Gas search for neutrino-hydrogen interactions with DUNE HPgTPC

– updated version (see **UPDATE** tag)

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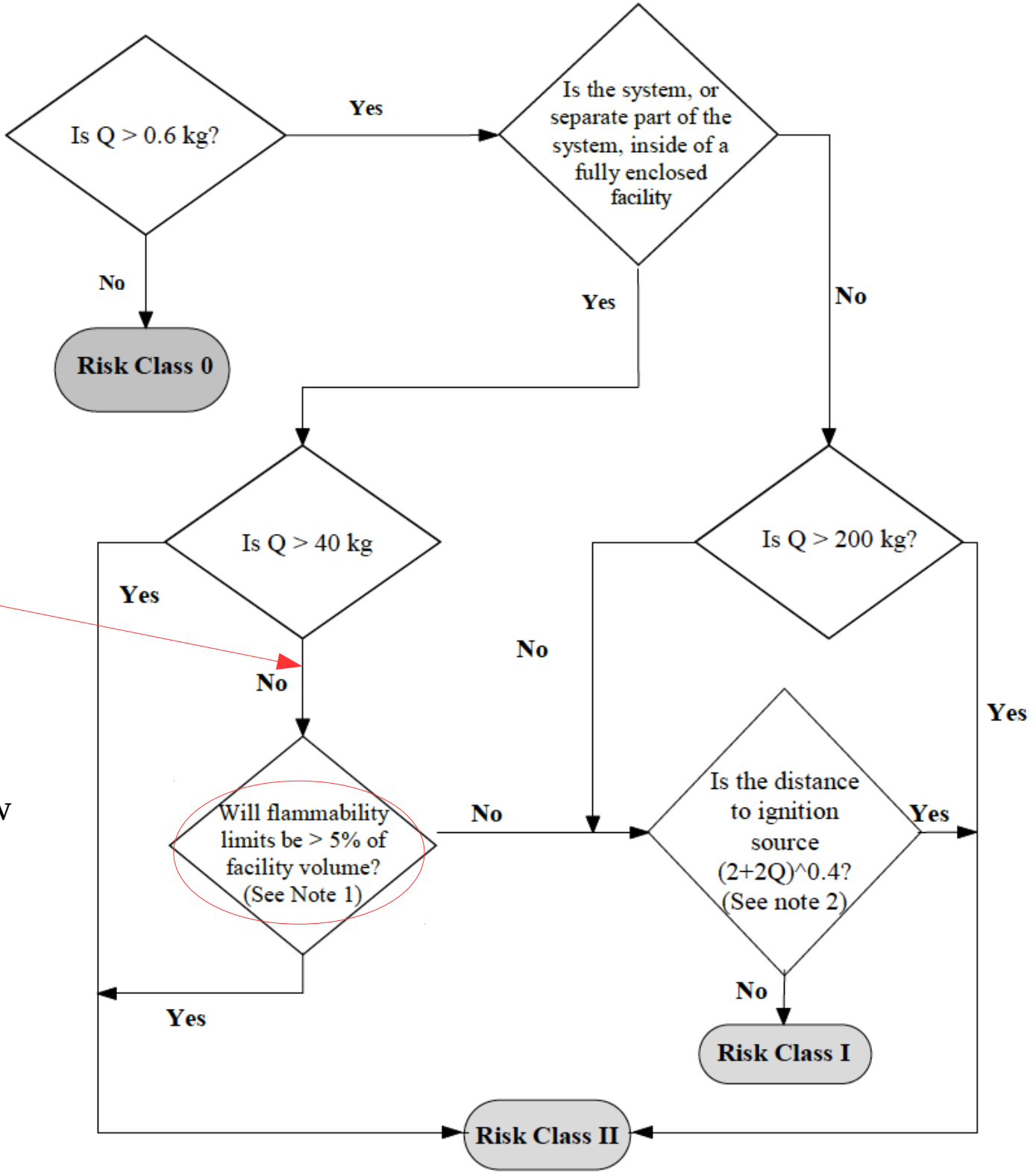
*with input from Diego Diaz and Philip Hamacher-Baumann

Recap

FESHM 6020.3

	100m^3 vol. allowed percentage
H2	49.22%
CH4	15.76%
C2H6	8.94%
C3H8	6.27%
iC4H10	4.47%
D2	49.26%



Interestingly, we can now proceed to next level...

Example 1

Two 81 SCF cylinders of a 50-50 mixture (by volume) of argon-ethane (Fermilab stock catalog number 1980-1095) will be used in a room whose volume is 9*15*20 ft^3 (2700 ft^3). This room, inside a larger building, contains no obvious fire hazards such as welding operations. The gas is to be supplied to drift chambers. First, to determine Q, it is recognized that only 40.5 SCF of a given cylinder is ethane. Thus, from Appendix 3 and Appendix 4;

$$Q = 2*40.5\ ft^3 *0.028(m^3/ft^3)*1.26(kg/m^3)*0.36(H_2\ equivalence\ factor)$$

$$Q = 1.03\ kg\ hydrogen\ equivalent\ inventory$$

Thus by box 1 in the flowchart, we exceed the limit for Risk Class 0 and must go to box 2. Continuing to box 2, we find the answer to be yes but the answer to the question in box 3 is negative. Doing the calculation prescribed in box 4 we find that 5% of 2700 ft^3 is 135 ft^3. Dividing 81/135 finds a maximum concentration of 60 %, which exceeds the flammability upper limit. Thus, any concentration below this limit is reachable with the available inventory, since no inventory controls have been specified. Therefore the answer to this question is affirmative and the Risk Class is II. If only a single cylinder was needed, the Ø.5 kg hydrogen equivalence would have rendered a Risk Class 0 determination.

Recap UPDATE

FESHM 6020.3 example

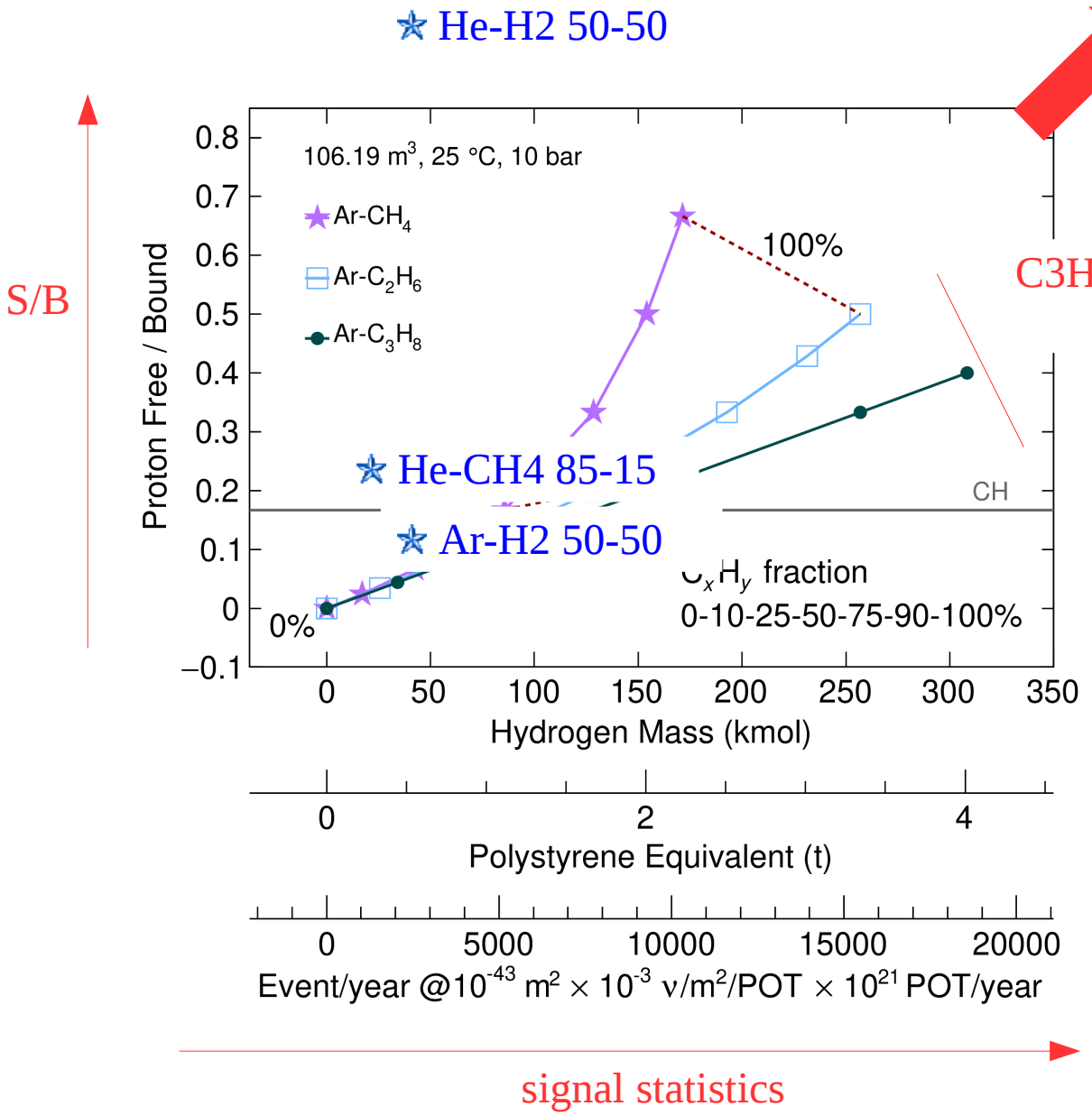
	flammability upper limit in % (from FESHM 6020.3 p17)	minimal facility volume (m^3) = gas volume at 1 bar/upper flam limit/5%
H2	75	1.31E+04
CH4	15	2.10E+04
C2H6	12.5	1.43E+04
C3H8	9.5	1.32E+04
D2	75	1.31E+04

