Electronic Supplementary Information

Hydrogen Bonds between Methanol and the Light Liquid Olefins 1-Pentene and 1-Hexene: From Novel Application to Fundamental Science

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I. FCC gasoline "*Extractive Refining*" experiment

The commercial FCC gasoline was purchased from a SINOPEC petroleum refinery, and the mass fractions of olefin in this gasoline is 49.3%, and the detailed olefin group composition of the commercial FCC gasoline is listed in Table S1T. Following the "*Extractive Refining*" process[S1] experiment, Gas Chromatography–Mass Spectrometry (GCMS) method was employed to quantify the level of olefins content in the purified FCC gasoline. The GCMS analyser was a SHIMADZU GCMS-QP2010 SE gas chromatography mass spectrometer.

Table S1. Olefin group composition of commercial FCC gasoline from SINOPEC petroleum refinery.

Olefin	Wt %
C4	10.2

C5	22.2
C6	10.8
C7	4.2
C8	1.9
Total	**49.3**

II. Computational Details

The full geometry optimization of 1-pentene, 1-hexene, methanol (MeOH) and their clusters has been carried out at the DFT level of theory in both gas phase and solution (SMD model,[S2] olefin or methanol as solvent) using the M06-2X[S3a] or wB97XD functional[S3b] and the 6-311+G** basis set with the help of the Gaussian-09[S4] program package. It was shown that the M06-2X functional describes reasonably the weak dispersion forces.[S5] The binding energies for the 1-hexene•••methanol associate in gas phase calculated using the M06-2X and wB97XD functionals are very similar (–19.6 *vs.* –19.9 kJ/mol). No symmetry operations have been applied. The Hessian matrix was calculated analytically in order to prove the location of correct minima (no imaginary frequencies). The topological analysis of the electron density distribution with help of the AIM method of Bader[S6] was performed using the program AIMAll.[S7] The atomic charges and bond orbital nature were analyzed by using the natural bond orbital (NBO) partitioning scheme.[S8]

For the clusters 1-hexene···MeOH, several initial geometries with various mutual positions of the 1-hexene and methanol molecules were used. The olefin···methanol binding energies were calculated at both M06-2X/6-311+G** and CCSD(T)/6-311+G**//M06-2X/6-311+G** levels as the difference between the enthalpy at 0 K of the cluster olefin···methanol and the sum of enthalpies of isolated olefin and MeOH. Counterpoise estimates of the basis set superposition

error (BSSE)[S9] were made using the Counterpoise keyword in Gaussian 09.

Magnetic shielding was calculated for the equilibrium geometries using the GIAO method[S10] at the M06-2X/6-311+G(2d,p)//6-311+G** level. The ^{1}H chemical shifts were estimated relative to TMS calculated at the same level of theory.

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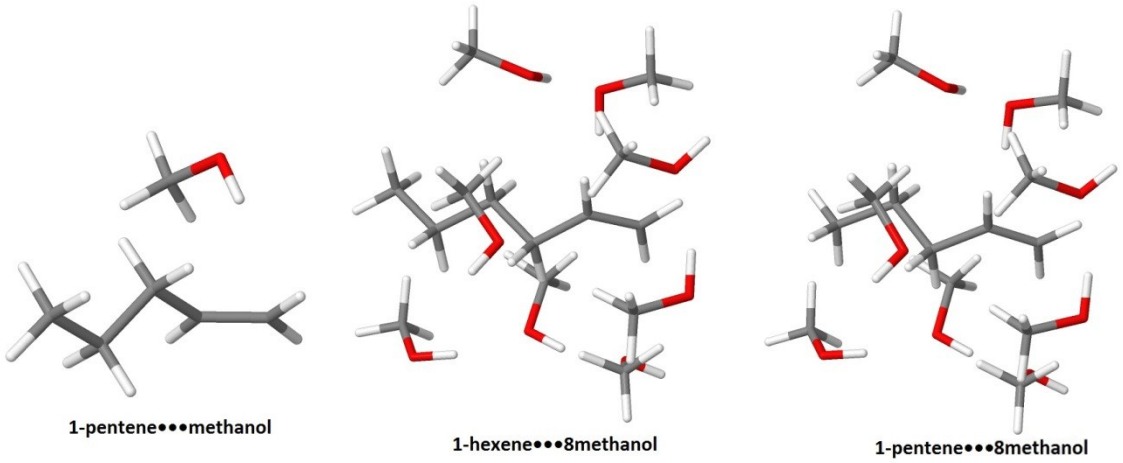

Fig. S1. Equilibrium structures of associates 1-pentene•••methanol, 1-hexene•••8methanol and 1-pentene•••8methanol.

