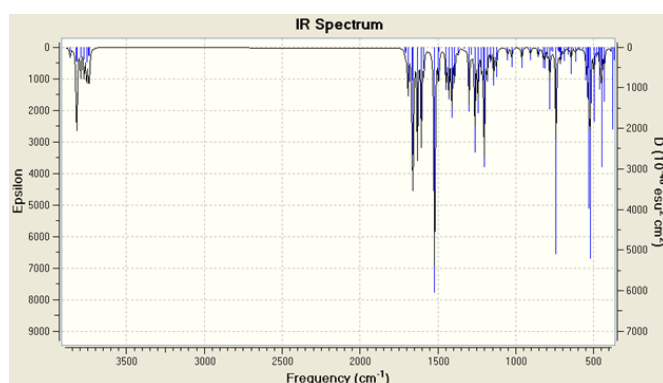


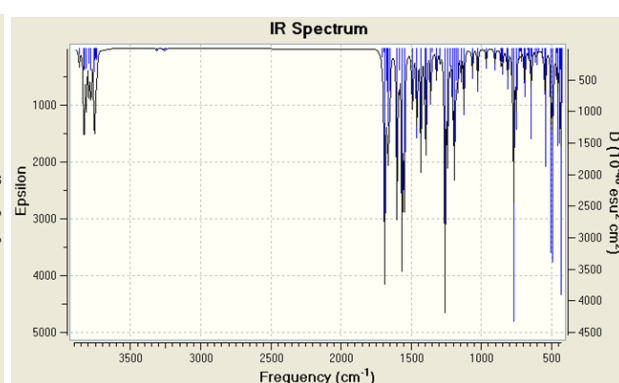
## Supplementary Information

**Table S1** Summary of the relevant data taken in 4 titrations for the system  $\text{Al}^{3+}$ –quercetin

$C_M$ , mol/dm <sup>3</sup>	$C_L$ , mol/dm <sup>3</sup>	pH <sub>range</sub>
$0.5 \cdot 10^{-3}$	$5 \cdot 10^{-3}$	2.0–3.6
$5 \cdot 10^{-3}$	$5 \cdot 10^{-3}$	1.6–2.8
$0.5 \cdot 10^{-3}$	$1 \cdot 10^{-3}$	2.1–3.4
$1 \cdot 10^{-3}$	$2 \cdot 10^{-3}$	1.8–3.2

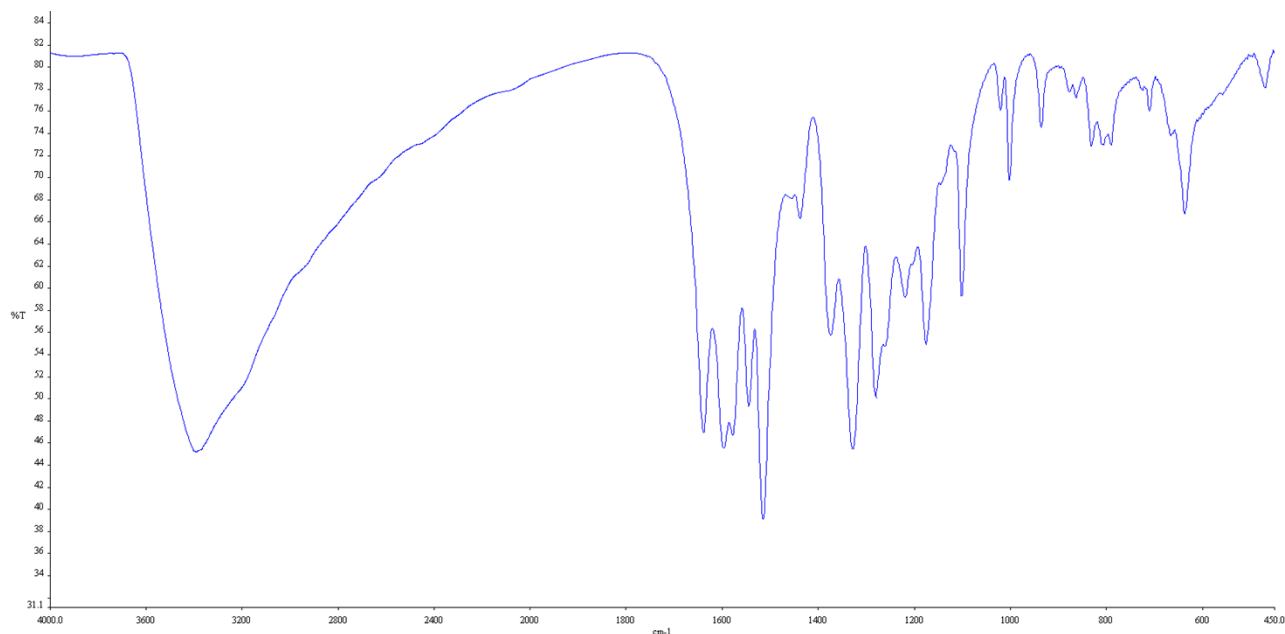


(a)

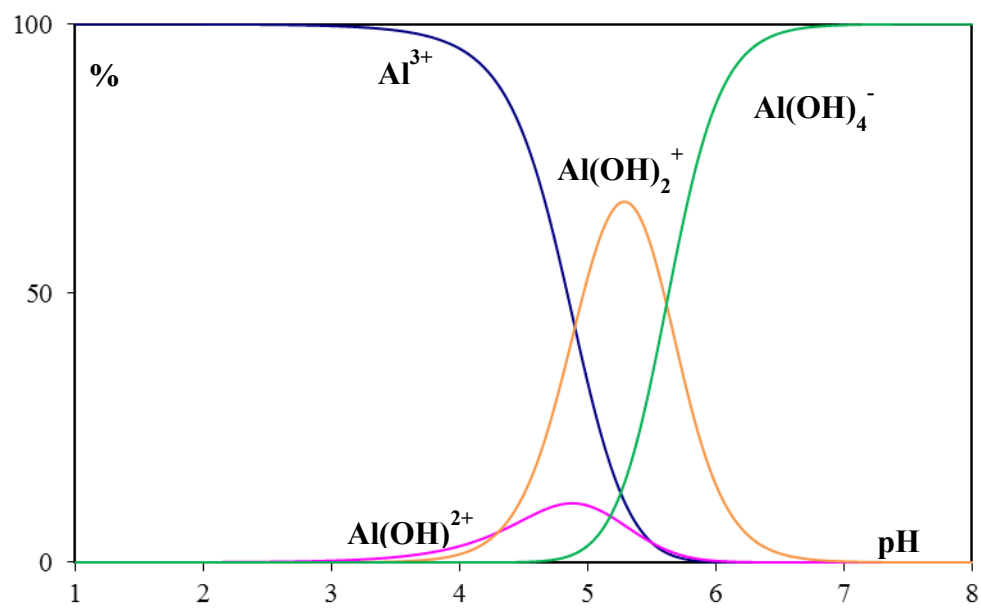


(b)

**Figure S1** The computed vibrational spectra of metallated complexes: **b3-4eq** (a) and **b4-5eq** (b)



**Figure S2** The experimental vibrational spectrum of metallated complex



**Figure S3** Distribution of Al(III) ion in the hydrolytical species for  $C_M = 5 \cdot 10^{-3} \text{ mol/dm}^3$