Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Electronic Supplementary Information

A two pocket Schiff-base molecule as chemosensor for Al^{3+}

Dinesh Maity, Sudipto Dey and Partha Roy*

Department of Chemistry, Jadavpur University, Jadavpur, Kolkata-700 032, India

E-mail: proy@chemistry.jdvu.ac.in

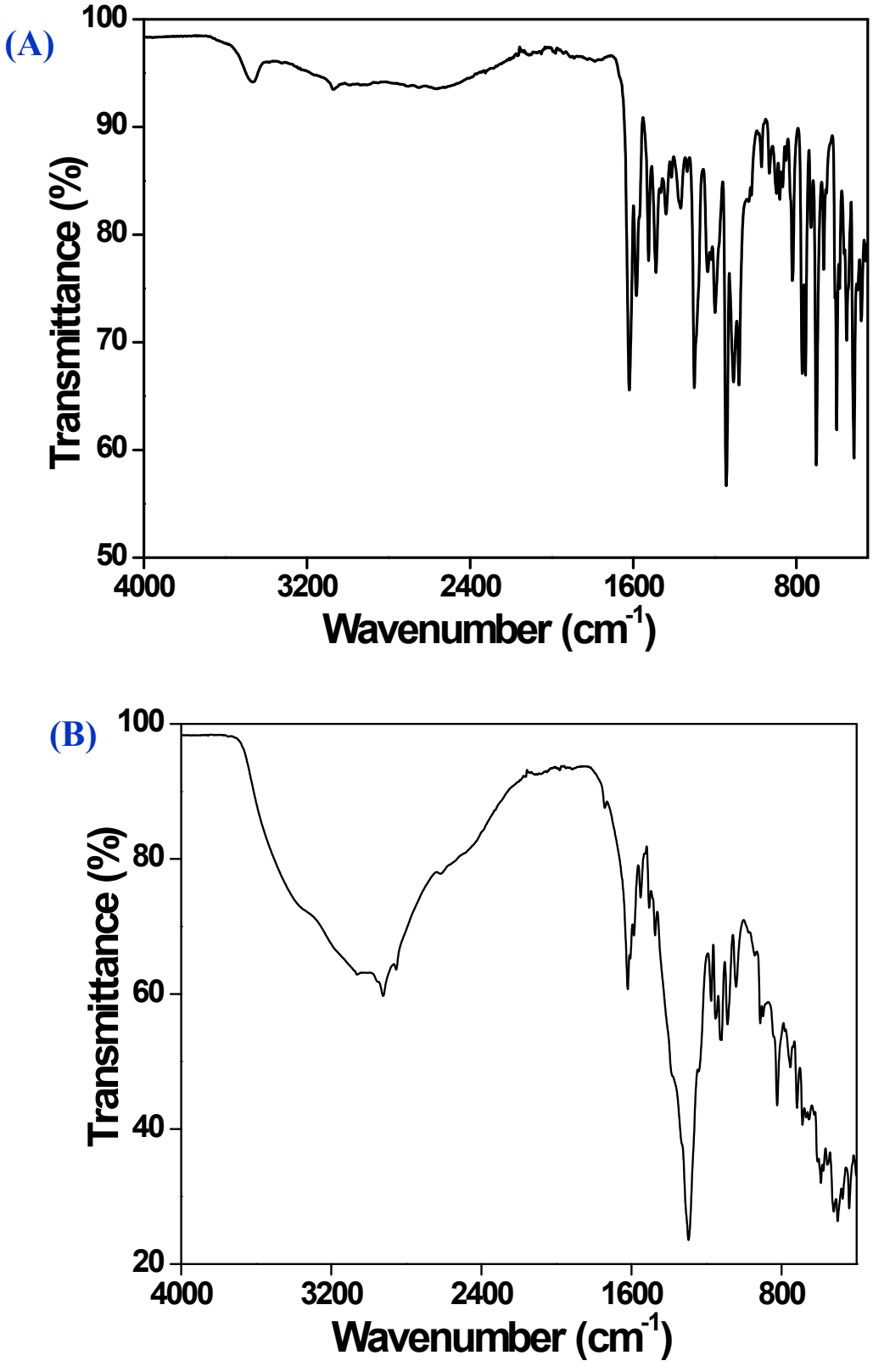

Fig. s1: FT-IR spectra of H_4L (A) and its complex with Al^{3+} (B).

