

Electronic Supplementary Information

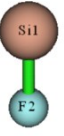
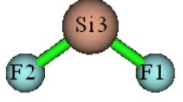
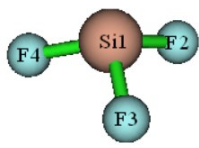
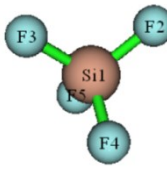
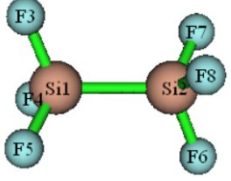
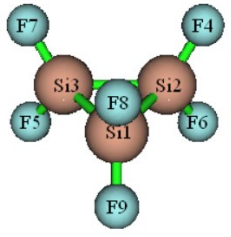
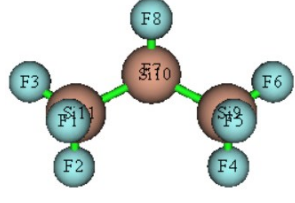
Chemical structure stabilities of Si_xF_y ($x \leq 6$, $y \leq 12$) series

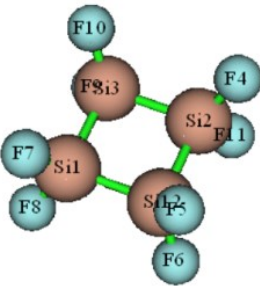
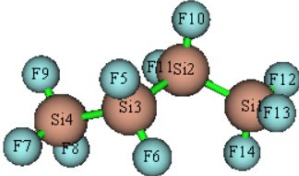
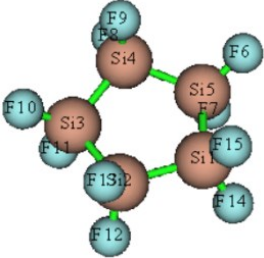
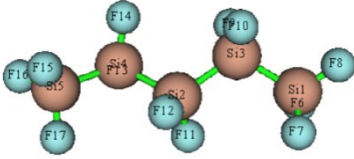
An-jiang Tang,^{*a} Qi-shan Huan,^b Shi-yun Tang,^a De-ju Wei,^a Jun-jiang Guo^a and Yu-han Zhao^a

^a School of Chemical Engineering, Guizhou Institute of Technology, Guiyang, China. E-mail: tangaj2000@163.com.

^b School of Chemistry and Chemical Engineering, Guizhou University, Guiyang, China.

Table S1. The optimised structural parameters of Si_xF_y ($x \leq 6, y \leq 12$) series

molecular	Structure diagram	Bond length R(Å)	Bond angle A(°)
SiF		R(2,1)1.626	/
SiF ₂		R(3,1)1.616; R(3,2)1.616	A(2,3,1)100.933
SiF ₃		R(4,1)1.600; R(3,1)1.600; R(2,1)1.600	A(2,1,3)108.019; A(2,1,4)108.019; A(3,1,4)108.019
SiF ₄		R(5,1)1.579; R(4,1)1.579; R(3,1)1.579; R(2,1)1.579	A(2,1,3)109.471; A(2,1,4)109.471; A(2,1,5)109.471; A(3,1,4)109.471; A(3,1,5)109.471; A(4,1,5)109.471
Si ₂ F ₆		R(8,2)1.593; R(7,2)1.593; R(6,2)1.593; R(5,1)1.593; R(4,1)1.593; R(3,1)1.593; R(2,1)2.317	A(1,2,6)110.557; A(1,2,7)110.557; A(1,2,8)110.494; A(6,2,7)108.385; A(6,2,8)108.374; A(7,2,8)108.399; A(2,1,3)110.556; A(2,1,4)110.492; A(2,1,5)110.558; A(3,1,4)108.374; A(3,1,5)108.386; A(4,1,5)108.399
Si ₃ F ₆		R(9,1)1.609; R(8,1)1.609; R(7,3)1.609; R(6,2)1.609; R(5,3)1.609; R(4,2)1.609; R(3,2)2.390; R(3,1)2.390; R(2,1)2.390	A(5,3,7)107.599; A(5,3,2)120.763; A(5,3,1)120.763; A(7,3,2)120.763; A(7,3,1)120.763; A(2,3,1)59.998; A(4,2,6)107.635; A(4,2,6)120.751; A(4,2,1)120.744; A(6,2,3)120.751; A(6,2,1)120.744; A(3,2,1)60.006; A(8,1,9)107.634; A(8,1,3)120.755; A(8,1,2)120.744; A(9,1,3)120.755; A(9,1,2)120.744; A(3,1,2)59.996
Si ₃ F ₈		R(11,10)2.336; R(11,3)1.593; R(11,1)1.595; R(11,2)1.595; R(10,9)2.336; R(10,8)1.608; R(10,7)1.608; R(9,6)1.593; R(9,5)1.595; R(9,4)1.595	A(2,11,1)107.982; A(2,11,3)108.460; A(2,11,10)110.226; A(1,11,3)108.460; A(1,11,10)110.226; A(3,11,10)111.394; A(7,10,8)108.268; A(7,10,9)107.593; A(7,10,11)107.593; A(8,10,9)107.593; A(8,10,11)107.593; A(9,10,11)117.888; A(4,9,5)107.982; A(4,9,6)108.460; A(4,9,10)110.226; A(5,9,6)108.460; A(5,9,10)110.226; A(6,9,10)111.394
Si ₄ F ₈		R(12,5)1.609; R(12,6)1.609; R(12,2)2.375; R(12,1)2.375; R(11,2)1.609;	A(6,12,5)108.342; A(6,12,2)114.482; A(6,12,1)114.401; A(5,12,2)114.459; A(5,12,1)114.464; A(2,12,1)90.000; A(9,3,10)108.342; A(9,3,2)114.421; A(9,3,1)114.492; A(10,3,2)114.443; A(10,3,1)114.449; A(2,3,1)90.000; A(4,2,11)108.342; A(4,2,12)114.403; A(4,2,3)114.473;

