

SUPPLEMENTARY INFORMATION

Sulfonium Cation $[\text{SF}_3]^+$ Complexes with Noble Gases

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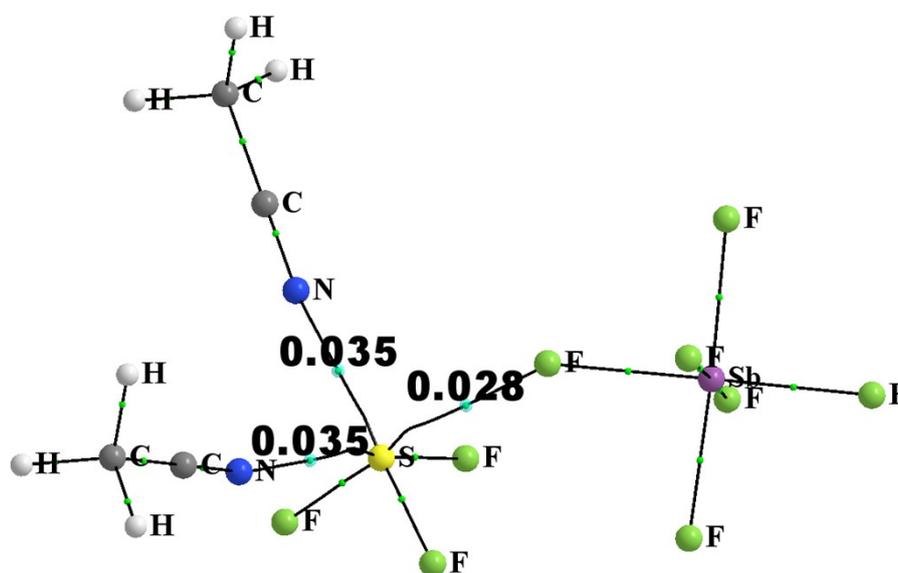
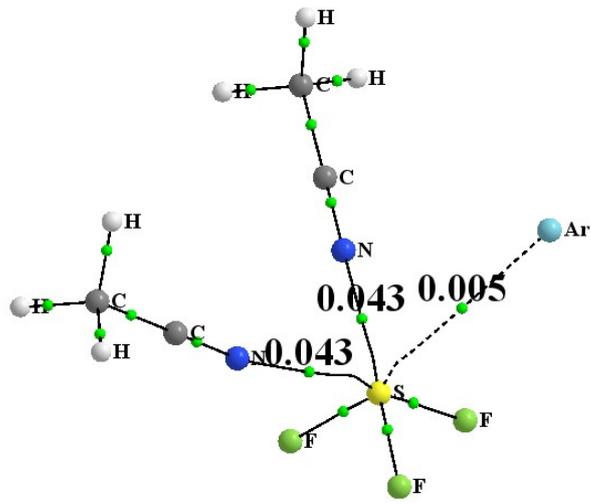
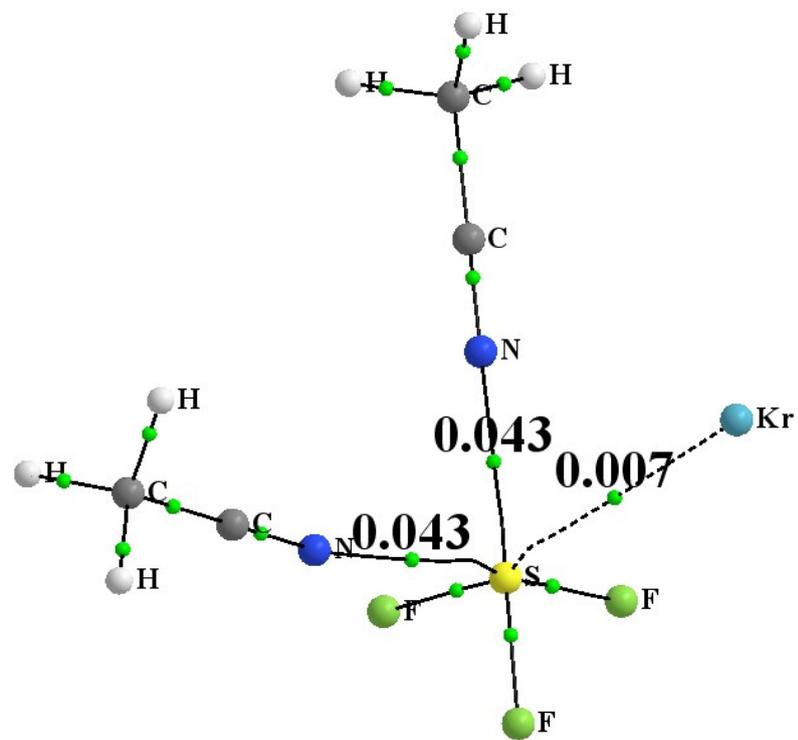


