ELECTRONIC SUPPLEMENTARY INFORMATION FOR

Acid-Base and Redox Performance of Carbon Nanotubes in the Methanol Conversion

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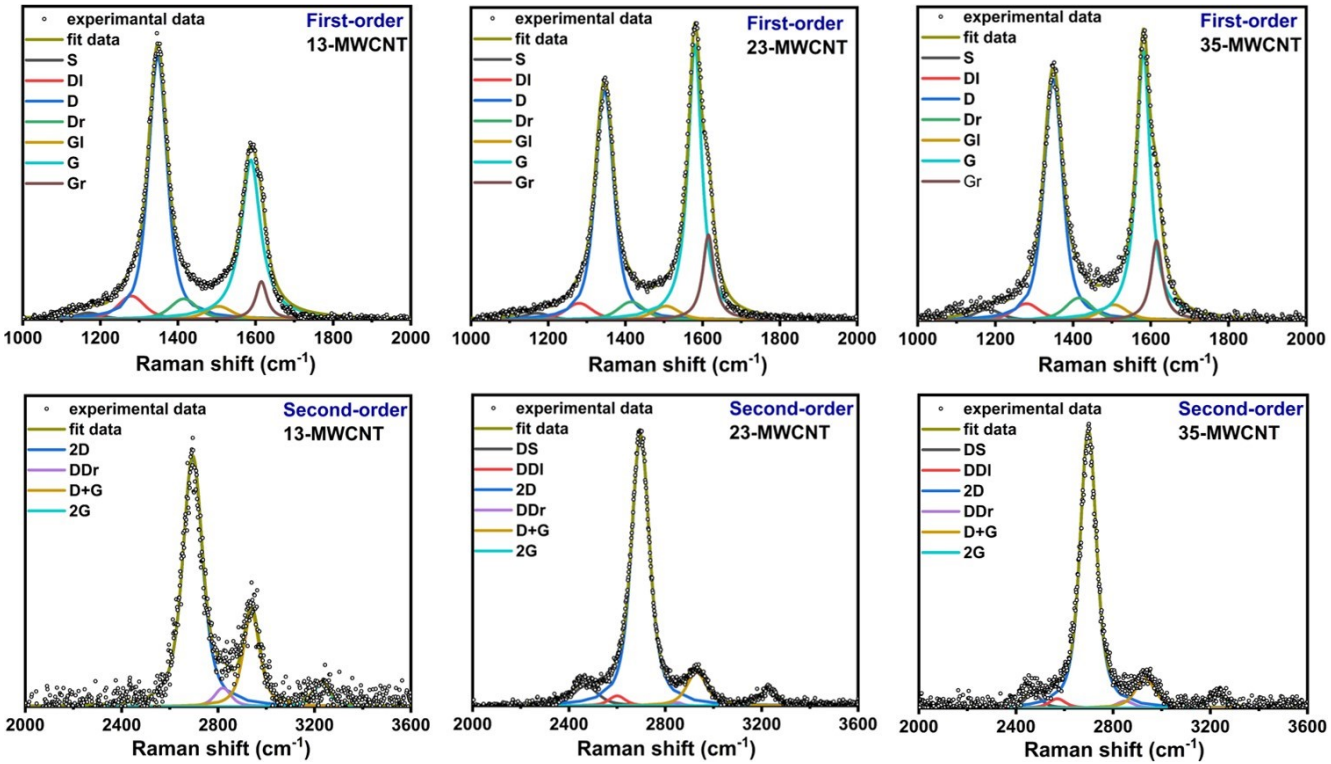

Figure S1. Deconvolution of Raman spectra of MWCNT samples.

Raman spectra of MWCNT samples were analyzed using Gaussians considered the deconvolution of the "D band region", which consists of a central D band and two satellite bands designed Dl (D-left) and Dr (D-right), at ~1250 cm^{-1} and ~1400 cm^{-1}, respectively. In the "G band region" the fitting considered two Lorentzian bands, G and Gr (G right) at ~1580 cm^{-1} and ~1610 cm^{-1}, respectively, and Gl (G left) near 1500 cm^{-1}. Also, the S-band near ~1150 cm^{-1} is presented. Dl, Dr, and Gr bands are assigned to the presence of low size aromatic domains, analogous structures to polycyclic aromatic hydrocarbons, and S and Gl bands refer to polyacetylene-like structures.

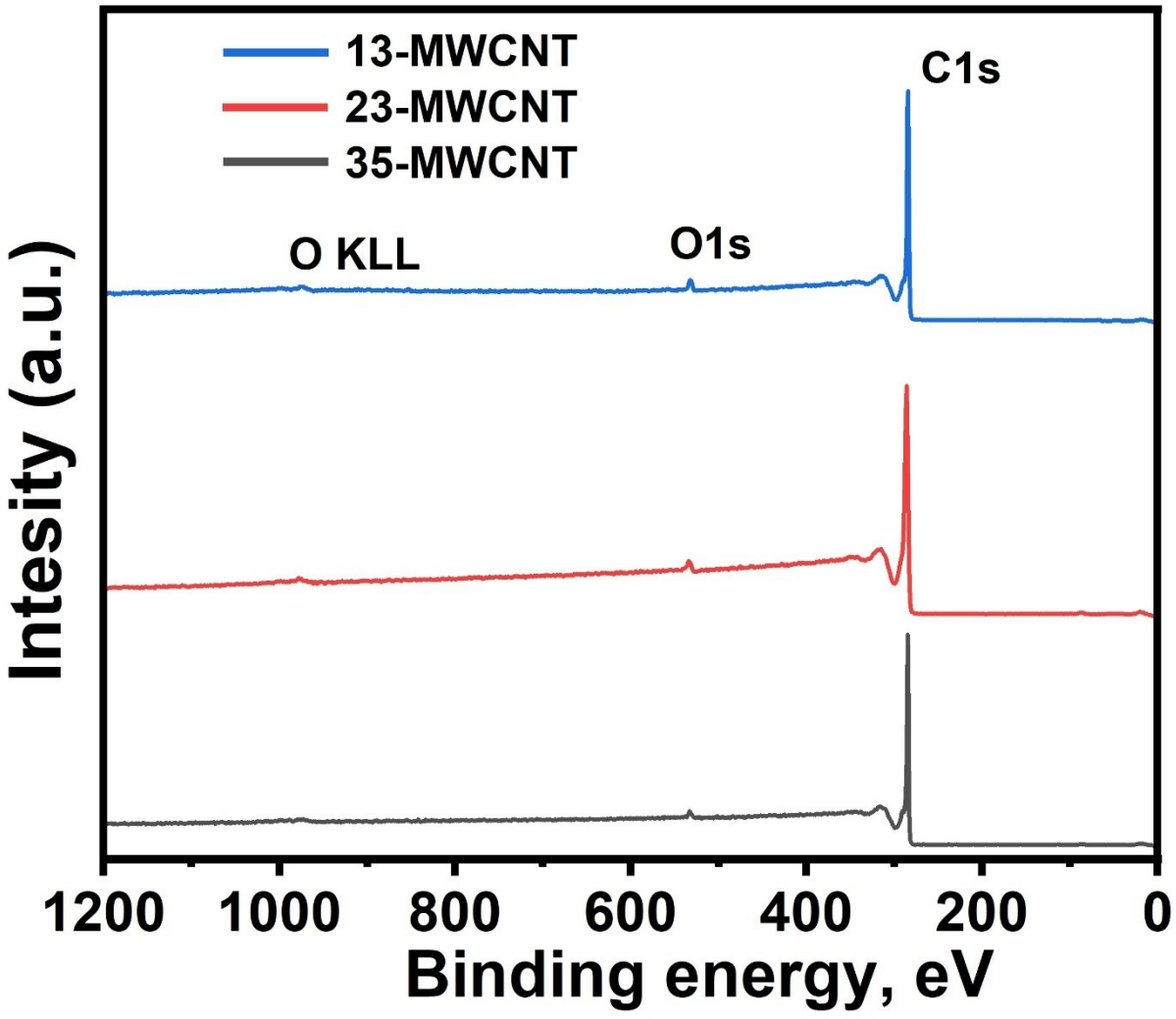

Figure S2. Survey XPS of MWCNT samples.

