Supporting Information

	Aluminium			Fluorine		
Orbital	Exponent	s co-eff.	p co-eff.	Exponent	s co-eff.	p co-eff.
1s	70510	0.000226		13770	0.000877	
	10080	0.0019		1589	0.00195	
	2131	0.0110		327.6	0.0486	
	547.5	0.0509		91.46	0.1691	
	163.1	0.1697		30.50	0.3707	
	54.48	0.3688		11.46	0.4165	
	19.05	0.3546		4.66	0.1316	
	5.402	0.0443				
2sp	139.6	-0.01120	0.0089	27.802	-0.16	0.123
	32.53	-0.1136	0.0606	6.8982	-0.5333	0.6004
	10.23	-0.0711	0.1974	2.095	1.362	1.509
	3.810	0.5269	0.3186			
	1.517	0.7675	0.2995			
3sp	0.59	1.0	1.0	0.6723	1.0	1.0
4sp	0.35	1.0	1.0	0.217	1.0	1.0
3d	0.51	1.0 (d co-eff.)		1.28	1.0 (d co-eff.)	

TABLE I: The basis sets used for aluminium and fluorine.

	Carbon			Chlorine		
Orbital	Exponent	s co-eff	p co-eff	Exponent	s co-eff	p co-eff
1s	4563.24	0.00196665		135320	0.000225	
	682.024	0.0152306		19440	0.00191	
	154.973	0.0761269		4130	0.0111	
	44.4553	0.260801		1074	0.04989	
	13.0290	0.616462		323.4	0.1703	
	1.82773	0.221006		111.1	0.3683	
				43.4	0.4036	
				18.18	0.1459	
2sp	20.9642	0.114660	0.0402487	324.8	-0.00763	0.00820
	4.80331	0.919999	0.237594	73.00	-0.0829	0.0605
	1.45933	-0.00303068	0.815854	23.71	-0.1046	0.2115
				9.138	0.2540	0.3765
				3.930	0.695	0.3967
				1.329	0.399	0.186
3sp	0.483456	1.0	1.0	4.755	-0.3740	-0.034
				1.756	-0.4754	0.1617
				0.785	1.3400	0.9250
4sp	0.145585	1.0	1.0	0.29	1.0	1.0
5sp				0.090	1.0	1.0
3d	0.626	1.0 (d co-eff)		0.50	1.0 (d co-eff)	

TABLE II: The basis sets used for carbon and chlorine.