Fig. S1. QTAIM molecular diagrams for fully optimized $[\text{SF}_3(\text{NCCH}_3)_2][\text{SbF}_6]$ complexes in PCM-model solvent (DCM) simulation. The density of the bond critical points (marked as green dots) is shown in au.

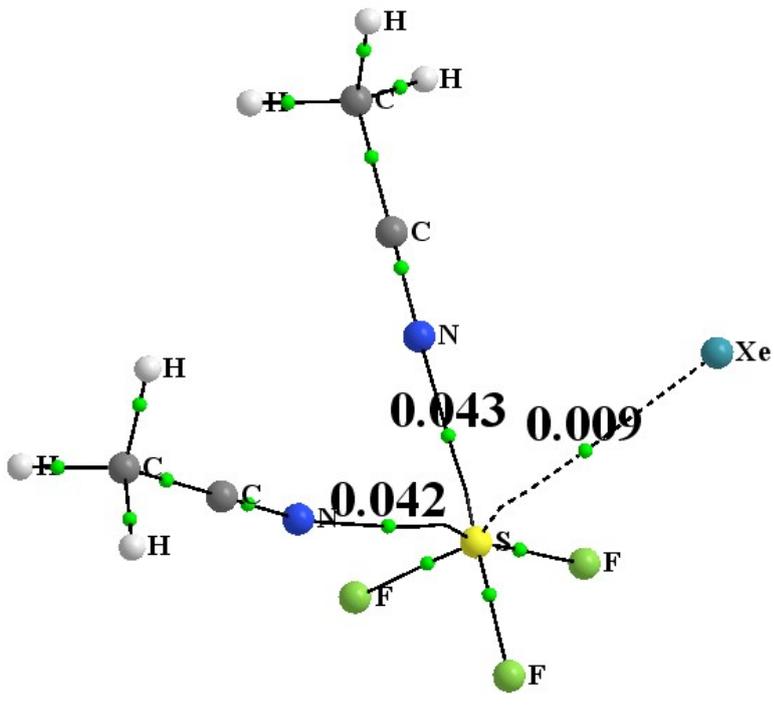
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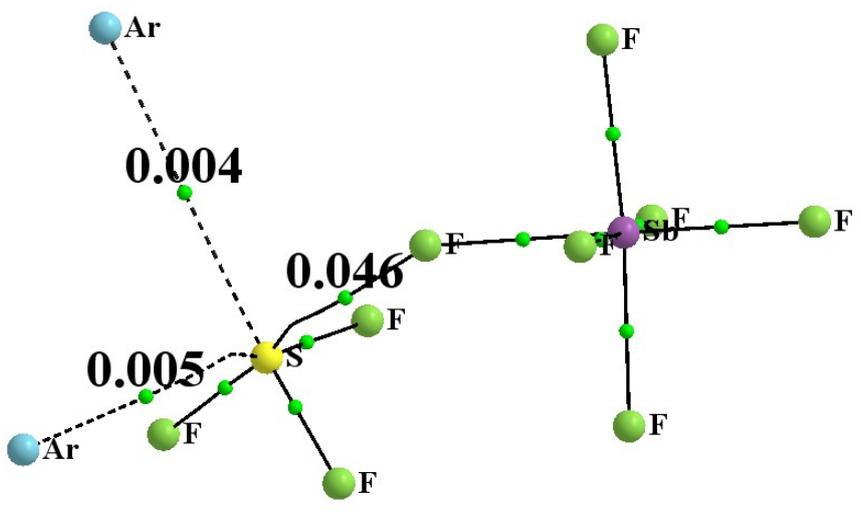
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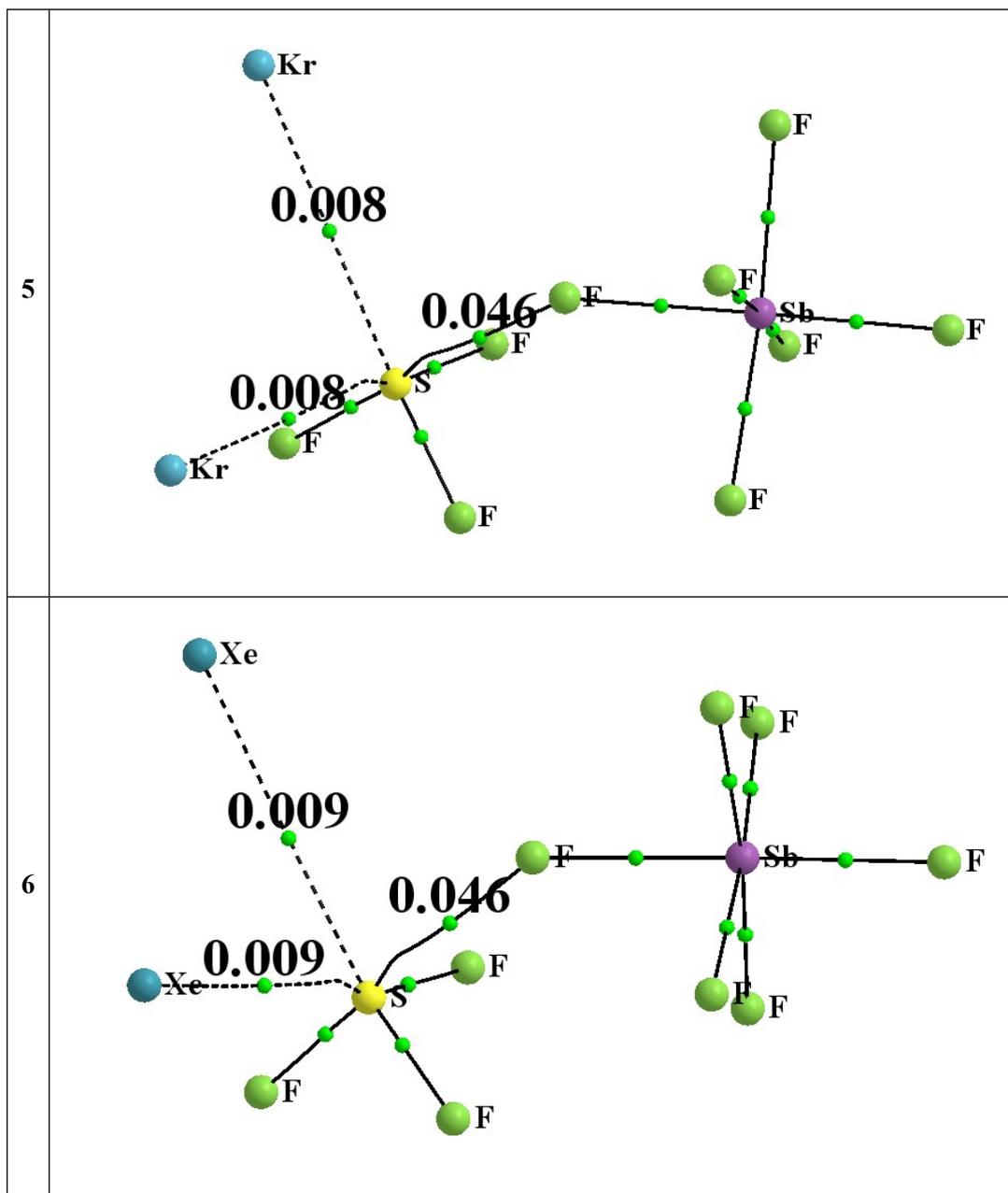


