
Al22	1.0	0.499311	0.240240	0.314002	Al
Al23	1.0	0.878954	0.247401	0.160352	Al
Al24	1.0	0.865546	0.227228	0.370896	Al
Al25	1.0	0.099310	0.767719	0.013284	Al
Al26	1.0	0.129852	0.746273	0.217808	Al
Al27	1.0	0.213769	0.586978	0.423923	Al
Al28	1.0	0.509477	0.745884	0.160709	Al
Al29	1.0	0.501723	0.755516	0.381262	Al
Al30	1.0	0.140656	0.751019	0.110238	Al
Al31	1.0	0.123964	0.748670	0.322216	Al
Al32	1.0	0.750431	0.748250	0.052716	Al
Al33	1.0	0.749996	0.748173	0.267106	Al
Al34	1.0	0.304434	0.248574	0.027808	Al
Al35	1.0	0.264936	0.249360	0.215914	Al
Al36	1.0	0.256962	0.254941	0.423897	Al

Coordinate for a calculated transition state of the initial CH_4 activation on a γ-Al_2O_3 (100) surface (**TS1**) in Figure S6.
Absolute Energy: –731.15875929 eV.

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	0.920240	0.400297	0.445216	H
H2	1.0	0.446076	0.056069	0.966456	H
H3	1.0	0.561919	0.045875	0.520166	H
H4	1.0	0.755645	0.658765	0.491000	H
H5	1.0	0.521510	0.642216	0.495072	H
H6	1.0	0.654002	0.584338	0.550936	H
H7	1.0	0.127609	0.406266	0.501422	H
H8	1.0	0.392015	0.762486	0.967252	H
H9	1.0	0.821895	0.302536	0.953363	H
H10	1.0	0.613689	0.868908	0.504787	H
C1	1.0	0.643463	0.633358	0.512911	C
O1	1.0	0.610577	0.276015	0.468214	O
O2	1.0	0.113988	0.596167	0.158018	O
O3	1.0	0.118020	0.571217	0.362424	O
O4	1.0	0.626232	0.911975	0.039562	O
O5	1.0	0.618653	0.917782	0.260709	O
O6	1.0	0.772178	0.407821	0.958558	O
O7	1.0	0.859057	0.408682	0.209112	O
O8	1.0	0.846876	0.404233	0.415123	O
O9	1.0	0.373672	0.114030	0.088357	O
O10	1.0	0.361968	0.081373	0.314132	O
O11	1.0	0.907286	0.090389	0.110455	O
O12	1.0	0.899208	0.102416	0.314982	O
O13	1.0	0.398394	0.408191	0.001087	O
O14	1.0	0.393592	0.423396	0.212612	O
O15	1.0	0.370005	0.441124	0.416136	O
O16	1.0	0.159311	0.915029	0.061107	O
O17	1.0	0.152807	0.901854	0.267916	O
O18	1.0	0.642895	0.580726	0.159124	O
O19	1.0	0.638874	0.587873	0.380216	O
O20	1.0	0.907042	0.411381	0.112283	O
O21	1.0	0.898203	0.404932	0.319865	O
O22	1.0	0.355829	0.063164	0.992858	O
O23	1.0	0.392555	0.080863	0.213547	O
O24	1.0	0.391845	0.111184	0.438487	O
O25	1.0	0.149614	0.601396	0.058658	O
O26	1.0	0.154973	0.595946	0.268258	O
O27	1.0	0.641762	0.919997	0.159435	O
O28	1.0	0.650073	0.900787	0.393952	O
O29	1.0	0.114311	0.910955	0.157936	O
O30	1.0	0.100448	0.915917	0.364996	O
O31	1.0	0.612412	0.592096	0.040479	O
O32	1.0	0.619561	0.585933	0.260068	O
O33	1.0	0.884407	0.109602	0.994427	O
O34	1.0	0.859028	0.093033	0.206950	O
O35	1.0	0.862193	0.087925	0.421755	O
O36	1.0	0.365508	0.419917	0.098834	O
O37	1.0	0.367960	0.407995	0.310923	O
O38	1.0	0.139875	0.249967	0.157440	O
O39	1.0	0.125166	0.246149	0.368439	O
O40	1.0	0.661563	0.272238	0.054814	O
O41	1.0	0.641205	0.250435	0.260303	O
O42	1.0	0.885766	0.751125	0.108905	O