DFT Calculations were performed using the US GAMESS program with the B3LYP exchange-correlation functional in the 6-31G(d, p) basis set with the Grimme dispersion correction.

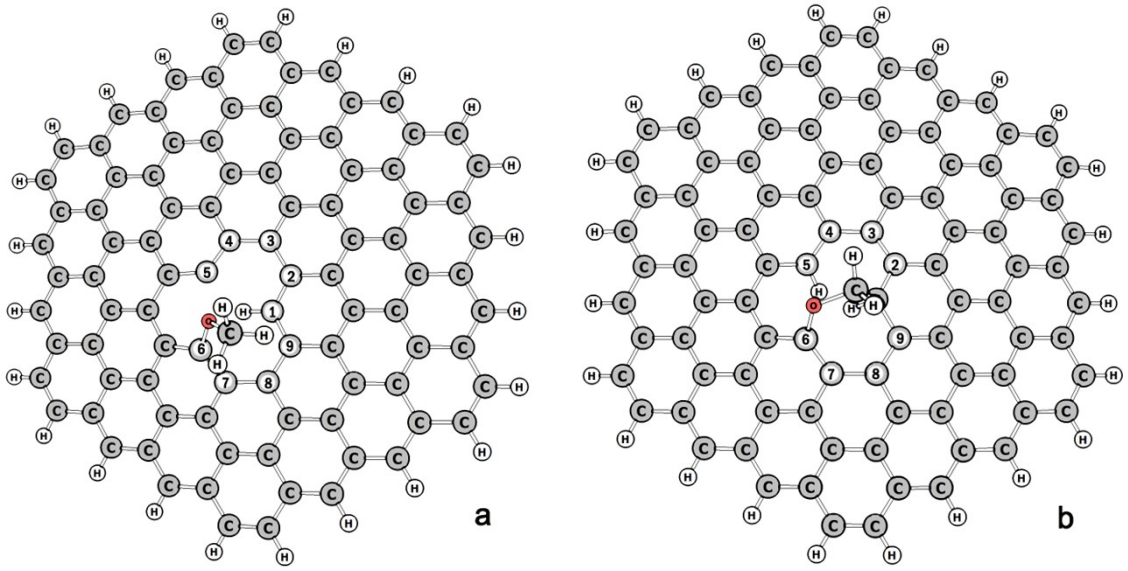

Figure S3. The equilibrium structure of the complex, which is formed at the step B (a) and C (b) of the methanol interaction with SV (PAH $C_{95}H_{24}$).

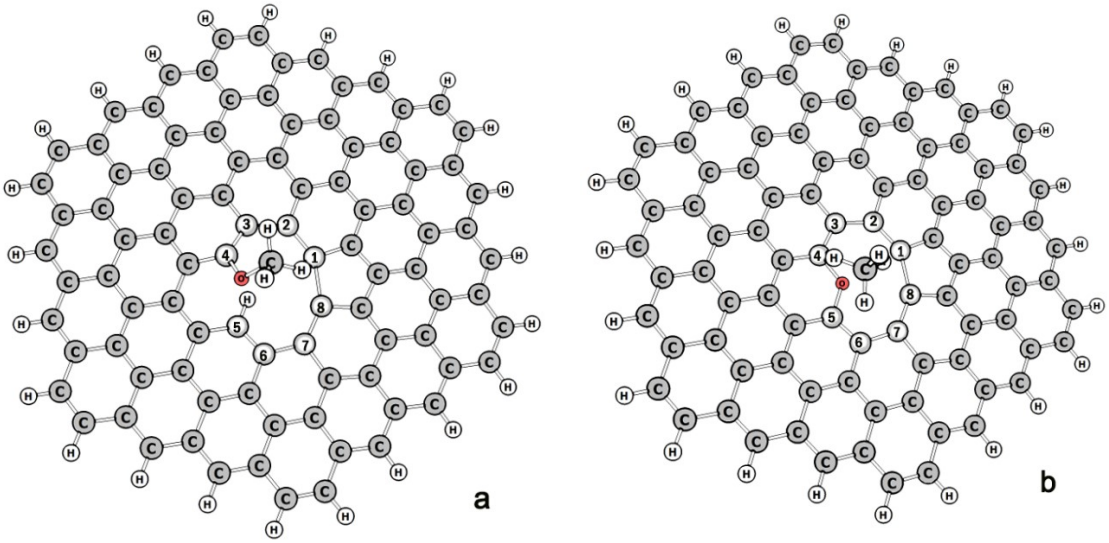

Figure S4. The equilibrium structure of the complex that is formed at steps B (a) and C (b) of the methanol interaction with DV (PAH $C_{94}H_{24}$).

Table S1. Thermochemical values (kJ/mol) for the CH_3OH molecule. E_0 (CH_3OH) = -303836.67, E_{ZPE} (CH_3OH) = 134.89, E_0+E_{ZPE} = (CH_3OH) = -303701.78 kJ/mol.

T, K; (CH_3OH)	Thermodynamic corrections			Electronic energy with thermodynamic corrections		
	E_{tot}	H_{corr}	G_{corr}	E_0+E_{tot}	E_0+H_{corr}	E_0+G_{corr}
273	142.67	144.94	81.14	-303694.00	-303691.73	-303755.53
373	146.51	149.61	57.03	-303690.16	-303687.06	-303779.64
473	151.17	155.10	31.55	-303685.50	-303681.57	-303805.12
573	156.66	161.42	4.82	-303680.01	-303675.25	-303831.85
673	162.90	168.50	-23.08	-303673.77	-303668.17	-303859.75
773	169.81	176.24	-52.09	-303666.86	-303660.43	-303888.76
873	177.30	184.56	-82.14	-303659.37	-303652.11	-303918.81
973	185.31	193.40	-113.17	-303651.36	-303643.27	-303949.84
1073	193.77	202.69	-145.14	-303642.90	-303633.98	-303981.81
1173	202.63	212.38	-177.99	-303634.04	-303624.29	-304014.66

Table S2. Thermochemical values (kJ/mol) for the CH_2O molecule. E_0 (CH_2O) = -300629.67, E_{ZPE} (CH_2O) = 70.22, E_0+E_{ZPE} = (CH_2O) = -300699.89 kJ/mol.

T, K; (CH_2O)	Thermodynamic corrections			Electronic energy with thermodynamic corrections		
	E_{tot}	H_{corr}	G_{corr}	E_0+E_{tot}	E_0+H_{corr}	E_0+G_{corr}
273	77.08	79.35	18.94	-300552.60	-300550.33	-300610.73
373	79.84	82.94	-3.77	-300549.83	-300546.73	-300633.44
473	82.98	86.91	-27.49	-300546.70	-300542.76	-300657.17
573	86.55	91.31	-52.11	-300543.13	-300538.36	-300681.78
673	90.54	96.13	-77.53	-300539.14	-300533.54	-300707.20
773	94.92	101.35	-103.70	-300534.76	-300528.32	-300733.37
873	99.65	106.91	-130.56	-300530.02	-300522.76	-300760.24
973	104.70	112.79	-158.09	-300524.97	-300516.88	-300787.76
1073	110.02	118.94	-186.23	-300519.65	-300510.73	-300815.90
1173	115.58	125.33	-214.96	-300514.10	-300504.34	-300844.63

Table S3. Thermochemical values (kJ/mol) for the H_2 molecule. E_0 (H_2) = -3094.26, E_{ZPE} (H_2) = 26.72, E_0+E_{ZPE} = (H_2) = -3067.54 kJ/mol.

