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PROPERTIES OF POTENTIAL ECO-FRIENDLY GAS REPLACEMENTS FOR PARTICLE DETECTORS IN HIGH-ENERGY PHYSICS

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Abstract

Modern gas detectors for detection of particles require F-based gases for optimal performance. Recent regulations demand the use of environmentally unfriendly F-based gases to be limited or banned. This review studies properties of potential eco-friendly gas candidate replacements.

Keywords: gas detectors, muon detectors, GEM, RPC, GWP, ODP, eco-friendly gas, Quantum chemistry, NWCHEM , RT-TDDFT, absorption spectrum, ionization energy

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1 Introduction

Many currently used refrigerant gases have a great impact on the environment since they either contribute largely to the greenhouse gas effect, or because they tear the ozone layer, or both. In an attempt to protect the environment, regulations preventing the production and use of certain refrigerant gases have been implemented [1].

Gas detectors are widespread for detection, tracking and triggering of charged particles such as muons in Nuclear and High Energy Physics (HEP). They are characterized by simple and reliable use, but utmost care must be taken to issues such as properties of gas interaction with materials, gas purification, gas mixture contaminants, etc. [2]-[8].

A large part of gas muon detectors used in HEP operates with mixtures containing the regulated refrigerants as quenching medium in applications where excellent time resolution and avalanche operation are necessary. Therefore, actions towards finding new mixtures must be undertaken. Gas Electron Multiplier (GEM) [9] detectors operate in experiments such as CMS (Compact Muon Solenoid) at the LHC (Large Hadron Collider) with an argon/CO_2 mixture [11]. However, for high time resolution applications an argon/CO_2/CF_4 mixture is used [12], where CF_4 has a Global-Warming Potential (GWP) of 7390 [13]. Resistive Plate Counters (RPC) [10] currently operate with a F-based R134a/Isobutane/SF_6 gas mixture, with typical GWP of 1430. Investigations into new gas mixtures has to be performed in order to keep the mixture properties while complying with the regulations. A few industrial refrigerant industrial replacements were proposed [14] as alternatives to R134a. A study of transport properties of currently used gas mixtures in HEP, and evaluation of transport properties of freon-less gas mixtures, was recently published [15][16].

The aim of this paper is to discuss some of the important properties of gases for particle gas detectors, to list and summarize basic properties of eco-friendly refrigerants from the literature, to discuss their properties for materials compatibility and safe use, and make a prediction on selected parameters crucial for the performance of gas detectors considered. While this study is aimed to GEM and RPC detectors, its findings can be considered for selection of ecogas replacement for other gas detectors.

2 Gas properties

For a gas mixture to be appropriate in a gas detector, first of all it has to comply with the regulations. Furthermore, its properties must also be appropriate for the specific

type of detectors. For example, a gas that is suitable for the RPC detectors may not be fully optimized for the GEM detectors. To better find the appropriate gas for a detector, an understanding of the influence of different parameters is required. This section aims to clarify the most essential parameters for gases.

2.1 Global-warming potential and Ozone depletion potential

In order to estimate the impact of a refrigerant on the environment, the effects have to be quantified. Two important effects are the contribution to the greenhouse effect and the depletion of the ozone layer. The first mentioned effect is measured in Global-Warming Potential (GWP), and is normalized to the effect of CO_2 (GWP = 1), while the effect on the ozone layer is measured in Ozone Depletion Potential (ODP), normalized to the effect of CCl_3F (ODP = 1). The effects of selected refrigerant candidates are listed in table 1.

2.2 Stopping power

When a particle passes through a medium, energy is transferred from the particle to the surroundings. The energy lost is typically defined as the stopping power expressed as $\frac{1}{\rho}\left\langle \frac{dE}{dx} \right\rangle$, where ρ denotes the density of the medium, E denotes energy, and x is length. This expression is itself dependent on the momentum p of the particle. In the next section it will be shown the particle will experience a minimum energy loss at around $p/Mc \approx 3$, where M is the particle mass, and c is the speed of light. By knowing the average minimum energy loss, we also know the minimum energy the particle loses by passing through a detector. The minimum mean ionization energies for the refrigerants under consideration are summarized in table 2.

2.3 Radiation length

The radiation length X_0 is a characteristic length of a medium. It describes both the mean distance required for a high energy electron to lose all but e^{-1} of its energy due to bremsstrahlung, and $^7/_9$ of the mean free path of a e^+e^- pair produced by a high-energy photon [18]. These quantities are also estimated and summarized in table 2.

2.4 Ion pair production

When an incoming particle passes through a medium, it will eventually interact with the medium and transfer some of its energy to ionize atoms. In this process, a pair con-

sisting of an ionized atom and a free electron is produced. The number of ionizations produced by an incoming particle per unit length is denoted by N_P, in units of cm^{-1}. Each produced ion pair will have an initial kinetic energy and can itself produce an ion pair, called secondary ion pair production. The sum of the primary and secondary ion pairs production per unit length is denoted N_T, and will be mainly depending on the material and the incoming particle energy and mass. This parameter is relevant in particle gas detectors as it determines both the number and the size of avalanches produced by a single incoming particle when the gas is under an amplifying electric field.

2.5 Drift velocity

In the absence of electric field, electrons move randomly in all direction having an average thermal energy $3/2KT$. In presence of an electric field, the electrons start to drift along the field direction with mean drift velocity v_d (the average distance covered by the drift electron per unit time). The drift velocity depends on the pressure, temperature and could be affected by the presence of pollutants like water or oxygen. Electric field lines are, in addition, deformed by any magnetic field applied to the gas volume. Finally, electronegative pollutants deplete the gas of electrons. Computer codes such as Magboltz [17] computes the drift velocity using montecarlo techniques, by tracing electrons at the microscopic level through numerous collisions with gas molecules.

2.6 Diffusion

Electrons and ions in a gas are subject only to an electric field and move on average along the electric field, but individual electrons deviate from the average due to scattering on the atoms of the gas. Scattering leads to variations in velocity, called longitudinal diffusion, and to lateral displacements, called transverse diffusion. The scattering process in each direction can, to a good approximation, be considered gaussian on a microscopic scale. In cold gases like carbon-dioxide for example, the diffusion is small, while the drift velocity is low and unsaturated for values of electric fields common in gas detectors; this implies a non linear space time relation. Warm gases, like argon for instance, have a higher diffusion; when mixed with polyatomic/organic gases having vibrational thresholds between 0.1 and 0.5 eV, diffusion is reduced in most cases, while the drift velocity is increased.

2.7 Townsend coefficients

The average distance an electron travels between ionizing collisions is called mean free path and its inverse is the number of ionizing collision per centimeter α (the first Townsend coefficient). This parameter determines the gas gain of the gas. If n_0 is the number of primary electron without amplification in uniform electric field, and n is the number of electrons after distance x under avalanche condition, then n is given by $n = n_0 e^{\alpha x}$ and the gas gain G is given by $G \equiv n_0/n = e^{\alpha x}$. The first Townsend coefficient depends on the nature of the gas, the electric field and pressure. To take into account the augmented emission of electrons by the cathode caused by impact of positive ions, it is customary to introduce η, Townsend's second ionization coefficient or attachment parameter, *i.e.*, the average number of electrons released from a surface by an incident positive ion, according to the formula

$$G \equiv \frac{e^{\alpha x}}{1 - \eta(e^{\alpha x} - 1)} \tag{1}$$

2.8 Lorentz angle

Because of the deflection effect exerted by a magnetic field perpendicular to the electric field and the motion of the electron, the electron moves in a helical trajectory resulting in a lowered drift velocity and transverse dispersion. Thus the arrival time of electrons at the anode changes and the spread in the drift time increases. The angle which the drifting electron swarm makes with the electric field is defined as the Lorentz angle of the particular gas or gas mixture under consideration. The Lorentz angle depends on both the electric field and the magnetic field. It is normally large at small electric fields but falls to smaller values for larger electric fields and is approximately linear with increasing magnetic field.

2.9 Hazards and flammability

Many refrigerants may constitute danger for the user and its environment. The greatest dangers involved are the flammability and toxicity. We have used two standards in categorizing the refrigerants in table 3 and 4. The Ashrae standard [19] gives each refrigerant a number denoting flammability from 1 (not flammable) to 3 (highly flammable), as well as a letter A (non-toxic) or B (Toxic). The Health Material Hazardous Material Information System (HMIS), rates Health/ Flammability/ and Physical hazards from 0 (low) to 4 (high).

2.10 Compatibility with materials

Some refrigerants are incompatible with certain materials, and can either react violently, or have long term effect. Some refrigerants may even produce toxic decomposition and/or polymerization. Known incompatibilities and toxic byproducts are summarized in Table 3 and 4.

2.11 Aging and longevity

Aging is defined (following [20]) the general deterioration of the detectors during their operation. The aging phenomenon is very complex and depends on several parameters. The commonly used variables include the cross-sections, electron/photon energies, electrostatic forces, dipole moments, chemical reactivity of atoms and molecules, etc. For a comprehensive (although non recent) collection see [21][22][23]. A more recent review of ageing effects in GEM detectors can be found in [24].

3 Estimation of Gas Parameters

3.1 Stopping power

Quantities such as the minimum ionization energy can be found if the stopping power is known. An approximate expression for moderately relativistic particles in the momentum region $0.1 \leq \beta\gamma = p/Mc \leq 1000$ can be found using the Bethe-Bloch equation, given by [30]

$$\frac{1}{\rho}\left\langle -\frac{dE}{dx}\right\rangle = Kz^2\frac{Z}{A}\frac{1}{\beta^2}\left[\frac{1}{2}\ln\frac{2m_ec^2\beta^2\gamma^2T_{max}}{I^2} - \beta^2 - \frac{\delta(\beta\gamma)}{2}\right] \tag{2}$$

where $\left\langle -\frac{dE}{dx}\right\rangle$ is the mean energy loss per length, ρ is the density of the medium, I is the mean excitation energy, and $\delta(\beta\gamma)$ is the density effect correction function to ionization energy loss. K is a constant given by $4\pi N_A r_e^2 m_e c^2$, and T_{max} is the maximum energy transfer in a single collision, given by

$$T_{max} = \frac{2m_ec^2\beta^2\gamma^2}{1 + 2\gamma m_e/M + (m_e/M)^2}, \tag{3}$$

where M is the mass of the incoming particle.

