SUPPORTING INFORMATION

Theoretical investigation of the OH-initiated atmospheric degradation mechanism of CX_2=CHX (X = H, F, Cl) by advanced quantum chemical and transition state theory methods.

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S1. Computational details for the Kinetics Model of barrierless OH-addition:

Variable Reaction Coordinate-Variational Transition State Theory (VRC-VTST) with a multifaceted dividing surface[1,2] was employed to evaluate the number of states $N^{\ddagger}_{outer}(E)$ and $N^{\ddagger}_{inner}(E)$ of the two transition state model,[3,4] in order to include fully anharmonic treatments of all the inter-fragment modes. Since the most computationally expensive step in the VRC-VTST calculations is the Monte Carlo sampling (in which thousands of energy calculations need to be performed to explore different configurations of the system and to obtain accurate number of accessible states of transitional modes), we tested several spin-unrestricted density functional methods (B3LYP-D3(BJ)[5], ωB97X-D[6], MN12-L[7], M06-L[8] and M08-HX[9]) in conjunction with the MG3S basis set[10], in order to find the one which best matches the reference jChS results. The reason for employing the jChS results as benchmark values is that several previous studies have shown that this composite scheme provides sub-chemical accuracy (~0.3 kcal mol^{-1}) for reaction energies and barriers over a large panel of different systems[11–14] in the absence of strong static correlation. Since the T1 diagnostic[15] for the species present in the bond association path was found to be less than 0.044, single-reference based composite schemes like jChS can be safely used without the risk of any unphysical bump.[16] Benchmark results for the three reactive systems are shown in Figure S1 for the OH addition to both carbon atoms of the double bond, and the Mean Unsigned Error (MUE) of different levels of theory with respect to the jChS reference is presented in Figure S2. Inspection of both Figures shows a remarkable agreement between M08-HX and jChS trends, with a MUE < 1 kcal mol^{-1} in the region 2.0-2.5 Å, where the most relevant dynamical bottleneck lies for this class of reactions. In addition to the above-mentioned density functionals, some exploratory computations for the reaction between OH and ethylene were also carried out at the rev-DSDPBEP86-D3[17] double-hybrid density functional theory, that was augmented by DFT-D3 dispersion with Becke-Johnson (BJ) damping, [18,19] in conjunction with the partially augmented jun-cc-pV(T+*d*)Z[20] basis set. Even though the computational cost of double-hybrid density functionals cannot be afforded in the VRC-VTST procedure, some points in the range 2.0 - 2.5 Å along the MEP were selected and the rev-DSDPBEP86 energies were compared to the jChS reference values to estimate the performance of this method which is supposed to be superior. Interestingly, an average accuracy close to that of the M08-HX functional was obtained (see Table S1), thus giving further confidence for the choice of this functional for the Monte Carlo sampling in the VRC-VTST computations.

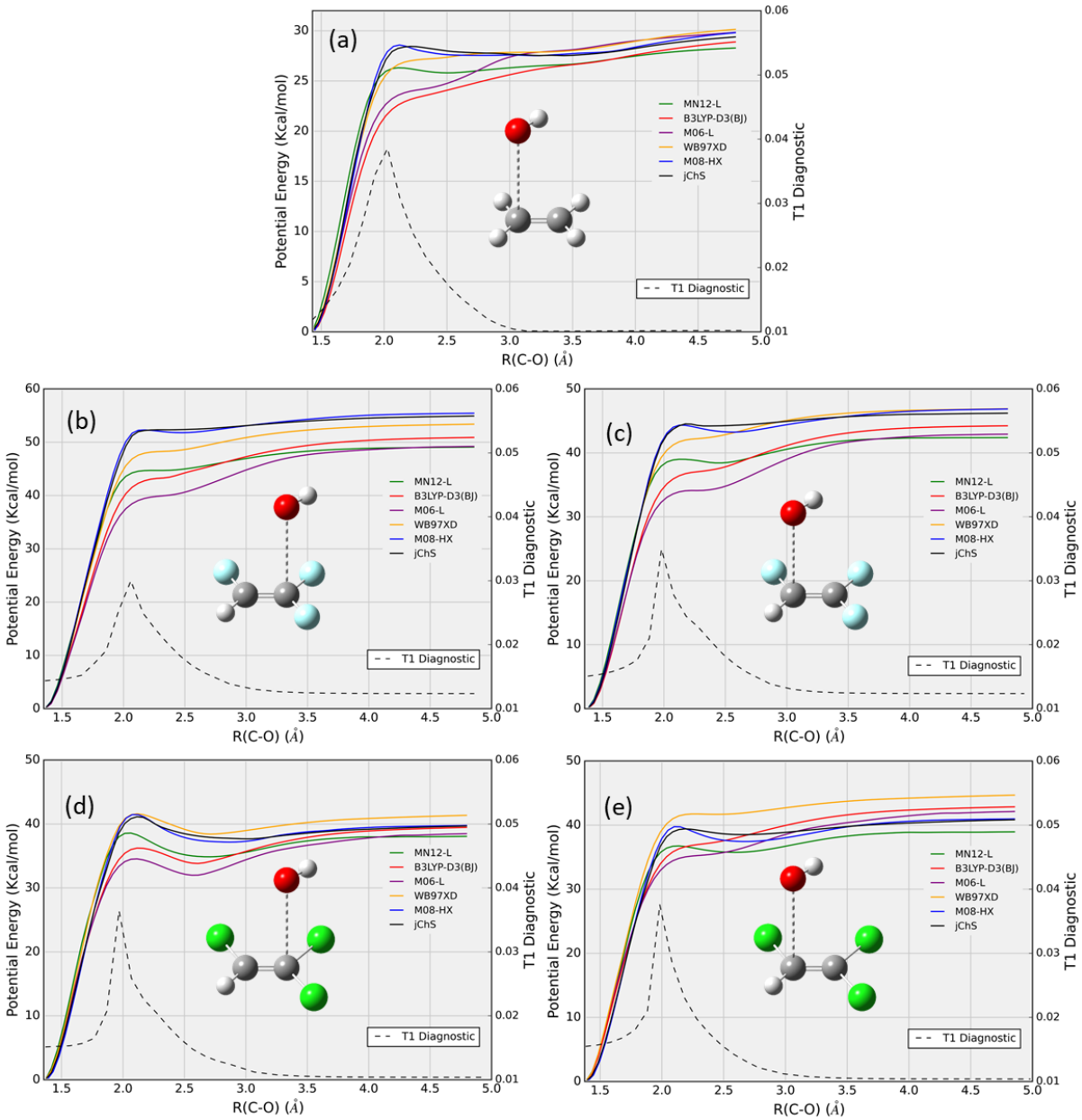

Figure S1. Potential energy (kcal mol^{-1}) along the C–O distance (Å) at different levels of theory for the addition of the OH radical to the C=C double bond of CH_2=CH_2 (a), CF_2=CHF (b, c) and CCl_2=CHCl (d, e). The zero of the energy is set to be the energy of the addition adduct.

Next, we setup the variable reaction coordinate for the multifaceted VRC-VTST calculations. We describe the adopted method with reference to the CF_2=CHF + OH reactive system, since the same setup was applied for the other systems. For the inner TS, we studied the addition to – CF_2 and – CHF fragments separately. In both cases a two-faceted dividing surface was obtained by placing two pivot points perpendicularly above and below the C atom, and a third pivot point in proximity to the O atom, as shown in Figure S3 (a, b). The distances between the pivot points 1, 2 and the C atom, and between pivot point 3 and O atom were 0.25 Å and 0.3 Å, respectively. Pivot points 1, 2 and 3 of the reactants were separated by distances

r_{13} and r_{23}, and the reaction coordinate s (r_{13} and r_{23}) was variationally minimized within the 1.9 Å ≤ s ≤ 3.0 Å interval, with a 0.1 Å step. The location of the pivot points was also varied during the minimization of the flux from its original location, up to a distance of 0.31 Å for the C atom and 0.36 Å for the O atom, with a 0.015 Å step, and a set of 1000 Monte Carlo sampling points over the multifaceted dividing surface was employed. All the calculated reactive fluxes were multiplied by a 0.9 factor to correct for recrossing dynamical effects, on the grounds of previous comparisons with trajectory simulations for prototypical systems.[21,22]

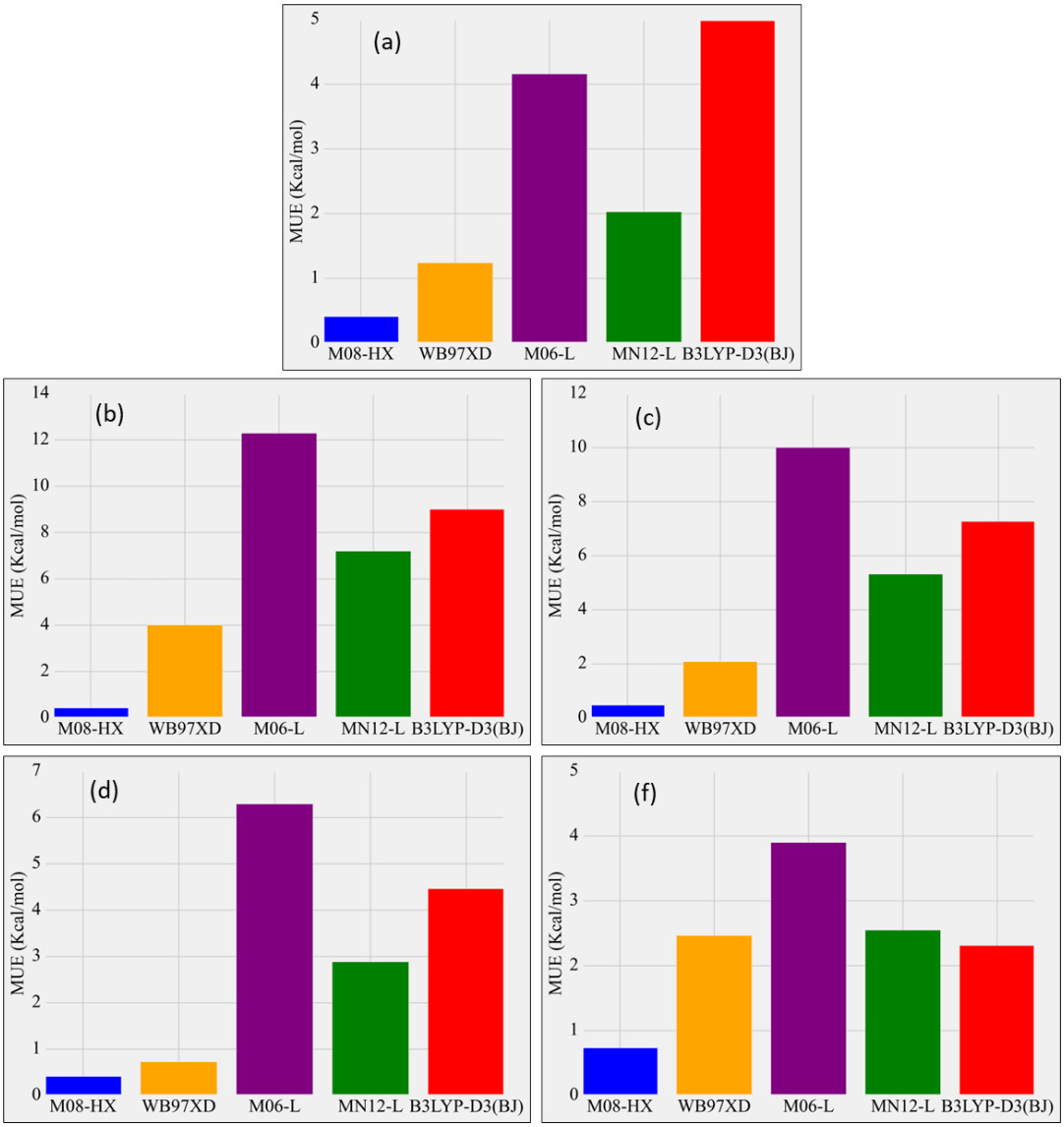

Figure S2. Potential Mean Unsigned Error (kcal mol-1) at different levels of theory compared to jChS method in the region 2.0-2.5 Å for the addition of the OH radical to the C=C double bond of CH_2=CH_2 (a), CF_2=CHF (b, c) and CCl_2=CHCl (d, e).

Table S1. CH_2=CH_2 + OH association relative energies in the 2.0-2.5 Å range. Values are given in kcal mol^{-1}.

distance (Å)	jChS	M08-HX[a]	revDSD[b]
2.0	26.78323	27.67038	27.83063
2.1	28.19802	28.57619	28.66596
2.2	28.43778	28.29279	28.46171
2.3	28.35288	27.95686	27.96769
2.4	28.17183	27.74198	27.49974
2.5	27.99021	27.60651	27.15564
MUE[c]	0	0.436644	0.571851

[a]M08HX/MG3S; [b]revDSD-PBEP86-D3(BJ)/jun-cc-pV(T+*d*)Z; [c]Mean Unsigned Error relative to jChS energies.

