Electronic Supplementary Material (ESI) for Polymer Chemistry.

RAFT synthesis of PVDF-*b*-PVAc block copolymers.

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SUPPORTING INFORMATION

RAFT Homopolymerization of VDF

Using the experimental setup described above, a typical polymerization (entry 1 in Table 1) of VDF was performed as follows: A solution of Trigonox 121 (158 mg, 6.87 10^{-4} mol) and CTA_{XA} (1.30 g, 6.25 10^{-3} mol) in DMC (60 mL), was degassed by N_2 bubbling during 30 min. This homogenous solution was introduced into the autoclave using a funnel, VDF gas (19.0 g, 2.97 10^{-1} mol) was transferred in the autoclave at low temperature, and the reactor was gradually heated to 73 °C. The reaction was stopped after 18 h. During the reaction, the pressure increased to a maximum of 25 bars and then decreased to 10 bars after 24 h. The autoclave was cooled down to room temperature (ca. 20 °C), purged from the residual monomers and DMC was removed under vacuum. The crude product was dissolved in 30 mL of warm THF (ca. 40 °C), and left under vigorous stirring for 30 minutes. This polymer solution was then precipitated from 400 mL of chilled hexane. The precipitated polymer (white powder) was filtered through a filter funnel and dried under vacuum ($15 \cdot 10^{-3}$ bar) for two hours at 50°C. The polymerization yield (65%) was determined gravimetrically (mass of dried precipitated polymers / mass of monomer introduced in the pressure reactor). Yields were used as conversion, since conversion is very difficult to measure accurately for VDF or other gaseous monomers.

DP and $M_{n(NMR)}$ calculations:

The degree of polymerization (DP) of PVDF can be calculated according to equations (S1) and (S2):[1]

$$(S1) \quad DP = \frac{\int_{2.70}^{3.19} \mathrm{CH_2\ (HT)} + \int_{2.28}^{2.43} \mathrm{CH_2(TT)} + \int_{4.02}^{4.17} \mathrm{CH_2(End-group)}}{2/3 \times \int_{1.19}^{1.24} \mathrm{CH_3\ (R-CTA_{XA})}}$$

$$(S2) \quad M_{n,NMR}(\mathrm{R}) = M_{n,CTA} + (DP \times M_{n,VDF})$$

Where $M_{n\ CTA}$ = 208.3 g.mol^{-1} and $M_{n\ VDF}$= 64.04 g.mol^{-1}

^{1}H NMR (400 MHz $(CD_3)_2CO$, δ (ppm)) : 1.19-1.24 (d, -CH(C**H$_3$**)(C=O)-, $^{3}J_{HH}$ = 7.1 Hz), 1.40-1.46 (t, -S(C=S)O-CH_2-C**H$_3$**, $^{3}J_{HH}$ = 7.2 Hz), 2.28-2.43 (m,-CF_2-C**H$_2$**-C**H$_2$**-CF_2-, VDF-VDF TT reverse addition), 2.70-3.19 (t, -CF_2-C**H$_2$**-CF_2-, VDF-VDF HT regular addition), 3.60-3.69 (s, -(C=O)-O-C**H$_3$**), 4.02-4.17 (t, -CF_2-C**H$_2$**-S(C=S)OEt, $^{3}J_{HF}$ = 18 Hz), 4.67-4.77 (q, (-S(C=S)O-C**H$_2$**-CH_3, $^{3}J_{HH}$ = 7.2 Hz), 6.05-6.45 (tt, $^{2}J_{HF}$ = 55 Hz , $^{3}J_{HH}$ = 4.6 Hz -CH_2-CF_2-**H**).

^{19}F NMR (376 MHz $(CD_3)_2CO$, δ (ppm)) : -115.63 (-CH_2-CF_2-C**F$_2$**-CH_2-CH_2-, VDF-VDF HH reverse addition), -114.29 ($^{2}J_{HF}$ = 55 Hz, -CH_2-C**F$_2$**-H), -113.34 (-CH_2-C**F$_2$**-CF_2-CH_2-CH_2-, HH reverse addition), -113.09 (CH_2-CF_2-**C**F$_2$**-CH_2-S-), -112.69 (-CH_2-**C**F$_2$**-CF_2-CH_2-S-), -94.79 (-CH_2-CH_2-C**F$_2$**-CH_2-, TT reverse addition), -93.50 (-CH_2-C**F$_2$**-CH_2-CH(CH_3)(C=O)-), -92.12 (-CH_2-C**F$_2$**-CH_2-CF_2H), -91.44 (-CH_2-CH_2-CF_2-CH_2-**C**F$_2$**-CH_2-CF_2-, regular VDF-VDF HT addition), -91.00 (-CH_2-C**F$_2$**-CH_2-, regular VDF-VDF HT addition).

Equations used to determine the proportion of the polymer chain end-groups:

1) PVDF:

$$(S3)\ (\%) - CF_2 - CH_2 - XA = \frac{\frac{1}{2}\int_{4.02}^{4.17} -CF_2 - CH_2 - XA}{\frac{1}{2}\int_{3.26}^{3.52} -CH_2 - CF_2 - XA + \int_{6.01}^{6.48} -CH_2 - CF_2H + \frac{1}{2}\int_{4.02}^{4.17} -CF_2 - CH_2 - XA}$$

$$(S4)\ (\%) - CH_2 - CF_2 - XA\ = \frac{\frac{1}{2}\int_{3.26}^{3.52} -CH_2 - CF_2 - XA}{\frac{1}{2}\int_{3.26}^{3.52} -CH_2 - CF_2 - XA + \int_{6.01}^{6.48} -CH_2 - CF_2H + \frac{1}{2}\int_{4.02}^{4.17} -CF_2 - CH_2 - XA}$$

$$(S5)\ (\%) - CH_2 - CF_2H\ = \frac{\int_{6.01}^{6.48} -CH_2 - CF_2H}{\frac{1}{2}\int_{3.26}^{3.52} -CH_2 - CF_2 - XA + \int_{6.01}^{6.48} -CH_2 - CF_2H + \frac{1}{2}\int_{4.02}^{4.17} -CF_2 - CH_2 - XA}$$

Note : -CF_2-CH_3 end groups were not taken into consideration in the calculation because, as described in a previous study,[2] irreversible transfer reactions between -$CH_2^{\bullet}$ radicals and solvent molecules were exclusively observed for targeted DP higher than 100.

2) PVAc:

$$(S6)\ (\%) - CH(OAc) - CH_2 - XA = \frac{\frac{1}{2}\int_{3.18}^{3.51} -CH(OAc) - CH_2 - XA}{\frac{1}{2}\int_{3.18}^{3.51} -CH(OAc) - CH_2 - XA + \int_{6.01}^{6.48} -CH_2 - CF_2H + \frac{1}{2}\int_{3.95}^{4.13} -CH_2 - (OAc)CH_2 + \int_{6.50}^{6.70} -CH_2 - CH(OAc) - XA}$$

$$(S7)\ (\%) - CH_2 - CH(OAc) - XA = \frac{\int_{6.50}^{6.70} -CH_2 - CH(OAc) - XA}{\frac{1}{2}\int_{3.18}^{3.51} -CH(OAc) - CH_2 - XA + \int_{6.01}^{6.48} -CH_2 - CF_2H + \frac{1}{2}\int_{3.95}^{4.13} -CH_2 - (OAc)CH_2 + \int_{6.50}^{6.70} -CH_2 - CH(OAc) - XA}$$

$$(S8)\ (\%) - CH_2 - (OAc)CH_2 = \frac{\frac{1}{2}\int_{3.95}^{4.13} -CH_2 - (OAc)CH_2}{\frac{1}{2}\int_{3.18}^{3.51} -CH(OAc) - CH_2 - XA + \int_{6.01}^{6.48} -CH_2 - CF_2H + \frac{1}{2}\int_{3.95}^{4.13} -CH_2 - (OAc)CH_2 + \int_{6.50}^{6.70} -CH_2 - CH(OAc) - XA}$$

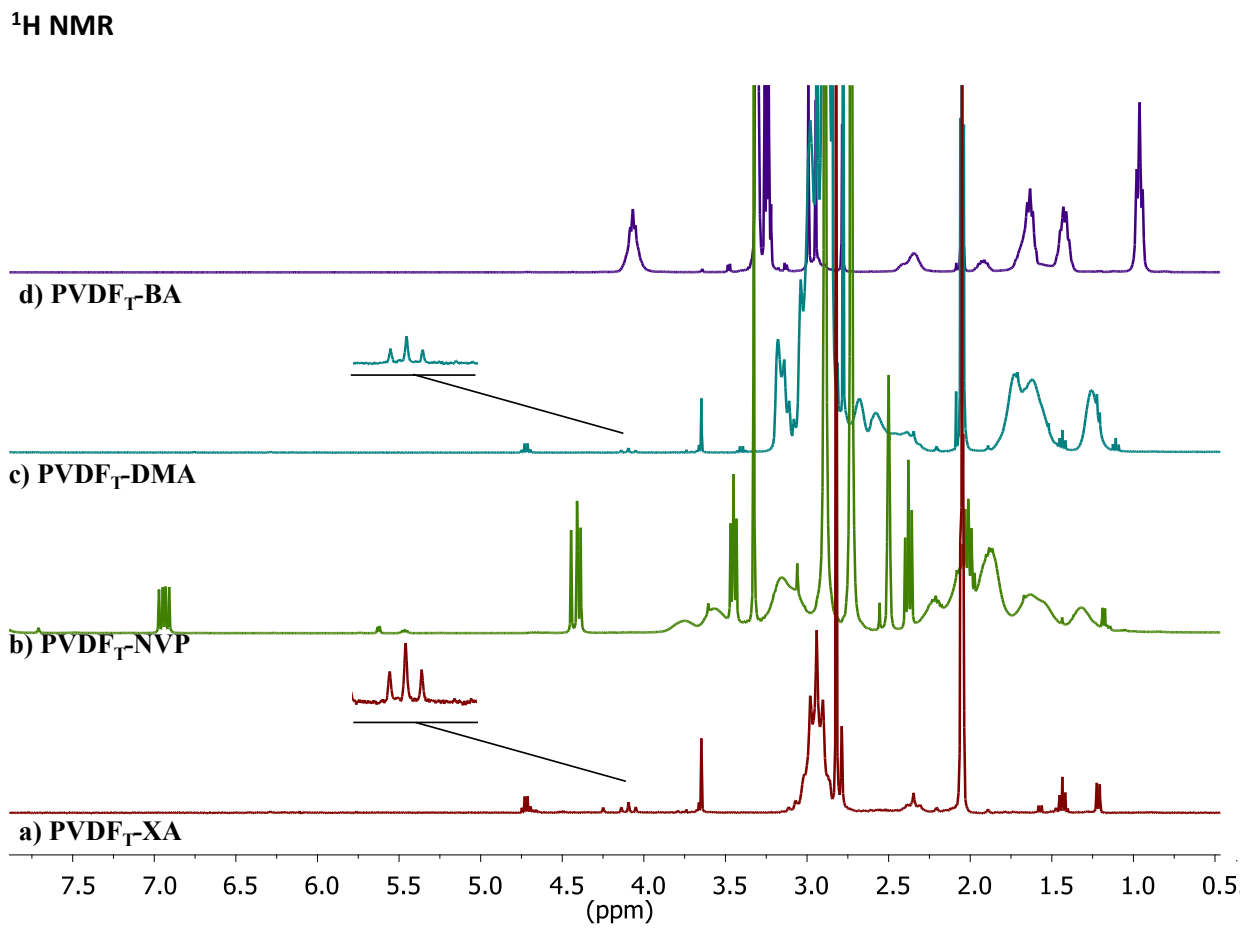


Figure S1. Expansion of the 0.5 to 8.5 ppm region of the ^{1}H NMR spectrum of : a) PVDF$_T$-XA (entry 1, Table 1), b) chain extension with NVP (entry 5, Table 1), c) chain extension with DMA (entry 6, Table 1), d) chain extension with BA (entry 7, Table 1). Spectra a), c) and d) recorded in $(CD_3)_2CO$, spectrum b) recorded in $(CD_3)_2SO$. All polymers were purified by precipitation in cold hexane.

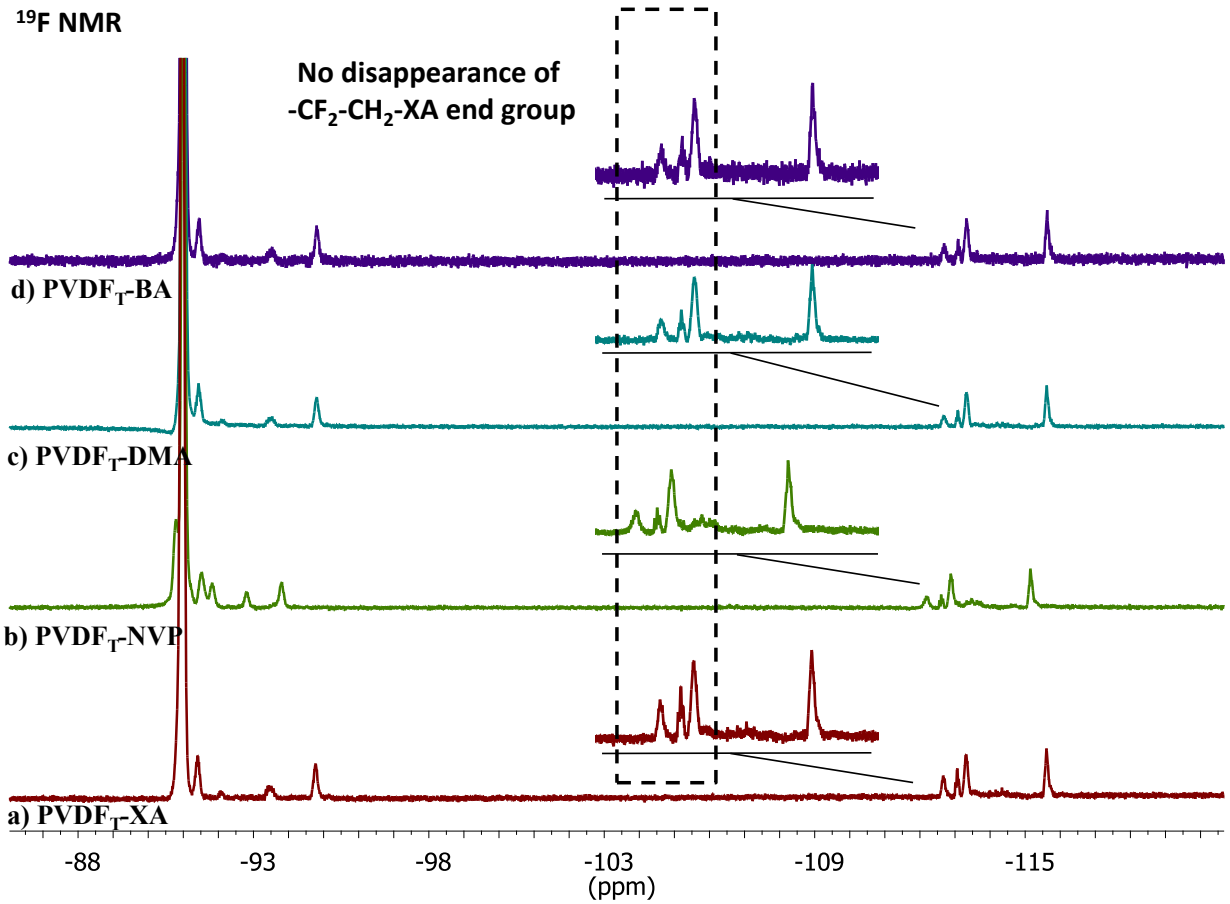


Figure S2. Expansion of the -86 to -120.5 ppm region of the ^{19}F NMR spectrum of : a) $PVDF_T$-XA (entry 1, Table 1), b) chain extension with NVP (entry 5, Table 1), c) chain extension with DMA (entry 6, Table 1), d) chain extension with BA (entry 7, Table 1). Spectra a), c) and d) recorded in $(CD_3)_2CO$, spectrum b) recorded in $(CD_3)_2SO$. All polymers were purified by precipitation in cold hexane.

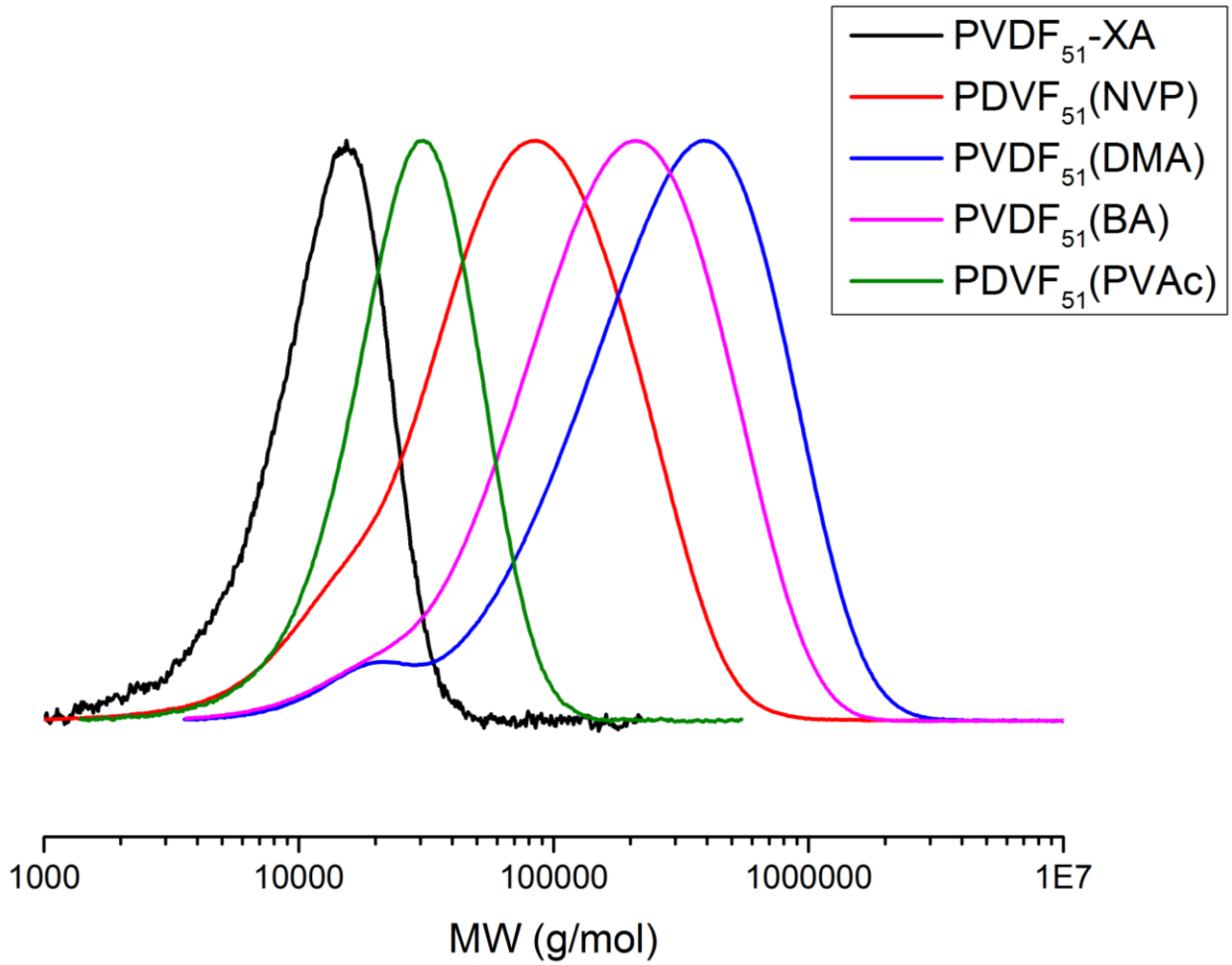


Figure S3. Normalized GPC traces (viscometric detector) of $PVDF_{51}$-XA (black trace) and of the polymers obtained by chain extension of this $PVDF_T$-XA with: 1) NVP: $PVDF_{51}$(NVP) (red trace), 2) DMA: $PVDF_{51}$(DMA) (blue trace), 3) BA: $PVDF_{51}$(BA) (pink trace), and 4) VAc: $PVDF_{51}$(PVAc) (green trace).

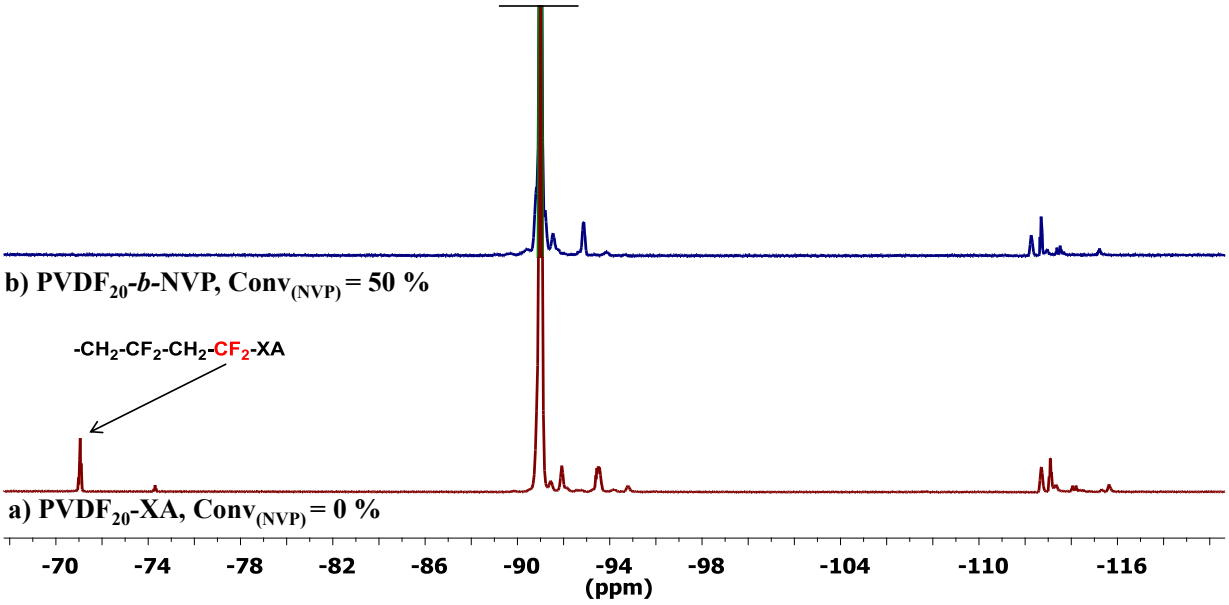


Figure S4. Expansion of the -68 to -118 ppm region of the ^{19}F NMR spectra of: a) $PVDF_{20}$-XA synthesized via RAFT polymerization (entry 3, Table 1) composed of 38 % of $PVDF_T$-XA, 47 % of $PVDF_H$-XA and 14 % of PVDF-H chains, b) $PVDF_{20}$-*b*-PNVP block copolymer synthesized *via* RAFT polymerization (polymerization time = 14 h, $Conv_{(NVP)}$ = 50%) (entry 17, Table 1). Spectrum a) recorded in $(CD_3)_2CO$ and spectrum b) recorded in $(CD_3)_2SO$.

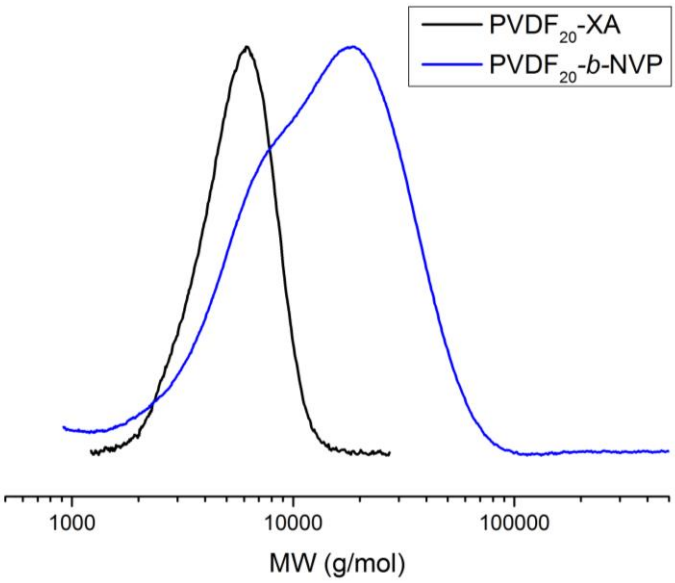


Figure S5. Normalized GPC traces (viscometric detector) of $PVDF_{20}$-XA (black trace) and of the polymers obtained by chain extension of this $PVDF_{20}$-XA composed of 38 % of $PVDF_T$-XA, 47 % of $PVDF_H$-XA and 14 % of PVDF-H chains (blue trace).

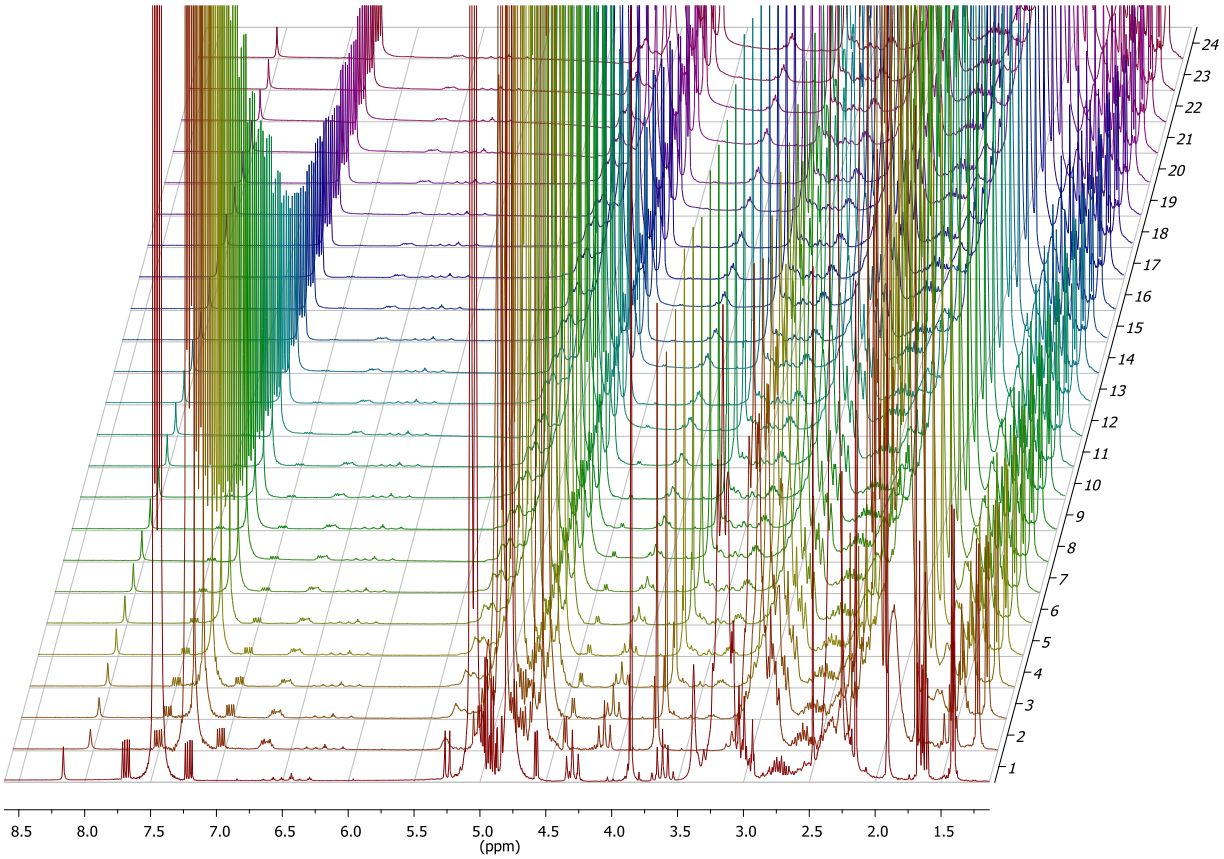


Figure S6. Stacked ^{1}H NMR spectra in deuterated DMF of the chain extension of $PVDF_{20}$-XA (entry 3, Table 1) with VAc (Target DP = 100) *via* RAFT polymerization (entry 16, Table 1).

