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

Supporting information for

Δ-Machine learning approach efficiently brings the DFT based potential energy surface to the CCSD(T) quality: a case for the OH + CH_3OH reaction

Kaisheng Song,[1] and Jun Li[1,*]

[1] *School of Chemistry and Chemical Engineering & Chongqing Key Laboratory of Theoretical and Computational Chemistry, Chongqing University, Chongqing 401331, P.R. China*

*: *Corresponding author, email:* jli15@cqu.edu.cn (JL).

SI. DFT calculations

As mentioned in text, how to choose an appropriate low-level method is one of the key problems we need to face. Thus, we should know the rules about how to define "an appropriate low-level method". First, the selected low-level method should be used to get convergent, correct, and smooth results in the same configuration space as the target high-level method. If not, the target high-level PES cannot be developed due to the uncovered or the nonconvergent configuration space. Second, the energy differences between the low- and the target high-level method in all configuration space should be small, smooth and nonnegative. The smaller the energy deviations between the low-level and the target high-level method, the fewer points are need to develop the correction PES and the cheaper the cost. The smooth and nonnegative requirements of the energy differences in all configuration space guarantee a highly accurate correction PES. Third, the selected low-level method should be highly efficient to reduce the cost as much as possible. In order to select an appropriate low-level method meeting all the demanding mentioned above, many DFT methods have been tested by G16. Table S2 displays the comparison of energy (in kcal mol^{-1}) and vibrational frequencies (in cm^{-1}) of the stationary points from 12 methods for the title reaction. Thanks to Ying Zhang for two candidate methods, UB3LYP/6-311+G(3df,2p) and UM05-2X/6-311+G(3df,2p), selected from 40 DFT methods. Compared with the target high-level (UCCSD(T)-F12a/AVTZ) method in Table S1, the molecular properties including energy and frequencies of stationary points from the UM05-2X/6-311+G(3df,2p) method were closer than others, particularly of which at TS1 and TS2. In addition to the molecular properties, several one-dimensional scans for each low-level method have also been performed to check if satisfy the requirements mentioned above, and we have found that none of the 12 methods could fulfill all the requirements with default settings, but lowering the energy convergence threshold to 10^{-6}, which is reliable and acceptable, could greatly improve the situation. Only the results from UM05-2X/6-311+G(3df,2p) were continuous, smooth and nonnegative. For the title reaction system, the high efficiency for UM05-2X/6-311+G(3df,2p) was apparently evident that only about 1~3 mins were needed for one single point energy calculation with 4 processors on a

slave node with Intel Xeon CPU E5-2682 V4 @2.5GHZ compared with the target high-level method (UCCSD(T)-F12a/AVTZ) taking about 30~70 mins for one single point energy calculation with 8 processors on the same node. Finally, UM05-2X/6-311+G(3df,2p) successfully passed in all tests and was chosen as the low-level method.

SII. Figures and Tables

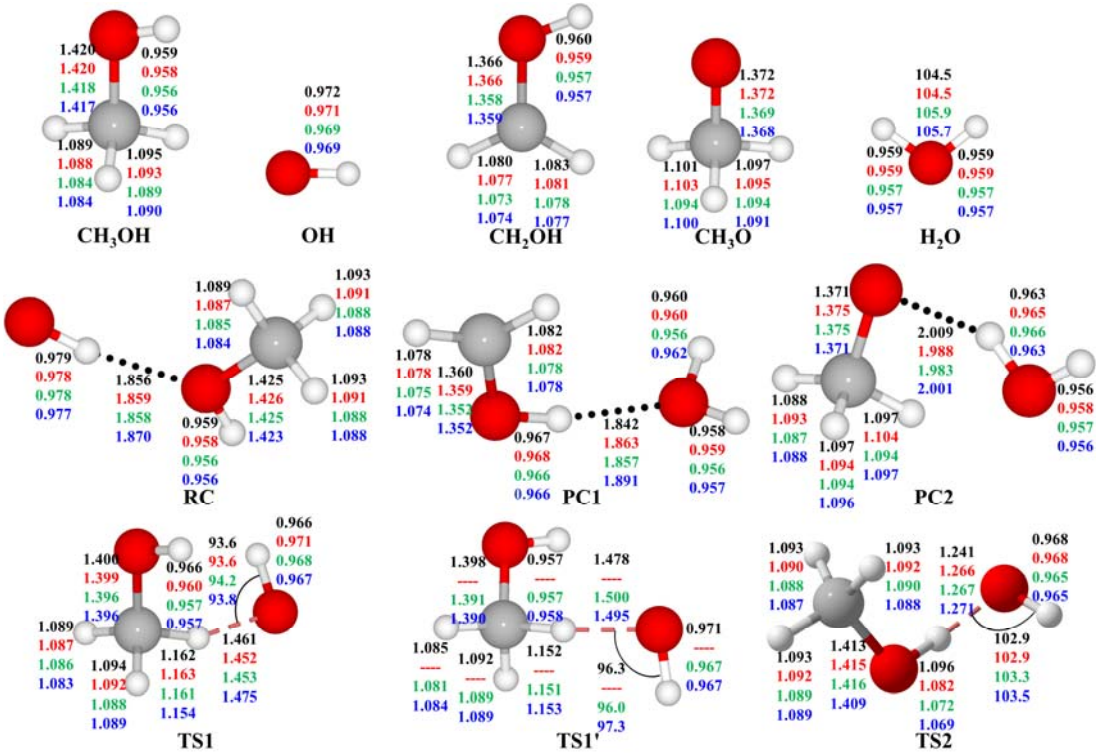

Figure S1. Comparison of geometries of the stationary points (angle in degree and distance in Å) obtained from different levels: PESH, UCCSD(T)-F12a/AVTZ, PESL, M05-2X/6-311+G(3df,2p), from top to bottom.