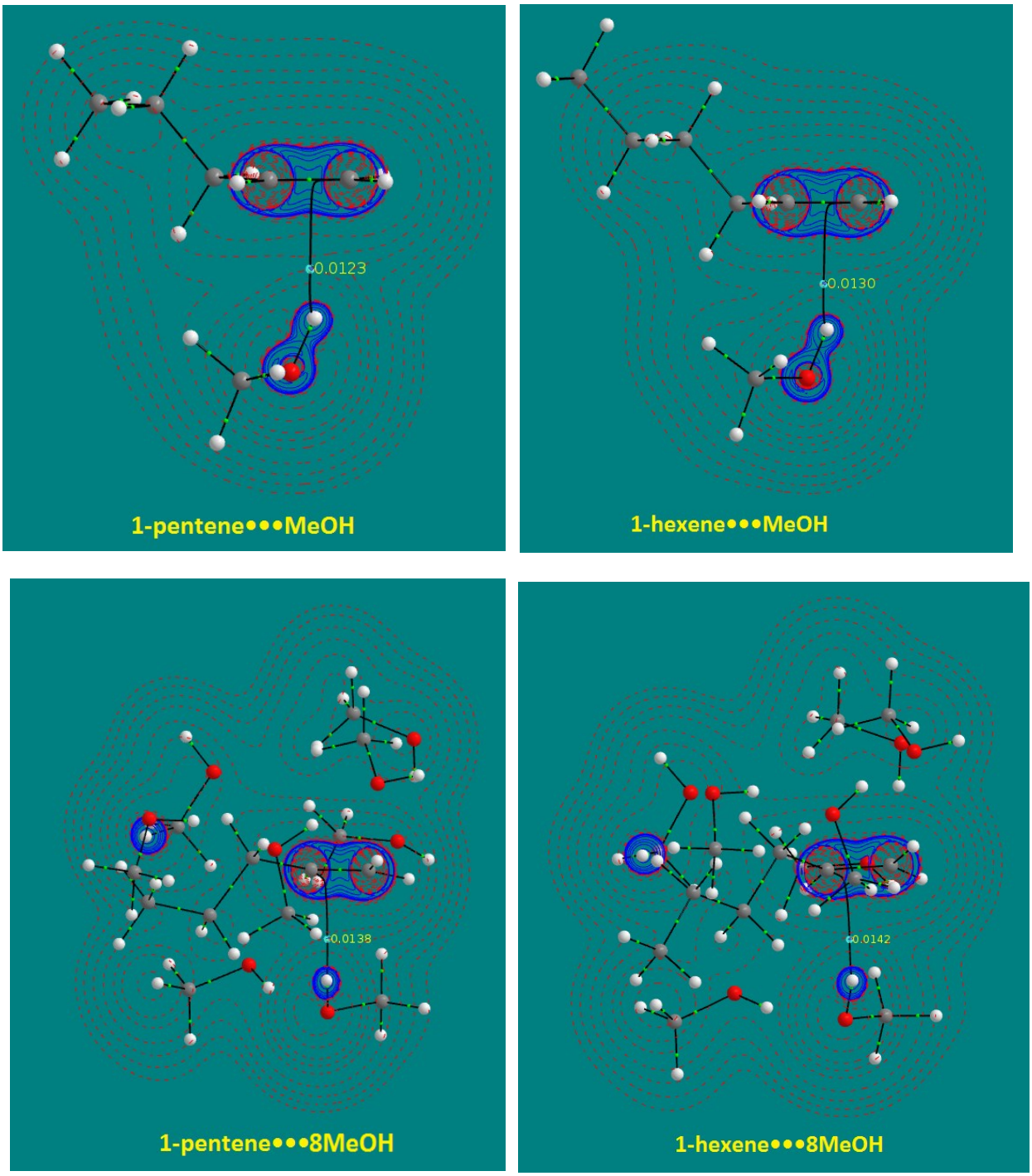

Fig. S2. Contour line diagrams of the Laplacian distribution $\nabla^2\rho(\mathbf{r})$ and selected bond paths in the plane formed by the carbon atoms of the C=C group and the hydroxyl hydrogen atom of the methanol for 1-pentene•••MeOH, 1-hexene•••MeOH, 1-pentene•••8MeOH and 1-hexene•••8MeOH associates. Dashed lines indicate charge depletion ($\nabla^2\rho(\mathbf{r}) > 0$), solid lines of the Laplacian distribution indicate charge concentration ($\nabla^2\rho(\mathbf{r}) > 0$). Electron density values (in e/Bohr^3) are indicated for the OH•••(C=C) BCP.