The mean excitation energy I for a composite medium can be approximated from the composite atoms by the relation[51].

$$I = \exp\left\{\left[\sum_j w_j(Z_j/A_j)\ln I_j\right] / \langle Z/A\rangle\right\} \tag{4}$$

Molecular name	Chemical formula	CAS	Refrigerant identifier	GWP	ODP
Chloropentafluoroethane	C_2ClF_5	76-15-3	R115	7370	0.44
Hexafluoroethane	C_2F_6	76-16-4	R116	-	-
2,2-Dicloro-1,1,1-trifluoroethane	$C_2HCl_2F_3$	306-83-2	R123	120	0
1-Chloro-3,3,3-Trifluoropropene	$C_3H_2ClF_3$	2730-43-0	R1233zd	4.7-7	0
2,3,3,3-Tetrafluoropropene	$C_3H_2F_4$	754-12-1	R1234yf	4	0
1,3,3,3 Tetrafluoropropene	$C_3H_2F_4$	29118-24-9	R1234ze	6	0
Trifluoroiodomethane	CF_3I	2314-97-8	R13I1	0	0
1,1,1,2-Tetrafluoroethane	CH_2FCF_3	811-97-2	R134a	1430	0
Tetrafluoromethane	CF_4	75-73-0	R14	7390	0
1,1,1-trifluoroethane	CH_3CF_3	420-46-2	R143a	4300	-
1,1-Difluoroethane	$C_2H_4F_2$	75-37-6	R152a	124	0
Octafluoropropane	C_3F_8	76-19-7	R218	-	-
Propane	C_3H_8	74-98-6	R290	3	0
Difluoromethane	CH_2F_2	75-10-5	R32	650	0
Isobutane	C_4H_{10}	75-28-5	R600a	3	0
Sulfur Hexafluoride	SF_6	2551-62-4	R7146	23000	0.04
Carbon Dioxide	CO_2	124-38-9	R744	1	0
Octafluorocyclobutane	C_4F_8	115-25-3	RC318	-	-
Pentafluoroethane	HF_2CF_3	354-33-6	R125	3400	0
Trifluoromethane	CHF_3	75-46-7	R23	0	0
R409 :	$CHClF_2$	75-45-6 2837-89-0 75-68-3	R22 (60%), R142b (25%), R124 (15%)	1700 - 620	0.5 / 0.065 / 0.02
R407c :	CH_2F_2, CF_3CHF_2, $CH2FCF_3$	75-10-5, 354-33-6, 811-97-2	R32 (21-25%), R125 (23-27%), R134a (50-54%)	650 3400 1430	0 0 0

Table 1: Summary of various refrigerant candidates.

Name	I	$-\left\langle \frac{dE}{dx} \right\rangle_{min}$	X_0	N_P
	[eV]	$\left[\text{MeV}\frac{\text{g}}{\text{cm}^2}\right]$	$\left[\frac{\text{g}}{\text{cm}^2}\right]$	$\left[\text{cm}^{-1}\right]$
R32	89.3602	1.80973	35.4581	49.2
R7146	127.401	1.67833	28.6027	92.0
R600a	47.848	2.24057	45.2260	81.0
R1234yf	91.9674	1.7734	35.8204	89.5
R152a	78.1889	1.88706	37.0969	67.1
R1234ze	91.9674	1.7734	35.8204	89.5
R115	116.695	1.69178	29.2197	98.4
R1233zd	106.689	1.73915	29.7636	105
R290	47.0151	2.26184	45.3725	65.2
R13|1	271.737	1.42486	11.5399	272
R134a	95.0294	1.76439	35.1542	81.6
R14	107.127	1.69909	33.9905	63.6
R123	125.275	1.69722	25.5416	98.4
R143a	87.8152	1.8126	35.8928	74.8
R744	88.7429	1.81124	36.1954	37.2
R23	99.9508	1.7402	34.5214	56.9
R116	105.075	1.70566	34.2947	93.3
RC318	101.578	1.71721	34.8435	123
R218	104.13	1.70873	34.439	117

Table 2: Minimum ionization, radiation length and number of primary ion pair creation for the considered refrigerants, as well as the approximated mean ionization energy used.

Refrigerant	Molecular weight	Density g/L	Boiling point degC	HMIS	Ashrae Safety Group
Material incompatibility					
Hazardous decomposition products and polymerization					
R115	154.4	6.623	-39.1	1/0/2	A1
Material is stable. However, avoid open flames and high temperatures. Incompatible with alkali or alkaline earth metals-powdered Al, Zn, Be, etc.					
Decomposition product are hazardous."FREON" 115 Fluorocarbon can be decomposed by high temperatures (open flames, glowing metal surfaces, etc.)forming hydrochloric and hydrofluoric acids, and possibly carbonyl halides. Thermal decomposition can yield toxic fumes of fluorides such as Hydrogen Fluoride, Hydrogen Chlo- ride, Carbon Monoxide and Chlorine.					
R116	138.01	5.734	-79	1/0/0	A1
May react violently with alkaline-earth and alkali metals Thermal decomposition yields toxic products which can be corrosive in the presence of moisture. If involved in a fire the following toxic and/or corrosive fumes may be produced by thermal decomposition: Carbonyl fluoride, Hydrogen fluoride, Carbon monoxide					
Thermal decomposition products: halogenated compounds, oxides of carbon					
R1233zd	130.5	6.10	-19	-	-
Incompatible with polyacrylate, Viton®, natural rubber, silicon rubber and other elastomers.					
Is considered non-toxic at less than 800 ppm[**?**]. Hazardous polymerization can occur. If involved in a fire, production under thermal decompose into pyrolysis products containing Hydrogen Fluoride, Carbon Monoxide, Carbonyl halides, and Hydrogen Chloride can occur [42].					
R1234yf	114.0	4.82	-29	0/2/2	-
Incompatible with alkali metals, Zn, Mg and other light metals.					
If involved in a fire, production under thermal decompose into pyrolysis products containing Fluorine, Carbon Monoxide, Carbonyl halides, and Hydrogen halides can occur. No toxic decomposition should happen under normal conditions.					
R1234ze	114.0	4.82	-29	1/0/0	-
Incompatible with strongly oxidizing materials and finely divided Mg and Al.					
If involved in a fire, production under thermal decompose into pyrolysis products containing Fluorine, Carbon Monoxide, Carbonyl halides, and Hydrogen halides can occur. Polymerization may also occur.					
R13I1	195.9	-	-22.5	-	-
Incompatible with active metals, fires of hydrides, and materials containing oxygen.					
Can decompose to Iodine, Hydrogen Fluoride, and Hydrogen Iodide.					
R134a	102.0	4.320[50]	-26.5	1/1/0	A1
Chemically reactive with K, Ca, powdered Al, Mg, Zn. Under high temperature/ high pressure, may react with Al surfaces.					
Under special circumstances (e.g. high temperature) Carbon monoxide, Carbonyl fluoride, Hydrogen fluoride can be produced. Under normal storage and use, no hazardous decomposition should be produced					
R14	88.0	3.65	-128	0/0/0	A1
Not compatible with aluminium, alloys containing more than 2% magnesium, alkali metals in powdered form and carbon dioxide above 1000 °C.					
If involved in a fire, production under thermal decompose into pyrolysis products containing hydrogen fluorid and carbonyl fluoride.					

Table 3: Chemical, physical and compatibility information of the refrigerants (Part 1).

Refrigerant	Molecular weight	Density g/L	Boiling point degC	HMIS	Ashare Safety Group
Material incompatibility					
Hazardous decomposition products and polymerization					
R143a	84.0	-	-47.6	-	A2
Can form explosive mixture with air. May react violently with oxidants. Air, Oxidiser. Non recommended: Hydrocarbon based lubricant, significant loss of mass by extraction or chemical reaction and Fluorocarbon based lubricant, significant loss of mass by extraction or chemical reaction.					
Thermal decomposition yields toxic products which can be corrosive in the presence of moisture.					
R125	120	1.24g/cm3	-48.5	1/1/0	A1
Under very high temperature and/or appropriate pressures freshly abraded aluminum surfaces may cause strongly exothermic reaction. Chemical reactive metals: potassium calcium powdered aluminum, magnesium and zinc.					
The product is stable. Do not mix with oxygen or air above atmospheric pressure. Any source of high temperatures, such as lighted cigarettes, flames, hot spots or welding may yield toxic and/or corrosive decomposition products.					
R22	86.45	3	-40.1	1/0/0	-
Chemically reactive metals: potassium, calcium, powdered aluminum, magnesium, and zinc, powdered metals, powdered metal salts					
Hazardous decomposition products: Halogens, halogen acids and possibly carbonyl halides. Carbon monoxide, Phosgene, Hydrogen chloride, Hydrogen fluoride, Carbonyl fluoride.					
R744	44	1.52	-78.5	1/0/0	A1
The product is stable under regular conditions					
Materials to avoid: strong oxidising agents, strong acids. Hazardous decomposition products: In combustion emits toxic fumes.					
R142b	100.5	4.18	-10	2/4/0	-
Materials to avoid: Light and/or alkaline metals, Alkaline earth metals, Powdered metals, Oxidizing agents, Chlorine, Powdered aluminum, magnesium, zinc, beryllium and their alloys.					
Hazardous decomposition products: Gaseous hydrogen fluoride (HF)., Gaseous hydrogen chloride (HCl)., Fluorophosgene, Phosgene					
R152a	66.1	2.738	-25	1/4/2	A2
Extremely reactive with oxiding materials , such as alkaline, alkaline earth metals, and other reactive chemicals, (i.e. Na, K, Ca, Mg, powdered Al, Zn), brass, and steel . Incompatible with amines, bases, and halogens.					
Under normal condition, hazardous decomposition and/or polymerization products should not be produced. If exposed to fire, hazardous products may be produced.					
R218	188.0	8.17 g/l gas	-36.7	-	A1
Stable under normal conditions materials with which gas mixture is incompatible: oxidizing materials and alkali and alkali earth metals. May react violently with chemical active metals as sodium, potassium and barium powdered magnesium, powdered aluminum and organometallics					
Thermal decomposition yields toxical products which can be corrosive in presence of moisture hazardous decomposition products: acid halides					
R23	70.0	-2.946 kg /m^3	-84.4	-	A1
Incompatible materials: metals,polystyrene, natural rubber, alloys of more than 2% magnesium in the presence of water, nitrosyl fluoride,N_2O_3, lime at dull red heat, and metals at elevated temperature					
Decomposition products: halogenated compounds, oxides of carbon, hydrogen fluoride, thermal decomposition may produce toxic fumes of fluorides. Decomposition products may include the following materials: carbon dioxide carbon monoxide halogenated compounds carbonyl halides.					

