SUPPORTING INFORMATION

Synthesis and Dielectric Properties of the Eco-friendly Insulating Gas Thiazyl Trifluoride

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Table S1. The MSDS information of the chemicals involved in the reaction.

	CAS number	Toxicity [a]
sulfur monochloride	10025-67-9	LD50 orally in Rabbit: 132 mg/kg
carbon tetrachloride	56-23-5	LC50 for mice: 9528 ppm (Svirbely); LD50 orally in rats, mice, dogs (g/kg): 2.92, 12.1-14.4, 2.3
1,4-Dioxane	123-91-1	LD50 orally in mice, rats (ml/kg): 5.7, 5.2 (Laug)
Benzene	71-43-2	LD50 orally in young adult rats: 3.8 ml/kg (Kimura)
Ammonia	7664-41-7	LD50 oral (rat) 350 mg/kg LC50 inhal (rat) 2000 ppm (4 h)
Silver(II) fluoride	7783-95-1	\[b]

[a] According to the Chemical Book.

[b] No related data.

Table S2. Reaction energy of radical decomposition of NSF_3

Reactant → Product	E_1[a] (Hartree)	E_2[b] (Hartree)[c]	E_2-E_1 (kcal/mol)
A →B + Frad	-752.32145	-752.228408	58.2163794
A →C + Nrad	-752.32145	-752.32145	77.7031802
C →D + Frad	-697.597739	-697.549037	30.4728414

[a] Energy of reactant.

[b] Energy of product.

[c] 1 Hartree = 2625.5 kJ/mol = 27.21 eV = 627.51 kcal/mol

Table S3. Physical and environmental properties of common dielectric gases

	NSF_3	CF_3I	c-C_4F_8	$C_5F_{10}O$	C_4F_7N	SF_6
Molecular Weight (MW)	103.07	195.91	200.3	266.03	195.04	146.05
Electric strength relative to SF_6 (Er)	1.35	1.23	1.25	1.2	2.17	1
Boiling point/°C	-27	-22.5	−6	26.5	−4.7	−63
Atmospheric lifetime (τ)/years	5	0.005	3200	0.04	35	3200
Global Warming Potential (GWP)	916	1~5	8700	1	2100	23900