T, K; (H_2)	Thermodynamic corrections			Electronic energy with thermodynamic corrections		
	E_{tot}	H_{corr}	G_{corr}	$E_0+ E_{tot}$	$E_0+ H_{corr}$	E_0+G_{corr}
273	32.39	34.66	-0.20	-3061.87	-3059.560	-3094.46
373	34.47	37.57	-13.45	-3059.79	-3056.69	-3107.71
473	36.55	40.48	-27.48	-3057.71	-3053.78	-3121.74
573	38.63	43.39	-42.14	-3055.63	-3050.87	-3136.40
673	40.71	46.30	-57.31	-3053.55	-3047.95	-3151.57
773	42.80	49.22	-72.91	-3051.46	-3045.04	-3167.17
873	44.90	52.15	-88.89	-3049.36	-3042.10	-3183.15
973	47.01	55.10	-105.21	-3047.25	-3039.16	-3199.47
1073	49.15	58.08	-121.83	-3045.11	-3036.18	-3216.09
1173	51.32	61.07	-138.74	-3042.94	-3033.18	-3233.00

General remarks

E_0 – the total electronic energy.

E_{ZPE} – zero-point energy of the molecule.

E_{tot} – total internal energy ($E_t + E_r + E_v + E_e$).

E_t – internal energy due to translation.

E_r – internal energy due to rotational motion.

E_v – internal energy due to vibrational motion.

E_e – internal energy due to electronic motion.

H_{corr} – correction to the enthalpy due to internal energy.

G_{corr} – correction to the Gibbs free energy due to internal energy.

PAH – polycyclic aromatic hydrocarbon.

SV – single vacancy.

DV – double vacancy.

Table S4. The thermochemical Gibbs energy values (kJ/mol) for CH_3OH, CH_2O, and H_2 molecules depend on the temperature and the Gibbs energy values of the reaction $CH_3OH \rightarrow CH_2O + H_2$. $\Delta G_{reac} = (G(CH_2O) + G(H_2)) - G(CH_3OH)$. $G(CH_2O) = E_0(CH_2O) + G_{corr}(CH_2O)$. $G(H_2) = E_0(H_2) + G_{corr}(H_2)$. $G(CH_3OH) = E_0(CH_3OH) + G_{corr}(CH_3OH)$.

Temperature (K)	$E_0 + G_{corr}$ (CH_3OH)	$E_0 + G_{corr}$ (CH_2O)	$E_0 + G_{corr}$ (H_2)	ΔG_{reac}	ΔG_{reac}*
273	-303755.53	-300610.73	-3094.46	50.34	62,38
373	-303779.64	-300633.44	-3107.71	38.49	51,25
473	-303805.12	-300657.17	-3121.74	26.21	39,65
573	-303831.85	-300681.78	-3136.40	13.67	27,76
673	-303859.75	-300707.20	-3151.57	0.98	15,67
773	-303888.76	-300733.37	-3167.17	-11.78	3,46
873	-303918.81	-300760.24	-3183.15	-24.58	-8,84
973	-303949.84	-300787.76	-3199.47	-37.39	-21,19
1073	-303981.81	-300815.90	-3216.09	-50.19	-33,57
1173	-304014.66	-300844.63	-3233.00	-62.97	-45,97
*ΔG_{reac} after the fitting. The Least square method was used to fit calculated data to experimental data.					

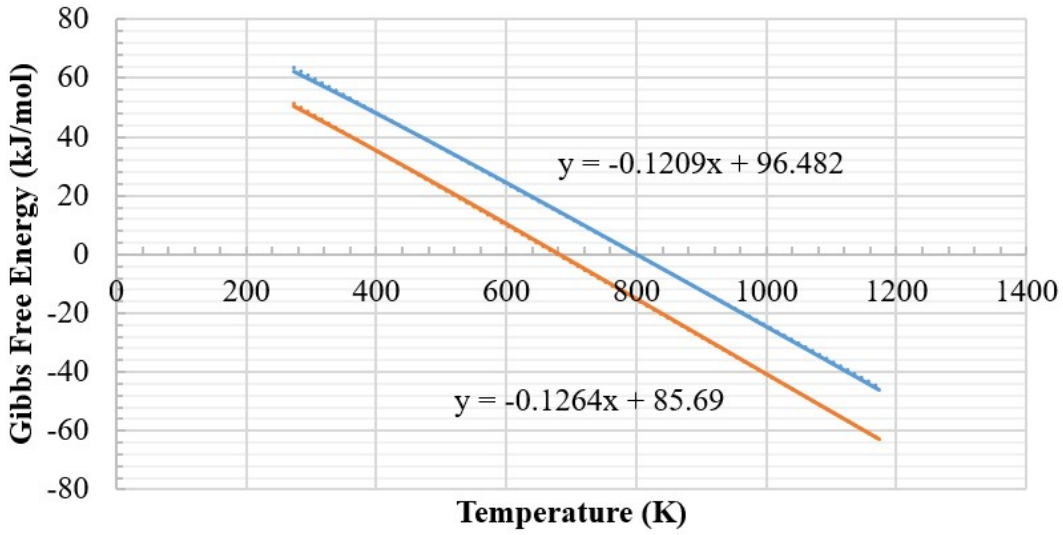

Figure S5. The equations of straight lines approximate calculated and experimental data of Gibbs energy values dependent on temperature for the reaction $CH_3OH \rightarrow CH_2O + H_2$. For experimental data: $\Delta G_{exp} = -0.1209T + 96.482$; for calculated data: $\Delta G_{calc} = -0.1264T + 85.69$.

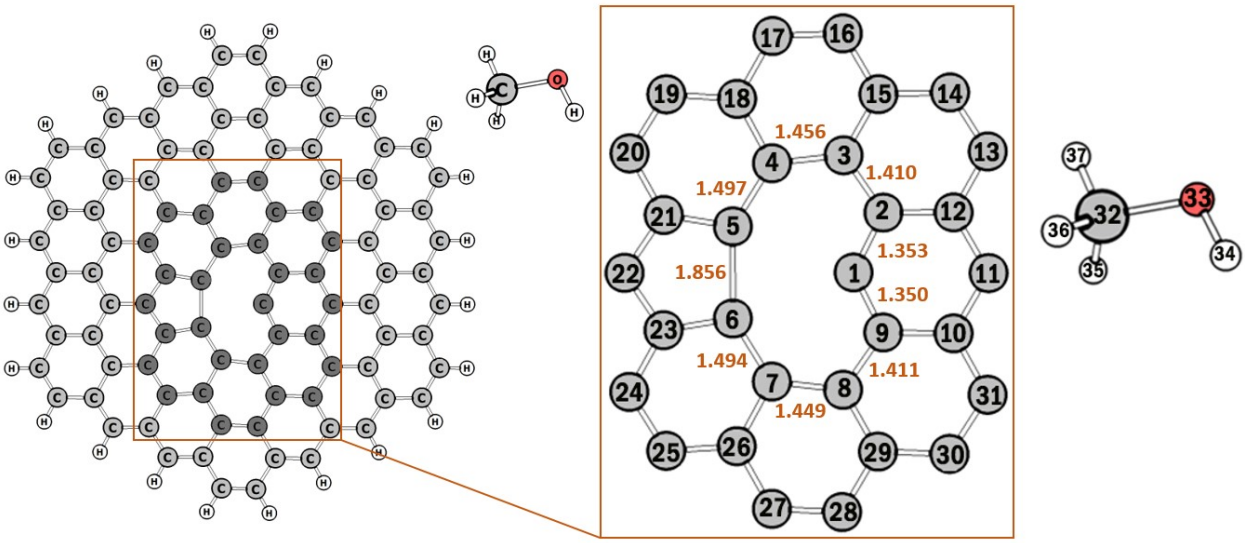

Figure S6. Structures of PAH with SV and methanol molecule, designation of atoms, and distance (Å) between C atoms of the catalyst reaction center.

