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Supplementary Material

Hybridizations and VALBOND parameters used around hypervalent centers.

molecule	bond	hybridization	K _{VALBOND}
XeF ₂	Xe-F	sp10.0	220.0
ClF ₃	Cl-F	sp10.0	220.0
ClF ₂ H	Cl-F	sp10.0	220.0
	Cl-H	sp3.0	220.0
ClF ₂ CH ₃	Cl-F	sp10.0	220.0
	Cl-C	sp3.0	220.0
ClF ₂ SiH ₃	Cl-F	sp10.0	220.0
	Cl-Si	sp3.0	220.0
SF ₄	S-F	sp5.0	220.0
SF ₆	S-F	sp50.0	220.0
XeF ₄	Xe-F	sp10.0	220.0
XeF ₆	Xe-F	sp10.0	220.0
PF ₅	P-F	sp10.0	220.0
PF ₄ H	P-F	sp10.0	220.0
	P-H	sp3.5	220.0
PF ₄ Me	P-F	sp10.0	220.0
	P-C	sp4.0	220.0
PF ₃ Me ₂	P-F	sp10.0	220.0
	P-C	sp4.0	220.0
PF ₂ Me ₃	P-F	sp10.0	220.0
	P-C	sp4.0	220.0
PNPOSI	Si-N	sp3.591	220.0
	Si-O	sp3.591	220.0
	Si-C	sp6.772	220.0
CINLIU	Si-F	sp5.122	220.0
	Si-C	sp2.922	220.0
DALFOL	Si-O	sp3.591	220.0
	Si-C	sp6.772	220.0
ADSBOP	P-O	sp2.410	220.0
	P-C	sp2.516	220.0

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MSPBZP	P-O	sp1.410	220.0
	P-C	sp2.516	220.0
MPHLPA	P-C	sp3.000	220.0
DULDIX	I-O	sp4.0	220.0
	I-C	sp4.0	220.0
BENICL	I-Cl	sp4.0	220.0
	I-C	sp4.0	220.0
JAGCUP	I-O	sp4.0	220.0
IBZDAC	I-O	sp4.0	220.0
	I-C	sp4.0	220.0
DUCCAF	I-O	sp5.0	220.0
	I-C	sp4.0	220.0
CESFEL	P-O	sp4.0	220.0
	P-N	sp4.0	220.0

nonstandard bond stretch parameters

Atom type, Atom type, force constant(kcal/mol Å), equilibrium distance (Å)

XCL	XF	300.0	1.698
XI	XCL	300.0	2.465
XE	XF	210.0	2.029
ST	XF	300.0	1.5467
PT	XF	300.0	1.55
PT	H	443.0	1.4
H	OT	505.0	0.948
H	ST	281.0	1.35
PT	OT	455.0	1.580
CF3	CT	208.0	1.520
CF3	XF	275.0	1.320
OE	XI	350.0	2.11
OS	XI	350.0	2.11
OT	XI	350.0	2.11
OS	PT	300.0	1.810
PT	NP	300.0	1.700
C6R	XI	300.0	2.09
MSI	XCL	300.0	2.07
MSI	HA	500.0	1.475
MSI	OE	390.0	1.64
MSI	NT	300.0	2.34
MSI	CT	295.0	1.874
MSI	C6R	295.0	1.853
MSI	XF	300.0	1.68

Results from selected NRT and NBO analyses. All calculations done at HF/6-311G** or HF/LANL1DZ

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Molecule	Resonance structure	Weight (%)	Hybridizations
XeF ₂		50	Xe-F: sp ^{99.99}
		50	
ClF ₃		40.22	Cl-F _{ax} : sp ^{11.34} Cl-F _{eq} : sp ^{9.61}
		40.22	
		19.08	
PCl ₅		33.63	P-Cl _{ax} : sp ^{2.86} d ^{1.86} P-Cl _{eq} : sp ^{3.00} d ^{0.61}
		33.63	
		3x(6.38)	
SF ₄		29.84	S-F _{ax} : sp ^{7.57} S-F _{eq} : sp ^{5.95}
		29.84	
		17.68	
		17.68	