Table 4: Chemical, physical and compatibility information of the refrigerants (Part 2).

Refrigerant	Molecular weight	Density g/L	Boiling point degC	HMIS	Ashare Safety Group
Material incompatibility					
Hazardous decomposition products and polymerization					
R290	44.1	1.86	-42	1/4/0	A3
Incompatible with acids, oxygen, oxidizing materials, copper, some plastics, Chlorine Dioxide.					
Under normal condition, hazardous decomposition and/or polymerization products should not be produced . May produce carbon monoxide and other toxic gasses under thermal decomposition.					
R32	52.0	11.4	-51.7	1/4/1	A2
incompatible with acids and oxidizing materials as Na, K, Ca, Zn, Mg, powdered Al, and other active metals. Incompatible with air and moisture.					
No hazardous decomposition/polymerization should be produced under normal conditions.					
R600a	58.1	8.93	-11.7	1/4/0	A3
Incompatible with oxiding materials, halogenated hydrocarbons, halogens, and metal catalysts.					
No hazardous decomposition/polymerization should be produced under normal conditions. May produce carbon monoxide and other toxic gasses under thermal decomposition.					
R7146	146.1	6.17	-63.7	1/0/0	-
Stable with most chemical, except metals other than aluminium, stainless steel, copper brass, silver, at elevated temperatures (¿204°C). Also reacts violently with disilane.					
Decomposes into Sulfur oxides and hydrogen fluorine.					

Table 5: Chemical, physical and compatibility information of the refrigerants (Part 3).

where w_j, Z_j, A_j and I_j is the fraction by weight, atomic number, atomic weight and mean ionization energy, respectively, of the j'th constituent. The shape of the $\delta(\gamma\delta)$ function for non-conducting materials can be approximated by

$$\delta(\gamma\delta) = \begin{cases} 2(\ln 10)X - \bar{C} & \text{if } X \geq X_1; \\ 2(\ln 10)X - \bar{C} & \text{if } X_0 \leq X < X_1; \\ 0 & \text{if } X < X_0; \end{cases} \tag{5}$$

where $X = \log_{10}(\gamma\delta)$. For finding an approximate expression for the parameters $\bar{C}$, X_0 and X_1 based on experimental fits, we refer to [52]. For gases with momenta below $\beta\gamma$, the density effect correlation function can be neglected. A plot of the calculated energy loss for different refrigerants is show in figure 1.

3.2 Radiation length

The radiation length of an atom can be found by [18]

$$X_0 = 716.405(\text{cm}^{-2}\text{mol})A/\left[Z^2(L_{rad} - f(z)) + ZL'_{rad}\right] \tag{6}$$

$$f(z) = z^2 \sum_{n=1}^{\infty} \frac{1}{n(n^2+z^2)} \approx 1.202z - 1.0369z^2 + \frac{1.008z^3}{1+z} \tag{7}$$

where L_1 and L_2 is given by table 3.2, $f(z)$ is the one-photon exchange approximation, and $z = \alpha Z$, α being the fine-structure constant and Z is the atomic number.

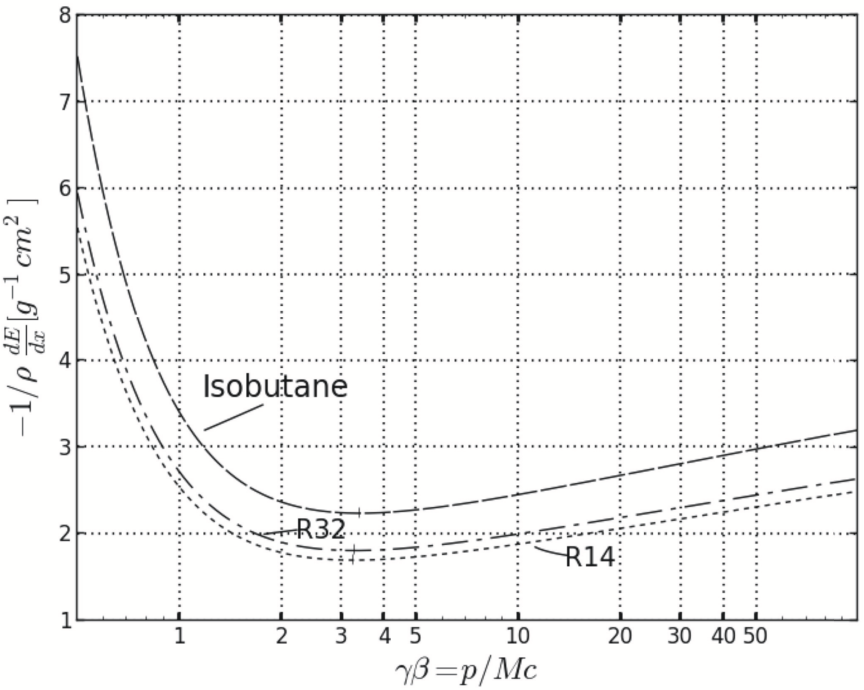


Figure 1: Energy loss as a function of the relativistic time dilation factor $\gamma\beta$ for various refrigerants.

Z	L_1	L_2
1	5.31	6.144
2	4.79	5.621
3	4.74	5.805
4	4.71	5.924
5$\geq$	$\ln(184.15Z^{-1/3})$	$\ln(1994Z^{-2/3})$

Table 6: L_1 and L_2 expressions for various atom numbers.

This formula, however, only holds for free atoms. When one wants to find the stopping power for a molecule, one has to take into account the influence from molecular bindings, crystal structures and polarization of the medium. By neglecting these effects, however, one can find an approximate expression by weighting the radiation length of the single atoms

$$\frac{1}{X_0} = \frac{1}{A_{molecule}} \sum_j \frac{A_j}{X_{0j}}, \tag{8}$$

where j reffers to the j'th atom's constituent.

3.3 Estimation of ionization pair production

In order to model the number of primary ionization caused by a single particle, the cross section for all the particle-atom interaction should be calculated. The number of primary electrons per unit length would then be the integral over energy across all the energy transfer cross sections. This is tedious work since all electron orbital transfers have to be considered. An easier, but approximate correlation between primary ionization and atom number has been found based on experimental data by [53]

$$N_P = 3.996 \frac{Z_m}{\bar{Z}^{0.4}} - 0.025 \left(\frac{Z_m}{\bar{Z}^{0.4}} \right) \text{cm}^{-1}, \tag{9}$$

which holds for normal pressure and temperature (NPT) (1 atm, 20°C). For different pressure and temperature, the number scales with the density. This value should only be taken as a rough estimation though. This formula has proven to work best for hydrocarbons and worst for molecules consisting mainly of fluorine, differing as much as 30% from the experimental value for CF_4.

The total number of ionization has proven to be more difficult to estimate. Whereas no general formula has been derived, the most straightforward method will be to use the cross sections used to calculate the primary ionization electrons, and use Monte Carlo simulations to track the production of secondary electrons from primary electrons. The total number of pair ionization turns out to be dependent on the incoming particle energy and mass, and a general expression can therefore be difficult to find. For an

incoming particle, $W = \frac{\Delta E}{N}$ defines the average energy cost to produce an ion pair. Luckily, this turns out to be a function slowly varying with particle energy[27], and can therefore be taken to be a constant in an energy interval. The total ionization per unit length can then be found by

$$N_T = \rho \frac{dE}{dx} \frac{1}{W} \tag{10}$$

If the W values for specific gases are know, the average W value for a gas mixture can be found by[53]

$$\bar{W} = \sum_m \left[f(n_m) Z(n_m) W(n_m) \right] \Big/ \sum_m \left[f(n_m) Z(n_m) \right] , \tag{11}$$

where n_m denotes the index of the molecule, and $f(n_m)$ denotes the relative number of molecules of the given sort in the mixture.

The value of W is difficult to predict, and there is not a direct way to give a proper estimate based on experimental data alone. A montecarlo simulation is in preparation which uses the photoabsorption ionization and relaxation (PAIR) model [53] and it will be the subject of a forthcoming paper.

4 Quantum chemistry calculations

In this section of the paper we describe the calculation of gas properties using the quantum chemistry calculation tool NWCHEM . The ionization energies, electron affinities and the absorption spectrums are calculated for several kinds of potential Eco-friendly gas replacements. The results are validated and compared with different methods or calculation schemes. In the last part, the problems related to the computation of the Townsend parameter and prop sects for future works are discussed.

Developments of quantum chemistry in the past few decades have improved the calculation to be accurate enough to be compared with real experiments. These calculations enable us to study gas properties from atom level, where the underlying theory is believed to be more fundamental and may therefore provide us more general descriptions of the chemical properties.

In the paper, we used the NWCHEM software [54] for computation, and the PYMOL [55] tool for visualization. The calculation determines the electronic structure of the molecule system and can provide basic information of the system like ground state energy, dipole momentum, charged density and molecular orbit. To obtain properties more suitable to be compared to experimental data, the software also provides frameworks to compute the absorption spectrum and the ionization energy.