		R(10,3)1.609; R(9,3)1.609; R(8,1)1.609; R(7,1)1.609; R(4,2)1.609; R(3,2)2.375; R(3,1)2.375	A(11,2,12)114.461; A(11,2,3)114.466; A(12,2,3)90.000; A(7,1,8)108.342; A(7,1,12)114.492; A(7,1,3)114.410; A(8,1,12)114.448; A(8,1,3)114.455; A(12,1,3)90.000
Si ₄ F ₁₀		R(14,1)1.595; R(13,1)1.595; R(12,1)1.594; R(11,2)1.612; R(10,2)1.608; R(9,4)1.595; R(8,4)1.595; R(7,4)1.594; R(6,3)1.612; R(5,3)1.608; R(4,3)2.336; R(3,2)2.356; R(2,1)2.336	A(3,4,7)113.045; A(3,4,8)109.371; A(3,4,9)109.376; A(7,4,8)108.305; A(7,4,9)108.357; A(8,4,9)108.273; A(2,3,4)114.469; A(2,3,5)110.198; A(2,3,6)106.220; A(4,3,5)109.141; A(4,3,6)108.634; A(5,3,6)107.948; A(1,2,3)114.450; A(1,2,10)109.141; A(1,2,11)108.633; A(3,2,10)110.202; A(3,2,11)106.240; A(10,2,11)107.945; A(2,1,12)113.027; A(2,1,13)109.387; A(2,1,14)109.380; A(12,1,13)108.358; A(12,1,14)108.307; A(13,1,14)108.268
Si ₅ F ₁₀		R(15,1)1.611; R(14,1)1.609; R(13,2)1.611; R(12,2)1.609; R(11,3)1.612; R(10,3)1.608; R(9,4)1.613; R(8,4)1.608; R(7,5)1.613; R(6,5)1.608; R(5,1)2.380; R(5,4)2.375; R(4,3)2.375; R(3,2)2.380; R(2,1)2.384	A(6,5,7)108.134; A(6,5,1)112.577; A(6,5,4)113.004; A(7,5,1)108.325; A(7,5,4)108.323; A(1,5,4)106.317; A(8,4,9)108.128; A(8,4,5)113.312; A(8,4,3)113.278; A(9,4,5)108.034; A(9,4,3)108.036; A(5,4,3)105.825; A(10,3,11)108.134; A(10,3,4)112.877; A(10,3,2)112.441; A(11,3,4)108.421; A(11,3,2)108.406; A(4,3,2)106.416; A(12,2,13)108.128; A(12,2,3)111.197; A(12,2,1)111.002; A(13, 2,3)109.669; A(13,2,1)109.645; A(3,2,1)107.193; A(14,1,15)108.129; A(14,1,5)111.413; A(14,1,2)111.175; A(15,1,5)109.502; A(15,1,2)109.474; A(5,1,2)107.131
Si ₅ F ₁₂		R(17,5)1.596; R(16,5)1.594; R(15,5)1.594; R(14,4)1.611; R(13,4)1.609; R(12,2)1.613; R(11,2)1.613; R(10,3)1.609; R(9,3)1.611; R(8,1) 1.594; R(7,1)1.596; R(6,1)1.594; R(5,4)2.339; R(4,2)2.354; R(3,1)2.339; R(3,2)2.354	A(4,5,15)110.648; A(4,5,16)113.022; A(4,5,17)108.19; A(15,5,16)108.271; A(15,5,17)108.171; A(16,5,17)108.402; A(2,4,5)115.066; A(2,4,13)109.555; A(2,4,14)106.280; A(5,4,13)108.837; A(5,4,14)108.881; A(13,4,14)107.989; A(2,3,1)115.080; A(2,3,9)106.269; A(2,3,10)109.558; A(1,3,9)108.875; A(1,3,10)108.837; A(9,3,10)107.989; A(3,2,4)115.919; A(3,2,11)106.572; A(3,2,12)109.964; A(4,2,11)109.958; A(4,2,12)106.571; A(11,2,12)107.608; A(3,1,6)110.645; A(3,1,7)108.208; A(3,1,8)113.014; A(6,1,7)108.173; A(6,1,8)108.272; A(7,1,8)108.400
Si ₆ F ₁₂		R(18,6)1.609; R(17,6)1.614; R(16,5)1.614; R(15,5)1.609; R(14,4)1.614;	A(17,6,18)108.440; A(17,6,5)106.920; A(17,6,1)106.926; A(18,6,5)110.641; A(18,6,1)110.694; A(5,6,1)112.980; A(15,5,16)108.454; A(15,5,6)110.729; A(15,5,4)110.683; A(16,5,6)106.786; A(16,5,4)106.816; A(6,5,4)113.117; A(13,4,14)108.434; A(13,4,5)110.688; A(13,4,3)110.768;