O43	1.0	0.882053	0.738707	0.321977	O
O44	1.0	0.327203	0.746235	0.998405	O
O45	1.0	0.367114	0.751074	0.213673	O
O46	1.0	0.344930	0.747810	0.429936	O
O47	1.0	0.893103	0.774880	0.999668	O
O48	1.0	0.894479	0.751045	0.210349	O
O49	1.0	0.949767	0.706879	0.425416	O
O50	1.0	0.389301	0.756959	0.101557	O
O51	1.0	0.385043	0.750348	0.318190	O
O52	1.0	0.107422	0.258430	0.057218	O
O53	1.0	0.114563	0.253782	0.264832	O
O54	1.0	0.636685	0.251026	0.161815	O
O55	1.0	0.630414	0.243521	0.369417	O
O56	1.0	0.117073	0.407649	0.464748	O
O57	1.0	0.640459	0.983044	0.500351	O
Al1	1.0	0.408163	0.927698	0.050890	Al
Al2	1.0	0.390853	0.921653	0.268445	Al
Al3	1.0	0.136249	0.423987	0.111240	Al
Al4	1.0	0.138404	0.412362	0.316438	Al
Al5	1.0	0.623802	0.412822	0.004500	Al
Al6	1.0	0.619066	0.426970	0.212547	Al
Al7	1.0	0.589616	0.410655	0.415413	Al
Al8	1.0	0.868619	0.920402	0.161249	Al
Al9	1.0	0.894893	0.893784	0.395571	Al
Al10	1.0	0.742888	0.961881	0.975011	Al
Al11	1.0	0.619449	0.075289	0.212131	Al
Al12	1.0	0.622716	0.084181	0.432368	Al
Al13	1.0	0.869795	0.579683	0.160712	Al
Al14	1.0	0.866937	0.579032	0.371240	Al
Al15	1.0	0.387853	0.579404	0.051866	Al
Al16	1.0	0.393587	0.577947	0.268850	Al
Al17	1.0	0.144303	0.080666	0.112388	Al
Al18	1.0	0.128708	0.073601	0.319764	Al
Al19	1.0	0.878989	0.205986	0.052359	Al
Al20	1.0	0.876852	0.255260	0.267273	Al
Al21	1.0	0.520766	0.269963	0.107407	Al
Al22	1.0	0.501603	0.242285	0.315711	Al
Al23	1.0	0.878590	0.253156	0.160588	Al
Al24	1.0	0.873496	0.231605	0.370736	Al
Al25	1.0	0.101318	0.765943	0.014800	Al
Al26	1.0	0.133436	0.748095	0.217851	Al
Al27	1.0	0.193733	0.603274	0.425551	Al
Al28	1.0	0.511702	0.749897	0.162104	Al
Al29	1.0	0.496121	0.753721	0.382436	Al
Al30	1.0	0.142457	0.753596	0.111988	Al
Al31	1.0	0.128607	0.751714	0.322341	Al
Al32	1.0	0.755689	0.746584	0.053224	Al
Al33	1.0	0.752683	0.752398	0.268505	Al
Al34	1.0	0.298903	0.238997	0.025993	Al
Al35	1.0	0.266690	0.252792	0.216001	Al
Al36	1.0	0.257031	0.265115	0.423848	Al

Coordinate for a γ-Al_2O_3 (100) surface with CH_3* and H* in Figure S6.
Absolute Energy: –735.48943316 eV.

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	0.920806	0.416708	0.445179	H
H2	1.0	0.454286	0.063327	0.966430	H
H3	1.0	0.319484	0.002360	0.433871	H
H4	1.0	0.610200	0.432055	0.533295	H
H5	1.0	0.429203	0.317138	0.519836	H
H6	1.0	0.607844	0.220170	0.544821	H
H7	1.0	0.131170	0.431022	0.500998	H
H8	1.0	0.403265	0.775152	0.968250	H
H9	1.0	0.823690	0.312047	0.951249	H
H10	1.0	0.565867	0.880729	0.500626	H
C1	1.0	0.566060	0.315602	0.519540	C
O1	1.0	0.629214	0.287386	0.469707	O
O2	1.0	0.120958	0.609141	0.158642	O
O3	1.0	0.123781	0.583731	0.362801	O
O4	1.0	0.633554	0.921791	0.040463	O
O5	1.0	0.624030	0.930817	0.261153	O
O6	1.0	0.775984	0.417061	0.958030	O
O7	1.0	0.864648	0.420422	0.209722	O
O8	1.0	0.850064	0.417351	0.414479	O
O9	1.0	0.379645	0.125096	0.088326	O
O10	1.0	0.365763	0.093327	0.314335	O
O11	1.0	0.913268	0.102080	0.110653	O
O12	1.0	0.902982	0.114064	0.315228	O
O13	1.0	0.404731	0.417564	0.001913	O
O14	1.0	0.398809	0.435425	0.213792	O
O15	1.0	0.383596	0.446087	0.420575	O
O16	1.0	0.165675	0.925754	0.061224	O
O17	1.0	0.157698	0.913849	0.268013	O
O18	1.0	0.648939	0.593536	0.160096	O
O19	1.0	0.642544	0.599670	0.380230	O
O20	1.0	0.913921	0.425834	0.113374	O
O21	1.0	0.901764	0.417868	0.319645	O
O22	1.0	0.363145	0.072478	0.992842	O
O23	1.0	0.397786	0.092710	0.213814	O
O24	1.0	0.367009	0.110529	0.437763	O
O25	1.0	0.156671	0.612322	0.059022	O
O26	1.0	0.159789	0.608008	0.268607	O
O27	1.0	0.647699	0.932317	0.160068	O
O28	1.0	0.652105	0.914421	0.392026	O
O29	1.0	0.120046	0.923033	0.158196	O
O30	1.0	0.105374	0.928505	0.364923	O
O31	1.0	0.619621	0.601400	0.040918	O
O32	1.0	0.625433	0.598184	0.260976	O
O33	1.0	0.890484	0.114251	0.993335	O
O34	1.0	0.864824	0.106006	0.207138	O
O35	1.0	0.868617	0.097643	0.422011	O
O36	1.0	0.372015	0.431685	0.099719	O
O37	1.0	0.372490	0.420723	0.312229	O
O38	1.0	0.146178	0.261689	0.157514	O
O39	1.0	0.126302	0.260623	0.368269	O
O40	1.0	0.670228	0.281948	0.054988	O
O41	1.0	0.645782	0.262523	0.260853	O
O42	1.0	0.891963	0.762955	0.109344	O