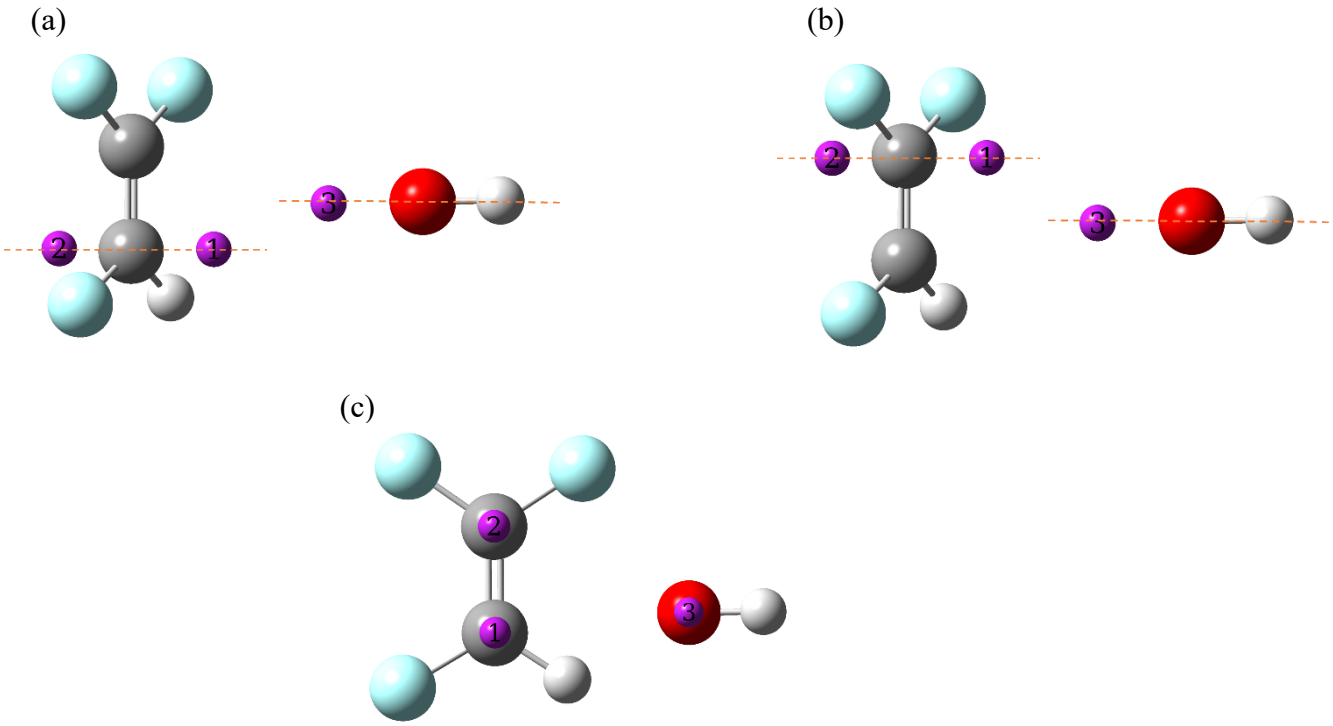

Figure S3. Location of the pivot points that define the two-faceted dividing surface of the inner transition states for the OH addition to the (a) CHF and (b) CF_2 groups and (c) for the outer transition state.

For the outer TS, the two-faceted dividing surface was obtained by employing as pivot points the C and O atoms, as shown in Figure S3 (c). The reaction coordinate, which was defined as the distance between the C atoms of CF_2=CHF moiety and the O atom of OH, was variationally minimized within the 3.5 Å ≤ s ≤ 6.0 Å interval, with a 0.1 Å step. For each of the two facets of the dividing surface, 1000 configurations were explored by Monte Carlo sampling, leading to 2000 single-point calculations for each step.

Table S2. Predicted Rate Coefficients for CX_2=CHX + OH (X = H, F and Cl) reactions with N_2 as Buffer Gas (T = 100 – 600 K).
$k(T) = A_1(T/300)^{n1} \exp(-E_1/RT) + A_2(T/300)^{n2} \exp(-E_2/RT)$ cm^3 $molecule^{-1}$ s^{-1}, where R = 1.987 cal mol^{-1} K^{-1} and T is in K.

Reaction	*Products*	*P (atm)*	A_1	n_1	E_1	A_2	n_2	E_2
CH_2=CH_2 + OH	Total (P-depend)	0.01	3.89E-12	-2.37	98.3	/	/	/
		0.1	5.04E-12	-1.42	-64.7	/	/	/
		1	4.48E-12	-0.53	-284.2	/	/	/
		HPL	3.65E-12	-1.04	-196.6	8.15E-13	2.02	-687.6
	C_2H_4OH	0.01	7.07E-12	-3.66	508.5	/	/	/
		0.1	5.26E-12	-1.55	-29.0	/	/	/
		1	4.67E-12	-0.63	-254.5	/	/	/
	$HOCHCH_2$ + H	0.01	1.68E-16	6.29	1025.7	/	/	/
		0.1	1.15E-15	4.70	2242.7	/	/	/
		1	6.62E-16	6.18	2337.5	/	/	/
	CH_2O + CH_3	0.01	1.74E-15	0.66	-293.6	3.80E-15	2.15	1933.9
		0.1	1.14E-16	-5.21	928.4	9.39E-16	2.65	-49.2
		1	1.83E-17	4.86	-1177.8	9.44E-14	0.21	4300.3
	$OCHCH_3$ + H	0.01	2.59E-17	2.05	-552.2	2.64E-18	6.27	-664.1
		0.1	5.97E-19	-7.42	1355.5	7.58E-18	4.94	-838.1
		1	6.79E-19	2.14	-317.0	4.48E-17	4.52	1199.1
	C_2H_3 + H_2O	P-indep	1.85E-14	5.47	1738.9	/	/	/
CF_2=CHF + OH	Total (P-independ)	HPL	3.04E-12	-1.78	-116.9	1.07E-12	1.54	-656.8
	CF_2(OH)CHF	0.01	2.35E-13	-9.75	1418.3	/	/	/
		0.1	3.90E-12	-5.37	834.1	/	/	/
		1	3.25E-11	-3.77	1397.6	1.10E-12	-7.50	1026.9
	$CF_2CHF(OH)$	0.01	1.20E-12	-7.90	1286.5	/	/	/
		0.1	4.25E-12	-4.28	683.1	/	/	/
		1	5.12E-11	-3.75	1748.4	1.28E-14	-6.50	909.1
	CHFCFO + HF	0.01	2.93E-12	-1.49	-26.5	2.25E-12	0.71	771.1
		0.1	1.80E-12	0.54	-159.8	1.65E-14	-1.32	-497.1
		1	1.52E-13	1.97	-581.5	1.89E-09	-3.27	5965.3
	CF_2O + CH_2F	0.01	3.39E-14	-1.43	-30.2	9.82E-15	1.92	-371.1
		0.1	1.30E-14	1.16	-425.2	3.85E-15	2.03	-380.8
		1	1.58E-15	2.83	-785.0	2.40E-11	-2.62	5932.3
	CH_2FCFO + F	0.01	2.05E-19	1.63	-583.6	8.19E-20	5.90	-879.3
		0.1	4.77E-20	5.72	-1422.8	3.11E-20	6.23	-199.6
		1	6.34E-21	6.84	-1600.9	4.42E-17	2.30	4186.5
	CF_2CHO + HF	0.01	2.34E-12	-0.33	60.2	7.30E-08	-4.72	10772.8
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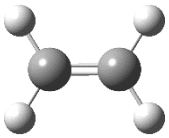
		1	7.09E-15	5.05	-1228.0	2.86E-09	-3.16	7266.8
	CF_3CHO + H	0.01	3.87E-13	0.63	-10.1	8.24E-10	-2.83	8276.2
		0.1	5.44E-11	-1.74	3871.5	6.23E-14	-0.61	760.43
		1	5.68E-13	3.79	3085.4	3.92E-15	0.45	1060.3
	CF_2H + CHFO	0.01	2.64E-15	0.87	-350.8	2.79E-14	1.13	2695.4
		0.1	3.00E-16	-7.65	1518.3	4.39E-15	1.90	333.0
		1	5.29E-17	4.25	-1006.4	8.59E-14	1.11	3668.0
	CHF_2CFO + H	0.01	1.14E-17	1.94	-554.3	5.39E-17	3.27	1571.3
		0.1	9.49E-19	-11.97	2473.7	8.51E-18	4.07	-419.14
		1	1.91E-19	6.40	-1479.7	5.41E-15	0.58	5055.0
	CF_3 + CH_2O	0.01	3.75E-13	-0.14	133.2	6.20E-07	-7.30	13965.9
		0.1	3.46E-11	-2.22	3789.0	3.86E-14	-0.48	587.4
		1	1.39E-16	7.56	-1419.4	1.13E-12	2.48	4091.26
	C_2F_3 + H_2O	P-indep	3.05E-17	7.02	4662.4	/	/	/
CCl_2=CHCl + OH	Total (P-independ)	HPL	5.63E-13	1.73	-590.7	5.67E-13	-1.35	-161.9

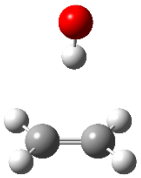
	$CHCl(OH)CCl_2$	0.01	3.47E-20	-8.23	459.7	/	/	/
		0.1	2.45E-17	-9.73	775.3	/	/	/
		1	4.30E-14	-9.26	1249.3	/	/	/
	$CHClCCl_2(OH)$	0.01	2.69E-22	-6.68	947.1	/	/	/
		0.1	4.62E-20	-9.71	910.4	/	/	/
		1	1.13E-15	-9.83	1708.8	/	/	/
	$CCl_2CHOH + Cl$	0.01	4.99E-13	1.56	-592.8	5.21E-13	-1.37	-174.4
		0.1	4.77E-13	1.58	-637.1	5.09E-13	-1.43	-155.8
		1	1.99E-12	0.91	953.7	1.23E-12	-0.54	-170.9
	$CCl_2CClOH + H$	0.01	3.11E-22	13.22	1365.8	/	/	/
		0.1	1.07E-22	13.98	725.8	/	/	/
		1	2.45E-22	13.42	1233.6	/	/	/
	$CHCl_2CClO + H$	0.01	2.89E-26	15.45	-3568.2	/	/	/
		0.1	3.22E-26	15.33	-3499.4	/	/	/
		1	4.83E-26	15.20	-3257.3	/	/	/
	$CHClO + CHCl_2$	0.01	2.06E-21	-0.77	110.1	2.45E-22	10.31	-2694.7
		0.1	8.95E-22	3.87	-1182.5	6.80E-22	9.88	-1939.3
		1	1.27E-21	5.99	-1445.6	3.17E-20	7.31	759.2
	$CHCl_2CHO + Cl$	0.01	3.10E-23	8.11	14621.8	/	/	/
		0.1	5.56E-23	7.62	14971.4	/	/	/
		1	5.77E-23	7.51	14994.9	/	/	/
	$CHClOCHCl + Cl$	0.01	9.95E-29	20.08	1853.6	/	/	/
		0.1	5.80E-29	20.66	1531.9	/	/	/
		1	7.87E-29	20.37	1717.7	/	/	/
	$CHClCClOH + Cl$	0.01	1.04E-13	2.18	-426.1	/	/	/
		0.1	1.03E-13	2.20	-430.7	/	/	/
		1	1.23E-13	2.04	-329.4	/	/	/
	$CHCl_2CO + HCl$	0.01	2.90E-23	13.65	-2865.5	/	/	/
		0.1	2.99E-23	13.67	-2846.0	/	/	/
		1	3.71E-23	13.75	-2698.5	/	/	/
	$CCl_2O + CH_2Cl$	0.01	7.58E-22	9.85	-2058.1	/	/	/
		0.1	9.51E-22	9.60	-1918.2	/	/	/
		1	1.62E-21	8.95	-1544.3	/	/	/
	$CH_2OCCl_2 + Cl$	0.01	2.32E-26	14.58	2074.0	/	/	/
		0.1	2.82E-26	14.31	2197.6	/	/	/
		1	4.03E-26	13.97	2430.7	/	/	/
	$CH_2ClCClO + Cl$	0.01	5.95E-29	19.98	6014.3	/	/	/
		0.1	4.21E-29	20.29	5807.2	/	/	/
		1	3.29E-29	20.49	5662.8	/	/	/
	$C_2Cl_3 + H_2O$	P-indep	4.35E-26	20.79	7242.7	/	/	/

Figure S4. Structures of the minima and transition states present in the PES for the CH_2=CH_2 + OH reaction.



Ethylene

Hydroxyl radical



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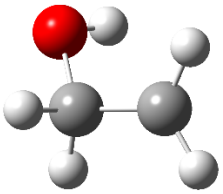

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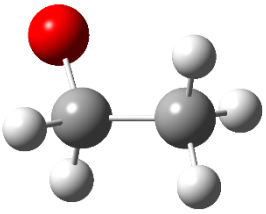

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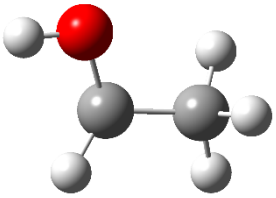

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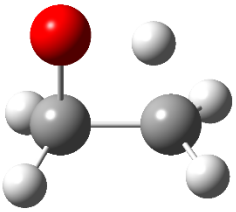

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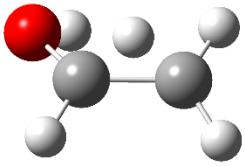

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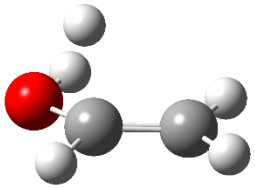

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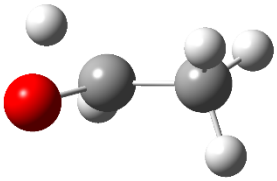

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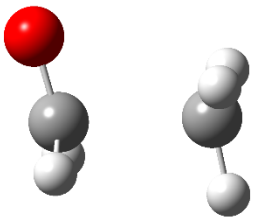

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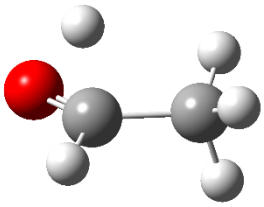

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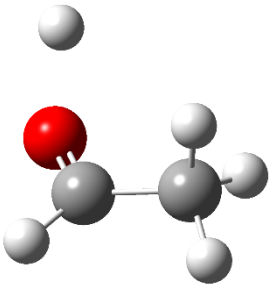

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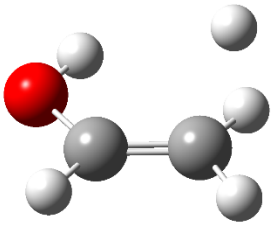

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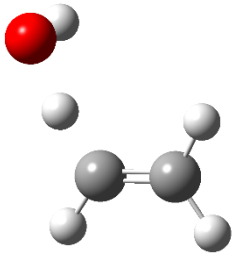

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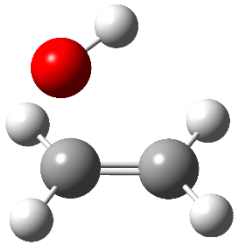

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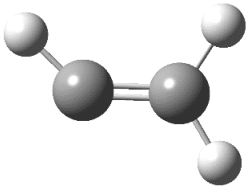
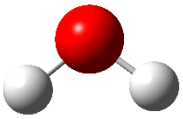
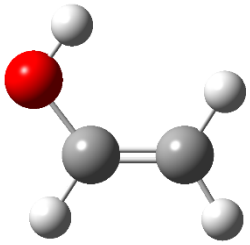


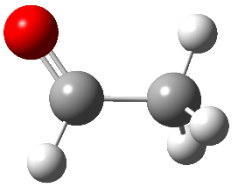
P1(CH_2CH)



P1(H_2O)



P2(CH_2CHOH)



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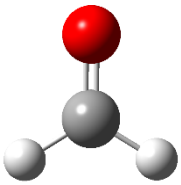
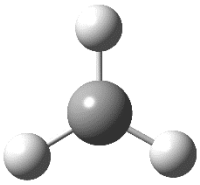
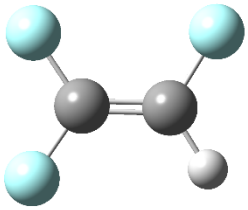


P4(CH_2O)



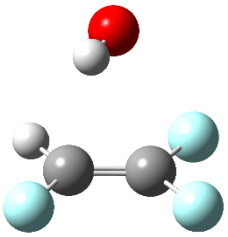
P4(CH_3)

Figure S5. Structures of the minima and transition states present in the PES for the CF_2=CHF + OH reaction.



