Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information for:

On the possible catalysis by single water molecules of gas-phase hydrogen abstraction reactions by OH radicals

Ditte Linde Thomsen[a], Theo Kurtén[b], Solvejg Jørgensen[a], Timothy J. Wallington[c], Signe Bang Baggesen[a], Cecilie Aalling[a],

and Henrik G. Kjaergaard[a]*

[a] Department of Chemistry, University of Copenhagen, Universitetsparken 5, DK-2100 Copenhagen Ø, Denmark.

[b] Laboratory of Physical Chemistry, Department of Chemistry, P.O. BOX 55, FI-00014 University of Helsinki, Finland

[c] Systems Analytics and Environmental Sciences Department, Ford Motor Company, Mail Drop RIC-2122, Dearborn, Michigan 48121-2053, USA

*Corresponding author:

Email: hgk @ chem.ku.dk

FAX: 45-35320322

Phone: 45-35320334

	ΔE_{TS}		
	B3LYP	CCSD(T)-F12	CBS-QB3
CH_4	2.3	6.7	4.1
CF_3H	0.0	4.9	3.2
CH_3OH	-2.3	-1.4	0.9
CH_3NH_2	-2.8	-0.4	1.1

Tabel S1: Electronic energy without ZPVE of the transistion state in the absence of water calculated in kcal/mol with respect to isolated reactants. Calculated with B3LYP/aug-cc-pVTZ and CCSD(T)-F12/VDZ-F12a on B3LYP/AVTZ optimized geometries, and with the composite CBS-QB3 method.

	$\Delta\Delta G_{TS}$		
	298 K	200 K	100 K
CH_4	-	-	-
CFH_3	-0.4	-0.9	-2.0
$(CH_3)_2CFH$	0.8	-0.1	-0.9
CF_3H	-	-	-
CH_3OH	1.4	0.4	-0.5
$(CH_3)_2CHOH$	-0.9	-1.5	-2.1
F_2CHOH	2.1	1.3	0.5
CH_3NH_2	0.8	0.0	-0.8
$(CH_3)_2CHNH2$	-0.6	-1.3	-1.9
F_2CHNH_2	-0.9	-1.9	-2.9
CH_3CHO	-2.0	-2.7	-3.2

Table S2: Temperature dependence of the change in Gibbs free energy ($\Delta\Delta G_{TS}$, in kcal/mol) of the transition state between hydrated and non-hydrated reactions ($\Delta\Delta G_{TS}= \Delta G_{TS,H2O} -\Delta G_{TS}$). Calculated with respect to the energy of $RH\cdots H_2O$ + OH for the hydrated reaction and relative to the isolated reactants for the non-hydrated reaction. Calculated with the CCSD(T)-F12a/cc-pVDZ-F12 electronic energies at the B3LYP/aug-cc-pVTZ structures and the B3LYP/ aug-cc-pVTZ thermodynamic corrections.

Tables of Energetics of all reactants, water adducts, reaction complexes and transition states

Reactants

	B3LYP					CCSD(T)-F12	
	E_{B3LYP}	$ZPVE_{B3LYP}$	H_{B3LYP}	G_{B3LYP}	S^2	$E_{CCSD(T)-F12}$	T1
CH_4	-40.53842	0.04455	-40.49007	-40.51250	-	-40.45303	0.009
CH_3F	-139.80443	0.03907	-139.76150	-139.78679	-	-139.60834	0.009
$(CH_3)_2CHF$	-218.47458	0.09539	-218.37316	-218.40647	-	-218.12748	0.010
CF_3H	-338.38137	0.02498	-338.35197	-338.38252	-	-337.96880	0.011
CH_3OH	-115.77676	0.05106	-115.72141	-115.74847	-	-115.59412	0.009
$(CH_3)_2CHOH$	-194.44282	0.10735	-194.32899	-194.36296	-	-194.11072	0.010
CF_2HOH	-314.35508	0.03663	-314.31340	-314.34507	-	-313.95491	0.011
CH_3NH_2	-95.90341	0.06372	-95.83529	-95.86263	-	-95.73312	0.009
$(CH_3)_2CH\ NH_2$	-174.56612	0.12018	-174.43940	-174.47344	-	-174.24740	0.009
CF_2HNH_2	-294.48037	0.04933	-294.42592	-294.45760	-	-294.09107	0.011
CH_3CHO	-153.89642	0.055201	-153.836377	-153.86616	-	-153.64020	0.014
OH	-75.768599	0.008418	-75.756877	-75.77711	0.7527	-75.66378	0.008
H_2O	-76.466197	0.021236	-76.441181	-76.46260	-	-76.36316	0.008

Table S3: Total electronic energies, zero point vibrational energies, enthalpies and Gibbs Free energies (hartree) of all reactants. All geometries are optimized using B3LYP/aug-cc-pVTZ and the B3LYP values corresponds to this level of theory. S^2 refers to the expectation value of the total spin before projection.. $E_{CCSD(T)-F12}$ refer to the electronic energy calculated with CCSD(T)-F12a/cc-pVDZ-F12 on the B3LYP/aug-cc-pVTZ geometries

Water adducts, $RH^{\cdots}H_2O$

	B3LYP					CCSD(T)-F12	
	E_{B3LYP}	$ZPVE_{B3LYP}$	H_{B3LYP}	G_{B3LYP}	S^2	$E_{CCSD(T)-F12}$	T1
CH_4	-	-	-	-		-	-
CH_3F	-216.27548	0.06236	-216.20617	-216.24275	-	-215.97783	0.0091
$(CH_3)_2CHF$	-294.94636	0.11883	-294.81757	-294.86263	-	-294.49792	0.010
CF_3H	-	-	-	-	-	-	-
CH_3OH	-192.25080	0.07524	-192.16781	-192.20574	-	-191.96629	0.009
$(CH_3)_2CHOH$	-270.91740	0.13155	-270.77591	-270.81986	-	-270.48392	0.009
CF_2HOH	-390.82975	0.06010	-390.76068	-390.80389	-	-390.32858	0.010
CH_3NH_2	-172.38001	0.08836	-172.28405	-172.32169	-	-172.10778	0.009
$(CH_3)_2CH\ NH_2$	-251.04229	0.14463	-250.88776	-250.93160	-	-250.62219	0.009
CF_2HNH_2	-370.95304	0.07333	-370.87097	-370.91373	-	-370.46221	0.010
OH	-152.24355	0.03290	-152.20465	-152.23638	0.7526	-152.03605	0.008148