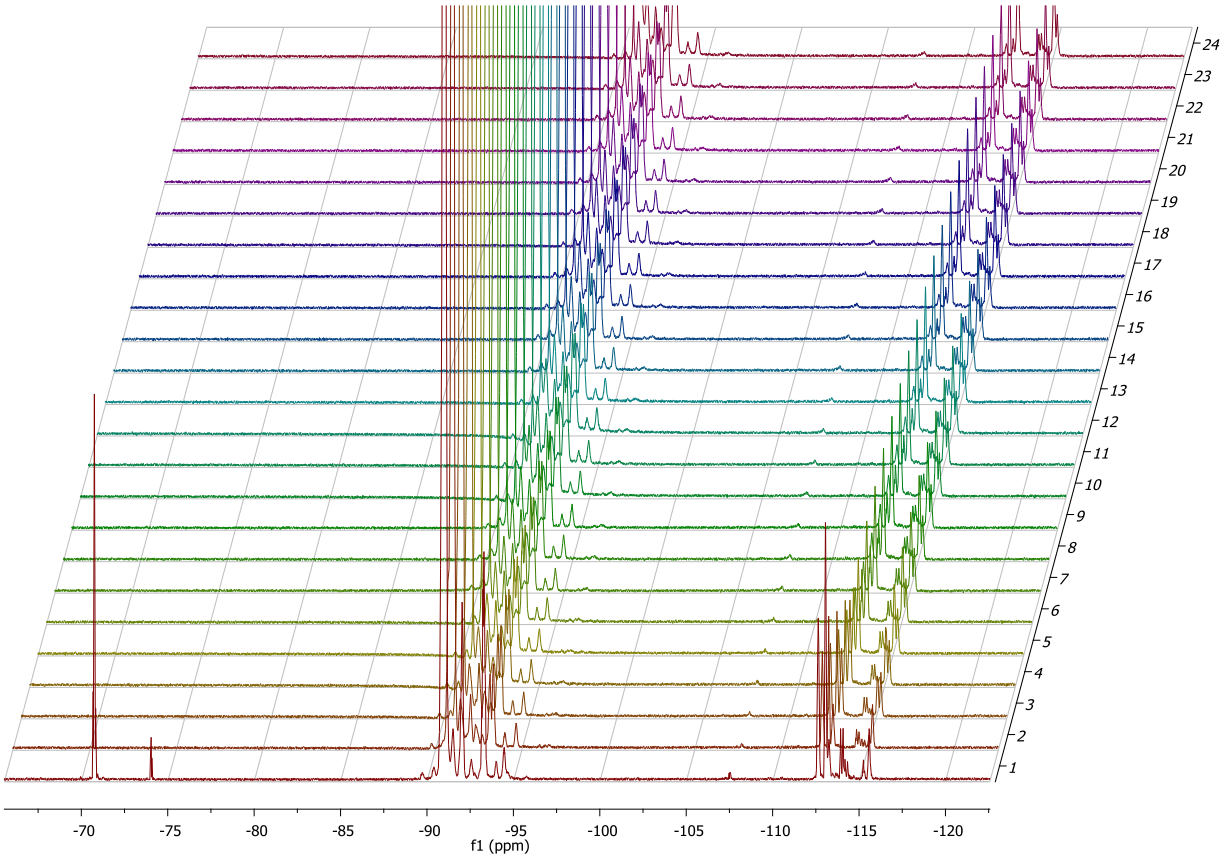


Figure S7. Stacked ^{19}F NMR spectra in deuterated DMF of the chain extension of $PVDF_{20}$-XA (entry 3, Table 1) with VAc (Target DP = 100) *via* RAFT polymerization (entry 16, Table 1).

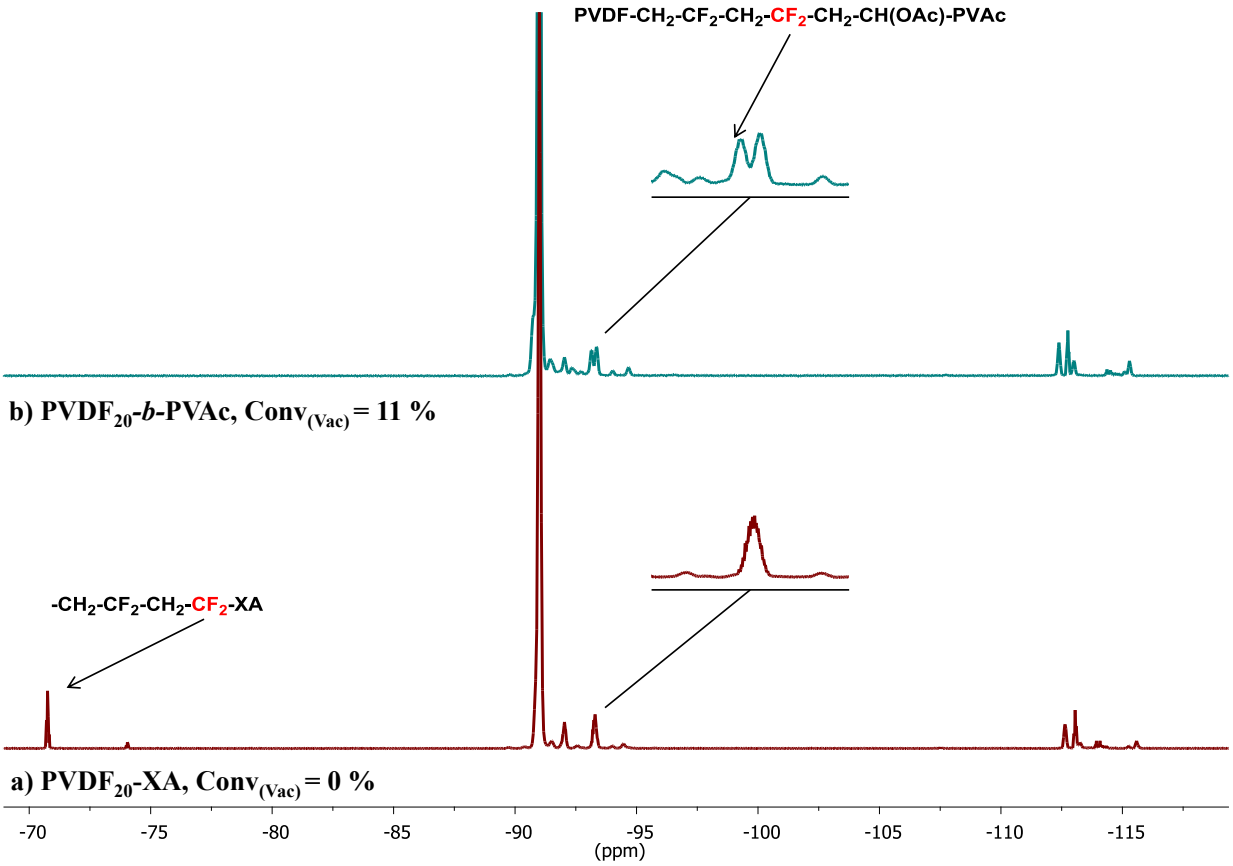


Figure S8. Expansion of the -68 to -118 ppm region of the ^{19}F NMR spectra of: a) $PVDF_{20}$-XA synthesized via RAFT polymerization (entry 3, Table 1) composed of 38 % of $PVDF_T$-XA, 47 % of $PVDF_H$-XA and 14 % of PVDF-H chains, b) $PVDF_{20}$-*b*-PVAc block copolymer synthesized *via* RAFT polymerization, (polymerization time = 2 min and 7 s, second point in the in situ NMR monitoring, $Conv_{(VAc)}$ = 11 %, entry 16, Table 1). Spectrum a) recorded in $(CD_3)_2CO$ and spectrum b) recorded in d_7-DMF.

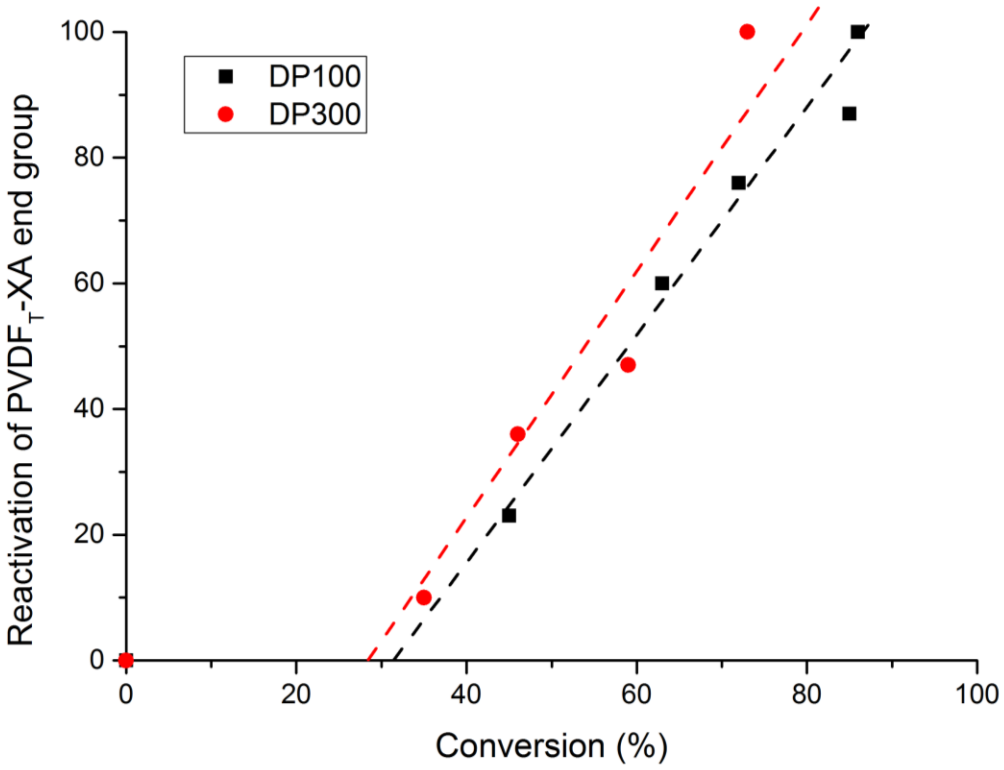


Figure S9. Reactivation of PVDF$_T$-XA (entry 1, Table 1) vs VAc conversion during the syntheses of PVAc block with VAc target DP = 100 (black squares) and 300 (red circles).

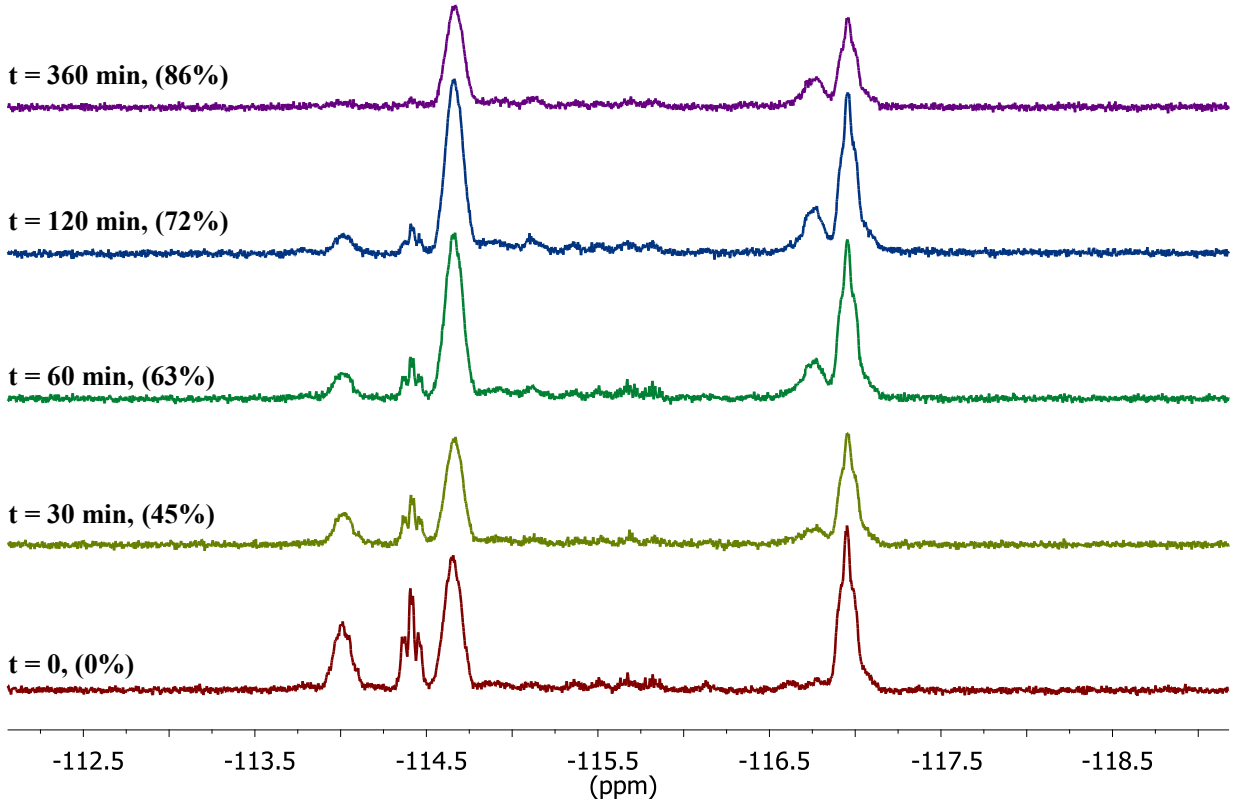


Figure S10. Expansion of selected ^{19}F NMR signals with conversion of $PVDF_{20}$-XA chain extension monitored by *in situ* NMR Spectroscopy recorded in d_7-DMF. The conversion of VAc is shown in brackets after the reaction time for each spectrum.

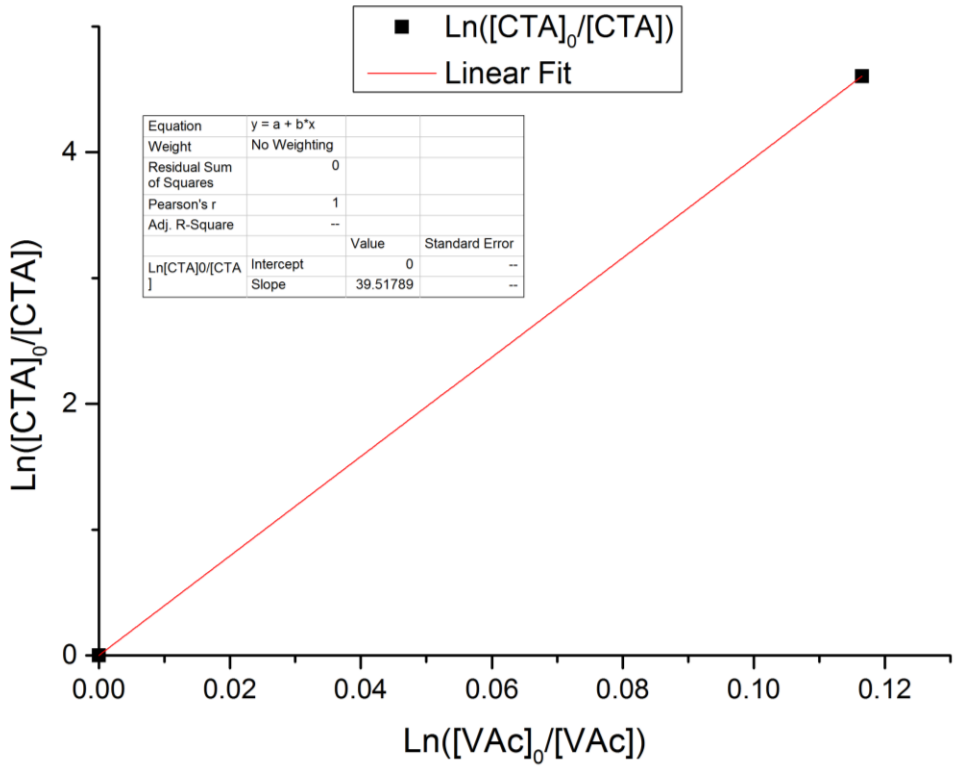


Figure S11. Determination of the apparent transfer constant of $PVDF_H$-XA macroCTA with VAc using O'Brien and Gornick's method.[3]

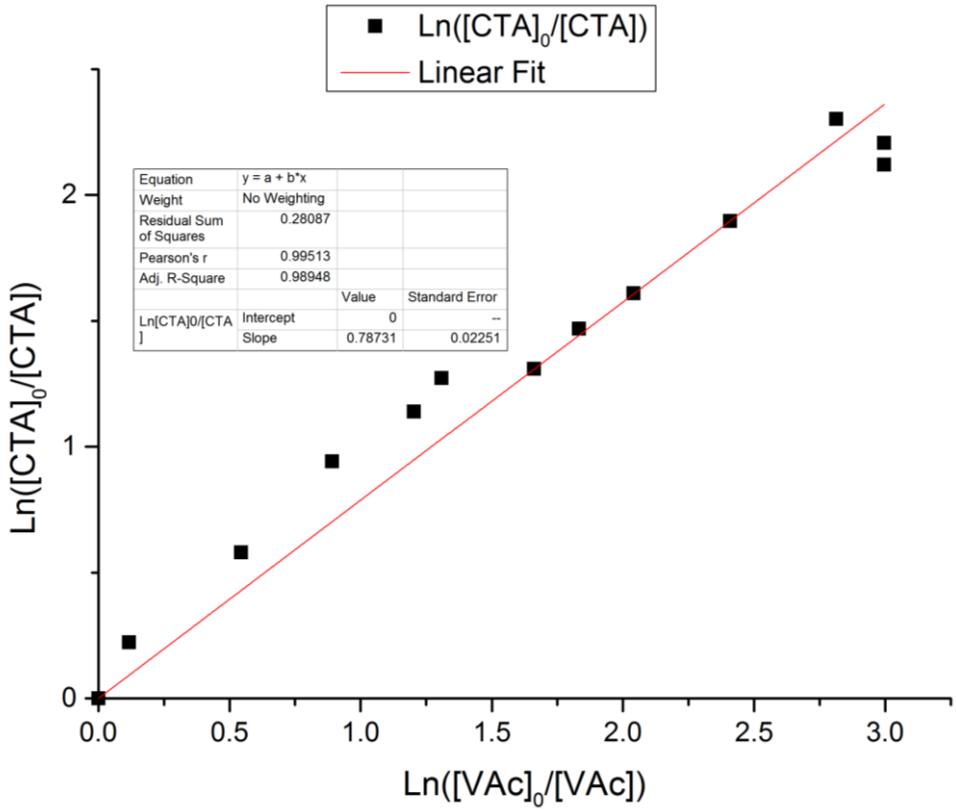


Figure S12. Determination of the apparent transfer constant of $PVDF_T$-XA macroCTA with VAc using O'Brien and Gornick's method.[2]

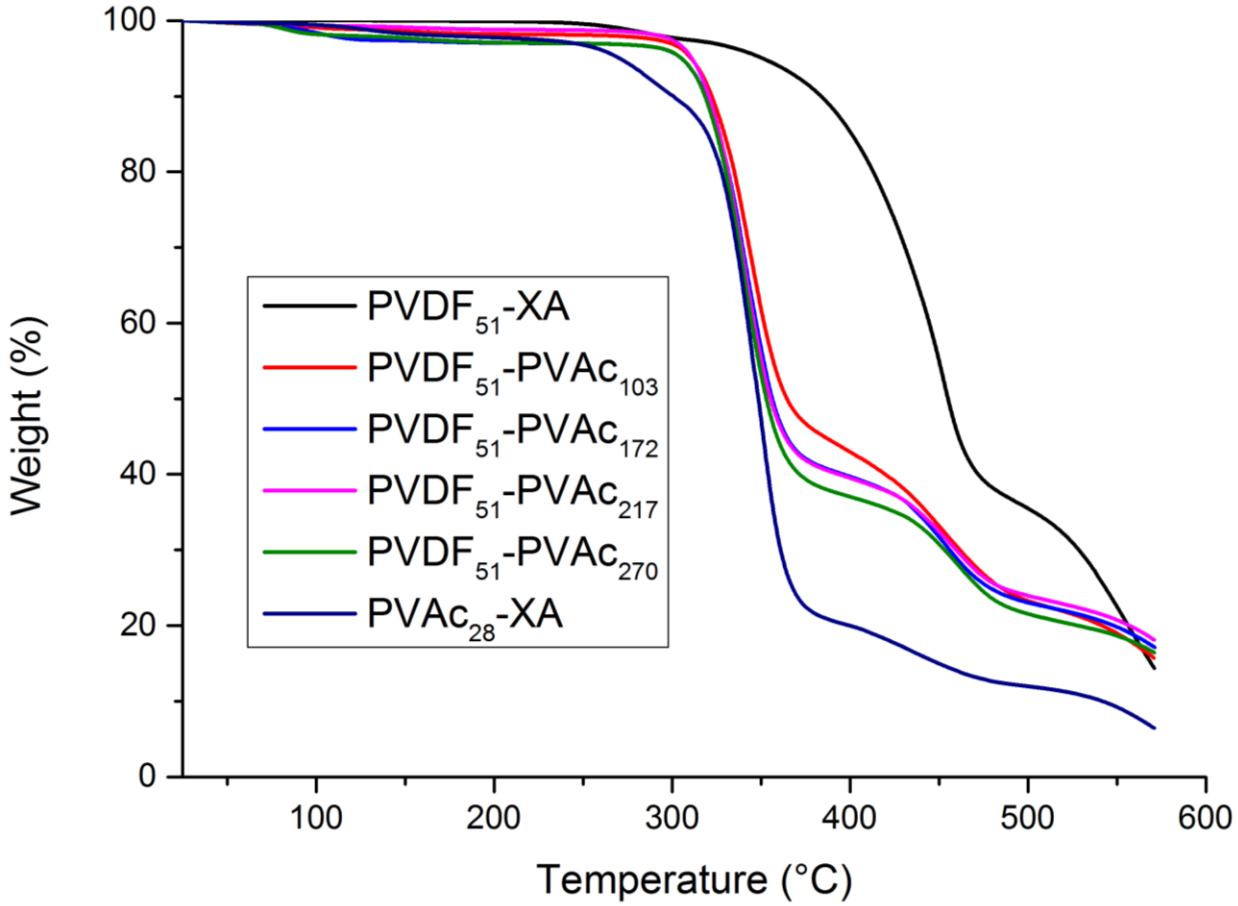


Figure S13. TGA thermograms of $PVDF_{51}$-XA (black), $PVAc_{28}$-XA (dark blue) homopolymer, $PVDF_{51}$-*b*-$PVAc_{103}$ (red), $PVDF_{51}$-*b*-$PVAc_{172}$ (blue), $PVDF_{51}$-*b*-$PVAc_{217}$ (pink) and $PVDF_{51}$-*b*-$PVAc_{270}$ (green).

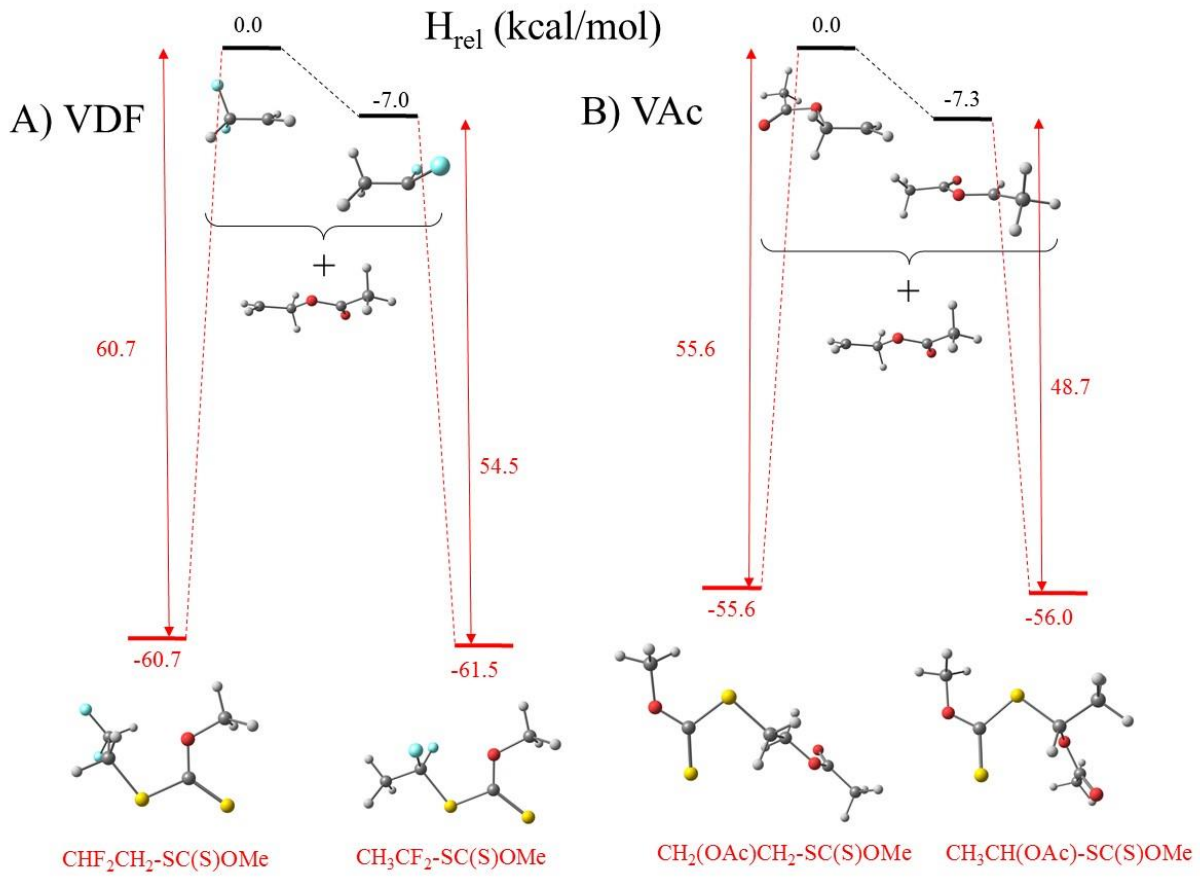


Figure S14. Relative energies and views of the optimized geometries of the isomeric $CHF_2CH_2^{\bullet}$ and $CH_3CF_2^{\bullet}$ radicals, the isomeric $CH_2(OAc)CH_2^{\bullet}$ and $CH_3CH(OAc)^{\bullet}$ radicals, the $(MeO)C(S)S^{\bullet}$ radical, and the corresponding adducts. The values are the standard enthalpies ($\Delta H°_{298.15}$) in kcal/mol.

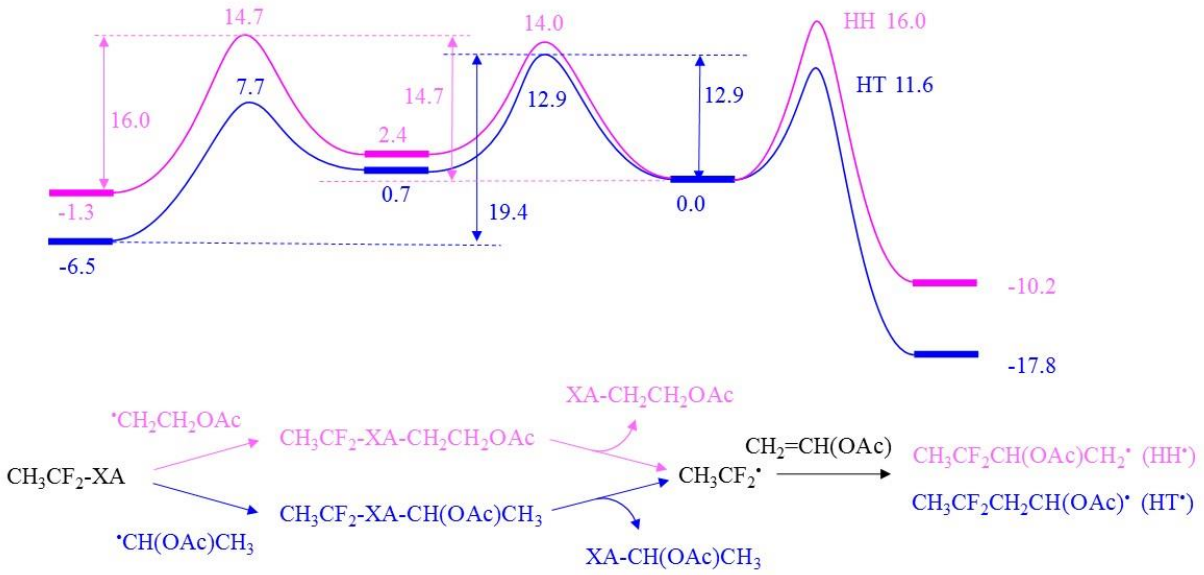


Figure S15. Energy profiles (ΔG at 343.5 K in kcal/mol) for the model $PVDF_H$-XA reactivation by both head and tail $PVAc^{\bullet}$ model radicals in the chain extension with VAc.

