Quantum chemical calculation of reactions in plasma important for the operation of RPC system

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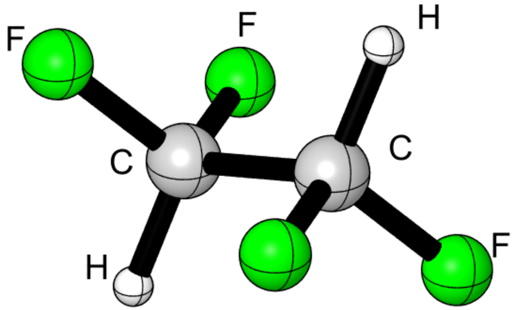
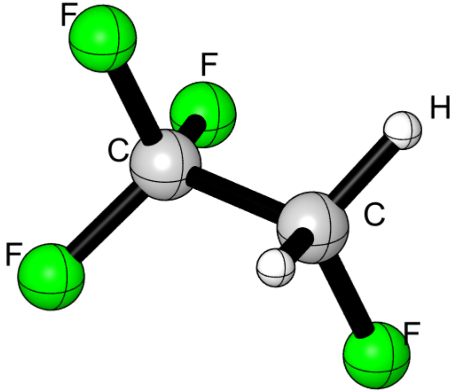
The aim Examine and compare how two basic processes in plasma affect the stability of CHF_2CHF_2 (HFE-134), CH_2FCF_3 (HFE-134a), $CF_3CH=CHF$ (HFO-1234ze(E)) and $(CF_3)_2CF\text{-}O\text{-}CH_3$ (HFE-347mmy1) molecules



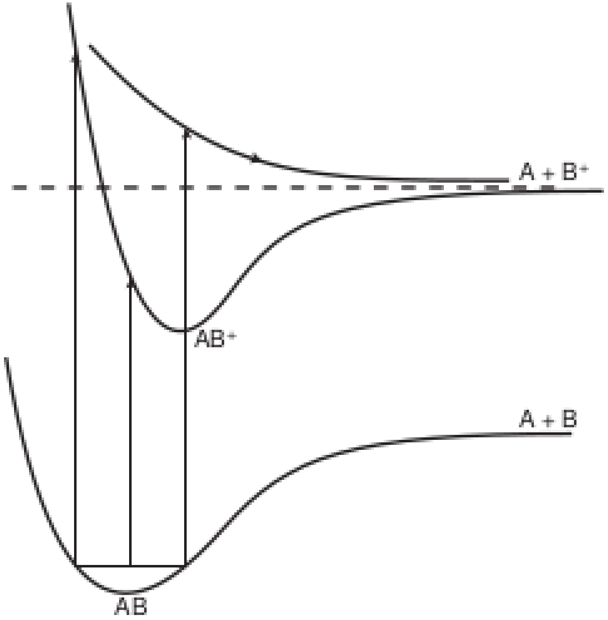
HFE-134



HFE-134a

We examine ionization and electron attachment processes by calculations at Density-functional theory (DFT) method using Gaussian 16 quantum chemical package.

We calculate Vertical and Adiabatic energy for ionization and electron attachment processes