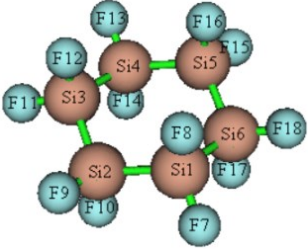
		R(13,4)1.609; R(12,3)1.614; R(11,3)1.609; R(10,2)1.614; R(9,2)1.609; R(8,1)1.614; R(7,1)1.609; R(6,5)2.366; R(6,1)2.367; R(5,4)2.366; R(4,3)2.366; R(3,2)2.366; R(2,1)2.366	A(14,4,5)106.860; A(14,4,3)106.817; A(5,4,3)113.021; A(11,3,12)108.441; A(11,3,4)110.697; A(11,3,2)110.640; A(12,3,4)106.926; A(12,3,2)106.920; A(4,3,2)112.978; A(9,2,10)108.455; A(9,2,3)110.729; A(9,2,1)110.687; A(10,2,3)106.783; A(10,2,1)106.808; A(3,2,1)113.122; A(7,1,8)108.433; A(7,1,6)110.764; A(7,1,2)110.683; A(8,1,6)106.820; A(8,1,2)106.869; A(6,1,2)113.019
--	---	--	--

Table S2. The theoretical and experimental frequency of optimised Si_xF_y ($x \leq 6$, $y \leq 12$) series

molecular	Theoretical value (vibration intensity>1)	Correction value (0.9614)	Experimental value	error
SiF	866.98(90)	833.51	/	/
SiF ₂	315.76(17); 835.25(106); 866.67(130)	303.57; 803.00; 833.22	855 ^[1]	2.34; 0.49
SiF ₃	278.40(10); 395.99(56); 827.18(59); 972.66(150)	267.65; 380.70; 795.25; 935.12	/	/
SiF ₄	378.48(45); 1046.15(201)	363.87; 1005.77	390; 1031 ^[2]	2.44
Si ₂ F ₆	98.08(4); 99.95(4); 300.76(27); 392.87(203); 822.33(229); 1005.23(282)	94.29; 96.09; 289.66; 377.71; 790.59; 966.43	104; 308; 992 ^[3-6]	7.69; 6.17; 2.77
Si ₃ F ₆	83.01(7); 302.20(63); 487.23(37); 861.92(232); 957.21(315)	79.81; 290.54; 468.42; 828.65; 920.26	/	/
Si ₃ F ₈	87.25(6); 118.21(4); 165.59(2); 230.23(4); 301.25(30); 310.68(44); 325.82(21); 356.21(16); 368.84(236); 491.43(24); 589.29(7); 837.87(151); 860.30(201); 909.34(2); 963.32(55); 994.80(74); 998.91(318); 1002.96(206)	83.88; 113.65; 159.20; 221.23; 289.60; 298.69; 313.24; 342.46; 354.60; 472.46; 566.54; 805.53; 827.09; 874.24; 926.14; 956.40; 960.35; 964.25	/	/
Si ₄ F ₈	91.14(9); 171.05(3); 305.12(102); 524.43(79); 886.95(243); 971.71(387)	87.62; 164.45; 293.34; 504.19; 852.71; 934.20	/	/
Si ₄ F ₁₀	91.63(6); 124.83(11); 235.09 (7); 296.31(94); 309.14(3); 316.21(14); 339.20(49); 348.93(245); 364.77(29); 464.09(19); 528.71(15); 611.84(4); 840.39(290); 846.97(53); 878.88(132); 955.53(29); 960.14(106); 994.23(52); 996.01(116); 998.13(281); 998.96(163)	92.90; 120.01; 226.02; 284.87; 297.21; 304.00; 326.11; 335.46; 350.69; 446.18; 508.30; 588.22; 807.95; 814.28; 844.96; 918.65; 923.08; 955.85; 957.56; 956.60; 960.40	/	/
Si ₅ F ₁₀	69.56(5) 84.80(3); 160.19(3); 167.75(3); 249.04(4); 254.86(5); 310.21(126); 320.98(9); 513.08(115); 852.93(43); 883.95(272); 915.45(2); 955.07(18); 958.14(12); 958.33(4); 959.04(29); 968.19(427)	66.87; 81.53; 154.01; 161.27; 239.43; 245.02; 298.24; 308.59; 493.28; 820.01; 849.83; 880.11; 918.20; 921.16; 921.34; 922.02; 930.82	/	/