Table S4: Total electronic energies, zero point vibrational energies, enthalpies and Gibbs Free energies (hartree) of all water adducts. All geometries are optimized using B3LYP/aug-cc-pVTZ and the B3LYP values corresponds to this level of theory. S^2 refers to the expectation value of the total spin before projection.. $E_{CCSD(T)-F12}$ refer to the electronic energy calculated with CCSD(T)-F12a/cc-pVDZ-F12 on the B3LYP/aug-cc-pVTZ geometries

Reactions complexes – without water

	B3LYP					CCSD(T)-F12	
	E_{B3LYP}	$ZPVE_{B3LYP}$	H_{B3LYP}	G_{B3LYP}	S^2	$E_{CCSD(T)-F12}$	T1
CH_4	-	-	-	-	-	-	-
CH_3F	-215.57850	0.049616	-215.52198	-215.55944	0.7526	-215.27835	0.009
$(CH_3)_2CHF$	-294.24963	0.10598	-294.13458	-294.17830	0.7526	-293.79806	0.009
CF_3H	-414.15158	0.03456	-414.10983	-414.14989	0.7526	-413.63483	0.010
CH_3OH	-191.55498	0.06227	-191.48571	-191.52304	0.7527	-191.26810	0.009
$(CH_3)_2CHOH$	-270.22160	0.11851	-270.09385	-270.13737	0.7527	-269.78530	0.009
CF_2HOH	-390.13256	0.04748	-390.07713	-390.11901	0.7526	-389.62842	0.010
CH_3NH_2	-171.68502	0.07570	-171.60273	-171.63818	0.7527	-171.41017	0.009
$(CH_3)_2CH\ NH_2$	-250.34728	0.13187	-250.20647	-250.24849	0.7527	-249.92431	0.009
CF_2HNH_2	-370.25650	0.06030	-370.18817	-370.22830	0.7543	-369.76009	0.016

Table S5: Total electronic energies, zero point vibrational energies, enthalpies and Gibbs Free energies (hartree) of all reaction complexes without water. All geometries are optimized using B3LYP/aug-cc-pVTZ and the B3LYP values corresponds to this level of theory. S^2 refers to the expectation value of the total spin before projection.. $E_{CCSD(T)-F12}$ refer to the electronic energy calculated with CCSD(T)-F12a/cc-pVDZ-F12 on the B3LYP/aug-cc-pVTZ geometries

Reactions complexes – with water

		B3LYP					CCSD(T)-F12	
X	**Y**	E_{B3LYP}	$ZPVE_{B3LYP}$	H_{B3LYP}	G_{B3LYP}	S^2	$E_{CCSD(T)-F12}$	T1
CH_4		-	-	-	-	-	-	-
CH_3F		-292.05598	0.07460	-291.97167	-292.01606	0.7527	-291.65240	0.009
$(CH_3)_2CHF$		-370.72703	0.13076	-370.58420	-370.63514	0.7527	-370.17278	0.009
CF_3H		-490.62910	0.05942	-490.55863	-490.60882	0.7527	-490.01051	0.010
CH_3OH		-268.03171	0.08710	-267.93473	-267.97993	0.7527	-267.64318	0.009
$(CH_3)_2CHOH$		-	-	-	-	-	-	-
CF_2HOH		-	-	-	-	-	-	-
CH_3NH_2		-248.16210	0.10029	-248.05219	-248.09669	0.7527	-247.78569	0.009
$(CH_3)_2CH\ NH_2$		-326.82428	0.15653	-326.65576	-326.70642	0.7527	-326.29985	0.009
CF_2HNH_2		-	-	-	-	-	-	-

Table S6: Total electronic energies, zero point vibrational energies, enthalpies and Gibbs Free energies (hartree) of all reaction complexes with water. All geometries are optimized using B3LYP/aug-cc-pVTZ and the B3LYP values corresponds to this level of theory. S^2 refers to the expectation value of the total spin before projection.. $E_{CCSD(T)-F12}$ refer to the electronic energy calculated with CCSD(T)-F12a/cc-pVDZ-F12 on the B3LYP/aug-cc-pVTZ geometries

Transition state – without water

	B3LYP/AVTZ					CCSD(T)-F12	
	E_{B3LYP}	$ZPVE_{B3LYP}$	H_{B3LYP}	G_{B3LYP}	S^2	$E_{CCSD(T)-F12}$	T1
CH_4	-116.30344	0.05074	-116.24714	-116.27925	0.7571	-116.10620	0.034
CH_3F	-215.57301	0.04590	-215.52127	-215.55525	0.7567	-215.26425	0.029
$(CH_3)_2CHF$	-294.24683	0.10493	-294.13358	-294.17396	0.7541	-293.79337	0.013
CF_3H	-414.14536	0.02999	-414.10843	-414.14660	0.7568	-413.61902	0.026
CH_3OH	-191.54897	0.06110	-191.48158	-191.51607	0.7540	-191.26006	0.014
$(CH_3)_2CHOH$	-270.21702	0.11767	-270.09092	-270.13107	0.7540	-269.77966	0.013
CF_2HOH	-390.12532	0.04404	-390.07408	-390.11263	0.7562	-389.61244	0.023
CH_3NH_2	-171.67643	0.07336	-171.59672	-171.63117	0.7551	-171.39750	0.018
$(CH_3)_2CH\ NH_2$	-250.34057	0.13017	-250.20190	-250.24205	0.7549	-249.91467	0.015
CF_2HNH_2	-370.24851	0.05569	-370.18538	-370.22411	0.7564	-369.74651	0.024
CH_3CHO	-229.67053	0.06567	-229.59805	-229.63462	0.7536	-229.30915	0.015