TFE

Hydroxyl radical



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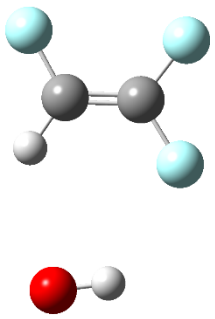
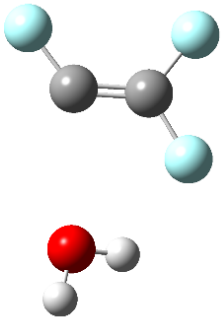


PRCabs



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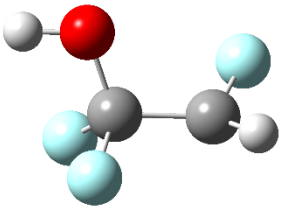

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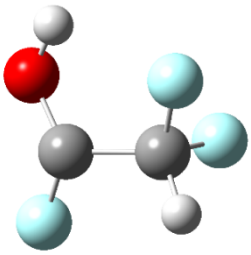

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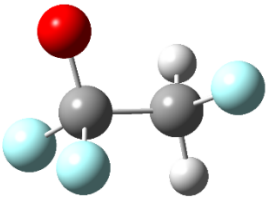

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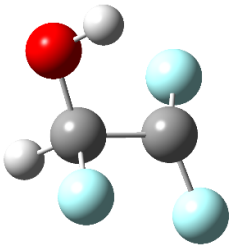

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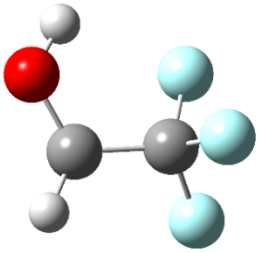

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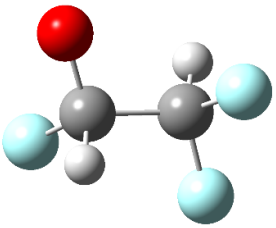

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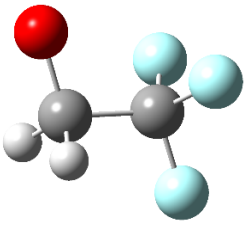

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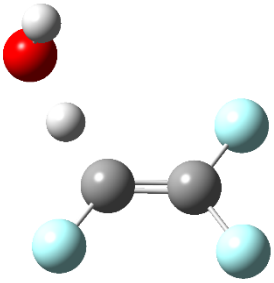

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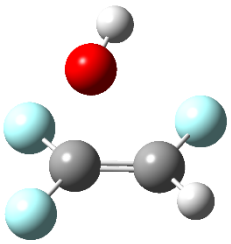

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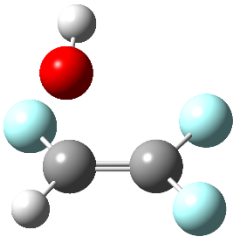

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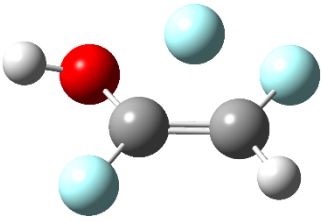

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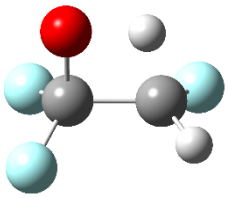

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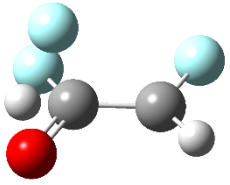

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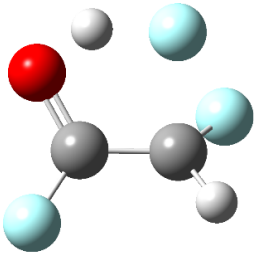

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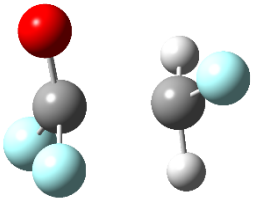

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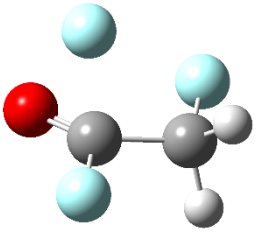

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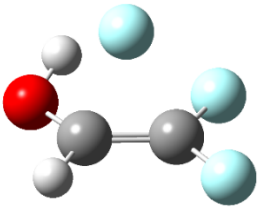

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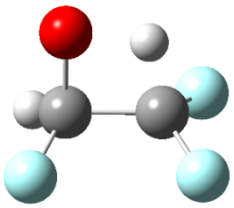

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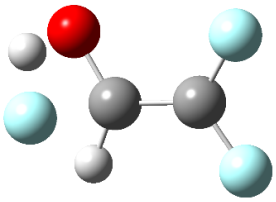

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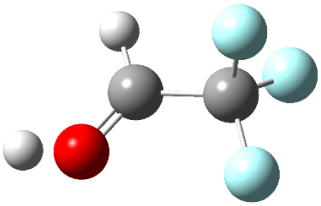

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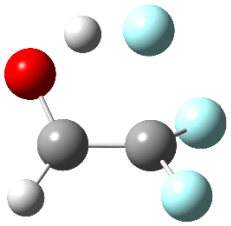

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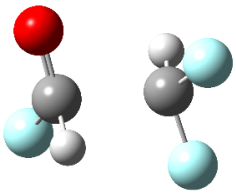

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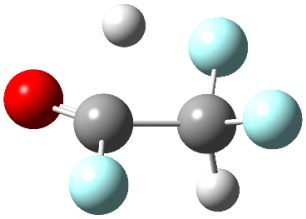

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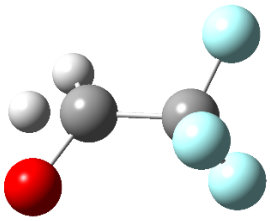

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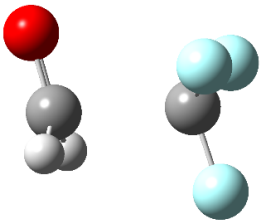

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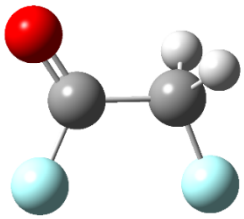

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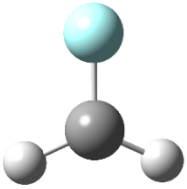

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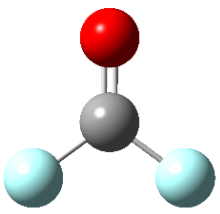

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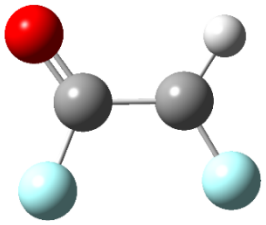

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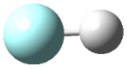
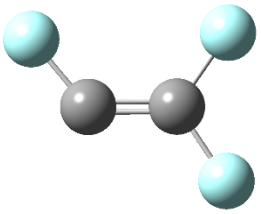
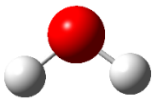


P3(HF)



P4(C_2F_3)



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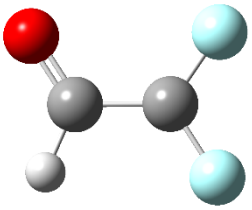

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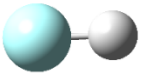
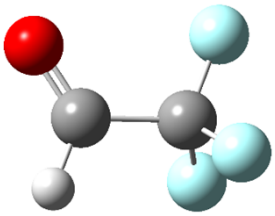


P5(HF)



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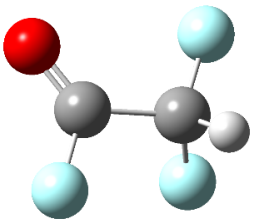
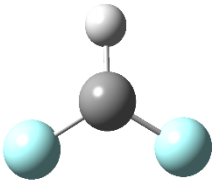
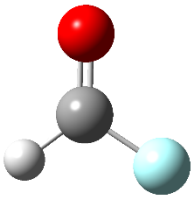


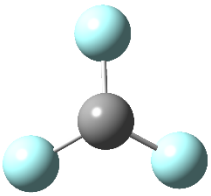
P7(CF2HCFO)



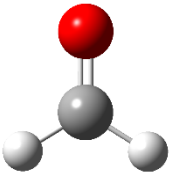
P8(CF_2H)



P8(CHFO)

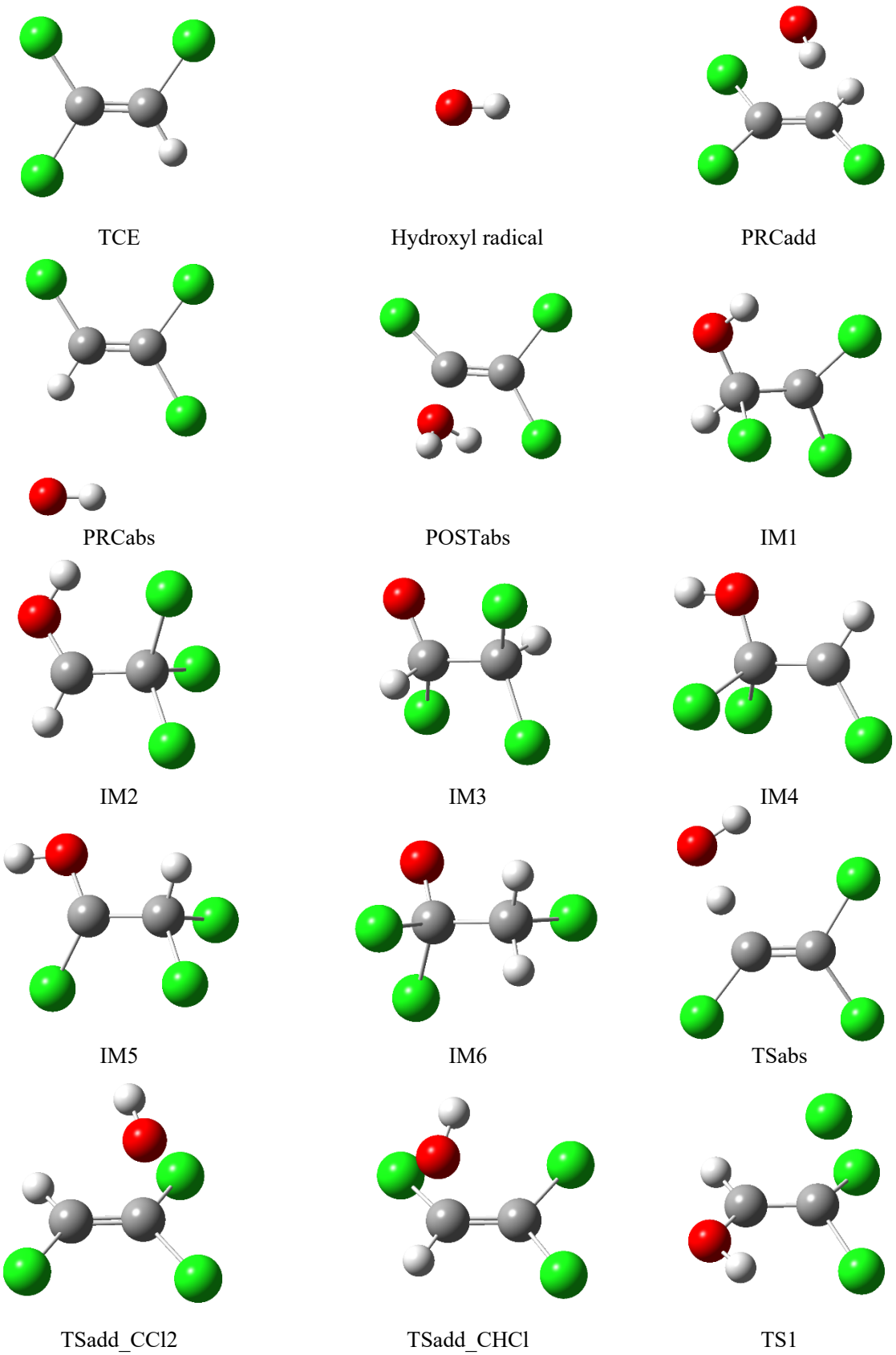


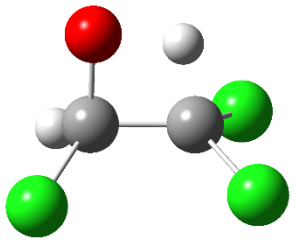
P9(CF_3)



P9(CH_2O)

Figure S6. Structures of the minima and transition states present in the PES for the CCl_2=CHCl + OH reaction.