O43	1.0	0.885777	0.753487	0.322731	O
O44	1.0	0.335771	0.756578	0.998919	O
O45	1.0	0.373262	0.763733	0.214218	O
O46	1.0	0.341864	0.767765	0.428459	O
O47	1.0	0.901048	0.781583	-0.000281	O
O48	1.0	0.900288	0.763616	0.210822	O
O49	1.0	0.954323	0.721193	0.424718	O
O50	1.0	0.395053	0.768540	0.102068	O
O51	1.0	0.389108	0.762285	0.318387	O
O52	1.0	0.111845	0.268335	0.057096	O
O53	1.0	0.119944	0.265090	0.265232	O
O54	1.0	0.641680	0.263530	0.162095	O
O55	1.0	0.633988	0.255726	0.370235	O
O56	1.0	0.115711	0.433238	0.464435	O
O57	1.0	0.638776	0.972081	0.499111	O
Al1	1.0	0.415591	0.938032	0.051018	Al
Al2	1.0	0.396086	0.934220	0.268303	Al
Al3	1.0	0.142218	0.436055	0.111207	Al
Al4	1.0	0.142748	0.425175	0.316518	Al
Al5	1.0	0.630292	0.422385	0.004623	Al
Al6	1.0	0.624646	0.439721	0.212925	Al
Al7	1.0	0.598674	0.419666	0.414565	Al
Al8	1.0	0.874628	0.932628	0.161255	Al
Al9	1.0	0.894226	0.905432	0.392905	Al
Al10	1.0	0.744590	0.970201	0.973157	Al
Al11	1.0	0.624848	0.087798	0.212247	Al
Al12	1.0	0.640832	0.075552	0.441410	Al
Al13	1.0	0.876165	0.592058	0.160951	Al
Al14	1.0	0.869910	0.589373	0.369804	Al
Al15	1.0	0.395006	0.590083	0.052282	Al
Al16	1.0	0.399207	0.589429	0.269270	Al
Al17	1.0	0.150830	0.092438	0.112353	Al
Al18	1.0	0.132979	0.086488	0.319347	Al
Al19	1.0	0.884415	0.209426	0.051011	Al
Al20	1.0	0.881350	0.266949	0.266954	Al
Al21	1.0	0.526935	0.280774	0.107071	Al
Al22	1.0	0.505964	0.253918	0.316323	Al
Al23	1.0	0.883750	0.265950	0.160372	Al
Al24	1.0	0.873677	0.241921	0.370820	Al
Al25	1.0	0.109101	0.776530	0.014627	Al
Al26	1.0	0.139485	0.759947	0.217543	Al
Al27	1.0	0.175511	0.635521	0.426826	Al
Al28	1.0	0.517217	0.762452	0.162268	Al
Al29	1.0	0.500324	0.764139	0.382083	Al
Al30	1.0	0.148203	0.765356	0.112013	Al
Al31	1.0	0.136194	0.764030	0.322135	Al
Al32	1.0	0.763408	0.756533	0.052927	Al
Al33	1.0	0.758065	0.765458	0.268358	Al
Al34	1.0	0.303104	0.247893	0.025366	Al
Al35	1.0	0.271816	0.264537	0.215925	Al
Al36	1.0	0.252243	0.284856	0.423719	Al

Coordinate for a calculated transition state from CH_3* on a γ-Al_2O_3 (100) surface (**TS3**) in Figure S6.
Absolute Energy: –734.90592846 eV.

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	0.878798	0.413373	0.449579	H
H2	1.0	0.452120	0.055973	0.966720	H
H3	1.0	0.316144	0.998889	0.431882	H
H4	1.0	0.535542	0.543100	0.533514	H
H5	1.0	0.479016	0.335993	0.529587	H
H6	1.0	0.667816	0.392185	0.559001	H
H7	1.0	0.174586	0.444668	0.498809	H
H8	1.0	0.399931	0.766877	0.968159	H
H9	1.0	0.824437	0.303567	0.952502	H
H10	1.0	0.529432	1.014650	0.509586	H
C1	1.0	0.583355	0.421278	0.527514	C
O1	1.0	0.669836	0.409237	0.481470	O
O2	1.0	0.118922	0.601528	0.158589	O
O3	1.0	0.122411	0.578516	0.362271	O
O4	1.0	0.631296	0.914454	0.040661	O
O5	1.0	0.622810	0.923657	0.261260	O
O6	1.0	0.777559	0.409065	0.959267	O
O7	1.0	0.862922	0.412872	0.210034	O
O8	1.0	0.860943	0.410207	0.412601	O
O9	1.0	0.377788	0.117161	0.088756	O
O10	1.0	0.367387	0.086839	0.314780	O
O11	1.0	0.911337	0.094688	0.111065	O
O12	1.0	0.902623	0.106943	0.315619	O
O13	1.0	0.403408	0.409843	0.001996	O
O14	1.0	0.398040	0.428328	0.213399	O
O15	1.0	0.391747	0.433740	0.417281	O
O16	1.0	0.163287	0.918036	0.061343	O
O17	1.0	0.157471	0.908251	0.267418	O
O18	1.0	0.647402	0.585604	0.160008	O
O19	1.0	0.644326	0.592268	0.376634	O
O20	1.0	0.912119	0.417707	0.113552	O
O21	1.0	0.900452	0.410379	0.319534	O
O22	1.0	0.360912	0.064984	0.993171	O
O23	1.0	0.396753	0.085903	0.214060	O
O24	1.0	0.365080	0.106808	0.435061	O
O25	1.0	0.154560	0.604239	0.059083	O
O26	1.0	0.158087	0.600886	0.267971	O
O27	1.0	0.645607	0.925268	0.160234	O
O28	1.0	0.647451	0.901646	0.387172	O
O29	1.0	0.118332	0.915209	0.158248	O
O30	1.0	0.107641	0.921669	0.364073	O
O31	1.0	0.617721	0.593891	0.041129	O
O32	1.0	0.624239	0.591678	0.260658	O
O33	1.0	0.888785	0.106469	0.993923	O
O34	1.0	0.862968	0.098772	0.207624	O
O35	1.0	0.865528	0.085909	0.419529	O
O36	1.0	0.370056	0.423646	0.099749	O
O37	1.0	0.372204	0.414393	0.311614	O
O38	1.0	0.144365	0.254120	0.157895	O
O39	1.0	0.126692	0.254223	0.367873	O
O40	1.0	0.667962	0.274343	0.055555	O
O41	1.0	0.644325	0.255806	0.262739	O
O42	1.0	0.889977	0.755460	0.109315	O