Table S7: Total electronic energies, zero point vibrational energies, enthalpies and Gibbs Free energies (hartree) of all transition states without water. All geometries are optimized using B3LYP/aug-cc-pVTZ and the B3LYP values corresponds to this level of theory. S^2 refers to the expectation value of the total spin before projection.. $E_{CCSD(T)-F12}$ refer to the electronic energy calculated with CCSD(T)-F12a/cc-pVDZ-F12 on the B3LYP/aug-cc-pVTZ geometries

Transition state – with water

	B3LYP/AVTZ					CCSD(T)-F12	
	E_{B3LYP}	$ZPVE_{B3LYP}$	H_{B3LYP}	G_{B3LYP}	S^2	$E_{CCSD(T)-F12}$	T1
CH_4	-192.77624	0.07445	-192.69255	-192.73692	0.7572	-192.47741	0.028
CH_3F	-292.04790	0.06971	-291.96945	-292.01090	0.7572	-291.63853	0.026
$(CH_3)_2CHF$	-370.72389	0.12714	-370.58555	-370.63311	0.7566	-370.16479	0.021
CF_3H	-490.62039	0.05366	-490.55609	-490.60547	0.7570	-489.99252	0.024
CH_3OH	-268.02794	0.08418	-267.93512	-267.97557	0.7565	-267.63270	0.025
$(CH_3)_2CHOH$	-346.69761	0.14256	-346.54392	-346.59085	0.7546	-346.15740	0.014
CF_2HOH	-466.59878	0.06642	-466.52200	-466.56816	0.7571	-465.98490	0.024
CH_3NH_2	-248.15662	0.09685	-248.05116	-248.09166	0.7566	-247.77302	0.025
$(CH_3)_2CH\ NH_2$	-326.82225	0.15458	-326.65661	-326.70314	0.7558	-326.29306	0.018
CF_2HNH_2	-446.72544	0.08025	-446.63520	-446.67984	0.7569	-446.12365	0.023
CH_3CHO	-306.15216	0.09094	-306.05169	-306.09538	0.7529	-305.68904	0.014

Table S8: Total electronic energies, zero point vibrational energies, enthalpies and Gibbs Free energies (hartree) of all transition states with water. All geometries are optimized using B3LYP/aug-cc-pVTZ and the B3LYP values corresponds to this level of theory. S^2 refers to the expectation value of the total spin before projection.. $E_{CCSD(T)-F12}$ refer to the electronic energy calculated with CCSD(T)-F12a/cc-pVDZ-F12 on the B3LYP/aug-cc-pVTZ geometries

Optimized geometries

All geometries are optimized on the B3LYP/aug-cc-pVTZ level of theory.

Reactants

CH_4

C,-0.13626834,-0.031446584,0.
H,0.2263798818,-1.0572102172,-0.0000008781
H,0.2263992503,0.4814281313,0.8883335575
H,0.2263978164,0.4814291453,-0.8883335575
H,-1.2242503085,-0.0314333954,0.0000008781

CH_3F

C,0.0,0.0,-0.6374804735
H,0.0000001243,1.0321167902,-0.986484557
H,-0.8938394222,-0.5160582875,-0.986484557
H,0.8938392979,-0.5160585027,-0.986484557
F,0.0,0.0,0.7543741445

$(CH_3)_2CHF$

C,0.,0.0348290701,0.3662511024
H,0.,0.1368866752,1.4544102242
F,0.,1.356710722,-0.1347691437
C,1.2726438926,-0.641919088,-0.0977431807
H,2.146044765,-0.0776739254,0.2270404423
H,1.3388534654,-1.6479818631,0.3189769317
H,1.2905493243,-0.7167418571,-1.1856747846
C,-1.2726438926,-0.641919088,-0.0977431807
H,-1.3388534654,-1.6479818631,0.3189769317
H,-2.146044765,-0.0776739254,0.2270404423
H,-1.2905493243,-0.7167418571,-1.1856747846

CF_3H

C,-0.3987037579,0.5217522264,-0.0220245556
H,-0.0357486953,1.0350094953,-0.9110291574
F,0.0373267054,1.1382650956,1.0863870404
F,0.0373031056,-0.7464296926,-0.0017444955
F,-1.7397361677,0.5100838153,-0.0017945019

CH_3OH

C,0.6668654019,-0.0202997308,-0.0000002012
H,1.0817192433,0.9855384458,-0.0000077328
H,1.0268582312,-0.5438879134,-0.8906375489
H,1.0268589693,-0.5438751419,0.8906443638

O,-0.7497580594,0.1202824659,-0.0000005066
H,-1.1496367864,-0.7537911256,0.000000459

$(CH_3)_2)CHOH$

C,0.0206460321,0.0579655019,0.3855996568
H,-0.8608684136,-0.4512081462,-0.0091742762
C,-0.1061797961,0.1619381313,1.9012497274
H,-1.0029637933,0.7184668105,2.1715023328
H,-0.1615433041,-0.827231517,2.3588981291
H,0.7590772567,0.6774704516,2.3270319202
C,1.2674784292,-0.7035787471,-0.0497384616
H,1.2603831485,-1.7229384093,0.3398873148
H,1.3261762378,-0.7494312368,-1.1366772487
H,2.1704028912,-0.2116161611,0.3223599328
O,-0.0337678772,1.3530063611,-0.2271977869
H,0.7220343889,1.868289971,0.0743140494

CF_2HOH

C,-0.0076432595,-0.0088324115,0.3333473625
H,-0.050191407,0.0366114945,1.4238688406
F,-0.258038473,1.2538017935,-0.1375955403
F,-0.9875081502,-0.8142247587,-0.1154588456
O,1.1658812959,-0.4897559501,-0.1693660463
H,1.8955209939,0.0673948323,0.1241382291