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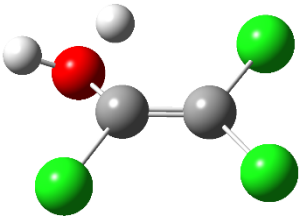

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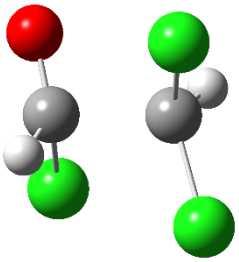

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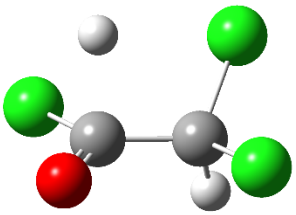

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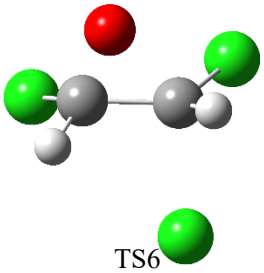

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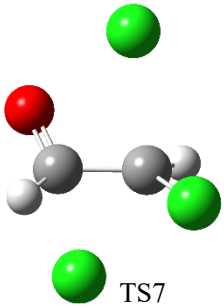

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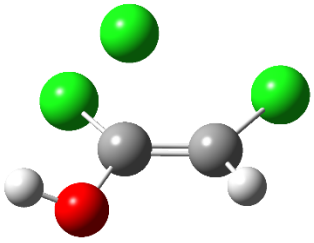
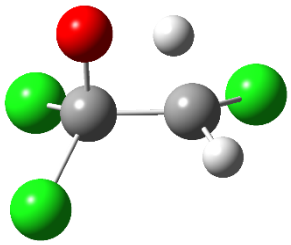


TS8



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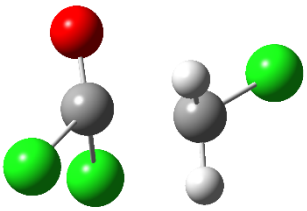
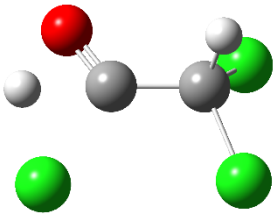


TS10



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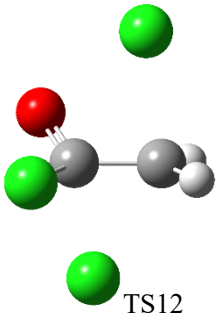
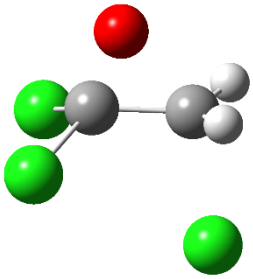
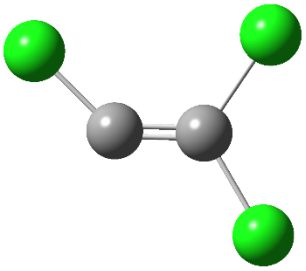


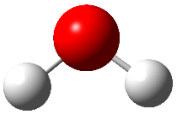
TS12



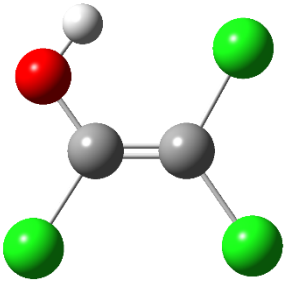
TS13



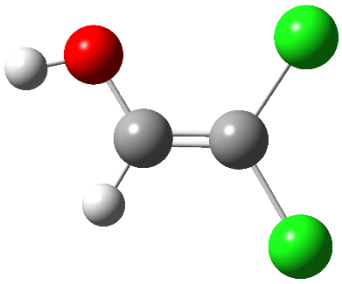
P1(C2Cl3)



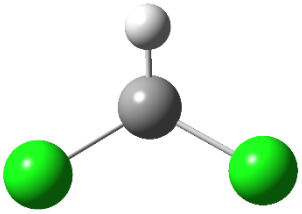
P1(H_2O)



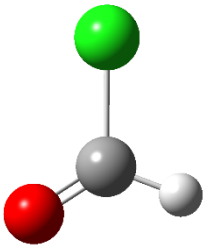
P2(CCl_2CClOH)



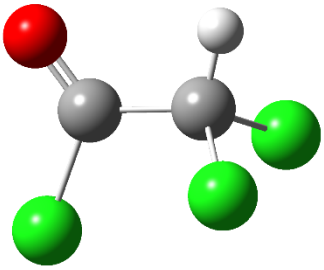
P3(CCl_2CHOH)



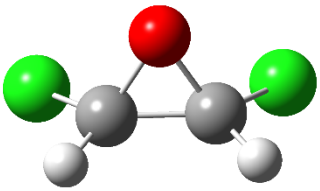
P4($CHCl_2$)



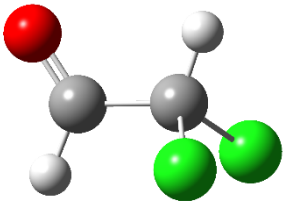
P4(CHClO)



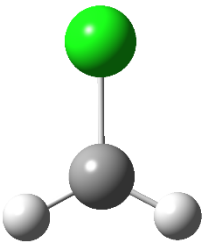
P5($CHCl_2CClO$)



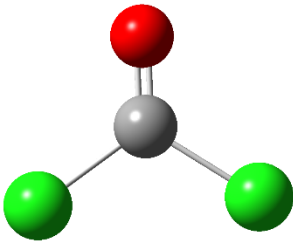
P6(CHCl(O)CHCl)



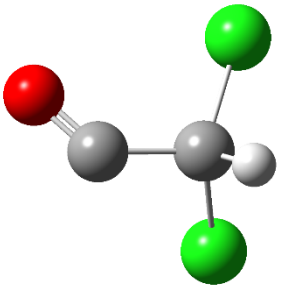
P7($CHCl_2CHO$)



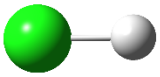
P8(CH_2Cl)



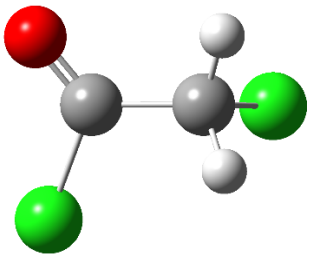
P8(CCl_2O)



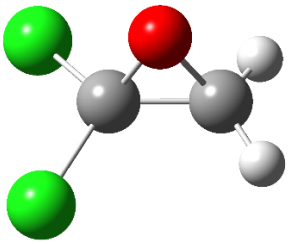
P9($CHCl_2CO$)



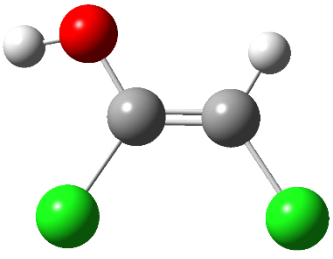
P9(HCl)



P10(CH2ClCClO)



P11($CH_2(O)CCl_2$)



P12(CHClCClOH)

S2. Cartesian coordinates and harmonic vibrational frequencies of equilibrium geometries at the rev-DSD-PBEP86-D3(BJ)/jun-cc-pV(T+d)Z level of theory

I. C_2H_4 + OH reaction:

```
Reactant1 C2H4

Geometry[angstrom]
C              0.00000000    0.00000000    0.00000000
H              0.00000000    0.00000000    1.08618000
H              0.96976012    0.00000000   -0.48923645
C             -1.12628419    0.00000000   -0.69328844
H             -2.09604397    0.00000000   -0.20405131
H             -1.12629538    0.00000000   -1.77946844
Frequencies[1/cm]
3157.35 3132.88 3073.47 3057.03
1657.29 1417.49 1337.74 1200.14
1032.24 975.26 959.10 799.16
!************************************************

Reactant2 OH
Geometry[angstrom]
O             0.00000000    0.00000000    0.00000000
H             0.00000000    0.00000000   -0.97015000
Frequencies[1/cm]
3700.73
!************************************************

Well PRCadd
Geometry[angstrom]
C            1.166598    0.666956    0.000084
C            1.166599   -0.666955    0.000078
H            1.169998    1.233114    0.924107
O           -2.184056   -0.000001   -0.000141
H           -1.208158    0.000002   -0.000175
H            1.170708    1.233122   -0.923931
H            1.170004   -1.233121    0.924096
H            1.170711   -1.233115   -0.923940
Frequencies[1/cm]
3675.08 3255.91 3228.06 3163.81
3147.14 1680.73 1485.19 1380.05
1248.11 1070.35 997.67 979.10
829.60 369.10 304.6717 115.65
89.79 69.99
!************************************************

Well IM1
Geometry[angstrom]
C            -1.233575   -0.272945   -0.012642
C             0.008579    0.540044    0.031808
H            -2.136337    0.118401   -0.460363
O             1.191797   -0.257716    0.043724
```

```
H             1.148794   -0.849117   -0.714163
H            -1.285539   -1.193287    0.553266
H             0.060945    1.127918    0.956249
H             0.027740    1.255216   -0.799773
Frequencies[1/cm]
3833.65 3282.28 3169.74 3039.75
3010.51 1503.38 1472.26 1411.05
1371.28 1190.61 1132.90 1106.16
961.08 837.24 530.29 425.3542
315.93 181.52
!************************************************

Well IM2
Geometry[angstrom]
C             1.182345   -0.199536   -0.000122
C            -0.173842    0.489510   -0.002933
H             1.986917    0.539066    0.032299
O            -1.253525   -0.365505   -0.005462
H            -0.310183    1.103534    0.904759
H             1.274294   -0.856015    0.866165
H             1.304320   -0.800393   -0.902754
H            -0.278167    1.197998   -0.838445
Frequencies[1/cm]
3139.13 3127.34 3050.95 2997.67
2954.10 1510.34 1498.64 1416.10
1407.03 1371.61 1260.70 1105.35
1071.10 906.33 877.14 473.67
390.93 225.36
!************************************************

Well IM3
Geometry[angstrom]
C            -1.225724   -0.164780    0.012291
C             0.090752    0.509181   -0.103740
H            -1.389922   -0.575111    1.018445
O             1.164453   -0.341376    0.021062
H             1.976464    0.172732    0.000195
H            -1.295409   -0.996169   -0.693552
H             0.233653    1.523352    0.255858
H            -2.030576    0.539802   -0.200746
Frequencies[1/cm]
3856.61 3161.04 3131.06 3079.60
2995.10 1502.82 1480.56 1462.89
1400.72 1285.37 1216.01 1070.63
1032.30 937.45 600.30 412.54
371.42 185.11
!************************************************
!                    Transition states
!************************************************

Barrier TSabs
Geometry[angstrom]
C           0.575866    0.574539   -0.019087
H           0.738329    1.639913    0.092058
```

```
H          -0.596972    0.274071   -0.187537
C           1.472416   -0.390763    0.004080
H           2.529228   -0.168230    0.119811
H           1.189320   -1.430996   -0.103925
O          -1.791131   -0.141038   -0.087562
H          -1.820549   -0.289106    0.870137
Frequencies[1/cm]
3776.75 3233.35 3210.35 3139.00
1755.32 1430.24 1307.95 1251.43
1146.46 989.24 935.27 851.35
807.24 617.21 293.47 153.12
137.41 -1680.76
!************************************************

Barrier TSadd
Geometry[angstrom]
C           1.140860   -0.447201   -0.029300
C           0.467460    0.714483    0.030255
H           1.356134   -0.922504   -0.977485
O          -1.459845   -0.153587   -0.055686
H          -1.305634   -0.972184    0.441130
H           1.456705   -0.961049    0.870708
H           0.222203    1.264044   -0.867406
H           0.299434    1.216694    0.972814
Frequencies[1/cm]
3765.10 3281.59 3249.70 3185.05
3160.60 1658.77 1486.40 1372.22
1253.80 1062.41 1032.16 964.53
833.23 711.60 380.65 222.48
97.87 -378.66
!************************************************

Barrier TS1
Geometry[angstrom]
C            -0.977200   -0.422125    0.000000
C             0.000000    0.712664    0.000000
H            -1.487365   -0.658600    0.926683
O             1.082926   -0.246403    0.000000
H             0.159810   -1.115340    0.000000
H            -1.487365   -0.658600   -0.926683
H             0.007358    1.330269    0.898392
H             0.007358    1.330269   -0.898392
Frequencies[1/cm]
3251.24 3137.69 3131.07 3075.4871
1987.36 1539.09 1439.89 1316.8692
1230.11 1161.98 1115.08 1095.9892
995.98 940.48 824.88 726.81
384.82 -2134.69
!************************************************

Barrier TS2
Geometry[angstrom]
C            -1.227267   -0.239404   -0.033737
C             0.047151    0.502998    0.025244
```

```
H            -2.077424    0.175220   -0.556548
O             1.249168   -0.174235    0.019952
H             1.115244   -1.018718   -0.429392
H            -1.221190   -1.285126    0.240871
H            -0.804012    0.430495    1.007884
H             0.074729    1.510445   -0.371471
Frequencies[1/cm]
3754.72 3283.62 3182.35 3163.25
2216.60 1446.73 1405.47 1331.35
1301.83 1215.57 1089.71 934.39
774.69 686.97 441.20 405.63
257.78 -1977.76
!************************************************

Barrier TS3
Geometry[angstrom]
C            -1.196931   -0.267678   -0.025597
C            -0.026830    0.393325   -0.140221
H            -2.123672    0.262358   -0.185775
O             1.209723   -0.165579   -0.037452
H             1.121562   -1.059699    0.310578
H            -1.240757   -1.293261    0.319973
H            -0.120999    1.281539    1.430984
H             0.028646    1.379815   -0.581237
Frequencies[1/cm]
3823.14 3279.39 3217.89 3171.4923
1633.89 1456.83 1352.13 1323.9516
1124.48 1080.59 964.17 836.9144
695.67 520.13 509.38 456.6279
400.73 -1165.971
!************************************************

Barrier TS4
Geometry[angstrom]
C             -1.217866   -0.174188   -0.000997
C              0.127227    0.477631   -0.029690
H             -1.990250    0.512306   -0.352024
O              1.255220   -0.316063    0.088983
H              0.958449    0.240720   -0.947270
H             -1.225930   -1.075849   -0.613736
H             -1.460853   -0.463252    1.028211
H              0.220656    1.493913    0.357077

Frequencies[1/cm]
3145.83 3105.54 3094.72 3028.39
2454.54 1495.26 1486.13 1416.46
1370.53 1193.69 1127.09 1078.23
915.77 897.37 623.89 429.1405
194.51 -2042.9926
!************************************************
Barrier TS5
Geometry[angstrom]
C            1.451622   -0.171158    0.000000
C           -0.530411    0.547659    0.000000
```

```
H            1.989906    0.768712    0.000009
O           -1.213066   -0.471678    0.000000
H           -0.341787    1.109540    0.931601
H            1.435465   -0.736695    0.920894
H            1.435469   -0.736680   -0.920903
H           -0.341789    1.109542   -0.931601
Frequencies[1/cm]
3289.89 3275.06 3109.46 2978.09
2921.11 1664.46 1499.73 1449.47
1433.61 1252.83 1138.48 934.82
667.47 593.93 552.65 296.38
149.64 -499.3037
!************************************************

Barrier TS6
Geometry[angstrom]
C           -1.185082   -0.169273    0.032266
C            0.225316    0.331397   -0.184516
H           -1.878174    0.651660    0.220145
O            1.217950   -0.338998    0.053662
H            0.313960    1.243295   -0.811258
H           -1.496498   -0.670781   -0.889601
H           -1.211548   -0.889527    0.848371
H            0.287261    1.404592    1.116540
Frequencies[1/cm]
3164.90 3123.76 3047.07 2895.12
1741.33 1489.51 1479.12 1408.62
1386.30 1161.56 1119.52 922.19
836.60 541.78 513.73 457.06
190.96 -1271.15
!************************************************

Barrier TS7
Geometry[angstrom]
C            1.206872   -0.186105    0.024751
C           -0.124363    0.482545   -0.044271
H            2.012255    0.529173    0.192321
O           -1.181181   -0.121410    0.149192
H           -1.489209   -1.231528   -0.734361
H            1.212010   -0.959894    0.791597
H            1.379519   -0.674196   -0.944931
H           -0.160182    1.529084   -0.381049

Frequencies[1/cm]
3161.99 3110.09 3016.30 3010.64
1730.67 1489.49 1465.94 1414.08
1383.42 1133.54 1109.52 949.26
765.79 654.87 487.50 229.24
53.30 -1999.20
!************************************************

Barrier TS8
Geometry[angstrom]
C           -1.132227   -0.104779   -0.196526
```

```
C             0.057531    0.471732    0.016389
H            -1.213889   -1.133293   -0.527063
O             1.258658   -0.153531    0.026478
H             1.129180   -1.089284   -0.167608
H            -1.678747   -0.780903    1.535273
H            -2.018707    0.510286   -0.236209
H             0.161072    1.519721    0.264605
Frequencies[1/cm]   17
3811.29 3274.64 3224.75 3168.95
1692.67 1458.09 1358.79 1338.73
1137.05 1019.83 970.51 923.32
795.73 497.35 492.54 375.89
259.65 -823.49

!************************************************
!                        Products
!************************************************
Bimolecular P1

Fragment1 CH2CH
Geometry[angstrom]
C             -0.703496   -0.145551    0.000000
H             -1.592782    0.465911   -0.000001
C              0.585470    0.030029    0.000000
H              1.020042    1.030514    0.000001
H              1.280894   -0.803288    0.000000
Frequencies[1/cm]
3264.21 3189.26 3088.38 1772.51 1415.02 1071.81
964.48 855.87 723.55
!*********
Fragment2 H2O
Geometry[angstrom]
O              0.000000    0.000000    0.117724
H              0.000000    0.759692   -0.470895
H              0.000000   -0.759692   -0.470895
Frequencies[1/cm]
3938.88 3824.01 1644.89
!************************************************

Bimolecular P2
Fragment1 HOCHCH2
Geometry[angstrom]
C          1.212835   -0.108845    0.000000
C          0.000000    0.444309    0.000000
H          2.087788    0.524084    0.000000
O         -1.192862   -0.213364    0.000000
H         -1.024878   -1.162488    0.000000
H          1.355193   -1.183552    0.000000
H         -0.152214    1.516084    0.000000
Frequencies[1/cm]
3817.08 3269.82 3216.35 3163.90
1702.39 1456.43 1356.52 1331.15
1123.44 999.94 962.98 829.9663
716.33 487.98 446.97
```

```
!*********
Fragment2 H
  Atom
!*************************************************

 Bimolecular P3
 Fragment1 OCHCH3
 RRHO
 Geometry[angstrom]
C            -1.167047   -0.149307   -0.000004
C             0.230605    0.400124   -0.000002
H            -1.702296    0.221714   -0.878770
O             1.233658   -0.277052    0.000000
H             0.307129    1.505890    0.000004
H            -1.153221   -1.237690   -0.000058
H            -1.702222    0.221604    0.878859
Frequencies[1/cm]
3165.25 3110.72 3044.26 2922.88
1789.19 1485.22 1474.17 1428.00
1389.96 1140.26 1138.38 899.13
778.13 507.49 158.00
!*********
Fragment2 H
  Atom
!*************************************************

Bimolecular P4
Fragment1 CH2O
Geometry[angstrom]
C            0.000000    0.000000   -0.530899
O            0.000000    0.000000    0.676285
H            0.000000    0.938533   -1.112441
H            0.000000   -0.938533   -1.112441
Frequencies[1/cm]
3001.58 2935.61 1783.59 1538.25
1268.07 1199.36
!*********
Fragment2 CH3
Geometry[angstrom]
C             0.000000    0.000000    0.000000
H             0.433510    0.987390    0.000000
H             0.638350   -0.869125    0.000000
H            -1.071860   -0.118264    0.000000
Frequencies[1/cm]
3319.40 3319.40 3136.92 1430.32
1430.32 501.29
```