Si ₅ F ₁₂	83.81(7); 91.79(2); 130.79(17); 245.12(29); 290.80(161); 306.66(33); 316.73(2); 317.47(29); 326.09(34); 330.25(214); 351.66(9); 368.91(12); 443.27(7); 491.64(34); 559.92(10); 632.54(3); 843.18(164); 844.06(220); 861.58(54); 883.24(165); 910.40(2); 948.43(26) 959.24(24); 961.53(160); 993.13(104); 993.70(106); 998.06(61); 998.69(292)	80.57; 88.25; 125.74; 235.66; 279.58; 294.82; 304.50; 305.22; 313.50; 317.50; 338.09; 354.67; 426.16; 472.66; 538.31; 608.12; 810.63; 811.48; 828.58; 849.15; 875.26; 911.82; 922.21; 924.41; 954.80; 955.34; 959.53; 960.14	/	/
Si ₆ F ₁₂	47.84(5); 101.83(3); 155.98(11); 201.03(10); 221.72(9); 325.66(156); 350.75(25); 482.70(130); 483.10(13); 847.00(158); 881.09(23); 881.20(234); 953.95(11); 954.50(121); 968.52(32)	45.99; 97.90; 149.89; 193.27; 213.16; 313.09; 337.21; 464.07; 464.45; 814.31; 847.08; 847.19; 916.34; 917.66; 931.14	/	/

Table S3. Si-Si and Si-F Mayer bond orders of Si_xF_y (x ≤ 6, y ≤ 12) series

Species	Si-Si bond order	Si-F bond order
SiF	/	B(1,2)0.9863
SiF ₂	/	B(1,3)1.0171; B(2, 3)1.0171
SiF ₃	/	B(1,2)0.9872; B(1,3)0.9872; B(2,3)0.9872
SiF ₄	/	B(1,2)1.0538; B(1,3)1.0538; B(1,4)1.0538; B(1,5)1.0538
Si ₂ F ₆	B(1,2)0.8471	B(1,3)1.0370; R(1,4)1.0370; B(1,5)1.0371; B(2,6)1.0370; B(2,7)1.0371; B(2,8)1.0370
Si ₃ F ₆	B(1,2)0.6521; B(1,3)0.6521; B(2,3)0.6520	B(1,8)1.0203; B(1,9)1.0203; B(2,4)1.0203; B(2,6)1.0203; B(3,5)1.0203; B(3,7)1.0203
Si ₃ F ₈	B(9,10)0.7884; B(10,11)0.7884	B(1,11)1.0354; B(2,11)1.0354; B(3,11)1.0366; B(4,9)1.0354; B(5,9)1.0354; B(6,9)1.0366; B(7,10)1.0217; B(8,10)1.0217
Si ₄ F ₈	B(1,2)0.0718; B(1,3)0.7614; B(2,3)0.7614; B(2,12)0.7614; B(3,12)0.0718	B(1,7)1.0233; B(1,8)1.0233; B(2,4)1.0232; B(2,11)1.0234; B(3,9)1.0233; B(3,10)1.0233; B(5,12)1.0233; B(6,12)1.0233
Si ₄ F ₁₀	B(1,2)0.7848; B(2,3)0.7312; B(3,4)0.7848	B(1,12)1.0409; B(1,13)1.0316; B(1,14)1.0324; B(2,10)1.0335; B(2,11)1.0157; B(3,5)1.0335; B(3,6)1.0157; B(4,7)1.0410; B(4,8)1.0324; B(4,9)1.0315
Si ₅ F ₁₀	B(1,2)0.7031; B(1,5)0.7086; B(2,3)0.7078; B(3,4)0.7133; B(4,5)0.7136	B(1,14)1.0337; B(1,15)1.0228; B(2,12)1.0327; B(2,13)1.0241; B(3,10)1.0403; B(3,11)1.0134; B(4,8)1.0427; B(4,9)1.0090; B(5,6)1.0409; B(5,7)1.0124
Si ₅ F ₁₂	B(1,3)0.7872; B(2,3)0.7288; B(2,4)0.7289; B(4,5)0.7872	B(1,6)1.0386; B(1,7)1.0264; B(1,8)1.0412; B(2,11)1.0224; B(2,12)1.0224; B(3,9)1.0152; B(3,10)1.0318; B(4,13)1.0317; B(4,14)1.0153; B(5,15)1.0386; B(5,16)1.0412; B(5,17)1.0263
Si ₆ F ₁₂	B(1,2)0.7177; B(1,6)0.7176; B(2,3)0.7178; B(3,4)0.7178; B(4,5)0.7178; B(5,6)0.7177	B(1,7)1.0346; B(1,8)1.0119; B(2,9)1.0346; B(2,10)1.0116; B(3,11)1.0341; B(3,12)1.0124; B(4,13)1.0346; B(4,14)1.0119; B(5,15)1.0346; B(5,16)1.0116; B(6,17)1.0124; B(6,18)1.0341