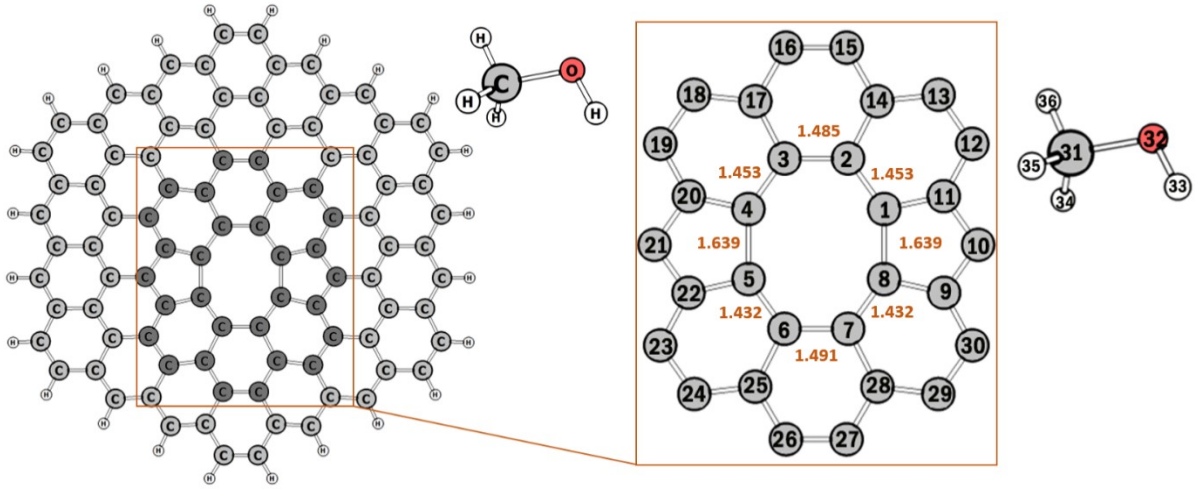

Figure S7. Structures of PAH with DV, methanol molecule, designation of atoms, and distance (Å) between C atoms of the catalyst reaction center.

Table S5. Atomic charge (a.u.) obtained by Mulliken analysis for calculated energy profile for CH_3OH dehydrogenation on PAH with SV. Designation of atoms according to Figure S6. **A** (starting point) – $C_{95}H_{24}$ + CH_3OH; **B** – first step (H(5)–$C_{95}H_{24}$–O(6)–CH_3); **C** – second step (H(5)–$C_{95}H_{24}$–O(6)–C(1)H_2–H(1)), bridge-structure formation; **D** – third step (H(5)–$C_{95}H_{24}$–H(1)•••CH_2O), physical adsorption of FA; **E** – fourth step (H(5)–$C_{95}H_{24}$–H(1) + CH_2O), FA desorption; **F** – fifth step ($C_{95}H_{24}$•••H_2), physical adsorption of H_2; **G** – final step, H_2 desorption. TS – transition state.

Atoms designation		Steps of methanol transformation on PAH with SV							
		A	**B**	**C**	**TS**	**D**	**E**	**F**	**G**
Atoms of the catalyst reaction center	C1	-0.187	-0.215	-0.320	-0.338	-0.297	-0.290	-0.193	-0.187
	C2	-0.041	0.056	-0.032	0.068	0.059	0.065	-0.39	-0.041
	C3	0.002	-0.008	0.024	-0.039	0.000	0.003	0.032	0.002
	C4	0.016	0.066	0.048	0.080	0.070	0.064	0.010	0.016
	C5	0.047	-0.199	0.303	-0.319	-0.294	-0.293	0.057	0.047
	C6	0.059	0.104	0.093	-0.135	-0.280	-0.298	0.044	0.059
	C7	0.011	0.046	0.078	0.088	0.073	0.080	0.015	0.011
	C8	0.030	0.003	0.064	0.014	0.016	0.022	0.005	0.030
	C9	-0.041	0.008	-0.042	0.062	0.064	0.075	-0.038	-0.041
	C10	0.060	0.029	0.080	0.035	0.010	0.015	0.040	0.060
	C11	0.035	0.006	-0.019	0.012	0.027	0.029	0.035	0.035
	C12	0.038	0.002	0.072	-0.007	-0.010	-0.008	0.062	0.038
	C13	-0.043	0.032	0.002	0.018	0.013	0.016	-0.025	-0.043
	C14	0.076	-0.005	0.013	0.013	0.017	0.018	0.002	0.076
	C15	0.045	0.054	0.024	0.058	0.046	0.045	0.062	0.045
	C16	-0.088	0.015	0.015	-0.004	-0.003	0.001	-0.108	-0.088
	C17	0.051	0.019	0.007	0.023	0.031	0.029	-0.002	0.051
	C18	0.063	-0.012	-0.001	-0.003	0.003	0.003	0.076	0.063
	C19	-0.070	0.034	0.023	0.006	0.000	0.002	-0.111	-0.070
	C20	0.027	0.018	-0.006	0.007	0.020	0.019	0.039	0.027
	C21	-0.052	0.027	0.079	0.092	0.071	0.062	-0.032	-0.052
	C22	-0.066	0.060	0.023	0.026	-0.010	-0.014	-0.064	-0.066
	C23	-0.034	0.040	0.017	0.029	0.068	0.076	-0.050	-0.034
	C24	0.038	0.026	0.016	0.026	0.030	0.028	0.029	0.038
	C25	-0.110	-0.039	-0.035	-0.034	-0.050	-0.051	-0.071	-0.110
	C26	0.075	0.021	0.029	0.045	0.039	0.035	0.063	0.075
	C27	-0.003	-0.016	-0.021	-0.036	-0.017	-0.017	0.051	-0.003
	C28	-0.109	-0.044	-0.044	-0.036	-0.044	-0.044	-0.088	-0.109
	C29	0.062	0.065	0.036	0.054	0.058	0.058	0.045	0.062
	C30	0.002	-0.038	-0.024	-0.046	-0.035	-0.035	0.077	0.002
	C31	-0.025	0.014	0.008	0.010	0.013	0.014	-0.043	-0.025
Atoms of the methanol molecule	C32	-0.074	-0.083	0.084	0.075	0.176	0.176	0.176	0.176*
	O33	-0.532	-0.497	-0.492	-0.382	-0.346	-0.340*	-0.340*	-0.340*
	H34	0.306	0.122	0.129	0.197	0.178	0.160	0.008	0.000**
	H35	0.089	0.018	0.125	0.151	0.158	0.158	-0.019	0.000**
	H36	0.090	0.028	0.131	0.103	0.085	0.082*	0.082*	0.082*

	H37	0.121	0.130	0.139	0.106	0.090	0.082*	0.082*	0.082*
* – charge on the atoms in the isolated CH_2O molecule. ** – charge on the atoms in the isolated H_2 molecule.									

The charge of the O(33) atom in the transition state is -0.382 a.u. and decreases in absolute value along the reaction coordinate (is -0.346 for adsorbed CH_2O molecule and -0.340 a.u. for isolated CH_2O molecule).