Here we first show the basic geometrical information for interested molecules. Then we describe the procedure to calculate the absorption spectrum and in the following we present the methods to calculate the ionization energy and the electron affinity. In the end, we discussed the possibility to estimate the Townsend parameter under some certain environment of particle detectors.

4.1 Molecules and their optimized geometries

The freon gases we have been interested in are R134a (CH_2FCF_3), R152a ($C_2H_4F_2$), HFO1234ze ($CFHCHCF_3$), HFO1234yf (CH_2CFCF_3), CF_3I and HFO1233zd ($CHClCFCF_3$). Meanwhile we choose R12(CCl_2F_2) to be the standard freon gas model. CH_4 and CF_4 are the molecules we were used to make a comparison between the NWCHEM calculated results and experimental results, in order to check the reliability of NWCHEM . Fig.(2) shows the optimized ground state geometries of gas molecules, where the green balls stand for carbon atoms, the grey balls stand for hydrogen atoms, the indigo balls stand for fluorine atoms, the brown balls stand for chlorine atoms, and purple ball for iodine. Fig.(3) shows the highest occupied molecular orbitals (HOMO) of gas molecules.

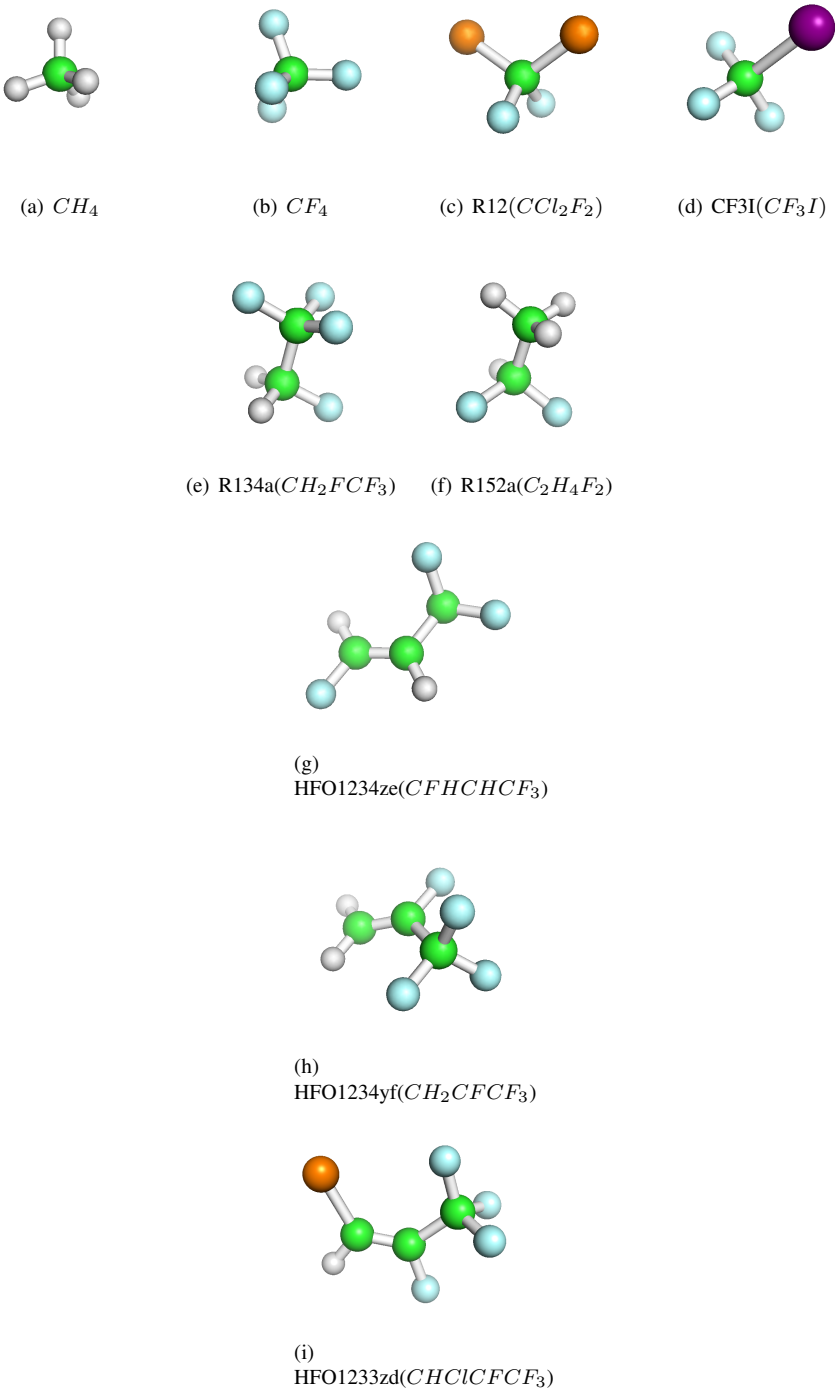
5 Calculation of absorption spectrum

The excitation energy of a molecule is one of the fundamental properties of molecular interactions one can get from experiment. To study these properties, we used the framework introduced in Ref.[56] to simulate the time-dependent response of molecules under external fields using quantum chemical calculations. The framework implemented is the Real-Time Time-Dependent Density Functional Theory (RT-TDDFT) [57] method within the NWCHEM , making it capable of doing the simulation beyond small perturbation from the ground state.

In our case, we are mostly interested in low excitations of small molecules. We therefore adopt the procedure as described in section 3 of the reference [56]. The choice of external field is δ-function-like electric field "kick"

$$\mathbf{E}(t) = \kappa \cdot exp\left[-(t-t_0)^2/2w^2\right]\hat{d}, \tag{12}$$

where t_0 is the center of pulse, w is the pulse width, which has dimensions of time, $\hat{d} = \hat{x}, \hat{y}, \hat{z}$ is the polarization of the pulse, and κ is the maximum field strength.



(a) CH_4 (b) CF_4 (c) R12(CCl_2F_2) (d) CF3I(CF_3I)

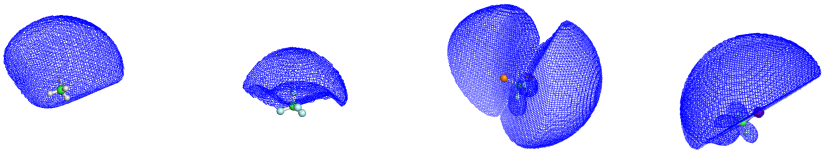
(e) R134a(CH_2FCF_3) (f) R152a($C_2H_4F_2$)

(g) HFO1234ze($CFHCHCF_3$)

(h) HFO1234yf(CH_2CFCF_3)

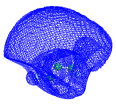
(i) HFO1233zd($CHClCFCF_3$)

Figure 2: Optimized ground state geometries of gas molecules.

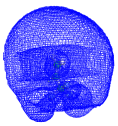


(a) CH_4 (b) CF_4 (c) R12(CCl_2F_2) (d) CF3I(CF_3I)

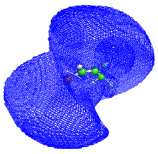
(e) R134a(CH_2FCF_3) (f) R152a($C_2H_4F_2$)



(g)
HFO1234ze($CFHCHCF_3$)



(h)
HFO1234yf(CH_2CFCF_3)



(i)
HFO1233zd($CHClCFCF_3$)

Figure 3: Highest Occupied Molecular Orbitals (HOMO) of gas molecules.

The system is then evolved in time, and the dipole moment can be calculated with respect to the added dipole coupling term

$$\mathbf{V}_{\mu\nu}^{app}(t) = -\mathbf{D}_{\mu\nu} \cdot \mathbf{E}(t), \tag{13}$$

where $\mathbf{D}$ is the transition dipole tensor of the system. Then we Fourier transform the dipole signals to construct the complex polarizability tensor $\alpha_{i,j}(\omega)$, and finally the dipole absorption spectrum is

$$S(\omega) = \frac{1}{3} Tr\left[\sigma(\omega)\right] = \frac{4\pi\omega}{3c} Tr\left[Im\left[\alpha_{i,j}(\omega)\right]\right]. \tag{14}$$

We first validate our calculation by repeating the calculation of CH_4 lowest excitation energy in Table (7) of the paper [56]. With the same basis set (6-311G) and functional (B3LYP), our calculation gives 11.16 eV excitation energy, which is consistent with the 11.13 eV in the paper. The small difference can come from other minor uncertainty sources like the choice of time separation in the simulation.

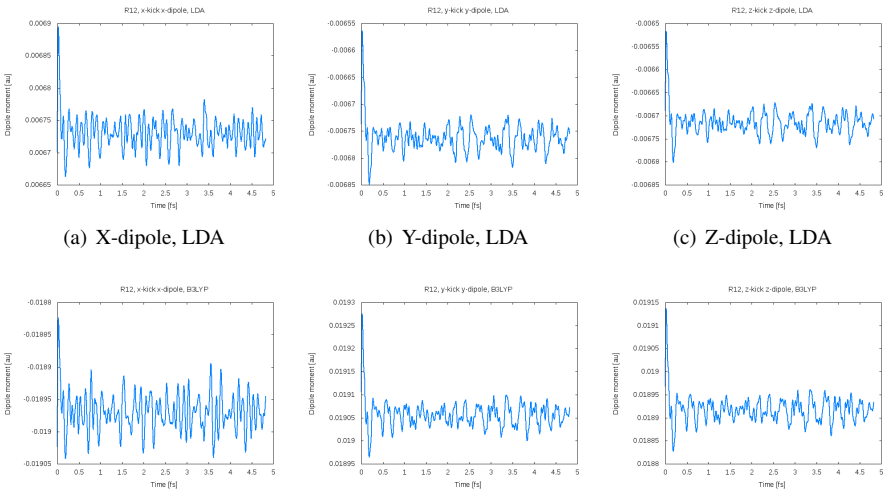
We further checked the dependence of wave function basis sets as well as density functional of our results. The dependence of basis sets is found to be much smaller than the functional one. Fig.(4) and Fig.(5) compares the results using two different functionals. As shown in the figures, although the strength varies large between the two functionals, the excitation energies are similar, especially the lowest one, which is also the same story as in the reference [56].