Minimal facility volume at maximal allowed mass

Just match the current hall size 1.3E4 m^3

Very large due to the small upper limit

Recap

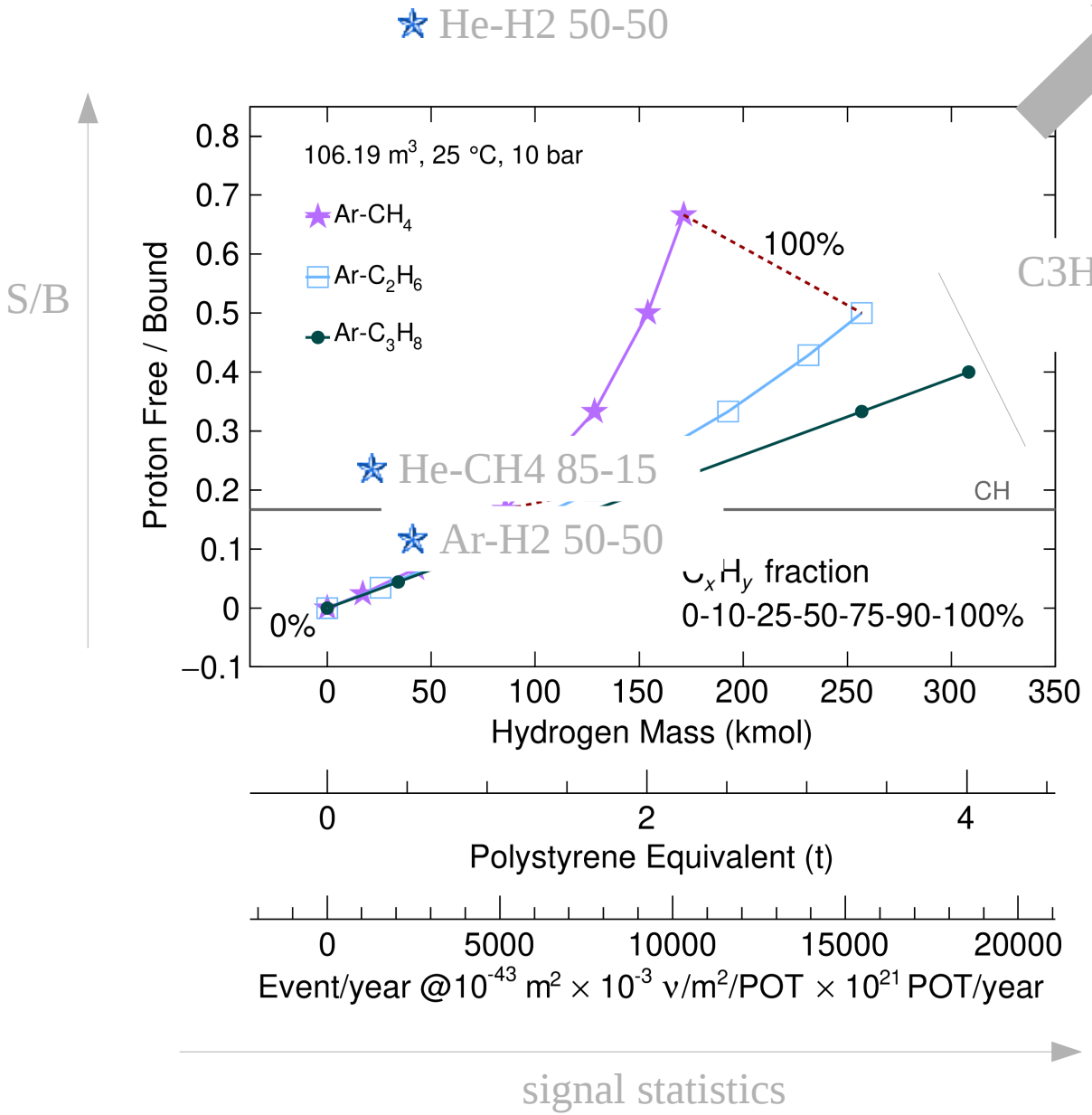


1) He-H2 50-50: proton free/bound ratio is 1, rate = 25%CH4, i.e. 0.5 t of polystyrene, giving 2.5k event/year.

2) Ar-H2 50-50: the rate is the same as 1), but the purity is lower with proton free/bound ratio 0.1, lower than P-50 (or CH, 0.16)

3) He-CH4 85-15: this is also allowed. The H event rate is 60% of 1). The proton free/bound ratio is 0.23, higher than P-50 or CH.

Introduce **H-index** = f/b * #H



Purpose of this talk:

- Discussion gas search strategy and possible candidates for nu-H program

Maximal hydrogen event rate with alkane

UPDATE

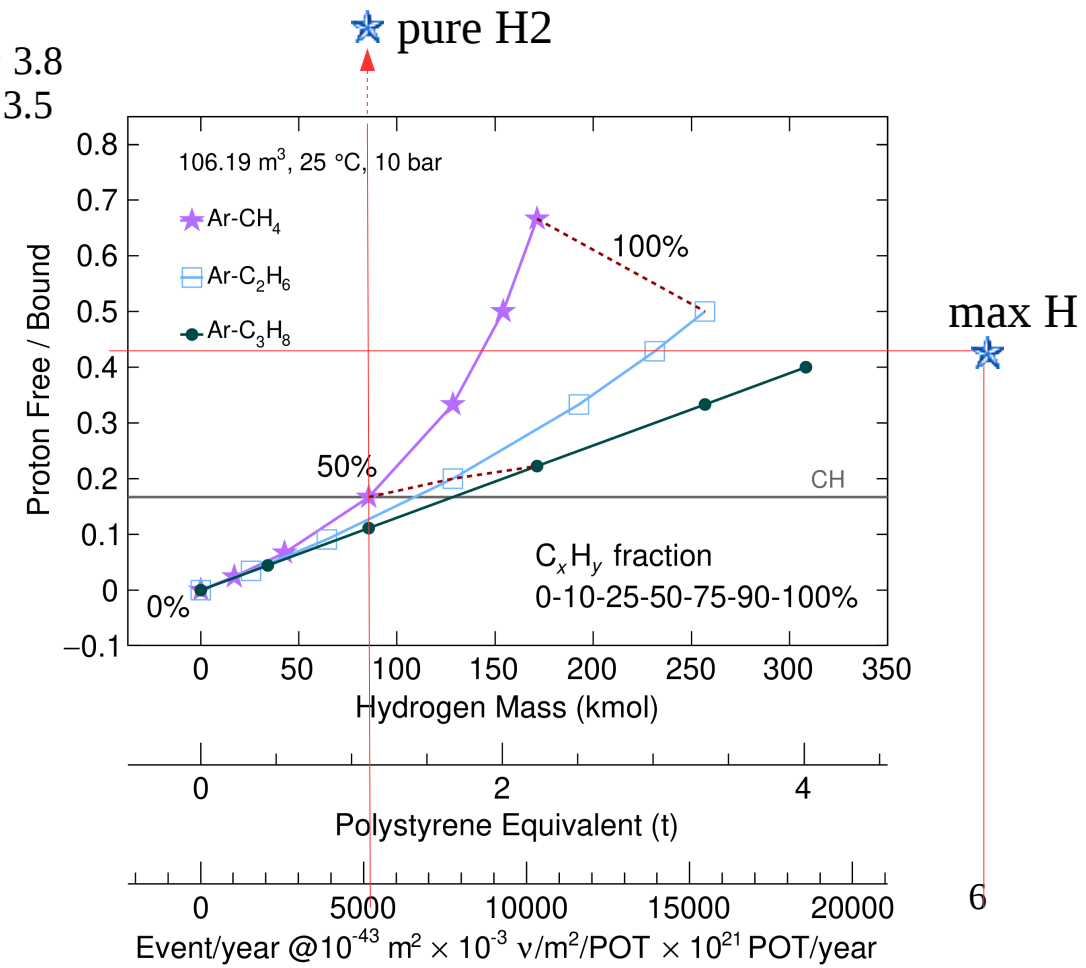
- CnH2n+2: most efficient hydrogen carrier
  - ✓ Large n → high H event rate
  - ✗ Large n → low vapor pressure
    - from propane (C3) on can't get to 10bar, last gas at 1bar is neopentane (C5)
- **Maximal H** achieved by towering partial pressure in 10bar :

  ~~17% neopentane (C5) + 35% isobutane (C4) + (1-17%-35%=) 48% propane (C3)~~ = C3.7H9.4
  - ~~f/b: 0.42, **H-index: 4.0**~~

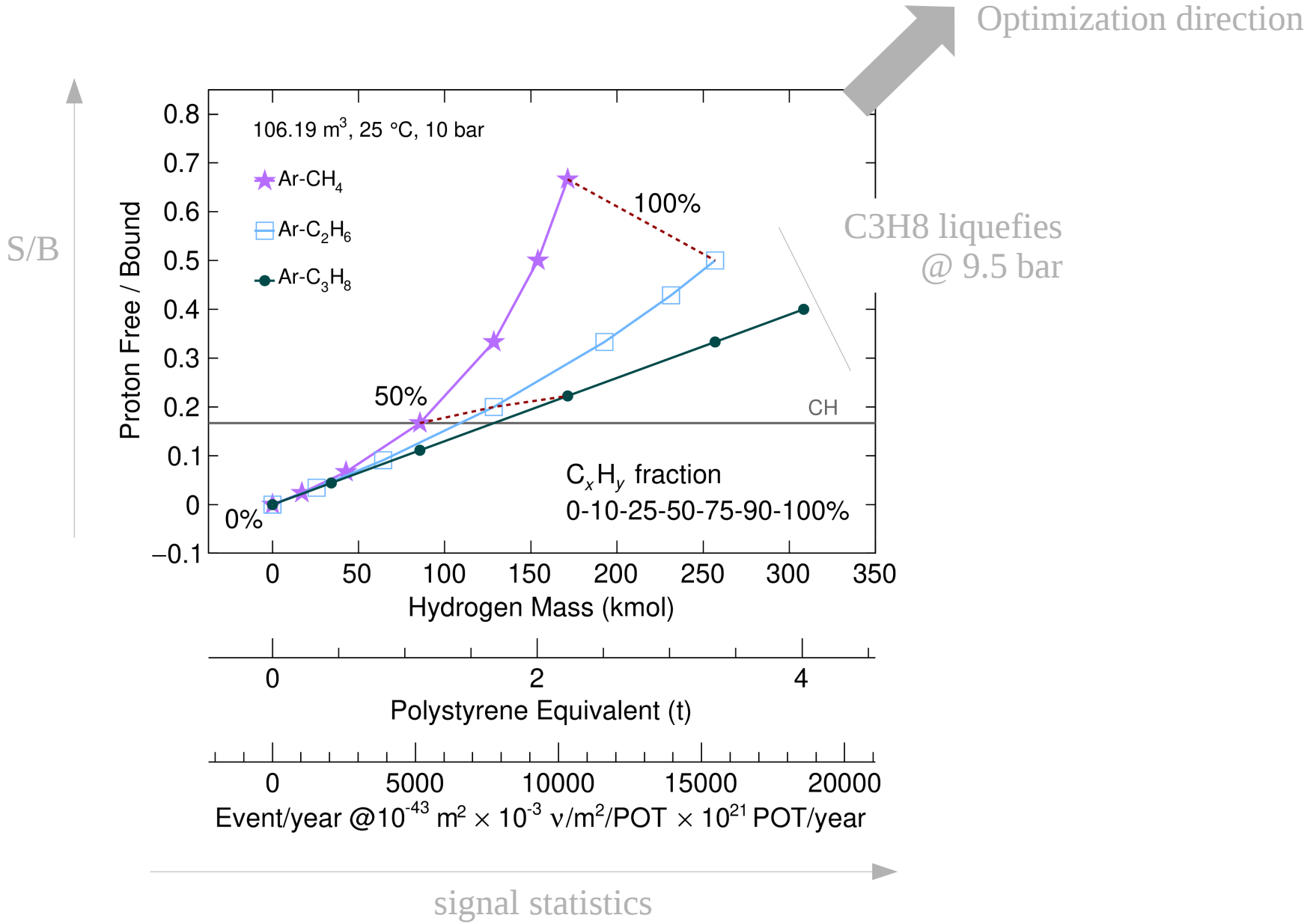
  1) 17% neopentane (C5) + 35% isobutane (C4) + 24% butane (C4) + (1-17%-35%-24%=) 24% propane (C3) = C3.9H9.9
     - f/b: 0.42, **H-index: 4.1**
  2) Other "towering":
     - 35% C4 + 65% C3 = C3.4H8.7, f/b: 0.43, H-index: 3.8
     - 95% C3 + 5% C2 = C3.0H7.9, f/b: 0.44, H-index: 3.5
- Corresponding **maximal event rate: ~25k/year**

	v.p. 25C (bar)	H-index= f/b * #H
C5H12, Neope	1.72	4.80
C5H12, isopar	0.92	4.80
iC4H10, CH(C	3.51	4.17
C4H10, butan	2.43	4.17
C3H8	9.52	3.56
C2H6	41.90	3.00
CH4	superc	2.67