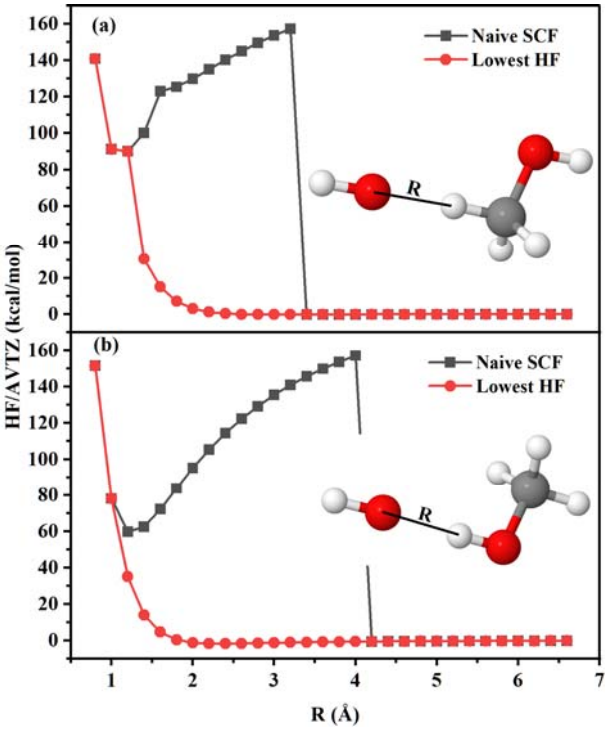

Figure S2. Comparison of the Hartree-Frock reference energies relative to the reactants CH_3OH and OH, calculated from the default SCF procedure and the lowest HF method for (a) and (b), respecitively.

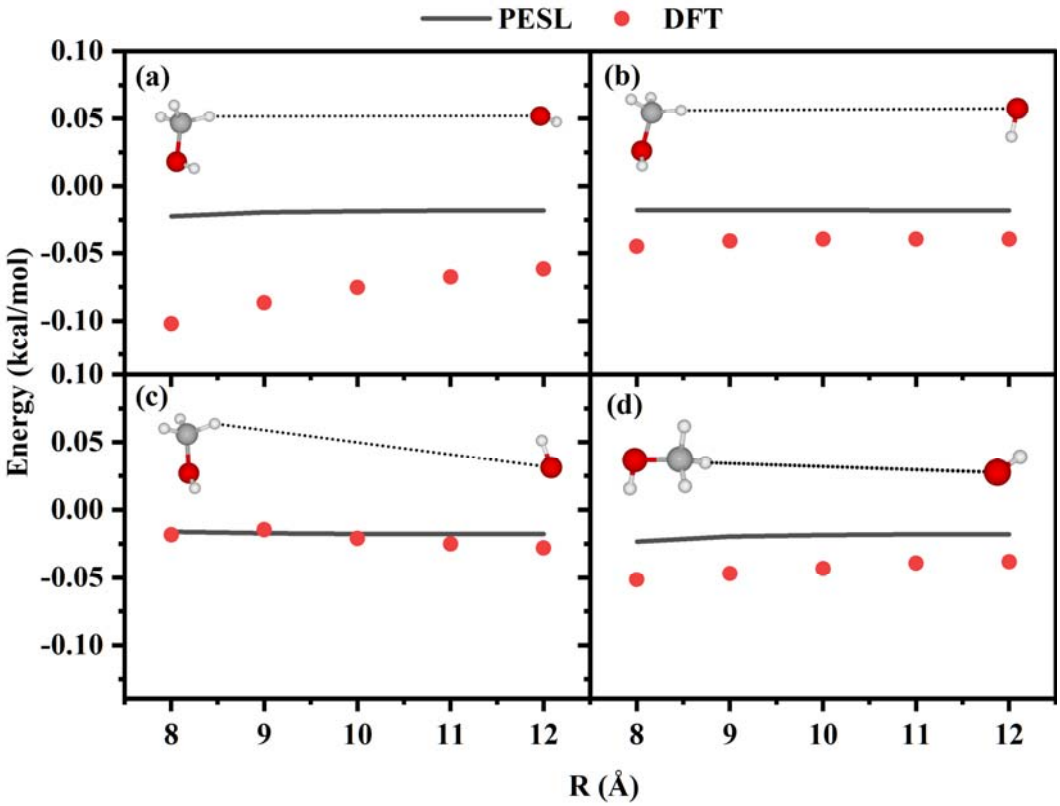

Figure S3. Four one-dimensional cuts for the long-range interaction between OH and CH_3OH at different orientations with other coordinates fixed at the equilibrium of the reactants.