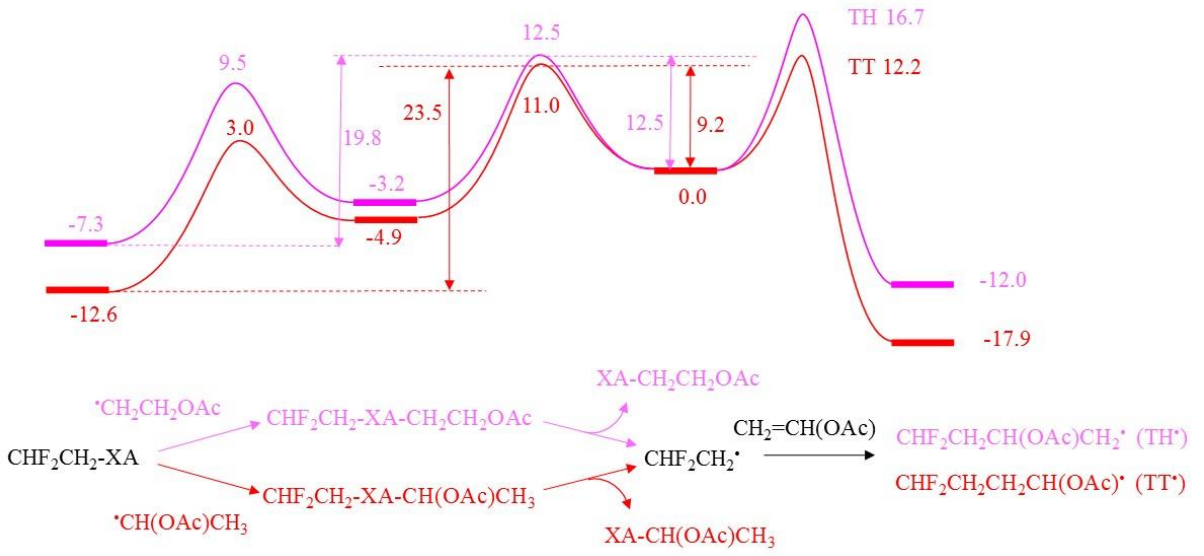


Figure S16. Energy profiles (ΔG at 343.5 K in kcal/mol) for the model $PVDF_T$-XA reactivation by both head and tail $PVAc^{\bullet}$ model radicals in the chain extension with VAc.

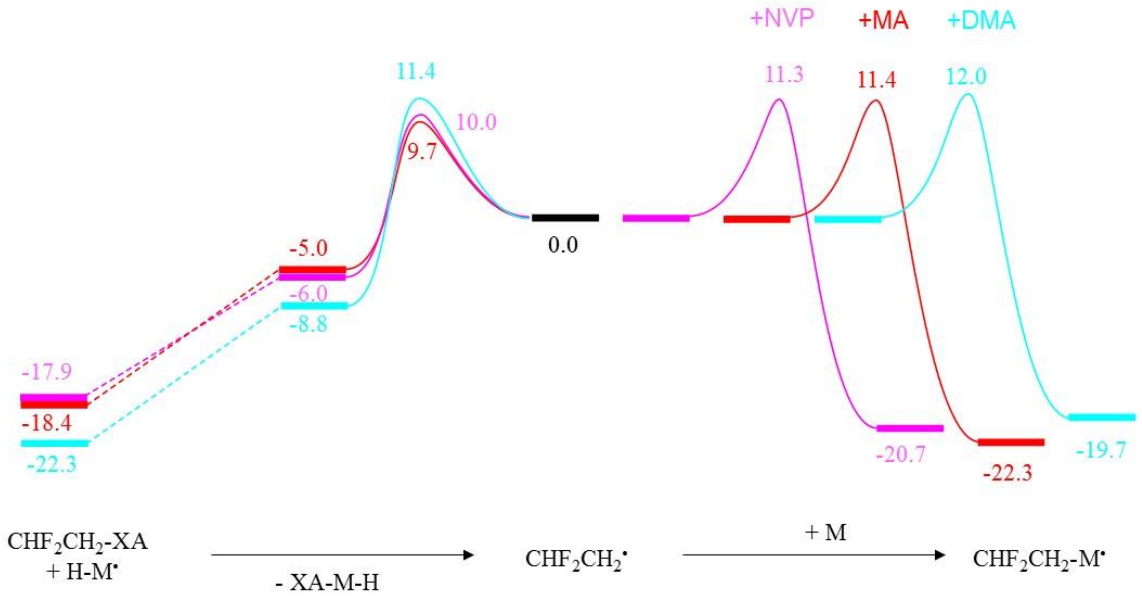


Figure S17. Energy profiles (ΔG at 343.5 K in kcal/mol) for the model $PVDF_T$-XA reactivation by the H-M$^{\bullet}$ model radicals in the chain extension with NVP, MA (model of BA), and DMA. Only the rate-determining transition state corresponding to the intermediate fragmentation was optimized.

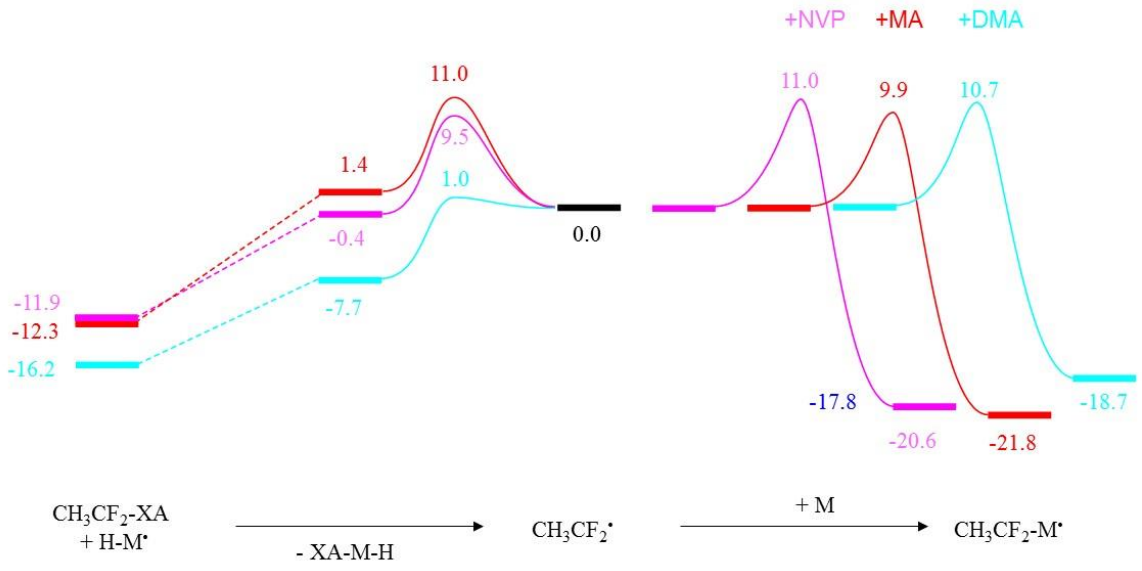


Figure S18. Energy profiles (ΔG at 343.5 K in kcal/mol) for the model $PVDF_H$-XA reactivation by the H-M$^{\bullet}$ model radicals in the chain extension with NVP, MA (model of BA), and DMA. Only the rate-determining transition state corresponding to the intermediate fragmentation was optimized.

Table S1. Energies, enthalpies, Gibbs energies of all optimized geometries (N-pyr = N-substituted pyrrolidone).

Compound	E (hartrees)	$H_{298.15}$ (hartrees)	$G_{298.15}$ (hartrees)	$G_{343.15}$ (hartrees)[a]
(a) Radicals				
$CH_3CF_2^{\bullet}$	-277.3942109	-277.341757	-277.374487	-277.379427
$CHF_2CH_2^{\bullet}$	-277.3819182	-277.330618	-277.363927	-277.368954
$CH_3CH(OAc)^{\bullet}$	-306.748937	-306.637180	-306.678902	-306.685199
$CH_3CH(OAc)^{\bullet}$ (in vinyl acetate, ε = 4.2)	-306.748869	-306.637110	-306.678314	-306.684533
$CH_3CH(OAc)^{\bullet}$ (in acetonitrile, ε = 35.7)	-306.748832	-306.637082	-306.678154	-306.684353
$AcOCH_2CH_2^{\bullet}$	-306.736664	-306.625483	-306.668129	-306.674566
$CH_3CH(N\text{-}pyr)^{\bullet}$	-364.248303	-364.086106	-364.128929	-364.135392
$CH_3CH(COOMe)^{\bullet}$	-306.752227	-306.639465	-306.679787	-306.685873
$CH_3CH(CONMe_2)^{\bullet}$	-326.159236	-326.004772	-326.048889	-326.055548
$(MeO)C(S)S^{\bullet}$	-949.138793	-949.081962	-949.119578	-949.125255
(b) Monomers				
CH_2=CH(OAc)	-306.174665	-306.072904	-306.111829	-306.117704
CH_2=CH(OAc) (in vinyl acetate, ε = 4.2)	-306.174615	-306.072872	-306.111505	-306.117336
CH_2=CH(OAc) (in acetonitrile, ε = 35.7)	-306.174590	-306.072872	-306.111386	-306.117199
CH_2=CH(N-pyr)	-363.667907	-363.515781	-363.556191	-363.562290
CH_2=CH(COOMe)	-306.170160	-306.067512	-306.105545	-306.111285
CH_2=CH($CONMe_2$)	-325.581015	-325.436666	-325.478491	-325.484804
(c) Chain transfer agents				
CH_3CF_2-SC(S)(OCH_3)	-1226.623079	-1226.509289	-1226.558343	-1226.565747
CHF_2CH_2-SC(S)(OCH_3)	-1226.623112	-1226.510636	-1226.559231	-1226.566565
$CH_3CH(OAc)$-SC(S)(OCH_3)	-1255.969930	-1255.796755	-1255.853426	-1255.861979
$AcOCH_2CH_2$-SC(S)(OCH_3)	-1255.969996	-1255.796001	-1255.853922	-1255.862664
$CH_3CH(N\text{-}pyr)$-SC(S)(OCH_3)	-1313.459406	-1313.236059	-1313.294756	-1313.303615
$CH_3CH(COOMe)$-SC(S)(OCH_3)	-1255.962630	-1255.788557	-1255.844913	-1255.853419
$CH_3CH(CONMe_2)$-SC(S)(OCH_3)	-1275.36569	-1275.149574	-1275.208001	-1275.216819
(d) VAc homopropagation				
d1. Head-to-tail				
$CH_3CH(OAc)^{\bullet\cdots}CH_2$=CH(OAc) TS	-612.9146473	-612.699775	-612.759644	-612.768680
$CH_3CH(OAc)^{\bullet\cdots}CH_2$=CH(OAc) TS (in vinyl acetate, ε = 4.2)	-612.9141652	-612.700268	-612.757935	-612.766639
$CH_3CH(OAc)^{\bullet\cdots}CH_2$=CH(OAc) TS (in acetonitrile, ε = 35.7)	-612.9140444	-612.700163	-612.757689	-612.766371
$CH_3CH(OAc)$-$CH_2CH(OAc)^{\bullet}$	-612.9604502	-612.742476	-612.802898	-612.812018
$CH_3CH(OAc)$-$CH_2CH(OAc)^{\bullet}$ (in vinyl acetate, ε = 4.2)	-612.9603017	-612.742385	-612.802230	-612.811262
$CH_3CH(OAc)$-$CH_2CH(OAc)^{\bullet}$ (in acetonitrile, ε = 35.7)	-612.9602412	-612.742284	-612.801606	-612.810560
d2. Head-to-head				

$CH_3CH(OAc)^{\bullet\cdots}CH(OAc)=CH_2$ TS	-612.912089	-612.697544	-612.757623	-612.766691
$CH_3CH(OAc)$-$CH(OAc)CH_2^{\bullet}$	-612.9550274	-612.737817	-612.797963	-612.807041
d3. Tail-to-tail				
$AcOCH_2CH_2^{\bullet\cdots}CH_2=CH(OAc)$ TS	-612.9068575	-612.69188	-612.755489	-612.765090
$AcOCH_2CH_2$-$CH_2CH(OAc)^{\bullet}$	-612.9593542	-612.740662	-612.802093	-612.811365
d4. Tail-to-head				
$AcOCH_2CH_2^{\bullet\cdots}CH(OAc)=CH_2$ TS	-612.9020385	-612.687388	-612.749543	-612.758924
$AcOCH_2CH_2$-$CH(OAc)CH_2^{\bullet}$	-612.9517277	-612.733705	-612.794286	-612.803430
(e) Other monomers homopropagation (all head-to-tail)				
$CH_3CH(N\text{-}pyr)^{\bullet\cdots}CH_2=CH(N\text{-}pyr)$ TS	-727.9168423	-727.600943	-727.664546	-727.674146
CH3CH(N-pyr)-CH2CH(N-pyr)$^{\bullet}$	-727.9554137	-727.636386	-727.698752	-727.708165
$CH_3CH(COOMe)^{\bullet\cdots}CH_2=CH(COOMe)$ TS	-612.9160239	-612.699270	-612.759524	-612.768618
$CH_3CH(COOMe)$-$CH_2CH(COOMe)^{\bullet}$	-612.9565734	-612.736780	-612.796156	-612.805118
$CH_3CH(CONMe_2)^{\bullet\cdots}CH_2=CH(CONMe_2)$ TS	-651.7337656	-651.433334	-651.500074	-651.510147
$CH_3CH(CONMe_2)$-$CH_2CH(CONMe_2)^{\bullet}$	-651.7734329	-651.469831	-651.535584	-651.545508
(e) VAc RAFT: MacroCTA degenerative and non-degenerative radical exchange				
e1. Head-head (degenerative)				
$CH_3CH(OAc)$-$SC(OMe)S^{\cdots\bullet}CH(OAc)CH_3$ TS	-1562.725753	-1562.438808	-1562.514567	-1562.526001
$CH_3CH(OAc)$-$SC^{\bullet}(OMe)S$-$CH(OAc)CH_3$	-1562.739448	-1562.450252	-1562.524707	-1562.535945
e2. Head-tail (non-degenerative)				
$CH_3CH(OAc)$-$SC(OMe)S^{\cdots\bullet}CH_2CH_2OAc$ TS	-1562.704885	-1562.418258	-1562.498879	-1562.511047
$CH_3CH(OAc)$-$SC^{\bullet}(OMe)S$-CH_2CH_2OAc	-1562.735275	-1562.445479	-1562.525252	-1562.537292
$CH_3CH(OAc)^{\bullet\cdots}SC(OMe)S$-$CH_2CH_2OAc$ TS	-1562.724235	-1562.436581	-1562.516658	-1562.528744
e3. Tail-tail (degenerative)				
$AcOCH_2CH_2$-$SC(OMe)S^{\cdots\bullet}CH_2CH_2OAc$ TS	-1562.702989	-1562.415461	-1562.494514	-1562.506446
$AcOCH_2CH_2$-$SC^{\bullet}(OMe)S$-CH_2CH_2OAc	-1562.724562	-1562.434221	-1562.511981	-1562.523717
(f) $PVDF_H$-XA reactivation				
f1. By VAc (head)				
CH_3CF_2-$SC(OMe)S^{\cdots\bullet}CH(OAc)CH_3$ TS	-1533.370507	-1533.144785	-1533.215404	-1533.226063
CH_3CF_2-$SC^{\bullet}(OMe)S$-$CH(OAc)CH_3$	-1533.384941	-1533.157036	-1533.226742	-1533.237263
$CH_3CF_2^{\bullet\cdots}SC(OMe)S$-$CH(OAc)CH_3$ TS	-1533.362805	-1533.136301	-1533.207169	-1533.217865
f2. By VAc (tail)				
CH_3CF_2-$SC(OMe)S^{\cdots\bullet}CH_2CH_2OAc$ TS	-1533.359134	-1533.133279	-1533.204875	-1533.215681
CH_3CF_2-$SC^{\bullet}(OMe)S$-CH_2CH_2OAc	-1533.382418	-1533.153724	-1533.224516	-1533.235201
$CH_3CF_2^{\bullet\cdots}SC(OMe)S$-$CH_2CH_2OAc$ TS	-1533.360834	-1533.13358	-1533.205937	-1533.216858
f3. By NVP (head)				
CH_3CF_2-$SC^{\bullet}(OMe)S$-$CH(N\text{-}pyr)CH_3$	-1590.875069	-1590.596986	-1590.66974	-1590.680721
$CH_3CF_2^{\bullet\cdots}SC(OMe)S$-$CH(N\text{-}pyr)CH_3$ TS	-1590.857208	-1590.580442	-1590.653796	-1590.664867

f4. By MA (head)				
CH_3CF_2- $SC^{\bullet}(OMe)S$-CH(COOMe)CH_3	-1533.373768	-1533.145211	-1533.216727	-1533.227521
$CH_3CF_2^{\bullet\cdots}SC(OMe)S$-CH(COOMe)$CH_3$ TS	-1533.355094	-1533.127949	-1533.201246	-1533.212309
f5. By DMA (head)				
CH_3CF_2-$SC^{\bullet}(OMe)S$-CH($CONMe_2$)CH_3	-1552.789602	-1552.519183	-1552.594241	-1552.605570
$CH_3CF_2^{\bullet\cdots}SC(OMe)S$-CH($CONMe_2$)$CH_3$ TS	-1552.774757	-1552.505650	-1552.580418	-1552.591703
(g) $PVDF_T$-XA reactivation				
g1. By VAc (head)				
CHF_2CH_2-$SC(OMe)S^{\cdots\bullet}CH(OAc)CH_3$ TS	-1533.368746	-1533.141749	-1533.212515	-1533.223196
CHF_2CH_2-$SC^{\bullet}(OMe)S$-CH(OAc)CH_3	-1533.383938	-1533.154939	-1533.225124	-1533.235717
$CHF_2CH_2^{\bullet\cdots}SC(OMe)S$-CH(OAc)$CH_3$ TS	-1533.354954	-1533.128909	-1533.19973	-1533.210419
g2. By VAc (tail)				
CHF_2CH_2-$SC(OMe)S^{\cdots\bullet}CH_2CH_2OAc$ TS	-1533.358868	-1533.131644	-1533.202796	-1533.213535
CHF_2CH_2-$SC^{\bullet}(OMe)S$-CH_2CH_2OAc	-1533.382549	-1533.152609	-1533.223061	-1533.233694
$CHF_2CH_2^{\bullet\cdots}SC(OMe)S$-$CH_2CH_2OAc$ TS	-1533.353517	-1533.126535	-1533.197946	-1533.208724
g3. By NVP (head)				
CHF_2CH_2-$SC^{\bullet}(OMe)S$-CH(N-pyr)CH_3	-1590.874868	-1590.595518	-1590.66815	-1590.679112
$CHF_2CH_2^{\bullet\cdots}SC(OMe)S$-CH(N-pyr)$CH_3$ TS	-1590.846518	-1590.570249	-1590.642649	-1590.653576
g4. By MA (head)				
CHF_2CH_2- $SC^{\bullet}(OMe)S$-CH(COOMe)CH_3	-1533.376416	-1533.146421	-1533.216746	-1533.227360
$CHF_2CH_2^{\bullet\cdots}SC(OMe)S$-CH(COOMe)$CH_3$ TS	-1533.346591	-1533.119745	-1533.192852	-1533.203886
g5. By DMA (head)				
CHF_2CH_2-$SC^{\bullet}(OMe)S$-CH($CONMe_2$)CH_3	-1552.783000	-1552.511104	-1552.585599	-1552.596843
$CHF_2CH_2^{\bullet\cdots}SC(OMe)S$-CH($CONMe_2$)$CH_3$ TS	-1552.746166	-1552.477343	-1552.553144	-1552.564585
(h) $PVDF_H^{\bullet}$ addition to monomer				
h1. To VAc (tail)				
$CH_3CF_2^{\bullet\cdots}CH_2$=CHOAc TS	-583.5661989	-583.411501	-583.467199	-583.475606
CH_3CF_2-$CH_2CH^{\bullet}$(OAc)	-583.6184335	-583.461508	-583.514463	-583.522456
h2. To VAc (head)				
$CH_3CF_2^{\bullet\cdots}$ CH(OAc)=CH_2 TS	-583.5632561	-583.408942	-583.460804	-583.468632
CH_3CF_2-CH(OAc)$CH_2^{\bullet}$	-583.6070571	-583.450876	-583.502591	-583.510396
h3. To NVP (tail)				
$CH_3CF_2^{\bullet\cdots}CH_2$=CH(N-pyr) TS	-641.0626328	-640.857376	-640.912834	-640.921204
CH_3CF_2-CH_2CH(N-pyr)$^{\bullet}$	-641.1172897	-640.909599	-640.963287	-640.971390
h4. To MA (tail)				
$CH_3CF_2^{\bullet\cdots}CH_2$=CH(COOMe) TS	-583.565874	-583.409888	-583.46379	-583.471926
CH_3CF_2-CH_2CH(COOMe)$^{\bullet}$	-583.6214092	-583.463503	-583.514737	-583.522470
h5. To DMA (tail)				

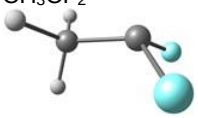
$CH_3CF_2^{\bullet}\cdots CH_2$=CH($CONMe_2$) TS	-602.9768097	-602.779299	-602.835686	-602.844196
CH_3CF_2-$CH_2CH(CONMe_2)^{\bullet}$	-603.0274511	-602.827802	-602.882699	-602.890985
(i) $PVDF_T^{\bullet}$ addition to monomer				
i1. To VAc (tail)				
$CHF_2CH_2^{\bullet}\cdots CH_2$=CHOAc TS	-583.5556446	-583.401323	-583.455898	-583.464135
CHF_2CH_2-$CH_2CH^{\bullet}$(OAc)	-583.6092704	-583.450861	-583.504152	-583.512195
i2. To VAc (head)				
$CHF_2CH_2^{\bullet}\cdots$ CH(OAc)=CH_2 TS	-583.549514	-583.395363	-583.448964	-583.457054
CHF_2CH_2-CH(OAc)$CH_2^{\bullet}$	-583.5993171	-583.441958	-583.494767	-583.502738
i3. To NVP (tail)				
$CHF_2CH_2^{\bullet}\cdots CH_2$=CH(N-pyr) TS	-641.0502614	-640.845362	-640.901730	-640.910238
CHF_2CH_2-CH_2CH(N-pyr)$^{\bullet}$	-641.1080386	-640.899154	-640.953059	-640.961200
i4. To MA (tail)				
$CHF_2CH_2^{\bullet}\cdots CH_2$=CH(COOMe) TS	-583.5518487	-583.396475	-583.450774	-583.458969
CHF_2CH_2-$CH_2CH(COOMe)^{\bullet}$	-583.6118974	-583.452544	-583.504878	-583.512777
i5. To DMA (tail)				
$CHF_2CH_2^{\bullet}\cdots CH_2$=CH($CONMe_2$) TS	-602.9642969	-602.767117	-602.823126	-602.831580
CHF_2CH_2-$CH_2CH(CONMe_2)^{\bullet}$	-603.0191477	-602.818125	-602.873759	-602.882156

[a]Extrapolation done on the basis of $G_{343.15} \approx H_{298.15} - 343.15 \cdot S_{298.15}$.

Table S2. Cartesian coordinates and views of all optimized geometries.