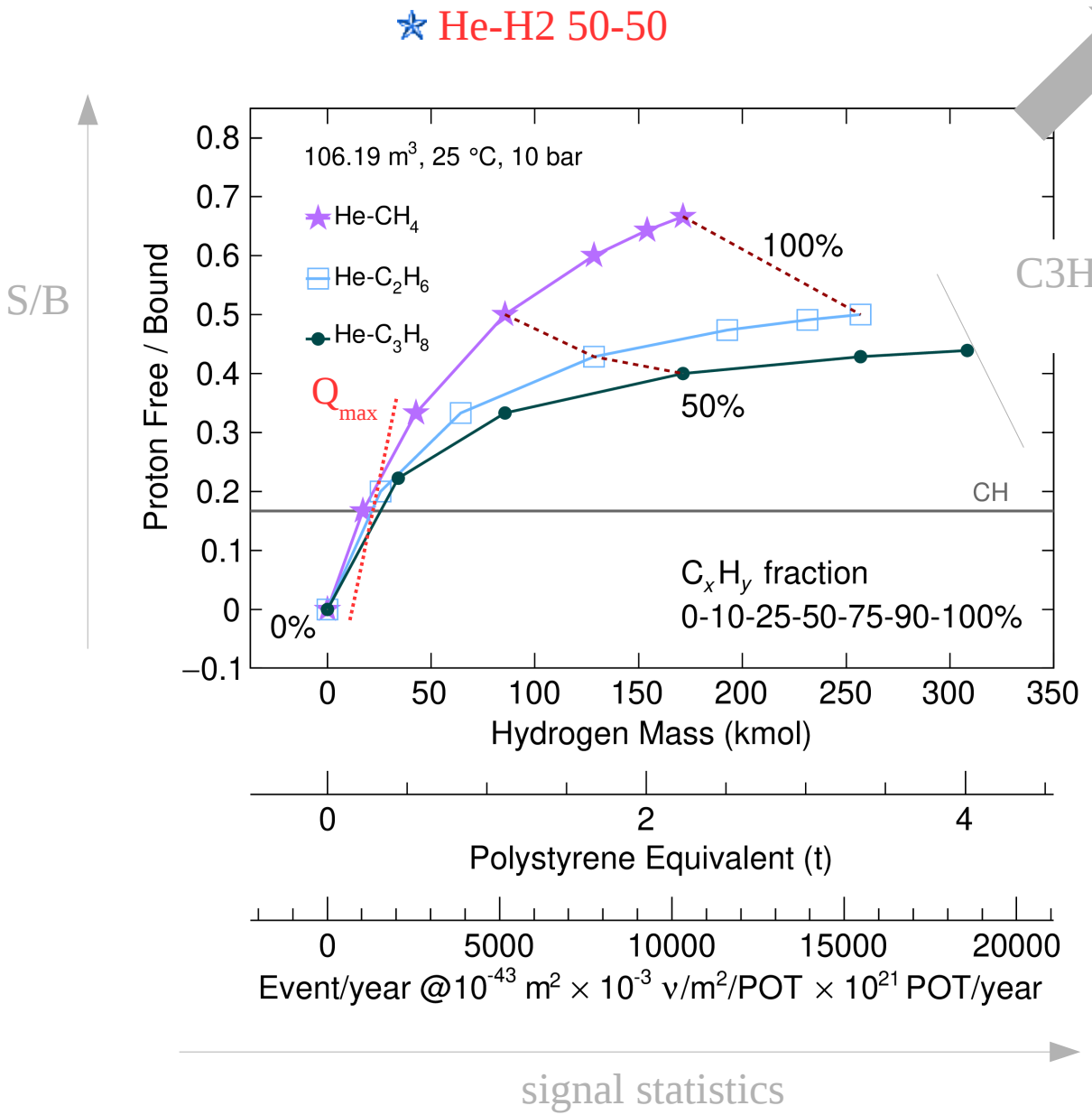
max H



Recap


Optimization direction
S/B
106.19 m^3, 25 °C, 10 bar
Ar-CH$_4$
Ar-C$_2$H$_6$
Ar-C$_3$H$_8$
100%
50%
0%
CH
C$_x$H$_y$ fraction
0-10-25-50-75-90-100%
Proton Free / Bound
Hydrogen Mass (kmol)
Polystyrene Equivalent (t)
Event/year @10^{-43} m^2 × 10^{-3} ν/m^2/POT × 10^{21} POT/year
C3H8 liquefies
@ 9.5 bar
signal statistics

He-base mixtures



C3H8 liquefies @ 9.5 bar

With He, the purity goes up very quickly at low alkane fraction.

The event rate is limited by Q_{max}.

Search for H-rich non-flammable gas

Safety Classification of Refrigerants[47]

Flammability in Air @ 60 °C & 101.3 kPa	**ASHRAE 34 Safety group**	
Higher Flammability LFL or $ETFL_{60}$ = 100 g/m^3 OR HOC = 19 MJ/kg[48]	A3	B3
Lower Flammability LFL or $ETFL_{60}$ > 100 g/m^3 & HOC < 19 MJ/kg[48]	A2	B2
Lower Flammability LFL or $ETFL_{60}$ > 100 g/m^3 & HOC < 19 MJ/kg[48] with a maximum burning velocity of = 10 cm/s	A2L	B2L
No flame Propagation	A1	B1
Flammability in Air @ 60 °C & 101.3 kPa	**Lower Toxicity OEL ≥ 400 ppm**[25]	**Higher Toxicity OEL < 400 ppm**[25]

LFL = Lower Flammability Limit

$ETFL_{60}$ = Elevated Temperature Flame Limit @ 60 °C

HOC = Heat Of Combustion

https://en.wikipedia.org/wiki/List_of_refrigerants

ASHRAE 34 Safety group

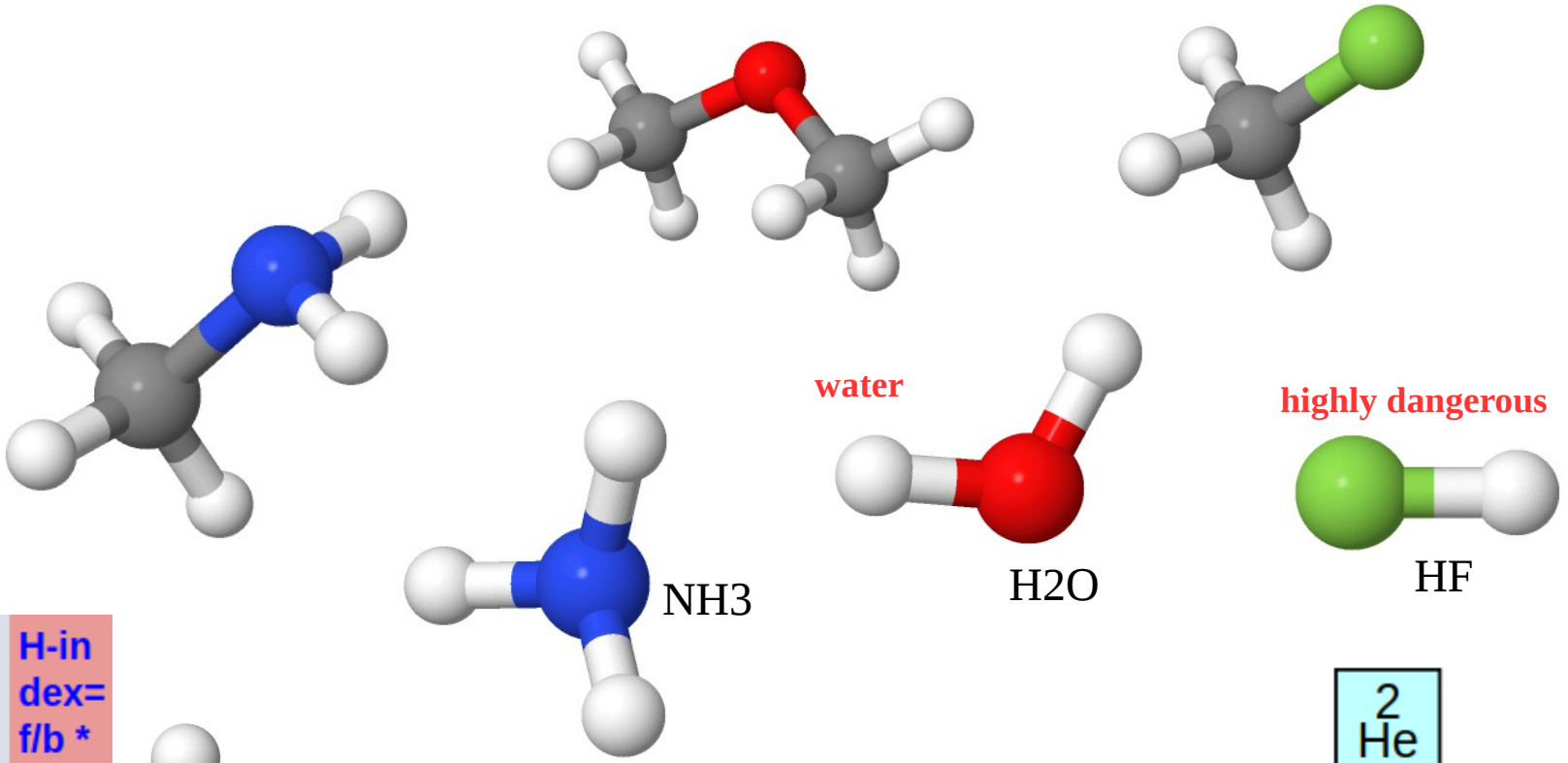
(ASH-ray) American Society of Heating, Refrigerating and Air-Conditioning Engineers