Table S2. The calculated parameters of the 1-pentene···methanol and 1-pentene···8methanol associates.

	1-pentene···methanol			1-pentene···8 methanol[a,c]
	Gas phase[a]	SMD (1-pentene as solvent)[b]	SMD (methanol as solvent)[b]	
E_b[d]	–19.4 (–17.1)[f]	–19.2	–13.6	
E_b[e]	–15.6	–13.8	–10.8	
l(OH···π)[g]	2.412	2.392	2.387	2.385
ρ[h]	0.082	0.088	0.083	0.093
$\nabla^2\rho$[i]	0.856	0.887	0.879	0.979
H_b[j]	0.010	0.011	0.011	0.010

[a] Isolated molecular associate without bulky solvent effects. [b] SMD solvation model. [c] Molecular associate with a 1-pentene molecule surrounded by 8 methanol molecules. [d, e] Binding energies (in kJ/mol) at the M06-2X/6-311+G and CCSD(T)/6-311+G**//M06-2X/6-311+G** levels, respectively. [f] BSSE corrected value. [g] Intermolecular OH···(C=C)$_{midpoint}$ distances (in Å). [h] Electron density (in e/Å^3) at the OH···(C=C) BCP. [i] Laplacian (in e/Å^5) at the OH···(C=C) BCP. [j] Energy density at the OH···(C=C) BCP (in Hartree/Å^3).**

Table S3. Cartesian atomic coordinates (Å) of the equilibrium structures.

1-hexene, gas phase

C	-2.545428	1.484526	-0.874100
C	-1.328810	1.028262	-0.599443
C	-0.563888	1.316034	0.658375
C	0.754281	2.047117	0.383145
C	1.577661	2.281216	1.647340
H	1.789713	1.316221	2.120668
H	0.980866	2.853120	2.366166
C	2.885927	3.015427	1.365064
H	3.469465	3.161261	2.276217
H	2.694510	3.999040	0.928340
H	3.502076	2.453183	0.658498
H	-1.182662	1.909843	1.338884
H	-0.341075	0.371826	1.170537
H	1.347613	1.466514	-0.333524
H	0.537909	3.006350	-0.100465
H	-3.042398	1.250363	-1.808095
H	-3.085434	2.107648	-0.167496
H	-0.817725	0.408059	-1.334800

1-hexene, SMD (1-hexene)

C	-2.547013	1.484039	-0.874214
C	-1.329549	1.028538	-0.598945
C	-0.564728	1.317928	0.658433
C	0.755181	2.046192	0.382557
C	1.579170	2.279149	1.646723
H	1.794041	1.313426	2.117510
H	0.982493	2.849321	2.367231
C	2.885371	3.016253	1.365555
H	3.470320	3.158888	2.277170
H	2.693208	4.002985	0.935052
H	3.503746	2.459283	0.656032
H	-1.182867	1.913950	1.337531
H	-0.343192	0.373476	1.170830
H	1.347152	1.463651	-0.333665
H	0.540640	3.006357	-0.100381
H	-3.043609	1.246675	-1.808570
H	-3.088769	2.109749	-0.170257
H	-0.818996	0.406148	-1.333282

1-hexene, SMD (MeOH)

C	-2.547915	1.479988	-0.876790
C	-1.329010	1.027479	-0.595500
C	-0.566988	1.325626	0.661411
C	0.754265	2.049819	0.381072
C	1.581426	2.274838	1.644296
H	1.799037	1.304846	2.105314
H	0.985435	2.838500	2.370831
C	2.885775	3.016240	1.365896
H	3.473758	3.147852	2.277907
H	2.690713	4.008569	0.948714
H	3.501715	2.467214	0.647502
H	-1.185354	1.926902	1.335901
H	-0.344248	0.383358	1.177528
H	1.341365	1.465618	-0.337877
H	0.542465	3.013869	-0.096487
H	-3.041655	1.234394	-1.811564
H	-3.091758	2.111734	-0.178697
H	-0.816426	0.399165	-1.324148