CH_3NH_2

C,0.7082279694,0.0001004587,0.0164626701
H,1.1146324158,0.8783834553,-0.4852397155
H,1.1150865163,-0.8767261272,-0.4874333878
H,1.0787602719,-0.0010851667,1.0490639455
N,-0.7499309198,-0.0000332287,-0.1184379199
H,-1.1548968444,-0.8131272709,0.3280235889
H,-1.1551374092,0.8124148794,0.3289858188

$(CH_3)_2)CHNH_2$

C,0.0000450607,0.024246739,0.3612319641
H,0.000016656,0.0381997592,1.4614285079
N,0.0008083436,1.3834596203,-0.1992900436
H,-0.8138919501,1.9027153242,0.1054613977
H,0.8163024125,1.9016574799,0.1051398266
C,1.262362253,-0.7002288968,-0.0957111836
H,2.1599702972,-0.1734119391,0.2351295172
H,1.3003216416,-1.7105180914,0.3136051085
H,1.2905523623,-0.7629407516,-1.1846326898
C,-1.2630448623,-0.6988408075,-0.0957883952
H,-1.3022266554,-1.7090323318,0.3136566873

H,-2.1600822393,-0.170937252,0.234866061
H,-1.2911713198,-0.7616468524,-1.1847047582

CF2HNH2

C,-0.0081795659,-0.0070181508,0.3522304461
H,-0.0880880064,0.0529269597,1.4365772987
N,1.3164770308,-0.1717133918,-0.0698482405
H,1.3971440556,-0.1685870949,-1.0791115309
H,1.9368235826,0.5128638561,0.3382941983
F,-0.6207291326,1.1332770268,-0.1590768226
F,-0.7641609642,-1.0461442051,-0.1014443491

H_2O

O,0.0,0.0,0.1164830922
H,0.0,0.7633767419,-0.4687600461
H,0.0,-0.7633767419,-0.4687600461

OH

O,0.0,0.0,0.1053101775
H,0.0,0.0,-0.8699981775

Water adducts, RH···H_2O

CH_4

No stationary structure localized

CH_3F

C,1.35812348,-0.4357927152,0.6563029381
H,0.6028760095,-1.2125835123,0.7547560046
H,2.0437674164,-0.6649217247,-0.1570469175
H,1.9004523795,-0.3028395555,1.5903153966
O,-1.9942334925,-0.2439078476,0.1021943309
H,-1.2500034055,0.3708521948,0.1164792436
F,0.7101485192,0.7717401748,0.3532754642
H,-2.7795806767,0.3037045158,0.0205246494

$(CH_3)_2CHF$

C,0.714434,0.001603,-0.301076
H,0.341248,-0.105282,-1.321057
O,-2.836287,-0.000178,-0.22553
H,-2.049028,-0.428845,0.135831
F,-0.153553,-0.811314,0.492183
C,2.108507,-0.570627,-0.178269
H,2.12366,-1.616164,-0.483519

H,2.795831,-0.016386,-0.818902
H,2.463198,-0.50038,0.850501
C,0.569685,1.430659,0.170755
H,1.176969,2.089046,-0.4521
H,-0.467695,1.75475,0.101773
H,0.903968,1.52905,1.204275
H,-3.571628,-0.57235,0.009333

CF_3H

No stationary structure localized

CH_3OH

C,1.5693889303,-0.4540348752,0.0103864987
H,1.3191433971,-1.1424123735,-0.7928559472
H,0.8018636056,1.2428883592,0.6496126489
O,-2.1423227698,-0.2011465792,0.071907517
H,-1.2276256163,0.105844534,-0.0391650724
O,0.6193860718,0.6134020568,-0.0537033699
H,-2.6122380138,0.1075944771,-0.7070795719
H,1.5111821716,-0.9880855865,0.9612146556
H,2.5872022235,-0.0886120127,-0.1420163587

$(CH_3)_2)CHOH$

C,-0.73393,-0.008371,-0.309601
H,-0.425434,-0.073307,-1.354074
H,0.03953,-0.815869,1.321511
O,2.921597,0.041826,-0.131746
H,2.045154,-0.3445,0.034643
O,0.237788,-0.824961,0.378548
C,-0.646887,1.441015,0.148401
H,0.367687,1.819937,0.032886
H,-1.320066,2.070621,-0.435371
H,-0.933882,1.532824,1.199557
C,-2.128404,-0.600448,-0.160293
H,-2.852551,-0.038481,-0.7519
H,-2.142786,-1.638189,-0.491675
H,-2.453949,-0.566995,0.8829
H,3.456555,-0.67414,-0.483932

CF_2HOH

C,-0.534815594,0.0016688365,-0.1675488719
H,0.2199993766,0.0114462108,-0.9481900536
H,-0.5948631033,-0.0474324872,1.7449635836
O,2.6389683564,0.0030942259,-0.3724403787
H,2.2674669727,-0.0169799933,0.516891108
O,0.0761805357,-0.0384306441,1.0489853113

H,3.5935008447,0.0140237488,-0.2609020781
F,-1.3330860611,1.1040965765,-0.2744273113
F,-1.3637853278,-1.0708234741,-0.3306433094

CH_3NH_2

N,-0.6883440098,0.7048003927,-0.0010188254
C,-1.4509031073,-0.5521045552,0.0033593301
H,-1.1646172488,-1.1445606125,-0.8643053891
H,-0.9076238584,1.2543433304,-0.8229529327
H,-0.927640842,1.2722105188,0.8029733001
O,2.0499209375,-0.2591503544,0.0100448057
H,1.1704105898,0.1723274944,0.0120159131
H,2.6905896188,0.455407551,0.0492947
H,-1.1867489398,-1.1251076967,0.8908895225
H,-2.53705314,-0.4174830686,-0.0118274242