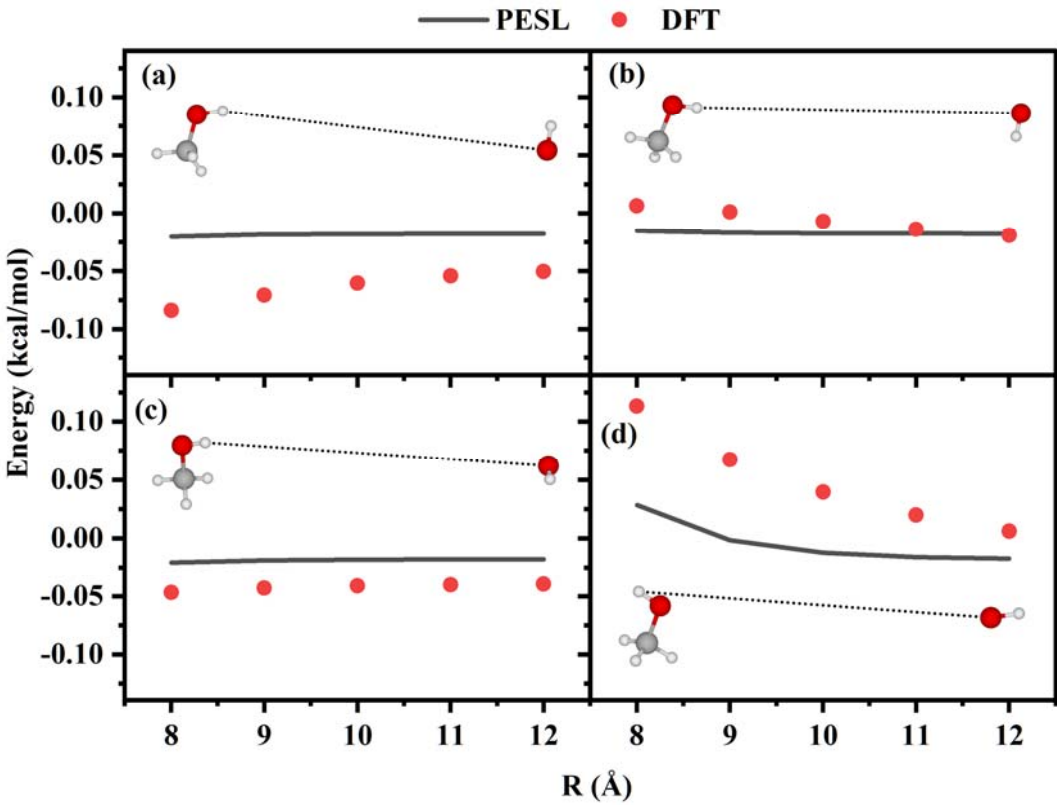

Figure S4. Four one-dimensional cuts for the long-range interaction at different orientations between OH and CH_3OH with other coordinates fixed at the equilibrium of the reactants.

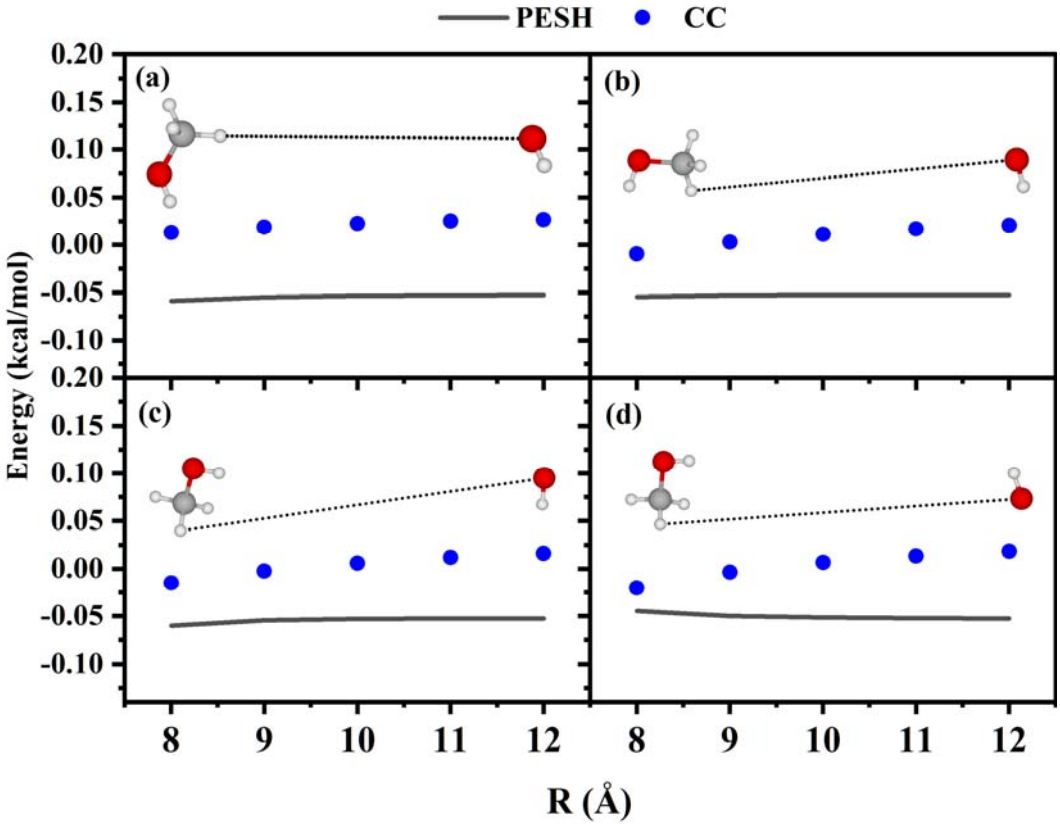

Figure S5. Four one-dimensional cuts at different orientations between CH_3OH and OH with other coordinates fixed at the equilibrium of the reactants.