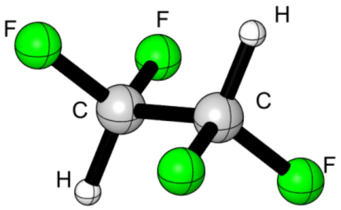


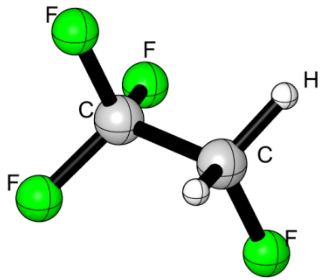
Ionization by losing electron

HFE-134

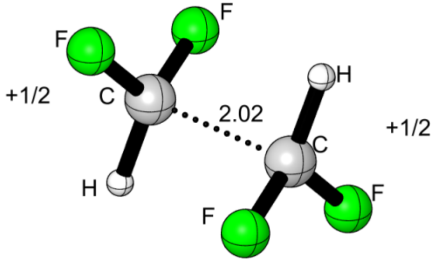
HFE-134a

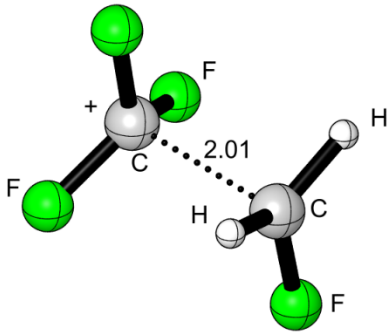
Ground state





Ionized state





Vertical energy	(eV)	12.69
Adiabatic energy	(eV)	11.44

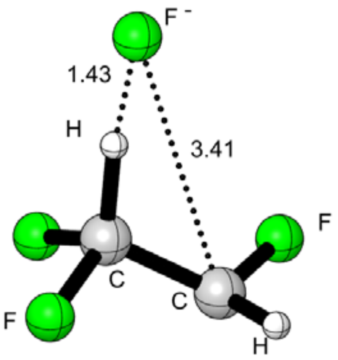
Vertical energy	(eV)	13.32
Adiabatic energy	(eV)	11.93

Ionization by attaching electron

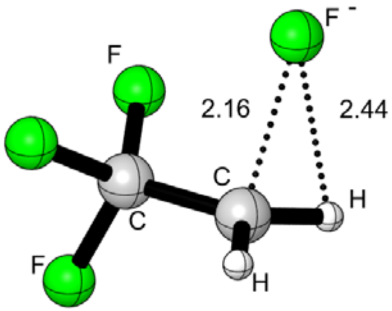
HFE-134

HFE-134a

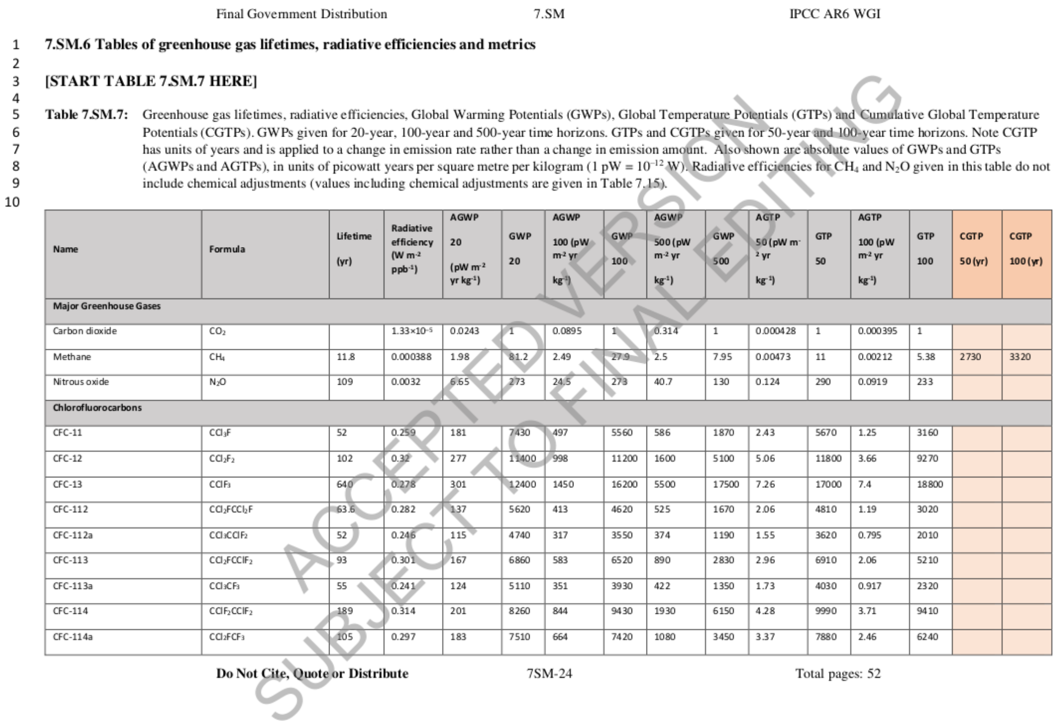
electron attached state



Vertical energy	(eV)	3.96
Adiabatic energy	(eV)	1.04



Vertical energy	(eV)	3.27
Adiabatic energy	(eV)	0.95



Final Government Distribution 7.SM IPCC AR6 WGI

7.SM.6 Tables of greenhouse gas lifetimes, radiative efficiencies and metrics

[START TABLE 7.SM.7 HERE]

Table 7.SM.7: Greenhouse gas lifetimes, radiative efficiencies, Global Warming Potentials (GWPs), Global Temperature Potentials (GTPs) and Cumulative Global Temperature Potentials (CGTPs). GWPs given for 20-year, 100-year and 500-year time horizons. GTPs and CGTPs given for 50-year and 100-year time horizons. Note CGTP has units of years and is applied to a change in emission rate rather than a change in emission amount. Also shown are absolute values of GWPs and GTPs (AGWPs and AGTPs), in units of picowatt years per square metre per kilogram (1 pW = 10^{-12} W). Radiative efficiencies for CH_4 and N_2O given in this table do not include chemical adjustments (values including chemical adjustments are given in Table 7.15).