The same calculation is performed to gas molecules of our interest. The optical absorption spectrums are compiled in Fig.(6).

In the Fig.(7) we put together all spectra of interesting molecules. Comparing to the R12, which is one of the Freon gas spectrum, we found the similarity between molecules are in good agreement with their structures. In other words, the absorption spectrum is closer to that of R12 if the candidate molecule is similar to the R12 molecular structure.

6 Calculation of the vertical ionization energy and the electron affinity

The vertical ionization energy and the electron affinity are another two important parameters closely related to experiments. In the case of small molecules, there is a simple way to do the estimation. The Koopman's theorem states that at in closed-shell Hartree-Fock (HF) theory, the negative value of the Highest Occupied Molecular Orbital (HOMO) energy is a good approximation of to the experimental ionization energy



(a) X-dipole, LDA (b) Y-dipole, LDA (c) Z-dipole, LDA

(d) X-dipole, B3LYP (e) Y-dipole, B3LYP (f) Z-dipole, B3LYP

Figure 4: R12(CCl_2F_2) dipole moment in the 3 kicked directions, using the 6-31 G* basis and LDA (top) and B3LYP (bottom) functionals.

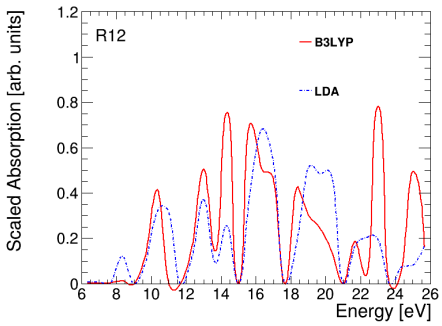
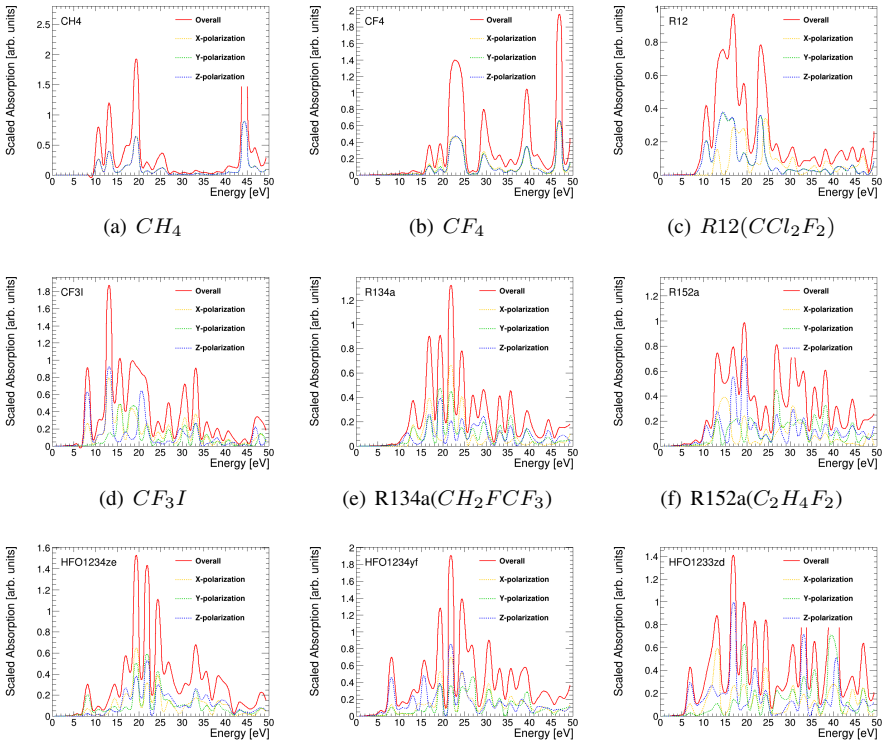


Figure 5: A comparison of R12(CCl_2F_2) absorption spectrum using different functionals.

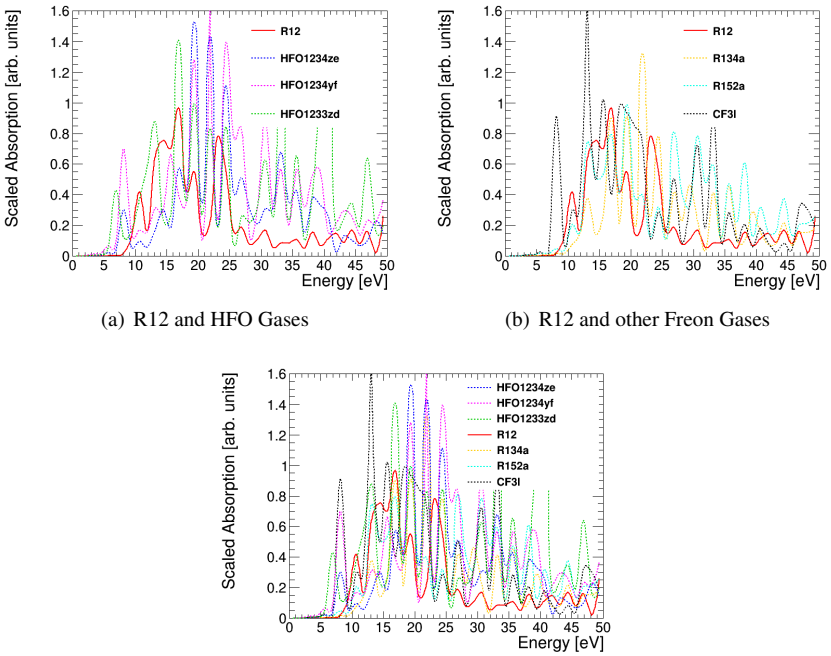


(a) CH_4 (b) CF_4 (c) $R12(CCl_2F_2)$

(d) CF_3I (e) R134a(CH_2FCF_3) (f) R152a($C_2H_4F_2$)

(g) HFO1234ze($CFHCHCF_3$) (h) HFO1234yf(CH_2CFCF_3) (i) HFO1233zd($CHClCFCF_3$)

Figure 6: Absorption spectrum of interested gas molecules. The calculation is performed in the AO basis, where the solid line corresponds to the overall dipole strength and the dashed lines correspond to polarizations in the coordinate basis directions.



(a) R12 and HFO Gases

(b) R12 and other Freon Gases

(c) All Freon Gases

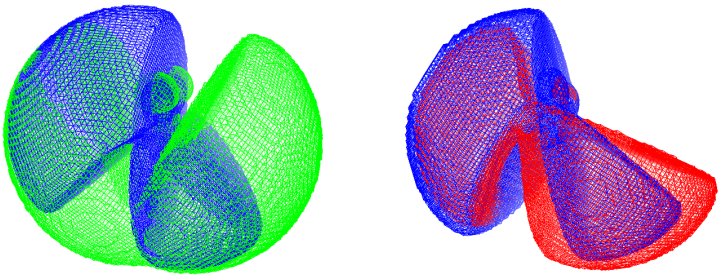
Figure 7: A comparison of absorption spectrum among molecules.

(IE). Similarly, it also suggests that the electron affinity (EA) is equal to the negative of the Lowest Unoccupied Molecular Orbital (LUMO) energy. However, the EA part of the prediction is in general not reliable because of the large effect of orbital relaxation on the LUMO eigenvalue [58, 59].

In this section, besides estimating the vertical ionization energy from the HOMO, we present a more direct way to do the calculation. In this calculation, we optimized the geometry of both the neutral gas molecule and the positive one charged ion accordingly, for the spin-Unrestricted Hartree-Fock (UHF) wave functions. Then the vertical ionization energy is calculated from the ground state energy of positively charged ion by subtracting that of the neutral molecule. The results are shown in Table.(7).

For the electron affinity calculation, we calculated the LUMO with two methods. The Hartree-Fock method, computes the closed-shell Restricted Hartree-Fock (RHF) wave functions, and the Density Functional Theory (DFT), computes the closed shell densities and Kohn-Sham orbitals in the Generalized Gradient Approximation. The results are also shown in Table.(8).

The Fig.(8) compares the HOMO (in blue) and LUMO (in green) of R12 on the left

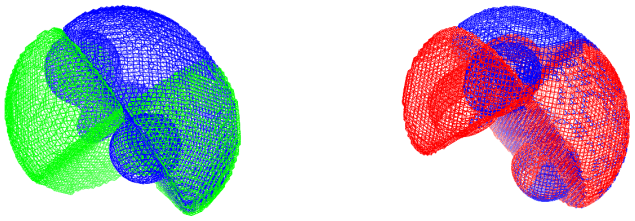


(a) R12 HOMO and LUMO (b) R12 and R12$^+$ HOMO

Figure 8: A comparison of R12(CCl_2F_2) HOMO (in blue) and LUMO (in green) for the neutral molecule (left plot) and the HOMO for neutral R12 molecule (in blue) and charged one R12 ion (in red, right plot) .

plot and the HOMO for neutral R12 molecule (in blue) and charged one R12 ion (in red) on the right plot. Similar plot for HFO1234ze is shown in Fig.(9). As can be seen from the HOMO plot, the molecular orbit between the neutral molecule and charged molecule are similar, especially for the R12, which has less atoms in the molecule. Since the Koopman's theorem will be exact when the molecular orbit for the neutral molecule and charged molecule are the same, we calculated the atom number averaged difference between our two methods, which reflect the difference of the molecular orbitals. The results are shown in Table.(8)

As the lowest excitation energy can be estimated from the energy gap between the HOMO and LUMO, we also make a comparison of these results to those obtained in the previous section. From the comparison in Table.(8), we see that, although the absolute values of the excitation energy have relatively large differences between the two approaches, the difference of the excitation energies among the molecules considered is only marginal.