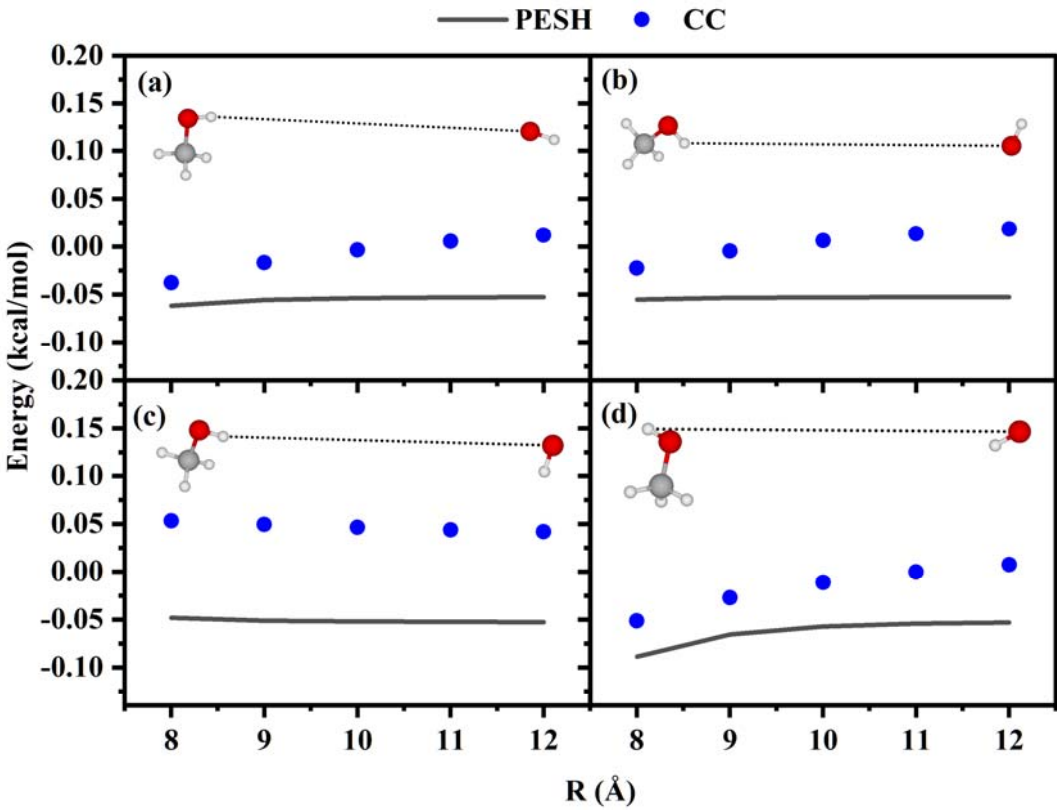

Figure S6. Four one-dimensional cuts for the interaction at different orientations between CH_3OH and OH with other coordinates fixed at the equilibrium of the reactants.

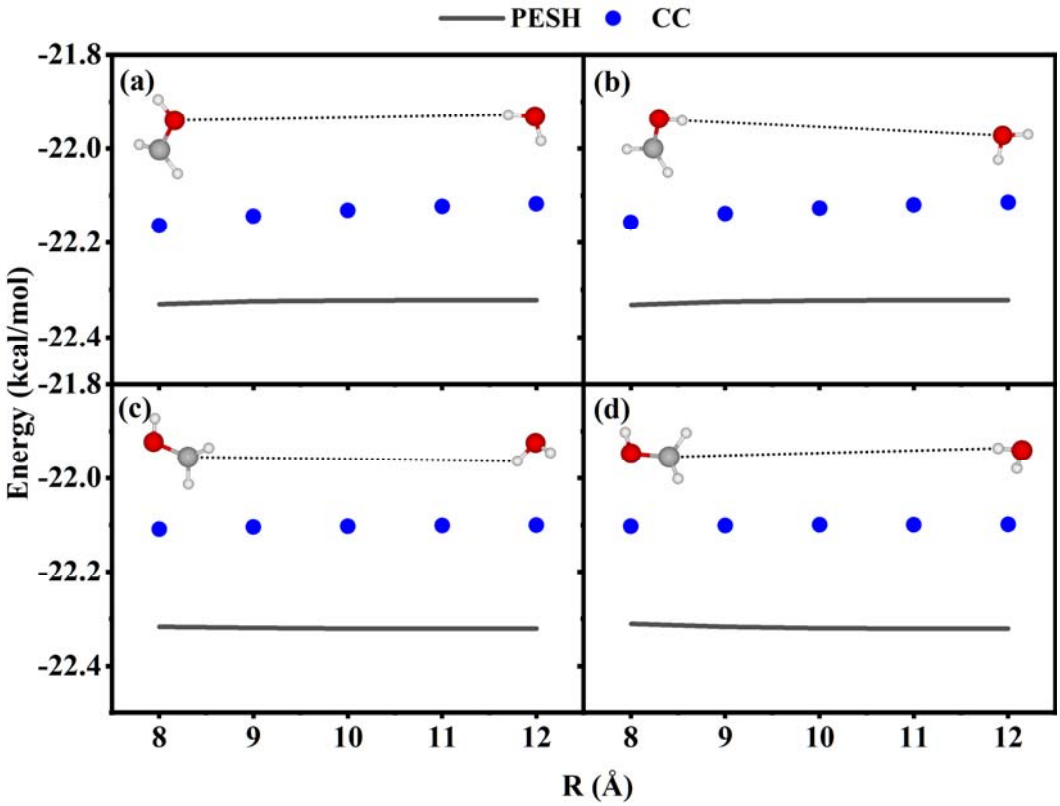

Figure S7. Four one-dimensional cuts for the long-range interaction at different orientations between CH_2OH and H_2O with other coordinates fixed at the equilibrium of the monomer.