Table S6. Atomic charge (a.u.) obtained by Mulliken analysis for calculated energy profile of methanol transformation on PAH with DV. Designation of atoms according to Figure S7. **A** starting point – $C_{94}H_{24}$ + CH_3OH; **B** – first step (H(5)–$C_{94}H_{24}$–O(4)–CH_3); **C** – second step ($C_{94}H_{24}$–O(4–5)•••CH_4), physical adsorption of methane and the oxygen atom is implemented in the PAH plane; **D** – final step, methane desorption.

Atoms designation		**Steps of methanol transformation on PAH with DV**			
		A	**B**	**C**	**D**
Atoms of the catalyst reaction center	C1	0.041	-0.009	0.065	0.067
	C2	-0.012	-0.001	0.035	0.035
	C3	-0.012	0.019	0.022	0.017
	C4	0.041	0.098	0.108	0.097
	C5	0.041	-0.234	0.130	0.110
	C6	-0.009	0.083	0.029	0.029
	C7	-0.009	-0.014	0.037	0.034
	C8	0.041	-0.004	0.070	0.070
	C9	-0.045	-0.004	-0.043	-0.043
	C10	-0.164	-0.116	-0.116	-0.116
	C11	-0.079	-0.032	-0.069	-0.068
	C12	0.002	0.016	0.022	0.023
	C13	-0.047	-0.048	-0.068	-0.068
	C14	0.132	0.084	0.073	0.072
	C15	-0.054	0.002	0.035	0.035
	C16	-0.054	-0.037	-0.094	-0.094
	C17	0.132	0.025	0.053	0.054
	C18	-0.147	0.008	0.044	0.042
	C19	0.002	-0.010	-0.036	-0.034
	C20	-0.079	0.010	0.037	0.038
	C21	-0.164	0.013	0.073	0.073
	C22	-0.045	0.061	0.057	0.054
	C23	0.008	0.007	-0.012	-0.011
	C24	-0.098	-0.050	-0.030	-0.031
	C25	0.141	0.064	0.074	0.075
	C26	-0.082	-0.074	-0.119	-0.120
	C27	-0.082	-0.033	-0.011	-0.011
	C28	0.141	0.096	0.082	0.082
	C29	-0.098	-0.097	-0.106	-0.106
	C30	0.008	0.027	0.027	0.027
Atoms of the methanol molecule	C31	-0.074	-0.087	-0.484	-0.472*
	O32	-0.532	-0.495	-0.562	-0.541
	H33	0.306	0.129	0.107	0.118*
	H34	0.089	0.129	0.117	0.118*
	H35	0.090	0.140	0.133	0.118*
	H36	0.121	0.123	0.111	0.118*
* – charge on the atoms in the isolated CH_4 molecule.					

XYZ coordinates of equilibrium structure of the $C_{96}H_{28}O$ complex, which is formed at the step B (a) of the methanol interaction with SV (PAH $C_{95}H_{24}$).

$C_{96}H_{28}O$

125

C	2.163814293	0.253384992	-3.134877195
H	3.144950212	0.565030798	-3.508295413
H	2.209218981	-0.786513486	-2.802080641
H	1.415623731	0.351176420	-3.922292883
O	1.727119936	1.127848012	-2.087633944
H	1.256035977	0.307329356	0.092069501
C	1.253588521	-0.750781670	-0.130676292
C	-1.225269547	-0.669060717	-0.179906915
C	-1.248857346	0.767531142	-0.268786075
C	-2.448013646	-1.371675487	-0.168934181
C	-2.485854371	1.478291508	-0.268982338
C	-3.692196158	-0.660476300	-0.173263954
C	3.699450888	-0.650987580	-0.540920890
C	-3.707953395	0.756298647	-0.208961679
C	3.734915638	0.777039592	-0.727090139
C	-4.923873721	-1.377176220	-0.134742128
C	4.924779139	-1.365846808	-0.417101823
C	-4.941684819	1.471392785	-0.186132350
C	4.945837898	1.484848129	-0.424906502
C	-6.155066536	-0.665929886	-0.114725433
C	6.158433160	-0.656371996	-0.325736582
C	-6.163892152	0.754976653	-0.133255251
C	6.159453414	0.762598669	-0.273415675
C	-7.393924380	-1.395681439	-0.072903304
C	7.393086736	-1.385234663	-0.222711758
C	-7.406194250	1.480545645	-0.099293539
C	7.391349478	1.485343093	-0.097190739
C	-8.624368464	-0.641042619	-0.051565784
C	8.615123558	-0.632929319	-0.081013865
C	-8.631181494	0.717891479	-0.060794473
C	8.613055220	0.724612171	-0.010787896
H	-9.560372078	-1.192546402	-0.021382041
H	9.548185829	-1.185083252	-0.010317943
H	-9.572198353	1.259522880	-0.041851058
H	9.547255968	1.266357015	0.112863611
C	-2.452538730	-2.804683976	-0.158359350
C	2.466860336	-2.819327754	-0.365103979
C	-2.474730492	2.901326677	-0.331023382
C	2.501302066	2.927201316	-0.751152269

C	-4.920677085	-2.801693356	-0.108076460
C	4.925351359	-2.797818800	-0.353975619
C	-4.939615308	2.895740102	-0.205991879
C	4.941052209	2.904655200	-0.340447100
C	-7.371294979	-2.783818145	-0.051745214
C	7.374932977	-2.775267968	-0.227508925
C	-7.389417911	2.869618609	-0.105110424
C	7.370430005	2.874226921	-0.024426431
C	-1.231156659	-3.522359610	-0.194542704
C	1.238585694	-3.522960766	-0.281331802
C	-1.254529334	3.623597653	-0.427322236
C	1.246998599	3.615885379	-0.637127648
C	-3.688352926	-3.515687887	-0.121002379
C	3.702330373	-3.525913367	-0.357029103
C	-3.712835545	3.613108012	-0.271617238
C	3.710739338	3.617476497	-0.424169317
C	-6.158463468	-3.516864411	-0.063775540
C	6.164181251	-3.511463526	-0.276610904
C	-6.180895036	3.610262232	-0.151094790
C	6.166093163	3.612679506	-0.118758267
H	-8.310075054	-3.331202064	-0.024372163
H	8.312578690	-3.319624004	-0.150958631
H	-8.332456423	3.409603358	-0.076049256
H	8.304719894	3.412860129	0.117156446
C	-1.229044184	-4.948788589	-0.164971666
C	1.237783698	-4.952092251	-0.232391414
C	-1.249433130	5.045511239	-0.390873537
C	1.233073337	5.028217778	-0.453211275
C	-3.686133349	-4.936515512	-0.088231412
C	3.700391146	-4.943667607	-0.271731106
C	-3.711021871	5.031505798	-0.263989602
C	3.689919376	5.028238823	-0.251847990
C	-6.128176098	-4.933263957	-0.025626946
C	6.138041628	-4.926037837	-0.218400037
C	-6.151494132	5.025432183	-0.134645896
C	6.124716026	5.022745031	0.000581001
C	-2.459193038	-5.651688939	-0.101513547
C	2.468785958	-5.656369193	-0.219138399
C	-2.480363442	5.747397466	-0.300254651
C	2.461245160	5.738309289	-0.306416919
C	-4.936188381	-5.645496982	-0.031557527
C	4.948689137	-5.647756768	-0.205057696
C	-4.958241864	5.738980968	-0.177085047
C	4.929815570	5.731997058	-0.051624540