O43	1.0	0.887045	0.749362	0.321828	O
O44	1.0	0.333178	0.748619	0.998977	O
O45	1.0	0.371977	0.756203	0.213879	O
O46	1.0	0.338046	0.758886	0.426954	O
O47	1.0	0.898593	0.773749	0.999710	O
O48	1.0	0.898611	0.756461	0.210598	O
O49	1.0	0.947432	0.718360	0.422907	O
O50	1.0	0.393158	0.760583	0.102026	O
O51	1.0	0.386234	0.754234	0.317219	O
O52	1.0	0.110337	0.260407	0.057483	O
O53	1.0	0.119167	0.258005	0.265454	O
O54	1.0	0.639892	0.256083	0.162776	O
O55	1.0	0.629883	0.242264	0.376539	O
O56	1.0	0.127497	0.439986	0.464820	O
O57	1.0	0.635859	0.035232	0.494013	O
Al1	1.0	0.413379	0.930428	0.051153	Al
Al2	1.0	0.395453	0.928106	0.268203	Al
Al3	1.0	0.140422	0.428367	0.111402	Al
Al4	1.0	0.142912	0.419303	0.316301	Al
Al5	1.0	0.629038	0.414635	0.005042	Al
Al6	1.0	0.623784	0.431925	0.213308	Al
Al7	1.0	0.605383	0.429000	0.418312	Al
Al8	1.0	0.872275	0.925268	0.161205	Al
Al9	1.0	0.892563	0.898062	0.388390	Al
Al10	1.0	0.742245	0.963489	0.973322	Al
Al11	1.0	0.623494	0.080991	0.212824	Al
Al12	1.0	0.633099	0.069319	0.429184	Al
Al13	1.0	0.874292	0.584561	0.160929	Al
Al14	1.0	0.870586	0.582597	0.368560	Al
Al15	1.0	0.393106	0.582370	0.052360	Al
Al16	1.0	0.397648	0.582274	0.268294	Al
Al17	1.0	0.149073	0.084927	0.112575	Al
Al18	1.0	0.134687	0.080473	0.318993	Al
Al19	1.0	0.882531	0.202754	0.051482	Al
Al20	1.0	0.879885	0.259388	0.267254	Al
Al21	1.0	0.525055	0.272929	0.107670	Al
Al22	1.0	0.505789	0.249104	0.319478	Al
Al23	1.0	0.882676	0.258400	0.160787	Al
Al24	1.0	0.882262	0.236028	0.371443	Al
Al25	1.0	0.106593	0.768630	0.014641	Al
Al26	1.0	0.138258	0.753806	0.217100	Al
Al27	1.0	0.163192	0.636842	0.426819	Al
Al28	1.0	0.515900	0.754681	0.162062	Al
Al29	1.0	0.495151	0.750105	0.380452	Al
Al30	1.0	0.146080	0.757648	0.111915	Al
Al31	1.0	0.137664	0.757421	0.321260	Al
Al32	1.0	0.761280	0.749215	0.052937	Al
Al33	1.0	0.756599	0.758637	0.267966	Al
Al34	1.0	0.301726	0.240482	0.025774	Al
Al35	1.0	0.271195	0.257790	0.216217	Al
Al36	1.0	0.251512	0.285227	0.423495	Al

Coordinate for a γ-Al_2O_3 (100) surface with CH_3OH* in Figure S6.
Absolute Energy: –735.56165834eV.

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	0.878798	0.413373	0.449579	H
H2	1.0	0.452120	0.055973	0.966720	H
H3	1.0	0.316144	0.998889	0.431882	H
H4	1.0	0.535542	0.543100	0.533514	H
H5	1.0	0.479016	0.335993	0.529587	H
H6	1.0	0.667816	0.392185	0.559001	H
H7	1.0	0.174586	0.444668	0.498809	H
H8	1.0	0.399931	0.766877	0.968159	H
H9	1.0	0.824437	0.303567	0.952502	H
H10	1.0	0.529432	1.014650	0.509586	H
C1	1.0	0.583355	0.421278	0.527514	C
O1	1.0	0.669836	0.409237	0.481470	O
O2	1.0	0.118922	0.601528	0.158589	O
O3	1.0	0.122411	0.578516	0.362271	O
O4	1.0	0.631296	0.914454	0.040661	O
O5	1.0	0.622810	0.923657	0.261260	O
O6	1.0	0.777559	0.409065	0.959267	O
O7	1.0	0.862922	0.412872	0.210034	O
O8	1.0	0.860943	0.410207	0.412601	O
O9	1.0	0.377788	0.117161	0.088756	O
O10	1.0	0.367387	0.086839	0.314780	O
O11	1.0	0.911337	0.094688	0.111065	O
O12	1.0	0.902623	0.106943	0.315619	O
O13	1.0	0.403408	0.409843	0.001996	O
O14	1.0	0.398040	0.428328	0.213399	O
O15	1.0	0.391747	0.433740	0.417281	O
O16	1.0	0.163287	0.918036	0.061343	O
O17	1.0	0.157471	0.908251	0.267418	O
O18	1.0	0.647402	0.585604	0.160008	O
O19	1.0	0.644326	0.592268	0.376634	O
O20	1.0	0.912119	0.417707	0.113552	O
O21	1.0	0.900452	0.410379	0.319534	O
O22	1.0	0.360912	0.064984	0.993171	O
O23	1.0	0.396753	0.085903	0.214060	O
O24	1.0	0.365080	0.106808	0.435061	O
O25	1.0	0.154560	0.604239	0.059083	O
O26	1.0	0.158087	0.600886	0.267971	O
O27	1.0	0.645607	0.925268	0.160234	O
O28	1.0	0.647451	0.901646	0.387172	O
O29	1.0	0.118332	0.915209	0.158248	O
O30	1.0	0.107641	0.921669	0.364073	O
O31	1.0	0.617721	0.593891	0.041129	O
O32	1.0	0.624239	0.591678	0.260658	O
O33	1.0	0.888785	0.106469	0.993923	O
O34	1.0	0.862968	0.098772	0.207624	O
O35	1.0	0.865528	0.085909	0.419529	O
O36	1.0	0.370056	0.423646	0.099749	O
O37	1.0	0.372204	0.414393	0.311614	O
O38	1.0	0.144365	0.254120	0.157895	O
O39	1.0	0.126692	0.254223	0.367873	O
O40	1.0	0.667962	0.274343	0.055555	O
O41	1.0	0.644325	0.255806	0.262739	O
O42	1.0	0.889977	0.755460	0.109315	O