A3: H2 and all alkane
(all LFL <= 5%, see later slides)

LFL is an important parameter in safety, but not considered in FESHM 6020.3

In mixture
`x% flammable A + (1-x%) non-fl. B`
if x < LFL, the mixture is non-flammable (assuming A and B stay together if leaked, namely both have similar density)

Search for H-rich non-flammable gas



water

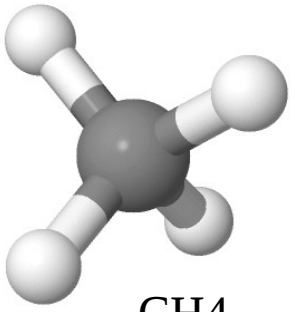
highly dangerous

NH3

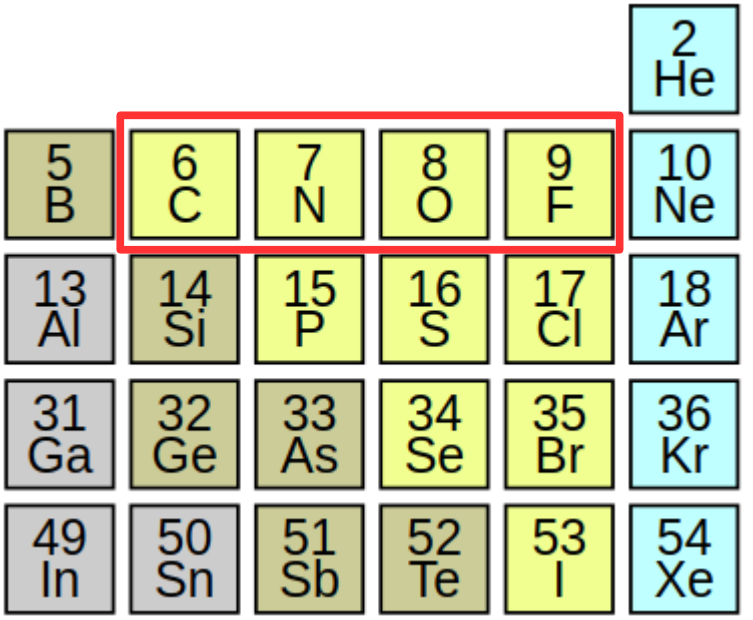
H2O

HF

	v.p. 25C (bar)	H-index= f/b * #H
C5H12, Neope	1.72	4.80
C5H12, isopar	0.92	4.80
iC4H10, CH(C	3.51	4.17
C4H10, butan	2.43	4.17
C3H8	9.52	3.56
C2H6	41.90	3.00
CH4	superc	2.67



CH4
H-index: 2.7
16%@Q_{max}



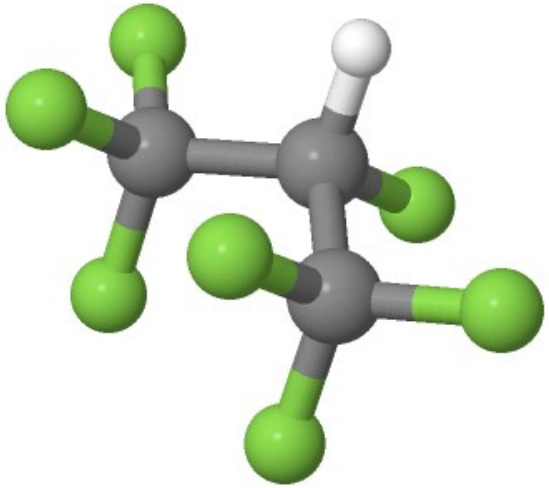
https://chemapps.stolaf.edu/jmol

Search for H-rich non-flammable gas: HFC (in collaboration with Diego)

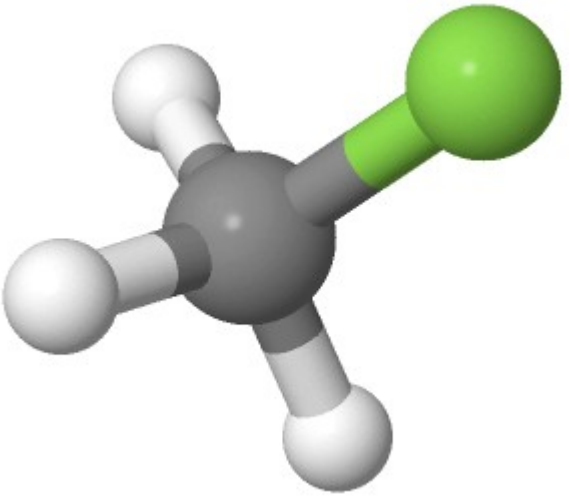
- Check the industry of refrigerants

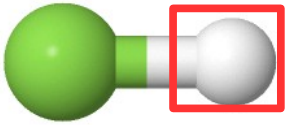
https://en.wikipedia.org/wiki/List_of_refrigerants

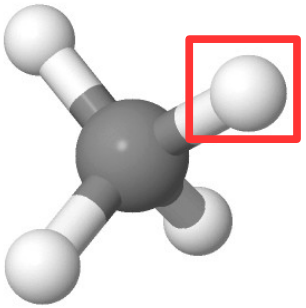
C3HF7 1,1,1,2,3,3,3-Heptafluoropropane

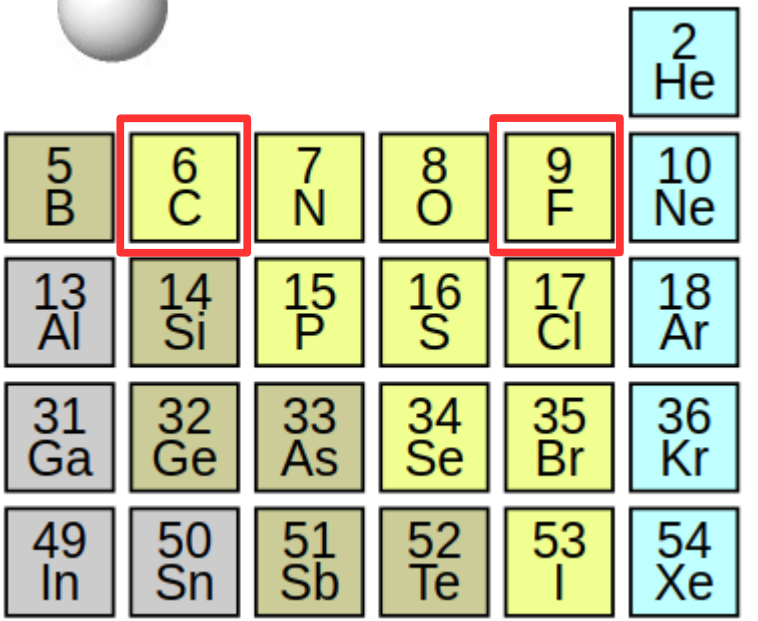


CH3F Fluoromethane









https://chemapps.stolaf.edu/jmol

Search for H-rich non-flammable gas: HFC (in collaboration with Diego)

Vol. % at Q_{max}

	code name: HFC-, R-		v.p. 25C (bar)	allowed percentage	ASHRAE 34 Safety group	flammablility lower limit %	fraction of Q at LFL	flammability upper limit in	H-index= f/b * #H
CH		H2	superc	49.2%	A3	4	8%	75	999.0
		C5H12, Neopentane, C(CH3)4, 2,2-Dimethy	1.72	3.8%	A3?	1.4	36%	7.5	4.80
		C5H12, isopantane, (CH3)2CHCH2CH3	0.92	0.0%	A3	1.4	7376%	8.3	4.80
	600a	iC4H10, CH(CH3)2CH3	3.51	4.5%	A3	1.8	40%	8.4	4.17
		C4H10, butane	2.43	4.7%	A3	1.8	38%	8.5	4.17
		C3H8	9.52	6.3%	A3	2.1	33%	9.5	3.56
		C2H6	41.90	8.9%	A3	3	34%	12.5	3.00
		CH4	superc	15.8%	A3	5	32%	15	2.67
HFC*	152a	C2H4F2 1,1-Difluoroethane	5.96	12.8%	A2	3.7	29%	18	0.53
	143a	C2H3F3 1,1,1-Trifluoroethane	12.62	16.0%	A2L	7	44%	17	0.23
	32	CH2F2 Difluoromethane	17.31	28.4%	A2L	13	46%	33	0.17
	245fa	C3H3F5, 1,1,1,3,3-Pentafluoropropane	1.48		B1				0.14
	134a	C2H2F4 1,1,1,2-Tetrafluoroethane, Norflurar	6.65		A1			x	0.08
	1234ze	C3H2F4, 1,3,3,3-Tetrafluoropropene	7.00	#DIV/0!	A2L	x	#DIV/0!	x	0.07
	1234yf	C3H2F4 2,3,3,3-Tetrafluoropropene	0.06	#VALUE	A2L		#VALUE!		0.07
	236fa	C3H2F6, 1,1,1,3,3,3-Hexafluoropropane	2.72		A1				0.06
	23	CHF3 Fluoroform	45.98		A1			35.3	0.03
	125	C2HF5 Pentafluoroethane	13.90		A1			x	0.02
	227ea	C3HF7, 1,1,1,2,3,3,3-Heptafluoropropane	4.55		A1				0.01

*less common ones in BACKUP

A1, B1: non-flammable
A2(L): low flammability

Search for H-rich non-flammable gas: HFC (in collaboration with Diego)

	code name: HFC-, R-		v.p. 25C (bar)	allowed percentage	ASHRAE 34 Safety group	flammablility lower limit %	fraction of Q at LFL	flammability upper limit in	H-index= f/b * #H
		H2	superc	49.2%	A3	4	8%	75	999.0
		C5H12, Neopentane, C(CH3)4, 2,2-Dimethy	1.72	3.8%	A3?	1.4	36%	7.5	4.80
		C5H12, isopantane, (CH3)2CHCH2CH3	0.92	0.0%	A3	1.4	7376%	8.3	4.80
CH	600a	iC4H10, CH(CH3)2CH3	3.51	4.5%	A3	1.8	40%	8.4	4.17
CH		C4H10, butane	2.43	4.7%	A3	1.8	38%	8.5	4.17
CH		C3H8	9.52	6.3%	A3	2.1	33%	9.5	3.56
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HFC*	152a	C2H4F2 1,1-Difluoroethane	5.96	12.8%	A2	3.7	29%	18	0.53
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HFC*	32	CH2F2 Difluoromethane	17.31	28.4%	A2L	13	46%	33	0.17
HFC*	245fa	C3H3F5, 1,1,1,3,3-Pentafluoropropane	1.48		B1				0.14
HFC*	134a	C2H2F4 1,1,1,2-Tetrafluoroethane, Norflura	6.65		A1			x	0.08
HFC*	1234ze	C3H2F4, 1,3,3,3-Tetrafluoropropene	7.00	#DIV/0!	A2L	x	#DIV/0!	x	0.07
HFC*	1234yf	C3H2F4 2,3,3,3-Tetrafluoropropene	0.06	#VALUE	A2L		#VALUE!		0.07
HFC*	236fa	C3H2F6, 1,1,1,3,3,3-Hexafluoropropane	2.72		A1				0.06
HFC*	23	CHF3 Fluoroform	45.98		A1			35.3	0.03
HFC*	125	C2HF5 Pentafluoroethane	13.90		A1			x	0.02
HFC*	227ea	C3HF7, 1,1,1,2,3,3,3-Heptafluoropropane	4.55		A1				0.01