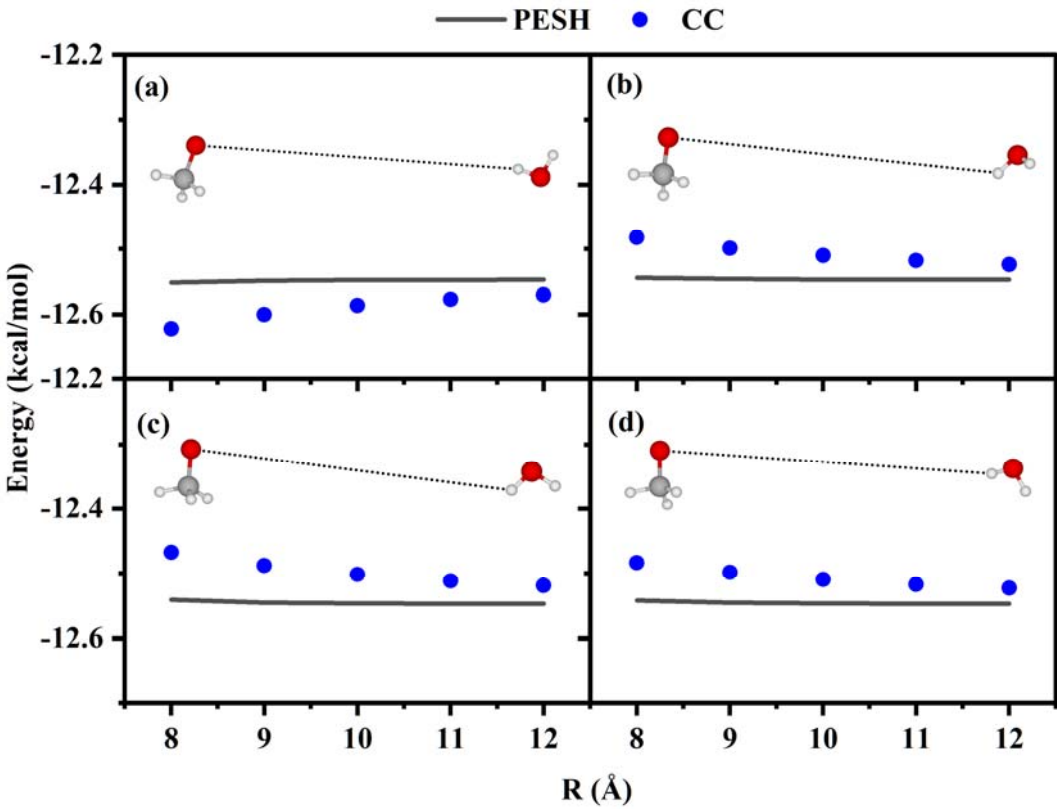

Figure S8. Four one-dimensional cuts for the long-range interaction at different orientations between CH_3O and H_2O with other coordinates fixed at the equilibrium of the monomer.

Table S1. Energies (kcal/mol) and vibrational harmonic frequencies (cm^{-1}) of the stationary points for the title reaction.

Species	Methods	Energy	Frequencies																	
			1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
$OH + CH_3OH$	*a*	0.00	3730	223	1053	1140	1191	1424	1485	1536	1550	3055	3118	3188	3904					
	b	0.00	3745	281	1060	1087	1183	1391	1463	1530	1532	3025	3086	3157	3867					
	c	0.00	3737	288	1061	1088	1179	1381	1483	1510	1520	3017	3077	3137	3863					
	d	0.00	3731	291	1063	1088	1178	1378	1480	1505	1515	3014	3073	3134	3859					
	e	0.00	3806	294	1074	1101	1198	1371	1506	1534	1541	3072	3123	3182	3929					
	f	0.00	3812	270	1081	1103	1205	1382	1500	1546	1546	3077	3124	3194	3926					
$H_2O + CH_2OH$	*a*	-22.11	1802	3874	3958	278	468	1103	1196	1391	1471	3175	3372	3891						
	b	-22.29	1672	3836	3942	462	547	1086	1207	1413	1529	3160	3312	3900						
	c	-22.10	1645	3831	3942	430	580	1063	1210	1374	1494	3149	3292	3859						
	d	-22.07	1643	3830	3940	434	576	1062	1209	1372	1492	3145	3289	3856						
	e	-22.55	1614	3895	3996	406	553	1066	1238	1359	1509	3205	3346	3922						
	f	-22.52	1625	3899	4015	450	525	1082	1237	1397	1542	3223	3383	3955						
$H_2O + CH_3O$	*a*	-13.52	1799	3870	3947	842	843	1081	1432	1440	1441	3069	3084	3085						
	b	-12.78	1650	3838	3951	636	636	1091	1363	1447	1447	2959	3056	3058						
	c	-12.55	1645	3831	3942	755	962	1116	1383	1386	1521	2940	3021	3065						

	d	-12.57	1643	3830	3940	756	965	1118	1380	1381	1518	2934	3018	3064						
	e	-13.44	1614	3895	3996	857	982	1138	1411	1416	1540	2998	3070	3112						
	f	-13.60	1613	3876	3983	711	712	1105	1433	1479	1479	3017	3110	3110						
RC	*a*	-6.95	49	57	160	258	478	527	1044	1157	1229	1345	1507	1567	1571	3080	3146	3172	3707	3951
	b	-6.60	21	61	74	207	479	548	1061	1125	1202	1391	1458	1525	1526	3051	3150	3176	3580	3907
	c	-6.53	54	86	199	304	411	616	1065	1088	1183	1381	1485	1513	1522	3034	3103	3149	3608	3872
	d	-6.54	i85	i34	192	278	398	610	1067	1082	1178	1375	1484	1506	1513	3029	3098	3144	3599	3866
	e	-6.81	i6	48	204	263	408	605	1078	1088	1203	1366	1510	1535	1542	3088	3148	3191	3653	3930
	f	-6.87	44	56	217	285	469	558	1078	1094	1233	1399	1490	1542	1554	3073	3179	3186	3615	3945
PC1	*a*	-31.13	107	137	225	288	404	542	594	988	1089	1286	1579	1711	1861	3235	3407	3460	3929	4111
	b	-28.79	36	50	133	180	221	300	504	678	1094	1223	1437	1535	1702	3181	3317	3808	3828	3955
	c	-28.69	71	90	171	191	239	295	548	760	1109	1227	1441	1494	1647	3140	3279	3702	3828	3935
	d	-28.70	104	125	194	201	243	307	543	765	1108	1226	1438	1492	1645	3137	3277	3700	3827	3933
	e	-28.76	24	83	135	158	201	290	520	739	1106	1257	1415	1509	1613	3194	3333	3764	3887	3987
	f	-28.90	60	83	135	141	213	300	438	755	1098	1272	1456	1546	1639	3213	3315	3771	3870	4026
PC2	*a*	-18.62	i20.4	94	136	146	281	303	819	852	1100	1422	1434	1475	1846	3024	3152	3171	3960	4087
	b	-17.61	96	108	125	168	289	385	734	782	1072	1373	1440	1453	1707	2908	3045	3149	3843	3972