$(CH_3)_2)CHNH_2$

N,-0.2016485734,-0.9161226244,0.4306888639
C,0.7081242975,-0.0020785038,-0.291861957
H,0.3877243789,-0.0263190542,-1.3366796529
H,-0.0599434557,-1.8724727407,0.1244879265
H,0.0023584965,-0.8967189921,1.4251150354
O,-2.8424591498,0.0566742625,-0.2723324693
H,-2.0069255591,-0.3553813503,0.0326016056
C,0.5077138359,1.4151975205,0.2347448511
H,1.1209062901,2.1235507889,-0.3225545997
H,-0.535121582,1.7171946456,0.150327214
H,0.8003938745,1.4808223036,1.286616896
C,2.1749646372,-0.4340554757,-0.2261505489
H,2.3052455403,-1.447104571,-0.6117761084
H,2.8074730948,0.231251486,-0.8167947758
H,2.5389492668,-0.415486875,0.8042517956
H,-3.5495253925,-0.4664118199,0.1135239238

CF_2HNH_2

N,-0.1723637907,-0.7527090375,0.4305511525
C,0.7644730601,0.0101578353,-0.2964111318
H,0.52242482,0.0487038403,-1.3571438559
H,-0.2924157844,-1.6742215926,0.0294509126
H,0.0983116834,-0.8364453018,1.4041891841
O,-3.0221342313,-0.0217219108,-0.1925263042
H,-2.1107330278,-0.0942604576,0.1323536452
H,-3.3259232749,0.8492663092,0.0769001648
F,0.7970747115,1.2739511017,0.2081552231
F,2.0576778341,-0.4674387863,-0.1848489903

OH

O,-0.3640798177,1.5141316321,0.2000097466
H,-0.067480124,0.5885635849,0.049333927
O,0.4350278602,-1.227695417,-0.1526250723
H,-0.2239763644,-1.865827304,-0.4429856682
H,0.9289317758,-1.6584206458,0.5518918568

Reactions complexes – without water

CH_4

No stationary structure localized

CH_3F

C,1.514417,0.39979,-0.0000002222
H,0.99423,1.355037,-0.033988
H,2.101707,0.313218,0.911804
H,2.144641,0.272811,-0.877751
O,-2.247252,0.188039,-0.000075
H,-1.354058,-0.213207,0.000904
F,0.55611,-0.625657,-0.000041

$(CH_3)_2CHF$

C,0.6427,-0.000009,-0.279923
H,0.134121,-0.001426,-1.245586
O,-3.134917,-0.001163,-0.255421
H,-2.248476,-0.003775,0.162847
F,-0.410414,-0.00762,0.688984
C,1.441606,-1.269486,-0.093857
H,0.801726,-2.145381,-0.192266
H,2.223991,-1.330365,-0.851548
H,1.911592,-1.286538,0.889856
C,1.426977,1.277996,-0.089866
H,2.208824,1.350086,-0.847116
H,0.777133,2.146798,-0.185837
H,1.896464,1.297476,0.894042

CF_3H

C,0.758419865,0.0029003696,0.2961435659
H,0.4222166321,0.00647807,1.3313756727
F,1.3164644372,1.1746309561,-0.0265519186
F,1.6506225856,-0.9709820027,0.0890746242
F,-0.2891893903,-0.2056488447,-0.5319338351
O,-3.3275636783,0.0084702724,0.188408616
H,-2.5347914513,-0.0902358206,-0.3721887251

CH_3OH

C,1.55355,-0.395167,0.016492
H,1.876266,-0.543557,1.049097
H,0.764122,1.396242,0.276534
O,-2.258284,-0.188942,0.013831
H,-1.312044,0.082963,-0.026699
O,0.479761,0.545458,-0.068269
H,2.404505,-0.079954,-0.59057
H,1.174034,-1.336815,-0.37181

$(CH_3)_2)CHOH$

C,-0.663103,-0.001882,-0.289279
H,-0.258613,-0.031936,-1.301906
H,0.20999,-0.326158,1.462455
O,3.172295,-0.026618,-0.234682
H,2.236462,-0.146431,0.051293
O,0.47232,-0.337956,0.535778
C,-1.153012,1.406923,0.014627
H,-0.341489,2.126546,-0.086417
H,-1.954183,1.692792,-0.668286
H,-1.545794,1.469441,1.032938
C,-1.752429,-1.055915,-0.151179
H,-2.575104,-0.853601,-0.838369
H,-1.35703,-2.047305,-0.368701
H,-2.159894,-1.06151,0.863208

CF_2HOH

C,-0.681428,0.001763,-0.280386
H,-0.299599,0.016554,-1.297975
H,0.022242,-0.150828,1.498691
O,3.216515,0.011707,-0.227704
H,2.298001,-0.04487,0.10676
O,0.35776,-0.135256,0.591335
F,-1.571731,-1.017653,-0.137357
F,-1.375633,1.146204,-0.033111

CH_3NH_2

N,0.538292,0.652061,-0.000088
C,1.450553,-0.501336,-0.000121
H,2.51085,-0.231582,-0.000869
H,1.252555,-1.112512,0.879264
H,1.251513,-1.113326,-0.878708
H,0.697972,1.234957,0.812817
H,0.697878,1.234942,-0.813024
O,-2.203454,-0.208467,0.000271

H,-1.254495,0.098845,-0.000312

(CH3)2)CHNH2

N,-0.339469,-0.834157,0.370937
C,0.671885,0.000156,-0.312645
H,0.414428,-0.027736,-1.374755
H,-0.251781,-1.804052,0.086758
H,-0.185939,-0.815785,1.37479
O,-3.032245,-0.012528,-0.195526
H,-2.102197,-0.308636,0.01336
C,0.537228,1.439292,0.173446
H,1.231713,2.091998,-0.35535
H,-0.474447,1.81051,0.014911
H,0.7647,1.509515,1.240746
C,2.098597,-0.527837,-0.147585
H,2.182039,-1.556264,-0.50398
H,2.809742,0.078908,-0.710891
H,2.399724,-0.508802,0.902764