O43	1.0	0.887045	0.749362	0.321828	O
O44	1.0	0.333178	0.748619	0.998977	O
O45	1.0	0.371977	0.756203	0.213879	O
O46	1.0	0.338046	0.758886	0.426954	O
O47	1.0	0.898593	0.773749	0.999710	O
O48	1.0	0.898611	0.756461	0.210598	O
O49	1.0	0.947432	0.718360	0.422907	O
O50	1.0	0.393158	0.760583	0.102026	O
O51	1.0	0.386234	0.754234	0.317219	O
O52	1.0	0.110337	0.260407	0.057483	O
O53	1.0	0.119167	0.258005	0.265454	O
O54	1.0	0.639892	0.256083	0.162776	O
O55	1.0	0.629883	0.242264	0.376539	O
O56	1.0	0.127497	0.439986	0.464820	O
O57	1.0	0.635859	0.035232	0.494013	O
Al1	1.0	0.413379	0.930428	0.051153	Al
Al2	1.0	0.395453	0.928106	0.268203	Al
Al3	1.0	0.140422	0.428367	0.111402	Al
Al4	1.0	0.142912	0.419303	0.316301	Al
Al5	1.0	0.629038	0.414635	0.005042	Al
Al6	1.0	0.623784	0.431925	0.213308	Al
Al7	1.0	0.605383	0.429000	0.418312	Al
Al8	1.0	0.872275	0.925268	0.161205	Al
Al9	1.0	0.892563	0.898062	0.388390	Al
Al10	1.0	0.742245	0.963489	0.973322	Al
Al11	1.0	0.623494	0.080991	0.212824	Al
Al12	1.0	0.633099	0.069319	0.429184	Al
Al13	1.0	0.874292	0.584561	0.160929	Al
Al14	1.0	0.870586	0.582597	0.368560	Al
Al15	1.0	0.393106	0.582370	0.052360	Al
Al16	1.0	0.397648	0.582274	0.268294	Al
Al17	1.0	0.149073	0.084927	0.112575	Al
Al18	1.0	0.134687	0.080473	0.318993	Al
Al19	1.0	0.882531	0.202754	0.051482	Al
Al20	1.0	0.879885	0.259388	0.267254	Al
Al21	1.0	0.525055	0.272929	0.107670	Al
Al22	1.0	0.505789	0.249104	0.319478	Al
Al23	1.0	0.882676	0.258400	0.160787	Al
Al24	1.0	0.882262	0.236028	0.371443	Al
Al25	1.0	0.106593	0.768630	0.014641	Al
Al26	1.0	0.138258	0.753806	0.217100	Al
Al27	1.0	0.163192	0.636842	0.426819	Al
Al28	1.0	0.515900	0.754681	0.162062	Al
Al29	1.0	0.495151	0.750105	0.380452	Al
Al30	1.0	0.146080	0.757648	0.111915	Al
Al31	1.0	0.137664	0.757421	0.321260	Al
Al32	1.0	0.761280	0.749215	0.052937	Al
Al33	1.0	0.756599	0.758637	0.267966	Al
Al34	1.0	0.301726	0.240482	0.025774	Al
Al35	1.0	0.271195	0.257790	0.216217	Al
Al36	1.0	0.251512	0.285227	0.423495	Al

S3.3 Optimized Structures and Energies for Figure S8

Coordinate for a γ-Al_2O_3 (100) surface with CH_4 σ-complex at a 6-coordinated Al site.
Absolute Energy: −751.20248905 eV.

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	0.000647	0.431891	0.446116	H
H2	1.0	0.397608	0.758756	0.963031	H
H3	1.0	0.870488	0.312798	0.966527	H
H4	1.0	0.573832	0.796423	0.505100	H
H5	1.0	0.272796	0.835634	0.398556	H
H6	1.0	0.274106	0.002458	0.462014	H
H7	1.0	0.843184	0.145696	0.447270	H
H8	1.0	0.848942	0.716110	0.448037	H
H9	1.0	0.658037	0.556409	0.550341	H
H10	1.0	0.575993	0.516356	0.612460	H
H11	1.0	0.454986	0.477515	0.556797	H
H12	1.0	0.630540	0.355652	0.570290	H
C1	1.0	0.580270	0.476538	0.572878	C
O1	1.0	0.658774	0.227307	0.468866	O
O2	1.0	0.620666	0.599222	0.455137	O
O3	1.0	0.118417	0.581923	0.150846	O
O4	1.0	0.127608	0.583215	0.361494	O
O5	1.0	0.624612	0.903348	0.044615	O
O6	1.0	0.621451	0.918417	0.263303	O
O7	1.0	0.849375	0.407438	-0.012199	O
O8	1.0	0.868542	0.407173	0.203658	O
O9	1.0	0.858931	0.430101	0.411832	O
O10	1.0	0.376508	0.097723	0.093119	O
O11	1.0	0.373472	0.092954	0.312919	O
O12	1.0	0.914556	0.091267	0.105388	O
O13	1.0	0.905570	0.102053	0.320048	O
O14	1.0	0.426961	0.420271	0.994823	O
O15	1.0	0.399640	0.417798	0.205912	O
O16	1.0	0.397411	0.404877	0.415910	O
O17	1.0	0.166605	0.910026	0.055735	O
O18	1.0	0.155206	0.917205	0.264850	O
O19	1.0	0.651776	0.575618	0.154193	O
O20	1.0	0.657389	0.643572	0.354562	O
O21	1.0	0.912459	0.395732	0.102188	O
O22	1.0	0.909678	0.413748	0.314137	O
O23	1.0	0.429336	0.081886	0.996628	O
O24	1.0	0.402379	0.081175	0.211801	O
O25	1.0	0.336166	0.092580	0.448538	O
O26	1.0	0.164857	0.592937	0.053537	O
O27	1.0	0.150858	0.599089	0.263520	O
O28	1.0	0.649046	0.917548	0.159010	O
O29	1.0	0.660241	0.932165	0.405259	O
O30	1.0	0.124011	0.910491	0.153193	O
O31	1.0	0.128808	0.921816	0.364706	O
O32	1.0	0.625024	0.599693	0.042269	O
O33	1.0	0.616713	0.587665	0.253960	O
O34	1.0	0.852600	0.112314	0.994526	O
O35	1.0	0.868774	0.091329	0.205271	O
O36	1.0	0.929182	0.113219	0.421156	O
O37	1.0	0.372846	0.402912	0.090047	O