Table S4. Natural population analysis results of Si_xF_y ($x \leq 6, y \leq 12$) series

Mol	Ato	No	Natural charge	Natural Population				Natural Electron Configuration
				Cor	Val	Ryd	Total	
SiF	Si	1	0.6518	9.9998	3.3111	0.0373	13.3482	3S(1.88)3p(1.43)4S(0.01)3d(0.02)4p(0.01)
	F	2	-0.6518	2.0000	7.6389	0.0129	9.6518	2S(1.94)2p(5.69)3d(0.01)
	Total		0.0000	11.9998	10.9500	0.0502	23.0000	
SiF ₂	F	1	-0.6609	2.0000	7.6485	0.0124	9.6609	2S(1.94)2p(5.71)3d(0.01)
	F	2	-0.6609	2.0000	7.6485	0.0124	9.6609	2S(1.94)2p(5.71)3d(0.01)
	Si	3	1.3219	9.9997	2.6160	0.0624	12.6782	3S(1.75)3p(0.87)4S(0.02)3d(0.03)4p(0.01)
	Total		0.0000	13.9997	17.9131	0.0872	32.0000	
SiF ₃	Si	1	1.8617	9.9996	2.0406	0.0982	12.1383	3S(0.98)3p(1.06)4S(0.03)3d(0.05)4p(0.02)
	F	2	-0.6206	2.0000	7.6117	0.0089	9.6206	2S(1.93)2p(5.68)3d(0.01)
	F	3	-0.6206	2.0000	7.6117	0.0089	9.6206	2S(1.93)2p(5.68)3d(0.01)
	F	4	-0.6206	2.0000	7.6117	0.0089	9.6206	2S(1.93)2p(5.68)3d(0.01)
	Total		0.0000	15.9995	24.8756	0.1249	41.0000	
SiF ₄	Si	1	2.4600	10.0000	1.4500	0.0901	11.5401	3S(0.53)3p(0.92)3d(0.06)4p(0.03)
	F	2	-0.6150	2.0000	7.6055	0.0095	9.6150	2S(1.92)2p(5.68)3d(0.01)
	F	3	-0.6150	2.0000	7.6055	0.0095	9.6150	2S(1.92)2p(5.68)3d(0.01)
	F	4	-0.6150	2.0000	7.6055	0.0095	9.6150	2S(1.92)2p(5.68)3d(0.01)
	F	5	-0.6150	2.0000	7.6055	0.0095	9.6150	2S(1.92)2p(5.68)3d(0.01)
	Total		0.0000	17.9999	31.8719	0.1282	50.0000	
Si ₂ F ₆	Si	1	1.8567	9.9996	2.0568	0.0869	12.1433	3S(0.86)3p(1.20)4S(0.01)3d(0.06)4p(0.02)
	Si	2	1.8567	9.9996	2.0569	0.0869	12.1434	3S(0.86)3p(1.20)4S(0.01)3d(0.06)4p(0.02)
	F	3	-0.6189	2.0000	7.6107	0.0082	9.6189	2S(1.91)2p(5.70)3d(0.01)
	F	4	-0.6189	2.0000	7.6108	0.0082	9.6189	2S(1.91)2p(5.70)3d(0.01)
	F	5	-0.6189	2.0000	7.6107	0.0082	9.6189	2S(1.91)2p(5.70)3d(0.01)
	F	6	-0.6189	2.0000	7.6107	0.0082	9.6189	2S(1.91)2p(5.70)3d(0.01)
	F	7	-0.6189	2.0000	7.6107	0.0082	9.6189	2S(1.91)2p(5.70)3d(0.01)
	F	8	-0.6189	2.0000	7.6108	0.0082	9.6189	2S(1.91)2p(5.70)3d(0.01)
	total		0.0000	31.9990	49.7779	0.2231	82.0000	
Si ₃ F ₆	Si	1	1.2290	9.9986	2.6850	0.0873	12.771	3S(1.13)3p(1.55)4S(0.01)3d(0.06)4p(0.02)
	Si	2	1.2290	9.9986	2.6850	0.0873	12.771	3S(1.13)3p(1.55)4S(0.01)3d(0.06)4p(0.02)
	Si	3	1.2290	9.9986	2.6850	0.0873	12.771	3S(1.13)3p(1.55)4S(0.01)3d(0.06)4p(0.02)
	F	4	-0.6145	2.0000	7.6067	0.0078	9.6145	2S(1.91)2p(5.70)3d(0.01)
	F	5	-0.6145	2.0000	7.6067	0.0078	9.6145	2S(1.91)2p(5.70)3d(0.01)
	F	6	-0.6145	2.0000	7.6067	0.0078	9.6145	2S(1.91)2p(5.70)3d(0.01)
	F	7	-0.6145	2.0000	7.6067	0.0078	9.6145	2S(1.91)2p(5.70)3d(0.01)
	F	8	-0.6145	2.0000	7.6067	0.0078	9.6145	2S(1.91)2p(5.70)3d(0.01)
	F	9	-0.6145	2.0000	7.6067	0.0078	9.6145	2S(1.91)2p(5.70)3d(0.01)
total		0.0000	41.9957	53.6954	0.3089	96.0000		
Si ₃ F ₈	F	1	-0.6212	2.0000	7.6131	0.0081	9.6212	2S(1.91)2p(5.70)3d(0.01)
	F	2	-0.6212	2.0000	7.6131	0.0081	9.6212	2S(1.91)2p(5.70)3d(0.01)
	F	3	-0.6173	2.0000	7.6093	0.0081	9.6173	2S(1.91)2p(5.70)3d(0.01)