*less common ones in BACKUP

A1, B1: non-flammable
A2(L): low flammability

Search for H-rich non-flammable gas: HFC (in collaboration with Diego)

Sorted by H-index

	code name: HFC-, R-		v.p. 25C (bar)	allowed percentage	ASHRAE 34 Safety group	flammablility lower limit %	fraction of Q at LFL	flammability upper limit in	H-index= f/b * #H
CH		H2	superc	49.2%	A3	4	8%	75	999.0
		C5H12, Neopentane, C(CH3)4, 2,2-Dimethy	1.72	3.8%	A3?	1.4	36%	7.5	4.80
		C5H12, isopantane, (CH3)2CHCH2CH3	0.92	0.0%	A3	1.4	7376%	8.3	4.80
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		C3H8	9.52	6.3%	A3	2.1	33%	9.5	3.56
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	134a	C2H2F4 1,1,1,2-Tetrafluoroethane, Norflura	6.65		A1			x	0.08
	1234ze	C3H2F4, 1,3,3,3-Tetrafluoropropene	7.00	#DIV/0!	A2L	x	#DIV/0!	x	0.07
	1234yf	C3H2F4 2,3,3,3-Tetrafluoropropene	0.06	#VALUE	A2L		#VALUE!		0.07
	236fa	C3H2F6, 1,1,1,3,3,3-Hexafluoropropane	2.72		A1				0.06
	23	CHF3 Fluoroform	45.98		A1			35.3	0.03
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	227ea	C3HF7, 1,1,1,2,3,3,3-Heptafluoropropane	4.55		A1				0.01

Flammability ~ H-index

*less common ones in BACKUP

A1, B1: non-flammable
A2(L): low flammability

Search for H-rich non-flammable gas: HFC (in collaboration with Diego)

Maximal H-index HFC by A2(L)-towering
0.35 bar C2H4F2 (LFL)
0.7 bar C2H3F3 (LFL)
0.75 bar C1H2F2 (remaining Q)
1.4 bar C3H3F5 (v.p.)
6.6 bar C2H2F4 (v.p.)
0.2 bar C3H2F6 (remaining fraction)
Name [4]C2H4F2[7]C2H3F3[8]C1H2F2[14]C3H3F5[66]C2H2F4[2]C3H2F6
Z 49.80
A 101.21
H 2.28
B 47.52,
Element H 0 2.28, Element C 2 2.09, Element F 4 3.89
purity: 0.047980
H-index: 0.109394

					flammability lower limit %	fraction of Q at LFL	flammability upper limit in	H-index= f/b * #H
					4	8%	75	999.0
					1.4	36%	7.5	4.80
					1.4	7376%	8.3	4.80
					1.8	40%	8.4	4.17
					1.8	38%	8.5	4.17
					2.1	33%	9.5	3.56
					3	34%	12.5	3.00
					5	32%	15	2.67
152a	C2H4F2 1,1-Difluoroethane	5.96	12.8%	A2	3.7	29%	18	0.53
143a	C2H3F3 1,1,1-Trifluoroethane	12.62	16.0%	A2L	7	44%	17	0.23
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A1, B1: non-flammable
A2(L): low flammability

Search for H-rich non-flammable gas: HFC (in collaboration with Diego)

All non-flammable HFC away from phase boundary
0.7 bar C3H3F5
4.5 bar C2H2F4
1.5 bar C3H2F6
3.3 bar CHF3
Name [7]C3H3F5[45]C2H2F4[15]C3H2F6[33]C1H1F3
Z 49.44
A 101.18
H 1.74
B 47.70,
Element H 0 1.74, Element C 2 1.89, Element F 4 4.04
purity: 0.036478
H-index: 0.063472

code name: HFC-, R-		v.p. 25C (bar)	allowed percentage	ASHRAE 34 Safety group	flammablility lower limit %	fraction of Q at LFL	flammability upper limit in	H-index= f/b * #H
					4	8%	75	999.0
					1.4	36%	7.5	4.80
					1.4	7376%	8.3	4.80
					1.8	40%	8.4	4.17
					1.8	38%	8.5	4.17
					2.1	33%	9.5	3.56
					3	34%	12.5	3.00
					5	32%	15	2.67
					3.7	29%	18	0.53
					7	44%	17	0.23
					13	46%	33	0.17
245fa	C3H3F5, 1,1,1,3,3-Pentafluoropropane	1.48		B1				0.14
134a	C2H2F4 1,1,1,2-Tetrafluoroethane, Norflurar	6.65		A1			x	0.08
1234ze	C3H2F4, 1,3,3,3-Tetrafluoropropene	7.00	#DIV/0!	A2L	x	#DIV/0!	x	0.07
1234yf	C3H2F4 2,3,3,3-Tetrafluoropropene	0.06	#VALUE	A2L		#VALUE!		0.07
236fa	C3H2F6, 1,1,1,3,3,3-Hexafluoropropane	2.72		A1				0.06
23	CHF3 Fluoroform	45.98		A1			35.3	0.03
125	C2HF5 Pentafluoroethane	13.90		A1			x	0.02
227ea	C3HF7, 1,1,1,2,3,3,3-Heptafluoropropane	4.55		A1				0.01

A1, B1: non-flammable
A2(L): low flammability

Search for H-rich non-flammable gas: HFC (in collaboration with Diego)

Single High-LFL Flammable Cocktail
1.3 bar CH2F2 (LFL)
0.7 bar C3H3F5
4.5 bar C2H2F4
1.5 bar C3H2F6
2 bar CHF3
Name [13]C1H2F2[7]C3H3F5[45]C2H2F4[15]C3H2F6[20]C1H1F3
Z 48.40
A 98.84
H 1.87
B 46.53,
Element H 0 1.87, Element C 2 1.89, Element F 4 3.91
purity: 0.040189
H-index: 0.075154

code name:		v.p.	allowed percent	ASHRAE 34	flammablility lower limit %	fraction of Q at LFL	flammability upper limit in	H-index= f/b * #H
					4	8%	75	999.0
					1.4	36%	7.5	4.80
					1.4	7376%	8.3	4.80
					1.8	40%	8.4	4.17
					1.8	38%	8.5	4.17
					2.1	33%	9.5	3.56
					3	34%	12.5	3.00
					5	32%	15	2.67
					3.7	29%	18	0.53
					7	44%	17	0.23
32	CH2F2 Difluoromethane	17.31	28.4%	A2L	13	46%	33	0.17
245fa	C3H3F5, 1,1,1,3,3-Pentafluoropropane	1.48		B1				0.14
134a	C2H2F4 1,1,1,2-Tetrafluoroethane, Norflurar	6.65		A1			x	0.08
1234ze	C3H2F4, 1,3,3,3-Tetrafluoropropene	7.00	#DIV/0!	A2L	x	#DIV/0!	x	0.07
1234yf	C3H2F4 2,3,3,3-Tetrafluoropropene	0.06	#VALUE	A2L		#VALUE!		0.07
236fa	C3H2F6, 1,1,1,3,3,3-Hexafluoropropane	2.72		A1				0.06
23	CHF3 Fluoroform	45.98		A1			35.3	0.03
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A1, B1: non-flammable
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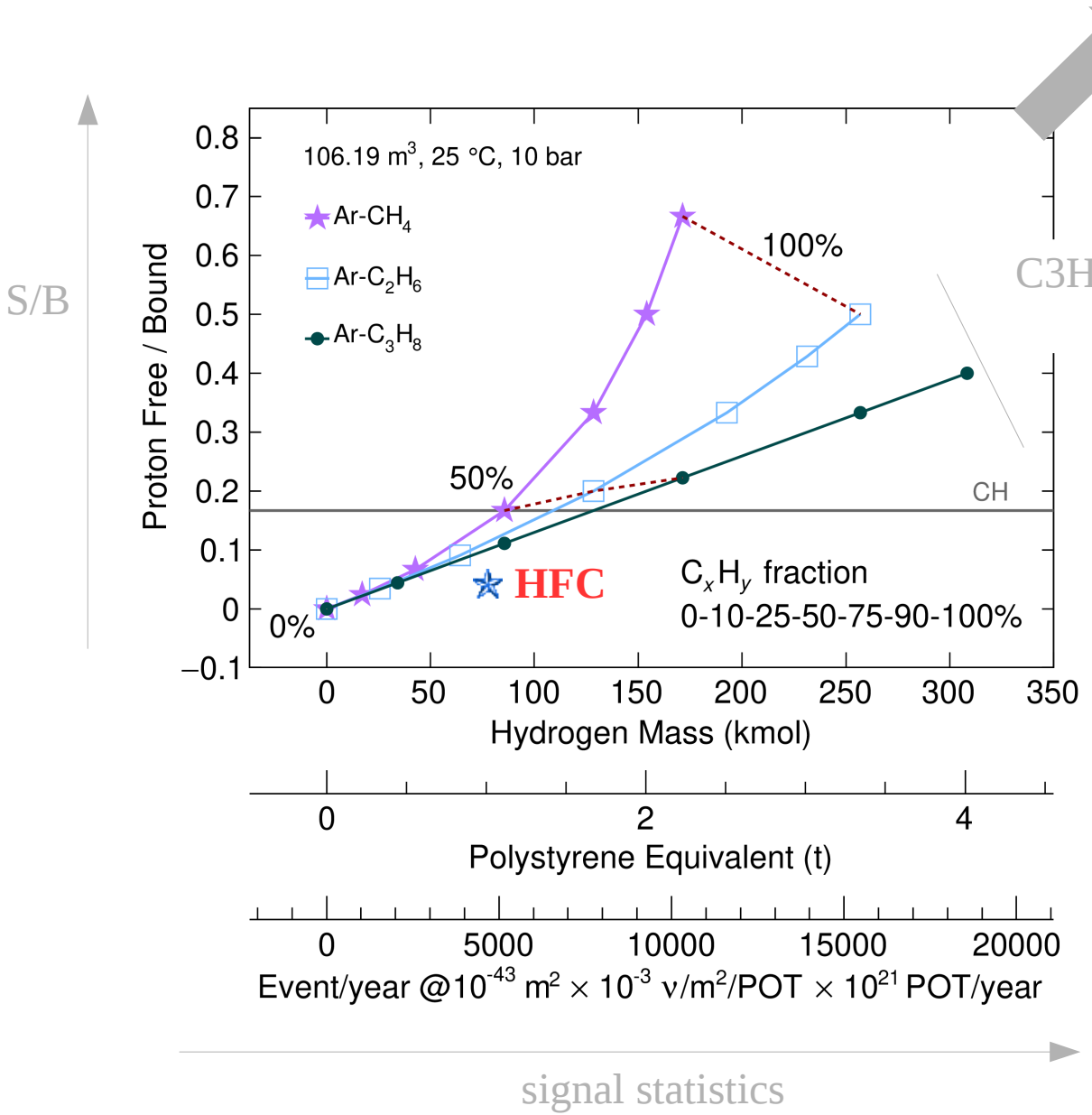
Search for H-rich non-flammable gas: HFC (in collaboration with Diego)