II. CF_2=CHF + OH reaction:

```
Reactant1 CF2=CHF
Geometry[angstrom]
C           0.00000000    0.00000000    0.00000000
```

```
H           0.00000000    0.00000000    1.08038000
F           1.19402608    0.00000000   -0.60246761
C          -1.10425239    0.00000000   -0.71665074
F          -2.30955047    0.00000000   -0.18684690
F          -1.14803019    0.00000000   -2.02813028
Frequencies[1/cm]
3177.73 1819.60 1345.90 1251.84
1158.33 931.11 800.92 615.46
594.72 476.25 309.89 218.83
!************************************************

Reactant2 OH
Geometry[angstrom]
O            0.00000000    0.00000000    0.00000000
H            0.00000000    0.00000000   -0.97015000
Frequencies[1/cm]
3700.73
!************************************************

Well PRCadd
Geometry[angstrom]
C          -0.603028   -0.459741   -0.701026
C           0.571387   -0.326831   -0.091530
F          -1.656300   -0.947702   -0.027874
H          -0.772429   -0.184916   -1.728281
F           1.639331    0.138791   -0.693875
F           0.806099   -0.653532    1.156025
O          -0.604613    2.044197    0.220661
H          -1.302991    1.712762    0.809840
Frequencies[1/cm]
3751.61 3286.66 1804.85 1390.88
1295.84 1178.72 947.51 777.22
630.45 593.89 489.74 425.45
313.99 234.67 162.19 89.03
63.53 49.76
!************************************************

Well PRCabs
Geometry[angstrom]
C          -0.997506    0.211970    0.000000
C          -0.798643   -1.098134   -0.000008
F           0.048975    1.047863   -0.000079
H          -1.979711    0.656621    0.000061
F          -1.792301   -1.975959    0.000045
F           0.369684   -1.695838   -0.000080
O          -4.360786   -0.184799   -0.000033
H          -4.069968   -1.113147   -0.000104
Frequencies[1/cm]
3745.18 3274.36 1835.28 1387.21
1273.51 1184.04 944.18 810.06
627.65 575.55 488.41 314.55
241.54 226.74 110.19 90.83
60.69 32.38
!************************************************
```

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Well POSTabs
Geometry[angstrom]
C           0.338198    0.824248   -0.176454
C           0.582701   -0.451933   -0.052228
F           1.139293    1.838829   -0.022091
H          -3.744262    0.352358    0.115914
F          -0.335295   -1.387413   -0.227771
F           1.754720   -0.983756    0.251513
O          -2.784068    0.346592    0.156298
H          -2.537047   -0.567920   -0.009062
Frequencies[1/cm]
3935.08 3820.63 1980.43 1641.59
1294.41 1252.97 949.23 627.73
571.73 491.12 310.07 217.42
172.86 139.34 79.90 54.64
44.92 9.05
!************************************************

Well IM1
Geometry[angstrom]
C        0.959183    0.687849   -0.061253
C       -0.377511    0.024771   -0.015271
F        2.001977   -0.129520    0.030183
H        1.117837    1.601634   -0.614217
F       -1.326093    1.001891   -0.058350
F       -0.560838   -0.617511    1.173164
O       -0.535789   -0.853445   -1.041353
H       -1.356969   -1.343534   -0.900775
Frequencies[1/cm]
3793.40 3251.36 1504.49 1354.20
1235.73 1204.95 1112.72 1104.98
865.41 661.95 617.88 557.18
503.11 430.02 333.62 290.95
219.23 79.46
!************************************************

Well IM2
Geometry[angstrom]
C                  -0.689454   -0.323074   -0.356560
C                   0.725185    0.183834   -0.330326
F                  -1.514689    0.759883   -0.449159
H                  -0.876593   -0.997303   -1.190731
F                   1.630443   -0.793945   -0.329930
F                  -1.014593   -0.969104    0.801194
O                   1.051975    1.134839    0.564767
H                   0.335954    1.782521    0.594955
Frequencies[1/cm]
3811.74 3145.55 1464.18 1384.32
1365.03 1334.54 1149.71 1106.01
1063.68 891.89 745.70 594.53
535.30 421.21 343.66 240.66
215.58 82.08
!************************************************
```

```
Well IM3
Geometry[angstrom]
C       -0.888588   -0.711335   -0.177267
C        0.440128    0.025042    0.062812
F       -1.944373    0.144174   -0.020166
H       -0.852544   -1.069376   -1.207978
F        0.563502    1.087995   -0.760669
F        1.444306   -0.832481   -0.265956
O        0.493776    0.391646    1.349382
H       -0.977814   -1.543214    0.520772
Frequencies[1/cm]
3158.26 3086.58 1500.03 1415.86
1322.15 1220.75 1157.24 1130.51
1124.67 918.47 847.79 620.51
537.43 506.95 386.51 330.83
220.21 105.41
!************************************************

Well IM4
Geometry[angstrom]
C          -0.704618    0.003003    0.331854
C           0.695297   -0.027736   -0.249503
F          -1.278195    1.181345   -0.094087
H          -0.680614    0.019239    1.424974
F           1.379794   -1.123876    0.049695
F           1.420652    1.053748   -0.016666
O          -1.446334   -1.085922   -0.045660
H          -1.393047   -1.184408   -1.004280
Frequencies[1/cm]
3805.08 3086.96 1462.73 1386.70
1326.03 1263.40 1259.53 1162.13
1068.32 962.80 643.38 556.76
497.04 424.65 384.79 332.68
212.36 72.08
!************************************************

Well IM5
Geometry[angstrom]
C          -0.911289   -0.729553   -0.158963
C           0.393780   -0.037218   -0.014764
F           0.753919    0.180168    1.270922
H          -0.980714   -1.781086    0.069390
F           1.379210   -0.738239   -0.582084
F           0.345712    1.183450   -0.596105
O          -2.043214   -0.019640    0.037720
H          -1.878092    0.910414   -0.163382
Frequencies[1/cm]
3800.34 3265.42 1496.63 1363.04
1264.49 1220.92 1162.43 1107.95
849.52 682.94 637.44 558.15
536.70 454.16 429.06 312.74
230.46 89.06
!************************************************
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```
Well IM6
Geometry[angstrom]
C          -0.672427   -0.010793    0.334317
C           0.740567    0.098431   -0.285024
F          -1.246704   -1.149913   -0.108232
H          -0.641970   -0.022594    1.424174
F           1.431483   -1.036777    0.082936
F          -1.414949    1.032161   -0.092238
O           1.332752    1.222501    0.090129
H           0.642649    0.107516   -1.383151
Frequencies[1/cm]
3130.49 2985.77 1396.26 1381.92
1287.99 1192.93 1156.89 1149.47
1113.51 1062.31 982.26 629.27
556.38 459.36 400.54 361.14
218.27 78.98
!************************************************

Well IM7
Geometry[angstrom]
C           -0.369331    0.003178    0.000002
C            0.969279    0.748384    0.000017
F           -1.365402    0.899336    0.000010
H            0.979649    1.366532    0.903808
F           -0.507347   -0.768292   -1.080454
F           -0.507364   -0.768334    1.080424
O            1.982753   -0.188359   -0.000001
H            0.979648    1.366577   -0.903743
Frequencies[1/cm]
3100.49 3033.94 1523.73 1494.30
1348.59 1302.22 1267.41 1184.72
1104.40 1025.45 836.02 643.00
552.94 540.86 409.26 353.29
231.53 119.11

!************************************************
!                    Transition states
!************************************************