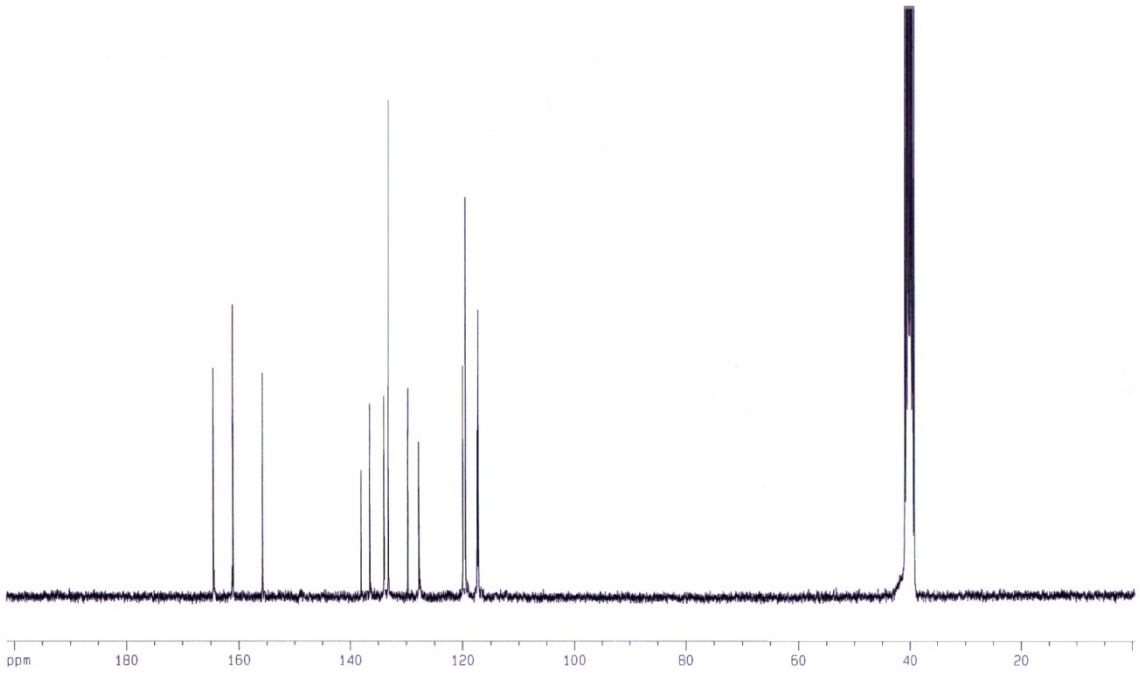

Fig. s2: ^{13}C NMR of H_4L in DMSO-d_6.