	F	4	-0.6212	2.0000	7.6131	0.0081	9.6212	2S(1.91)2p(5.70)3d(0.01)
	F	5	-0.6212	2.0000	7.6131	0.0081	9.6212	2S(1.91)2p(5.70)3d(0.01)
	F	6	-0.6173	2.0000	7.6093	0.0081	9.6173	2S(1.91)2p(5.70)3d(0.01)
	F	7	-0.6166	2.0000	7.6089	0.0078	9.6166	2S(1.90)2p(5.71)3d(0.01)
	F	8	-0.6166	2.0000	7.6089	0.0078	9.6166	2S(1.90)2p(5.71)3d(0.01)
	Si	9	1.9205	9.9994	1.9937	0.0864	12.0795	3S(0.83)3p(1.17)3d(0.06)4p(0.02)
	Si	10	1.1115	9.9992	2.8066	0.0827	12.8885	3S(1.12)3p(1.68)3d(0.06)4p(0.02)
	Si	11	1.9205	9.9994	1.9937	0.0864	12.0795	3S(0.83)3p(1.17)3d(0.06)4p(0.02)
	total		0.00000	45.9977	67.6827	0.3196	114.0000	
Si ₄ F ₈	Si	1	1.2255	29.9986	2.694	0.0819	12.7745	3S(1.05)3p(1.64)4S(0.01)3d(0.06)4p(0.02)
	Si	2	1.2255	9.9986	2.694	0.0819	12.7745	3S(1.05)3p(1.64)4S(0.01)3d(0.06)4p(0.02)
	Si	3	1.2255	9.9986	2.694	0.0819	12.7745	3S(1.05)3p(1.64)4S(0.01)3d(0.06)4p(0.02)
	F	4	-0.6128	2.0000	7.6051	0.0077	9.6128	2S(1.90)2p(5.70)3d(0.01)
	F	5	-0.6127	2.0000	7.6051	0.0077	9.6127	2S(1.90)2p(5.70)3d(0.01)
	F	6	-0.6128	2.0000	7.6051	0.0077	9.6128	2S(1.90)2p(5.70)3d(0.01)
	F	7	-0.6127	2.0000	7.6051	0.0077	9.6127	2S(1.90)2p(5.70)3d(0.01)
	F	8	-0.6127	2.0000	7.6051	0.0077	9.6127	2S(1.90)2p(5.70)3d(0.01)
	F	9	-0.6127	2.0000	7.6051	0.0077	9.6127	2S(1.90)2p(5.70)3d(0.01)
	F	10	-0.6127	2.0000	7.6051	0.0077	9.6127	2S(1.90)2p(5.70)3d(0.01)
	F	11	-0.6127	2.0000	7.6051	0.0077	9.6127	2S(1.90)2p(5.70)3d(0.01)
	Si	12	1.2255	9.9986	2.6940	0.0819	12.7745	3S(1.05)3p(1.64)4S(0.01)3d(0.06)4p(0.02)
	total		0.0000	55.9943	71.6168	0.3889	128.0000	
Si ₄ F ₁₀	Si	1	1.9185	9.9993	1.9955	0.0866	12.0815	3S(0.83)3p(1.17)4S(0.01)3d(0.06)4p(0.02)
	Si	2	1.1773	9.9989	2.7418	0.0821	12.8228	3S(1.10)3p(1.64)3d(0.06)4p(0.02)
	Si	3	1.1772	9.9989	2.7418	0.0821	12.8228	3S(1.10)3p(1.64)3d(0.06)4p(0.02)
	Si	4	1.9185	9.9993	1.9955	0.0866	12.0815	3S(0.83)3p(1.17)4S(0.01)3d(0.06)4p(0.02)
	F	5	-0.6150	2.0000	7.6073	0.0077	9.6150	2S(1.90)2p(5.70)3d(0.01)
	F	6	-0.6204	2.0000	7.6128	0.0077	9.6204	2S(1.90)2p(5.71)3d(0.01)
	F	7	-0.6178	2.0000	7.6098	0.0081	9.6178	2S(1.91)2p(5.70)3d(0.01)
	F	8	-0.6210	2.0000	7.613	0.0081	9.6210	2S(1.91)2p(5.70)3d(0.01)
	F	9	-0.6215	2.0000	7.6135	0.0081	9.6215	2S(1.91)2p(5.70)3d(0.01)
	F	10	-0.6150	2.0000	7.6073	0.0077	9.6150	2S(1.90)2p(5.70)3d(0.01)
	F	11	-0.6204	2.0000	7.6128	0.0077	9.6204	2S(1.90)2p(5.71)3d(0.01)
	F	12	-0.6178	2.0000	7.6098	0.0081	9.6178	2S(1.91)2p(5.70)3d(0.01)
	F	13	-0.6215	2.0000	7.6135	0.0081	9.6215	2S(1.91)2p(5.70)3d(0.01)
	F	14	-0.6210	2.0000	7.6130	0.0081	9.6210	2S(1.91)2p(5.70)3d(0.01)
total		0.0000	59.9963	85.5872	0.4165	46.0000		
Si ₅ F ₁₀	Si	1	1.2333	9.9987	2.6848	0.0832	12.7667	3S(1.08)3p(1.61)4S(0.01)3d(0.06)4p(0.02)
	Si	2	1.2334	9.9987	2.6847	0.0832	12.7666	3S(1.08)3p(1.61)4S(0.01)3d(0.06)4p(0.02)
	Si	3	1.2318	9.9986	2.6862	0.0834	12.7682	3S(1.07)3p(1.61)4S(0.01)3d(0.06)4p(0.02)
	Si	4	1.2308	9.9986	2.6871	0.0834	12.7692	3S(1.07)3p(1.61)4S(0.01)3d(0.06)4p(0.02)
	Si	5	1.2316	9.9986	2.6863	0.0834	12.7684	3S(1.07)3p(1.61)4S(0.01)3d(0.06)4p(0.02)
	F	6	-0.6134	2.0000	7.6058	0.0077	9.6134	2S(1.90)2p(5.70)3d(0.01)
	F	7	-0.6190	2.0000	7.6115	0.0076	9.6190	2S(1.90)2p(5.71)3d(0.01)