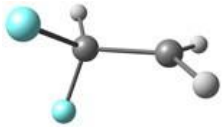
(a) Radicals

$CH_3CF_2^{\bullet}$



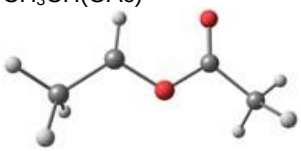
6	0.059485000	0.000229000	-0.305567000
6	-1.386581000	0.000075000	0.044979000
1	-1.526760000	0.000221000	1.137790000
1	-1.870565000	0.890101000	-0.366469000
1	-1.869553000	-0.890889000	-0.365766000
9	0.735032000	1.098602000	0.064360000
9	0.734907000	-1.098742000	0.064303000

$CHF_2CH_2^{\bullet}$



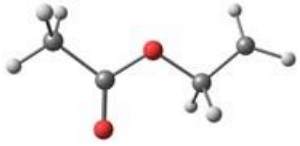
6	1.394001000	-0.107134000	-0.085236000
6	-0.012319000	0.007573000	0.354372000
1	1.605256000	-0.523019000	-1.065566000
1	-0.126101000	0.065360000	1.446414000
1	2.185777000	0.377679000	0.476297000
9	-0.595048000	1.137805000	-0.178214000
9	-0.733288000	-1.062544000	-0.096448000

$CH_3CH(OAc)^{\bullet}$



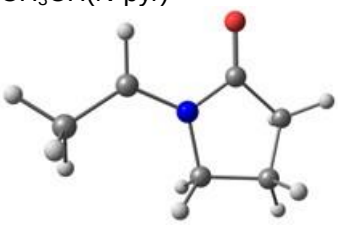
6	-1.317193000	0.378626000	0.127296000
1	-1.138269000	1.439541000	-0.011959000
6	-2.612320000	-0.308037000	-0.059108000
1	-2.688219000	-1.200343000	0.577045000
1	-3.435138000	0.367766000	0.196880000
1	-2.770382000	-0.643370000	-1.099745000
6	1.021800000	0.159756000	-0.010070000
6	2.102555000	-0.884143000	-0.016208000
1	3.059268000	-0.411321000	-0.244154000
1	2.161285000	-1.361742000	0.969438000
1	1.881530000	-1.669032000	-0.746692000
8	-0.211172000	-0.433592000	0.050058000
8	1.181282000	1.358753000	-0.036592000

$AcOCH_2CH_2^{\bullet}$



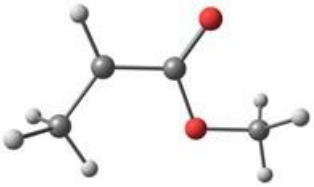
6	2.590296000	0.428611000	-0.053564000
1	2.563545000	1.366036000	-0.600509000
6	-0.972335000	-0.148153000	-0.005656000
1	3.548517000	0.027284000	0.260812000
6	1.372092000	-0.397371000	0.063337000
1	1.372485000	-1.008668000	0.977953000
1	1.254996000	-1.110042000	-0.772854000
8	0.224291000	0.475481000	0.073181000
6	-2.097558000	0.852835000	0.012625000
1	-1.978617000	1.571953000	-0.805039000
1	-3.049920000	0.329379000	-0.084528000
1	-2.078954000	1.420145000	0.949875000
8	-1.097669000	-1.351933000	-0.076451000

$CH_3CH(N\text{-}pyr)^{\bullet}$



6	1.604229000	0.573915000	0.058455000
6	-0.799941000	0.867325000	0.001853000
6	0.003647000	-1.358441000	0.174567000
6	-2.016788000	-0.037628000	0.109161000
6	-1.477724000	-1.429332000	-0.228391000
1	0.159975000	-1.677167000	1.217567000
1	0.646067000	-1.976840000	-0.462951000
1	-2.402551000	0.017944000	1.137908000
1	-2.814038000	0.311917000	-0.553885000
1	-2.001034000	-2.242239000	0.284891000
1	-1.555828000	-1.609778000	-1.307192000
8	-0.769686000	2.087317000	-0.063960000
7	0.330620000	0.055363000	0.026685000
1	1.635803000	1.654445000	-0.026985000
6	2.807955000	-0.285920000	-0.062264000
1	2.921980000	-0.740047000	-1.063883000
1	3.707209000	0.311757000	0.118402000
1	2.817288000	-1.115585000	0.660730000

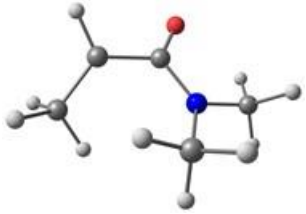
$CH_3CH(COOMe)^{\bullet}$



6	-0.072335000	0.527703000	-0.000007000
6	1.378554000	0.516345000	-0.000018000
8	-0.762975000	1.545644000	0.000018000
8	-0.611279000	-0.741331000	-0.000013000
6	-2.054762000	-0.771908000	0.000002000
1	-2.454698000	-0.268927000	-0.893760000
1	-2.324426000	-1.835020000	-0.000041000
1	-2.454677000	-0.269009000	0.893820000
1	1.833847000	1.509781000	0.000009000

6	2.237822000	-0.696024000	0.000000000
1	1.642705000	-1.617667000	-0.000288000
1	2.908037000	-0.705031000	-0.881227000
1	2.907570000	-0.705330000	0.881586000

$CH_3CH(CONMe_2)^{\bullet}$



6	-2.320376000	0.525191000	0.432044000
1	-3.085277000	0.026269000	1.046289000
1	-1.715383000	1.150478000	1.095816000
1	-2.872779000	1.189726000	-0.252335000
6	-1.507709000	-0.484340000	-0.302939000
1	-2.029606000	-1.285350000	-0.822810000
8	0.321146000	-1.914228000	-0.111385000
6	-0.073003000	-0.741279000	-0.142815000
7	0.789292000	0.321432000	0.045065000
6	2.169585000	0.035726000	0.375848000
1	2.830113000	0.183514000	-0.492808000
1	2.510965000	0.697421000	1.183631000
1	2.238993000	-1.006218000	0.693664000
6	0.513301000	1.667827000	-0.405670000
1	0.538473000	2.393450000	0.421005000
1	1.264983000	1.978402000	-1.147544000
1	-0.465479000	1.717353000	-0.888088000

$(MeO)C(S)S^{\bullet}$

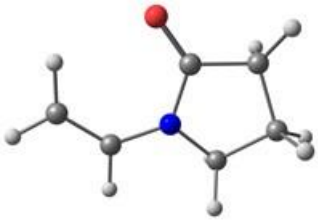
16	1.736278000	-0.629578000	-0.000015000
6	0.122262000	-0.147474000	0.000058000
8	-0.840806000	-1.050048000	0.000022000
16	-0.059249000	1.524074000	-0.000003000
6	-2.203329000	-0.590138000	-0.000024000
1	-2.405410000	0.006032000	-0.896070000
1	-2.405500000	0.005896000	0.896092000
1	-2.808709000	-1.497813000	-0.000123000

(b) Monomers

$CH_2=CH(OAc)$

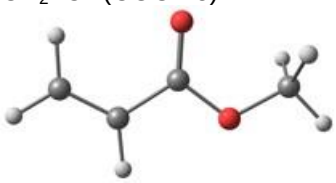
6	-1.405642000	0.278115000	-0.000006000
1	-1.228064000	1.350183000	0.000023000
6	-2.598642000	-0.307743000	0.000029000
1	-2.705080000	-1.388925000	0.000009000
1	-3.495708000	0.302694000	0.000116000
6	0.943656000	0.169181000	-0.000018000
6	2.071051000	-0.823171000	0.000023000
1	3.023078000	-0.290578000	-0.000909000
1	2.002784000	-1.468808000	0.882637000
1	2.001784000	-1.470211000	-0.881468000
8	-0.257894000	-0.489091000	-0.000078000
8	1.050228000	1.372510000	0.000005000

$CH_2=CH(N\text{-}pyr)$



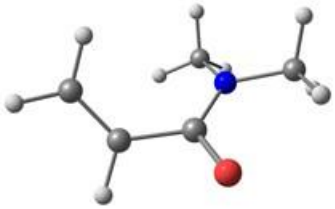
6	-2.686331000	-0.133135000	0.037509000
1	-3.651156000	-0.631901000	0.045072000
1	-2.647440000	0.948852000	0.061135000
6	-1.578855000	-0.884401000	0.003226000
1	-1.649499000	-1.971584000	-0.016936000
6	0.169019000	0.877452000	-0.014475000
6	0.852539000	-1.387584000	-0.143278000
6	1.688522000	0.867245000	-0.136517000
6	2.087518000	-0.560326000	0.239250000
1	0.913661000	-1.754316000	-1.180439000
1	0.703727000	-2.255138000	0.511245000
1	1.944277000	1.107677000	-1.178398000
1	2.125534000	1.646414000	0.494482000
1	2.992374000	-0.914470000	-0.264226000
1	2.255703000	-0.629824000	1.320706000
8	-0.552422000	1.859212000	0.036674000
7	-0.251755000	-0.442130000	-0.000047000

$CH_2=CH(COOMe)$



6	2.485397000	-0.007753000	-0.000081000
1	3.431200000	-0.543770000	-0.000088000
1	2.510442000	1.080322000	-0.000318000
6	1.314034000	-0.647934000	0.000107000
6	0.042467000	0.113825000	0.000027000
1	1.240816000	-1.733426000	0.000118000
8	-0.063509000	1.324420000	0.000076000
8	-1.015214000	-0.729120000	-0.000013000
6	-2.292455000	-0.085382000	-0.000056000
1	-3.031182000	-0.889324000	0.000507000
1	-2.408895000	0.544089000	0.888622000
1	-2.409261000	0.543173000	-0.889324000

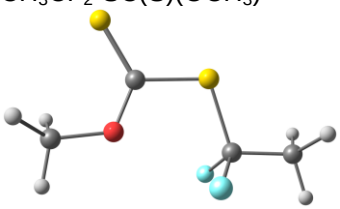
$CH_2=CH(CONMe_2)$



6	-2.285341000	0.589878000	0.452633000
1	-1.795719000	1.178881000	1.226516000
1	-3.360473000	0.720320000	0.346714000
6	-1.614308000	-0.278807000	-0.308982000
1	-2.142507000	-0.898765000	-1.032580000
8	0.060136000	-1.891137000	-0.045550000
6	-0.186688000	-0.688020000	-0.121408000
7	0.785252000	0.273756000	0.000771000
6	2.138636000	-0.154695000	0.296292000
1	2.802518000	0.020042000	-0.563145000
1	2.534216000	0.402383000	1.156494000
1	2.118720000	-1.222293000	0.522099000
6	0.628090000	1.675839000	-0.325983000
1	0.786279000	2.314114000	0.556132000
1	1.367026000	1.966992000	-1.086977000
1	-0.370242000	1.865952000	-0.721553000

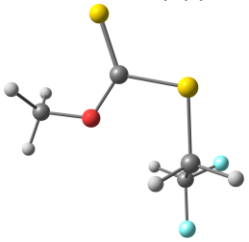
(c) Chain transfer agents

CH_3CF_2-SC(S)(OCH_3)



6	-1.739920000	0.093570000	-0.000102000
6	-3.070870000	-0.619464000	-0.000207000
1	-3.858173000	0.141307000	-0.000444000
1	-3.174583000	-1.241038000	-0.893661000
1	-3.174924000	-1.240682000	0.893459000
9	-1.641560000	0.894919000	-1.093022000
9	-1.642260000	0.895670000	1.092355000
16	-0.382514000	-1.168765000	0.000561000
6	1.124096000	-0.245886000	0.000132000
8	0.933171000	1.065294000	0.000332000
16	2.556679000	-1.052479000	-0.000251000
6	2.090846000	1.914417000	0.000030000
1	2.696436000	1.728319000	-0.892552000
1	2.696846000	1.728387000	0.892371000
1	1.691865000	2.930133000	0.000106000

CHF_2CH_2-SC(S)(OCH_3)

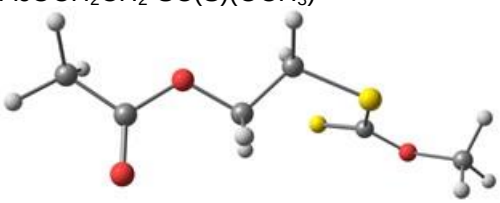


6	-1.388504000	-0.272977000	0.878223000
6	-2.139901000	0.290759000	-0.311861000
1	-1.514938000	0.912329000	-0.965455000
16	0.039507000	-1.312514000	0.424652000
6	1.315328000	-0.152852000	0.073669000
8	0.907451000	1.115151000	0.186556000
16	2.818127000	-0.673688000	-0.340214000
6	1.871772000	2.153075000	-0.054321000
1	2.256150000	2.082942000	-1.076646000
1	2.705447000	2.065589000	0.649297000
1	1.325110000	3.085697000	0.097855000
1	-1.061251000	0.538475000	1.533052000
1	-2.065970000	-0.928721000	1.436919000
9	-2.670438000	-0.720824000	-1.051412000
9	-3.171613000	1.053457000	0.158884000

$CH_3CH(OAc)$-SC(S)(OCH_3)

16	0.785871000	1.772068000	0.822287000
6	1.633161000	0.530039000	0.166306000
8	2.917159000	0.702222000	-0.161754000
6	3.701159000	-0.358456000	-0.721666000
1	3.291733000	-0.685763000	-1.684825000
1	3.763931000	-1.209083000	-0.032518000
16	1.013752000	-1.108091000	-0.177284000
6	-0.719661000	-0.997320000	0.375073000
1	4.693935000	0.070739000	-0.869132000
1	-0.744433000	-0.383305000	1.282664000
6	-1.257925000	-2.397547000	0.608134000
1	-1.239612000	-2.989968000	-0.313033000
1	-0.676975000	-2.914787000	1.378618000
1	-2.293346000	-2.309588000	0.951967000
6	-2.544085000	0.372869000	-0.225708000
6	-3.124393000	1.178155000	-1.353549000
1	-4.108624000	1.550717000	-1.065002000
1	-2.460932000	2.025709000	-1.561926000
1	-3.191369000	0.578525000	-2.266485000
8	-1.457775000	-0.331055000	-0.654280000
8	-2.954108000	0.338425000	0.912044000

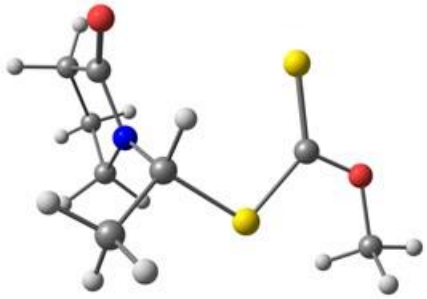
$AcOCH_2CH_2$-SC(S)(OCH_3)



16	1.496067000	1.940834000	0.081796000
6	2.171592000	0.446881000	-0.015408000
8	3.406804000	0.308853000	-0.501811000
6	4.040069000	-0.973135000	-0.600643000
1	3.474955000	-1.641675000	-1.260851000
1	4.156688000	-1.432729000	0.388072000
16	1.417223000	-1.090809000	0.487952000
6	-0.223927000	-0.556829000	1.047017000

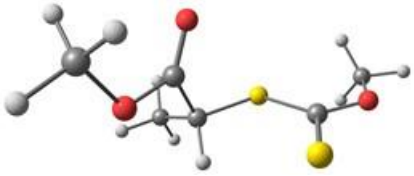
1	5.022193000	-0.770774000	-1.031746000
1	-0.112606000	0.423904000	1.523602000
6	-3.522347000	-0.079958000	-0.369307000
1	-0.529547000	-1.294490000	1.797703000
6	-1.219998000	-0.497307000	-0.097615000
1	-1.328475000	-1.466839000	-0.597714000
1	-0.914674000	0.243393000	-0.845289000
8	-2.473006000	-0.110403000	0.488157000
6	-4.773084000	0.372499000	0.335333000
1	-4.661645000	1.416105000	0.651292000
1	-5.623037000	0.284481000	-0.343142000
1	-4.943463000	-0.225051000	1.236901000
8	-3.432157000	-0.374653000	-1.540228000

CH_3CH(N-pyr)-SC(S)(OCH_3)



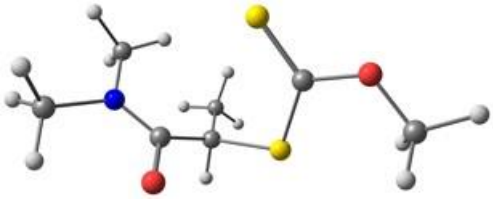
16	-1.171040000	-1.921352000	0.625972000
6	-1.925753000	-0.583858000	0.059034000
8	-3.137397000	-0.686940000	-0.503307000
6	-3.844980000	0.459395000	-0.988379000
1	-3.293553000	0.953273000	-1.797586000
1	-4.040903000	1.175075000	-0.180893000
16	-1.296722000	1.084157000	0.110607000
6	0.376871000	0.910448000	0.883172000
1	-4.789695000	0.068209000	-1.371207000
1	0.286033000	0.174768000	1.692436000
6	0.742944000	2.290757000	1.429388000
1	0.811076000	3.044958000	0.636618000
1	0.004865000	2.628175000	2.164253000
1	1.718237000	2.219297000	1.923363000
7	1.352544000	0.374054000	-0.020467000
6	3.221985000	-0.835196000	-0.738678000
1	4.182086000	-0.365012000	-0.483943000
1	3.403626000	-1.908495000	-0.845860000
6	2.555048000	-0.175637000	-1.948289000
1	1.916840000	-0.901508000	-2.465141000
1	3.264921000	0.228701000	-2.676494000
6	1.674963000	0.923408000	-1.328512000
1	2.221330000	1.877145000	-1.238992000
1	0.761122000	1.111608000	-1.904438000
6	2.258974000	-0.577168000	0.414044000
8	2.288660000	-1.063353000	1.530208000

CH_3CH(COOMe)-SC(S)(OCH_3)



16	-0.790895000	1.824988000	-0.796460000
6	-1.601251000	0.533117000	-0.183868000
8	-2.870727000	0.671862000	0.209027000
6	-3.602870000	-0.425340000	0.767438000
1	-3.123359000	-0.791724000	1.682986000
1	-3.701809000	-1.242843000	0.042846000
16	-0.950862000	-1.108342000	0.014499000
6	0.746553000	-0.921083000	-0.607406000
1	-4.588747000	-0.019653000	1.001942000
1	0.693154000	-0.360108000	-1.546681000
6	1.329793000	-2.321057000	-0.838994000
1	1.375228000	-2.894693000	0.093412000
1	0.730035000	-2.877730000	-1.566114000
1	2.347023000	-2.221046000	-1.231783000
6	3.594548000	1.115977000	0.512444000
1	4.368202000	1.470960000	-0.170809000
1	3.092603000	1.959259000	0.996959000
1	4.026740000	0.469636000	1.283317000
6	1.624070000	-0.140107000	0.370313000
8	1.468054000	-0.058185000	1.566274000
8	2.665671000	0.385393000	-0.299583000

$CH_3CH(CONMe_2)$-SC(S)(OCH_3)

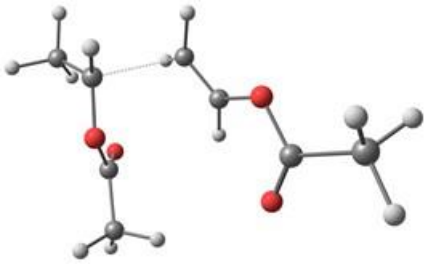


6	-1.697839000	0.550607000	-0.113274000
6	0.613747000	-0.488744000	2.235624000
1	1.657960000	-0.531108000	2.564705000
1	0.258506000	0.542603000	2.301423000
1	0.023024000	-1.096508000	2.929991000
16	-0.700311000	1.860458000	-0.073707000
8	-2.967706000	0.720032000	-0.497302000
6	-3.876488000	-0.383666000	-0.593652000
1	-3.525421000	-1.118427000	-1.327898000
1	-4.015307000	-0.866364000	0.381280000
16	-1.280988000	-1.118635000	0.283326000
6	0.470041000	-1.066811000	0.830046000
1	0.639493000	-2.151769000	0.912364000
8	1.216252000	-1.406051000	-1.389479000
6	1.406317000	-0.749426000	-0.370121000
7	2.506037000	0.050203000	-0.227943000
6	3.476506000	0.022079000	-1.311980000
1	3.318614000	0.858316000	-2.008469000
1	4.487274000	0.100809000	-0.893071000
1	3.370063000	-0.912546000	-1.864054000
6	2.695143000	1.130342000	0.723963000
1	3.427384000	0.870158000	1.502369000
1	3.072930000	2.008117000	0.184325000
1	1.750317000	1.424221000	1.176996000
1	-4.819240000	0.053783000	-0.927643000

d) VAc homopropagation

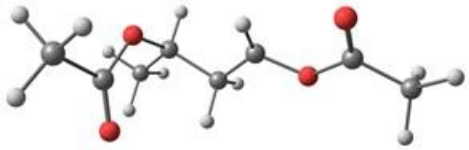
d1. Head-to-tail

$CH_3CH(OAc)^{\bullet}\cdots CH_2$=CH(OAc) TS



6	1.585616000	1.206690000	-0.081789000
6	1.748714000	-0.991150000	0.850453000
1	1.286717000	-1.524968000	1.679046000
8	1.415706000	0.349645000	0.967002000
6	1.027754000	2.559345000	0.261910000
1	1.234246000	2.823681000	1.303026000
1	1.444391000	3.306578000	-0.416206000
1	-0.061205000	2.524481000	0.129841000
8	2.082749000	0.896587000	-1.142456000
6	0.272262000	-1.797956000	-0.828491000
1	1.086446000	-1.760358000	-1.543804000
1	0.118100000	-2.717326000	-0.270105000
6	-0.715046000	-0.882302000	-0.935531000
1	-0.673852000	0.011444000	-1.548993000
8	-1.848290000	-1.006850000	-0.153999000
6	-2.632677000	0.098327000	0.001637000
8	-2.355471000	1.188865000	-0.446976000
6	-3.868914000	-0.245186000	0.783617000
1	-4.415463000	0.669691000	1.017497000
1	-4.507505000	-0.912143000	0.192457000
1	-3.605369000	-0.777333000	1.703555000
6	3.127114000	-1.381848000	0.437861000
1	3.210354000	-2.474689000	0.436010000
1	3.376659000	-0.996250000	-0.554397000
1	3.879992000	-0.994299000	1.145501000

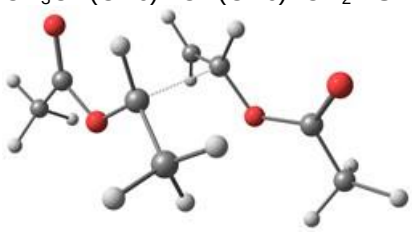
$CH_3CH(OAc)\text{-}CH_2CH(OAc)^{\bullet}$



6	2.300214000	0.918783000	-0.308441000
6	1.443043000	-1.147908000	0.636123000
1	1.199128000	-1.406068000	1.674221000
8	1.903950000	0.224824000	0.781204000
6	2.709419000	2.315094000	0.086155000
1	3.457118000	2.282794000	0.885517000
1	3.109970000	2.834625000	-0.785793000
1	1.841500000	2.860522000	0.474042000
8	2.316478000	0.484886000	-1.441508000
6	0.159853000	-1.228968000	-0.193441000
1	0.394530000	-0.972286000	-1.239711000
1	-0.171698000	-2.279308000	-0.200965000
6	-0.918975000	-0.370389000	0.351819000
1	-0.769250000	0.572728000	0.866304000
8	-2.157112000	-0.573616000	-0.204718000
6	-3.145756000	0.333092000	0.077085000
8	-2.970809000	1.310851000	0.767287000
6	-4.432294000	-0.080173000	-0.579188000
1	-5.183536000	0.694890000	-0.419722000
1	-4.280994000	-0.244134000	-1.651530000
1	-4.784119000	-1.026359000	-0.151444000
6	2.547945000	-2.068798000	0.139338000
1	2.225039000	-3.112276000	0.235870000
1	2.790506000	-1.867566000	-0.907045000
1	3.451052000	-1.937519000	0.745432000

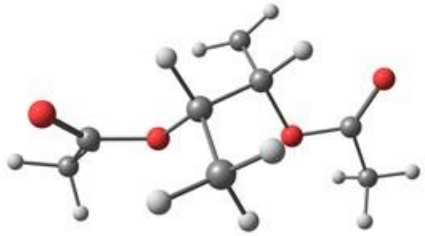
d2. Head-to-head

$CH_3CH(OAc)^{\bullet}\cdots CH(OAc)=CH_2$ TS



6	-2.773507000	0.063602000	-0.005780000
6	-0.631297000	0.904839000	-0.502962000
1	-0.958836000	0.802941000	-1.536589000
8	-1.648893000	0.717263000	0.413413000
6	-3.717819000	-0.138414000	1.146155000
1	-3.903746000	0.810253000	1.661014000
1	-4.655406000	-0.556931000	0.776892000
1	-3.270997000	-0.823118000	1.876049000
8	-2.961765000	-0.278824000	-1.151943000
6	-0.262887000	-1.977206000	-0.140054000
1	-0.316709000	-2.352841000	0.877522000
1	-0.998185000	-2.310816000	-0.863925000
6	0.615473000	-0.991753000	-0.479736000
1	0.889760000	-0.751514000	-1.503399000
8	1.604430000	-0.679069000	0.457869000
6	2.761318000	-0.131341000	-0.005727000
8	2.963125000	0.142864000	-1.167991000
6	3.736620000	0.057138000	1.123330000
1	4.605401000	0.610430000	0.763321000
1	3.265141000	0.587723000	1.956828000
1	4.056051000	-0.921740000	1.499675000
6	0.283897000	2.009877000	-0.114927000
1	0.669795000	1.861975000	0.901108000
1	1.127670000	2.063655000	-0.809479000
1	-0.235907000	2.981661000	-0.131595000

$CH_3CH(OAc)\text{-}CH(OAc)CH_2^{\bullet}$

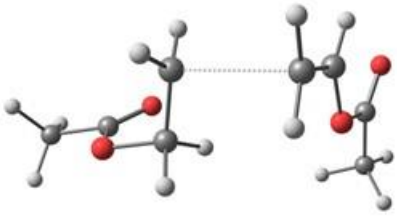


6	2.761344000	0.252559000	-0.016055000
6	0.663808000	-0.858993000	0.143249000
1	1.221990000	-1.651063000	-0.372552000
8	1.412485000	0.370565000	0.003260000
6	3.409410000	1.606962000	-0.130769000
1	3.221893000	2.182645000	0.783015000
1	4.484549000	1.484422000	-0.271043000
1	2.978114000	2.171134000	-0.964005000
8	3.349907000	-0.804481000	0.060437000

6	-0.526674000	-0.276381000	-2.005524000
1	0.304146000	0.346073000	-2.322979000
1	-1.344357000	-0.466049000	-2.693500000
6	-0.662554000	-0.674446000	-0.583317000
1	-1.233375000	-1.609406000	-0.509468000
8	-1.423422000	0.340585000	0.155713000
6	-2.768947000	0.230615000	0.082548000
8	-3.346060000	-0.638671000	-0.535819000
6	-3.434606000	1.335645000	0.860673000
1	-4.513100000	1.170353000	0.875330000
1	-3.042734000	1.376306000	1.882247000
1	-3.215792000	2.300643000	0.389317000
6	0.516817000	-1.207332000	1.615248000
1	0.018945000	-0.395317000	2.153493000
1	-0.078402000	-2.120818000	1.731285000
1	1.503260000	-1.384685000	2.053816000

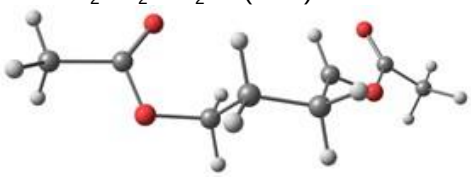
d3. Tail-to-tail

$AcOCH_2CH_2^{\bullet}\cdots CH_2=CH(OAc)$ TS



6	-1.079938000	1.851066000	-0.341750000
1	-0.961182000	1.465779000	-1.350932000
6	-2.877603000	-0.735904000	-0.160422000
1	-1.461750000	2.866520000	-0.251415000
6	-1.370253000	0.875549000	0.738228000
1	-1.345864000	1.338999000	1.729492000
1	-0.674837000	0.030909000	0.706296000
8	-2.730935000	0.341872000	0.639061000
6	-4.321112000	-1.168441000	-0.207659000
1	-4.922816000	-0.391932000	-0.693889000
1	-4.403000000	-2.100487000	-0.769307000
1	-4.715812000	-1.299130000	0.805284000
8	-1.967667000	-1.271563000	-0.758472000
6	1.249030000	2.334449000	0.072840000
1	1.161314000	3.220415000	-0.546856000
1	1.000207000	2.425889000	1.126231000
6	1.987461000	1.297832000	-0.375639000
1	2.386047000	1.193212000	-1.380399000
8	2.202538000	0.215302000	0.446743000
6	2.948065000	-0.824018000	-0.055650000
8	3.459081000	-0.807533000	-1.149494000
6	3.002208000	-1.946840000	0.938694000
1	3.741841000	-2.680770000	0.615027000
1	3.246766000	-1.569658000	1.936683000
1	2.017805000	-2.426533000	0.999216000

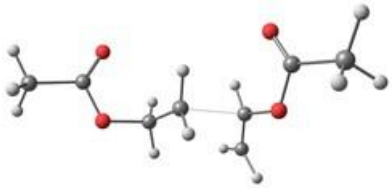
$AcOCH_2CH_2$-$CH_2CH(OAc)^{\bullet}$



6	-0.907968000	1.234132000	-0.632528000
1	-1.113525000	0.516149000	-1.436841000
6	-3.376731000	-0.581019000	0.068485000
1	-1.438592000	2.161989000	-0.881431000
6	-1.463356000	0.679053000	0.671644000
1	-1.268987000	1.363702000	1.505100000
1	-1.024730000	-0.298961000	0.897630000
8	-2.897271000	0.557474000	0.621923000
6	-4.882666000	-0.586490000	0.090353000
1	-5.270558000	0.282773000	-0.451945000
1	-5.249100000	-1.506339000	-0.367939000
1	-5.243570000	-0.513063000	1.122175000
8	-2.675742000	-1.465499000	-0.374120000
6	0.596910000	1.513884000	-0.550952000
1	0.913723000	2.017851000	-1.484021000
1	0.808200000	2.235888000	0.253765000
6	1.396950000	0.284715000	-0.325306000
1	1.182931000	-0.684892000	-0.766567000
8	2.695175000	0.502462000	0.065444000
6	3.563382000	-0.559424000	0.047307000
8	3.250567000	-1.664616000	-0.329540000
6	4.908360000	-0.138833000	0.568159000
1	5.621162000	-0.952244000	0.423653000
1	5.255541000	0.765285000	0.057166000
1	4.836385000	0.097182000	1.636628000

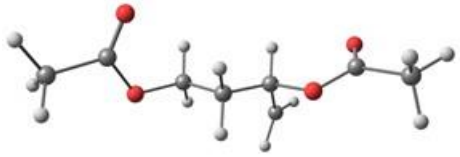
d4. Tail-to-head

$AcOCH_2CH_2^{\bullet}\cdots CH(OAc)=CH_2$ TS



6	-0.212966000	0.198998000	-0.463050000
1	-0.094283000	-0.770697000	0.016145000
6	-3.240276000	-0.414406000	0.122840000
1	0.116080000	0.270795000	-1.498046000
6	-1.363446000	1.040378000	-0.040465000
1	-1.282420000	2.059547000	-0.429923000
1	-1.462534000	1.063628000	1.050369000
8	-2.621590000	0.549213000	-0.595335000
6	-4.513493000	-0.846420000	-0.558483000
1	-4.281834000	-1.285357000	-1.535505000
1	-5.027095000	-1.580815000	0.064056000
1	-5.162266000	0.017917000	-0.735968000
8	-2.818421000	-0.860376000	1.168562000
6	1.563877000	2.488035000	0.239474000
1	2.043320000	2.961169000	-0.612318000
1	0.930118000	3.089440000	0.882735000
6	1.661831000	1.150085000	0.453438000
1	1.369532000	0.657661000	1.377124000
8	2.591164000	0.445351000	-0.303100000
6	2.884544000	-0.830179000	0.090353000
8	2.379296000	-1.370638000	1.046422000
6	3.907994000	-1.432043000	-0.830421000
1	4.157043000	-2.437188000	-0.487278000
1	3.514359000	-1.473215000	-1.852216000
1	4.807994000	-0.807969000	-0.853681000