CF_2HNH_2

N,-0.386427,-0.64369,0.592511
C,0.523285,0.007553,-0.258606
H,0.1511,0.059954,-1.278442
H,-0.727176,-1.520627,0.229877
H,-0.06073,-0.72114,1.547863
O,-2.489802,0.00161,-0.340574
H,-2.535591,0.72229,0.308399
F,0.754429,1.26414,0.213257
F,1.762916,-0.60779,-0.288706

Reactions complexes – with water

CH_4

No stationary structure localized

CH_3F

C,1.710358,-0.751132,0.064966
H,2.220258,-0.888498,1.015939
H,0.751802,-1.265446,0.056916
H,2.338692,-1.078912,-0.760183
O,-1.861605,-1.41831,-0.050552
H,-1.799197,-0.434539,0.02153
O,-1.277795,1.317147,0.126124
H,-1.601786,2.015584,-0.449311

H,-0.315118,1.297838,0.020438
F,1.473155,0.630008,-0.099967

$(CH_3)_2CHF$

C,-1.0331521125,0.1680637436,0.0371515829
H,-0.2007144213,0.8691744014,0.1046550062
O,2.3504694082,1.7168475742,0.0967812709
H,2.4886662566,0.7383728364,0.0626142409
O,2.3673261161,-1.0790545239,-0.0282436372
H,2.8535390555,-1.6202802244,-0.6561771166
H,1.4261920938,-1.2641537503,-0.174522909
F,-0.4266196394,-1.0898163862,-0.3131500025
C,-1.6977826846,-0.011421336,1.3819821858
H,-0.9743740431,-0.3345566407,2.1293680167
H,-2.1253166051,0.9367510471,1.7106449576
H,-2.4980489775,-0.7498433723,1.3228398829
C,-1.9670182068,0.5445787282,-1.0889265768
H,-2.4055861736,1.5236100888,-0.8915698669
H,-1.4288095698,0.5981868712,-2.0343274407
H,-2.7739044966,-0.1830360572,-1.1831235941

CF_3H

C,1.072619,0.11275,0.016663
H,0.456531,1.009123,0.078398
O,-1.617642,1.755686,0.050252
H,-2.237197,0.987903,0.032641
O,-2.796979,-0.795636,-0.089
H,-3.241879,-1.223319,0.649298
H,-1.979328,-1.288735,-0.223619
F,0.301658,-0.962675,-0.283012
F,2.00374,0.226157,-0.936254
F,1.681617,-0.134802,1.182965

CH_3OH

C,-1.6567157578,-0.8770096635,0.2231996928
H,-0.9098699539,-1.4996781911,-0.2714432153
H,-1.7954885955,0.5515632257,-1.1289557682
O,2.173533479,-1.1787424542,-0.142278919
H,1.8908520569,-0.2344759167,-0.0591293398
O,1.065253825,1.3786299751,0.0582428152
H,1.2059687247,2.0206981349,0.7588959107
H,0.10663299,1.1883667353,0.033426992
O,-1.5594182895,0.4927922791,-0.1985190767
H,-1.4692572574,-0.8858919818,1.2938290053
H,-2.6569322214,-1.2713841428,0.037491903

$(CH_3)_2)CHOH$

No stationary structure localized

CF_2HOH

No stationary structure localized

CH_3NH_2

N,-1.5557686877,0.4676740459,-0.2799590402
C,-1.6088644439,-0.9048276861,0.2541728527
H,-2.5051056264,-1.4578347737,-0.040429424
H,-0.7309711618,-1.4518975188,-0.085197647
H,-1.5727447047,-0.8644840305,1.3419094943
H,-1.6131773318,0.4551052326,-1.2918115776
H,-2.3465747856,1.0105544763,0.0457380525
O,2.1856498205,-1.1700911492,-0.1251309963
H,1.8904150612,-0.2268889527,-0.0470247127
O,1.076945711,1.3665037992,0.0828842355
H,1.2125048414,1.9406864188,0.8409639792
H,0.1079673078,1.1688561381,0.0334257837

$(CH_3)_2)CHNH_2$

N,-0.5565896489,1.1993376702,-0.275443764
C,-1.0704923764,-0.1814020297,-0.113381258
H,-0.3549548371,-0.8297364907,-0.623952486
H,-0.618286793,1.4843081986,-1.2475766473
H,-1.136017429,1.8482990488,0.2485313102
O,2.6124899665,-1.5674264914,-0.3935238125
H,2.5682438376,-0.5905550182,-0.2301765809
O,2.2235092336,1.1389082474,0.0722842548
H,2.5461111258,1.5941052628,0.8541554729
H,1.2405027918,1.2623096176,0.0444792802
C,-1.0656559528,-0.5400005737,1.3685297737
H,-1.3876851505,-1.5705549823,1.5158704531
H,-0.0688408528,-0.4326519829,1.7946657032
H,-1.7501726893,0.1052349521,1.9266266372
C,-2.4498320854,-0.3804408956,-0.7427775173
H,-2.438530641,-0.1261245936,-1.8041340493
H,-2.773661618,-1.4186233341,-0.6537597701
H,-3.1969368811,0.2480153947,-0.2512819999

CF_2HNH_2

No stationary structure localized

Transition states – without water

CH_4

C,0.6293767827,0.6027737294,-0.0163602243
H,-0.5233065309,0.269296974,-0.1927526575
H,0.6841844935,1.017313303,0.9851478809
H,0.8030115768,1.3445416988,-0.7905767244
O,-1.7733372025,-0.1708971822,-0.2907584591
H,-1.774873359,-0.7980487142,0.4500358521
H,1.2342571094,-0.2893563087,-0.1432130277

CH_3F

C,-0.5938712444,0.6185707034,0.0001036771
H,0.5594081999,0.3564104224,0.0004198311
H,-0.7844831181,1.1793432252,-0.9134541952
H,-0.7847768308,1.1798285981,0.9133053654
O,1.8874352922,-0.0774044761,0.0005411772
H,1.7165244772,-1.0342059643,-0.000879357
F,-1.3141337761,-0.5471355087,0.0002935015