H	-7.071133660	-5.474113583	0.012787560
H	7.082186284	-5.461780856	-0.162215800
H	-7.092934679	5.565271155	-0.074058062
H	7.057185726	5.564578542	0.141134488
C	-2.450296481	-7.089637794	-0.042367822
C	2.460945561	-7.091041451	-0.120871976
C	-2.468714882	7.179990174	-0.215172176
C	2.443681720	7.167504356	-0.150732580
C	-4.896032008	-7.087121728	0.027280940
C	4.909194090	-7.087186642	-0.097183421
C	-4.914140888	7.179927532	-0.113311071
C	4.879148758	7.167220959	0.080703166
C	-1.238111597	-7.769421858	-0.043839904
C	1.246163916	-7.769594478	-0.072395648
C	-1.249172520	7.849728054	-0.191125063
C	1.231093752	7.846427858	-0.154931228
C	-3.721219374	-7.770048763	0.025344319
C	3.733212572	-7.768406338	-0.058209172
C	-3.737380852	7.861408219	-0.125907654
C	3.702945208	7.846283687	0.032466670
H	-5.839444739	-7.623438785	0.083764918
H	5.852785381	-7.623407597	-0.036212029
H	-5.855746242	7.715841545	-0.034846469
H	5.813985831	7.700789199	0.224588954
H	-1.240302965	-8.855095463	0.007440245
H	1.246352308	-8.853886574	0.004344844
H	-1.242563174	8.933690081	-0.103174731
H	1.227168745	8.927986140	-0.042762646
H	-3.718562073	-8.855543328	0.077520993
H	3.731179974	-8.850642774	0.035819698
H	-3.734440172	8.946137039	-0.055410594
H	3.687290345	8.927011863	0.144836531
C	0.004061451	-2.818840363	-0.234390448
C	-0.013358610	2.916453844	-0.522557404
C	0.005187176	-5.659297591	-0.170946676
C	-0.007810450	5.741046301	-0.376548084
C	0.005027192	-7.090871375	-0.101355302
C	-0.009968573	7.166808128	-0.250839087
C	2.466028834	-1.390515085	-0.365786706
C	2.647357348	1.576242762	-1.190969157
C	0.015719064	-1.399871948	-0.171055362
C	-0.123165310	1.556317475	-0.383829551

XYZ coordinates of equilibrium structure of the $C_{96}H_{28}O$ complex, which is formed at the step C (b) of the methanol interaction with SV (PAH $C_{95}H_{24}$).

$C_{96}H_{28}O$

125

C	1.177018632	0.025654580	-2.292999821
H	1.780119128	-0.472665536	-3.059309243
H	1.491921681	0.057646436	-0.222921794
H	0.147930652	0.115611414	-2.644011027
O	1.643130691	1.355670737	-2.096291784
H	0.811568154	1.166864374	0.382496944
C	1.285817968	-0.721469054	-0.938297043
C	-1.174571675	-0.667643829	-0.317877078
C	-1.215041941	0.792972280	-0.218348681
C	-2.416560638	-1.370352797	-0.270842185
C	-2.455567108	1.487695115	-0.342017589
C	-3.658453558	-0.656183508	-0.251872942
C	3.736363976	-0.697068896	-0.890149428
C	-3.677920233	0.764087884	-0.319713204
C	3.729229110	0.774043702	-0.900949176
C	-4.891376959	-1.371005745	-0.183540432
C	4.975161913	-1.397275199	-0.677370278
C	-4.914738077	1.475118725	-0.309755126
C	4.938286555	1.471234133	-0.523406539
C	-6.124736818	-0.660690641	-0.164648320
C	6.182109293	-0.675634469	-0.480960875
C	-6.137134491	0.758069892	-0.231363052
C	6.160507061	0.752267230	-0.392940341
C	-7.363160444	-1.389397285	-0.069789481
C	7.411103527	-1.392080131	-0.294629159
C	-7.381710712	1.482815950	-0.205631870
C	7.381639481	1.469596454	-0.151614930
C	-8.594425505	-0.636354845	-0.047461598
C	8.618875109	-0.636932144	-0.081852617
C	-8.604023668	0.720540763	-0.112000700
C	8.604630267	0.720280184	-0.014881178
H	-9.528402605	-1.186376409	0.028182128
H	9.549361022	-1.183294788	0.048534841
H	-9.545750982	1.261882162	-0.085406531
H	9.524635290	1.271899561	0.162441915
C	-2.421291125	-2.796324343	-0.266016551
C	2.526760788	-2.855474884	-0.707879707
C	-2.463350483	2.913274465	-0.362828105

C	2.496496889	2.936584442	-0.637311824
C	-4.888097740	-2.794921108	-0.121391222
C	4.977220734	-2.821601706	-0.580053832
C	-4.924125447	2.902423783	-0.344556311
C	4.938162025	2.889738194	-0.355165520
C	-7.339737418	-2.775748673	0.003351833
C	7.406440130	-2.788511160	-0.277810435
C	-7.373115589	2.871398155	-0.262735394
C	7.362566970	2.859114892	-0.036678088
C	-1.200648392	-3.516570609	-0.333784799
C	1.275020441	-3.536884032	-0.576474528
C	-1.248774022	3.643782938	-0.378665402
C	1.248101013	3.617403232	-0.426031997
C	-3.659835206	-3.508134266	-0.161145356
C	3.759241593	-3.556663949	-0.593144223
C	-3.701793709	3.622892888	-0.372475285
C	3.714881413	3.619354804	-0.364503665
C	-6.127384843	-3.509050836	-0.018300582
C	6.214128600	-3.529503389	-0.385421194
C	-6.167518574	3.615157131	-0.327362382
C	6.165073591	3.593133068	-0.114781004
H	-8.278328294	-3.320324036	0.077989065
H	8.344506811	-3.318323759	-0.126655188
H	-8.316776168	3.409999031	-0.243939792
H	8.293109234	3.390148353	0.148885173
C	-1.195567957	-4.941796914	-0.244700357
C	1.274510576	-4.945282342	-0.409493739
C	-1.239722080	5.063971104	-0.356095962
C	1.242845161	5.031678164	-0.279938962
C	-3.654434898	-4.925573394	-0.078638458
C	3.746541507	-4.964618323	-0.415647909
C	-3.699613285	5.043802447	-0.374586373
C	3.698659451	5.025931718	-0.141772612
C	-6.094399896	-4.920471386	0.067785151
C	6.182334188	-4.944741441	-0.259382847
C	-6.141984946	5.031285599	-0.351856288
C	6.129670459	5.003917153	0.059562542
C	-2.423932491	-5.640665345	-0.104057202
C	2.512057546	-5.657505336	-0.344778576
C	-2.470716965	5.764798630	-0.350584418
C	2.473441215	5.736454022	-0.154044721
C	-4.900064453	-5.632459739	0.051427281
C	4.996259923	-5.664774997	-0.265029794
C	-4.948863324	5.750425659	-0.366357717