	[c]	-17.62	i70	91	111	184	347	423	894	1007	1116	1376	1394	1512	1659	2934	3030	3086	3748	3915
	[d]	-17.71	45	82	112	179	336	413	873	1014	1121	1368	1391	1509	1655	2929	3025	3085	3745	3913
	[e]	-18.86	i14	43	111	195	285	337	687	1056	1211	1385	1464	1515	1624	3013	3044	3141	3803	3967
	[f]	-18.84	90	125	148	176	314	373	798	812	1081	1461	1504	1513	1674	3005	3138	3237	3778	3942
TS1	[a]	1.39	i624	86	117	276	355	782	984	1124	1184	1382	1406	1420	1475	1597	3156	3203	3764	3921
	[b]	1.30	i934	108	209	277	434	704	980	1094	1143	1288	1364	1393	1521	1709	3073	3204	3703	3913
	[c]	1.39	i696	i31	166	172	388	740	1015	1065	1141	1355	1389	1440	1475	1573	3048	3153	3733	3843
	[d]	1.23	i653	99	155	251	423	755	1027	1077	1147	1350	1397	1450	1477	1597	3051	3153	3731	3841
	[e]	0.88	i1016	93	170	241	433	739	947	1080	1156	1354	1409	1442	1508	1649	3104	3203	3812	3909
	[f]	0.72	i811	77	179	215	414	745	997	1107	1178	1380	1424	1451	1552	1697	3138	3222	3817	3970
TS2	[a]	3.87	i1553	71	143	228	253	818	1054	1092	1102	1376	1491	1551	1623	1624	3028	3105	3115	3830
	[b]	3.82	i1759	134	186	315	335	846	1059	1089	1112	1385	1548	1571	1616	1757	2921	3071	3167	3805
	[c]	3.86	i1494	172	200	272	451	780	1046	1153	1182	1337	1457	1481	1523	1624	3030	3111	3118	3783
	[d]	4.18	i2262	127	174	229	395	776	1033	1124	1171	1305	1445	1465	1511	1625	3016	3090	3112	3783
	[e]	2.16	i1533	108	183	233	422	789	1071	1148	1189	1308	1477	1495	1533	1652	3077	3139	3157	3847
	[f]	2.04	i1522	106	198	279	353	857	1079	1113	1160	1350	1618	1684	1695	1818	3102	3117	3193	3886

[a] This work, PESH-PIP; [b] This work, PESH; [c] This work, UCCSD(T)-F12a/AVTZ; [d] This work, UCCSD(T)-F12a/AVDZ; [e] This work, M05-2X/6-311+G(3df,2p); [f] This work, PESL; [g] See http://cccbdb.nist.gov/ and ATcT.

Table S2. Comparison of energies (kcal/mol) and vibrational harmonic frequencies (cm^{-1}) of the stationary points for the title reaction at selected several DFT methods.

Species	Method	Energy	Frequencies																	
			1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
$OH + CH_3OH$	*a*	0.00	3697	291	1039	1076	1171	1366	1477	1498	1509	2994	3039	3108	3829					
	b	0.00	3864	295	1100	1125	1221	1414	1536	1554	1564	3087	3135	3198	4004					
	c	0.00	3796	298	1074	1107	1196	1379	1502	1527	1536	2998	3051	3114	3938					
	d	0.00	3779	310	1071	1100	1180	1368	1476	1501	1509	3080	3138	3199	3912					
	e	0.00	3773	291	1070	1098	1193	1368	1502	1533	1540	3080	3129	3188	3898					
	f	0.00	3759	275	1060	1109	1175	1346	1467	1483	1495	3009	3068	3136	3922					
	g	0.00	3770	304	1070	1110	1181	1370	1486	1511	1519	3039	3092	3150	3901					
	h	0.00	3754	277	1053	1111	1167	1350	1462	1471	1486	2977	3033	3099	3903					
	i	0.00	3799	290	1073	1105	1206	1365	1523	1554	1567	3104	3146	3190	3918					
	j	0.00	3832	286	1079	1124	1194	1390	1498	1520	1531	3057	3116	3180	3962					
	k	0.00	3722	291	1043	1077	1174	1366	1481	1500	1511	2991	3037	3107	3855					
	l	0.00	3806	294	1074	1101	1198	1371	1506	1534	1541	3072	3123	3182	3929					
H_2O+CH_2OH	*a*	-21.97	1627	3797	3900	414	529	1053	1199	1356	1482	3133	3272	3822						
	b	-17.38	1675	3962	4065	416	575	1091	1257	1402	1540	3220	3361	3999						
	c	-21.59	1634	3900	4005	443	587	1072	1255	1369	1507	3122	3265	3927						
	d	-22.58	1612	3872	3977	413	562	1061	1236	1358	1487	3204	3352	3906						
	e	-22.14	1611	3864	3962	402	560	1064	1232	1357	1506	3209	3347	3893						
	f	-22.44	1607	3874	3998	370	477	1047	1241	1337	1468	3153	3297	3899						
	g	-21.72	1620	3868	3971	408	581	1063	1236	1359	1494	3162	3300	3896						
	h	-21.94	1613	3861	3982	392	510	1041	1238	1340	1458	3103	3243	3887						
	i	-21.83	1598	3887	3972	404	644	1063	1240	1354	1525	3222	3354	3922						
	j	-18.33	1653	3919	4029	414	565	1071	1253	1381	1509	3191	3334	3954						