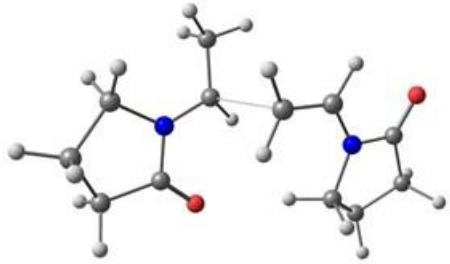
$AcOCH_2CH_2$-CH(OAc)$CH_2^{\bullet}$



6	-0.289765000	0.215484000	-0.435059000
1	-0.431054000	-0.855514000	-0.250870000
6	-3.298967000	-0.444626000	0.189831000
1	-0.328107000	0.378942000	-1.520497000
6	-1.414459000	0.989996000	0.238708000
1	-1.311781000	2.067957000	0.076031000
1	-1.435891000	0.785960000	1.315575000
8	-2.690373000	0.647797000	-0.331065000
6	-4.621871000	-0.685545000	-0.487485000
1	-4.473889000	-0.823612000	-1.564147000
1	-5.093222000	-1.571322000	-0.058989000
1	-5.274167000	0.185145000	-0.358392000
8	-2.829642000	-1.118410000	1.081360000
6	1.450855000	2.032837000	-0.226406000
1	1.145912000	2.474654000	-1.173171000
1	2.178368000	2.557780000	0.384643000
6	1.078017000	0.631745000	0.094154000
1	1.149551000	0.466445000	1.176881000
8	2.029874000	-0.298373000	-0.533786000
6	3.198857000	-0.470860000	0.122783000
8	3.489371000	0.098055000	1.153625000
6	4.071185000	-1.463870000	-0.601291000
1	5.012377000	-1.580579000	-0.061699000
1	3.560229000	-2.430159000	-0.674893000
1	4.264736000	-1.119207000	-1.622963000

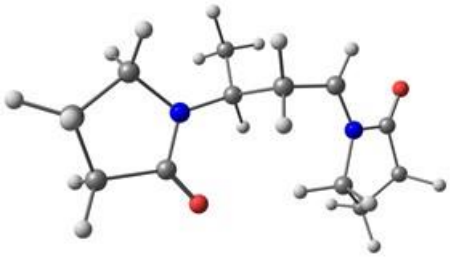
(e) Other monomers homopropagation (all head-to-tail)

CH_3CH(N-pyr)$^{\bullet\cdots}CH_2$=CH(N-pyr) TS



6	1.470492000	1.201836000	0.806511000
6	-2.337504000	-1.113711000	-0.331740000
6	-3.579840000	0.846176000	0.155031000
6	-3.719941000	-1.570948000	0.102856000
6	-4.308004000	-0.344157000	0.803976000
1	-4.149517000	1.270064000	-0.686002000
1	-3.388609000	1.656636000	0.868575000
1	-4.292184000	-1.852817000	-0.793119000
1	-3.649555000	-2.461221000	0.735093000
1	-5.394775000	-0.259482000	0.706507000
1	-4.071804000	-0.378302000	1.874220000
8	-1.387239000	-1.813493000	-0.668296000
7	-2.327490000	0.269254000	-0.321547000
6	-1.345165000	2.427899000	-1.091900000
1	-1.871623000	2.548622000	-2.054052000
1	-1.887372000	3.025285000	-0.347532000
1	-0.349680000	2.870340000	-1.205714000
6	-1.202333000	0.996909000	-0.692370000
1	-0.499944000	0.378994000	-1.245529000
6	0.164856000	1.045372000	1.176431000
1	-0.348891000	1.899834000	1.608120000
1	-0.236578000	0.065415000	1.420779000
1	1.952568000	2.173240000	0.726782000
7	2.293792000	0.171608000	0.390077000
6	3.610251000	0.394140000	0.009127000
8	4.138726000	1.492306000	-0.060227000
6	1.934176000	-1.242330000	0.432174000
1	0.933586000	-1.407435000	0.014691000
1	1.930046000	-1.595145000	1.476083000
6	3.043108000	-1.911413000	-0.396875000
1	2.728532000	-1.970158000	-1.445560000
1	3.248449000	-2.930544000	-0.055215000
6	4.238198000	-0.964935000	-0.258996000
1	4.872610000	-1.220210000	0.602354000
1	4.888958000	-0.918687000	-1.137368000

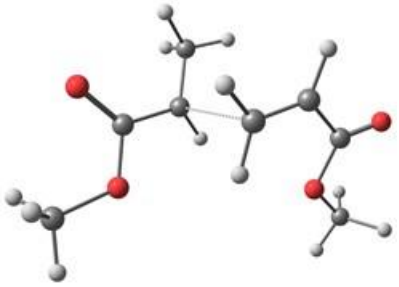
CH3CH(N-pyr)-CH2CH(N-pyr)$^{\bullet}$



6	1.367141000	1.193609000	0.745124000
6	-2.389073000	-1.099413000	-0.277665000
6	-3.394249000	0.998502000	0.163722000
6	-3.869776000	-1.368288000	-0.039765000
6	-4.366476000	-0.093929000	0.648818000
1	-3.787829000	1.534596000	-0.714462000
1	-3.190626000	1.746319000	0.941230000
1	-4.347589000	-1.529134000	-1.016419000
1	-4.005811000	-2.282733000	0.544567000
1	-5.407905000	0.153406000	0.420975000
1	-4.280766000	-0.202341000	1.736737000
8	-1.518566000	-1.923463000	-0.538278000
7	-2.193687000	0.251227000	-0.177050000
6	-0.959946000	2.149561000	-1.174981000
1	-1.470714000	2.020722000	-2.136054000
1	-1.487474000	2.924381000	-0.603626000
1	0.052488000	2.517410000	-1.374033000
6	-0.880568000	0.834177000	-0.408935000
1	-0.354901000	0.093009000	-1.024553000
6	-0.088864000	0.967900000	0.927580000
1	-0.509871000	1.797881000	1.512343000
1	-0.275072000	0.048971000	1.502339000
1	1.815918000	2.178438000	0.668003000
7	2.208892000	0.172962000	0.368459000
6	3.531546000	0.410491000	0.002114000
8	4.026506000	1.523633000	-0.100297000
6	1.906397000	-1.255558000	0.486233000
1	0.909559000	-1.490954000	0.095455000
1	1.934980000	-1.552437000	1.546862000
6	3.034194000	-1.919944000	-0.317085000
1	2.728423000	-2.014947000	-1.365867000

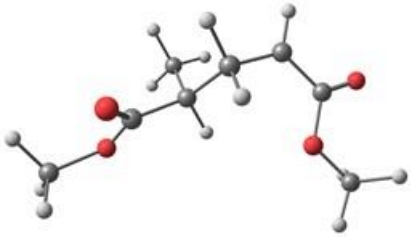
1	3.260662000	-2.923742000	0.055519000
6	4.201830000	-0.938714000	-0.195646000
1	4.825763000	-1.147524000	0.686200000
1	4.867878000	-0.912363000	-1.063574000

$CH_3CH(COOMe)^{\bullet}\cdots CH_2{=}CH(COOMe)$ TS



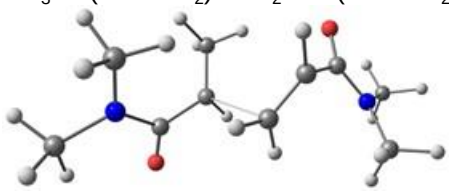
6	1.448646000	-0.941874000	-0.987474000
6	-0.971993000	-2.170293000	1.017545000
1	-1.396714000	-2.382077000	2.012138000
1	-1.562752000	-2.735834000	0.289815000
1	0.061267000	-2.533003000	1.022834000
6	-1.038529000	-0.712937000	0.732800000
1	-0.392153000	-0.030139000	1.279381000
6	0.226674000	-0.381177000	-1.205002000
1	-0.517737000	-0.910135000	-1.796076000
1	0.074163000	0.683500000	-1.051000000
1	1.661918000	-1.969868000	-1.270672000
6	2.572938000	-0.257613000	-0.333837000
8	3.684207000	-0.739689000	-0.204323000
8	2.242819000	0.977899000	0.119513000
6	3.315539000	1.689342000	0.741622000
1	3.708780000	1.130309000	1.597406000
1	4.132900000	1.857949000	0.032131000
1	2.891220000	2.641205000	1.067708000
8	-3.204624000	-0.811477000	-0.260265000
8	-2.271564000	1.201846000	0.222798000
6	-3.449530000	1.813172000	-0.307817000
1	-3.287007000	2.890170000	-0.229583000
1	-3.604230000	1.523151000	-1.352890000
1	-4.333747000	1.517674000	0.267496000
6	-2.277515000	-0.157210000	0.193752000

$CH_3CH(COOMe)\text{-}CH_2CH(COOMe)^{\bullet}$



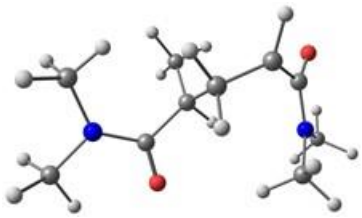
6	-1.583188000	1.234258000	-0.489422000
6	0.953965000	1.637622000	1.225656000
1	1.611168000	1.332411000	2.045402000
1	1.417164000	2.489510000	0.711764000
1	0.003979000	1.977034000	1.653474000
6	0.716229000	0.474036000	0.252517000
1	0.255115000	-0.354901000	0.807353000
6	-0.213020000	0.852588000	-0.923476000
1	0.249742000	1.672452000	-1.485474000
1	-0.264942000	-0.011122000	-1.599141000
1	-1.892626000	2.275603000	-0.450041000
6	-2.603987000	0.291838000	-0.075176000
8	-3.732596000	0.603150000	0.281578000
8	-2.173471000	-1.000270000	-0.124153000
6	-3.152721000	-1.965882000	0.262342000
1	-3.482016000	-1.796852000	1.293531000
1	-4.029157000	-1.914902000	-0.392985000
1	-2.664546000	-2.938539000	0.171353000
8	2.386888000	-0.014768000	-1.453262000
8	2.799041000	-0.554566000	0.698681000
6	4.075026000	-1.054734000	0.282308000
1	4.561332000	-1.418333000	1.189648000
1	3.954151000	-1.868229000	-0.440658000
1	4.670418000	-0.261067000	-0.180955000
6	2.036250000	-0.044965000	-0.292419000

$CH_3CH(CONMe_2)^{\bullet}\cdots CH_2{=}CH(CONMe_2)$ TS



6	1.201225000	0.280466000	1.150487000
6	-0.828087000	1.756348000	-0.959599000
1	-1.022493000	2.094286000	-1.989944000
1	-1.499303000	2.321153000	-0.307721000
1	0.207370000	2.037529000	-0.724850000
6	-1.002705000	0.269363000	-0.892824000
1	-0.395944000	-0.276799000	-1.613121000
6	0.249182000	-0.640759000	0.811903000
1	-0.616340000	-0.788230000	1.453212000
1	0.476617000	-1.465243000	0.140532000
1	0.971854000	1.055333000	1.881105000
6	2.415743000	0.580472000	0.344319000
8	2.576627000	1.736783000	-0.062412000
8	-2.558447000	-1.365803000	-1.505037000
6	-2.297085000	-0.434982000	-0.732841000
7	-3.188923000	-0.052006000	0.248092000
7	3.290695000	-0.428994000	0.038838000
6	-4.496184000	-0.675944000	0.274085000
1	-4.647442000	-1.229930000	1.212376000
1	-5.289445000	0.081291000	0.191929000
1	-4.559287000	-1.368076000	-0.567397000
6	-2.927304000	0.895229000	1.307856000
1	-3.471214000	1.842036000	1.162971000
1	-3.252838000	0.470284000	2.268584000
1	-1.861587000	1.114044000	1.382947000
6	3.304203000	-1.731018000	0.672363000
1	3.095761000	-2.533875000	-0.049997000
1	4.293956000	-1.921744000	1.112112000
1	2.558980000	-1.770302000	1.468699000
6	4.398604000	-0.142845000	-0.851123000
1	5.356479000	-0.190583000	-0.312889000
1	4.427393000	-0.872773000	-1.671661000
1	4.264083000	0.862773000	-1.253568000

$CH_3CH(CONMe_2)\text{-}CH_2CH(CONMe_2)^{\bullet}$

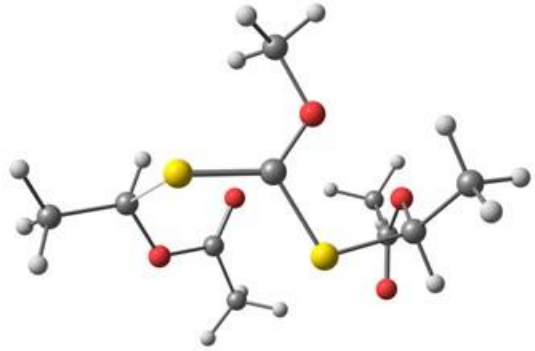


6	-1.410483000	1.222088000	-1.059102000
6	0.630486000	1.579716000	1.295024000
1	1.031778000	1.280149000	2.270135000
1	1.257512000	2.390387000	0.908845000
1	-0.371347000	1.993821000	1.458410000
6	0.525178000	0.372865000	0.354117000
1	-0.232083000	-0.289604000	0.788624000
6	0.007946000	0.738801000	-1.064570000
1	0.637241000	1.511867000	-1.524897000
1	0.120659000	-0.155286000	-1.698823000
1	-1.625234000	2.221036000	-1.432259000
6	-2.503080000	0.685589000	-0.230131000
8	-3.200706000	1.498059000	0.395948000
8	1.516609000	-1.781725000	0.521059000
6	1.724049000	-0.587142000	0.296358000
7	2.984113000	-0.137299000	-0.007560000
7	-2.680812000	-0.670603000	-0.115785000
6	4.082568000	-1.085660000	0.022117000
1	4.525338000	-1.199757000	-0.977880000
1	4.867615000	-0.739567000	0.708984000
1	3.693413000	-2.048084000	0.357690000
6	3.352444000	1.206452000	-0.395316000
1	3.953770000	1.701621000	0.382119000
1	3.953919000	1.173778000	-1.314902000
1	2.474610000	1.818298000	-0.595048000
6	-2.053044000	-1.644295000	-0.988868000
1	-1.142220000	-2.081512000	-0.552799000
1	-2.765182000	-2.455026000	-1.186603000
1	-1.805535000	-1.184609000	-1.950240000
6	-3.625211000	-1.174241000	0.861277000
1	-4.476666000	-1.666255000	0.368954000
1	-3.140813000	-1.903043000	1.525419000
1	-3.992248000	-0.328595000	1.446186000

(e) VAc RAFT: MacroCTA degenerative and non-degenerative radical exchange

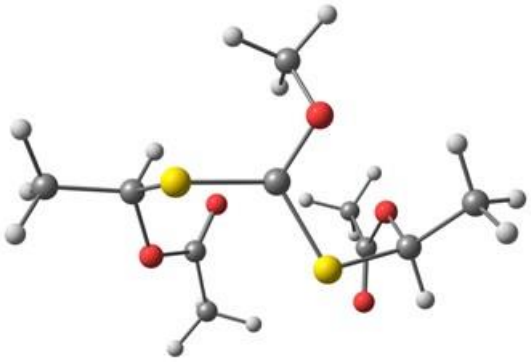
e1. Head-head (degenerative)

$CH_3CH(OAc)$-$SC(OMe)S^{\cdots\bullet}CH(OAc)CH_3$ TS



6	2.484098000	-0.634868000	-0.807774000
16	0.758250000	-0.816034000	-1.444623000
6	-0.180960000	-1.581485000	-0.160883000
8	0.530849000	-1.862155000	0.940834000
6	-0.169013000	-2.373907000	2.077021000
1	-0.678820000	-3.312201000	1.831528000
1	-0.903807000	-1.643071000	2.430188000
16	-1.813456000	-1.780317000	-0.369799000
6	-3.109910000	0.257929000	0.250744000
1	0.600663000	-2.538623000	2.834236000
1	-2.898234000	0.223497000	1.317010000
6	-4.449524000	-0.095994000	-0.284456000
1	-4.414418000	-0.228481000	-1.371996000
1	-4.800497000	-1.028683000	0.169608000
1	-5.192928000	0.687867000	-0.065654000
6	-1.456133000	1.931427000	0.173091000
6	-0.937187000	3.047801000	-0.683223000
1	-0.869458000	3.958807000	-0.079124000
1	0.078405000	2.799082000	-1.014533000
1	-1.574573000	3.221512000	-1.552164000
8	-2.533016000	1.323890000	-0.404024000
8	-1.001898000	1.588893000	1.246889000
1	2.939535000	-0.051260000	-1.618502000
6	3.220501000	-1.937079000	-0.571368000
1	3.231539000	-2.530763000	-1.490514000
1	4.255159000	-1.718911000	-0.281348000
1	2.744822000	-2.516430000	0.222909000
8	2.535368000	0.131487000	0.393425000
6	2.470767000	1.482868000	0.256890000
6	2.379114000	2.150350000	1.596391000
1	2.737810000	3.178769000	1.517602000
1	1.318734000	2.159686000	1.883004000
1	2.937499000	1.599264000	2.357655000
8	2.451365000	2.042797000	-0.819342000

$CH_3CH(OAc)$-$SC^{\bullet}(OMe)S$-$CH(OAc)CH_3$

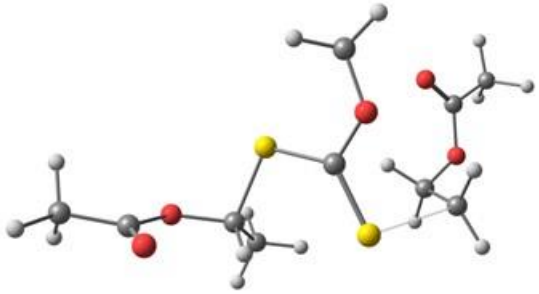


6	2.390269000	-0.770216000	-0.746858000
16	0.700746000	-0.972511000	-1.473603000
6	-0.309847000	-1.398123000	-0.103627000
8	0.266174000	-2.158392000	0.865893000
6	-0.239975000	-1.940444000	2.183307000
1	-1.300121000	-2.219706000	2.243923000
1	-0.115569000	-0.889424000	2.470503000
16	-2.031944000	-1.525126000	-0.454149000
6	-2.711617000	0.062155000	0.209069000
1	0.344999000	-2.585770000	2.843524000
1	-2.382463000	0.178715000	1.245176000
6	-4.220491000	0.025272000	0.071484000
1	-4.513700000	-0.083392000	-0.978298000
1	-4.637415000	-0.810360000	0.642954000

1	-4.645767000	0.959046000	0.455164000
6	-1.288298000	1.962896000	0.037324000
6	-0.822127000	3.039773000	-0.898905000
1	-0.801684000	3.994006000	-0.363978000
1	0.205465000	2.809012000	-1.205332000
1	-1.457367000	3.110411000	-1.783860000
8	-2.219378000	1.170634000	-0.548844000
8	-0.890352000	1.809362000	1.176330000
1	2.903210000	-0.209079000	-1.538144000
6	3.092605000	-2.074974000	-0.431888000
1	3.146819000	-2.693557000	-1.333160000
1	4.112584000	-1.864873000	-0.087756000
1	2.555107000	-2.626333000	0.342818000
8	2.375741000	0.022247000	0.439736000
6	2.447706000	1.371158000	0.275698000
6	2.393525000	2.077022000	1.598211000
1	2.884767000	3.048433000	1.508804000
1	1.335852000	2.233523000	1.847110000
1	2.854099000	1.479959000	2.389596000
8	2.520295000	1.906708000	-0.810351000

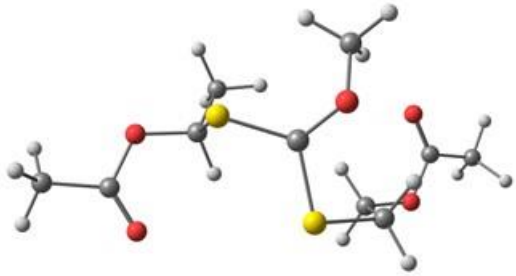
e2. Head-tail (non-degenerative)

$CH_3CH(OAc)$-$SC(OMe)S^{\cdots\bullet}CH_2CH_2OAc$ TS



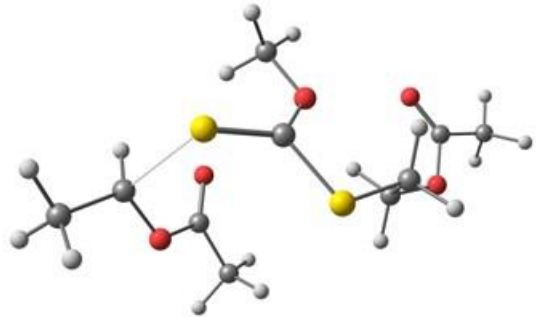
6	2.540046000	-0.980503000	1.626213000
6	2.600000000	-1.370777000	0.196440000
16	0.037699000	-0.548209000	1.997506000
6	-0.144136000	0.685336000	0.907536000
8	0.558313000	1.807988000	1.103484000
6	0.638137000	2.818384000	0.090540000
1	-0.356568000	3.201594000	-0.167950000
1	1.151197000	2.424411000	-0.793608000
16	-1.117138000	0.647043000	-0.576228000
6	-2.166296000	-0.858930000	-0.317340000
1	2.403225000	-2.436702000	0.050860000
1	1.236112000	3.616893000	0.533717000
1	-2.332828000	-0.926998000	0.763225000
1	2.717376000	-1.725249000	2.397932000
1	2.777441000	0.049040000	1.878839000
1	1.906426000	-0.779809000	-0.413014000
8	3.940691000	-1.172342000	-0.364566000
6	4.180885000	0.036720000	-0.906156000
8	3.365386000	0.935520000	-0.976806000
6	5.602382000	0.124364000	-1.400716000
1	5.736071000	1.048967000	-1.964853000
1	6.288641000	0.115133000	-0.545897000
1	5.846940000	-0.741738000	-2.023949000
6	-1.553798000	-2.107141000	-0.907124000
1	-2.226406000	-2.956499000	-0.738195000
1	-1.389043000	-1.994591000	-1.983585000
1	-0.600398000	-2.313418000	-0.412242000
8	-3.390613000	-0.601646000	-0.999395000
6	-4.390313000	-0.022592000	-0.264110000
6	-5.592638000	0.223097000	-1.131372000
1	-5.354558000	0.988269000	-1.879302000
1	-5.867747000	-0.687959000	-1.672644000
1	-6.423419000	0.562826000	-0.511125000
8	-4.289658000	0.241322000	0.909518000

$CH_3CH(OAc)$-$SC^{\bullet}(OMe)S$-CH_2CH_2OAc



6	-2.012421000	-0.334956000	-1.621921000
6	-2.118961000	-1.324307000	-0.471687000
16	-0.267504000	0.059512000	-2.000967000
6	0.067682000	1.197458000	-0.698850000
8	-0.795690000	2.247455000	-0.630925000
6	-1.063212000	2.760603000	0.678949000
1	-0.130263000	3.002164000	1.202688000
1	-1.650441000	2.034420000	1.253808000
16	1.749297000	1.445094000	-0.231030000
6	2.028728000	-0.061301000	0.825192000
1	-1.691025000	-2.293874000	-0.742876000
1	-1.645949000	3.673111000	0.528864000
1	1.603037000	-0.911536000	0.281445000
1	-2.443739000	-0.744961000	-2.541603000
1	-2.521808000	0.603167000	-1.381341000
1	-1.610001000	-0.929452000	0.413508000
8	-3.498837000	-1.588104000	-0.152030000
6	-4.071759000	-0.762206000	0.753397000
8	-3.493477000	0.154338000	1.299551000
6	-5.509589000	-1.143554000	0.982472000
1	-5.944481000	-0.487685000	1.738127000
1	-6.071971000	-1.057593000	0.046042000
1	-5.576155000	-2.187820000	1.306144000
6	1.477278000	0.082278000	2.225272000
1	1.650752000	-0.841465000	2.791307000
1	1.958995000	0.914102000	2.749935000
1	0.398935000	0.267482000	2.184909000
8	3.444033000	-0.211497000	0.910303000
6	4.016080000	-1.165748000	0.117179000
6	5.512211000	-1.122255000	0.256362000
1	5.893191000	-0.203856000	-0.205350000
1	5.800766000	-1.101663000	1.312101000
1	5.948601000	-1.988894000	-0.242634000
8	3.389801000	-1.924118000	-0.584566000

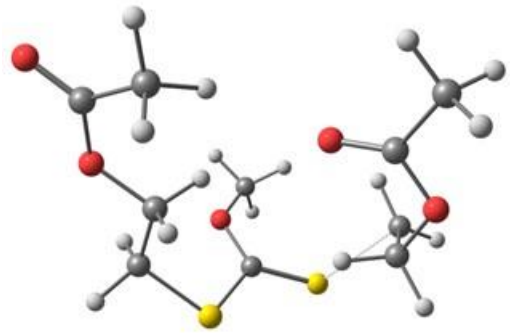
$CH_3CH(OAc)^{\bullet\cdots}SC(OMe)S$-$CH_2CH_2OAc$ TS



6	1.860870000	-0.736996000	-1.401607000
6	2.190774000	0.618716000	-0.793178000
16	0.081408000	-0.940065000	-1.768784000
6	-0.621634000	-1.353390000	-0.197375000
8	0.273400000	-1.273797000	0.793658000
6	-0.168326000	-1.504130000	2.137410000
1	-0.609756000	-2.502268000	2.230570000
1	-0.899858000	-0.741072000	2.419604000
16	-2.230310000	-1.725237000	-0.073418000
6	-3.608988000	0.308464000	0.428050000
1	1.862557000	1.430937000	-1.448917000
1	0.735928000	-1.417625000	2.742512000
1	-3.450100000	0.284885000	1.503514000
1	2.362548000	-0.857356000	-2.369132000
1	2.178195000	-1.543395000	-0.734710000
1	1.726083000	0.716123000	0.192090000
8	3.617028000	0.783101000	-0.678651000
6	4.187660000	0.286942000	0.446864000
8	3.573202000	-0.279394000	1.324041000
6	5.671015000	0.545232000	0.442160000
1	6.113230000	0.139580000	1.353348000
1	6.131249000	0.079942000	-0.436442000
1	5.865037000	1.621550000	0.378484000
6	-4.919961000	-0.047865000	-0.170124000
1	-5.679733000	0.727773000	0.022575000
1	-4.835044000	-0.172938000	-1.255425000
1	-5.284806000	-0.986623000	0.260432000
8	-2.984883000	1.355557000	-0.212531000
6	-1.915135000	1.940314000	0.401724000
6	-1.341088000	3.018381000	-0.472054000
1	-0.899226000	2.563944000	-1.367083000
1	-2.126868000	3.702991000	-0.808129000
1	-0.574855000	3.564670000	0.080462000
8	-1.509157000	1.611997000	1.496014000

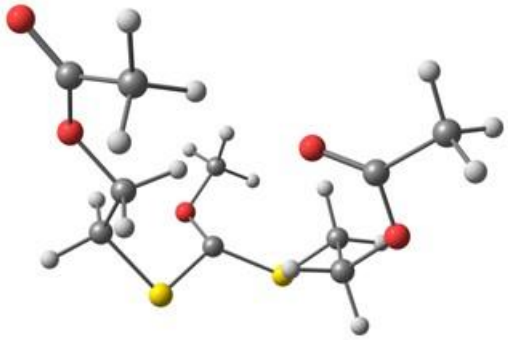
e3. Tail-tail (degenerative)