	F	8	-0.6130	2.0000	7.6053	0.0077	9.6130	2S(1.90)2p(5.70)3d(0.01)
	F	9	-0.6199	2.0000	7.6124	0.0076	9.6199	2S(1.90)2p(5.71)3d(0.01)
	F	10	-0.6135	2.0000	7.6059	0.0077	9.6135	2S(1.90)2p(5.70)3d(0.01)
	F	11	-0.6188	2.0000	7.6113	0.0076	9.6188	2S(1.90)2p(5.71)3d(0.01)
	F	12	-0.6149	2.0000	7.6073	0.0077	9.6149	2S(1.90)2p(5.70)3d(0.01)
	F	13	-0.6167	2.0000	7.6091	0.0076	9.6166	2S(1.90)2p(5.71)3d(0.01)
	F	14	-0.6147	2.0000	7.6071	0.0077	9.6147	2S(1.90)2p(5.70)3d(0.01)
	F	15	-0.6169	2.0000	7.6093	0.0076	9.6169	2S(1.90)2p(5.71)3d(0.01)
	total		0.0000	69.9931	89.5140	0.4929	160.0000	
Si ₅ F ₁₂	Si	1	1.9196	9.9993	1.9950	0.0861	12.0804	3S(0.83)3p(1.16)3d(0.06)4p(0.02)
	Si	2	1.2372	9.9987	2.6829	0.0812	12.7628	3S(1.08)3p(1.60)3d(0.05)4p(0.02)
	Si	3	1.17805	9.9989	2.7407	0.0823	12.8220	3S(1.10)3p(1.64)3d(0.06)4p(0.02)
	Si	4	1.1781	9.9989	2.7407	0.0823	12.8219	3S(1.10)3p(1.64)3d(0.06)4p(0.02)
	Si	5	1.9196	9.9993	1.9950	0.0861	12.0805	3S(0.83)3p(1.16)3d(0.06)4p(0.02)
	F	6	-0.6201	2.0000	7.6121	0.0081	9.6201	2S(1.91)2p(5.70)3d(0.01)
	F	7	-0.6227	2.0000	7.6147	0.0080	9.6227	2S(1.91)2p(5.70)3d(0.01)
	F	8	-0.6177	2.0000	7.6096	0.0080	9.6177	2S(1.91)2p(5.70)3d(0.01)
	F	9	-0.6193	2.0000	7.6117	0.0077	9.6193	2S(1.90)2p(5.71)3d(0.01)
	F	10	-0.6163	2.0000	7.6086	0.0077	9.6162	2S(1.90)2p(5.71)3d(0.01)
	F	11	-0.6202	2.0000	7.6126	0.0076	9.6202	2S(1.90)2p(5.71)3d(0.01)
	F	12	-0.6202	2.0000	7.6126	0.0076	9.6202	2S(1.90)2p(5.71)3d(0.01)
	F	13	-0.6163	2.0000	7.6086	0.0077	9.6163	2S(1.90)2p(5.71)3d(0.01)
	F	14	-0.6193	2.0000	7.6117	0.0077	9.6201	2S(1.90)2p(5.71)3d(0.01)
	F	15	-0.6201	2.0000	7.6121	0.0081	9.6201	2S(1.91)2p(5.70)3d(0.01)
	F	16	-0.6176	2.0000	7.6096	0.0080	9.6176	2S(1.91)2p(5.70)3d(0.01)
	F	17	-0.6227	2.0000	7.6147	0.0080	9.6227	2S(1.91)2p(5.70)3d(0.01)
	total		0.0000	73.9949	103.4928	0.5122	178.0000	
Si ₆ F ₁₂	Si	1	1.2335	9.9986	2.6838	0.0840	12.7665	3S(1.07)3p(1.62)4S(0.01)3d(0.06)4p(0.02)