(a) HFO1234ze HOMO and LUMO (b) HFO1234ze and HFO1234ze^{+} HOMO

Figure 9: A comparison of HFO1234ze($CFHCHCF_3$) HOMO (in blue) and LUMO (in green) for the neutral molecule (left plot) and the HOMO for neutral HFO1234ze molecule (in blue) and charged one HFO1234ze ion (in red, right plot) .

Molecule	GS energy Neutral [au.]	GS energy Charged [au.]	IE1 from GS [eV]	HOMO HF [au.]	HOMO DFT [au.]	IEa HF [eV]	IEb DFT [eV]	(IE1-IEm)/N [eV]
CH_4	-40.20	-39.77	11.78	-0.51	-0.52	13.99	14.21	0.46
CF_4	-435.65	-435.18	12.61	-0.57	-0.58	15.65	15.65	0.61
R12	-1150.28	-1149.90	10.24	-0.39	-0.39	10.72	10.72	0.10
R134a	-474.66	-474.21	12.40	-0.38	-0.38	10.29	10.28	0.26
R152a	-276.95	-276.55	10.78	-0.37	-0.37	10.15	10.06	0.09
CF_3I	-7222.45	-7222.10	9.62	-0.34	-0.34	9.12	9.12	0.05
HFO1234ze	-512.50	-512.16	9.34	-0.29	-0.29	7.89	7.88	0.16
HFO1234yf	-512.50	-512.16	9.37	-0.29	-0.30	7.84	8.03	0.16
HFO1233zd	-971.39	-971.05	9.23	-0.25	-0.25	6.82	6.82	0.27

Table 7: Results of ionization energy calculation. GS stands for Ground state, IE1 stands for the IE calculated from the GS difference, N stands for the number of atoms in the molecule, and IEm stands for the mean value of IEa, IEb, which are IE calculated with the HF and DFT method accordingly.

Molecule	LUMO HF [au.]	LUMO DFT [au.]	HOMO HF [au.]	HOMO DFT [au.]	EA HF [eV]	EA DFT [eV]	Lowest Excitation -(HOMO-LUMO)[eV]	Lowest Excitation Spectrum [eV]
CH_4	0.16	0.09	-0.51	-0.52	-4.40	-2.53	17.56	11.17
CF_4	0.35	0.35	-0.57	-0.58	-9.53	-9.54	25.18	17.02
R12	0.09	0.09	-0.39	-0.39	-2.32	-2.32	13.04	10.69
R134a	0.16	0.16	-0.38	-0.38	-4.45	-4.47	14.74	13.11
R152a	0.18	0.18	-0.37	-0.37	-4.93	-4.96	15.05	14.66
CF_3I	0.07	0.07	-0.34	-0.34	-1.87	-1.87	11.00	8.21
HFO1234ze	0.05	0.05	-0.29	-0.29	-1.46	-1.49	9.36	8.21
HFO1234yf	0.05	0.06	-0.29	-0.30	-1.40	-1.58	9.42	8.21
HFO1233zd	0.07	0.07	-0.25	-0.25	-1.90	-1.91	8.72	6.94

Table 8: Results of electron affinity calculation and the lowest excitation. The lowest excitation energy from the absorption for all molecules except for the CH_4, which is directly read out from the calculation, are obtained from the mean value of a Gaussian fit to the lowest peak in the spectrum.

7 Estimation of the first Townsend parameter

Following Ref. [60], we express the dependance of the first Townsend parameter α as a function of the reduced electric field E/p

$$\frac{\alpha}{p} = Ae^{-Bp/E} \tag{15}$$

where A and B are parameters depending on the gas type and electric field range, and p the gas pressure.

The reference [60] shows that the first Townsend coefficient at high reduced electric field depends almost entirely on the mean free path of the electrons. The mean free path, which is defined as

$$\lambda_m = \frac{1}{n\sigma}, \tag{16}$$

where n is the number of atoms per unit volume and σ is the total cross section for electron collision with atoms, can be calculated if the environment of gas molecule is provided. Firstly, the n is dependent on the gas pressure and can be put by hand. Secondly, the $\sigma(v)$, which is a function of electron velocity v, can be calculated from the NIST website [61]. Then, noting that at high reduced electric field, the first Townsend coefficient can be expressed as a combination of two components:

$$\begin{aligned} \alpha_1 = Ap \cdot exp\left(\frac{-Bp}{E}\right), E < E_m \\ \alpha_2 = n\sigma, E > E_m \end{aligned} \tag{17}$$

where E_m is the electric field that drifting an electron over λ_m and reach the ionization energy (I_0) of the gas. Therefore, we can estimate with two free parameters A, B, which need to be determined from experiments.

For real gases, we cannot take the free path lengths as a constant and the ionization cross section is only a fraction of the total cross section. In that case the estimation needs to be modified and use the following equation:

$$\alpha(r) = Ap \cdot exp\left(\frac{-Bp}{E(r)}\right)\left(1 - exp\left(-\frac{I_0 n\sigma}{eE(r)}\right)\right) + n\sigma_i exp\left(-\frac{I_0 n\sigma}{eE(r)}\right). \tag{18}$$

Numerous measurements of the Townsend coefficients are available for standard gas mixtures, such as those reviewed in [62].

Conclusions

Currently used F-based gases today used in HEP gas detectors are being phased out by industry and replaced by eco-friendly substitute gases. This study has reported on a general survey of industrially available replacements for HEP gases, discussed their physical properties, materials compatibility and safety issues. Parameters of interest for their use in HEP detectors have been computed following different approaches ranging from parametrizations to quantum chemical calculations: ionization energy, electronegativity, number of primary pairs. Statistical methods to compute amplification parameters of the ionization shower production such as the Townsend coefficients were investigated and preliminary results reported. Promising candidates with lower GWP are identified for further studies.

Acknowledgements

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8 Appendix - Datasheets

R125
National Refrigerants. http://www.refrigerants.com/msds/r125.pdf
Dupont http://www2.dupont.com/inclusive-innovations/en-us/sites/default/files/Pentafluoroethane%20%28R125%29%20Product%20Safety%20Summary.pdf
http://www.raprec.com/download/resources/msds/R-125%20MSDS.pdf
BOC gases https://www.boconline.co.uk/internet.lg.lg.gbr/en/images/r125410_55984.pdf
R23
Matheson trigas https://www.mathesongas.com/pdfs/msds/MAT09970.pdf
AIRGAS https://www.airgas.com/msds/001078.pdf
PRAXAIR http://www.praxair.com/ /media/North%20America/US/Documents/SDS/Halocarbon%2023%20CHF3%20Safety%20Data%20Sheet%20SDS%20P4668.ashx
Arkema http://www.lskair.com/MSDS/R23%20MSDS.pdf
National Refrigerants. http://www.refrigerants.com/msds/r23.pdf
BOC gases https://www.boconline.co.uk/internet.lg.lg.gbr/en/images/r23410_64635.pdf
Airliquid http://www.first.ethz.ch/infrastructure/Chemicals/Gases/MSDS_TriFluoroMethane.pdf
R143
Dupont http://www.raprec.com/download/resources/msds/R-143a%20MSDS.pdf
Air Liquide http://www.msds-al.co.uk/assets/file_assets/SDS_118-CLP-TRIFLUOROETHANE_R143a.pdf
Air Liquide Gas Encyclopedia http://encyclopedia.airliquide.com/encyclopedia.asp?GasID=114
Rivoira http://www.rivoiragas.it/wp-content/uploads/files/r407c%202009%20en.pdf
R14
AIRGAS https://www.airgas.com/msds/002847.pdf
PRAXAIR http://www.praxair.com/ /media/North%20America/US/Documents/SDS/Halocarbon %2014%20CF4%20Safety%20Data%20Sheet%20SDS%20P4665.ashx
Matheson trigas https://www.mathesongas.com/pdfs/msds/MAT02100.pdf
Lynde http://www.linde-gas.it/internet.lg.lg.ita/it/images/1062_R14_CF4335_68692.pdf
Air Liquide http://www.msdshazcom.com/MSDS/A/Air%20Liquide/116_AL_EN_Tetrafluoromethane%20%28R14%29.pdf
BOC gases http://www.google.ch/url?sa=t&rct=j&q=&esrc=s&source=web&cd=2&ved=0CCQQFjAB&url=http%3A%2F%2Fwww.chemicalsfinder.com%2Fdownload.php%3Ffile
%3DTVNEUy8xNTQ5M19CT0MtR2FzZXMtVUtfSGFsb2NhcmJvbi0xNF92Mi5wZGY%3D&ei=shoQVPTSHInTaPXdgfAJ&usg=AFQjCNHT1X1rbxqJpstbO8oM9G1M4wSCWg&sig2=kzAZpbdDJ6406R860FyCew
Spectra Gases Material safety data sheet http://www.spectragases.com.cn/pdfs/MSDS/pure%20gases/MSDS_Tetrafluoromethane-1028_121305.pdf
R7146
Airgas Material safety data sheet https://www.airgas.com/msds/001048.pdf
PRAXAIR safety data sheet http://www.praxair.com/ /media/North%20America/US/Documents/SDS/Sulfur%20Hexafluoride%20SF6%20Safety%20Data%20Sheet%20SDS%20P4657.ashx
Air Liquide material data sheet http://mfc.engr.arizona.edu/safety/MSDS%20FOLDER/SF6%20-%20MSDS%20Air%20Liquide.pdf
Concorde material data sheet http://www.concordegas.com/Images-%281%29/pdf/SF6-MSDS-English.aspx
AFROX material data sheet http://www.afrox.co.za/internet.global.corp.zaf/en/images/Sulphur_Hexafluoride266_27767.pdf
R407c
National Refrigerants. Material safety data sheet http://www.refrigerants.com/msds/r407c.pdf
Rivoira Material safety data sheet http://www.rivoiragas.it/wp-content/uploads/files/r407c%202009%20en.pdf
Honeywell Material safety data sheet http://msds-resource.honeywell.com/ehswww/hon/result/ result_single.jsp?P_LANGU=E&P_SYS=1&C001=
MSDS&C997=C100%3BESDS_US%2BC102%3BUS%2B1000&C100=*&C101=*&C102=*&C005=000000009894&C008=&C006=HON&C013=+
Harp Material safety data sheet http://www.harpintl.com/downloads/pdf/msds/harp-r407c-sds-clp.pdf
BOC gases Material safety data sheet https://www.boconline.co.uk/internet.lg.lg.gbr/en/images/r407c410_55995.pdf
R142b
AIRGAS Material safety data sheet https://www.airgas.com/msds/007729.pdf
National Refrigerants. Material safety data sheet http://www.refrigerants.com/msds/nri-142b.pdf
BOC gases Material safety data sheet https://www.boconline.co.uk/internet.lg.lg.gbr/en/images/r142b410_55987.pdf
Air Liquide material data sheet http://www.msds-al.co.uk/assets/file_assets/SDS_025-CLP- CHLORODIFLUOROETHANE.pdf
Solvay Chemical material data sheet http://www.solvaychemicals.us/SiteCollectionDocuments/sds/P19446-USA_CN_EN.pdf

Table 9: Gas data sheets (1).