$AcOCH_2CH_2$-SC(OMe)S$^{\cdots\bullet}CH_2CH_2OAc$ TS



6	1.174883000	-2.093457000	-1.027259000
6	1.775069000	-0.770839000	-0.574634000
16	-0.566135000	-1.897719000	-1.542925000
6	-1.452006000	-1.873738000	-0.018638000
8	-0.707078000	-2.264287000	1.023543000
6	-1.327877000	-2.335933000	2.312697000
1	-2.157667000	-3.050392000	2.296852000
1	-1.705066000	-1.353890000	2.614942000
16	-3.029427000	-1.376418000	0.026507000
6	-2.960954000	1.164792000	0.490276000
1	1.801063000	-0.060660000	-1.411715000
1	-0.538546000	-2.671408000	2.988223000
1	-2.392510000	1.081336000	1.412644000
6	-0.543548000	3.124209000	0.088368000
1	1.700350000	-2.482932000	-1.906352000
1	1.234882000	-2.840350000	-0.231581000
1	-4.033047000	1.315423000	0.590582000
6	-2.252725000	1.668602000	-0.712272000
1	-2.917571000	1.757728000	-1.574748000
1	-1.399159000	1.033879000	-0.972298000
8	-1.743778000	3.029984000	-0.506651000
6	-0.138928000	4.565519000	0.257103000
1	-0.841645000	5.069274000	0.930453000
1	0.868965000	4.618070000	0.671862000
1	-0.180925000	5.087471000	-0.704599000
8	0.119496000	2.167167000	0.446669000
1	1.170160000	-0.327443000	0.225757000
8	3.092342000	-1.071680000	-0.106984000
6	3.949977000	-0.077829000	0.266306000
8	5.016980000	-0.391942000	0.735803000
6	3.515875000	1.349375000	0.034883000
1	4.269425000	2.003586000	0.476433000
1	3.458456000	1.555705000	-1.041935000
1	2.529543000	1.572660000	0.458155000

$AcOCH_2CH_2$-SC$^{\bullet}$(OMe)S-CH_2CH_2OAc



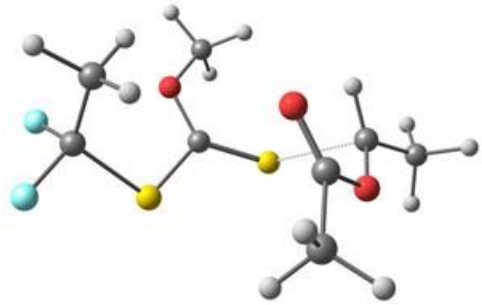
6	1.105603000	-2.165526000	-0.857540000
6	1.785960000	-0.831348000	-0.597178000
16	-0.599212000	-1.942185000	-1.482278000
6	-1.469632000	-1.680107000	0.023882000
8	-1.231282000	-2.630513000	0.970448000
6	-1.496689000	-2.265996000	2.324173000
1	-2.548936000	-1.987125000	2.457359000
1	-0.852751000	-1.432538000	2.635434000
16	-3.050503000	-0.893556000	-0.066419000
6	-2.615598000	0.844962000	0.344169000
1	1.909013000	-0.279722000	-1.539290000
1	-1.269238000	-3.151432000	2.922411000
1	-1.949684000	0.848254000	1.212284000

6	-0.484601000	3.132262000	0.145948000
1	1.642946000	-2.738875000	-1.620466000
1	1.059232000	-2.768959000	0.053363000
1	-3.560723000	1.327013000	0.622213000
6	-1.969434000	1.560771000	-0.830167000
1	-2.658030000	1.627733000	-1.677171000
1	-1.055914000	1.045017000	-1.140024000
8	-1.660342000	2.927543000	-0.482557000
6	-0.271249000	4.595523000	0.422037000
1	-1.123419000	5.004423000	0.975059000
1	0.648134000	4.729967000	0.993830000
1	-0.204260000	5.145566000	-0.523409000
8	0.290607000	2.241833000	0.436859000
1	1.179796000	-0.214984000	0.079774000
8	3.055580000	-1.133486000	-0.009135000
6	3.960341000	-0.149637000	0.259729000
8	4.989098000	-0.454445000	0.814045000
6	3.620964000	1.256111000	-0.174493000
1	4.426139000	1.912781000	0.158915000
1	3.545369000	1.314119000	-1.267894000
1	2.664494000	1.601069000	0.236120000

(f) PVDF$_H$-XA reactivation

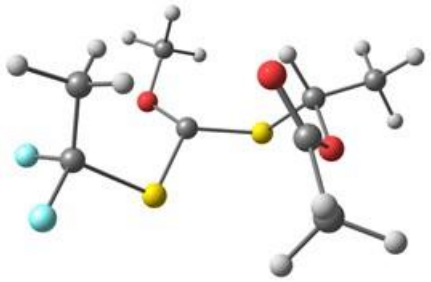
f1. By VAc (head)

CH_3CF_2-SC(OMe)S$^{\cdots}$$^{\bullet}$CH(OAc)$CH_3$ TS



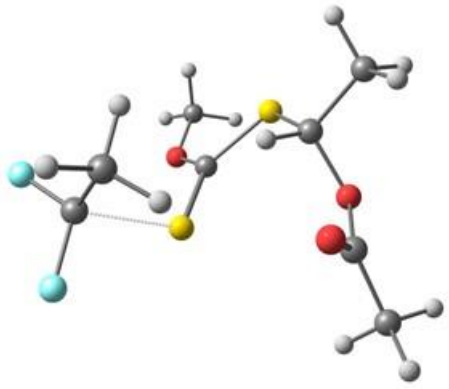
6	2.631789000	0.626291000	-0.004428000
6	2.245614000	0.952316000	1.412421000
16	1.237574000	0.183351000	-1.149409000
6	0.438628000	-1.210421000	-0.420109000
8	1.190649000	-1.836660000	0.500124000
6	0.660599000	-3.018859000	1.104559000
1	0.456753000	-3.779652000	0.343124000
1	-0.265552000	-2.799011000	1.646731000
16	-1.099380000	-1.608451000	-0.888296000
6	-2.867047000	-0.312835000	0.346836000
1	1.870910000	0.056296000	1.909685000
1	1.467682000	1.718290000	1.433283000
1	3.140978000	1.309913000	1.933114000
9	3.590601000	-0.332482000	-0.028429000
9	3.156826000	1.731873000	-0.615829000
1	1.437841000	-3.359358000	1.791940000
1	-2.461394000	-0.464299000	1.344458000
6	-4.094682000	-1.009228000	-0.113766000
1	-4.198041000	-0.946472000	-1.203751000
1	-4.058109000	-2.064834000	0.173447000
1	-5.000723000	-0.565739000	0.330669000
6	-1.861329000	1.809714000	0.480968000
6	-1.788312000	3.119120000	-0.246631000
1	-1.393393000	3.886638000	0.422064000
1	-1.101772000	3.007067000	-1.095582000
1	-2.765098000	3.412634000	-0.640465000
8	-2.771353000	0.980152000	-0.113920000
8	-1.201745000	1.488885000	1.445518000

CH_3CF_2-SC$^{\bullet}$(OMe)S-CH(OAc)CH_3



6	2.446529000	0.687510000	0.057042000
6	2.024708000	0.774162000	1.498028000
16	1.132993000	0.180444000	-1.149749000
6	0.358864000	-1.165179000	-0.329670000
8	1.214652000	-2.152369000	0.055545000
6	0.727989000	-3.100497000	1.004515000
1	-0.088126000	-3.700217000	0.585318000
1	0.376139000	-2.598837000	1.915963000
16	-1.284003000	-1.568720000	-0.840820000
6	-2.306785000	-0.470065000	0.229808000
1	1.771519000	-0.221749000	1.868041000
1	1.158881000	1.429962000	1.614074000
1	2.872203000	1.162997000	2.073007000
9	3.526355000	-0.129229000	-0.063293000
9	2.831113000	1.916014000	-0.404318000
1	1.578959000	-3.743813000	1.240409000
1	-1.842546000	-0.425366000	1.219239000
6	-3.725861000	-1.003885000	0.262880000
1	-4.150842000	-1.049569000	-0.745941000
1	-3.750579000	-2.005939000	0.702223000
1	-4.349660000	-0.337493000	0.868580000
6	-1.748799000	1.843432000	0.400110000
6	-1.769520000	3.132116000	-0.370713000
1	-1.560179000	3.964449000	0.303470000
1	-0.991820000	3.088408000	-1.142539000
1	-2.730213000	3.272570000	-0.874509000
8	-2.337107000	0.852161000	-0.319532000
8	-1.269737000	1.689006000	1.503771000

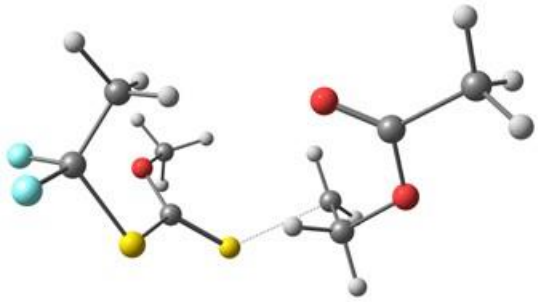
$CH_3CF_2^{\bullet}$$^{\cdots}$SC(OMe)S-CH(OAc)$CH_3$ TS



6	-2.605402000	-1.237757000	0.342422000
6	-1.915576000	-1.896165000	1.483795000
16	-0.887221000	0.093253000	-1.049302000
6	-0.334732000	1.549934000	-0.510241000
8	-1.000952000	2.670340000	-0.843101000
6	-0.581430000	3.951332000	-0.370650000
1	0.426755000	4.197460000	-0.727342000
1	-0.610403000	4.001897000	0.725158000
16	1.084004000	1.821781000	0.543166000
6	1.657979000	0.126508000	0.877225000
1	-1.622629000	-1.141539000	2.219359000
1	-1.021724000	-2.417318000	1.129329000
1	-2.583832000	-2.620792000	1.975176000
9	-3.622263000	-0.435194000	0.679503000
9	-2.989002000	-2.070809000	-0.634342000
1	-1.299430000	4.660021000	-0.788606000
1	0.782002000	-0.495127000	1.087958000
6	2.627844000	0.154035000	2.045426000
1	3.509974000	0.760811000	1.814790000
1	2.145594000	0.552045000	2.944217000
1	2.950265000	-0.872579000	2.247986000
6	2.132643000	-1.708395000	-0.529792000
6	2.692246000	-2.080650000	-1.872504000
1	2.782406000	-3.165957000	-1.942106000
1	2.005780000	-1.722743000	-2.649000000
1	3.660966000	-1.600176000	-2.039327000
8	2.304890000	-0.378804000	-0.294626000
8	1.594275000	-2.463483000	0.250235000

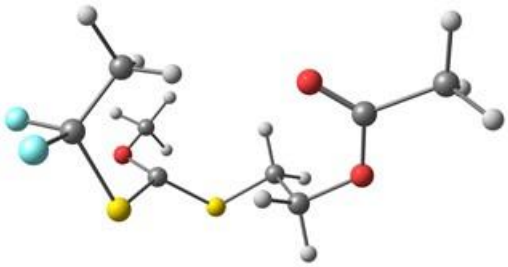
f2. By VAc (tail)

CH_3CF_2-SC(OMe)S$^{\cdots}$$^{\bullet}CH_2CH_2OAc$ TS



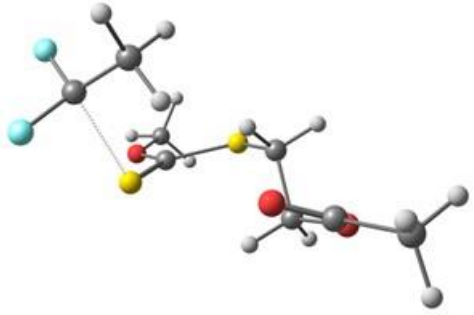
6	-1.986383000	-1.704741000	-0.103089000
6	-1.101769000	-1.951224000	1.088143000
16	-1.460683000	-0.309307000	-1.217688000
6	-1.427676000	1.127251000	-0.199055000
8	-2.159570000	1.010754000	0.915439000
6	-2.234085000	2.141694000	1.791874000
1	-2.669622000	2.999338000	1.268534000
1	-1.239326000	2.414517000	2.159599000
16	-0.532626000	2.437598000	-0.664103000
6	1.917944000	1.937660000	0.083007000
1	-0.057669000	-2.058107000	0.784283000
1	-2.877682000	1.820413000	2.613095000
1	1.660718000	1.621389000	1.090491000
6	3.458109000	-0.789031000	0.328245000
1	2.299245000	2.949907000	-0.029829000
6	2.296592000	0.890903000	-0.899154000
1	2.487677000	1.308744000	-1.890653000
1	1.529545000	0.113262000	-0.968658000
8	3.558927000	0.242038000	-0.531793000
6	4.816426000	-1.372547000	0.621946000
1	5.470391000	-0.603830000	1.048032000
1	4.712896000	-2.204066000	1.320913000
1	5.284986000	-1.719319000	-0.305582000
8	2.411592000	-1.190203000	0.798830000
1	-1.185695000	-1.119321000	1.790033000
1	-1.444185000	-2.869426000	1.578279000
9	-1.945058000	-2.771743000	-0.954530000
9	-3.277262000	-1.548997000	0.278840000

CH_3CF_2-SC$^{\bullet}$(OMe)S-CH_2CH_2OAc



6	-1.924309000	-1.695600000	-0.051083000
6	-1.037428000	-1.807435000	1.159081000
16	-1.515169000	-0.315692000	-1.223349000
6	-1.303567000	1.043480000	-0.134993000
8	-2.412857000	1.348417000	0.592598000
6	-2.250021000	2.220073000	1.710345000
1	-1.991896000	3.236028000	1.390669000
1	-1.471862000	1.848264000	2.390096000
16	-0.174317000	2.320791000	-0.600193000
6	1.430330000	1.651830000	-0.005723000
1	0.015177000	-1.874656000	0.873870000
1	-3.215942000	2.224937000	2.221053000
1	1.279010000	1.184865000	0.971849000
6	3.434563000	-0.722862000	0.343753000
1	2.080503000	2.526720000	0.116987000
6	2.048071000	0.668162000	-0.987837000
1	2.191081000	1.133643000	-1.967355000
1	1.420524000	-0.221505000	-1.092671000
8	3.368719000	0.286410000	-0.553360000
6	4.866209000	-1.043947000	0.678661000
1	5.388845000	-0.142517000	1.015723000
1	4.895768000	-1.809828000	1.455094000
1	5.384592000	-1.404021000	-0.217164000
8	2.463214000	-1.288174000	0.801764000
1	-1.179253000	-0.934752000	1.801292000
1	-1.331862000	-2.705960000	1.712378000
9	-1.815271000	-2.810607000	-0.832216000
9	-3.225685000	-1.611418000	0.332617000

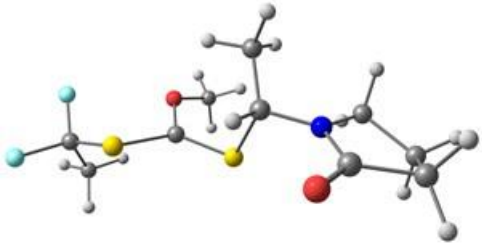
$CH_3CF_2^{\bullet\cdots}SC$(OMe)S-$CH_2CH_2OAc$ TS



6	1.360508000	2.537070000	0.225118000
6	0.205969000	2.675628000	1.152092000
16	1.141405000	0.311829000	-1.071980000
6	1.635829000	-1.090446000	-0.361449000
8	2.913809000	-1.487045000	-0.502385000
6	3.406819000	-2.656800000	0.151987000
1	2.879052000	-3.557601000	-0.186555000
1	3.325680000	-2.567781000	1.242567000
16	0.643273000	-2.168492000	0.663800000
6	-0.952675000	-1.307525000	0.750962000
1	-0.727999000	2.479622000	0.617736000
1	4.458930000	-2.722625000	-0.133163000
1	-0.769423000	-0.242576000	0.922366000
6	-3.527225000	0.128197000	-0.140049000
1	-1.438215000	-1.740075000	1.634599000
6	-1.836315000	-1.509659000	-0.474278000
1	-1.859180000	-2.561681000	-0.772545000
1	-1.480540000	-0.888364000	-1.301701000
8	-3.206962000	-1.186828000	-0.168361000
6	-5.001144000	0.308228000	0.108051000
1	-5.309935000	-0.248760000	0.998811000
1	-5.222263000	1.369684000	0.229702000
1	-5.569802000	-0.091939000	-0.739120000
8	-2.725956000	1.022738000	-0.304081000
1	0.307885000	1.957953000	1.971132000
1	0.171959000	3.690095000	1.580047000
9	1.332216000	3.361094000	-0.830454000
9	2.565703000	2.586860000	0.807233000

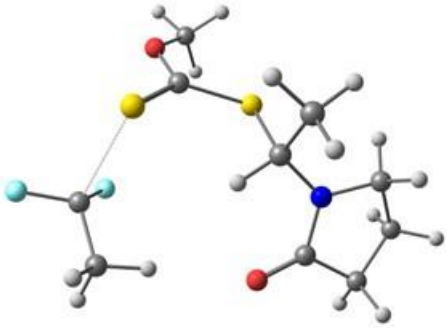
f3. By NVP (head)

CH_3CF_2-SC$^{\bullet}$(OMe)S-CH(N-pyr)CH_3



9	-4.475546000	-1.782985000	0.056268000
9	-4.216662000	0.182062000	0.982559000
6	-3.826694000	-0.587353000	-0.066400000
6	-1.194625000	0.430283000	-0.273274000
6	3.608193000	-1.236354000	0.017725000
6	3.616002000	1.143150000	0.060689000
6	5.001423000	-0.785819000	-0.401153000
6	4.822560000	0.686994000	-0.778640000
1	3.929895000	1.573952000	1.024707000
1	2.998055000	1.887407000	-0.456510000
1	5.672349000	-0.916945000	0.459522000
1	5.378340000	-1.420526000	-1.208074000
1	5.709054000	1.300086000	-0.589548000
1	4.577561000	0.771522000	-1.844047000
8	3.200463000	-2.376020000	0.153695000
7	2.869400000	-0.091423000	0.264695000
6	1.190166000	0.715782000	1.891641000
1	1.776340000	0.381578000	2.757494000
1	1.420485000	1.770362000	1.701352000
1	0.128856000	0.639881000	2.146941000
6	-4.203070000	0.079295000	-1.362890000
1	-3.670023000	1.027016000	-1.464162000
1	-3.957572000	-0.569954000	-2.206418000
1	-5.281220000	0.272423000	-1.349623000
16	-2.041489000	-1.058879000	0.098207000
8	-1.726077000	1.540536000	0.320964000
6	-1.277224000	2.808196000	-0.149376000
1	-0.218110000	2.967632000	0.083678000
1	-1.417314000	2.898751000	-1.234539000
16	0.441756000	0.322063000	-0.838958000
6	1.511554000	-0.153910000	0.691986000
1	1.299074000	-1.211652000	0.879202000
1	-1.890767000	3.548083000	0.370597000

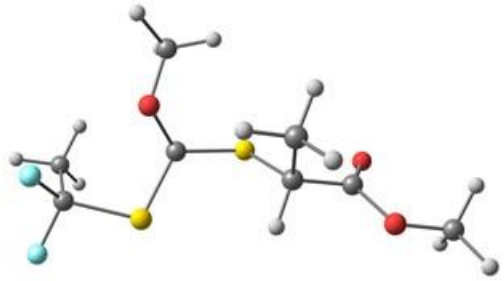
$CH_3CF_2^{\bullet}$···SC(OMe)S-CH(N-pyr)CH_3 TS



9	4.013539000	1.879536000	-0.002503000
9	2.456517000	1.199403000	-1.386386000
6	2.694415000	1.711120000	-0.169118000
6	1.400784000	-1.424773000	0.177849000
6	-2.434791000	1.368968000	-0.203875000
6	-3.582678000	-0.692541000	0.078857000
6	-3.843992000	1.567398000	-0.744354000
6	-4.373022000	0.144441000	-0.942568000
1	-4.120489000	-0.786742000	1.035079000
1	-3.368728000	-1.705428000	-0.285320000
1	-4.418454000	2.125712000	0.008120000
1	-3.819857000	2.174954000	-1.653287000
1	-5.453865000	0.052814000	-0.799452000
1	-4.138166000	-0.201453000	-1.956054000
8	-1.543107000	2.199554000	-0.139798000
7	-2.351512000	0.069377000	0.249150000
6	-1.428767000	-1.134870000	2.202220000
1	-1.917879000	-0.440398000	2.896836000
1	-2.063194000	-2.019354000	2.078574000
1	-0.476236000	-1.445884000	2.641261000
6	1.855378000	2.881014000	0.196221000
1	0.795232000	2.635291000	0.084734000
1	2.052374000	3.164961000	1.234041000
1	2.091287000	3.741488000	-0.450760000
16	2.003242000	-0.394017000	1.315621000
8	2.253232000	-2.219511000	-0.493500000
6	1.798534000	-3.069643000	-1.546518000
1	1.075063000	-3.808823000	-1.179924000
1	1.352586000	-2.486810000	-2.362266000
16	-0.300484000	-1.567535000	-0.324540000
6	-1.168426000	-0.432061000	0.879896000
1	-0.482871000	0.413819000	1.010385000
1	2.693540000	-3.580052000	-1.908587000

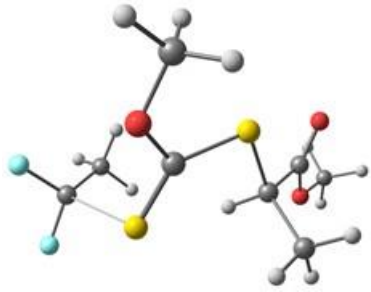
f4. By MA (head)

CH_3CF_2- SC$^{\bullet}$(OMe)S-CH(COOMe)CH_3



9	-3.932043000	-1.950021000	0.060452000
9	-3.675019000	-0.104041000	1.205799000
6	-3.356084000	-0.711850000	0.034819000
6	-0.808563000	0.477729000	-0.282704000
6	1.859448000	0.786550000	1.614990000
1	2.486457000	0.343766000	2.397977000
1	2.238944000	1.788842000	1.386178000
1	0.838316000	0.877736000	1.998681000
6	-3.887869000	0.088379000	-1.124199000
1	-3.414028000	1.072088000	-1.147492000
1	-3.693008000	-0.432518000	-2.064433000
1	-4.967814000	0.212418000	-0.989514000
16	-1.542909000	-1.092924000	-0.029245000
8	-1.311769000	1.470222000	0.510282000
6	-1.010347000	2.813684000	0.134097000
1	0.065466000	3.012477000	0.193421000
1	-1.352758000	3.019492000	-0.888519000
16	0.781865000	0.538821000	-1.003058000
6	1.876482000	-0.098438000	0.369559000
1	1.533648000	-1.107735000	0.627585000
8	3.658657000	0.327979000	-1.230863000
6	3.271801000	-0.209785000	-0.216304000
1	-1.550556000	3.445199000	0.843399000
8	4.046794000	-0.983364000	0.568507000
6	5.402757000	-1.127552000	0.122504000
1	5.900064000	-0.153186000	0.079410000
1	5.887195000	-1.774216000	0.856292000
1	5.433113000	-1.583146000	-0.872367000

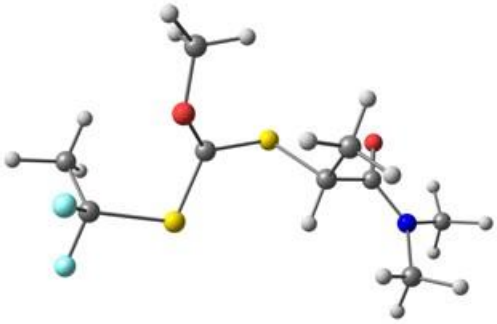
$CH_3CF_2^{\bullet\cdots}$SC(OMe)S-CH(COOMe)CH_3 TS



9	-3.308292000	-2.370953000	0.749848000
9	-3.903741000	-0.930722000	-0.790903000
6	-2.871230000	-1.582903000	-0.243728000
6	-0.855021000	1.380300000	0.274497000
6	2.003966000	0.482083000	1.976648000
1	2.462588000	-0.381762000	2.470426000
1	2.716633000	1.313690000	1.979181000
1	1.113322000	0.771777000	2.542371000
6	-1.974043000	-2.254756000	-1.222299000
1	-1.579794000	-1.518710000	-1.928515000
1	-1.140682000	-2.726624000	-0.695472000
1	-2.519540000	-3.027305000	-1.786923000
16	-1.518258000	0.146432000	1.154373000
8	-1.645954000	2.405860000	-0.088052000
6	-1.141605000	3.494158000	-0.865380000
1	-0.328103000	4.013426000	-0.344341000
1	-0.792666000	3.153930000	-1.848716000
16	0.810093000	1.483505000	-0.350296000
6	1.602902000	0.103313000	0.548923000
1	0.864429000	-0.708773000	0.586998000
8	3.308669000	0.284272000	-1.182639000
6	2.802517000	-0.334640000	-0.271841000
1	-1.989869000	4.169755000	-0.993416000
8	3.255723000	-1.519334000	0.177681000
6	4.423889000	-2.013364000	-0.493011000
1	5.254436000	-1.307627000	-0.390579000
1	4.662672000	-2.961408000	-0.007934000
1	4.219751000	-2.165806000	-1.557599000

f5. By DMA (head)

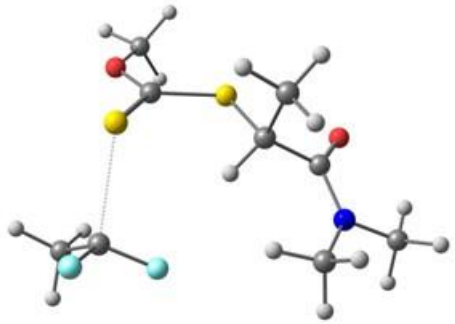
CH_3CF_2-SC$^{\bullet}$(OMe)S-CH(CONMe$_2$)CH_3



9	-3.948484000	-2.137986000	-0.230803000
9	-3.811275000	-0.495439000	1.207620000
6	-3.485632000	-0.863914000	-0.058060000
6	-1.063489000	0.596398000	-0.254052000
6	1.678910000	1.052520000	1.626442000
1	2.332975000	0.613554000	2.392206000
1	2.050546000	2.056582000	1.395135000
1	0.670990000	1.132452000	2.046891000
6	-4.133686000	0.064911000	-1.049973000
1	-3.750704000	1.078898000	-0.917576000
1	-3.932278000	-0.271536000	-2.069575000
1	-5.213907000	0.061542000	-0.868458000
16	-1.650891000	-1.056162000	-0.228578000
8	-1.648828000	1.416814000	0.670876000
6	-1.489611000	2.821776000	0.472208000
1	-0.437228000	3.118497000	0.542512000
1	-1.876770000	3.123904000	-0.509792000
16	0.512051000	0.897038000	-0.944097000
6	1.661900000	0.196768000	0.362204000
1	1.282854000	-0.807323000	0.578624000
8	3.319537000	1.013979000	-1.150278000
6	3.033520000	0.162016000	-0.311192000
7	3.917351000	-0.813582000	0.068625000
6	3.690336000	-1.835057000	1.069493000
1	4.504442000	-1.824095000	1.807908000
1	2.754271000	-1.673734000	1.604807000
1	3.661972000	-2.836002000	0.613891000

6	5.216572000	-0.857575000	-0.577683000
1	5.367037000	-1.829593000	-1.067622000
1	5.255135000	-0.061245000	-1.322610000
1	6.020101000	-0.711657000	0.157773000
1	-2.070220000	3.298245000	1.265837000