Barrier TSabs
Geometry[angstrom]
C           0.335787    0.480548   -0.092784
C          -0.761813   -0.246323   -0.012138
F          -0.764810   -1.558158   -0.055584
H           1.471637   -0.090742   -0.230240
F          -1.977503    0.244882    0.088200
F           0.362912    1.798485   -0.013199
O           2.501451   -0.618406   -0.030822
H           2.487517   -0.734242    0.931583
Frequencies[1/cm]
3781.01 1926.80 1372.99 1337.23
1242.36 1044.07 975.94 762.85
647.46 583.26 492.74 407.84
```

283.17 229.78 116.04 104.00
81.30 -1982.43
!**

Barrier TSadd-CF_2
Geometry[angstrom]
C   -0.791502   -0.109526   -0.696306
C   0.387020   -0.354207   -0.102026
F   -1.923326   -0.266988   -0.010480
H   -0.877768   0.259634   -1.703897
F   1.515949   -0.314592   -0.751718
F   0.505746   -0.862642   1.093122
O   0.350431   1.716897   0.320607
H   -0.384103   1.785600   0.950714
Frequencies[1/cm]
3764.64 3293.03 1775.24 1409.98
1308.96 1193.16 968.42 784.61
733.18 639.29 493.18 481.48
355.16 261.70 244.52 174.08
141.00 -386.28
!**

Barrier TSadd-CHF
Geometry[angstrom]
C   0.596417   -0.132691   -0.653131
C   -0.641465   -0.165035   -0.140554
F   1.497754   -1.021005   -0.238339
H   0.842031   0.435910   -1.533077
F   -1.601990   0.612078   -0.556963
F   -1.002092   -0.918385   0.863983
O   1.020864   1.532868   0.541034
H   1.218286   1.033301   1.348797
Frequencies[1/cm]
3764.22 3295.02 1780.41 1408.40
1313.48 1193.85 967.30 888.32
756.01 635.59 563.57 493.74
310.68 238.91 211.49 136.01
104.70 -433.23
!**

Barrier TS1
Geometry[angstrom]
C   0.502515   -0.235312   -0.181459
C   -0.759936   0.082840   -0.627340
F   -0.313889   1.384165   0.828499
F   -1.792154   -0.577481   -0.161967
O   0.746469   -1.177502   0.691599
H   1.597851   -1.011283   1.120511
F   1.540516   0.365864   -0.709101
H   -0.935337   0.793193   -1.417385
Frequencies[1/cm]
3787.38 3291.05 1761.82 1472.07
1354.81 1240.21 1188.81 960.31
806.44 618.02 558.85 486.43

```
411.93 304.34 254.19 245.63
167.76 -273.79
!************************************************

Barrier TS2
Geometry[angstrom]
C        -0.903702   -0.520585    0.347233
C         0.457565    0.007887   -0.013098
F        -1.961499    0.259769    0.120289
H        -0.986473   -1.143656    1.234927
F         1.391295   -0.050257    0.956756
F         0.474362    1.257799   -0.500398
O         0.637871   -0.958161   -0.972047
H        -0.577097   -1.320676   -0.653186
Frequencies[1/cm]
3163.11 2035.70 1434.90 1293.52
1189.54 1186.03 1168.73 1124.36
929.33 863.93 680.41 632.15
523.90 481.64 357.23 221.73
150.95 -2128.58
!************************************************

Barrier TS3
Geometry[angstrom]
C         -0.959472   -0.404905    0.569181
C          0.247859    0.284413    0.239505
F         -2.029374   -0.208040   -0.159410
H         -0.996013   -1.189707    1.307351
F          0.111703    1.276019   -0.601127
F          1.165470   -1.002809   -0.827404
O          1.289369    0.227404    0.984857
H          1.720551   -0.493105    0.253132
Frequencies[1/cm]
3281.77 2208.83 1602.67 1451.79
1338.47 1232.06 938.49 907.90
813.57 658.55 590.60 531.22
481.98 349.03 249.21 175.76
118.62 -1443.00
!************************************************

Barrier TS4
Geometry[angstrom]
C                  0.453932   -0.698996    0.315796
C                 -0.736930   -0.077370   -0.113768
F                  1.399067   -0.959010   -0.564995
H                  0.487521   -1.303634    1.211849
F                  1.205563    1.039826    0.655525
F                 -1.897089   -0.480412    0.348401
O                 -0.677354    1.026690   -0.754002
H                  0.261423    1.344670   -0.342381
Frequencies[1/cm]
3241.61 2286.57 1673.64 1509.85
1319.24 1251.59 1129.38 996.37
967.68 860.02 651.59 505.28
```

466.05 448.69 341.32 253.83
143.33 -753.49
!**

Barrier TS5
Geometry[angstrom]
C   1.038210   0.699366   -0.209211
C   -0.610993   -0.102538   0.164324
F   2.004294   -0.186355   -0.017017
H   0.859240   0.906969   -1.261906
F   -0.651966   -1.059520   -0.785130
F   -1.409598   0.901314   -0.275502
O   -0.496321   -0.364012   1.342166
H   1.063459   1.525206   0.492752
Frequencies[1/cm]
3248.29 3108.29 1622.66 1497.30
1225.94 1221.12 1165.03 1113.61
889.66 785.75 630.46 577.44
538.90 321.26 278.62 193.28
86.71 -536.39
!**

Barrier TS6
Geometry[angstrom]
C   -0.975272   -0.644705   -0.313633
C   0.370669   -0.240664   0.238398
F   -1.938927   0.227583   0.097340
H   -0.919260   -0.661896   -1.402128
F   0.750164   1.263443   -0.750580
F   1.305105   -1.079761   -0.204176
O   0.587478   0.489906   1.188430
H   -1.200011   -1.646523   0.062837
Frequencies[1/cm]
3144.72 3077.00 1652.41 1487.81
1433.67 1276.32 1192.06 1145.72
999.20 886.03 641.04 483.45
464.26 308.06 247.20 206.95
102.98 -738.18
!**
Barrier TS7
Geometry[angstrom]
C   0.704531   0.082977   -0.681279
C   -0.536660   -0.236290   -0.181696
F   0.331041   1.385283   0.783746
H   0.779714   0.736160   -1.535967
F   -1.639569   0.265038   -0.632783
F   -0.703981   -1.088804   0.785840
O   1.825928   -0.502256   -0.290342
H   1.718209   -0.851889   0.605320
Frequencies[1/cm]
3778.86 3276.02 1740.70 1443.39
1386.49 1349.64 1205.70 923.61
892.89 637.79 555.85 491.46
431.81 310.72 247.93 228.17

144.28 -387.42
!**

Barrier TS8
Geometry[angstrom]
C   0.760681   -0.271376   -0.401095
C   -0.628368   -0.036779   0.125651
F   1.536968   0.847881   -0.359553
H   0.873984   -0.742583   -1.376348
F   -1.622671   -0.652523   -0.508401
F   -0.978067   1.189086   0.479199
O   1.008886   -1.136217   0.676329
H   -0.165030   -0.778755   1.117166
Frequencies[1/cm]
3138.07 2039.74 1442.79 1350.80
1292.58 1223.55 1141.24 1085.86
1039.72 978.38 706.74 629.36
541.19 457.92 369.24 226.85
116.55 -2346.01
!**

Barrier TS9
Geometry[angstrom]
C   -0.475843   -0.060671   -0.630778
C   0.824724   0.021534   -0.100409
F   -1.736926   -0.826108   0.695795
H   -0.672462   -0.907290   -1.283038
F   1.695755   -0.926612   -0.253473
F   1.231187   0.981789   0.656144
O   -1.273953   0.963688   -0.538850
H   -1.939356   0.370987   0.094759
Frequencies[1/cm]
3176.50 2246.74 1648.01 1474.98
1384.57 1306.28 1036.77 937.63
816.35 720.10 637.63 482.05
478.09 429.68 243.92 135.52
74.65 -1316.60
!**

Barrier TS10
Geometry[angstrom]
C   -0.412877   0.003123   -0.004186
C   0.968983   -0.644242   0.062889
F   -0.387258   1.193311   -0.585146
H   0.969280   -1.688436   0.400392
F   -1.252676   -0.793841   -0.680360
F   -0.902114   0.146261   1.240021
O   1.984474   -0.018433   -0.176358
H   2.696723   0.771027   0.887611
Frequencies[1/cm]
3060.54 1768.04 1401.71 1324.70
1209.55 1179.64 956.40 857.57
707.28 601.10 538.53 529.30
432.32 325.23 262.52 163.74

54.27 -1947.79
!**

Barrier TS11
Geometry[angstrom]
C   -0.509137   -0.211286   0.076047
C   0.665024   -1.005871   0.012547
F   -0.839114   0.503261   1.105600
H   0.629558   -2.033769   -0.330042
F   0.475541   1.318638   -0.656997
F   -1.543370   -0.521940   -0.636889
O   1.775942   -0.375691   0.203880
H   1.390066   0.642601   -0.137995
Frequencies[1/cm]
3203.50 1934.02 1618.25 1441.76
1381.29 1280.44 1232.60 932.02
763.08 739.37 708.16 609.37
476.74 437.98 362.81 246.30
181.93 -1123.42
!**

Barrier TS12
Geometry[angstrom]
C   -0.812917   -0.017811   0.349238
C   0.979501   0.146718   -0.353998
F   -1.315926   -1.133910   -0.145148
H   -0.640434   -0.042947   1.422304
F   1.472105   -1.041791   0.137874
F   -1.486472   1.028295   -0.076891
O   1.369470   1.201602   0.094654
H   0.657804   -0.016651   -1.393483
Frequencies[1/cm]
3170.34 3011.21 1632.23 1370.48
1316.06 1223.01 1189.67 1137.97
1002.68 964.44 644.07 587.22
378.34 351.59 299.72 164.15
60.64 -478.71
!**

Barrier TS13
Geometry[angstrom]
C   0.705893   -0.021424   -0.364184
C   -0.775968   0.149818   0.037121
F   1.231041   -1.134099   0.188038
H   0.775106   -0.094712   -1.452476
F   -1.408646   -1.042344   -0.082260
F   1.402015   1.046011   0.061581
O   -1.369032   1.185060   0.033863
H   -0.422102   0.017760   1.637724
Frequencies[1/cm]
3101.24 1845.91 1390.90 1378.17
1191.46 1171.75 1107.88 961.49
725.27 624.74 599.68 567.99
482.37 462.39 360.32 224.74

75.45 -1235.92
!**
Barrier TS14
Geometry[angstrom]
C   0.399062   -0.012737   -0.008187
C   -0.961063   -0.662926   -0.073998
F   1.339163   -0.877730   -0.415086
H   -1.009343   -1.702876   0.244402
F   0.472057   1.078732   -0.773265
F   0.696728   0.351293   1.249576
O   -2.057784   0.136224   0.087266
H   -1.727913   -0.303595   -1.000453
Frequencies[1/cm]
3143.41 2494.22 1402.11 1302.85
1203.85 1187.42 1178.10 917.46
858.04 690.68 671.73 548.69
518.66 423.93 331.25 227.40
93.59 -2126.79

!**
Barrier TS15
Geometry[angstrom]
C   -0.542284   -0.017227   -0.000001
C   1.434966   0.675039   -0.000010
F   -1.306058   1.056887   -0.000006
F   -0.716117   -0.728933   1.084249
O   2.101782   -0.350353   -0.000002
H   1.237230   1.232488   0.934261
F   -0.716140   -0.728958   -1.084231
H   1.237259   1.232495   -0.934284
Frequencies[1/cm]
2976.13 2910.31 1665.86 1499.77
1311.00 1285.29 1249.14 1159.75
980.94 644.65 628.94 531.81
516.44 311.40 183.26 143.38
72.04 -418.40

!**
!   Products
!**

Bimolecular P1
Fragment1 CH2FCFO
Geometry[angstrom]
C   0.741724   -0.734759   0.000071
C   -0.621765   -0.077193   0.000002
F   1.767889   0.173727   -0.000077
H   0.812167   -1.363570   -0.889299
F   -0.558418   1.259219   0.000046
O   -1.653669   -0.662242   -0.000061
H   0.812198   -1.363304   0.889630
Frequencies[1/cm]
3137.47 3084.26 1893.06 1490.37
1408.71 1283.21 1257.68 1116.90

```
1044.90 842.26 632.62 551.16
495.47 255.35 43.70
!*********
Fragment2 F
Atom
!************************************************

Bimolecular P2
Fragment1 CF2O
Geometry[angstrom]
C          0.000000    0.142570    0.000000
F         -1.061750   -0.633097    0.000000
F          1.061756   -0.633085    0.000000
O         -0.000007    1.317527    0.000000
Frequencies[1/cm]
1960.46 1255.37 974.05 782.11
619.26 584.49
!*********
Fragment2 CH2F
Geometry[angstrom]
C          0.027407    0.656474    0.000000
F          0.027407   -0.683287    0.000000
H         -0.205551    1.105372    0.953901
H         -0.205551    1.105372   -0.953901
Frequencies[1/cm]
3319.15 3161.74 1484.88 1187.01
1185.09 602.98
!************************************************

Bimolecular P3
Fragment1 CHFCFO
Geometry[angstrom]
C           -0.740425   -0.611887    0.000000
C            0.496646    0.135021    0.000000
F           -1.861843    0.071571    0.000000
H           -0.823315   -1.686887    0.000000
F            1.537586   -0.732754    0.000000
O            0.650537    1.312341    0.000000
Frequencies[1/cm]
3273.97 1929.25 1479.06 1255.43
1147.85 943.53 695.88 659.27
480.58 454.75 253.92 192.73
!*********
Fragment2 HF
Geometry[angstrom]
F          0.000000    0.000000    0.092108
H          0.000000    0.000000   -0.828968
Frequencies[1/cm]
4123.19
!************************************************

Bimolecular P4
Fragment1 C2F3
Geometry[angstrom]
```

```
C           0.775619   -0.599412   -0.000002
C          -0.415499   -0.062054    0.000000
F           1.947314   -0.030663    0.000001
F          -1.527374   -0.765269    0.000001
F          -0.660020    1.236909    0.000000
Frequencies[1/cm]
1976.50 1312.10 1251.46 953.81 629.27 574.58
490.73 298.36 214.46
!*********
Fragment2 H2O
Geometry[angstrom]
O              0.000000    0.000000    0.117724
H              0.000000    0.759692   -0.470895
H              0.000000   -0.759692   -0.470895
Frequencies[1/cm]
3938.88 3824.01 1644.89
!************************************************

Bimolecular P5
Fragment1 CF2CHO
Geometry[angstrom]
C              0.000000    0.403943    0.000000
C             -0.626498   -0.874684    0.000000
F              1.283931    0.587769    0.000000
H             -1.726417   -0.822115    0.000000
F             -0.677169    1.523055    0.000000
O              0.003068   -1.918856    0.000000
Frequencies[1/cm]
3012.98 1685.82 1521.05 1434.86
1325.59 954.99 875.45 647.43
484.10 353.17 244.74 219.66
!*********
Fragment2 HF
Geometry[angstrom]
F          0.000000    0.000000    0.092108
H          0.000000    0.000000   -0.828968
Frequencies[1/cm]
4123.19
!************************************************