	Si	2	1.2332	9.9986	2.6841	0.0841	12.7668	3S(1.07)3p(1.62)4S(0.01)3d(0.06)4p(0.02)
	Si	3	1.2337	9.9986	2.6837	0.0841	12.7664	3S(1.07)3p(1.62)4S(0.01)3d(0.06)4p(0.02)
	Si	4	1.2335	9.9986	2.6838	0.0841	12.7665	3S(1.07)3p(1.62)4S(0.01)3d(0.06)4p(0.02)
	Si	5	1.2333	9.9986	2.6841	0.0841	12.7668	3S(1.07)3p(1.62)4S(0.01)3d(0.06)4p(0.02)
	F	6	1.2337	9.9986	2.6836	0.0841	12.7663	3S(1.07)3p(1.62)4S(0.01)3d(0.06)4p(0.02)
	F	7	-0.6127	2.0000	7.6051	0.0076	9.6127	2S(1.90)2p(5.70)3d(0.01)
	F	8	-0.6207	2.0000	7.6132	0.0075	9.6208	2S(1.90)2p(5.71)3d(0.01)
	F	9	-0.6127	2.0000	7.6052	0.0076	9.6127]2S(1.90)2p(5.70)3d(0.01)
	F	10	-0.6208	2.0000	7.6132	0.0075	9.6208	2S(1.90)2p(5.71)3d(0.01)
	F	11	-0.6127	2.0000	7.6052	0.0076	9.6127	2S(1.90)2p(5.70)3d(0.01)
	F	12	-0.6207	2.0000	7.6132	0.0076	9.6207	2S(1.90)2p(5.71)3d(0.01)
	F	13	-0.6127	2.0000	7.6051	0.0076	9.6127	2S(1.90)2p(5.70)3d(0.01)
	F	14	-0.6208	2.0000	7.6132	0.0075	9.6208	2S(1.90)2p(5.71)3d(0.01)
	F	15	-0.6127	2.0000	7.6052	0.0075	9.6127	2S(1.90)2p(5.70)3d(0.01)
	F	16	-0.6208	2.0000	7.6133	0.0075	9.6208	2S(1.90)2p(5.71)3d(0.01)
	F	17	-0.6207	2.0000	7.6132	0.0075	9.6207	2S(1.90)2p(5.71)3d(0.01)

	F	18	-0.6127	2.0000	7.6052	0.0076	9.6128	2S(1.90)2p(5.70)3d(0.01)
	total		0.0000	83.9916	107.4133	0.5951	192.0000	

References

- 1 J. M. Bassler, P. L. Timms, J. L. Margrave, *Inorg Chem*, 1966, **5**, 729-732.
- 2 W. D. Reents, D. L. Wood, A. M. Mujsee, *Analytical Chemistry*, 1985, **57**, 104-109.
- 3 E. Hengge, S. Waldhor, *Z Naturforsch B: Chem Sci*, 1974, **B29**, 437-437.
- 4 T. Noda, H. Suzuki, H. Araki, et al, *Journal of Nuclear Materials*, 1996, **233**, 1496-1499.
- 5 J. L. Lyman, B. E. Newnam, T. Noda, et al, *The Journal of Physical Chemistry A*, 1999, **103**, 4227-4232.
- 6 Lyman, L. John, *Journal of Physical & Chemical Reference Data*, 2001, **30**, 165-186.