Name	Formula	Lifetime (yr)	Radiative efficiency (W m^{-2} ppb^{-1})	AGWP 20 (pW m^{-2} yr kg^{-1})	GWP 20	AGWP 100 (pW m^{-2} yr kg^{-1})	GWP 100	AGWP 500 (pW m^{-2} yr kg^{-1})	GWP 500	AGTP 50 (pW m^{-2} yr kg^{-1})	GTP 50	AGTP 100 (pW m^{-2} yr kg^{-1})	GTP 100	CGTP 50 (yr)	CGTP 100 (yr)
Major Greenhouse Gases															
Carbon dioxide	CO_2		1.33×10^{-5}	0.0243	1	0.0895	1	0.314	1	0.000428	1	0.000395	1		
Methane	CH_4	11.8	0.000388	1.98	81.2	2.49	27.9	2.5	7.95	0.00473	11	0.00212	5.38	2730	3320
Nitrous oxide	N_2O	109	0.0032	6.65	273	24.5	273	40.7	130	0.124	290	0.0919	233		
Chlorofluorocarbons															
CFC-11	CCl_3F	52	0.259	181	7430	497	5560	586	1870	2.43	5670	1.25	3160		
CFC-12	CCl_2F_2	102	0.32	277	11400	998	11200	1600	5100	5.06	11800	3.66	9270		
CFC-13	$CClF_3$	640	0.278	301	12400	1450	16200	5500	17500	7.26	17000	7.4	18800		
CFC-112	CCl_2FCCl_2F	63.6	0.282	137	5620	413	4620	525	1670	2.06	4810	1.19	3020		
CFC-112a	CCl_3CClF_2	52	0.246	115	4740	317	3550	374	1190	1.55	3620	0.795	2010		
CFC-113	CCl_2FCClF_2	93	0.301	167	6860	583	6520	890	2830	2.96	6910	2.06	5210		
CFC-113a	CCl_3CF_3	55	0.241	124	5110	351	3930	422	1350	1.73	4030	0.917	2320		
CFC-114	$CClF_2CClF_2$	189	0.314	201	8260	844	9430	1930	6150	4.28	9990	3.71	9410		
CFC-114a	CCl_2FCF_3	105	0.297	183	7510	664	7420	1080	3450	3.37	7880	2.46	6240		

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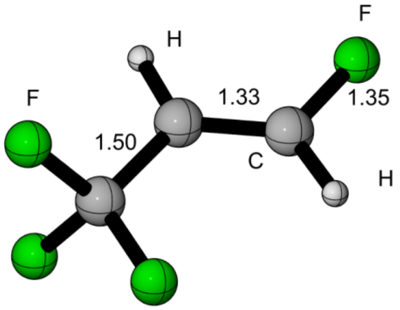
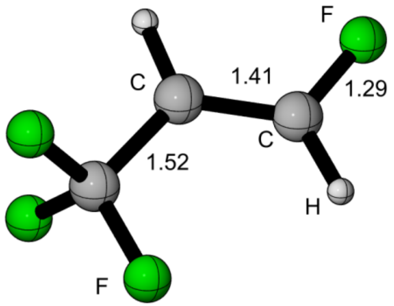
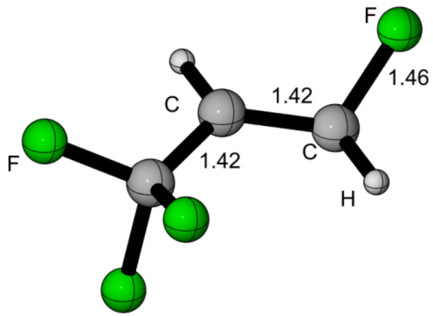
We examine how two basic processes in plasma affect the stability of $CF_3CH=CHF$ (HFO-1234ze(E)) molecule