C	4.944501477	5.721712229	0.049792142
H	-7.034493131	-5.460045765	0.157954843
H	7.122959876	-5.472849497	-0.121178839
H	-7.084675237	5.572796641	-0.339315063
H	7.068324614	5.531041813	0.212770894
C	-2.412351031	-7.071573677	0.019577007
C	2.498311658	-7.084824354	-0.155537571
C	-2.458299805	7.197327470	-0.279239545
C	2.455935163	7.167379000	0.011192933
C	-4.855170430	-7.069677904	0.169694192
C	4.947327695	-7.096454176	-0.087330195
C	-4.905416234	7.193975132	-0.348060583
C	4.896152736	7.155026544	0.221137942
C	-1.196541535	-7.748354258	0.017810567
C	1.285988974	-7.753987740	-0.065071364
C	-1.238083616	7.862942093	-0.173260275
C	1.246413416	7.847700136	-0.000738428
C	-3.678614099	-7.749861023	0.157510955
C	3.766950257	-7.767477108	-0.041557211
C	-3.730635242	7.878842364	-0.299986191
C	3.721444422	7.838065987	0.197933989
H	-5.795047526	-7.604671750	0.277012953
H	5.886698125	-7.632221352	0.023894559
H	-5.848762202	7.732852095	-0.357572487
H	5.833447160	7.685363002	0.368919744
H	-1.191854510	-8.829704802	0.126821998
H	1.285104113	-8.832405607	0.073066955
H	-1.233246345	8.948177176	-0.103239632
H	1.243442527	8.929089555	0.115556553
H	-3.672488793	-8.832063852	0.257823261
H	3.754792888	-8.844369421	0.103306494
H	-3.732681846	8.965248521	-0.267999665
H	3.711401684	8.916920409	0.329412403
C	0.025917151	-2.813041454	-0.509683831
C	-0.023064394	2.942427870	-0.290193896
C	0.038024421	-5.649792958	-0.264724503
C	0.001586971	5.750810980	-0.256076753
C	0.040295781	-7.072599606	-0.110877138
C	0.001304015	7.175977774	-0.143934038
C	2.558384337	-1.464365627	-0.876884072
C	2.618136935	1.611426777	-1.196738800
C	0.012856432	-1.409351046	-0.554153452
C	-0.088070856	1.584633407	-0.014679147

XYZ coordinates of equilibrium structure of the $C_{95}H_{28}O$ complex that is formed at steps B (a) of the methanol interaction with DV (PAH $C_{94}H_{24}$).

$C_{95}H_{28}O$

124

O	1.004170242	-1.113179222	1.628175164
H	1.433817063	-1.040792937	-0.740071148
C	-1.049836628	-0.707806939	0.377237836
C	-0.898769148	0.740286804	0.139108215
C	-2.306785655	-1.410042686	0.174968531
C	-2.213917624	1.435653687	0.029658003
C	-3.523480209	-0.691112737	0.039589367
C	3.487970185	-0.712396352	-0.369872238
C	-3.479436525	0.726026432	0.005748859
C	3.345224172	0.747205332	-0.266039900
C	-4.776050874	-1.397927900	-0.030549902
C	4.767190211	-1.404513221	-0.307209029
C	-4.737953931	1.429055369	-0.088969140
C	4.667487238	1.443467606	-0.267871721
C	-5.998708681	-0.687441144	-0.111997318
C	5.976950717	-0.686613179	-0.298656145
C	-5.978121022	0.723915128	-0.136235138
C	5.920235041	0.731654593	-0.296900747
C	-7.252063112	-1.400326086	-0.172896402
C	7.235796112	-1.385997504	-0.314687274
C	-7.228637685	1.439347248	-0.211622358
C	7.178273212	1.437479568	-0.311708325
C	-8.478801349	-0.651005294	-0.234932586
C	8.455916397	-0.635099248	-0.336846459
C	-8.465247987	0.701982806	-0.251377509
C	8.421738663	0.716568730	-0.337816565
H	-9.415787876	-1.199962169	-0.269804909
H	9.398655714	-1.173085908	-0.359525845
H	-9.392140189	1.266355282	-0.294717525
H	9.340141464	1.296790105	-0.358648325
C	-2.372545772	-2.839054636	0.184823647
C	2.413615795	-2.894977883	-0.241288313
C	-2.322224284	2.860678993	-0.056253473
C	2.376822667	2.937423396	-0.154507444
C	-4.815753238	-2.819450011	-0.022595909
C	4.833509510	-2.829000159	-0.323468604
C	-4.780617805	2.848082110	-0.138154208
C	4.785738705	2.862946170	-0.244428884

C	-7.259158067	-2.782940694	-0.179130581
C	7.269566417	-2.775396909	-0.322545393
C	-7.231358795	2.818803434	-0.242123821
C	7.219712550	2.822126485	-0.298416451
C	-1.178997980	-3.586626086	0.212084263
C	1.241175009	-3.611398265	0.091847677
C	-1.144433553	3.615035514	-0.080549858
C	1.236438979	3.723828785	-0.136541908
C	-3.608730735	-3.545061696	0.057572048
C	3.649724073	-3.588484622	-0.270964254
C	-3.571621218	3.569842390	-0.119099218
C	3.612576668	3.622116664	-0.204182798
C	-6.062697430	-3.524413186	-0.119391929
C	6.089640373	-3.529063305	-0.329426110
C	-6.030998215	3.552212034	-0.214288643
C	6.043303347	3.565466651	-0.267442248
H	-8.206924253	-3.312728779	-0.233962687
H	8.230137035	-3.284306487	-0.319330776
H	-8.175771304	3.353626283	-0.291914610
H	8.179069547	3.332185693	-0.305663880
C	-1.191963458	-5.011476443	0.067492789
C	1.247053546	-5.027323578	-0.006003849
C	-1.175471264	5.055905350	-0.131076789
C	1.244624464	5.120903013	-0.159819605
C	-3.633473337	-4.967267341	-0.020790739
C	3.681229538	-5.006657072	-0.243083215
C	-3.608406910	4.994307111	-0.172492604
C	3.660699035	5.053137107	-0.209505181
C	-6.063852766	-4.932921888	-0.163935613
C	6.105021322	-4.948620487	-0.339632430
C	-6.038911219	4.957837660	-0.260476274
C	6.078829912	4.981822119	-0.260697125
C	-2.422343453	-5.702334559	-0.025855790
C	2.470722013	-5.727310147	-0.176306787
C	-2.407500456	5.742165694	-0.168435829
C	2.474825697	5.809244935	-0.192002889
C	-4.884174292	-5.662207316	-0.138038956
C	4.938514401	-5.695760625	-0.314329550
C	-4.862706635	5.688273394	-0.239417160
C	4.922623475	5.735791842	-0.238853635
H	-7.014664268	-5.453280289	-0.241602174
H	7.066456585	-5.454578612	-0.368211267
H	-6.992997210	5.475544785	-0.315384434
H	7.048808576	5.473526853	-0.277627293

C	-2.429764078	-7.135050085	-0.149676879
C	2.468882077	-7.163506713	-0.252836210
C	-2.427568395	7.181808080	-0.217654035
C	2.478763664	7.246629397	-0.213404274
C	-4.868011653	-7.099260556	-0.245739108
C	4.914635178	-7.137679901	-0.367585336
C	-4.862642353	7.127921806	-0.286141574
C	4.920966249	7.180339018	-0.244932598
C	-1.224874846	-7.830388892	-0.187948408
C	1.259026379	-7.843995567	-0.227584732
C	-1.232621040	7.897139492	-0.222992733
C	1.265381684	7.924953681	-0.217105734
C	-3.703768016	-7.799528601	-0.253272438
C	3.745095622	-7.831747908	-0.355254520
C	-3.707675616	7.839455994	-0.271326913
C	3.766536213	7.898860692	-0.234795411
H	-5.820053553	-7.615470087	-0.334254201
H	5.860952863	-7.666500235	-0.433570300
H	-5.822314430	7.635580213	-0.335161282
H	5.882365603	7.687396856	-0.260358316
H	-1.237134607	-8.912503685	-0.297253283
H	1.255175508	-8.928473846	-0.309137919
H	-1.263480755	8.983452268	-0.259305812
H	1.264025446	9.012195616	-0.241437419
H	-3.711342902	-8.881758044	-0.349872417
H	3.751934113	-8.917027910	-0.414318714
H	-3.729286109	8.925213728	-0.310152182
H	3.798537611	8.984902438	-0.242170515
C	0.043470900	-2.908670572	0.398530181
C	0.086021446	2.929726996	-0.089270539
C	0.021655287	-5.738216008	0.014270947
C	0.018350717	5.813338479	-0.157327050
C	0.017626129	-7.163523093	-0.123763455
C	0.016065509	7.242170983	-0.196685878
C	2.375909183	-1.511973718	-0.498877174
C	2.112276891	1.528933862	-0.138571166
C	0.008634019	-1.533328710	0.815346178
C	0.347929018	1.528565659	-0.027343004
C	0.771668048	-0.093682437	2.610232084
H	-0.282969558	-0.048193847	2.892793353
H	1.381932190	-0.378006835	3.469068181
H	1.088978532	0.882382869	2.237094228

XYZ coordinates of equilibrium structure of the $C_{95}H_{28}O$ complex that is formed at C (b) of the methanol interaction with DV (PAH $C_{94}H_{24}$).