MeOH, gas phase

O	1.698592	-3.230905	-0.993473
H	2.373614	-3.821816	-1.331649
C	1.692668	-3.305724	0.419437
H	1.454007	-4.313283	0.775816
H	0.917495	-2.624766	0.768180
H	2.648861	-2.991439	0.850802

MeOH, SMD (1-hexene)

O	1.698067	-3.229730	-0.996138
H	2.375121	-3.823834	-1.328341
C	1.691696	-3.304661	0.419552
H	1.454419	-4.313540	0.773648
H	0.916597	-2.624461	0.771534
H	2.649338	-2.991708	0.848858

MeOH, SMD (1-pentene)

O	1.698067	-3.229730	-0.996138
H	2.375121	-3.823834	-1.328341
C	1.691696	-3.304661	0.419552
H	1.454419	-4.313540	0.773648
H	0.916597	-2.624461	0.771534
H	2.649338	-2.991708	0.848858

MeOH, SMD (MeOH)

O	1.698374	-3.230281	-0.998275
H	2.378625	-3.826553	-1.328141
C	1.689072	-3.302782	0.424940
H	1.455086	-4.314034	0.769426
H	0.914010	-2.622058	0.776583
H	2.650071	-2.992224	0.844580

1-hexene···MeOH, gas phase (the most stable O–H···(C=C) associate)

C	-2.583466	1.961247	-1.109224
C	-1.312282	1.569035	-1.076180
C	-0.516618	1.332884	0.173508
C	0.732984	2.216661	0.239745
C	1.571059	1.957697	1.489379
H	1.861800	0.902047	1.514194
H	0.954044	2.128924	2.377924
C	2.816360	2.838528	1.548874
H	3.404452	2.640968	2.447112
H	2.544643	3.897281	1.552049
H	3.459021	2.663162	0.682080
O	-2.365566	-1.409936	-0.411542
H	-2.598394	-0.482093	-0.516222
C	-1.600000	-1.788053	-1.536100
H	-2.162297	-1.684793	-2.470656
H	-1.334154	-2.836926	-1.406828
H	-0.674044	-1.205396	-1.618671
H	-1.148829	1.510921	1.049564
H	-0.212584	0.279463	0.216867
H	1.347595	2.043803	-0.651998
H	0.431951	3.269740	0.209194
H	-3.103336	2.127026	-2.045625
H	-3.139890	2.141091	-0.193546
H	-0.784981	1.413080	-2.017109

1-hexene···MeOH, SMD (1-hexene) (the most stable O–H···(C=C) associate)

C	-3.068706	1.315266	0.725851
C	-1.902161	0.733950	0.453976
C	-0.834664	0.433748	1.463829
C	0.520432	1.049912	1.096690
C	1.596947	0.751201	2.137494
H	1.703980	-0.333918	2.244939
H	1.269079	1.128753	3.112788
C	2.944310	1.369363	1.776776
H	3.703264	1.144528	2.529695
H	2.864866	2.456902	1.695331
H	3.304740	0.990713	0.816294
O	-1.284283	4.061523	0.520272
H	-1.708972	3.242688	0.241710
C	-1.418702	4.154312	1.924556
H	-2.465494	4.260191	2.231365
H	-0.878645	5.046081	2.244863
H	-0.985598	3.287982	2.440153
H	-1.154595	0.783988	2.451122
H	-0.713541	-0.654187	1.537666
H	0.839208	0.663524	0.121142
H	0.413530	2.134116	0.978646
H	-3.805276	1.500814	-0.048717
H	-3.330925	1.607271	1.739560
H	-1.681405	0.449378	-0.574558

1-hexene···MeOH, SMD (MeOH) (the most stable O–H···(C=C) associate)

C	-2.614706	1.879913	-1.024565
C	-1.328213	1.534965	-1.003969
C	-0.512682	1.330955	0.238360
C	0.737822	2.215839	0.259476
C	1.590791	2.002170	1.507289
H	1.865503	0.943743	1.578002
H	0.992304	2.230472	2.396156
C	2.852320	2.860183	1.502209
H	3.446141	2.705016	2.406424
H	2.602022	3.923614	1.444706
H	3.483645	2.619927	0.641707
O	-2.543408	-1.464270	-0.599613
H	-2.665821	-0.506132	-0.583015
C	-1.596225	-1.758489	-1.620906
H	-1.922355	-1.370903	-2.590655
H	-1.516588	-2.843976	-1.687038
H	-0.609037	-1.349981	-1.383179
H	-1.130169	1.527923	1.121017
H	-0.197108	0.280747	0.291260