R134a
Honeywell Material safety data sheet https://www.conncoll.edu/media/website-media/offices/ehs/ envhealthdocs/Genetron_R-134a.pdf
National Refrigerants. Material safety data sheet http://www.refrigerants.com/msds/r134a.pdf
R124
AIRGAS Material safety data sheet https://www.airgas.com/msds/001135.pdf
Arkema Material Safety Data Sheet http://www.hudsontech.com/wp-content/themes/hudson/pdfs/ msds/R-124/ARKEMA_R-124.pdf
Honeywell Material safety data sheet http://www.honeywell.com/sites/docs/doc19194b8-fb3eb4d751-3e3e4447ab3472a0c2a5e5fdc1e6517d.pdf
BOC gases Material safety data sheet https://www.boconline.co.uk/internet.lg.lg.gbr/en/images/r124410_55983.pdf
Actrol Material safety data sheet http://webcache.googleusercontent.com/search?q=cache:KUwNl9lnEIUJ:https://go.lupinsys. com/actrol/harms/public/materials/85cd6647d2c675a5fc02bf5367e562d8-published/attachments_api/997a373e34311b7c499864235208d0ef/search_api/R124_Refrigerant-MSDS.pdf+&cd=5&hl=it&ct=clnk&gl=ch&client= firefox-a
Advanced Specialty Gases Material safety data sheet http://www.advancedspecialtygases.com/pdf/R-124_MSDS.pdf
Honeywell Material safety data sheet http://www.3eonline.com/ImageServer/NewPdf/9c88917e-07a6-4217-ac6e-07efa24eabb0/9c88917e-07a6-4217-ac6e-07efa24eabb0.pdf
R123
Global Refrigerant Material safety data sheet http://www.globalrefrigerants.com.sg/docs%5Cglobal_r123_msds.pdf
National Refrigerants. Material safety data sheet http://www.refrigerants.com/msds/nri-r123.pdf
BOC gases Material safety data sheet https://www.boconline.co.uk/internet.lg.lg.gbr/en/images/r123410_55982.pdf
AFROX material data sheet http://www.afrox.co.za/internet.global.corp.zaf/en/images/R123266_27717.pdf
AIRGAS Material safety data sheet https://www.inrf.uci.edu/wordpress/wp-content/uploads/trifluoroethaneHalocarbon-r-123.pdf
Air Liquide material data sheet http://docs.airliquide.com.au/MSDSCalgaz/50106.pdf
Refrigerant inc. material data sheet http://www.refrigerantsinc.com/images/R123_MSDS.pdf
Honeywell Material safety data sheet http://msds-resource.honeywell.com/ehswww/hon/result/result_single.jsp?P_LANGU=E&P_SYS=1&C001=MSDS&C997=C100%3BESDS_US%2BC102%3BUS%2B1000&C100=*&C101=*&C102=*&C005=000000009885&C008=&C006=HON&C013=+
Honeywell Material safety data sheet http://www.3eonline.com/ImageServer/NewPdf/5cb53264-dd88-47f3-b77d-7fbff54287d7/5cb53264-dd88-47f3-b77d-7fbff54287d7.pdf
R290
National Refrigerants. Material safety data sheet http://www.refrigerants.com/MSDS/nri-R290.pdf
Kaltis Material safety data sheet http://www.kaltis.com/PDF/R290%20_Propane_%20MSDS.pdf
Global Refrigerant Material safety data sheet http://www.globalrefrigerants.com.sg/docs/global_r290_msds.pdf
Lynde Material safety data sheet http://www.lindecanada.com/internet.lg.lg.can/en/images/Propane_EN135_104332.pdf
AIRGAS Material safety data sheet https://www.airgas.com/msds/001135.pdf
AmeriGas Propane, L.P. Material safety data sheet http://www.amerigas.com/pdfs/AmeriGas-Propane-MSDS.pdf
BOC gases Material safety data sheet https://www.boconline.co.uk/internet.lg.lg.gbr/en/images/r124410_55983.pdf
Advanced Gas Technologies Material safety data sheet http://www.fieldenvironmental.com/assets/files/MSDS%20Sheets/MSDS%20Sheets%202012/4%20CarbonDioxide.pdf
AFROX material data sheet http://www.afrox.co.za/internet.global.corp.zaf/en/images/R409A266_27725.pdf
Honeywell Material safety data sheet http://www.honeywell.com/sites/docs/doc19194b8-fb3eb4d751-3e3e4447ab3472a0c2a5e5fdc1e6517d.pdf
Energas Material safety data sheet http://energas.co.uk/pdfs/013-Migweld.pdf
Calor Material safety data sheet https://www.calor.co.uk/media/wysiwyg/PDF/propane_safety_data_sheet.pdf
Unitor Material safety data sheet http://www.wilhelmsen.com/services/maritime/companies/buss/DocLit/MaterialSafety/Documents/MSDS/Refrigeration/REFRIGERANT_R_290_Italian.pdf
R125
National Refrigerants. Material safety data sheet http://www.refrigerants.com/msds/r125.pdf
Dupont Material data sheet http://www2.dupont.com/inclusive-innovations/en-us/sites/default/files/Pentafluoroethane%20%28R125%29%20Product%20Safety%20Summary.pdf
BOC gases Material safety data sheet https://www.boconline.co.uk/internet.lg.lg.gbr/en/images/r125410_55984.pdf
AFROX material data sheet http://www.afrox.co.za/internet.global.corp.zaf/en/images/NAF_S125266_27697.pdf

Table 10: Gas data sheets (2).

R218
AIRGAS http://webcache.googleusercontent.com/search?q=cache:TdB2lKIW34AJ:www.airgasrefrigerants.com
/admin/includes/doc_view.php%3FID%3D242+&cd=8&hl=it&ct=clnk&gl=ch&client=firefox-a
Spectra Gases http://www.spectragases.com.cn/pdfs/MSDS/pure%20gases/MSDS_Octafluoropropane1059_020507.pdf
BOC gases https://www.boconline.co.uk/internet.lg.lg.gbr/en/images/perfluoropropane410_64742.pdf
Tygris http://www.tygrisindustrial.com/product/static/assets/downloads/coshh/R218_5060253470215.pdf
Lynde http://msds.lindeus.com/files/msds/WPS_LIND_022_NA_MSDS_FINAL_REV_8_31_10.pdf
R318
Lynde http://msds.lindeus.com/files/msds/WPS_LIND_021_NA_MSDS_FINAL_REV_8_31_10.pdf
Matheson tri-gas http://www.nfc.umn.edu/assets/pdf/msds/octafluorocyclobutane.pdf
Spectra Gases http://www.spectragases.com.cn/pdfs/MSDS/pure%20gases/MSDS_Octafluorocyclobutane-1057_121305.pdf
Carboline http://www.google.ch/url?sa=t&rct=j&q=&esrc=s&source=web&cd=4&ved=0CDYQFjAD&url=http%3A%2F%2Fmsds.carboline.com
%2Fservlet%2FFeedFile%2F1%2Fprod%2FR318%2FBB3C031D1577B6D885257B830054E154%2FR318B1NL_2_USANSI.pdf
&ei=9lwRVO35BJPnaKW7geAO&usg=AFQjCNGHlgVYKj9–VNkldq-WxyPfMJN8g&sig2=wQ871i2BYRipK5OffyzBMw
R600a
Harp International http://www.harpintl.com/downloads%5Cpdf%5Cmsds%5CHARP-R600a-CLP.pdf
National Refrigerants. http://www.refrigerants.com/MSDS/nri-R600a.pdf
Global refrigerants http://globalrefrigerants.com.sg/docs/global_r600a_msds.pdf
Kaltis http://www.kaltis.com/PDF/R600a%20_Isobutane_%20MSDS.pdf
Frigostar Refrigerants http://www.soos.hu/WEBSET_DOWNLOADS/603/R600a_-_MSDS_EN.pdf
PRAXAIR http://www.praxair.com/ /media/North%20America/US/Documents/SDS/Isobutane%20C4H10%20Safety%20Data%20Sheet%20SDS%20P4613.ashx
A-Gas UK Limited http://www.climatecenter.co.uk/wcsstore7.00.00.749/ExtendedSitesCatalogAssetStore/images/products/AssetPush/DTP_AssetPushHighRes/std.lang.all/_h/&s/R600a_Isobutane_H&S.pdf
HFO1234ze
Honeywell http://msds-resource.honeywell.com/ehswww/hon/result/result_single.jsp?P_LANGU=E&P_SYS=1&C001=MSDS&C997=C100%3BE%2BC
101%3BSDS_US%2BC102%3BUS%2B1000&C100=*&C101=*&C102=*&C005=000000014785%20%20&C008=&C006=HON&C013=+
Harp International Material safety data sheet http://www.harpintl.com/downloads/pdf/msds/Solstice-1234ze-SDS-CLP.pdf
R13I1
Matheson tri-gas safety data sheet https://www.mathesongas.com/pdfs/msds/00229444.pdf
IODEAL Brand safety data sheet http://coupp-docdb.fnal.gov/cgi-bin/RetrieveFile?docid=163;filename=2.3%20CF3I%20MSDS.pdf;version=2
Lookchem safety data sheet http://www.lookchem.com/msds/2011-06%2F2%2F171441%282314-97-8%29.pdf
National Industrial Chemicals Notification and Assessment Scheme (NICNAS) http://www.nicnas.gov.au/__data/assets/pdf_file/0011/9101/NA334FR.PDF
AlfaAesar safety data sheet http://www.alfa.com/content/msds/british/41479.pdf
http://www.alfa.com/content/msds/british/39665.pdf
Strem Chemicals, Inc safety data sheet http://www.strem.com/catalog/msds/09-7680
Pfaltz - Bauer safety data sheet https://www.pfaltzandbauer.com/MSDS/T23585%20%20SDS%20%20051613.PDF
HFO1233zd
Honeywell safety data sheet http://www.ozoneprogram.ru/upload/files/2/2013_honeywell.pdf
HFO1234yf
Honeywell http://msds-resource.honeywell.com/ehswww/hon/result/result_single.jsp?P_LANGU=E&P_SYS=1&C001=MSDS&C997
=C100;E%2BC101;SDS_US%2BC102;US%2B1000&C100=*&C101=*&C102=*&C005=000000011078&C008&C006=HON&C013
http://www.idsrefrigeration.co.uk/docs/Solstice%20yf%20MSDS%20version%203.2.pdf
Harp International Material safety data sheet http://www.harpintl.com/downloads/pdf/msds/harp-hfo-1234yf-clp.pdf
BOC gases Material safety data sheet https://www.boconline.co.uk/internet.lg.lg.gbr/en/images/tetrafluoropropene-r1234yf-sg-155410_90007.pdf
National Refrigerants Material safety data sheet http://www.nationalref.com/pdf/19%20SDSR1234yf.pdf
Gerling Holz+co Material safety data sheet http://www.ghc.de/media/en/downloads/msds/0070.pdf
Friedrichs Kä%ltemittel Gmbh http://www.friedrichs-kaeltemittel.de/download/deutsch/kaeltemittel/r1234yf/ENG%20-%20R1234yf-2013-08-09%20-%20Friedrichs%20Kaeltemittel.pdf