$(CH_3)_2CHF$

C,0.332572,-0.000014,-0.068579
H,-0.657496,-0.000233,-0.573716
O,-2.452472,-0.000155,-0.457755
H,-2.396262,-0.000546,0.515372
F,0.035863,-0.000382,1.313369
C,1.068508,1.278032,-0.398494
H,1.251132,1.339242,-1.471671
H,0.483037,2.145859,-0.098902
H,2.02849,1.305644,0.119722
C,1.069319,-1.277467,-0.398991
H,0.484398,-2.145786,-0.099748
H,1.252002,-1.338136,-1.472189
H,2.029308,-1.304673,0.119233

CF_3H

C,0.2791613971,-0.0148752603,0.0000006803
H,-0.9404206935,-0.1653738219,0.0009302856
F,0.5678437276,1.2876565113,-0.0026645824
O,-2.2314528483,-0.1914425913,0.001629324
H,-2.4401661733,0.7577769923,-0.000587601
F,0.7849778977,-0.5881489908,-1.0872093606
F,0.7860986927,-0.5839498393,1.0888932541

CH_3OH

C,0.784993,0.697843,0.002045
H,0.997973,1.156714,-0.960589

H,-0.298771,0.82474,0.211816
H,1.340783,1.216912,0.787051
O,-1.936173,-0.025192,0.041352
H,-1.444951,-0.741096,-0.402212
O,1.132626,-0.672525,-0.095336
H,1.123387,-1.062588,0.783532

$(CH_3)_2)CHOH$

C,0.0000804823,-0.2568119712,0.0043578607
H,-0.0368608377,-0.5168061586,1.0870325149
C,1.4514208792,-0.043060654,-0.3807700768
H,2.0350776043,-0.9409109052,-0.1783826382
H,1.5292441745,0.194132683,-1.4431402799
H,1.8801322684,0.780569777,0.1884413909
C,-0.6804798322,-1.3728152992,-0.772891208
H,-0.1734969866,-2.3230462332,-0.6037282013
H,-1.7197921034,-1.4932354676,-0.4598713798
H,-0.661774112,-1.1555632504,-1.8426548986
O,-0.3699353448,0.3733073262,2.7143250941
H,-0.4927205054,1.1235541814,2.1016409643
O,-0.6742111767,0.9969670151,-0.168750835
H,-1.6240748274,0.8409721489,-0.1816405639

CF_2HOH

C,-0.3220064943,-0.0319240926,-0.1116335104
H,0.8233562742,-0.0673498408,-0.345978192
O,2.245611309,0.1226176416,-0.3988135799
H,2.5166450184,-0.4932927125,0.303561957
O,-0.8495823145,1.1728777133,-0.421956219
H,-0.2814699627,1.8738458572,-0.0789699311
F,-0.9534940297,-0.9724127063,-0.8205350322
F,-0.4605098004,-0.3354768598,1.2096735076

CH_3NH_2

N,-1.1504071354,-0.6041864763,-0.0319654656
C,-0.6272242505,0.7453987324,0.0120320613
H,-0.9925135689,1.3545617075,0.8446427412
H,0.4903200965,0.7159686712,0.1253100489
H,-0.8245745373,1.2583663808,-0.9268875267
H,-1.3509163034,-0.9799849358,0.8835131351
H,-1.9717790729,-0.6944798856,-0.611255329
O,1.9211120968,-0.1726719412,-0.0155632418
H,1.3424586751,-0.9114942529,-0.2785654234

$(CH_3)_2)CHNH_2$

N,-0.068623,-0.228099,1.342683

C,0.308382,-0.011397,-0.05292
H,-0.640776,-0.099202,-0.649846
H,-0.065232,-1.209198,1.590339
H,0.542301,0.261993,1.983579
O,-2.360237,-0.086703,-0.523944
H,-2.156539,0.00013,0.427427
C,0.81318,1.411316,-0.241566
H,0.983763,1.624804,-1.295944
H,0.090707,2.132724,0.139141
H,1.759663,1.556339,0.287892
C,1.26543,-1.063935,-0.611309
H,0.862279,-2.06873,-0.475722
H,1.433386,-0.913697,-1.678538
H,2.230758,-1.010755,-0.100789

CF_2HNH_2

N,-0.6815072044,1.3213009352,-0.0014070471
C,-0.2863812076,-0.0126362505,0.0094806966
H,0.8927414001,-0.0860722517,-0.0436783144
H,-0.3101664981,1.830516897,-0.7900627212
H,-1.6834305068,1.4400556396,0.0873475544
O,2.2837249424,0.0014065344,-0.0799667482
H,2.4378206764,0.3269989292,0.8231599585
F,-0.7234768974,-0.6291906731,1.1291970469
F,-0.7269697045,-0.7730637601,-1.0486904256

Transition states – with water

CH_4

C,2.0727059417,-0.6469752898,0.0010448063
H,2.6134074976,-0.7247655153,0.939368095
H,1.2363873763,0.2264876743,0.1922948394
H,1.5344193274,-1.5542466767,-0.2535162809
O,0.2448255784,1.0563961234,0.3632339834
H,-0.501706908,0.4604885493,0.1568565734
O,-2.1648722137,-0.5464987301,-0.2148762326
H,-2.7553474932,-0.5507701658,0.5451792519
H,-2.6694860528,-0.1478601183,-0.9309870967
H,2.6844019463,-0.2745088509,-0.8149729391

CH_3F

C,-1.5523498252,0.0860408006,0.087570165
H,-1.9736426777,0.1420104778,1.0881838441
H,-0.7041783885,0.965605223,0.0105963612

H,-2.2584177795,0.2732822267,-0.7181088314
O,0.3051140435,1.7854316894,-0.0506051168
H,1.0258497327,1.1258347371,0.0253025068
O,1.9613589179,-0.6081418521,0.1254866853
H,2.5881442712,-0.8640096082,-0.5576577124
H,1.1854196938,-1.1667987989,-0.0065901174
F,-0.9423579881,-1.1378678953,-0.0978967844

