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Theoretical Study of the Gas-Phase Reaction: $SF_6 + CO^+ \Leftarrow SF_5^+ + FCO$

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Two sets of basis functions were used in this work, a small basis (B0) and a larger one, with extra diffuse and polarization functions (B1). The effective core potential (ECP) used was SBKJC potential[21] for all atoms.

Table S1. Small Basis Set (B0)

Atom	Function	Exponent	Coefficient
CARBON	S	0.038875	1.000000
	S	0.112798	1.000000
	S	0.327290	1.000000
	S	1.116069	-0.093440
		3.931696	-0.134350
		13.850610	-0.004060
		48.793033	-0.001890
	P	0.128347	1.000000
	P	0.420634	1.000000
	P	1.364696	0.214740
		4.490295	0.055280
		14.774539	0.012870
	D	0.511867	1.000000
OXYGEN	S	0.179148	1.000000
	S	0.481294	1.000000
	S	1.293032	1.000000
	S	3.414395	-0.080010
		8.879166	-0.116351
		23.090350	0.004502
		60.046660	-0.004333
	P	0.198142	1.000000
	P	0.693275	1.000000
	P	2.329895	0.327622
		7.995507	0.091601
		27.438202	0.018310
	D	1.160205	1.000000

Atom	Function	Exponent	Coefficient
FLUORINE	S	0.274726	1.000000
	S	0.884323	1.000000
	S	2.846573	1.000000
	S	9.542028	-0.132409
		30.811976	-0.007367
		99.494352	-0.001405
		321.275271	-0.000427
	P	0.268811	1.000000
	P	0.936091	1.000000
	P	3.134847	0.298814
		10.733386	0.083031
		36.749988	0.016849
	D	1.403647	1.000000
SULFUR	S	0.180126	1.000000
	S	0.555085	1.000000
	S	1.710576	1.000000
	S	5.298288	-0.018630
		16.502688	0.007291
		51.401259	0.000940
		160.100548	0.000032
	P	0.084825	1.000000
	P	0.235876	1.000000
	P	0.650758	0.382423
		1.911477	-0.041052
		5.614597	-0.014522
	D	0.526495	1.000000

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Table S2. Larger Basis Set (B1): Small Basis Set plus extra diffuse and polarization functions

Atom	Function	Exponent	Coefficient
CARBON	S	0.013397	1.000000
	P	0.039162	1.000000
	D	0.128347	1.000000
	F	0.128347	1.000000
OXYGEN	S	0.066683	1.000000
	P	0.056630	1.000000
	D	0.693275	1.000000
	F	0.693275	1.000000
FLUORINE	S	0.085347	1.000000
	P	0.077193	1.000000
	D	0.936091	1.000000
	F	0.936091	1.000000
SULFUR	S	0.058452	1.000000
	P	0.305047	1.000000
	D	0.235876	1.000000
	F	0.235876	1.000000