	k	-22.15	1627	3823	3926	415	531	1054	1204	1356	1484	3129	3271	3850						
	l	-22.20	1614	3895	3996	406	553	1066	1238	1359	1509	3205	3346	3922						
$H_2O + CH_3O$	*a*	-14.85	1627	3797	3900	667	956	1103	1353	1363	1510	2887	2964	3007						
	b	-12.49	1675	3962	4065	749	1011	1155	1446	1447	1565	3032	3100	3140						
	c	-14.51	1634	3900	4005	789	977	1151	1390	1392	1535	2912	2986	3032						
	d	-13.56	1612	3872	3977	875	972	1138	1379	1385	1509	3006	3082	3127						
	e	-13.32	1611	3864	3962	869	980	1135	1409	1415	1539	3005	3077	3119						
	f	-14.98	1607	3874	3998	834	963	1142	1348	1352	1498	2924	2996	3039						
	g	-13.10	1620	3868	3971	389	969	1135	1385	1387	1519	2965	3039	3080						
	h	-14.52	1613	3861	3982	-363	957	1138	1333	1342	1491	2885	2957	2999						
	i	-11.18	1598	3887	3972	996	1024	1138	1451	1465	1569	3045	3115	3151						
	j	-12.51	1653	3919	4029	731	981	1158	1396	1398	1534	2983	3060	3103						
	k	-15.03	1627	3823	3926	663	959	1107	1355	1366	1512	2880	2961	3005						
	l	-13.44	1614	3895	3996	857	982	1138	1411	1416	1540	2998	3070	3112						
RC	*a*	-4.73	80	108	203	225	318	455	1029	1080	1165	1359	1468	1496	1505	3013	3074	3120	3738	3775
	b	-3.31	34	65	115	131	282	390	1124	1145	1222	1444	1536	1554	1565	3081	3126	3189	3852	3943
	c	-5.96	i16	52	232	288	398	623	1085	1099	1200	1381	1504	1527	1537	3016	3078	3128	3645	3937
	d	-6.68	i34	54	198	284	373	594	1076	1084	1184	1361	1480	1504	1509	3099	3167	3212	3611	3917
	e	-6.78	47	57	200	285	398	610	1074	1086	1197	1364	1506	1534	1540	3097	3156	3197	3605	3899
	f	-3.78	41	102	134	205	294	497	1098	1121	1173	1380	1466	1484	1496	3002	3058	3128	3744	3810
	g	-6.71	46	80	207	285	446	624	1077	1097	1185	1365	1489	1516	1520	3054	3118	3158	3603	3904
	h	-5.34	106	139	201	215	333	451	1059	1097	1165	1349	1456	1469	1480	2992	3059	3109	3782	3851
	i	-6.84	83	124	204	318	489	673	1073	1081	1210	1365	1525	1570	1574	3114	3168	3203	3544	3909
	j	-3.17	39	64	112	132	289	398	1114	1137	1196	1424	1499	1520	1532	3047	3103	3167	3818	3872

	k	-5.04	84	112	209	232	332	458	1033	1080	1169	1360	1472	1498	1508	3010	3073	3119	3768	3814
	l	-6.81	i6	48	204	263	408	605	1078	1088	1203	1366	1510	1535	1542	3088	3148	3191	3653	3930
PC1	*a*	-27.90	55	64	90	174	354	435	865	985	1102	1351	1364	1506	1644	2885	2979	3033	3674	3872
	b	-23.62	61	70	96	178	346	430	973	1041	1151	1443	1452	1564	1690	3031	3109	3156	3874	4040
	c	-27.37	i36	83	97	226	388	423	864	1021	1150	1382	1397	1523	1656	2907	2996	3055	3811	3977
	d	-29.09	83	128	145	155	194	292	516	725	1094	1256	1414	1488	1607	3199	3345	3751	3874	3979
	e	-28.75	55	91	109	185	350	404	828	1044	1159	1395	1431	1529	1623	3004	3080	3143	3770	3938
	f	-29.02	36	55	106	188	360	455	878	1032	1143	1336	1364	1494	1621	2923	3004	3067	3764	3969
	g	-28.45	i190	45	75	119	191	338	625	1044	1191	1357	1428	1496	1622	2971	3016	3107	3787	3947
	h	-28.33	40	120	131	198	232	357	645	1051	1189	1311	1373	1467	1619	2893	2932	3030	3742	3952
	i	-28.54	13	104	143	185	363	443	878	1056	1190	1427	1497	1537	1610	3046	3105	3175	3785	3947
	j	-24.39	67	77	92	180	358	445	924	1016	1151	1390	1404	1530	1669	2981	3071	3125	3801	3999
	k	-28.28	53	67	87	178	357	447	867	992	1108	1353	1367	1509	1649	2879	2974	3029	3705	3898
	l	-28.76	24	83	135	158	201	290	520	739	1106	1257	1415	1509	1613	3194	3333	3764	3887	3987
PC2	*a*	-19.07	64	89	158	183	246	291	479	767	1100	1219	1421	1483	1628	3125	3260	3613	3792	3891
	b	-16.83	72	85	151	178	223	281	540	767	1137	1277	1464	1542	1677	3211	3347	3819	3957	4057
	c	-18.72	65	77	147	203	249	290	551	764	1121	1274	1431	1508	1634	3114	3251	3757	3891	3993
	d	-19.10	i61	92	111	189	314	336	689	1053	1195	1351	1436	1483	1622	3025	3066	3161	3787	3959
	e	-18.55	55	85	143	174	215	279	518	735	1111	1249	1421	1507	1611	3202	3338	3714	3857	3954
	f	-19.88	57	76	147	201	245	276	414	747	1095	1262	1401	1470	1605	3143	3282	3701	3864	3983
	g	-18.40	101	141	207	219	245	351	662	676	1103	1252	1418	1495	1613	3142	3278	3766	3834	3947
	h	-19.46	65	120	199	224	259	322	537	696	1090	1259	1419	1464	1610	3086	3222	3698	3849	3967
	i	-16.29	52	151	192	208	268	339	666	715	1121	1255	1436	1535	1595	3208	3342	3734	3869	3956
	j	-16.54	65	87	160	189	252	292	524	786	1121	1273	1451	1510	1654	3182	3321	3724	3912	4018