$CH_3CF_2^{\bullet\cdots}SC(OMe)S\text{-}CH(CONMe_2)CH_3$ TS

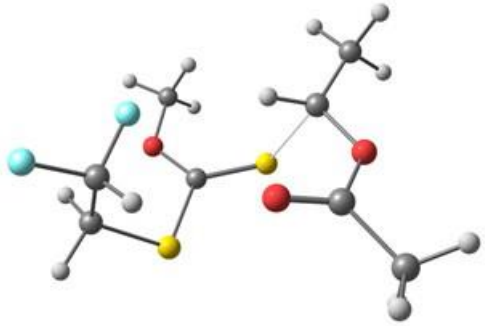


9	0.714187000	2.336078000	-0.692617000
9	2.309871000	3.052832000	0.629650000
6	1.993559000	2.139690000	-0.300010000
6	1.508887000	-1.352628000	0.266536000
6	-1.389988000	-0.739676000	2.078307000
1	-1.963449000	0.091497000	2.507995000
1	-1.962992000	-1.663140000	2.211403000
1	-0.443764000	-0.815224000	2.622583000
6	2.962956000	2.023181000	-1.420548000
1	3.957913000	1.812273000	-1.020469000
1	2.667401000	1.201941000	-2.079156000
1	3.001615000	2.953890000	-2.008194000
16	1.972363000	-0.010164000	1.122362000
8	2.473622000	-2.161773000	-0.213171000
6	2.145642000	-3.331864000	-0.966277000
1	1.537175000	-4.027790000	-0.375563000
1	1.615335000	-3.075382000	-1.892061000
16	-0.140170000	-1.839999000	-0.164546000
6	-1.121957000	-0.487727000	0.593892000
1	-0.512259000	0.411292000	0.462836000
8	-2.868399000	-1.502113000	-0.685605000
6	-2.432779000	-0.461941000	-0.192458000
7	-3.104940000	0.726171000	-0.271391000
6	-2.687569000	1.985381000	0.314277000
1	-3.236850000	2.201827000	1.243221000
1	-1.617843000	2.001699000	0.524689000
1	-2.893438000	2.797384000	-0.394726000
6	-4.417954000	0.732065000	-0.892071000
1	-4.444695000	1.454927000	-1.718453000
1	-4.621885000	-0.269557000	-1.273665000
1	-5.190703000	1.010979000	-0.161710000
1	3.104831000	-3.795178000	-1.207045000

(g) $PVDF_T$-XA reactivation

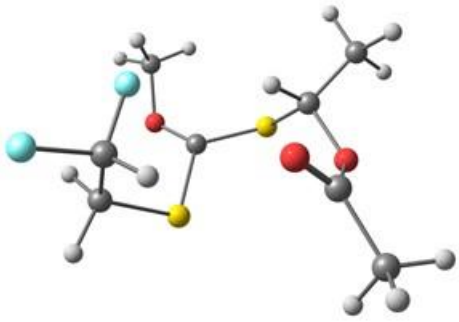
g1. By VAc (head)

$CHF_2CH_2\text{-}SC(OMe)S^{\cdots\bullet}CH(OAc)CH_3$ TS



6	-2.456219000	-1.184842000	-0.558141000
6	-1.785572000	-1.705876000	0.698885000
16	-1.284594000	-0.357433000	-1.685112000
6	-0.949761000	1.159089000	-0.838840000
8	-2.035850000	1.630968000	-0.204965000
6	-1.895098000	2.813913000	0.581560000
1	-1.565173000	3.654137000	-0.039183000
1	-1.169687000	2.658153000	1.387771000
16	0.559162000	1.836606000	-0.859586000
6	1.990764000	0.702654000	0.928572000
1	-0.899851000	-2.320118000	0.502317000
1	-2.888509000	3.003824000	0.993958000
1	1.155196000	0.155267000	1.358067000
6	2.628533000	1.849840000	1.622257000
1	3.252991000	2.433104000	0.934770000
1	1.862435000	2.509710000	2.040066000
1	3.276147000	1.510579000	2.448154000
6	2.518763000	-1.346005000	-0.109036000
6	3.535671000	-1.957929000	-1.027353000
1	4.551769000	-1.675910000	-0.736683000
1	3.420825000	-3.043455000	-1.025994000
1	3.365198000	-1.584823000	-2.045062000
8	2.883943000	-0.069958000	0.225098000
8	1.502405000	-1.873648000	0.283888000
1	-3.277137000	-0.513204000	-0.291449000
1	-2.859964000	-2.031381000	-1.123965000
9	-2.702003000	-2.439671000	1.402011000
9	-1.402863000	-0.661063000	1.497191000

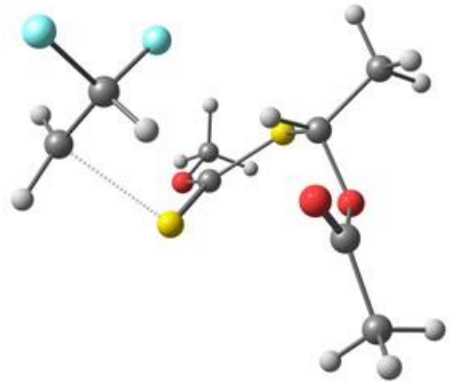
$CHF_2CH_2\text{-}SC^{\bullet}(OMe)S\text{-}CH(OAc)CH_3$



6	2.240232000	1.067198000	-0.776957000
6	1.847419000	1.628313000	0.574579000
16	0.879978000	0.227872000	-1.661288000
6	0.689680000	-1.210031000	-0.675659000
8	1.808263000	-1.973473000	-0.550257000
6	1.979074000	-2.640484000	0.704397000
1	1.142621000	-3.319815000	0.908135000
1	2.066812000	-1.905542000	1.512719000

16	-0.895799000	-1.952926000	-0.520195000
6	-1.741969000	-0.790290000	0.635128000
1	0.942198000	2.245479000	0.555835000
1	2.904998000	-3.213954000	0.613272000
1	-0.970087000	-0.266324000	1.206941000
6	-2.714621000	-1.552750000	1.514190000
1	-3.456048000	-2.086338000	0.908920000
1	-2.181453000	-2.277535000	2.136923000
1	-3.244507000	-0.849243000	2.166383000
6	-2.191675000	1.480913000	0.036726000
6	-2.990002000	2.322386000	-0.919570000
1	-2.928692000	3.370859000	-0.622988000
1	-2.572810000	2.204325000	-1.926830000
1	-4.032215000	1.991313000	-0.954298000
8	-2.488137000	0.168939000	-0.132111000
8	-1.387432000	1.902742000	0.841074000
9	1.637307000	0.608649000	1.467493000
9	2.893501000	2.371681000	1.050073000
1	2.553020000	1.890716000	-1.427887000
1	3.081649000	0.376750000	-0.658153000

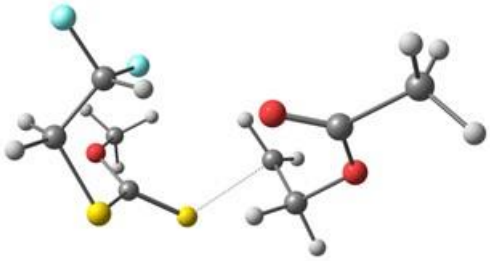
$CHF_2CH_2^{\bullet\cdots}SC(OMe)S\text{-}CH(OAc)CH_3$ TS



6	1.598314000	-2.434420000	-0.830300000
6	2.347515000	-1.670857000	0.189020000
16	-0.307153000	-0.742437000	-1.527901000
6	-1.620392000	-0.708380000	-0.529641000
8	-2.645075000	-1.538582000	-0.776395000
6	-3.797347000	-1.571779000	0.071383000
1	-4.316072000	-0.605211000	0.072353000
1	-3.526378000	-1.850298000	1.097098000
16	-1.836597000	0.321248000	0.903183000
6	-0.249860000	1.215963000	1.015189000
1	2.674847000	-0.678899000	-0.145779000
1	-4.446576000	-2.336500000	-0.359485000
1	0.555174000	0.494729000	0.854055000
6	-0.155876000	1.860543000	2.386524000
1	-0.961786000	2.585080000	2.545693000
1	-0.191143000	1.101495000	3.174489000
1	0.804374000	2.382665000	2.452619000
6	0.989641000	2.418499000	-0.599776000
6	0.850543000	3.370309000	-1.753719000
1	1.840030000	3.698125000	-2.076520000
1	0.349421000	2.853715000	-2.580762000
1	0.231342000	4.229132000	-1.477113000
8	-0.218812000	2.214993000	-0.006625000
8	2.017690000	1.894637000	-0.231707000
9	1.568106000	-1.500789000	1.313280000
9	3.465283000	-2.370833000	0.597775000
1	1.994794000	-2.471931000	-1.840557000
1	0.985826000	-3.266121000	-0.494373000

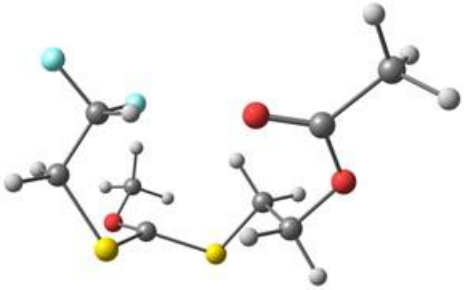
g2. By VAc (tail)

$CHF_2CH_2\text{-}SC(OMe)S^{\cdots\bullet}CH_2CH_2OAc$ TS



6	-1.586477000	1.899325000	0.894516000
6	-0.526845000	2.207685000	-0.148272000
16	-1.366787000	0.253017000	1.647614000
6	-1.914134000	-0.843610000	0.375112000
8	-2.865782000	-0.306816000	-0.393848000
6	-3.333624000	-1.062624000	-1.515511000
1	-3.786691000	-2.002192000	-1.181679000
1	-2.507847000	-1.284027000	-2.199546000
16	-1.240086000	-2.343889000	0.219069000
6	1.075547000	-1.786052000	-0.836300000
1	0.501437000	2.089661000	0.211834000
1	-4.075105000	-0.423868000	-1.999518000
1	0.727257000	-0.875819000	-1.317174000
6	3.437028000	0.140846000	-0.001549000
9	-0.687930000	1.388223000	-1.234409000
9	-0.715916000	3.493294000	-0.574409000
1	-1.497057000	2.613630000	1.719976000
1	-2.582642000	1.991140000	0.452815000
1	1.178553000	-2.668430000	-1.464140000
6	1.910903000	-1.655268000	0.383568000
1	2.074069000	-2.617186000	0.876568000
1	1.474476000	-0.943897000	1.090746000
8	3.265709000	-1.191536000	0.056110000
6	4.857462000	0.481479000	-0.373734000
1	5.042954000	0.188916000	-1.413821000
1	5.015325000	1.555800000	-0.264778000
1	5.563080000	-0.074032000	0.252117000
8	2.562276000	0.958341000	0.210495000

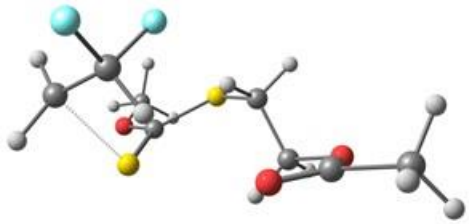
$CHF_2CH_2\text{-}SC^{\bullet}(OMe)S\text{-}CH_2CH_2OAc$



6	-1.735014000	1.773367000	0.881136000
6	-0.661367000	2.225491000	-0.086743000
16	-1.415576000	0.139085000	1.633324000
6	-1.711989000	-0.919343000	0.269021000
8	-2.964305000	-0.849368000	-0.256315000

6	-3.062636000	-1.023592000	-1.673620000
1	-2.693963000	-2.010398000	-1.978122000
1	-2.494229000	-0.240926000	-2.190001000
16	-0.746984000	-2.372213000	0.051847000
6	0.850355000	-1.667732000	-0.533767000
1	0.358342000	2.148052000	0.306435000
1	-4.125881000	-0.937420000	-1.911532000
1	0.633959000	-0.721808000	-1.038701000
6	3.317881000	0.265102000	-0.040100000
9	-0.721020000	1.480122000	-1.239870000
9	-0.915192000	3.523565000	-0.436578000
1	-1.783176000	2.480720000	1.716030000
1	-2.706821000	1.760313000	0.376897000
1	1.256020000	-2.379324000	-1.262787000
6	1.827995000	-1.467027000	0.614271000
1	2.009261000	-2.407540000	1.143386000
1	1.453246000	-0.714145000	1.314051000
8	3.116224000	-1.063000000	0.106686000
6	4.698514000	0.536458000	-0.574289000
1	4.821308000	0.059442000	-1.552983000
1	4.849107000	1.613250000	-0.664343000
1	5.452111000	0.105452000	0.093654000
8	2.492474000	1.112975000	0.229361000

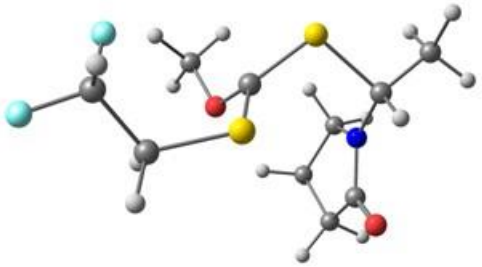
$CHF_2CH_2^{\bullet\cdots}SC(OMe)S\text{-}CH_2CH_2OAc$ TS



6	-0.404403000	2.913549000	0.441843000
6	0.877672000	2.610126000	-0.229117000
16	-1.197724000	0.595666000	1.356835000
6	-2.187003000	-0.303858000	0.390383000
8	-3.516602000	-0.151157000	0.493244000
6	-4.417418000	-0.878532000	-0.346790000
1	-4.320107000	-1.959999000	-0.190100000
1	-4.252403000	-0.640025000	-1.404591000
16	-1.676543000	-1.478099000	-0.845447000
6	0.134078000	-1.334742000	-0.851766000
1	1.580672000	2.032090000	0.382274000
1	-5.415034000	-0.552863000	-0.045507000
1	0.396693000	-0.272823000	-0.842574000
6	3.015939000	-1.189545000	0.355624000
9	0.644630000	1.903628000	-1.389975000
9	1.509741000	3.778176000	-0.611442000
1	-0.369157000	3.329455000	1.444431000
1	-1.252631000	3.178124000	-0.183306000
1	0.421701000	-1.761407000	-1.820826000
6	0.821377000	-2.100460000	0.271792000
1	0.451227000	-3.128302000	0.332254000
1	0.681285000	-1.586992000	1.227263000
8	2.225863000	-2.224993000	-0.019179000
6	4.451958000	-1.466693000	0.000722000
1	4.551624000	-1.594766000	-1.082858000
1	5.075154000	-0.635823000	0.334655000
1	4.783604000	-2.398934000	0.470517000
8	2.604876000	-0.189364000	0.902529000

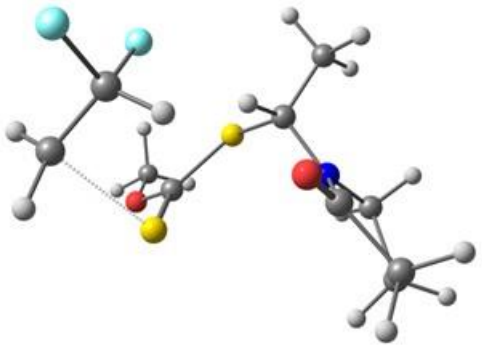
g3. By NVP (head)

$CHF_2CH_2\text{-}SC^{\bullet}(OMe)S\text{-}CH(N\text{-}pyr)CH_3$



6	2.807695000	0.951856000	0.736220000
6	3.996170000	0.087651000	0.372613000
16	1.379571000	0.008089000	1.360646000
6	0.631234000	-0.546505000	-0.123075000
8	0.629989000	0.350248000	-1.155174000
6	0.908161000	-0.206296000	-2.444483000
1	0.202914000	-1.012320000	-2.683462000
1	1.933555000	-0.590868000	-2.474833000
16	-0.458124000	-1.896274000	-0.070609000
6	-2.079145000	-1.216917000	0.690007000
1	4.328378000	-0.563238000	1.192606000
1	0.791895000	0.612692000	-3.159440000
1	-1.866237000	-1.012419000	1.744399000
6	-3.101923000	-2.332813000	0.533865000
1	-3.306800000	-2.551614000	-0.520438000
1	-2.740383000	-3.252242000	1.007074000
1	-4.040822000	-2.042653000	1.020402000
9	3.704413000	-0.704371000	-0.701412000
9	5.034976000	0.901306000	0.013137000
1	3.096607000	1.638191000	1.539036000
1	2.498560000	1.537931000	-0.134703000
7	-2.470481000	0.027649000	0.123614000
6	-2.918688000	2.313562000	-0.062805000
1	-3.973329000	2.532627000	0.157004000
1	-2.346691000	3.224307000	0.135869000
6	-2.725398000	1.730674000	-1.464833000
1	-1.705647000	1.937560000	-1.808889000
1	-3.426747000	2.123019000	-2.207762000
6	-2.883113000	0.214782000	-1.258441000
1	-3.924746000	-0.112476000	-1.405753000
1	-2.245267000	-0.375326000	-1.927941000
6	-2.465169000	1.194531000	0.865773000
8	-2.179799000	1.275836000	2.048470000

$CHF_2CH_2^{\bullet\cdots}SC(OMe)S\text{-}CH(N\text{-}pyr)CH_3$ TS

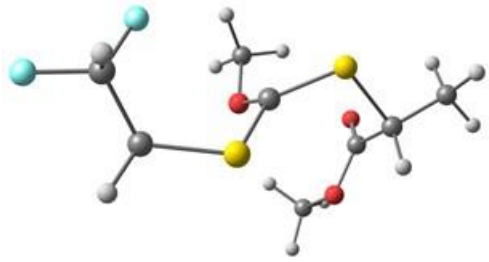


6	-3.033248000	-0.901667000	-1.020586000

6	-2.588005000	-1.780748000	0.080501000
16	-0.835912000	0.483671000	-1.573292000
6	-0.559013000	1.761819000	-0.573010000
8	-1.044720000	2.970067000	-0.908322000
6	-0.875372000	4.106494000	-0.056947000
1	0.186074000	4.349139000	0.077223000
1	-1.344342000	3.943158000	0.921076000
16	0.313058000	1.728573000	0.974642000
6	0.786394000	-0.048425000	1.219933000
1	-1.682071000	-2.355351000	-0.143976000
1	-1.376679000	4.927286000	-0.574083000
1	-0.108606000	-0.645465000	1.019798000
6	1.190068000	-0.164566000	2.690011000
1	2.051739000	0.466998000	2.936337000
1	0.356935000	0.114674000	3.342704000
1	1.455406000	-1.207669000	2.894600000
9	-2.339609000	-1.026012000	1.209955000
9	-3.589381000	-2.668124000	0.427448000
1	-3.065768000	-1.311337000	-2.025653000
1	-3.707358000	-0.083951000	-0.782310000
7	1.798379000	-0.500864000	0.313094000
6	2.956312000	-1.913257000	-1.145495000
1	3.539694000	-2.690892000	-0.632834000
1	2.725497000	-2.287241000	-2.147125000
6	3.651058000	-0.549565000	-1.116936000
1	3.346722000	0.042811000	-1.987450000
1	4.743553000	-0.612302000	-1.116386000
6	3.110243000	0.111552000	0.162138000
1	3.751378000	-0.102860000	1.032722000
1	3.017235000	1.200391000	0.071458000
6	1.670806000	-1.699972000	-0.357300000
8	0.718852000	-2.460070000	-0.282909000

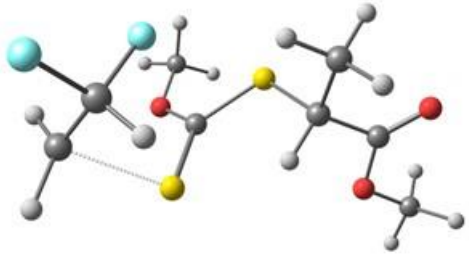
g4. By MA (head)

CHF_2CH_2- SC$^{\bullet}$(OMe)S-CH(COOMe)CH_3



6	2.742505000	-0.665564000	-0.856574000
6	3.704023000	0.239866000	-0.115492000
16	1.258137000	0.192650000	-1.476682000
6	0.318920000	0.389793000	-0.009118000
8	0.320431000	-0.689617000	0.817342000
6	0.101400000	-0.428970000	2.210974000
1	-0.924377000	-0.088453000	2.386321000
1	0.819563000	0.314901000	2.573118000
16	-0.859430000	1.654369000	0.082038000
6	-2.480836000	0.937546000	-0.586164000
1	3.990212000	1.132216000	-0.688949000
1	0.266260000	-1.384898000	2.714162000
1	-2.371237000	0.860709000	-1.671737000
6	-3.578356000	1.910827000	-0.183883000
1	-3.705708000	1.908691000	0.902776000
1	-3.342831000	2.927550000	-0.517139000
1	-4.529584000	1.615613000	-0.642779000
6	-2.418487000	-2.732439000	-0.391234000
1	-2.227749000	-3.374249000	-1.253397000
1	-1.652470000	-2.887379000	0.375490000
1	-3.404053000	-2.939093000	0.037202000
9	3.159949000	0.649828000	1.066287000
9	4.834894000	-0.472180000	0.176256000
1	3.244066000	-1.074831000	-1.739816000
1	2.442092000	-1.490531000	-0.203812000
6	-2.695443000	-0.436991000	0.001804000
8	-3.107746000	-0.665589000	1.121538000
8	-2.350113000	-1.389268000	-0.884117000

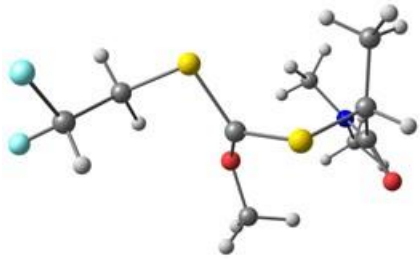
$CHF_2CH_2^{\bullet\cdots}$SC(OMe)S-CH(COOMe)$CH_3$ TS



6	3.373198000	-0.101370000	1.094878000
6	3.174488000	-1.293283000	0.247725000
16	0.897567000	0.710708000	1.581868000
6	0.325646000	1.425231000	0.207131000
8	0.759489000	2.654099000	-0.101927000
6	0.314851000	3.330315000	-1.283627000
1	-0.772083000	3.474698000	-1.270993000
1	0.608539000	2.781076000	-2.186370000
16	-0.786550000	0.727405000	-0.991405000
6	-1.200284000	-0.915447000	-0.283194000
1	2.579045000	-2.080849000	0.728718000
1	0.817101000	4.299308000	-1.261341000
1	-0.704122000	-0.913037000	0.698720000
6	-0.698890000	-2.039481000	-1.176745000
1	-1.184418000	-2.012279000	-2.156776000
1	0.383938000	-1.961805000	-1.302448000
1	-0.938888000	-3.005357000	-0.716632000
6	-4.488223000	-0.244507000	1.256090000
1	-4.612827000	0.332988000	2.173710000
1	-5.009837000	0.238637000	0.423334000
1	-4.885375000	-1.257079000	1.380598000
9	2.551737000	-0.946181000	-0.929016000
9	4.385355000	-1.854204000	-0.108837000
1	3.618314000	-0.248393000	2.142391000
1	3.720899000	0.808998000	0.615761000
6	-2.709253000	-0.966333000	-0.084922000
8	-3.480416000	-1.550476000	-0.814947000
8	-3.076521000	-0.282870000	1.011948000

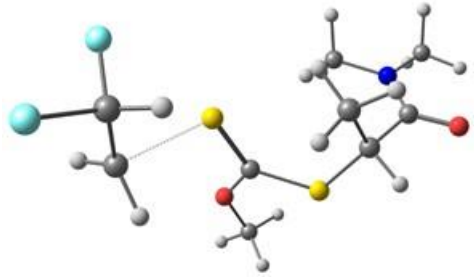
g5. By DMA (head)

CHF_2CH_2-SC$^{\bullet}$(OMe)S-CH($CONMe_2$)CH_3



6	2.842524000	-0.488228000	0.869511000
6	0.477343000	0.169315000	-0.430577000
6	-2.125583000	2.326296000	0.811556000
1	-3.078843000	2.301954000	1.356013000
1	-1.326417000	2.076016000	1.514544000
1	-1.951312000	3.355249000	0.479729000
6	3.912152000	-0.258545000	-0.178146000
1	3.511961000	-0.201827000	-1.199885000
16	1.531532000	0.780730000	0.835791000
8	0.263525000	-1.176566000	-0.392627000
6	-0.216321000	-1.792130000	-1.595581000
1	-1.235724000	-1.468094000	-1.833037000
1	0.445053000	-1.557686000	-2.438793000
16	-0.530651000	1.271728000	-1.306081000
6	-2.182735000	1.408341000	-0.406217000
1	-2.751291000	1.912453000	-1.197020000
8	-3.556167000	-0.286782000	-1.332981000
6	-2.916565000	0.061710000	-0.339051000
7	-2.907742000	-0.696051000	0.801310000
1	3.305344000	-0.444585000	1.861149000
1	2.383356000	-1.470641000	0.731987000
9	4.807780000	-1.290514000	-0.118157000
9	4.587484000	0.893922000	0.084350000
6	-3.764013000	-1.868463000	0.839295000
1	-3.177455000	-2.791904000	0.723222000
1	-4.286958000	-1.911753000	1.803565000
1	-4.484511000	-1.803595000	0.022878000
6	-1.993732000	-0.578327000	1.919717000
1	-2.511405000	-0.249730000	2.832603000
1	-1.538637000	-1.557702000	2.117287000
1	-1.177188000	0.107747000	1.703784000
1	-0.200534000	-2.866589000	-1.396473000

$CHF_2CH_2^{\bullet}\cdots SC(OMe)S\text{-}CH(CONMe_2)CH_3$ TS

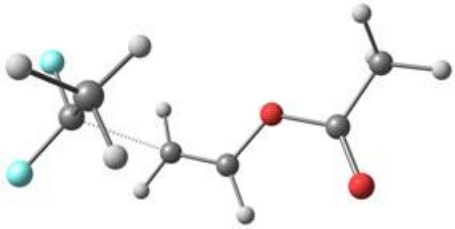


6	-3.659677000	0.308624000	-0.243969000
6	-0.276766000	1.459540000	0.206390000
6	0.495630000	-1.632112000	-1.124201000
1	0.935272000	-2.525414000	-1.585541000
1	0.205230000	-1.870422000	-0.100734000
1	-0.408499000	-1.366411000	-1.679932000
6	-3.933658000	-1.143373000	-0.239399000
1	-3.263155000	-1.719424000	-0.892075000
16	-1.270114000	0.328996000	0.891181000
8	-0.543932000	2.752743000	0.463423000
6	0.256959000	3.822490000	-0.052551000
1	1.298579000	3.732996000	0.277405000
1	0.217963000	3.856260000	-1.147958000
16	1.082999000	1.248182000	-0.910384000
6	1.541822000	-0.526761000	-1.227036000
1	1.796336000	-0.420867000	-2.287264000
8	3.797411000	-1.190652000	-1.452379000
6	2.919856000	-0.906600000	-0.638800000
7	3.120889000	-0.962461000	0.706985000
1	-4.146974000	0.913382000	0.514872000
1	-3.398681000	0.784525000	-1.184274000
9	-5.227089000	-1.394757000	-0.656789000
9	-3.829792000	-1.644591000	1.030541000
6	4.441500000	-1.325685000	1.189425000
1	4.856638000	-0.518089000	1.808161000
1	4.387705000	-2.236860000	1.800962000
1	5.088345000	-1.500437000	0.328511000
6	2.145362000	-0.672686000	1.734992000
1	2.078794000	-1.517666000	2.434485000
1	2.435220000	0.220083000	2.307888000
1	1.150532000	-0.502490000	1.321941000
1	-0.187758000	4.730001000	0.360677000

(h) $PVDF_H^{\bullet}$ addition to monomer

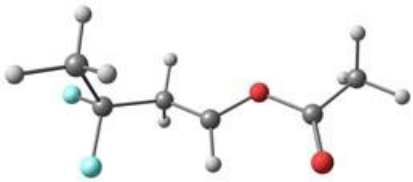
h1. To VAc (tail)