C3H8 liquefies @ 9.5 bar

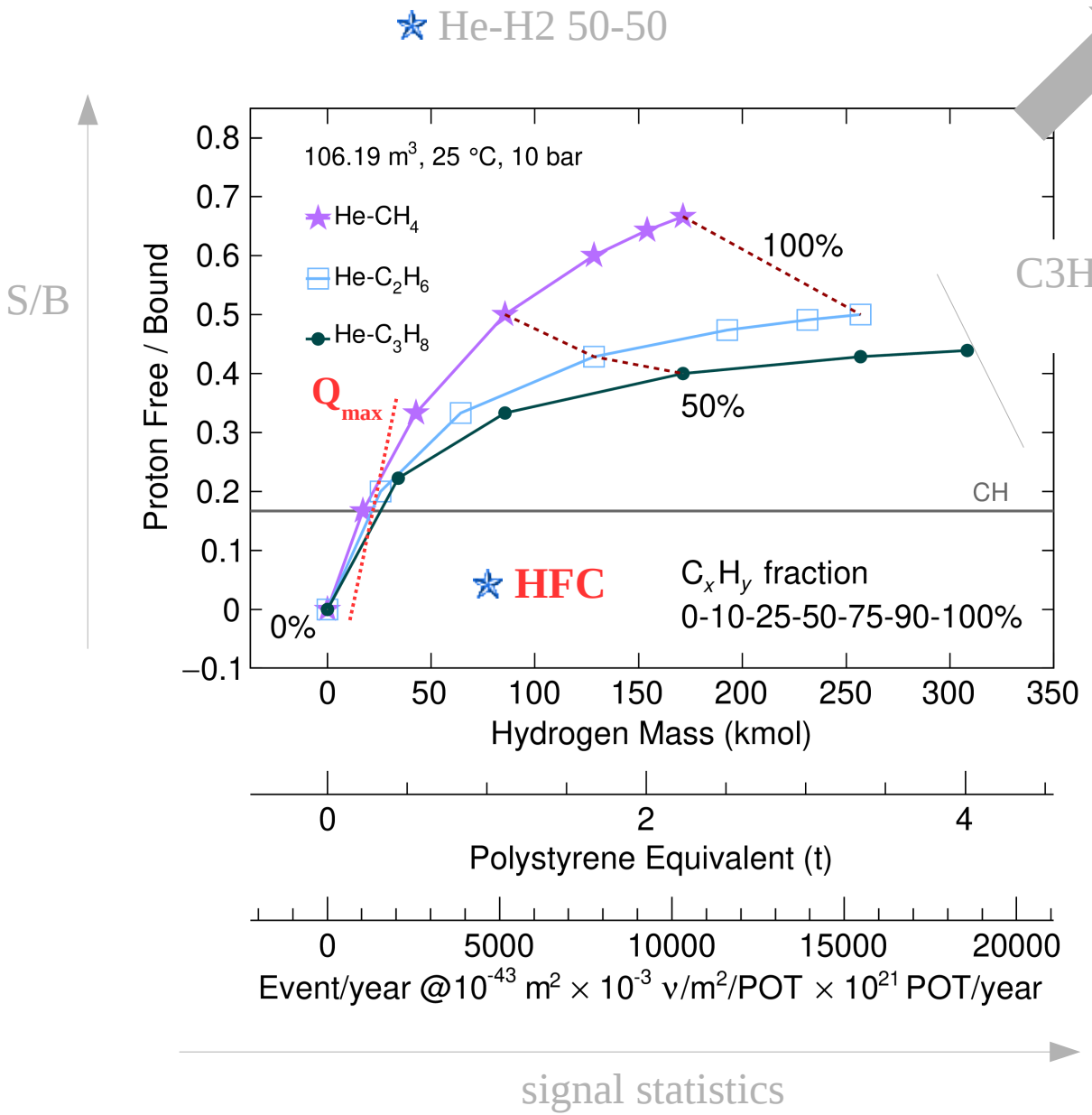
HFC cocktail
H: [1.74 ~ 1.87 ~ 2.28]
f/b: [0.036 ~ 0.040 ~ 0.048]
H-index: [0.06 ~ 0.08 ~ 0.11]

P-10
H-index: 0.010

P-50
H-index: 0.33

CH
H-index: 0.17

Search for H-rich non-flammable gas: HFC (in collaboration with Diego)



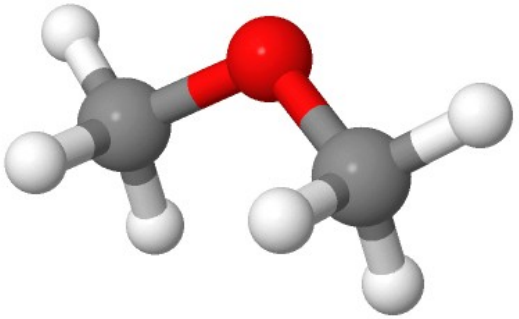
HFC cocktail
H: [1.74 ~ 1.87 ~ 2.28]
f/b: [0.036 ~ 0.040 ~ 0.048]
H-index: [0.06 ~ 0.08 ~ 0.11]

He-CH4 85-15
H: 0.60, f/b: 0.23 → H-index: 0.14

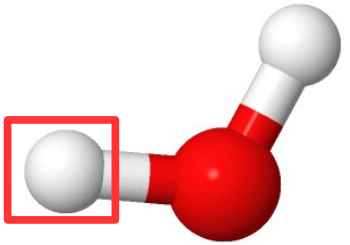
He-CH4 90-10
H:0.40, f/b: 0.17 → H-index: 0.067

HFC cocktail ~ He-CH4 10-15%
(better than P-10)
event rate OR purity
Not both

Search for H-rich non-flammable gas: CHO

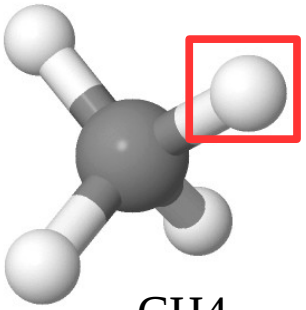


CH3OCH3 Dimethyl ether (DME)
v.p. 5.9 bar
H-index: 1.8
Flammable 3.4-18% (A3)
9.4%@Q_{max}

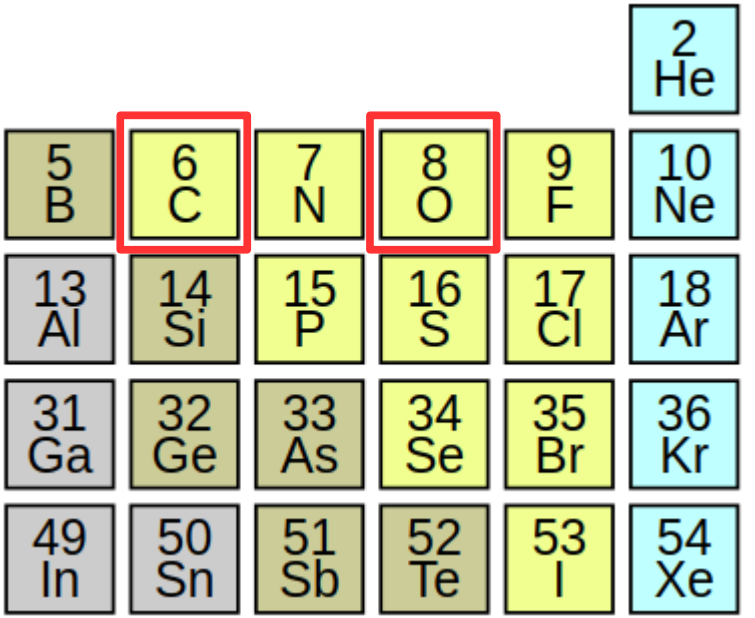


H2O

Any other CHO gas?



CH4
H-index: 2.7
16%@Q_{max}

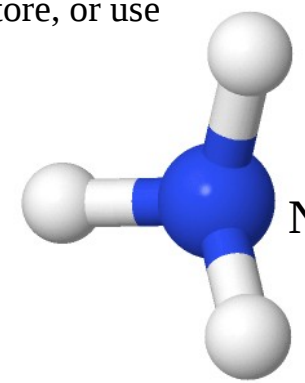


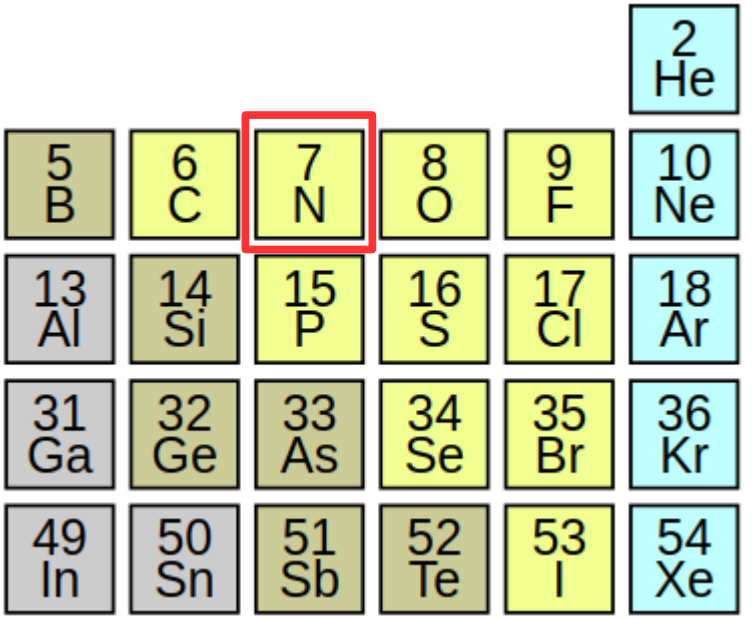
https://chemapps.stolaf.edu/jmol

Search for H-rich non-flammable gas: CHN

v.p. 10 bar
H-index: 1.3
Flammable 15-30% (B2L)
44%@Q_{max}
694kg in 100m3 10bar
"It is classified as an **extremely hazardous substance** in the United States, and is subject to strict reporting requirements by facilities which produce, store, or use it in significant quantities." [wiki]