O38	1.0	0.369439	0.417061	0.305235	O
O39	1.0	0.144400	0.248091	0.153272	O
O40	1.0	0.137443	0.259692	0.362830	O
O41	1.0	0.646442	0.254074	0.053410	O
O42	1.0	0.651521	0.251663	0.258874	O
O43	1.0	0.899196	0.750876	0.103411	O
O44	1.0	0.902983	0.765765	0.320709	O
O45	1.0	0.338669	0.753537	0.995096	O
O46	1.0	0.363729	0.749509	0.207348	O
O47	1.0	0.344124	0.756078	0.418599	O
O48	1.0	0.908621	0.753784	0.994218	O
O49	1.0	0.912066	0.750947	0.202258	O
O50	1.0	0.925551	0.743724	0.420244	O
O51	1.0	0.391618	0.748743	0.099374	O
O52	1.0	0.378565	0.753182	0.307377	O
O53	1.0	0.129561	0.248455	0.049615	O
O54	1.0	0.117719	0.250326	0.262123	O
O55	1.0	0.648983	0.246209	0.160587	O
O56	1.0	0.647111	0.272644	0.366905	O
O57	1.0	0.126317	0.426998	0.456738	O
O58	1.0	0.541827	0.908124	0.506370	O
Al1	1.0	0.401861	0.921285	0.052225	Al
Al2	1.0	0.393965	0.930145	0.267270	Al
Al3	1.0	0.142309	0.418910	0.106183	Al
Al4	1.0	0.143593	0.422899	0.311547	Al
Al5	1.0	0.645422	0.424806	0.009250	Al
Al6	1.0	0.627990	0.425741	0.209596	Al
Al7	1.0	0.628495	0.398498	0.430223	Al
Al8	1.0	0.875979	0.916140	0.159125	Al
Al9	1.0	0.897715	0.929024	0.382263	Al
Al10	1.0	0.650718	0.075065	0.009500	Al
Al11	1.0	0.630716	0.068353	0.213099	Al
Al12	1.0	0.567775	0.045835	0.458439	Al
Al13	1.0	0.878867	0.583495	0.160017	Al
Al14	1.0	0.880217	0.590776	0.366740	Al
Al15	1.0	0.399561	0.582899	0.050109	Al
Al16	1.0	0.389785	0.583874	0.261335	Al
Al17	1.0	0.147760	0.075825	0.108720	Al
Al18	1.0	0.144175	0.084508	0.317994	Al
Al19	1.0	0.902547	0.237668	0.049419	Al
Al20	1.0	0.883336	0.249930	0.265298	Al
Al21	1.0	0.514640	0.254474	0.111582	Al
Al22	1.0	0.510793	0.259101	0.316501	Al
Al23	1.0	0.886213	0.248304	0.156924	Al
Al24	1.0	0.874555	0.261556	0.368724	Al
Al25	1.0	0.110109	0.754742	0.010838	Al
Al26	1.0	0.132613	0.761471	0.215760	Al
Al27	1.0	0.251242	0.563824	0.418507	Al
Al28	1.0	0.521506	0.745543	0.160587	Al
Al29	1.0	0.571231	0.737221	0.408888	Al
Al30	1.0	0.144454	0.747515	0.108852	Al
Al31	1.0	0.144293	0.759536	0.317597	Al
Al32	1.0	0.777551	0.751864	0.046971	Al
Al33	1.0	0.694025	0.740907	0.293842	Al
Al34	1.0	0.333444	0.251690	0.025708	Al
Al35	1.0	0.271245	0.249691	0.213155	Al
Al36	1.0	0.233931	0.263123	0.423719	Al

Coordinate for a calculated transition state of the CH_4 activation on a γ-Al_2O_3 (100) surface (**TS1**) in Figure S8.
Absolute Energy: –748.39713689 eV.