$C_{95}H_{28}O$

124

O	1.207009243	-0.863347869	-0.310239284
H	2.509920248	-0.973473408	2.711332558
C	-1.080619124	-0.675380245	-0.216435093
C	-0.920252182	0.781856706	-0.212640262
C	-2.340203889	-1.380680960	-0.188752806
C	-2.238313424	1.474213085	-0.194041728
C	-3.559718566	-0.660400854	-0.173130705
C	3.487946317	-0.670857520	-0.246206243
C	-3.505616722	0.758827300	-0.179722441
C	3.316147252	0.784499356	-0.243550981
C	-4.810299491	-1.369140647	-0.155536167
C	4.757314709	-1.375066097	-0.227508817
C	-4.767861939	1.463722058	-0.168926740
C	4.641551884	1.481010295	-0.245849073
C	-6.032952984	-0.656021678	-0.148859653
C	5.963873490	-0.651132757	-0.228267539
C	-6.009073704	0.756858770	-0.156380882
C	5.896887060	0.768259423	-0.242620154
C	-7.287685461	-1.368880086	-0.133939334
C	7.224071460	-1.351412154	-0.217372802
C	-7.260609856	1.474076394	-0.149852848
C	7.154415690	1.478144210	-0.250264155
C	-8.514095814	-0.616269654	-0.128687281
C	8.440515013	-0.593670012	-0.227085467
C	-8.498277683	0.737290417	-0.136679847
C	8.399101433	0.757865422	-0.243848780
H	-9.453099726	-1.162511507	-0.117248801
H	9.386682773	-1.127001766	-0.220737575
H	-9.425969593	1.302828107	-0.131503364
H	9.316257333	1.340085193	-0.250546522
C	-2.399353001	-2.815575756	-0.174082816
C	2.420461542	-2.906286977	-0.231748896
C	-2.350586248	2.901504327	-0.188991296
C	2.349983513	2.985872424	-0.232381397
C	-4.848934182	-2.792786343	-0.144109528
C	4.831357892	-2.805589000	-0.208188312
C	-4.811415303	2.884228782	-0.169391207
C	4.759814937	2.903075727	-0.250062854

C	-7.296635863	-2.752334802	-0.123159641
C	7.264474049	-2.741314755	-0.198190192
C	-7.263933477	2.854777349	-0.154046627
C	7.193687578	2.862180969	-0.261141207
C	-1.219603637	-3.581539634	-0.183922288
C	1.220235323	-3.627089843	-0.218867291
C	-1.171761569	3.657186537	-0.197538326
C	1.211180515	3.774787530	-0.219727210
C	-3.641250895	-3.523116170	-0.150105821
C	3.655985018	-3.580971915	-0.205641271
C	-3.601877577	3.607749234	-0.177118891
C	3.586557979	3.665787394	-0.242727725
C	-6.098786679	-3.496983831	-0.125601445
C	6.087331300	-3.502128436	-0.190808067
C	-6.063322167	3.589022340	-0.161163040
C	6.015694325	3.606374868	-0.258853641
H	-8.246460441	-3.280886719	-0.110699577
H	8.227590868	-3.244530510	-0.188948402
H	-8.209695862	3.390697410	-0.150074710
H	8.153246503	3.372812923	-0.267877019
C	-1.226883396	-5.009173479	-0.156329286
C	1.226356135	-5.036846478	-0.180014091
C	-1.204622675	5.098144362	-0.194390183
C	1.217236835	5.169748072	-0.218273036
C	-3.666424123	-4.948715090	-0.130456717
C	3.676345308	-5.000820781	-0.176231664
C	-3.640306178	5.032953738	-0.174110253
C	3.633583344	5.097758196	-0.242632345
C	-6.100862113	-4.908280178	-0.108270799
C	6.100636272	-4.924764779	-0.167323181
C	-6.073081192	4.996550405	-0.158698494
C	6.051080762	5.023334236	-0.261909420
C	-2.458915651	-5.696025305	-0.130996152
C	2.463705981	-5.728580050	-0.165408930
C	-2.438734713	5.781866688	-0.182259340
C	2.447076948	5.856300662	-0.230839712
C	-4.922021817	-5.642279271	-0.108301822
C	4.937940217	-5.682389475	-0.158451871
C	-4.896458062	5.727475335	-0.163793034
C	4.894935953	5.780370507	-0.253567097
H	-7.055193444	-5.428978297	-0.092987900
H	7.064639545	-5.427548860	-0.154049737
H	-7.028755404	5.514718187	-0.151931614
H	7.021080429	5.514203054	-0.269679242

C	-2.465654206	-7.133395527	-0.105057581
C	2.460468151	-7.165810474	-0.133818589
C	-2.459209929	7.221680233	-0.179811876
C	2.448937719	7.293212419	-0.229929263
C	-4.907822521	-7.084938871	-0.085543433
C	4.913660604	-7.127428048	-0.132558961
C	-4.896554504	7.168584580	-0.159276382
C	4.891256087	7.225837136	-0.254955745
C	-1.257792364	-7.830386135	-0.101622911
C	1.244509641	-7.842408103	-0.116511814
C	-1.265228021	7.939009565	-0.190334532
C	1.234721782	7.971633547	-0.215954240
C	-3.747160305	-7.793163981	-0.082789867
C	3.745839354	-7.827293104	-0.120955050
C	-3.740070891	7.879403426	-0.166920601
C	3.736407966	7.945055338	-0.243907242
H	-5.863181047	-7.602462241	-0.068239201
H	5.863486174	-7.655196988	-0.121950745
H	-5.856101358	7.678201270	-0.149450699
H	5.850956027	7.735775178	-0.265157645
H	-1.274471972	-8.917243445	-0.080380050
H	1.245401972	-8.929654456	-0.093277530
H	-1.298955900	9.025821021	-0.188810254
H	1.231642224	9.058915990	-0.215058198
H	-3.767544286	-8.879415959	-0.063789259
H	3.762986979	-8.913675069	-0.101133552
H	-3.760531243	8.965807205	-0.164265518
H	3.767467028	9.031364871	-0.245392748
C	0.007344835	-2.904121286	-0.218516732
C	0.062093404	2.979561130	-0.210465241
C	-0.007365935	-5.735867705	-0.155772388
C	-0.010998332	5.858019509	-0.205201504
C	-0.008631187	-7.165570264	-0.124544287
C	-0.014183782	7.286709339	-0.203614702
C	2.382948990	-1.502712734	-0.266494601
C	2.067536368	1.579089664	-0.235516649
C	0.034810121	-1.507282283	-0.251252712
C	0.340755606	1.581072366	-0.220984166
C	1.449951923	-0.759938395	2.863630911
H	0.861036793	-1.645520856	2.612799951
H	1.276154516	-0.494065386	3.908049852
H	1.154798081	0.068925035	2.218647449