H	1.340596	2.007831	-0.632792
H	0.437513	3.268518	0.198003
H	-3.149311	2.018163	-1.958932
H	-3.171487	2.039159	-0.104069
H	-0.804076	1.390974	-1.949085

1-hexene···MeOH, SMD (MeOH) (the C–H···O associate)

C	0.186736	3.127354	-0.455967
C	0.085993	1.971816	0.195817
C	1.243292	1.099700	0.582289
C	1.179555	-0.273658	-0.096045
C	2.321611	-1.194119	0.326375
H	2.291806	-1.327477	1.413453
H	3.277935	-0.711041	0.096258
C	2.254565	-2.554699	-0.361605
H	3.077658	-3.203461	-0.051589
H	2.306890	-2.444412	-1.448772
H	1.317366	-3.066587	-0.123532
O	-2.661531	-0.345158	0.097419
H	-2.371947	-0.100856	-0.788195
C	-3.896868	-1.047778	-0.010278
H	-4.664059	-0.431817	-0.487677
H	-4.218578	-1.290356	1.002492
H	-3.778186	-1.976216	-0.575994
H	2.184487	1.597780	0.326818
H	1.235979	0.951543	1.669127
H	0.221180	-0.750405	0.142128
H	1.202395	-0.137809	-1.183989
H	-0.690839	3.708234	-0.721094
H	1.154443	3.531558	-0.742885
H	-0.901605	1.598266	0.465560

1-hexene···8MeOH, gas phase

C	0.872792	1.315224	1.457557
C	0.793112	0.404467	0.488858
C	-0.454487	0.053622	-0.262854
C	-0.918171	-1.379534	0.021378
C	-2.143517	-1.762266	-0.803004
H	-1.889081	-1.720527	-1.868370
H	-2.926425	-1.010534	-0.659623
C	-2.676921	-3.148515	-0.454243
H	-3.548978	-3.404411	-1.059674
H	-2.973039	-3.198045	0.598277
H	-1.914627	-3.916417	-0.616922
O	2.510214	3.459373	-0.339029
H	3.001720	2.746717	0.091647
C	2.117712	2.973669	-1.606705

H	2.981533	2.735619	-2.238670
H	1.543753	3.762000	-2.098835
H	1.493901	2.075200	-1.527864
H	-1.261107	0.746826	-0.009027
H	-0.260055	0.159106	-1.337647
H	-0.093660	-2.076296	-0.174778
H	-1.154210	-1.478109	1.089491
H	1.815588	1.519348	1.953660
H	0.006481	1.905187	1.744883
H	1.685818	-0.162007	0.220624
O	-1.758280	3.413789	0.842785
H	-1.773754	4.170731	1.432911
C	-0.860482	3.678334	-0.241839
H	-1.191244	4.547725	-0.815854
H	-0.883796	2.799632	-0.885367
H	0.162783	3.820396	0.113222
O	1.467833	-1.747609	2.662711
C	2.706582	-1.144940	3.020187
H	0.877746	-1.038828	2.375241
H	3.387576	-1.951557	3.289243
H	2.588182	-0.477570	3.878291
H	3.128506	-0.583571	2.179083
O	-5.169473	0.037327	-1.209021
C	-5.789133	-0.840283	-0.298279
H	-4.577148	0.605056	-0.695466
H	-6.575223	-1.376080	-0.832213
H	-6.246772	-0.305415	0.542420
H	-5.085360	-1.582891	0.102887
O	2.482194	-2.758646	0.292273
H	1.994381	-2.577334	1.113113
C	2.084903	-4.009539	-0.230235
H	2.228063	-4.818400	0.492994
H	2.705761	-4.215437	-1.103372
H	1.034121	-4.006148	-0.546965
O	1.640624	-0.117998	-2.955243
H	1.335439	0.037631	-3.851608
C	1.474022	-1.494650	-2.639484
H	0.417761	-1.786510	-2.651167
H	1.864183	-1.640872	-1.631223
H	2.032601	-2.136277	-3.328524
O	-3.561866	1.302984	0.713863
H	-3.074172	2.141694	0.723260
C	-3.214872	0.562427	1.869939
H	-2.139002	0.612702	2.069243
H	-3.484594	-0.480777	1.691643