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	0.026189	0.433421	0.450212	H
H2	1.0	0.398855	0.757379	0.963082	H
H3	1.0	0.894729	0.344723	0.967341	H
H4	1.0	0.598421	0.894456	0.534915	H
H5	1.0	0.257766	0.897019	0.417964	H
H6	1.0	0.274648	0.065829	0.486932	H
H7	1.0	0.954007	0.082717	0.447181	H
H8	1.0	0.812876	0.702044	0.439219	H
H9	1.0	0.633206	0.523465	0.544152	H
H10	1.0	0.623490	0.492217	0.611751	H
H11	1.0	0.441411	0.471270	0.573039	H
H12	1.0	0.603044	0.327710	0.568296	H
C1	1.0	0.576010	0.453975	0.574674	C
O1	1.0	0.482589	0.319493	0.456514	O
O2	1.0	0.632966	0.647085	0.454898	O
O3	1.0	0.119668	0.590114	0.152744	O
O4	1.0	0.117249	0.590767	0.359327	O
O5	1.0	0.626910	0.905441	0.044722	O
O6	1.0	0.626775	0.915136	0.258141	O
O7	1.0	0.861351	0.415211	0.995009	O
O8	1.0	0.872077	0.411700	0.203548	O
O9	1.0	0.853343	0.418993	0.416726	O
O10	1.0	0.378944	0.099917	0.094561	O
O11	1.0	0.378045	0.082484	0.311465	O
O12	1.0	0.918910	0.094138	0.106398	O
O13	1.0	0.905683	0.100703	0.323911	O
O14	1.0	0.427686	0.420730	0.995336	O
O15	1.0	0.406355	0.415174	0.202513	O
O16	1.0	0.404228	0.539084	0.393395	O
O17	1.0	0.168888	0.912177	0.056337	O
O18	1.0	0.163219	0.904896	0.262140	O
O19	1.0	0.652928	0.574055	0.151643	O
O20	1.0	0.672061	0.577329	0.351893	O
O21	1.0	0.917910	0.400899	0.104405	O
O22	1.0	0.921721	0.400627	0.317983	O
O23	1.0	0.430105	0.083178	0.997887	O
O24	1.0	0.405620	0.082237	0.210736	O
O25	1.0	0.210782	0.099411	0.457455	O
O26	1.0	0.165545	0.595702	0.054526	O
O27	1.0	0.158491	0.595447	0.262470	O
O28	1.0	0.652132	0.917404	0.156818	O
O29	1.0	0.627177	0.884931	0.386508	O
O30	1.0	0.121300	0.907660	0.154001	O
O31	1.0	0.117935	0.914966	0.362639	O
O32	1.0	0.625765	0.602105	0.041302	O
O33	1.0	0.623248	0.589464	0.250298	O
O34	1.0	0.855605	0.116109	0.995921	O
O35	1.0	0.872661	0.087679	0.205558	O
O36	1.0	0.873713	0.079283	0.419435	O
O37	1.0	0.374520	0.407013	0.090803	O
O38	1.0	0.374381	0.406966	0.299092	O
O39	1.0	0.146774	0.250119	0.155443	O
O40	1.0	0.178438	0.264193	0.369042	O

O41	1.0	0.647871	0.257377	0.054727	O
O42	1.0	0.657716	0.249536	0.258774	O
O43	1.0	0.899771	0.750965	0.104078	O
O44	1.0	0.897721	0.761458	0.315313	O
O45	1.0	0.340002	0.753625	0.995223	O
O46	1.0	0.372257	0.747469	0.207205	O
O47	1.0	0.326936	0.804970	0.430118	O
O48	1.0	0.911185	0.757333	0.994372	O
O49	1.0	0.901561	0.748720	0.205271	O
O50	1.0	0.913932	0.733431	0.416469	O
O51	1.0	0.392965	0.750638	0.099307	O
O52	1.0	0.386940	0.747519	0.309279	O
O53	1.0	0.132347	0.250659	0.051806	O
O54	1.0	0.120649	0.242758	0.265096	O
O55	1.0	0.656409	0.244749	0.160507	O
O56	1.0	0.630428	0.265979	0.368422	O
O57	1.0	0.149447	0.453056	0.457008	O
O58	1.0	0.558335	0.954826	0.506033	O
Al1	1.0	0.404599	0.924666	0.052731	Al
Al2	1.0	0.396702	0.926194	0.265061	Al
Al3	1.0	0.147967	0.421061	0.108533	Al
Al4	1.0	0.154435	0.415781	0.317333	Al
Al5	1.0	0.647586	0.424493	0.009532	Al
Al6	1.0	0.634694	0.421106	0.208904	Al
Al7	1.0	0.605399	0.453006	0.420077	Al
Al8	1.0	0.877685	0.919518	0.157900	Al
Al9	1.0	0.873802	0.909642	0.375199	Al
Al10	1.0	0.653503	0.078451	0.009998	Al
Al11	1.0	0.633036	0.072738	0.211124	Al
Al12	1.0	0.555080	0.841396	0.451699	Al
Al13	1.0	0.877749	0.578853	0.156624	Al
Al14	1.0	0.882200	0.572409	0.365846	Al
Al15	1.0	0.400930	0.584638	0.049606	Al
Al16	1.0	0.395624	0.579225	0.259007	Al
Al17	1.0	0.151252	0.078551	0.110227	Al
Al18	1.0	0.154581	0.091275	0.327359	Al
Al19	1.0	0.905042	0.242535	0.050306	Al
Al20	1.0	0.889378	0.242958	0.270702	Al
Al21	1.0	0.515320	0.259253	0.113241	Al
Al22	1.0	0.511511	0.250713	0.315791	Al
Al23	1.0	0.895419	0.248722	0.159261	Al
Al24	1.0	0.846512	0.247320	0.376547	Al
Al25	1.0	0.112690	0.757479	0.010751	Al
Al26	1.0	0.139759	0.751755	0.213823	Al
Al27	1.0	0.222814	0.615121	0.419530	Al
Al28	1.0	0.524952	0.744980	0.158844	Al
Al29	1.0	0.514195	0.707386	0.364928	Al
Al30	1.0	0.146484	0.750076	0.108068	Al
Al31	1.0	0.135328	0.760623	0.315297	Al
Al32	1.0	0.778756	0.753624	0.046702	Al
Al33	1.0	0.758950	0.747739	0.264493	Al
Al34	1.0	0.334732	0.252989	0.026774	Al
Al35	1.0	0.275441	0.250879	0.216883	Al
Al36	1.0	0.284089	0.282759	0.434177	Al

Coordinate for a γ-Al_2O_3 (100) surface with CH_3* and H* in Figure S8.
Absolute Energy: –750.95318799 eV.

