

Table 1 : List of transitions frequencies of SF₆-Rg (Rg = Ar, Kr, Xe) hetero dimers assigned and used to simulate the rovibrational parallel and perpendicular band contours.

	E _i (eV)	1/n _{eff}		β(Å ⁻¹)
SF ₆	15.7	1.0744		
Ne	21.565	1.2590	SF ₆ -Ne	4.411
Ar	15.760	1.0760	SF ₆ -Ar	4.065
Kr	14.000	1.0414	SF ₆ -Kr	3.949
Xe	12.130	0.9442	SF ₆ -Xe	3.816

Table 2: Ionization potential and effective principle quantum number for rare gases and SF₆ for calculating model repulsive forces and repulsive β parameters related to SF₆-Rg heterodimers

	C ₆ ^{Rg-Rg} <i>calculated</i>			C ₆ ^{SF₆-Rg} <i>From combining rules (CR)</i>			C ₆ ^{SF₆-Rg} <i>CR (mean)</i>	
	Tao	Vydrov	Kumar	Tao	Vydrov	Kumar		
Ne-Ne	7.33	6.35	6.38	SF ₆ -Ne	65.5	61.0	61.1	63.3(6)
Ar-Ar	67.7	64.42	64.30	SF ₆ -Ar	199.1	194.3	194.1	196.7(20)
Kr-Kr	133	130.1	129.6	SF ₆ -Kr	279.1	276.1	275.5	277.4(27)
Xe-Xe	296	-	285.9	SF ₆ -Xe	416.4	416.4	409.2	412.8(41)
SF ₆ -SF ₆	-	585.8	-					

Table 3: C₆^{SF₆-Rg} coefficients (in atomic units) derived from calculated C₆^{Rg-Rg} and C₆^{SF₆-SF₆} coefficients and combining rules. CR mean values are obtained by averaging sets from three distinct studies.