Ground state



Ionized state



electron attached -abstracted state

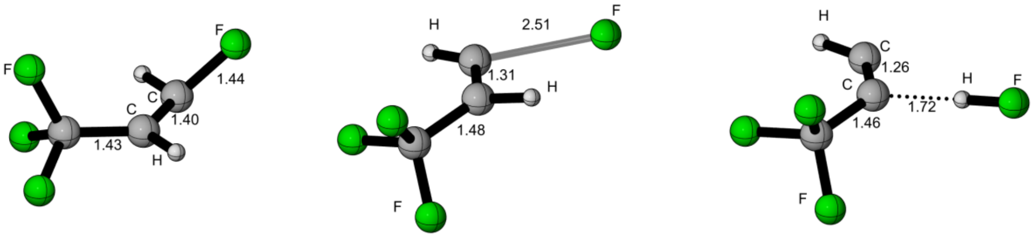
Vertical energy	(eV)	10.80
Adiabatic energy	(eV)	10.47

Vertical energy	(eV)	1.44
Adiabatic energy	(eV)	0.44

CHF_2CHF_2	**HFO**
$CHF_2CHF_2 + e^- \rightarrow 2\ CH_2F^{+1/2} + 2\ e^-$	$HFO + e^- \rightarrow HFO^{+1} + e^- + e^-$
$CHF_2CHF_2 + e^- \rightarrow {\cdot}CHF_2CHF + F^-$	$HFO + e^- \rightarrow HFO^{-1}$

CH_2FCF_3	**HFO**
$CH_2FCF_3 + e^- \rightarrow {\cdot}CH_2F + CF_3^+ + 2\ e^-$	$HFO + e^- \rightarrow HFO^{+1} + e^- + e^-$
$CH_2FCF_3 + e^- \rightarrow {\cdot}CH_2FCF_2 + F^-$	$HFO + e^- \rightarrow HFO^{-1}$