	k	-19.50	63	89	159	184	254	294	483	784	1103	1223	1422	1485	1629	3121	3258	3643	3815	3915
	l	-18.86	i14	43	111	195	285	337	687	1056	1211	1385	1464	1515	1624	3013	3044	3141	3803	3967
TS1	*a*	-3.43	i821	110	175	243	411	748	1037	1126	1159	1363	1444	1457	1499	1794	2999	3053	3082	3760
	b	7.52	i2444	134	192	223	444	800	1089	1168	1214	1317	1423	1503	1513	1561	3093	3155	3173	3930
	c	1.92	i1561	114	182	224	420	782	1080	1143	1186	1320	1466	1480	1522	1568	3001	3064	3087	3855
	d	-6.68	i890	77	160	226	438	715	956	1076	1148	1340	1393	1425	1481	1716	3117	3220	3789	3895
	e	2.17	i1583	115	182	228	415	781	1066	1141	1184	1293	1473	1494	1530	1630	3084	3145	3163	3818
	f	0.43	i1638	126	187	238	426	761	1077	1130	1161	1331	1427	1438	1482	1564	3008	3077	3101	3824
	g	1.91	i1288	118	185	228	408	781	1081	1134	1173	1303	1456	1472	1511	1714	3042	3108	3124	3815
	h	-0.66	i1515	120	186	232	411	756	1076	1128	1155	1335	1422	1426	1476	1693	2977	3045	3068	3821
	i	5.56	i1691	136	194	247	406	793	1075	1127	1191	1262	1490	1515	1529	1559	3106	3159	3172	3820
	j	7.32	i1581	123	186	237	421	797	1093	1154	1185	1334	1467	1482	1522	1628	3060	3135	3150	3879
	k	-3.53	i788	109	174	246	407	752	1042	1130	1162	1373	1448	1459	1501	1847	2997	3051	3080	3785
	l	-6.81	i1016	93	170	241	433	739	947	1080	1156	1354	1409	1442	1508	1649	3104	3203	3812	3909
TS2	*a*	-2.27	i171	109	141	224	395	517	1037	1071	1151	1362	1449	1476	1490	2730	3030	3119	3687	3820
	b	4.25	i1219	106	143	278	440	750	893	1108	1190	1209	1384	1426	1508	1546	3122	3229	3905	3987
	c	-0.41	i301	67	134	212	404	707	1082	1121	1176	1373	1418	1478	1505	2001	3027	3129	3813	3921
	d	0.35	i1511	121	186	246	419	764	1069	1136	1168	1312	1446	1464	1499	1675	3088	3160	3176	3826
	e	0.77	i945	87	164	229	423	734	956	1076	1151	1352	1408	1446	1506	1660	3111	3207	3783	3880
	f	-1.97	i581	111	141	264	442	770	1069	1116	1156	1260	1339	1375	1460	1527	3042	3158	3813	3884
	g	0.57	i755	95	163	224	421	730	999	1076	1156	1352	1402	1448	1489	1769	3068	3164	3774	3884
	h	-2.48	i355	53	117	243	424	754	1052	1121	1162	1320	1360	1416	1454	1646	3006	3116	3798	3874
	i	3.84	i1885	128	196	242	452	718	815	1071	1146	1353	1402	1439	1539	1613	3140	3219	3778	3904
	j	3.06	i354	72	139	213	397	718	1082	1128	1176	1379	1415	1482	1500	1974	3087	3191	3843	3942

[k]	-2.48	i168	109	141	225	398	530	1044	1072	1154	1362	1448	1480	1492	2714	3027	3117	3715	3845
[l]	0.88	i1533	108	183	233	422	789	1071	1148	1189	1308	1477	1495	1533	1652	3077	3139	3157	3847

[a] B3LYP/AVTZ; [b] BH-HLYP/AVTZ; [c] BMK/AVTZ; [d] M05-2X/AVDZ; [e] M05-2X/AVTZ; [f] M05/AVTZ; [g] M06-2X/AVTZ; [h] M06/AVTZ; [i] M06-HF/AVTZ; [j] PBE0/AVTZ; [k] B3LYP/6-311+G(3df,2p); [l] M05-2X/6-311+G(3df,2p).

Table S3 Most experimental overall rate constants of the title reaction at around 298 K.

Authors	Year	Methods	T(K)	k (10^{-12} $cm^3molecule^{-1}s^{-1}$)
Campbell	1976	RR	292	0.94
Overend	1978	FP/RA	296	1.06
Ravishankara	1978	FP/RF	298	1
Hagele	1983	LP/RF	295	0.78±0.15
Tuazon	1983	RR	300±3	0.9±0.07
Greenhill	1986	FP/RA	298	0.86
Wallington	1987	FP/RF	296	0.861±0.047
Pagsberg	1988	PR/TAS		0.88
Hess and Lin	1989	LP/LIF	298	0.943
McCaulley	1989	DF/LIF	298	1.01±0.1
Nelson	1990	PR-RA	298±2	0.9±0.09
Nelson	1990	RR	298±2	0.93±0.22
Picquet	1998	RR	298±4	0.86±0.08
Oh	2001	RR	298±2	0.96±0.1
Oh	2001	RR	298±2	0.84±0.07
Sorensen	2002	RR	296±2	0.79±0.05
Sorensen	2002	RR	296±2	0.82±0.05
Jimenez	2003	LP/LIF	298	0.93±0.11
Dillon	2005	PLP/PLIF	298	0.93±0.07
Atkinson	2006	Fitting	298	0.9
Srinivasan	2007	RST/MASD	298	1.0
Gomez Martin	2014	LP/LIF	295	1.13
Liu	2019	S/UV LA	300	0.877

RR: Relative rate method.
FP/RA: Flash photolysis/resonance absorption.
FP/RF: Flash photolysis/resonance fluorescence.
LP/RF: Laser photolysis/resonance fluorescence.
PR/TAS: Pulse radiolysis combined with transient absorption spectrophotometry
LP/LIF: Laser photolysis/laser-induced fluorescence
DF/LIF: Discharge flow/laser-induced fluorescence.
PR-RA: The absolute technique of pulse radiolysis combined with kinetic UV spectroscopy && a conventional photolytic relative rate method
PLP/PLIF: Pulsed laser photolysis technique coupled with pulsed laser induced fluorescence
RST/MASD: The reflected shock tube technique with multipass absorption spectrometric detection of OH radicals at 308 nm
S/UV LA: shock tube/UV laser absorption