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	0.018659	0.441341	0.456484	H
H2	1.0	0.396617	0.756631	0.965021	H
H3	1.0	0.913047	0.373586	0.970718	H
H4	1.0	0.610094	0.807523	0.487339	H
H5	1.0	0.259443	0.851052	0.403042	H
H6	1.0	0.172607	0.028528	0.477112	H
H7	1.0	0.999976	0.106528	0.451805	H
H8	1.0	0.826800	0.782912	0.444653	H
H9	1.0	0.609816	0.494704	0.509246	H
H10	1.0	0.668849	0.429763	0.598238	H
H11	1.0	0.441206	0.447640	0.583623	H
H12	1.0	0.559712	0.267039	0.562060	H
C1	1.0	0.557311	0.382484	0.580671	C
O1	1.0	0.439885	0.135680	0.443514	O
O2	1.0	0.608765	0.547465	0.476415	O
O3	1.0	0.119572	0.599833	0.155885	O
O4	1.0	0.121768	0.592975	0.363410	O
O5	1.0	0.627135	0.911220	0.041974	O
O6	1.0	0.627002	0.923190	0.258495	O
O7	1.0	0.874551	0.420502	0.002429	O
O8	1.0	0.870043	0.416423	0.206732	O
O9	1.0	0.858386	0.431637	0.415948	O
O10	1.0	0.379939	0.103152	0.095185	O
O11	1.0	0.376632	0.093406	0.312637	O
O12	1.0	0.917596	0.101707	0.108880	O
O13	1.0	0.908708	0.106270	0.320023	O
O14	1.0	0.406429	0.427847	0.999530	O
O15	1.0	0.402956	0.427771	0.210723	O
O16	1.0	0.393644	0.430909	0.411054	O
O17	1.0	0.167517	0.916115	0.058191	O
O18	1.0	0.160761	0.914427	0.265007	O
O19	1.0	0.651847	0.586313	0.157272	O
O20	1.0	0.644632	0.606122	0.370795	O
O21	1.0	0.917723	0.410806	0.108311	O
O22	1.0	0.912397	0.415169	0.317811	O
O23	1.0	0.422548	0.083041	0.997688	O
O24	1.0	0.403253	0.089844	0.212260	O
O25	1.0	0.118965	0.128333	0.468248	O
O26	1.0	0.165103	0.600909	0.058219	O
O27	1.0	0.159273	0.605512	0.265935	O
O28	1.0	0.650616	0.928006	0.157993	O
O29	1.0	0.644553	0.933446	0.372563	O
O30	1.0	0.120761	0.914754	0.155706	O
O31	1.0	0.121626	0.925044	0.363199	O
O32	1.0	0.625053	0.598836	0.039273	O
O33	1.0	0.626933	0.593122	0.257710	O
O34	1.0	0.866154	0.110763	0.999445	O
O35	1.0	0.869907	0.098680	0.207084	O
O36	1.0	0.856272	0.096967	0.419399	O
O37	1.0	0.378054	0.418458	0.098018	O
O38	1.0	0.372528	0.421724	0.308622	O
O39	1.0	0.146801	0.256840	0.157136	O
O40	1.0	0.138420	0.258409	0.369361	O

O41	1.0	0.650324	0.261917	0.054156	O
O42	1.0	0.652586	0.257939	0.260915	O
O43	1.0	0.894606	0.756826	0.105122	O
O44	1.0	0.894002	0.759586	0.317537	O
O45	1.0	0.337574	0.757889	0.997131	O
O46	1.0	0.374127	0.757712	0.210583	O
O47	1.0	0.345146	0.770613	0.416247	O
O48	1.0	0.913754	0.756619	0.994484	O
O49	1.0	0.902060	0.757962	0.206904	O
O50	1.0	0.906001	0.763497	0.415806	O
O51	1.0	0.395535	0.757413	0.100705	O
O52	1.0	0.387564	0.760003	0.312053	O
O53	1.0	0.131864	0.255772	0.055817	O
O54	1.0	0.122257	0.256447	0.265624	O
O55	1.0	0.648912	0.256938	0.161991	O
O56	1.0	0.645380	0.275047	0.369947	O
O57	1.0	0.141894	0.446816	0.462597	O
O58	1.0	0.680925	0.897137	0.478258	O
Al1	1.0	0.406235	0.928963	0.051925	Al
Al2	1.0	0.398017	0.934822	0.264729	Al
Al3	1.0	0.150562	0.428572	0.109922	Al
Al4	1.0	0.146215	0.423928	0.317330	Al
Al5	1.0	0.643734	0.422636	0.001164	Al
Al6	1.0	0.631146	0.432472	0.210985	Al
Al7	1.0	0.618220	0.446698	0.417087	Al
Al8	1.0	0.876516	0.928446	0.157049	Al
Al9	1.0	0.881298	0.932924	0.370419	Al
Al10	1.0	0.655377	0.088956	0.006114	Al
Al11	1.0	0.631458	0.082842	0.211296	Al
Al12	1.0	0.629114	0.042928	0.432439	Al
Al13	1.0	0.877531	0.585657	0.156945	Al
Al14	1.0	0.873272	0.595735	0.370579	Al
Al15	1.0	0.403281	0.582318	0.051935	Al
Al16	1.0	0.398286	0.584928	0.263727	Al
Al17	1.0	0.151614	0.086111	0.110169	Al
Al18	1.0	0.149257	0.092855	0.320634	Al
Al19	1.0	0.901074	0.249687	0.050123	Al
Al20	1.0	0.885393	0.257991	0.267627	Al
Al21	1.0	0.520553	0.262018	0.110102	Al
Al22	1.0	0.512509	0.260087	0.318156	Al
Al23	1.0	0.892419	0.257243	0.159697	Al
Al24	1.0	0.877104	0.263165	0.373740	Al
Al25	1.0	0.112918	0.759456	0.012585	Al
Al26	1.0	0.140009	0.759069	0.214470	Al
Al27	1.0	0.245611	0.577827	0.420652	Al
Al28	1.0	0.521713	0.756699	0.159419	Al
Al29	1.0	0.514481	0.769730	0.368375	Al
Al30	1.0	0.147397	0.756941	0.109414	Al
Al31	1.0	0.138547	0.762609	0.317648	Al
Al32	1.0	0.775033	0.754565	0.045179	Al
Al33	1.0	0.761861	0.757790	0.263305	Al
Al34	1.0	0.323506	0.250956	0.023721	Al
Al35	1.0	0.273407	0.258909	0.215559	Al
Al36	1.0	0.268238	0.260468	0.431301	Al