start	TS	end structure

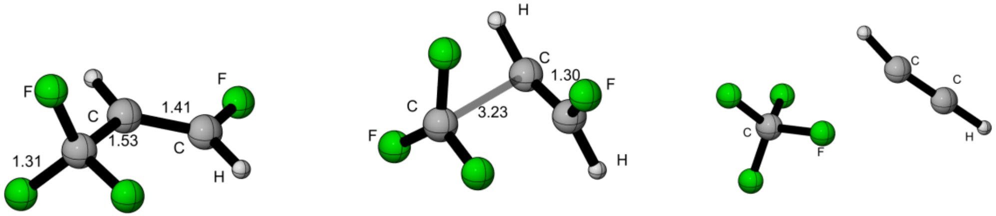


HFO^{-1}

$[CHF{=}CH\text{-}CF_3]^{-1}$ → TS → $[CH{=}C\text{-}CF_3]^{-1}$ + HF

$E_a = 1.08$ eV

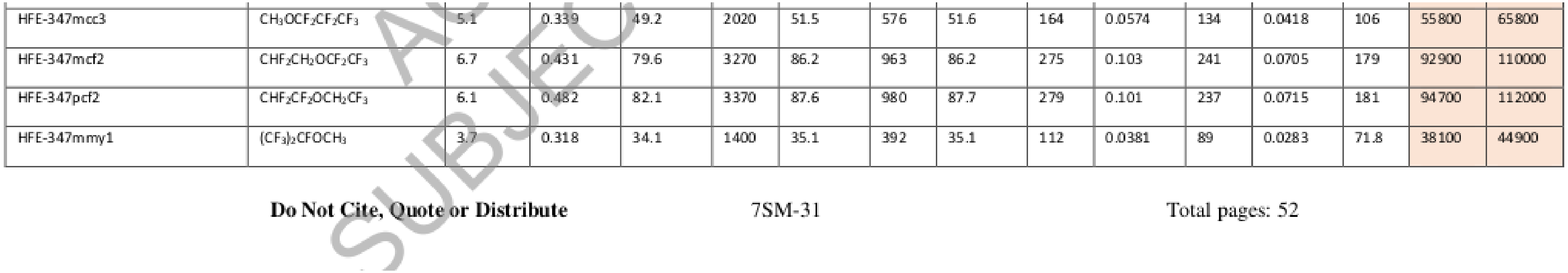
start	TS	end structure



HFO^{+1}

$[CHF{=}CH\text{-}CF_3]^{+1}$ → TS → $CF_4 + C_2H_2^{+1}$

$E_a = 2.64$ eV



HFE-347mcc3	$CH_3OCF_2CF_2CF_3$	5.1	0.339	49.2	2020	51.5	576	51.6	164	0.0574	134	0.0418	106	55800	65800
HFE-347mcf2	$CHF_2CH_2OCF_2CF_3$	6.7	0.431	79.6	3270	86.2	963	86.2	275	0.103	241	0.0705	179	92900	110000
HFE-347pcf2	$CHF_2CF_2OCH_2CF_3$	6.1	0.482	82.1	3370	87.6	980	87.7	279	0.101	237	0.0715	181	94700	112000
HFE-347mmy1	$(CF_3)_2CFOCH_3$	3.7	0.318	34.1	1400	35.1	392	35.1	112	0.0381	89	0.0283	71.8	38100	44900

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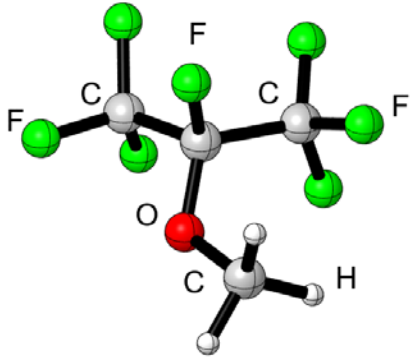
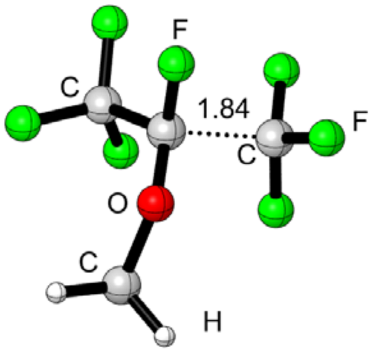
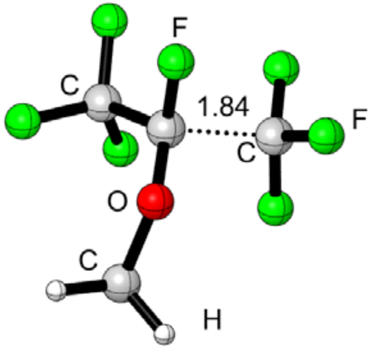
We examine how two basic processes in plasma affect the stability of $(CF_3)_2CF\text{-}O\text{-}CH_3$ (HFE-347mmy1) molecule