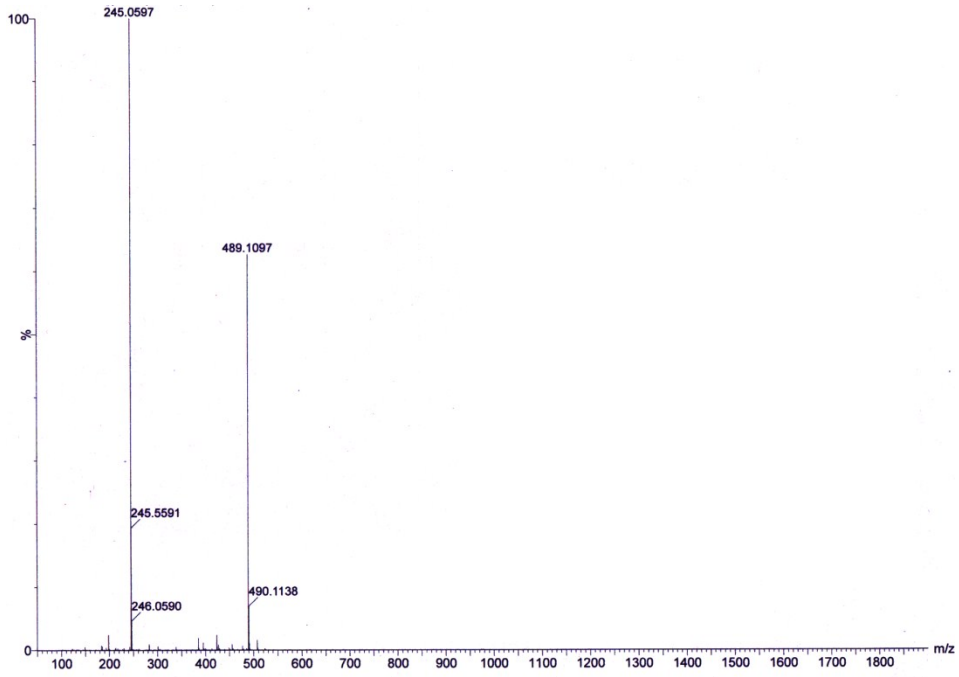

Fig. s3: ESI mass spectrum of H_4L in methanol.

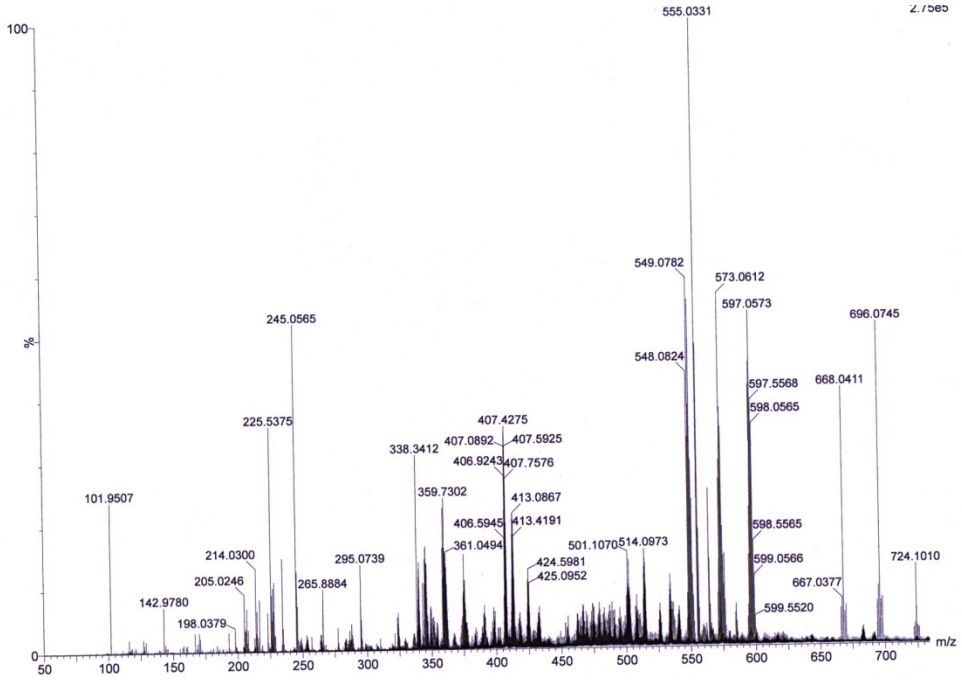

Fig. s4: ESI mass spectrum of H_4L in the presence of Al^{3+} in methanol.