H	-3.757950	0.919482	2.750768
O	3.990575	1.103868	0.415964
H	4.787960	1.066460	0.948946
C	4.103889	0.163812	-0.659298
H	5.059829	0.276230	-1.177582
H	3.299501	0.382787	-1.361914
H	3.989869	-0.862176	-0.295469

1-pentene, gas phase

C	-2.494513	-0.919470	-0.282612
C	-1.235143	-1.340601	-0.259648
C	-0.183504	-0.848357	0.690036
C	0.986382	-0.171273	-0.033424
C	2.069560	0.296228	0.934988
H	2.478691	-0.546734	1.498230
H	1.664272	1.011614	1.655263
H	2.894795	0.780817	0.409706
H	-0.630748	-0.148227	1.403158
H	0.205968	-1.692740	1.272117
H	1.413720	-0.870908	-0.759454
H	0.603146	0.677596	-0.607809
H	-3.209965	-1.300691	-1.001583
H	-2.850855	-0.176642	0.424612
H	-0.912276	-2.085442	-0.985769

1-pentene, SMD (1-pentene)

C	-2.496626	-0.919990	-0.280429
C	-1.235647	-1.338321	-0.260841
C	-0.183344	-0.848066	0.688990
C	0.988297	-0.172903	-0.033789
C	2.068750	0.296626	0.935637
H	2.478394	-0.544497	1.502102
H	1.663773	1.015582	1.653153
H	2.895733	0.779453	0.410162
H	-0.629121	-0.147818	1.402892
H	0.204594	-1.694727	1.268867
H	1.417928	-0.874061	-0.757235
H	0.607379	0.676116	-0.610029
H	-3.211819	-1.301804	-1.000632
H	-2.856041	-0.179870	0.429056
H	-0.912719	-2.080550	-0.990095

1-pentene, SMD (MeOH)

C	-2.508264	-0.911144	-0.315591
C	-1.254572	-1.351986	-0.255721
C	-0.193522	-0.798646	0.648470
C	0.993880	-0.222112	-0.131122
C	2.084174	0.306799	0.795752

H	2.473387	-0.491530	1.434546
H	1.694251	1.095498	1.445707
H	2.922425	0.722302	0.231024
H	-0.623900	-0.024462	1.292327
H	0.176041	-1.598214	1.302655
H	1.406126	-0.997759	-0.785454
H	0.635656	0.582188	-0.782254
H	-3.231137	-1.343492	-0.999987
H	-2.852176	-0.101613	0.323431
H	-0.945869	-2.164729	-0.913203

1-pentene···MeOH, gas phase (the most stable O–H···(C=C) associate)

C	-2.473318	1.139248	-0.681534
C	-1.251465	0.642208	-0.856849
C	-0.076056	0.912024	0.035248
C	1.089775	1.558418	-0.720706
C	2.294916	1.800869	0.183738
H	2.656848	0.861812	0.610159
H	2.031415	2.462159	1.013100
H	3.118729	2.261977	-0.364030
O	-1.914781	-1.448261	1.519886
H	-2.203743	-0.665456	1.040703
C	-1.611374	-2.443835	0.565611
H	-2.486912	-2.721018	-0.031623
H	-1.274018	-3.323406	1.113461
H	-0.808564	-2.131760	-0.113778
H	-0.384859	1.554908	0.866125
H	0.265909	-0.030559	0.481053
H	1.377073	0.913036	-1.557567
H	0.751369	2.502828	-1.157730
H	-3.282002	0.917745	-1.368074
H	-2.697101	1.799241	0.152221
H	-1.064213	-0.003008	-1.714955

1-pentene···MeOH, SMD (1-pentene) (the most stable O–H···(C=C) associate)

C	-2.439811	-0.279751	-0.905381
C	-1.235313	-0.588957	-1.380711
C	-0.240397	-1.476783	-0.693869
C	1.117309	-0.793648	-0.489142
C	2.108441	-1.697154	0.238032
H	2.280808	-2.622493	-0.319050
H	1.733628	-1.970941	1.228565
H	3.072755	-1.202758	0.372553
O	-0.756534	1.899504	0.891103
H	-1.119391	1.474272	0.106276
C	-0.993963	1.042036	1.989646
H	-2.064216	0.908530	2.183458