Ground state



Ionized state

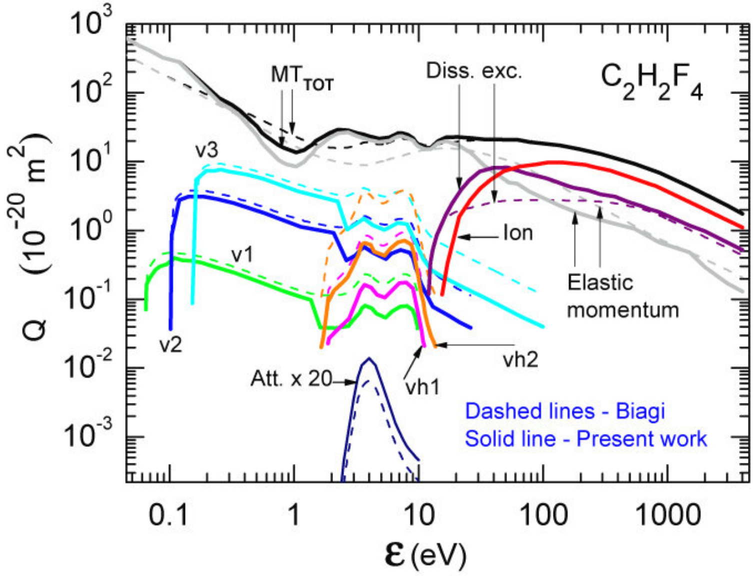


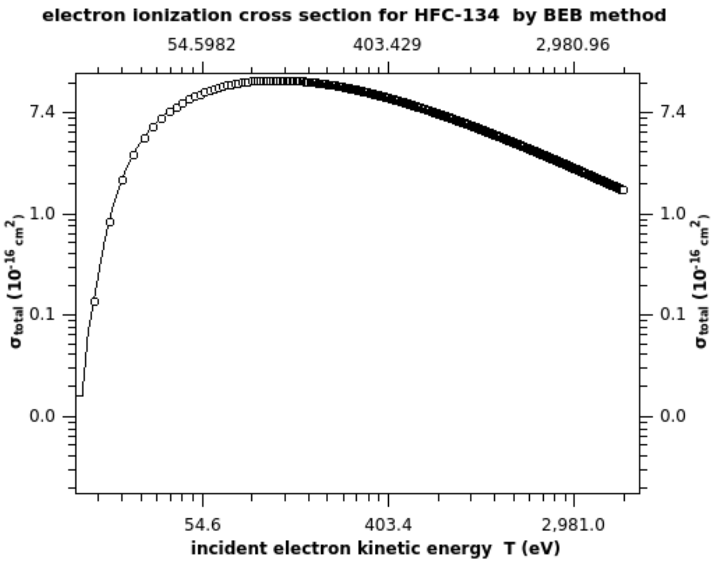
electron attached -abstracted state

Vertical energy	(eV)	11.39
Adiabatic energy	(eV)	11.01

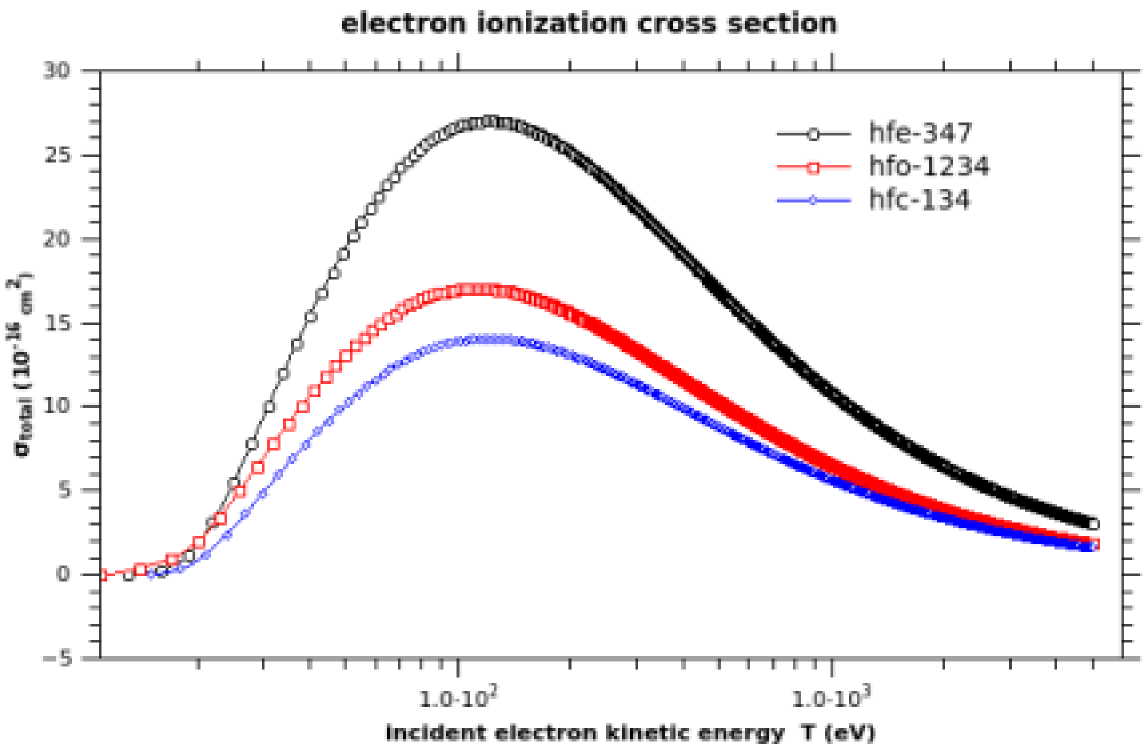
Vertical energy	(eV)	3.21
Adiabatic energy	(eV)	0.39

Experimental (well known, from literature) and calculated electron induced ionization cross-section for HFE-134 molecule





Comparison of calculated electron induced ionization cross-section for HFE-134/ HFE-134a, HFO-1234 and HFE-347 moleculs



Summary

- Quantum-Chemically analyze of behavior of gases which should be important for function of PRC detector, two already in use, one in experantally phase and for one completely novel is performed.
- We calculate values of energy for adiabatic and vertical transitions of both investigated processe in plasma
- For same molecules cross section for electron induced ionization is calculated
- We get better insight in different processes in RPC detectors