$(CH_3)_2CHF$

C,-0.8356534112,-0.049633797,0.0385774823
H,-0.0571917818,0.8267377801,0.1451980482
O,0.9579928918,1.8055980784,0.2632446751
H,1.7170082574,1.1904163293,0.1793278279
O,2.7256861436,-0.4846110476,-0.0837412148
H,3.3052872016,-0.5888320842,-0.8438814829
H,1.9398191231,-1.0136339872,-0.276169334
F,-0.0780072744,-1.176877087,-0.3520170433
C,-1.4351037774,-0.3096588739,1.3944915058
H,-0.6610823064,-0.5740471053,2.112859703
H,-1.9432312748,0.5857180039,1.7510488449
H,-2.1598745667,-1.1253307287,1.338861797
C,-1.7818168512,0.3111521481,-1.0750086499
H,-2.3094557127,1.2316816591,-0.8273103707
H,-1.2387560751,0.4660909283,-2.0056466221
H,-2.5160715857,-0.4845132162,-1.2218251666

CF_3H

C,0.9492079724,-0.0460645973,-0.0006060757
H,0.0368338309,0.8083476849,-0.0049040154
O,-0.9576171119,1.5668359595,-0.0134821724
H,-1.6935347203,0.9185032145,-0.0039428828
O,-3.0872524468,-0.3626928283,0.0086784469
H,-3.3088845195,-0.8756678537,0.7918262488
H,-3.2503083418,-0.9403674405,-0.7432253875
F,0.7522567284,-0.9265878012,-0.984099618
F,2.1125332262,0.5736659461,-0.1839890529
F,0.9636523826,-0.6876702841,1.1684325089

CH_3OH

C,1.4346252317,0.1236945068,0.3268521058
H,0.6610547096,0.9849919052,0.1105813474
H,1.1229964466,-1.0638348985,-1.1892184408
O,-0.4377196524,1.8425626079,-0.1675925813
H,-1.1280599699,1.1538443788,-0.0764496778
O,-1.8444787374,-0.7300253393,0.0319740383
H,-2.3269734951,-1.1236669378,0.7641355725

H,-0.9623305812,-1.1346738649,0.0366028163
O,1.0015098882,-1.0931246038,-0.2344436258
H,1.4811453923,0.0059811933,1.4058219397
H,2.3843667676,0.4699120522,-0.0837594943

$(CH_3)_2)CHOH$

C,0.836809,-0.009429,0.018584
H,0.109936,0.838824,0.11076
H,0.208399,-0.834869,-1.658964
O,-1.24683,1.889652,0.191338
H,-1.886282,1.144357,0.128679
O,-2.534524,-0.645433,-0.171026
H,-2.969952,-1.19953,0.482263
H,-1.650956,-1.030583,-0.318524
O,0.195716,-1.063905,-0.723244
C,1.125235,-0.544068,1.40657
H,1.529979,0.246962,2.036763
H,0.214517,-0.916448,1.874241
H,1.84838,-1.360258,1.357764
C,2.064173,0.509105,-0.710287
H,1.802529,0.884857,-1.701563
H,2.513412,1.333308,-0.156573
H,2.807838,-0.282786,-0.820596

CF_2HOH

C,0.8395452349,-0.0291191297,0.0025939853
H,0.0160200537,0.9211458945,-0.0038991336
H,0.7694422837,-1.9418718254,-0.1219581146
O,-0.9245776716,1.7326350146,-0.0161953951
H,-1.6890391088,1.1186391604,-0.0602859564
O,-2.7483306727,-0.4982793767,-0.0851422214
H,-3.3202008995,-0.6858172705,0.6652019869
H,-1.9966406569,-1.099131966,-0.0039079799
O,0.1539558144,-1.1999030234,-0.0212140726
F,1.6068191726,0.0910456098,1.1065948444
F,1.6505274502,0.1039119124,-1.066759943

CH_3NH_2

N,1.130568254,-0.9876762781,-0.129773301
C,1.4431735797,0.3934499658,0.1554268328
H,2.1817468937,0.8442447782,-0.5100227076
H,0.4913401661,1.0729575256,0.0109649791
H,1.7285482565,0.5238079183,1.1960134217
H,1.2815416373,-1.2329750164,-1.0984774492
H,1.634150945,-1.6394441071,0.4556520475
O,-0.7355870036,1.7749063973,-0.1413802428

H,-1.3105249816,0.9823388402,-0.0983385495
O,-1.7600969935,-0.951531197,0.0027306514
H,-2.1494518572,-1.2933354114,0.8122824558
H,-0.8026568963,-1.1531164154,0.0505728619

(CH3)2)CHNH2

N,0.106699,-1.168743,-0.633124
C,0.813286,-0.054019,0.002026
H,0.069869,0.814481,0.055719
H,0.107986,-1.079465,-1.64254
H,0.534057,-2.058855,-0.402353
O,-1.058027,1.877568,0.109437
H,-1.781388,1.213463,0.069611
O,-2.623609,-0.525694,-0.130682
H,-3.045153,-0.96033,0.615473
H,-1.743458,-0.950092,-0.242262
C,1.17219,-0.409934,1.434381
H,1.585832,0.454155,1.951627
H,0.294632,-0.746603,1.985898
H,1.921757,-1.207458,1.458014
C,1.994365,0.474119,-0.805645
H,1.684617,0.75054,-1.814425
H,2.420195,1.360495,-0.335157
H,2.778208,-0.285116,-0.882343

CF_2HNH_2

N,0.231534,-1.011703,-0.823751
C,0.802109,-0.03762,0.016305
H,0.075012,0.955355,0.0455
H,0.098291,-0.649421,-1.759689
H,0.791649,-1.858275,-0.851985
O,-0.871086,1.825491,-0.050341
H,-1.640745,1.222497,0.030606
O,-2.595219,-0.50638,-0.001591
H,-2.97536,-0.881767,0.797923
H,-1.782229,-1.007437,-0.178363
F,0.939722,-0.52593,1.265268
F,2.030326,0.411908,-0.376391