Fig. S2 QAIM molecular diagrams for fully optimized complexes with one or two noble gases in PCM-model solvent (DCM) simulation. The density of the bond critical points (marked as green dots) is shown in au.

Table S1. QTAIM parameters (au) within complexes at the bond critical point of S...Ng bond paths.

	ρ	-G/V	H
1	0.005	1.333	0.001
2	0.007	1.666	0.001
3	0.009	1.250	0.001
4	0.004	1.500	0.001
	0.005	1.500	0.001
5	0.008	1.250	0.001
	0.008	1.250	0.001
6	0.009	1.200	0.001
	0.009	1.200	0.001

Coordinates of studied compounds

1	S	12.27074400	9.52457800	5.02137400
	F	11.70250100	9.54606900	3.61873200
	F	13.26005200	8.38191100	4.78175200
	F	13.30520500	10.63015500	4.79806000
	N	10.64342600	7.72781200	5.25019400
	C	9.86194800	6.92678700	5.48524100
	C	8.87050000	5.90774000	5.77617800
	H	9.35502900	4.93448900	5.80306500
	H	8.10943800	5.91685600	4.99929600
	H	8.41332500	6.11627800	6.74065200
	N	10.71012400	11.37574200	5.27519100
	C	9.91688200	12.17009900	5.49287100
	C	8.91021200	13.18014800	5.76240900
	H	9.37740000	14.16212300	5.75707800
	H	8.14333300	13.13505000	4.99246700
	H	8.46415000	12.99159600	6.73615200
	Ar	12.83147500	9.54376700	8.52944600

2	S	12.28660600	9.52695500	4.99976000
	F	11.72733500	9.53625400	3.59304000
	F	13.28532000	8.38951600	4.77279200
	F	13.31483900	10.63862100	4.77585600
	N	10.66788200	7.72609600	5.23686100
	C	9.87807600	6.93676600	5.48344600
	C	8.87579300	5.93275300	5.78896100
	H	9.33960700	4.94918900	5.77898100
	H	8.08813600	5.97411000	5.04011700
	H	8.45731200	6.13062200	6.77302400
	N	10.71049900	11.36433000	5.24214800
	C	9.91859900	12.15444500	5.47936600
	C	8.91350800	13.15920500	5.77313900
	H	9.37543600	14.14355300	5.75689400
	H	8.12865700	13.11027000	5.02179900
	H	8.49183600	12.96842300	6.75726000
	Kr	12.68630400	9.53009300	8.54671400
3	S	12.27126500	9.52951600	5.01252900
	F	11.72294200	9.54032900	3.60042200
	F	13.26484400	8.38599000	4.79306800
	F	13.30794900	10.63458600	4.79463500
	N	10.64536600	7.72896600	5.24495100
	C	9.86178800	6.93124200	5.48439400
	C	8.86776100	5.91632700	5.78099900
	H	9.34391200	4.93860400	5.78238400
	H	8.09010100	5.94416900	5.02118000
	H	8.43328000	6.11374700	6.75820600
	N	10.70679300	11.37988600	5.24544600
	C	9.91094600	12.16809400	5.47581600
	C	8.90102400	13.17045500	5.76130200
	H	9.36045000	14.15601000	5.74851700
	H	8.12219000	13.11934800	5.00385900
	H	8.47205600	12.97871000	6.74208900
	Xe	12.86307900	9.53522500	8.57036000
4	Sb	14.94808100	9.58992000	8.64005000
	F	13.29208100	9.57796500	7.61134100
	F	15.58975600	8.29745500	7.43659700
	F	14.21921000	8.23382000	9.70813200
	F	16.55101200	9.59934000	9.60576400
	F	15.54901700	10.93814800	7.47883800
	F	14.17664100	10.88733700	9.74994400
	S	12.46704400	9.49490500	5.49930900
	F	11.95070400	9.44200300	4.07101800
	F	13.36482400	8.29091900	5.40642800
	F	13.48851000	10.57711400	5.27611800
	Ar	10.03208800	6.94338000	5.93160000
	Ar	10.22292000	12.23569500	6.29961800

5	Sb	14.94000300	9.52813800	8.64574000
	F	13.27172300	9.56367400	7.63638300
	F	15.40889400	8.01600100	7.63554900
	F	14.08651300	8.42812000	9.89920300
	F	16.55629300	9.49469600	9.58779200
	F	15.65337900	10.62581700	7.29796800
	F	14.34384200	11.04796100	9.56572900
	S	12.44171700	9.59579500	5.52457400
	F	11.91495900	9.62002600	4.09805100
	F	13.47353400	8.51916100	5.31111900
	F	13.33189500	10.80389500	5.40132000
	Kr	10.35706300	6.85473700	5.82748600
	Kr	10.07207100	12.00997900	6.28384200
	6	Sb	14.81775600	9.50399800
F		13.17312400	9.51509400	7.56741300
F		14.98443600	7.68593500	8.18266700
F		13.79787600	9.06017500	10.12020200
F		16.42169600	9.50024800	9.57612900
F		15.68407700	9.94393500	7.00141100
F		14.53438500	11.32689700	8.94736800
S		12.61850600	9.67844800	5.36643200
F		12.26725700	9.79219100	3.89145900
F		13.73835800	8.68299700	5.20183000
F		13.43668900	10.94134600	5.44679600
Xe		9.85540500	11.56110700	6.67428600
Xe		10.37192500	6.90622700	5.87110600