Bimolecular P6
Fragment1 CF3CHO
Geometry[angstrom]
C             0.361049    0.005729   -0.000003
C            -1.065946   -0.571660   -0.000009
F             0.376100    1.328217   -0.000106
H            -1.092790   -1.674184   -0.000002
F             1.016179   -0.436790    1.084001
F             1.016261   -0.436964   -1.083885
O            -2.044336    0.122450   -0.000002
Frequencies[1/cm]
3003.58 1822.18 1411.14 1330.09
1213.14 1190.46 981.85 852.48
711.02 533.66 530.09 432.07
```

```
312.26 253.40 72.76
!*********
Fragment2 H
Atom
!**************************************************

Bimolecular P7
Fragment1 CF2HCFO
Geometry[angstrom]
C            0.690835   -0.134275    0.353336
C           -0.767828    0.188190    0.017909
F            1.444165    0.959278    0.160055
H            0.797624   -0.477517    1.384123
F           -1.513992   -0.908227    0.230469
F            1.116322   -1.113762   -0.481197
O           -1.219266    1.214803   -0.349442
Frequencies[1/cm]
3112.83 1923.02 1430.12 1382.16
1202.74 1171.22 1109.95 932.25
754.77 609.57 568.41 427.45
311.83 229.68 50.89
!*********
Fragment2 H
Atom
!**************************************************

Bimolecular P8
Fragment1 CHFO
Geometry[angstrom]
C            0.126360    0.378401    0.000042
F           -1.089403   -0.195971   -0.000007
O            1.129218   -0.246515   -0.000047
H            0.012723    1.465452    0.000181
Frequencies[1/cm]
3126.12 1865.88 1374.87 1081.07
1036.58 665.54
!*********
Fragment2 CF2H
Geometry[angstrom]
C           -0.000004    0.487635   -0.150309
F            1.093737   -0.241925    0.028225
H           -0.000007    1.428868    0.393798
F           -1.093734   -0.241928    0.028225
Frequencies[1/cm]
3155.10 1348.89 1200.27 1184.80
1030.52 553.92
!**************************************************

Bimolecular P9
Fragment1 CH2O
Geometry[angstrom]
C          -0.530909    0.000000    0.000000
H          -1.112400   -0.938548    0.000000
O           0.676281   -0.000001    0.000000
```

```
H          -1.112393    0.938550    0.000000
Frequencies[1/cm]
3001.74 2935.72 1783.55 1538.22
1268.08 1199.32
!*********
Fragment2 CF3
Geometry[angstrom]
C          -0.000013    0.000010    0.324772
F           1.024191   -0.726495   -0.072169
F          -1.141257   -0.523722   -0.072173
F           0.117075    1.250210   -0.072173
Frequencies[1/cm]
1271.46 1271.36 1099.93 708.52
511.52 511.50
!************************************************
```

III. CCl_2=CHCl + OH reaction:

```
Reactant1 CCl2=CHCl
Geometry[angstrom]
C       0.00000000    0.00000000    0.00000000
H       0.00000000    0.00000000    1.08234000
Cl      1.53551603    0.00000000   -0.74837788
C      -1.14020942   -0.00000000   -0.67559018
Cl     -2.64453008   -0.00000000    0.15522967
Cl     -1.23605065    0.00000000   -2.38102928
Frequencies[1/cm]
3142.38 1639.95 1230.07 941.39
851.23 819.56 632.95 470.86
383.71 265.26 193.45 163.61
!************************************************

Reactant2 OH
Geometry[angstrom]
O            0.00000000    0.00000000    0.00000000
H            0.00000000    0.00000000   -0.97015000
Frequencies[1/cm]
3700.73
!************************************************

Well PRCadd
Geometry[angstrom]
C           0.594024    0.421130   -0.801263
Cl          2.194392   -0.123527   -0.509787
H           0.501243    1.284770   -1.441769
C          -0.486210   -0.159638   -0.269367
Cl         -0.427273   -1.523056    0.761465
Cl         -2.052767    0.454876   -0.613543
O           0.323346    1.990704    1.533127
H           1.121126    1.479665    1.752217
Frequencies[1/cm]
3745.54 3250.33 1648.24 1276.48
957.92 858.38 808.72 642.29
479.02 392.61 305.21 279.10
```

213.55 173.65 136.63 89.46
44.32 38.73
!**

Well PRCabs
Geometry[angstrom]
C   -0.048061   0.858482   0.000201
C   -0.144695   -0.473019   0.000082
H   0.915403   1.348579   0.000448
O   3.336994   1.401684   -0.000129
H   3.257210   0.431385   -0.000373
Cl   -1.413263   1.891129   -0.000048
Cl   -1.617376   -1.340505   -0.000335
Cl   1.282873   -1.450990   0.000339
Frequencies[1/cm]
3729.47 3231.08 1642.64 1300.77
947.00 860.54 836.69 641.91
467.16 390.03 281.47 263.43
207.20 173.05 98.00 91.14
56.38 14.03
!**

Well POSTabs
Geometry[angstrom]
C   0.725330   0.215316   -0.547532
C   -0.361473   -0.414781   -0.205156
H   -0.975535   2.419995   0.510833
O   -0.208481   2.871779   0.877244
H   -0.535635   3.740129   1.128101
Cl   -0.368591   -1.870025   0.727172
Cl   -1.918066   0.185390   -0.659014
Cl   2.345238   0.041249   -0.311732
Frequencies[1/cm]
3922.15 3806.51 1888.10 1644.64
897.37 873.60 609.58 498.70
398.26 264.70 224.63 189.52
163.57 128.93 75.94 73.43
32.71 13.72
!**

Well IM1
Geometry[angstrom]
C   0.828991   -0.088886   0.728114
C   -0.605816   0.100637   0.366539
H   0.923059   -0.869159   1.478266
O   1.440208   1.045652   1.204763
H   1.318312   1.757511   0.562839
Cl   -1.019453   1.472035   -0.559872
Cl   -1.588201   -1.277180   0.230695
Cl   1.719296   -0.743331   -0.744184
Frequencies[1/cm]
3785.14 3161.14 1437.76 1307.18
1238.73 1190.25 1087.39 971.49
650.58 639.46 476.43 454.84

412.43 318.35 270.85 202.44
134.11 67.02
!**

Well IM2
Geometry[angstrom]
C   0.807100   -0.020374   1.276983
C   -0.103336   -0.020062   0.119081
H   0.447536   0.347170   2.225761
O   2.135337   0.082914   1.090839
H   2.361805   -0.261946   0.214955
Cl   0.486355   -1.175590   -1.120858
Cl   -1.727835   -0.466598   0.647392
Cl   -0.177027   1.612429   -0.676170
Frequencies[1/cm]
3752.49 3254.33 1451.37 1352.30
1222.92 1062.74 866.55 682.36
580.07 559.82 461.80 436.96
325.61 299.15 264.59 236.04
188.40 104.85
!**

Well IM3
Geometry[angstrom]
C   -0.656963   -0.658766   -0.328638
C   0.499821   0.077008   0.388232
H   0.345282   0.055329   1.463407
O   -0.660258   -1.973621   -0.092209
H   -0.531637   -0.546075   -1.417159
Cl   -2.219788   0.135294   0.109217
Cl   0.568871   1.769203   -0.121116
Cl   2.028051   -0.741540   0.031537
Frequencies[1/cm]
3156.05 2988.44 1289.19 1246.56
1192.35 1148.51 1091.61 990.98
823.17 760.86 733.03 449.55
355.00 333.99 314.63 250.31
172.79 62.38
!**

Well IM4
Geometry[angstrom]
C   -0.878313   -0.058918   0.929019
C   0.505990   0.006994   0.418267
H   -1.042853   -0.269203   1.973588
O   1.339040   0.014769   1.503308
H   2.252268   0.036864   1.190602
Cl   0.756424   1.479112   -0.603838
Cl   0.868850   -1.423288   -0.650695
Cl   -2.195145   -0.030782   -0.114547
Frequencies[1/cm]
3804.70 3261.97 1404.09 1301.63
1138.17 1093.79 898.04 724.04
550.19 507.79 425.52 382.75

```
369.43 290.34 270.10 185.00
154.63 51.14
!************************************************

Well IM5
Geometry[angstrom]
C          -0.874151   -0.012963    0.589829
C           0.597419    0.179806    0.576887
H           0.909760    0.556589    1.546546
O          -1.524244    0.990084    1.222463
H          -2.475793    0.867013    1.120368
Cl          1.443800   -1.342949    0.277000
Cl         -1.638854   -0.691097   -0.796695
Cl          1.102135    1.425497   -0.624242
Frequencies[1/cm]
3815.06 3158.31 1397.15 1311.02
1232.80 1201.59 1078.88 825.00
692.83 623.54 548.84 460.62
381.52 325.77 265.07 170.85
155.51 68.27
!************************************************

Well IM6
Geometry[angstrom]
C          -0.412712   -0.072344    0.268990
C           0.692657   -0.857520   -0.474782
H           0.619997   -1.903333   -0.185971
O          -0.218656   -0.226448    1.576425
Cl          2.321398   -0.272786   -0.107906
Cl         -1.978648   -0.793889   -0.275814
Cl         -0.404693    1.656862   -0.184052
H           0.502616   -0.739070   -1.538567
Frequencies[1/cm]
3188.11 3115.22 1463.68 1314.50
1247.42 1076.33 969.02 903.10
797.77 756.06 600.39 421.50
343.23 307.42 264.55 232.56
149.21 104.04

!************************************************
!                   Transition states
!************************************************