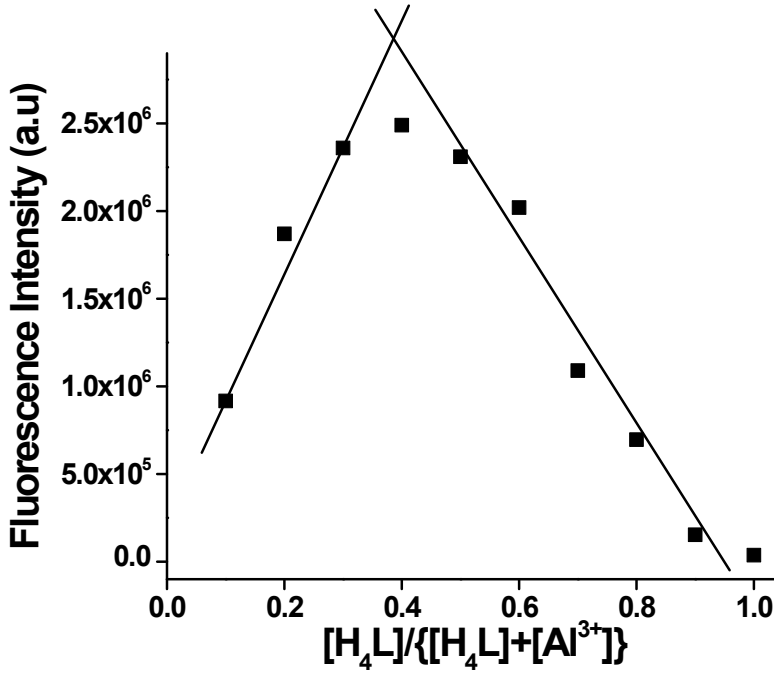

Fig. s5: Job's Plot showing 1:2 (ligand/metal) complex formation

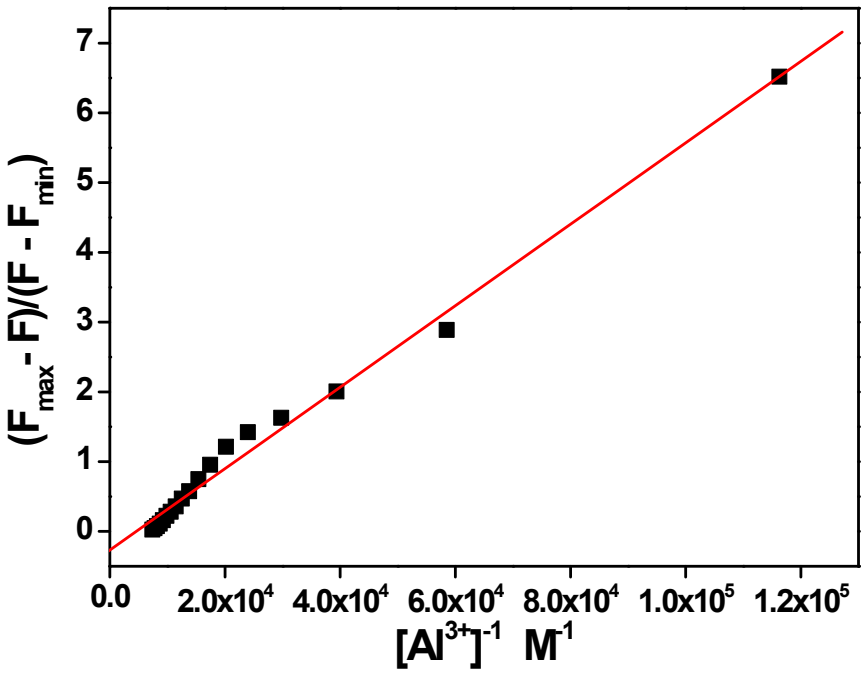

Fig. s6: Plot of $(F_{max} - F_0)/(F - F_0)$ vs. $1/[Al^{3+}]$. Binding constant, K has been determined from the slope as 1.712 x10^4 M^{-1}.