Replace CH2F2 in previous
HFC Single High-LFL Cocktail
1.3 bar NH3 (LFL)
0.7 bar C3H3F5
4.5 bar C2H2F4
1.5 bar C3H2F6
2 bar CHF3
Name
[13]NH3[7]C3H3F5[45]C2H2F4[15]C3H2F6[20]C1H1F3
Z 46.32
A 94.29
H 2.00
B 44.32,
Element H 0 2.00, Element C 2 1.76,
Element N 3 0.13, Element F 5 3.65
purity: 0.045126
H-index: 0.090253
→ slight improvement (wrt 0.075154)



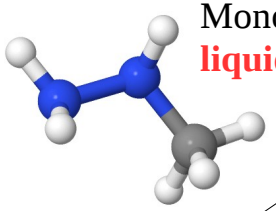


https://chemapps.stolaf.edu/jmol

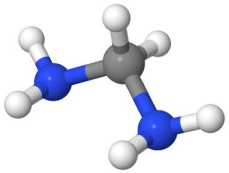
Search for H-rich non-flammable gas: CHN

CH6N2 isomers

H-index: 1.8

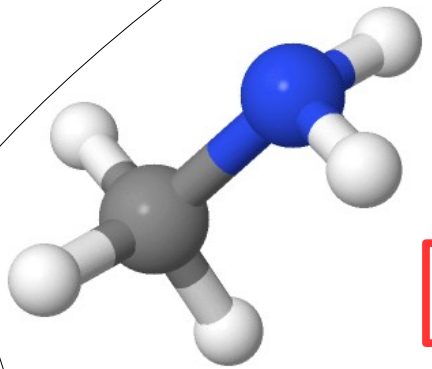


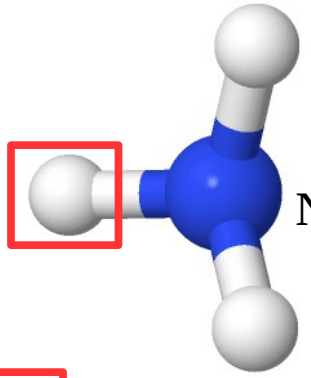
CH2(NH2)2
Monomethylhydrazine
liquid



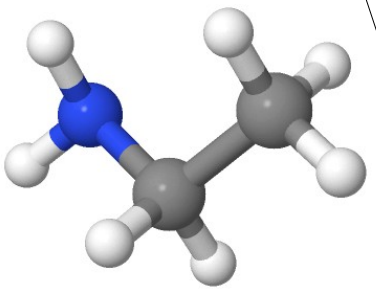
NH2CH2NH2
Methanediamine

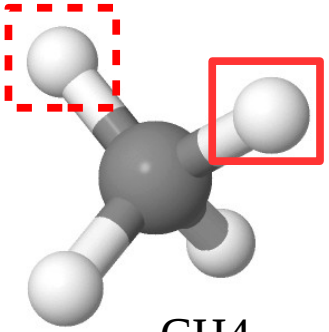
CH3NH2 Methylamine:
v.p. 3.5 bar
H-index: 1.9
In the United States, methylamine is **controlled as a List 1 precursor chemical** by the Drug Enforcement Administration [wiki]





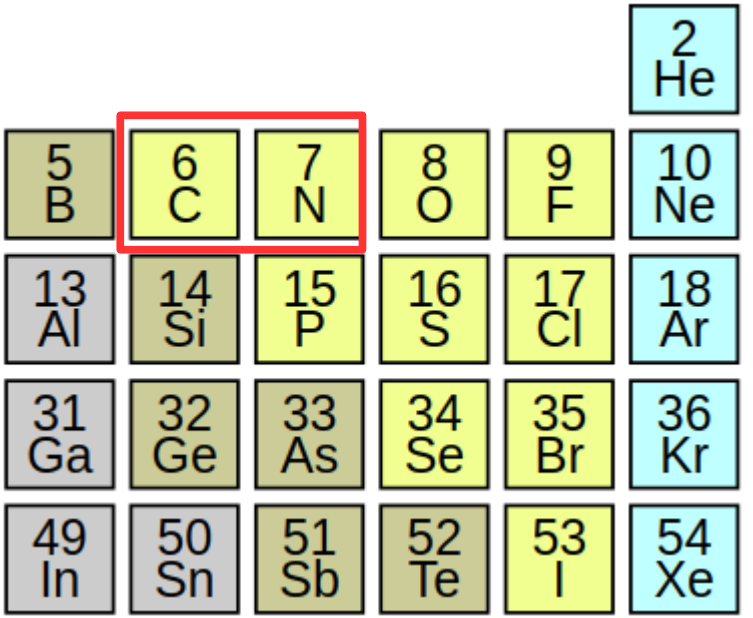
NH3





CH4

C2H5NH2 Ethylamine
v.p. 1.4 bar
H-index: 2.6
Flammable 3.5 – 14%



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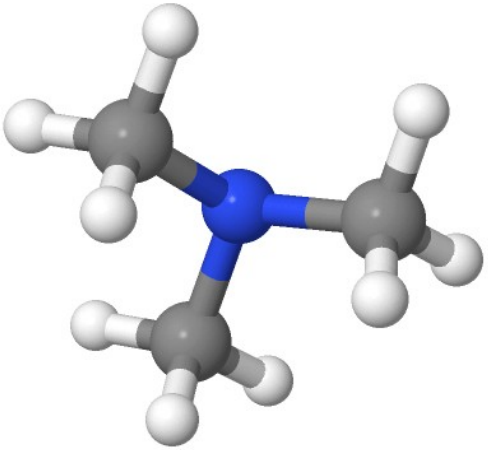
Search for H-rich non-flammable gas: CHN



N(CH3)3 Trimethylamine (TMA)

v.p. 2.2 bar

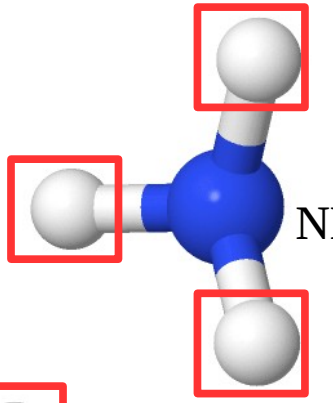
H-index: 3.2 (between C2H6 and C3H8)

Flammable 2 – 11.6% (too low LFL)

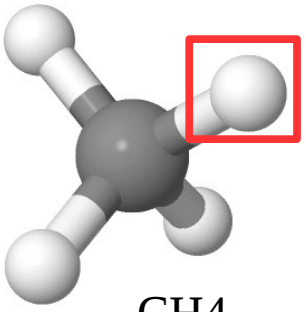
At lower concentrations, it has a "fishy" odor, the odor associated with rotting fish (wiki)

Xe-TMA 6.2% at 10 bar **(> LFL?!)**

JINST 8 (2013) P01012, arXiv:1210.3287



NH3



CH4

					2 He
5 B	6 C	7 N	8 O	9 F	10 Ne
13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe

https://chemapps.stolaf.edu/jmol

Summary and discussions (1)

code name: HFC-, R-		v.p. 25C (bar)	allowed percentage	ASHRAE 34 Safety group	flammablility lower limit %	fraction of Q at LFL	flammability upper limit in	H-index= f/b * #H
	H2	superc	49.2%	A3	4	8%	75	999.0
	C5H12, Neope	1.72	3.8%	A3?	1.4	36%	7.5	4.80
	C5H12, isopar	0.92	0.0%	A3	1.4	7376%	8.3	4.80
600a	iC4H10, CH(C	3.51	4.5%	A3	1.8	40%	8.4	4.17
	C4H10, butane	2.43	4.7%	A3	1.8	38%	8.5	4.17
	C3H8	9.52	6.3%	A3	2.1	33%	9.5	3.56
	C2H6	41.90	8.9%	A3	3	34%	12.5	3.00
	CH4	superc	15.8%	A3	5	32%	15	2.67
	CH3OCH3, sir	5.90	9.4%	A3	3.4	36%	18	1.80
	NH3	10.03	43.9%	B2L	15	34%	30	1.29
152a	C2H4F2 1,1-D	5.96	12.8%	A2	3.7	29%	18	0.53
143a	C2H3F3 1,1,1-	12.62	16.0%	A2L	7	44%	17	0.23
32	CH2F2 Difluor	17.31	28.4%	A2L	13	46%	33	0.17
245fa	C3H3F5, 1,1,1	1.48		B1				0.14
134a	C2H2F4 1,1,1,	6.65		A1			x	0.08
1234ze	C3H2F4, 1,3,3	7.00	#DIV/0!	A2L	x	#DIV/0!	x	0.07
1234yf	C3H2F4 2,3,3	0.06	#VALUE	A2L		#VALUE!		0.07
236fa	C3H2F6, 1,1,1	2.72		A1				0.06
23	CHF3 Fluorofc	45.98		A1			35.3	0.03
125	C2HF5 Pentaf	13.90		A1			x	0.02
227ea	C3HF7, 1,1,1,2	4.55		A1				0.01

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1234ze	C3H2F4, 1,3,3	7.00	#DIV/0!	A2L	x	#DIV/0!	x	0.07
1234yf	C3H2F4 2,3,3	0.06	#VALUE	A2L		#VALUE!		0.07
236fa	C3H2F6, 1,1,1	2.72		A1				0.06
23	CHF3 Fluorofc	45.98		A1			35.3	0.03
125	C2HF5 Pentaf	13.90		A1			x	0.02
227ea	C3HF7, 1,1,1,2	4.55		A1				0.01

Flammability hierarchy
A3 → (B → A)2 → (B → A)1

Corresponding H-index hierarchy
A2: below 1
A1: below 0.1

Summary and discussions (1)

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134a	C2H2F4 1,1,1,	6.65		A1			x	0.08
1234ze	C3H2F4, 1,3,3	7.00	#DIV/0!	A2L	x	#DIV/0!	x	0.07
1234yf	C3H2F4 2,3,3	0.06	#VALUE	A2L		#VALUE!		0.07
236fa	C3H2F6, 1,1,1	2.72		A1				0.06
23	CHF3 Fluorofc	45.98		A1			35.3	0.03
125	C2HF5 Pentaf	13.90		A1			x	0.02
227ea	C3HF7, 1,1,1,2	4.55		A1				0.01

At lower flammability limit, most of the gas use up only 30-40% Q_{max}

Assume LFL constant (generally not true):

15% NH3 + 13% CH2F2 ~ 80% Q_{max}

Leaving 7.2 bar 20% Q_{max} to fill up

Summary and discussions (2)