Barrier TSabs
Geometry[angstrom]
C           0.000000    0.000000    0.000000
C           0.000000    0.000000    1.320834
H           1.076838    0.000000    1.934812
Cl          1.473012    0.000000   -0.894307
Cl         -1.433946    0.000000   -0.942102
Cl         -1.332713    0.000000    2.354143
O           2.207623   -0.000130    2.411515
H           2.735380   -0.000265    1.596704
Frequencies[1/cm]
```

3762.73 1874.91 1423.50 975.85
902.62 839.13 770.09 677.83
476.39 450.94 349.94 279.67
215.09 165.80 123.86 106.68
49.46 -2013.23
!**

Barrier TSadd-CHCl
Geometry[angstrom]
C   -0.611981   -0.616897   -0.474166
C   0.505766   0.083102   -0.198176
H   -0.543798   -1.569588   -0.973705
O   -0.534126   -1.689261   1.318222
H   -0.780491   -0.960004   1.908818
Cl   0.494703   1.662060   0.446173
Cl   2.041983   -0.626572   -0.431786
Cl   -2.169945   0.096657   -0.452437
Frequencies[1/cm]
3763.15 3264.06 1593.30 1275.31
976.11 913.98 860.98 744.10
644.89 476.76 398.06 286.43
219.23 179.01 176.47 129.56
89.75 -515.01
!**

Barrier TSadd-CCl_2
Geometry[angstrom]
C   0.672139   -0.830163   -0.365888
C   -0.398255   -0.034786   -0.135117
H   0.530632   -1.877172   -0.588652
O   -0.237159   -0.479043   1.849182
H   -0.618011   -1.371009   1.868759
Cl   2.277297   -0.291587   -0.270456
Cl   -1.973336   -0.650529   -0.494222
Cl   -0.283881   1.663894   -0.004000
Frequencies[1/cm]
3762.14 3244.48 1572.21 1289.21
965.19 877.94 802.22 771.03
636.75 407.31 365.14 296.30
258.39 231.18 196.49 155.69
131.37 -629.10
!**

Barrier TS1
Geometry[angstrom]
C   0.738742   -0.168881   1.242660
C   -0.147490   -0.279910   0.180843
H   0.396382   0.185774   2.204193
O   2.038703   -0.354225   1.145303
H   2.261726   -0.624382   0.238877
Cl   0.383692   -1.157820   -1.213468
Cl   -1.827333   -0.365995   0.531371
Cl   0.119214   1.874706   -0.502992
Frequencies[1/cm]

3700.91 3251.65 1582.14 1386.79
1289.05 1205.02 970.43 868.31
631.73 569.84 477.73 304.57
300.75 250.42 229.39 162.74
129.27 -329.19
!**

Barrier TS2
Geometry[angstrom]
C 0.682066 -0.850605 -0.060821
C -0.565473 -0.030088 0.216837
H -0.382905 -0.518671 1.402516
O 0.664303 -1.297384 1.273214
H 0.555542 -1.647167 -0.790054
Cl -2.035383 -0.681607 -0.449932
Cl -0.481354 1.695421 0.258571
Cl 2.152818 0.034955 -0.498890
Frequencies[1/cm]
3140.76 2058.68 1315.42 1258.41
1148.12 1074.23 998.36 886.34
832.67 761.41 503.82 460.92
398.60 277.17 236.59 173.81
76.32 -2222.95
!**

Barrier TS3
Geometry[angstrom]
C 0.641494 -0.584055 0.072740
C -0.530616 0.079846 -0.019506
H 0.612162 -0.624412 1.905745
O 0.686171 -1.915892 -0.144580
H 1.442458 -2.283612 0.328976
Cl -2.005010 -0.781575 -0.023808
Cl -0.634274 1.779923 -0.002943
Cl 2.156387 0.252265 -0.055453
Frequencies[1/cm]
3805.13 1657.37 1282.01 1197.79
1003.24 830.62 674.25 594.73
519.40 499.25 407.82 368.21
296.76 260.99 257.04 181.94
113.23 -1223.03
!**

Barrier TS4
Geometry[angstrom]
C 0.826038 -0.783142 0.432838
C -0.617205 0.109076 -0.407775
H 0.565139 -0.456462 1.448847
O 0.706045 -1.938698 0.048244
H -0.310060 0.002994 -1.441517
Cl -0.624862 1.749263 0.125860
Cl -2.052733 -0.764868 -0.030010
Cl 2.256628 0.192514 -0.127829
Frequencies[1/cm]

3192.25 3005.68 1464.92 1258.79
1244.31 1072.04 959.14 864.96
735.40 683.42 437.78 350.08
332.76 270.95 218.56 149.97
55.06 -727.29
!**

Barrier TS5
Geometry[angstrom]
C   -0.657431   -0.746574   0.132351
C   0.521804   0.095284   -0.420588
H   0.387104   0.138572   -1.500587
O   -0.614115   -1.921094   0.324507
H   -0.523423   -0.135863   1.665465
Cl   2.046944   -0.715629   -0.083236
Cl   0.525847   1.754622   0.184488
Cl   -2.227909   0.094759   -0.161929
Frequencies[1/cm]
3126.76 1837.31 1251.83 1230.30
984.39 850.04 795.59 736.86
611.78 519.39 488.14 407.07
329.21 307.99 247.09 174.30
54.48 -1198.23
!**

Barrier TS6
Geometry[angstrom]
C   -0.820859   -0.405214   0.772759
C   0.477371   0.428902   0.637665
H   -0.724512   -1.339062   1.320997
O   -0.994557   0.728412   1.449500
H   1.135670   0.550843   1.481822
Cl   0.626603   1.607879   -0.593973
Cl   1.679992   -1.251213   -0.053549
Cl   -1.741522   -0.661442   -0.697265
Frequencies[1/cm]
3260.08 3147.87 1330.63 1295.79
1240.65 1133.81 1107.24 904.94
810.31 679.39 513.77 430.93
337.78 256.57 207.93 151.76
97.62 -1030.73
!**

Barrier TS7
Geometry[angstrom]
C   0.267713   -0.707703   0.647160
C   0.004692   0.402055   -0.298312
H   -0.017851   0.203978   -1.357224
O   -0.457580   -1.730585   0.477150
H   0.639282   -0.437474   1.637110
Cl   2.139007   -0.658938   -0.281923
Cl   0.109189   2.010610   0.177654
Cl   -2.165563   -0.415668   -0.259859
Frequencies[1/cm]

3280.54 3106.17 1448.14 1331.01
1263.43 1150.17 1035.80 974.14
887.03 546.22 508.17 438.81
318.88 267.62 196.90 163.73
85.49 -580.09
!**

Barrier TS8
Geometry[angstrom]
C 0.749625 0.288517 0.864289
C -0.397599 -0.405539 0.532806
H 0.732293 0.921825 1.738518
O -1.333250 -0.534720 1.472877
H -2.196590 -0.642142 1.049508
Cl -0.423181 -1.542237 -0.755930
Cl -1.147914 1.563703 -0.542546
Cl 2.160397 0.255017 -0.051737
Frequencies[1/cm]
3777.14 3250.09 1522.24 1326.79
1236.79 1209.68 928.64 744.25
646.67 500.01 430.07 364.97
311.09 267.23 194.38 160.70
109.74 -334.2849
!**

Barrier TS9
Geometry[angstrom]
C -0.474563 -0.068194 0.282850
C 0.762782 -0.927747 0.117208
H 0.585233 -1.016255 1.411935
O -0.508153 -0.342955 1.639941
Cl 2.278635 -0.256788 -0.327622
Cl -1.900411 -0.711595 -0.574075
Cl -0.308960 1.654141 -0.078188
H 0.573189 -1.922360 -0.273767
Frequencies[1/cm]
3179.17 2031.22 1273.44 1153.55
1130.11 1033.89 942.28 870.71
765.52 646.36 491.26 470.34
372.67 288.53 253.96 166.27
100.20 -2115.30
!**

Barrier TS10
Geometry[angstrom]
C -0.552822 0.000114 0.451108
C 0.830662 -0.885046 -0.497008
O -0.275580 -0.221156 1.606833
Cl -0.446284 1.668114 -0.217695
H 0.511686 -0.654472 -1.506363
H 0.670716 -1.895304 -0.142558
Cl 2.364667 -0.251234 -0.100911
Cl -1.956313 -0.850491 -0.324356
Frequencies[1/cm]

3266.02 3140.73 1524.97 1432.57
1119.69 1086.06 835.32 790.50
719.21 545.98 461.52 398.02
301.92 248.40 205.84 148.05
96.88 -531.12
!**

Barrier TS11
Geometry[angstrom]
C   -0.839646   -0.131089   0.574860
C   0.628371   -0.128176   0.891680
H   -1.344640   -0.420241   1.498287
O   1.305688   -1.151087   1.131921
H   2.185308   -0.633347   0.393839
Cl   2.055363   0.550033   -0.632575
Cl   -1.253748   -1.338340   -0.660740
Cl   -1.390940   1.483477   0.131742
Frequencies[1/cm]
3103.27 1686.45 1572.55 1218.61
1205.49 969.95 858.07 819.06
706.37 530.82 500.31 449.52
319.42 262.37 177.83 64.80
40.97 -1869.84
!**

Barrier TS12
Geometry[angstrom]
C   0.158981   0.085738   0.265964
C   -0.251844   -0.781602   -0.836883
H   -0.415696   -1.819590   -0.601049
O   -0.498016   -0.043167   1.326165
Cl   1.907012   -1.031166   0.030079
Cl   -2.295165   -0.283973   -0.115398
Cl   0.688741   1.715564   -0.192003
H   -0.152991   -0.467122   -1.868281
Frequencies[1/cm]
3330.78 3192.76 1475.53 1302.88
1179.90 1083.91 1015.51 892.41
651.02 554.87 536.97 432.04
350.29 285.75 222.76 207.63
105.90 -875.90
!**

Barrier TS13
Geometry[angstrom]
C   0.599546   0.000000   0.348624
C   -0.663487   0.000000   1.214759
O   0.960727   0.000000   1.617827
H   -0.997028   0.936134   1.631491
Cl   -2.160285   0.000000   -0.344107
Cl   0.924022   -1.455542   -0.580473
H   -0.997028   -0.936134   1.631491
Cl   0.924021   1.455542   -0.580473
Frequencies[1/cm]

```
3331.35 3198.04 1443.25 1288.51
1180.08 1139.77 1002.22 863.41
771.29 545.04 511.54 400.27
332.95 265.07 253.87 141.12
107.37 -902.46

!************************************************
!                        Products
!************************************************

Bimolecular P1
Fragment1 C2Cl3
Geometry[angstrom]
C             -0.673316    0.461346    0.000000
C             -0.673316    0.461346    1.303370
Cl             0.458685    0.461346   -1.201614
Cl            -2.140195    0.461346    2.204270
Cl             0.781516    0.461346    2.240009
Frequencies[1/cm]
1884.21 906.92 866.12 611.44 500.94 399.29 265.25
212.11 132.31
!*********
Fragment2 H2O
Geometry[angstrom]
O              0.000000    0.000000    0.117724
H              0.000000    0.759692   -0.470895
H              0.000000   -0.759692   -0.470895
Frequencies[1/cm]
3938.88 3824.01 1644.89
!************************************************

Bimolecular P2
Fragment1 CCl2CClOH
Geometry[angstrom]
C            0.658546   -0.588260    0.000041
C           -0.493925    0.103029   -0.000006
H           -0.143305   -2.296407    0.000194
O            0.754227   -1.931117    0.000147
Cl          -1.989509   -0.766871    0.000079
Cl          -0.600501    1.807802   -0.000139
Cl           2.185408    0.174170   -0.000033
Frequencies[1/cm]
3741.86 1684.53 1344.71 1193.58
996.19 832.05 576.80 539.23
419.46 407.34 367.26 286.83
264.28 181.11 125.66
!*********
Fragment2 H
Atom
!************************************************

 Bimolecular P3
 Fragment1 CCl2CHOH
 Geometry[angstrom]
```

```
 C          0.00000000    0.00000000    0.00000000
 C          0.00000000    0.00000000    1.32654000
 H          0.94464266    0.00000000   -0.53633430
 O         -1.14806471   -0.00000260   -0.70910351
 H         -0.96278322    0.00001595   -1.64733380
 Cl        -1.44747018    0.00000126    2.24024109
 Cl         1.47423418   -0.00000334    2.21065727
 Frequencies[1/cm]
3831.80 3107.12 1714.67 1305.18
1238.40 1158.62 955.46 858.38
646.88 469.95 452.77 274.27
268.85 195.43 178.35
!*********
Fragment2 Cl
Atom
!************************************************

Bimolecular P4
Fragment1 CHClO
Geometry[angstrom]
C           0.000000    0.794514    0.000000
H          -0.887695    1.434923    0.000000
O           1.128644    1.157770    0.000000
Cl         -0.478909   -0.909657    0.000000
Frequencies[1/cm]
3083.44 1809.83 1341.02 954.82
745.52 460.18
!*********
Fragment2 CHCl2
Geometry[angstrom]
C          -0.011637    0.693622    0.000000
H           0.465474    1.661062    0.000000
Cl         -0.011637   -0.171259    1.463221
Cl         -0.011637   -0.171259   -1.463221
Frequencies[1/cm]
3244.20 1254.82 909.96 773.34
485.67 307.80
!************************************************

Bimolecular P5
Fragment1 CHCl2CClO
Geometry[angstrom]
C           0.618659   -0.000003    0.604829
C          -0.909786   -0.000005    0.629977
H           0.963068   -0.000009    1.634131
O          -1.533134   -0.000015    1.643525
Cl         -1.666698    0.000009   -0.954359
Cl          1.217137    1.468288   -0.175494
Cl          1.217136   -1.468287   -0.175510
Frequencies[1/cm]
3168.74 1818.33 1266.95 1256.25
1100.90 818.45 802.66 643.02
593.17 508.33 414.18 261.18
174.64 167.13 50.69
```

```
!*********
Fragment2 H
Atom
!************************************************

Bimolecular P6
Fragment1 CHClOCHCl
Geometry[angstrom]
C          -0.731125    0.750650    0.378937
C           0.731126    0.750649    0.378937
H          -1.293988    1.406052    1.031952
O          -0.000002    1.387902   -0.653010
H           1.293989    1.406057    1.031944
Cl          1.644023   -0.674209   -0.040796
Cl         -1.644023   -0.674210   -0.040796
Frequencies[1/cm]
3194.53 3183.97 1389.45 1324.62
1287.49 1130.77 1125.92 957.22
830.02 821.55 681.14 485.89
430.68 325.64 160.79
!*********
Fragment2 Cl
Atom
!************************************************

Bimolecular P7
Fragment1 CHCl2CHO
Geometry[angstrom]
C           1.348766   -0.000080    0.380835
C           0.038982   -0.000014   -0.393718
H           0.214339   -0.000021   -1.464557
O           2.419274   -0.000129   -0.169346
H           1.229246   -0.000077    1.477983
Cl         -0.856502    1.467886    0.041724
Cl         -0.856690   -1.467786    0.041725
Frequencies[1/cm]
3174.71 2991.84 1792.66 1402.49
1248.27 1230.75 1080.82 1015.09
796.63 751.58 443.22 325.25
284.30 255.4050 83.11
!*********
Fragment2 Cl
Atom
!************************************************

Bimolecular P8
Fragment1 CCl2O
Geometry[angstrom]
C           0.000000    0.000000    0.495138
Cl          0.000000    1.444513   -0.481746
Cl          0.000000   -1.444513   -0.481746
O           0.000000    0.000000    1.676067
Frequencies[1/cm]
1837.87 854.54 591.20 578.20
```

```
445.43 304.80
!*********
Fragment2 CH2Cl
Geometry[angstrom]
C           0.000000   -1.111876    0.000000
H           0.000001   -1.615000    0.951240
H           0.000001   -1.615000   -0.951240
Cl          0.000000    0.582427    0.000000
Frequencies[1/cm]
3351.35 3200.34 1437.69 1009.38
857.15 123.25
!*************************************************

Bimolecular P9
Fragment1 CHCl2CO
Geometry[angstrom]
C           0.093406   -0.005453    0.567133
C          -0.686229   -1.305786    0.350390
H           0.237145    0.152596    1.631513
O          -1.617431   -1.510375   -0.336745
Cl         -0.732234    1.418649   -0.094346
Cl          1.688660   -0.254070   -0.166988
Frequencies[1/cm]
3162.17 1926.46 1258.49 1216.05
843.66 798.01 697.80 601.28
371.03 279.27 201.92 73.70
!*********
Fragment2 HCl
Geometry[angstrom]
H           0.000000    0.000000   -1.205622
Cl          0.000000    0.000000    0.070919
Frequencies[1/cm]
3006.48
!*************************************************

Bimolecular P10
Fragment1 CH2ClCClO
Geometry[angstrom]
C          -0.646480    0.630187    0.046909
C           0.709061    0.608455    0.720487
H           1.072587    1.629840    0.794323
O          -1.167169    1.594239   -0.414769
Cl          1.863854   -0.332380   -0.251628
H           0.634048    0.142318    1.700690
Cl         -1.437076   -0.959262    0.029203
Frequencies[1/cm]
3187.11 3112.42 1832.94 1476.31
1299.37 1214.61 1061.31 947.38
799.35 641.27 577.35 455.10
357.40 174.36 54.63
!*********
Fragment2 Cl
Atom
!*************************************************
```

```
Bimolecular P11
Fragment1 CH2OCCl2
Geometry[angstrom]
C          -0.000010    0.234184   -0.016674
C           0.000045    1.568254   -0.601647
O           0.000023    1.317550    0.836801
H           0.929323    1.970777   -0.986440
Cl         -1.455861   -0.743994   -0.029754
Cl          1.455830   -0.744044   -0.029750
H          -0.929195    1.970850   -0.986459
Frequencies[1/cm]
3246.96 3138.44 1522.07 1354.03
1172.96 1117.57 1080.14 997.29
822.71 756.63 515.91 435.96
358.07 308.46 278.78
!*********
Fragment2 Cl
Atom
!************************************************

Bimolecular P12
Fragment1 CHClCClOH
Geometry[angstrom]
C           0.00000000    0.00000000    0.00000000
C           0.00000000    0.00000000    1.32531000
H           0.93998943    0.00000000   -0.53513079
O           1.14801537   -0.04965008    2.02663019
H           0.99530296    0.21365134    2.93628589
Cl         -1.44000211    0.02648288    2.27017387
Cl         -1.42354721   -0.02189715   -0.94807389
Frequencies[1/cm]
3798.79 3152.96 1707.93 1284.72
1186.94 1171.16 884.03 787.81
647.47 515.24 473.31 385.64
254.36 173.82 161.82
!*********
Fragment2 Cl
Atom
```

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