Table 11: Gas data sheets (3).

R116
Matheson tri-gas safety data sheet https://www.mathesongas.com/pdfs/msds/MAT10860.pdf
PRAXAIR safety data sheet http://www.praxair.com/ /media/North%20America/US/Documents/SDS/Halocarbon%20116%20C2F6%20Safety%20Data%20Sheet%20SDS%20P4670.ashx
HYNOTE GAS safety data sheet http://www.uacj.mx/IIT/CICTA/Documents/Gases/Hexafluoroethane.pdf
Spectra Gases Material safety data sheet http://www.spectragases.com.cn/pdfs/MSDS/pure%20gases/MSDS_Hexafluoroethane-1058_092605.pdf
BOC gases Material safety data sheet https://www.boconline.co.uk/internet.lg.lg.gbr/en/images/sg_064_hexafluoroethane_r116410_64639.pdf
National Refrigerants Material safety data sheet http://www.refrigerants.com/msds/r116.pdf
AIRGAS Material safety data sheet https://www.airgas.com/msds/001053.pdf
Dupont Material data sheet http://www.raprec.com/download/resources/msds/R-116%20MSDS.pdf
Air Products and Chemicals,Inc Material data sheet http://cleanroom.ien.gatech.edu/media/uploads/msds/350.pdf
PRAXAIR Material safety data sheet http://www.praxair.com/ /media/North%20America/US/Documents/SDS/Halocarbon%20116%20C2F6%20Safety%20Data%20Sheet%20SDS%20P4670.ashx
SPECIALTY CHEMICAL PRODUCT Material data sheet http://www.chemadvisor.com/Matheson/database/msds/00232361000800003.PDF
R32
National Refrigerants Material safety data sheet http://www.refrigerants.com/msds/nri-r32.pdf
BOC gases Material safety data sheet https://www.boconline.co.uk/internet.lg.lg.gbr/en/images/sg_152-r32-difluoromethane-v1.51410_39651.pdf
AIRGAS Material safety data sheet https://www.airgas.com/msds/001054.pdf
Spectra Gases Material safety data sheet http://www.spectragases.com.cn/pdfs/MSDS/pure%20gases/MSDS_Difluoromethane-1029_121305.pdf
Matheson tri-gas safety data sheet https://www.mathesongas.com/pdfs/msds/MAT14937.pdf
Harp International Material safety data sheet http://www.harpintl.com/downloads/pdf/msds/harp-r410a-sds-clp.pdf
Dupont Material data sheet http://www2.dupont.com/inclusive-innovations/en-us/sites/default/files/Difluoromethane%20%28R32%29%20Product%20Safety%20Summary.pdf
R115
National Refrigerants Material safety data sheet http://www.refrigerants.com/msds/nri-r115.pdf
AIRGAS Material safety data sheet https://www.airgas.com/msds/009900.pdf
Air Liquide material data sheet http://www.msds-al.co.uk/assets/file_assets/SDS_030-CLP-CHLOROPENTAFLUOROETHANE.pdf
Dupont Material data sheet http://www.raprec.com/download/resources/msds/R-115%20MSDS.pdf
Zep Inc. Material data sheet http://www.zepprofessional.com/msds/eng/R115_ENG_USA.pdf
PRAXAIR Material safety data sheet http://www.praxair.ca/ /media/North%20America/Canada/Documents%20en/Safety%20Data%20Sheets%20en/Halocarbon%20115%20SDS%20E4669.ashx
Apolllo Scientific Limited Material safety data sheet http://www.apolloscientific.co.uk/downloads/msds/PC2020_msds.pdf
Matheson tri-gas safety data sheet https://www.mathesongas.com/pdfs/msds/MAT04810.pdf

Table 12: Gas data sheets (5).

R22
National Refrigerants Material safety data sheet http://www.refrigerants.com/msds/r22.pdf
BOC gases Material safety data sheet https://www.boconline.co.uk/internet.lg.lg.gbr/en/images/sg-027-r22-chlorodifluoromethane-v1.3410_39623.pdf
Harp International Material safety data sheet http://www.harpintl.com/downloads/pdf/msds/HARP-R22-SDS-CLP.pdf
AIRGAS Material safety data sheet https://www.airgas.com/msds/001016.pdf
Remtec Material safety data sheet http://www.remtec.net/docs/msds-r-22-remtec.pdf
AFROX material data sheet http://www.afrox.co.za/internet.global.corp.zaf/en/images/R22266_27716.pdf
Gasco material data sheet http://site.jjstech.com/pdf/Gasco/MSDS-Freon-R22-in-Air.pdf
Dupont Material data sheet http://www.pchetz.com/_Uploads/dbsAttachedFiles/freon22msds.pdf
SRF LIMITED Material data sheet http://www.siggases.com/images/products/MSDS-%20FLORON%20R22.pdf
Lynde Material data sheet http://msds.lindeus.com/files/msds/WPS_LIND_011_CHLORODIFLUOROMETHANE_%28Halocarbon_R22%29_NA_MSDS_FINAL_REV_8_25_10.pdf
Unitor Material data sheet http://www.wilhelmsen.com/services/maritime/companies/buss/DocLit/MaterialSafety/Documents/MSDS/Refrigeration/UNICOOL_R_22_English.pdf
A-GAS Material data sheet http://www.airefrig.com.au/file/msds/Agas_R22_MSDS_100708.pdf
Technical Chemical Company Material data sheet http://www.technicalchemical.com/msds/6230.pdf
Praxair Material data sheet http://www.praxair.com/ /media/North%20America/US/Documents/SDS/Halocarbon%2022%20CHCIF2%20Safety%20Data%20Sheet%20SDS%20P4667.ashx
Refron Material data sheet http://www.acsrefrigerant.com/pdf/REFRON_MSDS_R-22.pdf
Honeywell Material data sheet http://www.honeywell.com/sites/docs/doc19194b8-fb3eb861e4-3e3e4447ab3472a0c2a5e5fdc1e6517d.pdf
Patton LTD Material data sheet http://www.pattonnz.com/pdf/MSDS/MSDS_2013/Refrigerants/Refrigerant%20R22%20-%20MSDS.pdf
Coregas PTY LTD Material data sheet http://www.bjhowes.com.au/R22%20-%20CHLORODIFLUOROMETHANE%20REFRIGERANT%20GAS%5B1%5D.pdf
R152
Dupont Material data sheet http://www.raprec.com/download/resources/msds/R-152a%20MSDS.pdf
BOC gases Material safety data sheet https://www.boconline.co.uk/internet.lg.lg.gbr/en/images/sg-045-r152a-11-difluoroethane-v1.3410_39625.pdf
National Refrigerants Material safety data sheet http://www.refrigerants.com/msds/r152a.pdf
Electron Microscopy Sciences Material safety data sheet http://www.emsdiasum.com/microscopy/technical/msds/70837.pdf
Matheson tri-gas safety data sheet https://www.mathesongas.com/pdfs/msds/MAT26280.pdf
Lynde Material safety data sheet http://www.abellolinde.es/internet.lg.lg.esp/en/images/Gas%20Refrigerante%20R152a_FDS_7071_01_00FDS_SG_045_01_00302_89373.pdf
Air liquide Material safety data sheet http://www.msds-al.co.uk/assets/file_assets/SDS_045-CLP-DIFLUOROETHANE.pdf
AIRGAS Material safety data sheet https://www.airgas.com/msds/001029.pdf
SIDS Initial Assessment Report For SIAM 22 Paris, France, 18-21 April 2006 http://www.chem.unep.ch/irptc/sids/OECDSIDS/75376.pdf

Table 13: Gas data sheets (6).

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