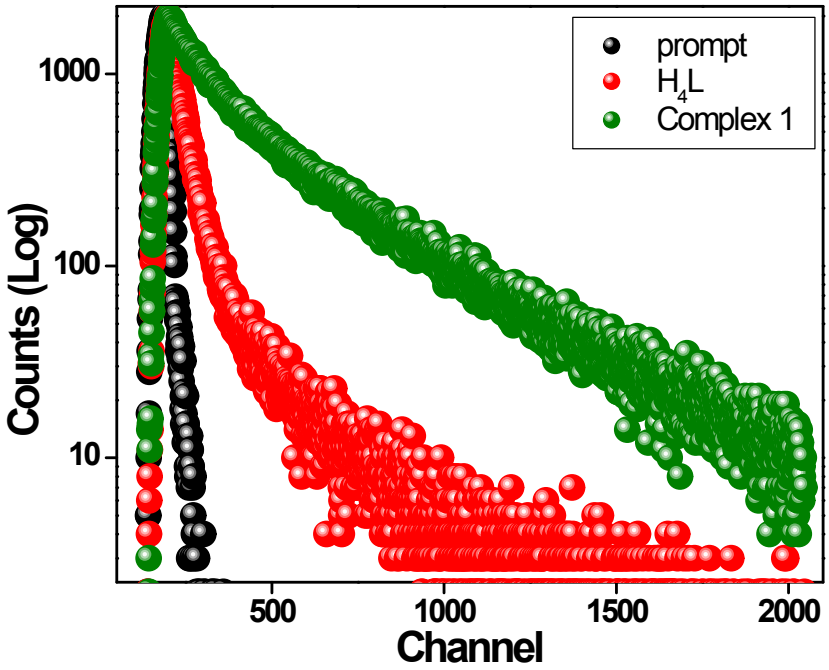

Fig. s7: Fluorescence decay patterns of H_4L and complex 1.

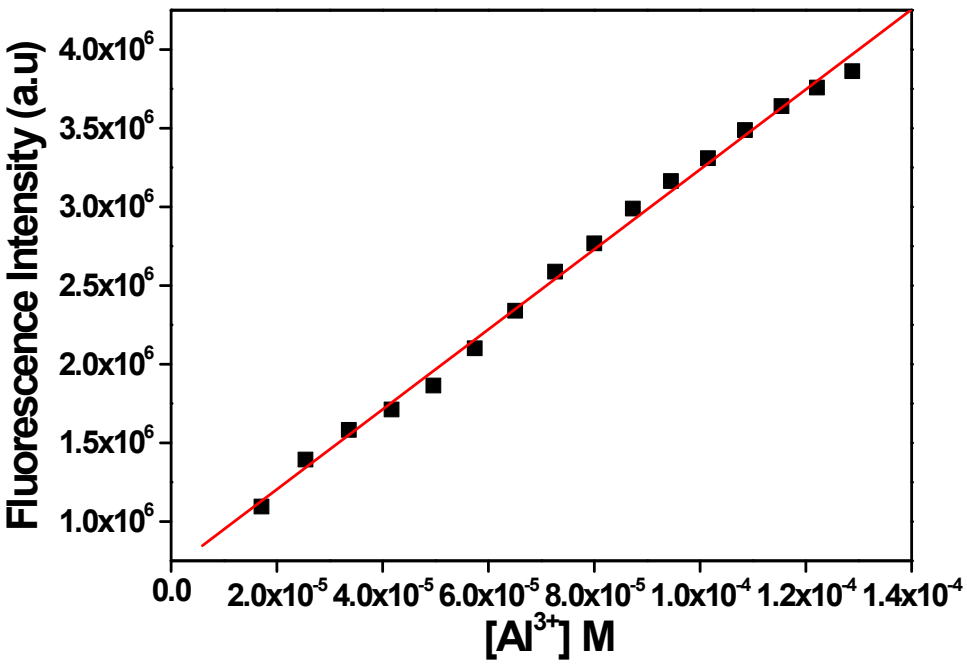

Fig. s8: Linear dynamic plot of F.I. (at 485 nm) vs. $[Al^{3+}]$ for the determination of S (slope). Slope = $2.5419\times10^{10} \pm 0.0425$ and R = 0.99805.