$CH_3CF_2^{\bullet}\cdots CH_2$=CHOAc TS



6	-2.304435000	0.200626000	0.085604000
6	-1.734179000	1.105977000	1.118348000
1	-0.971224000	1.745085000	0.666082000
1	-1.270895000	0.513112000	1.911850000
6	-0.562982000	-1.168903000	-0.865639000
1	-1.216667000	-2.007816000	-0.649618000
1	-0.743631000	-0.601125000	-1.774132000
6	0.610590000	-1.071270000	-0.210127000
1	0.917582000	-1.674682000	0.638788000
8	1.510930000	-0.090828000	-0.578164000
6	2.668503000	0.012869000	0.145203000
8	2.928934000	-0.686412000	1.096340000
6	3.536583000	1.098900000	-0.424023000
1	4.428657000	1.210218000	0.194032000
1	3.825520000	0.845893000	-1.450544000
1	2.985944000	2.044904000	-0.466038000
1	-2.515554000	1.742477000	1.560467000
9	-2.822705000	0.831186000	-0.984960000
9	-3.204309000	-0.683334000	0.554683000

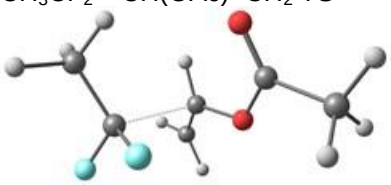
$CH_3CF_2\text{-}CH_2CH^{\bullet}(OAc)$



6	2.124552000	-0.045160000	0.009035000
6	2.246930000	0.045240000	1.511313000
1	2.216747000	-0.955144000	1.953768000
1	1.424625000	0.639660000	1.919918000
6	0.833644000	-0.651214000	-0.532629000
1	0.979083000	-0.756726000	-1.622688000
1	0.719159000	-1.664670000	-0.128581000
6	-0.360802000	0.162258000	-0.206352000
1	-0.448430000	1.229917000	-0.375726000
8	-1.529647000	-0.542631000	-0.084166000
6	-2.701812000	0.168402000	0.011895000
8	-2.745652000	1.375326000	-0.025094000
6	-3.863952000	-0.769164000	0.169909000
1	-4.790430000	-0.193461000	0.192026000
1	-3.888798000	-1.489618000	-0.654974000
1	-3.762011000	-1.341535000	1.099169000
1	3.199018000	0.519914000	1.765905000
9	3.173077000	-0.786166000	-0.482282000
9	2.258263000	1.218158000	-0.523691000

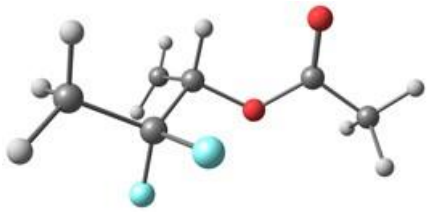
h2. To VAc (head)

$CH_3CF_2^{\bullet}$··· CH(OAc)=CH_2 TS



6	-1.394511000	-0.489168000	-0.176924000
6	-1.763098000	-1.351670000	0.980319000
1	-2.339602000	-0.769763000	1.705608000
1	-0.852874000	-1.722861000	1.458418000
6	-0.743941000	2.374375000	0.220156000
1	-0.559679000	2.888263000	-0.718214000
1	-1.561367000	2.714184000	0.847124000
6	-0.063892000	1.248540000	0.553788000
1	-0.081300000	0.798633000	1.543443000
8	1.056920000	0.921689000	-0.202097000
6	1.808543000	-0.132454000	0.219154000
8	1.574824000	-0.766741000	1.224375000
6	2.934258000	-0.386137000	-0.741274000
1	3.639453000	-1.091559000	-0.298960000
1	2.523167000	-0.811845000	-1.664308000
1	3.438392000	0.548548000	-1.005457000
1	-2.376069000	-2.203736000	0.650300000
9	-0.623332000	-1.103511000	-1.095944000
9	-2.437582000	0.084581000	-0.796000000

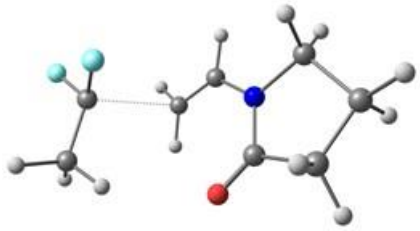
CH_3CF_2-CH(OAc)$CH_2^{\bullet}$



6	1.353415000	-0.364753000	0.038529000
6	2.606352000	-0.311129000	-0.803088000
1	3.114307000	0.648873000	-0.671769000
1	2.359103000	-0.443211000	-1.860660000
6	0.789799000	2.086152000	0.068739000
1	1.385270000	2.242254000	0.963374000
1	0.389757000	2.949317000	-0.454099000
6	0.323080000	0.723761000	-0.282310000
1	0.051487000	0.643662000	-1.342002000
8	-0.869729000	0.419512000	0.490254000
6	-1.952007000	-0.007011000	-0.211888000
8	-2.001544000	-0.069640000	-1.420077000
6	-3.063102000	-0.383002000	0.729988000
1	-3.972877000	-0.578408000	0.160084000
1	-2.776689000	-1.282895000	1.286303000
1	-3.232220000	0.413489000	1.461570000
1	3.276514000	-1.117278000	-0.490206000
9	0.750204000	-1.584497000	-0.127071000
9	1.697609000	-0.275379000	1.365536000

h3. To NVP (tail)

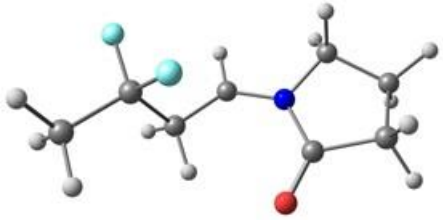
$CH_3CF_2^{\bullet}$···CH_2=CH(N-pyr) TS



6	-2.627696000	1.483018000	-0.113349000
1	-1.640195000	1.952531000	-0.079863000
6	-2.466532000	0.014317000	-0.278036000
6	-0.857651000	-0.762541000	1.467394000
1	-1.618153000	-1.449786000	1.825505000
1	-0.857215000	0.256652000	1.832719000
6	0.197560000	-1.270992000	0.790927000
1	0.224039000	-2.324254000	0.518050000
6	1.469753000	0.806287000	0.321202000
6	2.353617000	-1.252954000	-0.435869000
6	2.756631000	1.116287000	-0.433061000
6	3.490127000	-0.224032000	-0.493495000
1	1.989504000	-1.517183000	-1.441211000
1	2.643827000	-2.179982000	0.072871000
1	2.482323000	1.483634000	-1.432487000
1	3.307780000	1.917569000	0.067878000
1	4.112255000	-0.348085000	-1.385218000
1	4.135839000	-0.338546000	0.385407000
8	0.704256000	1.620375000	0.819222000
7	1.304531000	-0.565750000	0.315338000
9	-3.598023000	-0.702992000	-0.133267000
9	-1.855383000	-0.354543000	-1.418265000
1	-3.147383000	1.692576000	0.826133000

1	-3.212583000	1.913603000	-0.941424000

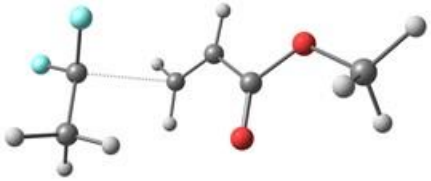
CH_3CF_2-CH_2CH(N-pyr)$^{\bullet}$



6	-3.435717000	0.865568000	-0.139385000
1	-3.111082000	1.907082000	-0.221168000
6	-2.236949000	-0.054013000	-0.137196000
6	-1.253833000	0.150497000	1.018507000
1	-1.809259000	-0.043597000	1.946804000
1	-0.926795000	1.194222000	1.019301000
6	-0.075635000	-0.753750000	0.933270000
1	-0.206116000	-1.824593000	1.054878000
6	1.598570000	0.909299000	0.150647000
6	2.072797000	-1.400740000	-0.078042000
6	2.939115000	0.786308000	-0.557070000
6	3.392938000	-0.642400000	-0.255564000
1	1.708192000	-1.824153000	-1.025934000
1	2.139334000	-2.215922000	0.653012000
1	2.779171000	0.948994000	-1.633103000
1	3.623269000	1.565283000	-0.207850000
1	4.016399000	-1.083854000	-1.039234000
1	3.963698000	-0.665614000	0.680594000
8	1.021791000	1.947977000	0.446428000
7	1.134126000	-0.379731000	0.392790000
1	-4.074906000	0.621565000	-0.993333000
1	-4.012055000	0.742807000	0.782646000
9	-1.563277000	0.092804000	-1.326983000
9	-2.682366000	-1.360864000	-0.111748000

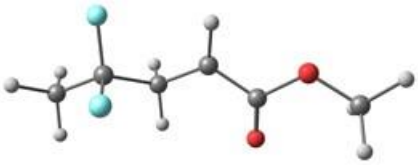
h4. To MA (tail)

$CH_3CF_2^{\bullet\cdots}CH_2$=CH(COOMe) TS



6	2.001610000	1.449351000	-0.573498000
1	0.936615000	1.695318000	-0.616268000
6	2.189128000	0.176313000	0.169602000
6	0.408385000	-1.425595000	-0.911698000
1	1.117334000	-2.244864000	-0.827112000
1	0.506877000	-0.751673000	-1.759546000
6	-0.659182000	-1.327336000	-0.098297000
6	-1.619358000	-0.223488000	-0.264712000
1	-0.836605000	-2.026216000	0.715352000
8	-1.495449000	0.723562000	-1.024459000
8	-2.685475000	-0.379478000	0.552965000
6	-3.667651000	0.655268000	0.463294000
1	-4.447476000	0.387980000	1.179305000
1	-3.231386000	1.627575000	0.716563000
1	-4.080555000	0.712688000	-0.549561000
1	2.379467000	1.340052000	-1.593881000
1	2.546547000	2.272104000	-0.084478000
9	1.766536000	0.186092000	1.438600000
9	3.415572000	-0.363061000	0.104004000

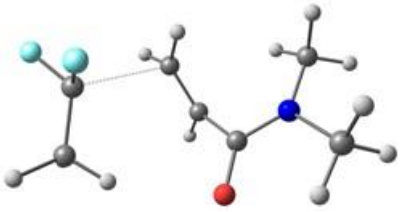
CH_3CF_2-CH_2CH(COOMe)$^{\bullet}$



6	3.285981000	0.804252000	-0.091035000
1	3.127550000	1.787069000	0.362668000
6	2.045815000	-0.046184000	0.053455000
6	0.787829000	0.510805000	-0.605394000
1	1.015821000	0.638610000	-1.677266000
1	0.562388000	1.506589000	-0.206605000
6	-0.393756000	-0.368251000	-0.437174000
6	-1.689888000	0.207633000	-0.143273000
1	-0.300807000	-1.445273000	-0.544708000
8	-1.908180000	1.403329000	0.009564000
8	-2.654019000	-0.743356000	-0.058177000
6	-3.958731000	-0.240846000	0.234678000
1	-4.612177000	-1.114789000	0.273930000
1	-3.966623000	0.286828000	1.194845000
1	-4.293208000	0.453094000	-0.544521000
1	3.539261000	0.934650000	-1.147374000
1	4.118523000	0.307850000	0.416070000
9	2.299009000	-1.292862000	-0.478599000
9	1.794698000	-0.244790000	1.389080000

h5. To DMA (tail)

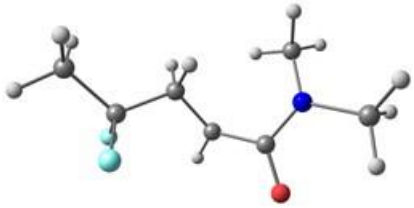
$CH_3CF_2^{\bullet\cdots}CH_2$=CH($CONMe_2$) TS



6	-0.348524000	-0.425783000	-1.341985000
6	2.314572000	-0.014269000	0.271010000
6	0.489013000	-1.312093000	-0.755440000
1	1.233660000	-1.851172000	-1.337177000
1	0.334051000	-1.650960000	0.267065000
1	-0.178910000	-0.108236000	-2.370086000
6	-1.293829000	0.452418000	-0.593275000
8	-1.134563000	1.675692000	-0.664161000
7	-2.275505000	-0.113602000	0.175309000
6	-2.647836000	-1.512256000	0.145218000
1	-2.473549000	-1.994446000	1.118415000
1	-3.716920000	-1.610960000	-0.093214000
1	-2.070468000	-2.038163000	-0.616763000
6	-3.110417000	0.750961000	0.985593000
1	-4.150694000	0.735191000	0.629594000
1	-3.098923000	0.420858000	2.033426000
1	-2.720926000	1.768006000	0.913236000
9	1.934242000	0.012320000	1.558989000
9	3.430449000	-0.754966000	0.154464000
6	2.347093000	1.308511000	-0.402451000

1	1.340709000	1.740473000	-0.417386000
1	3.032929000	1.993468000	0.118877000
1	2.691430000	1.184499000	-1.432955000

CH_3CF_2-$CH_2CH(CONMe_2)^{\bullet}$

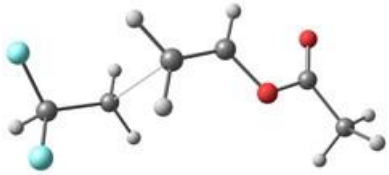


6	-0.111302000	0.433768000	-0.785236000
6	2.182360000	-0.063878000	0.112219000
6	0.822006000	-0.627447000	-0.304891000
1	1.025538000	-1.370801000	-1.094867000
1	0.400413000	-1.173815000	0.547205000
1	0.305978000	1.244514000	-1.376556000
6	-1.457325000	0.700173000	-0.267933000
8	-1.804225000	1.874498000	-0.097273000
7	-2.267670000	-0.359475000	0.090061000
6	-2.149021000	-1.685145000	-0.476457000
1	-1.986739000	-2.451758000	0.295787000
1	-3.068985000	-1.947139000	-1.021133000
1	-1.324208000	-1.723502000	-1.191709000
6	-3.517020000	-0.069217000	0.763156000
1	-4.372417000	-0.139837000	0.073367000
1	-3.676558000	-0.781066000	1.584039000
1	-3.469784000	0.947922000	1.156277000
9	2.719984000	0.609342000	-0.962284000
9	1.992529000	0.868698000	1.099197000
6	3.187198000	-1.086166000	0.592929000
1	3.394921000	-1.819205000	-0.192421000
1	4.117338000	-0.573463000	0.855122000
1	2.807993000	-1.606395000	1.477701000

(i) $PVDF_T^{\bullet}$ addition to monomer

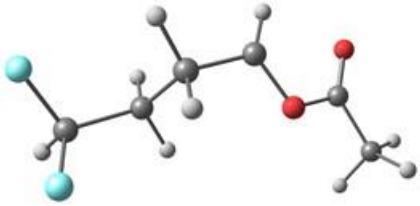
i1. To VAc (tail)

$CHF_2CH_2^{\bullet\cdots}CH_2$=CHOAc TS



6	-1.798123000	0.066931000	1.123956000
6	-0.442862000	-0.470412000	-0.841534000
1	-1.139469000	-1.283581000	-1.011611000
1	-0.718966000	0.515245000	-1.202456000
6	0.818012000	-0.749251000	-0.461401000
1	1.192049000	-1.727302000	-0.172675000
8	1.737101000	0.271585000	-0.359380000
6	2.994965000	-0.046952000	0.084980000
8	3.329064000	-1.163850000	0.401802000
6	3.858387000	1.181447000	0.105769000
1	4.844727000	0.924258000	0.494476000
1	3.951450000	1.589933000	-0.906880000
1	3.398623000	1.957389000	0.727562000
1	-1.643156000	-0.839788000	1.700707000
6	-3.117038000	0.248248000	0.480899000
9	-3.502107000	-0.902773000	-0.162800000
1	-1.265940000	0.959401000	1.438603000
9	-3.064069000	1.253352000	-0.453059000
1	-3.933112000	0.507294000	1.179624000

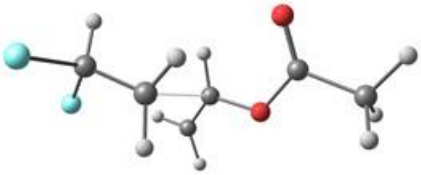
CHF_2CH_2-$CH_2CH^{\bullet}$(OAc)



6	-1.364040000	-0.055276000	0.693837000
6	-0.700139000	-0.558712000	-0.605838000
1	-1.229094000	-1.454335000	-0.951531000
1	-0.832690000	0.212150000	-1.377847000
6	0.736382000	-0.881452000	-0.454376000
1	1.143381000	-1.838912000	-0.145752000
8	1.561771000	0.205771000	-0.294753000
6	2.866895000	-0.019608000	0.062008000
8	3.311802000	-1.122419000	0.281045000
6	3.623409000	1.277003000	0.114320000
1	4.613732000	1.099886000	0.536800000
1	3.727358000	1.686698000	-0.897569000
1	3.082535000	2.018284000	0.711739000
1	-1.301893000	-0.820673000	1.477870000
6	-2.818716000	0.303347000	0.499273000
9	-3.515560000	-0.783776000	0.044482000
1	-0.837749000	0.833591000	1.062954000
9	-2.941009000	1.289292000	-0.442472000
1	-3.307789000	0.655040000	1.419571000

i2. To VAc (head)

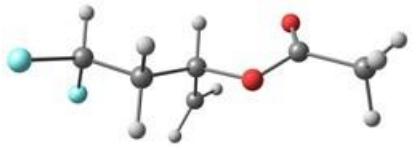
$CHF_2CH_2^{\bullet\cdots}$ CH(OAc)=CH_2 TS



6	-0.952576000	-0.555990000	-0.516344000
6	-2.243159000	-0.481557000	0.204570000
1	-2.150607000	-0.634508000	1.289777000
6	-0.132924000	2.236778000	0.055617000
1	0.190695000	2.800390000	-0.814486000
1	-1.008335000	2.571514000	0.599421000
6	0.446880000	1.055344000	0.381377000
1	0.298880000	0.537871000	1.325566000
8	1.612053000	0.702648000	-0.287424000
6	2.297325000	-0.386246000	0.170371000
8	1.928264000	-1.067139000	1.099929000
6	3.541736000	-0.596169000	-0.643803000
1	4.087509000	-1.457441000	-0.256056000
1	3.278773000	-0.761666000	-1.694557000
1	4.172906000	0.298360000	-0.604148000
9	-2.851168000	0.728232000	-0.004145000

9	-3.112205000	-1.444958000	-0.267011000
1	-0.305612000	-1.392124000	-0.262598000
1	-0.960094000	-0.228897000	-1.553281000

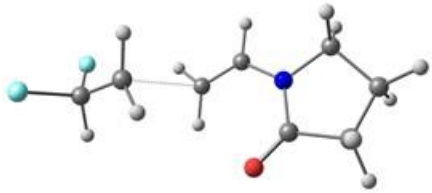
CHF_2CH_2-CH(OAc)$CH_2^{\bullet}$



6	-1.051803000	-0.639923000	-0.209126000
6	-2.367283000	-0.196985000	0.390092000
1	-2.307549000	0.023509000	1.466373000
6	0.010981000	1.637255000	-0.562270000
1	-0.595594000	1.785319000	-1.450314000
1	0.654242000	2.441448000	-0.218974000
6	0.108920000	0.304843000	0.079931000
1	0.256949000	0.425780000	1.162287000
8	1.296775000	-0.409995000	-0.416107000
6	2.465885000	-0.093138000	0.185888000
8	2.568596000	0.715141000	1.084098000
6	3.602941000	-0.873168000	-0.420944000
1	4.512482000	-0.695332000	0.155085000
1	3.368411000	-1.942386000	-0.441649000
1	3.756177000	-0.552562000	-1.457862000
9	-2.837459000	0.921921000	-0.239385000
9	-3.293362000	-1.185792000	0.211333000
1	-0.815561000	-1.627832000	0.203012000
1	-1.192982000	-0.757569000	-1.290852000

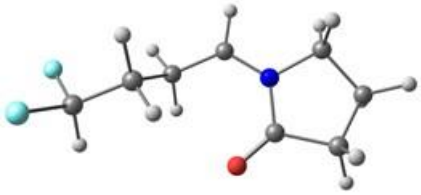
i3. To NVP (tail)

$CHF_2CH_2^{\bullet\cdots}CH_2$=CH(N-pyr) TS



9	4.375938000	0.828201000	0.756925000
9	3.740084000	-0.943267000	-0.388294000
6	3.353742000	0.326285000	-0.026934000
1	3.311092000	0.940618000	-0.936996000
6	2.082653000	0.288381000	0.720794000
1	1.475644000	1.186413000	0.764196000
1	2.008849000	-0.422307000	1.539170000
6	0.584013000	-0.833171000	-0.939414000
1	1.398400000	-1.531980000	-1.096290000
1	0.593409000	0.115347000	-1.461611000
6	-0.525577000	-1.266706000	-0.296562000
1	-0.556397000	-2.264179000	0.139166000
6	-1.899205000	0.798357000	-0.344891000
6	-2.816692000	-1.145189000	0.653754000
6	-3.280259000	1.167052000	0.181543000
6	-3.977759000	-0.178193000	0.386553000
1	-2.583726000	-1.215752000	1.728030000
1	-3.013258000	-2.158416000	0.283827000
1	-3.147493000	1.713559000	1.126312000
1	-3.784125000	1.842130000	-0.516166000
1	-4.708010000	-0.177956000	1.201480000
1	-4.499138000	-0.474165000	-0.531578000
8	-1.098950000	1.545165000	-0.884842000
7	-1.696190000	-0.545706000	-0.069648000

CHF_2CH_2-CH_2CH(N-pyr)$^{\bullet}$



9	3.750353000	0.976686000	0.918517000
9	3.784525000	-0.744771000	-0.463064000
6	3.050949000	0.347766000	-0.074411000
1	2.989884000	1.031305000	-0.933973000
6	1.701967000	-0.086617000	0.441744000
1	1.149412000	0.810031000	0.741825000
1	1.868370000	-0.707428000	1.331540000
6	0.894296000	-0.854727000	-0.622674000
1	1.481079000	-1.723963000	-0.943875000
1	0.762713000	-0.200487000	-1.493512000
6	-0.427623000	-1.347937000	-0.147731000
1	-0.543529000	-2.362933000	0.219366000
6	-1.679326000	0.794879000	-0.294040000
6	-2.775355000	-1.120517000	0.562901000
6	-3.098710000	1.207561000	0.067270000
6	-3.862311000	-0.112583000	0.171480000
1	-2.669911000	-1.209952000	1.655037000
1	-2.953112000	-2.123597000	0.157192000
1	-3.069595000	1.746447000	1.025741000
1	-3.491792000	1.902252000	-0.681308000
1	-4.683627000	-0.093178000	0.894683000
1	-4.281582000	-0.382813000	-0.805059000
8	-0.794108000	1.521770000	-0.729805000
7	-1.548953000	-0.559147000	-0.007932000

i4. To MA (tail)

$CHF_2CH_2^{\bullet\cdots}CH_2$=CH(COOMe) TS

9	3.965149000	-1.080016000	-0.275093000
9	3.302863000	0.996999000	0.057180000
6	2.930964000	-0.314276000	0.216297000
1	2.851243000	-0.518995000	1.292749000
6	1.687225000	-0.588141000	-0.536190000
1	1.058796000	-1.421064000	-0.237821000
1	1.641246000	-0.249365000	-1.567184000
6	0.125425000	1.141330000	0.437264000
1	0.898177000	1.862477000	0.189534000
1	0.229408000	0.574625000	1.360361000
6	-1.035310000	1.070835000	-0.246686000
6	-2.083973000	0.122402000	0.172783000
1	-1.228988000	1.676436000	-1.129101000
8	-1.990613000	-0.681903000	1.082748000
8	-3.188397000	0.251403000	-0.597838000

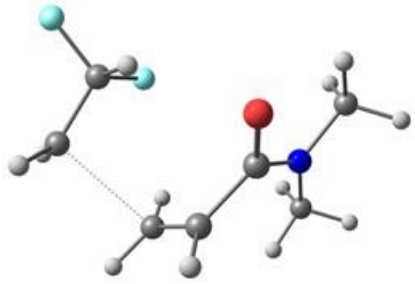
6	-4.261400000	-0.630735000	-0.257662000
1	-5.065188000	-0.407054000	-0.961877000
1	-3.948621000	-1.676260000	-0.351154000
1	-4.593693000	-0.458137000	0.771604000

CHF_2CH_2-$CH_2CH(COOMe)^{\bullet}$

9	3.814240000	0.835375000	-0.640718000
9	3.305035000	-0.797572000	0.755452000
6	2.873427000	-0.109914000	-0.347080000
1	2.826654000	-0.819086000	-1.186770000
6	1.553357000	0.562327000	-0.049872000
1	1.255721000	1.138124000	-0.934615000
1	1.727756000	1.277180000	0.764960000
6	0.459178000	-0.448314000	0.329941000
1	0.827203000	-1.033647000	1.188304000
1	0.277376000	-1.153342000	-0.491102000
6	-0.825666000	0.199293000	0.685540000
6	-2.050812000	-0.141311000	-0.010086000
1	-0.871735000	0.942333000	1.479660000
8	-2.138819000	-0.947094000	-0.928429000
8	-3.113137000	0.548448000	0.480049000
6	-4.356081000	0.258030000	-0.161427000
1	-5.102462000	0.875822000	0.342181000
1	-4.311496000	0.504683000	-1.228095000
1	-4.607255000	-0.803794000	-0.062188000

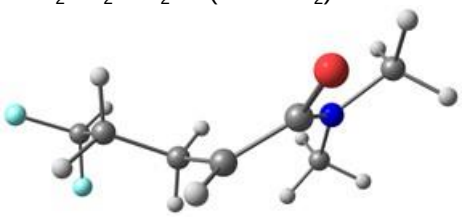
i5. To DMA (tail)

$CHF_2CH_2^{\bullet}\cdots CH_2$=CH(CONMe$_2$) TS



6	-0.553526000	1.469780000	0.794822000
6	2.440968000	1.026482000	-0.007744000
6	0.197442000	1.965793000	-0.217368000
1	0.659797000	2.946915000	-0.137139000
1	0.200605000	1.499166000	-1.199312000
1	-0.553668000	1.958157000	1.768792000
6	-1.143271000	0.096776000	0.811029000
8	-0.738822000	-0.691797000	1.671369000
7	-2.076420000	-0.248335000	-0.124492000
6	-2.695742000	0.668683000	-1.057738000
1	-2.414384000	0.435250000	-2.095147000
1	-3.789921000	0.597589000	-0.979569000
1	-2.396873000	1.694016000	-0.833783000
6	-2.545419000	-1.619651000	-0.168467000
1	-3.625232000	-1.666239000	0.030816000
1	-2.354937000	-2.057447000	-1.157897000
1	-2.010305000	-2.188558000	0.593871000
6	2.137054000	-0.422530000	0.009205000
1	1.559923000	-0.742121000	0.884721000
1	2.728723000	1.498447000	0.927063000
1	2.849219000	1.438919000	-0.928101000
9	1.423645000	-0.762688000	-1.117759000
9	3.306081000	-1.154353000	-0.032938000

CHF_2CH_2-$CH_2CH(CONMe_2)^{\bullet}$



6	0.552810000	0.602628000	0.905033000
6	-1.800112000	0.639721000	0.025351000
6	-0.579682000	-0.221838000	0.387224000
1	-0.905776000	-0.955079000	1.144337000
1	-0.262148000	-0.801525000	-0.490073000
1	0.324891000	1.390275000	1.621693000
6	1.889651000	0.724685000	0.311795000
8	2.393758000	1.850988000	0.218549000
7	2.510846000	-0.398558000	-0.193132000
6	2.204715000	-1.745469000	0.237183000
1	1.888641000	-2.384060000	-0.600863000
1	3.093623000	-2.206226000	0.694103000
1	1.414363000	-1.735952000	0.991303000
6	3.751863000	-0.230959000	-0.920867000
1	4.616895000	-0.538186000	-0.313184000
1	3.740451000	-0.838998000	-1.835578000
1	3.861154000	0.824523000	-1.176869000
6	-2.965146000	-0.184308000	-0.469501000
1	-2.745986000	-0.750539000	-1.387490000
1	-1.539412000	1.369020000	-0.751200000
1	-2.145650000	1.204390000	0.900923000
9	-3.343715000	-1.084399000	0.491562000
9	-4.033133000	0.628576000	-0.719437000

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