UPDATE

code name: HFC-, R-		v.p. 25C (bar)	allowed percentage	ASHRAE 34 Safety group	flammablility lower limit %	fraction of Q at LFL	flammability upper limit in	H-index= f/b * #H
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	C2H6	41.90	8.9%	A3	3	34%	12.5	3.00
	CH4	superc	15.8%	A3	5	32%	15	2.67
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134a	C2H2F4 1,1,1,	6.65		A1			x	0.08
1234ze	C3H2F4, 1,3,3	7.00	#DIV/0!	A2L	x	#DIV/0!	x	0.07
1234yf	C3H2F4 2,3,3	0.06	#VALUE	A2L		#VALUE!		0.07
236fa	C3H2F6, 1,1,1	2.72		A1				0.06
23	CHF3 Fluorofo	45.98		A1			35.3	0.03
125	C2HF5 Pentaf	13.90		A1			x	0.02
227ea	C3HF7, 1,1,1,2	4.55		A1				0.01

17%

35%

24%

24%

Maximal H Cocktail
1.7 bar neopentane (C5)
3.5 bar isobutane (C4)
2.4 bar butane (C4)
2.4 bar propane (C3)
Name
[17]C5H12[59]C4H10[24]C3H8
Z 33.44
A 57.02
H 9.86
B 23.58,
Element H 0 9.86, Element C 2 3.93
purity: 0.418151
H-index: 4.122969

Summary and discussions (2)

code name: HFC-, R-		v.p. 25C (bar)	allowed percentage	ASHRAE 34 Safety group	flammablility lower limit %	fraction of Q at LFL	flammability upper limit in	H-index= f/b * #H	
	H2	superc	49.2%	A3	4	8%	75	999.0	
	C5H12, Neope	1.72	3.8%	A3?	1.4	36%	7.5	4.80	
	C5H12, isopar	0.92	0.0%	A3	1.4	7376%	8.3	4.80	
600a	iC4H10, CH(C	3.51	4.5%	A3	1.8	40%	8.4	4.17	
	C4H10, butane	2.43	4.7%	A3	1.8	38%	8.5	4.17	
	C3H8	9.52	6.3%	A3	2.1	33%	9.5	3.56	
	C2H6	41.90	8.9%	A3	3	34%	12.5	3.00	
	CH4	superc	15.8%	A3	5	32%	15	2.67	
	CH3OCH3, sir	5.90	9.4%	A3	3.4	36%	18	1.80	
	NH3	10.03	43.9%	B2L	15	34%	30	1.29	
152a	C2H4F2 1,1-D	5.96	12.8%	A2	3.7	29%	18	0.53	
143a	C2H3F3 1,1,1-	12.62	16.0%	A2L	7	44%	17	0.23	
32	CH2F2 Difluor	17.31	28.4%	A2L	13	46%	33	0.17	13%
245fa	C3H3F5, 1,1,1	1.48		B1				0.14	7%
134a	C2H2F4 1,1,1,	6.65		A1			x	0.08	45%
1234ze	C3H2F4, 1,3,3	7.00	#DIV/0!	A2L	x	#DIV/0!	x	0.07	
1234yf	C3H2F4 2,3,3,	0.06	#VALUE	A2L		#VALUE!		0.07	
236fa	C3H2F6, 1,1,1	2.72		A1				0.06	15%
23	CHF3 Fluorofc	45.98		A1			35.3	0.03	20%
125	C2HF5 Pentaf	13.90		A1			x	0.02	
227ea	C3HF7, 1,1,1,2	4.55		A1				0.01	

Single High-LFL Flammable HFC Cocktail
1.3 bar CH2F2 (LFL)
0.7 bar C3H3F5
4.5 bar C2H2F4
1.5 bar C3H2F6
2 bar CHF3
Name [13]C1H2F2[7]C3H3F5[45]C2H2F4[15]C3H2F6[20]C1H1F3
Z 48.40
A 98.84
H 1.87
B 46.53,
Element H 0 1.87, Element C 2 1.89, Element F 4 3.91
purity: 0.040189
H-index: 0.075154

Summary and discussions (3)

1. Survey on HFC
   - Refrigerant industry
   - HFC has quite some non-flammable gas, but all with low H-index (necessarily)
   - One particular A2L (low flammability low toxicity) gas with high LFL (lower flammability limit):
     - CH2F2 Difluoromethane, 13% LFL
     - Can be cooked for non-flammable mixtures
   - **HFC cocktails ~ He-CH4 10-15%**
     - **Event rate OR purity, not both.**
     - **Need to consider realistic tracking and DUNE ND run plan**
   - Only looked at saturated HFC, non-saturated ones are more H-efficient
     - C2H2F2 H-index: 0.13, better than C2H2F4 (0.08), worse than CH2F2 (0.17), very flammable, allowed fraction is 2% by Q

2. Probed CHN
   - NH3 (B2L: low flammability *high* toxicity) has the highest H-index (1.29) among all low flammability gas, and even higher LFL (15%) than CH2F2
   - Generally, NH2 is more H-efficient than F when replacing H in alkane, but need a new strategy to explore as the industry is changed (refrigerant → drug); **might have surprises**

3. Briefly looked at CHO
   - CHO is mostly liquid except DME (CH3OCH3) which is A3 (high flammability)
   - OH is between NH2 and F in terms of H-efficiency; surprises?

Summary and discussions (3)

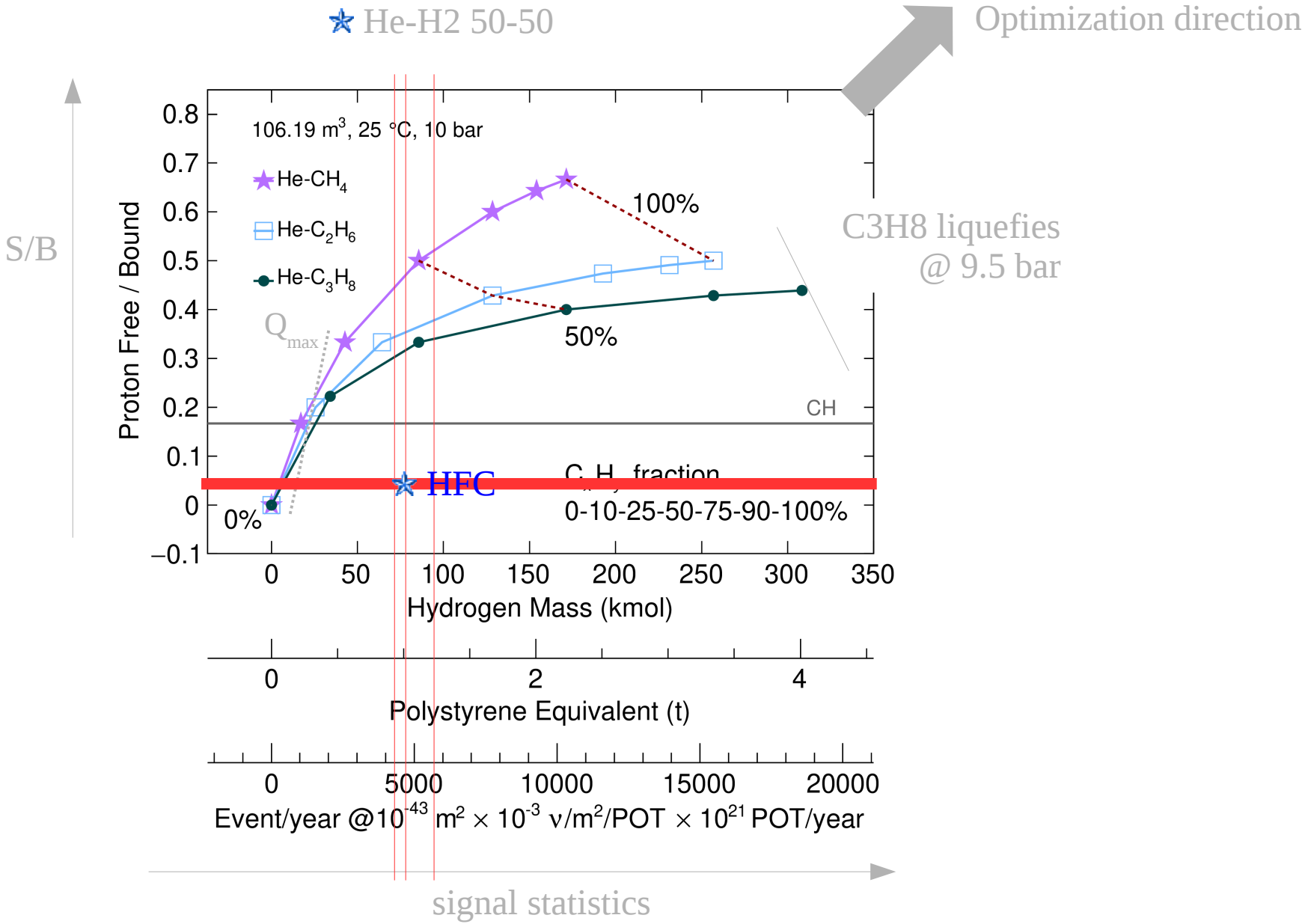
4. Need to sync with FNAL safety people
   - Regulation details: how much parametric overlap between FESHM 6020.3 and ASHRAE 34?
   - **Refine gas search strategy: safety vs. tracking vs. possible run plan**

5. TPC gas properties benchmarking
   - Ionization density can be large enough to enable μ/π separation outside dE/dx crossing?
   - 3-body attachment at high pressure, etc.

BACKUP

code name: HFC-, R-		v.p. 25C (bar)	allowed percentage	ASHRAE 34 Safety group	flammability lower limit %	fraction of Q at LFL	flammability upper limit in	H-index= f/b * #H
41	CH3F Fluoromethane	36.64	#VALUE	x	5.6	#VALUE	22.2	0.60
161	C2H5F Fluoroethane	9.43	#VALUE	x	x	#VALUE	17.3	1.19
152	C2H4F2 1,2-Difluoroethane	7.18	#VALUE	x		#VALUE!		0.53
	C2H2F2, 1,1-Difluoroethylene	40.04	2.0%	xx		0%		0.13
143	C2H3F3 1,1,2-TRIFLUOROETHANE	x	14.5%	x		0%		0.23
134	C2H2F4 1,1,2,2-Tetrafluoroethane	x	30.4%	x		0%	x	0.08
281	C3H7F, 1-Fluoropropane	x	#DIV/0!	x		#DIV/0!		1.81
272	C3H6F2, Difluoropropane		#DIV/0!	x		#DIV/0!		1.00
263	C3H5F3, Trifluoropropane		#DIV/0!	x		#DIV/0!		0.56
254cb	C3H4F4, 1,1,2,2-Tetrafluoropropane		#DIV/0!	x		#DIV/0!		0.30
245eb	C3H3F5, 1,1,1,2,3-Pentafluoropropane		#DIV/0!	x		#DIV/0!		0.14

Search for H-rich non-flammable gas: HFC



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