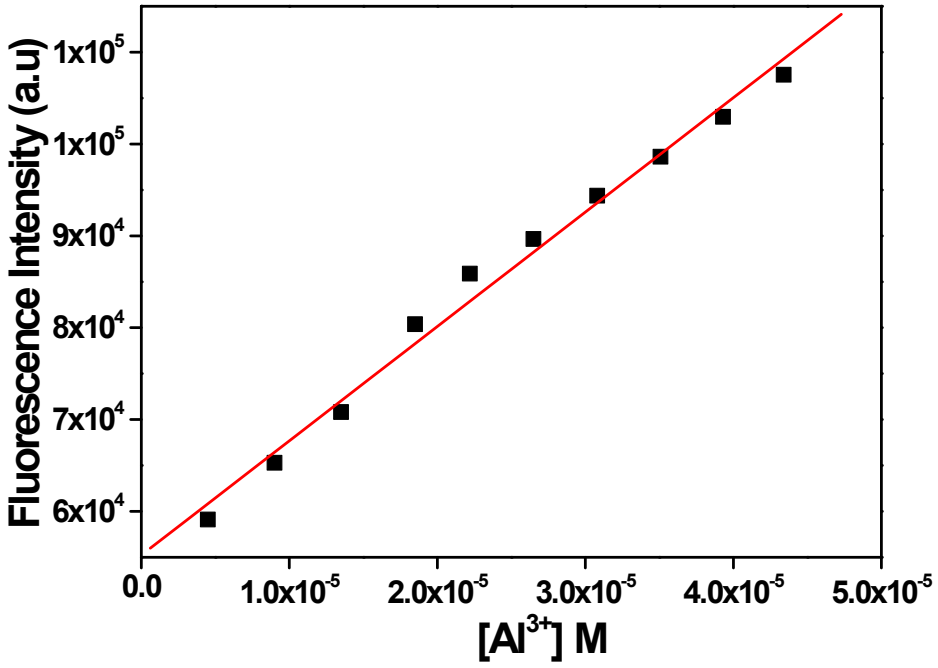

Fig. s9: Determination of Sb1 of the blank. Standard Deviation = 1824.68 and R = 0.99445.

Table s1: Selected bond lengths and bond angles for Lig and Lig-Al^{3+} complex in the ground state calculated at B3LYP Levels.

	Bond	Bond length(Å)	Bond angle	Angle(degree)
H_4L	O35-H55	0.9627	O35-C24-C22	117.728
	C24-O35	1.3636	C22-C20-N17	122.575
	C22-C24	1.4108	C20-N17-C14	122.295
	C20-C22	1.4603	N17-C14-C13	113.879
	C20-H44	1.0915	C14-C13-O16	119.442
	N17-C20	1.2827	O19-C1-C6	119.655
	C14-C13	1.4170	C6-N18-C21	122.062
	C13-O16	1.3444	N18-C21-C23	123.387
	O16-H42	0.9755	C21-C23-C33	121.037
	O19-H43	0.9743	C23-C33-O34	123.966
	C1-C6	1.4162		
	C6-N18	1.4013		
	N18-C21	1.2822		
	C21-H45	1.0981		
	C21-C23	1.4574		
	C23-C33	1.4129		
	C33-O34	1.3624		
	O34-H54	0.9618		
	Bond	Bond length(Å)	Bond angle	Angle (degree)
H_4L -Al^{3+} complex	Al37-O28	1.8200	N17-Al37-O28	109.500
	O28-C27	1.8412	O16-Al37-O28	109.500
	C27-C22	1.3371	O28-C27-C22	134.954
	C22-C20	1.3370	C22-C20-N17	120.001
	C20-N17	1.2660	C20-N17-C6	129.002
	N17-C6	1.2661	O16-C1-C6	111.002
	C6-C1	1.3369	N18-Al36-O34	103.838
	C1-O16	1.2250	O34-Al36-O35	141.128

	Al37-O16	1.7122	O34-C29-C21	124.303
	Al37-N17	1.8560	C21-C19-N18	120.006
	Al36-O34	1.1695	C19-N18-C12	129.003
	O34-C29	1.3550	O35-C11-C12	110.997
	C29-C21	1.3369		
	C21-C19	1.3370		
	C19-N18	1.2660		
	N18-C12	1.2660		
	C12-C11	1.3370		
	C11-O35	1.2250		
	O35-Al36	1.8917		
	Al36-N18	1.8561		