H	-0.544303	1.508031	2.867268
H	-0.533272	0.055539	1.852962
H	-0.646624	-1.807151	0.268341
H	-0.089192	-2.378839	-1.300007
H	1.523387	-0.507857	-1.465295
H	0.977850	0.136255	0.071495
H	-3.116476	0.369595	-1.450620
H	-2.794969	-0.684113	0.038949
H	-0.922319	-0.168975	-2.336383

1-pentene···MeOH, SMD (MeOH) (the most stable O–H···(C=C) associate)

C	1.850833	-0.061797	-0.539452
C	0.531840	-0.033659	-0.721956
C	-0.488180	-0.337297	0.335253
C	-1.425890	-1.478222	-0.072913
C	-2.484103	-1.757014	0.989361
H	-3.103371	-0.872465	1.164579
H	-2.018679	-2.032687	1.940114
H	-3.143595	-2.575397	0.690641
O	0.750627	2.865899	0.753600
H	1.157119	2.006310	0.584066
C	0.081691	3.266184	-0.437557
H	0.773995	3.322749	-1.282910
H	-0.335519	4.257221	-0.256636
H	-0.735526	2.582913	-0.689019
H	0.016397	-0.585215	1.275229
H	-1.090889	0.562076	0.519254
H	-1.909583	-1.221901	-1.021525
H	-0.833295	-2.381026	-0.254500
H	2.540033	0.165467	-1.346401
H	2.282395	-0.321647	0.424501
H	0.139410	0.222538	-1.706319

1-pentene···8MeOH, gas phase

C	0.413733	1.196902	1.385569
C	0.545962	0.272807	0.435024
C	-0.580502	-0.337719	-0.343083
C	-0.729801	-1.836791	-0.055932
C	-1.805064	-2.480866	-0.925658
H	-1.531391	-2.430566	-1.983534
H	-2.760341	-1.958340	-0.824561
H	-1.955248	-3.531664	-0.668201
O	1.659345	3.664677	-0.349189
H	2.274439	3.054262	0.080389
C	1.345282	3.115472	-1.613076
H	2.227601	3.050600	-2.260759
H	0.621663	3.780167	-2.090150

H	0.907093	2.114186	-1.527508
H	-1.523692	0.169611	-0.118840
H	-0.382843	-0.198186	-1.413076
H	0.237645	-2.328477	-0.210125
H	-0.979120	-1.973153	1.003422
H	1.282397	1.596889	1.897439
H	-0.558545	1.608052	1.643539
H	1.542870	-0.104263	0.200804
O	-2.468569	2.997720	0.971141
H	-2.575887	3.784461	1.509697
C	-1.673401	3.310899	-0.178785
H	-2.163988	4.070215	-0.793159
H	-1.588781	2.389629	-0.755488
H	-0.670775	3.635630	0.107931
O	1.628908	-1.681305	2.640116
C	2.686155	-0.804691	3.015077
H	0.895750	-1.130213	2.337104
H	3.535370	-1.429061	3.290703
H	2.402982	-0.189916	3.873860
H	2.972645	-0.154852	2.181012
O	-4.933270	-0.828641	-1.327455
C	-5.620472	-1.750467	-0.513077
H	-4.478283	-0.211637	-0.736125
H	-6.347421	-2.274145	-1.135619
H	-6.157167	-1.254288	0.303357
H	-4.943561	-2.500333	-0.080051
O	2.908979	-2.425150	0.303211
H	2.376297	-2.368619	1.114344
C	2.833095	-3.732090	-0.227945
H	3.201395	-4.482545	0.478611
H	3.461735	-3.761862	-1.119142
H	1.809135	-3.997328	-0.518914
O	1.589393	-0.000186	-2.936307
H	1.282389	0.115836	-3.838054
C	1.719421	-1.389701	-2.663271
H	0.755325	-1.906024	-2.730753
H	2.093293	-1.481286	-1.642443
H	2.431803	-1.868292	-3.342945
O	-3.779627	0.575841	0.785399
H	-3.468929	1.489587	0.890114
C	-3.316839	-0.204119	1.872481
H	-2.247429	-0.050444	2.053202
H	-3.476486	-1.253572	1.616916
H	-3.870001	0.020927	2.789657
O	3.541878	1.660025	0.479687

H	4.320569	1.784318	1.026599
C	3.863624	0.774995	-0.600547
H	4.786276	1.084860	-1.098440
H	3.044423	0.835043	-1.317463
H	3.953340	-0.256837	-0.246842