

Supplemental File

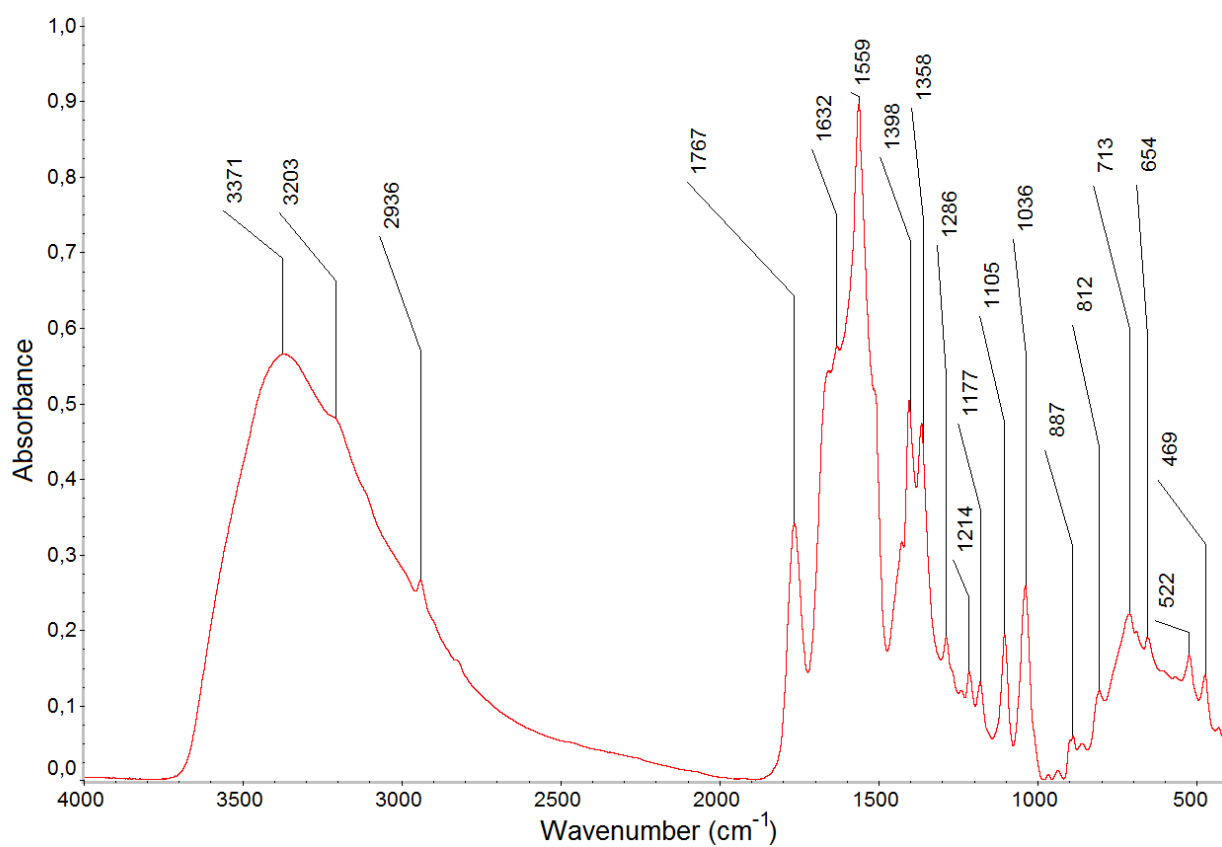


Fig. S1. FTIR spectra of [MgCefTria]·3H₂O

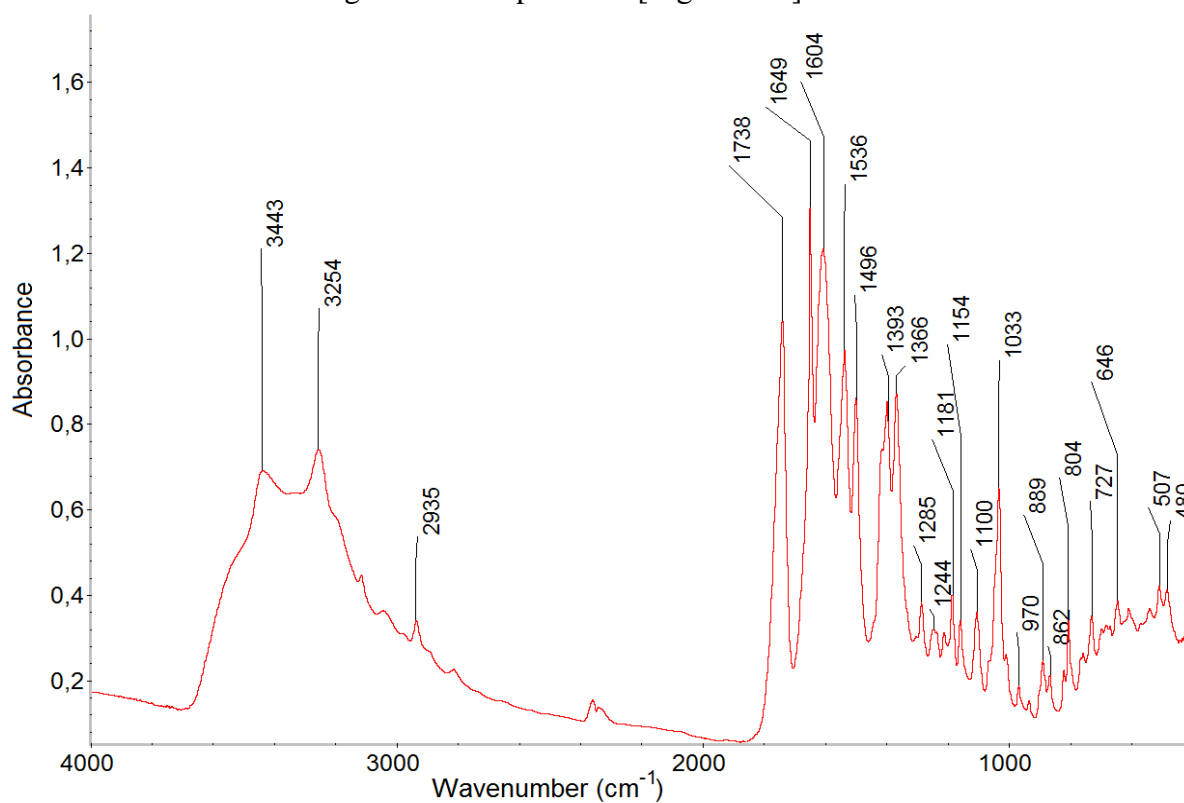


Fig. S2. FTIR spectra of Na₂CefTria·3.5H₂O

The favorable coordination of Mg(II) compound, E= -333.0611008421

C	1.988933622078	0.648313991713	0.994332539562
C	3.039815464632	1.072187647493	-0.033002934011
C	1.744528024234	-0.092283306974	-1.590470507293
O	2.215531112978	0.567857379739	2.263134551965
O	3.919521635235	1.887669536144	0.220770566908
N	0.783829107634	0.243774476873	0.564721980726
N	0.626970736742	0.006356259994	-0.801175327614
N	2.916789345658	0.388172119838	-1.250151648428
C	-0.773200605660	0.012066361016	-1.226409552447
S	1.605491245258	-1.068877613531	-3.114937346566
C	1.683357749232	-2.791686277738	-2.358513506951
C	0.475624526800	-3.169444285573	-1.520088629336
H	2.621354775792	-2.876213481716	-1.787465355197
H	1.764694793189	-3.435552681467	-3.258639404505
C	0.571428357723	-3.274768416533	-0.162594352915
C	1.901724758150	-3.238793224515	0.652293048701
C	-0.791014196627	-3.424177133462	-2.333768757933
S	-2.428636028894	-3.300905252507	-1.485187056305
O	1.921740468115	-2.453551585903	1.678814080228
O	2.804864177735	-3.985308487218	0.261909776863
C	-1.909606865127	-4.072158327138	0.094898641964
N	-0.621021424742	-3.522331947398	0.593695250730
C	-1.151639960477	-3.014846563646	1.752359024226
O	-0.693980683668	-2.288809443983	2.648110267808
C	-2.585979122812	-3.516622994425	1.410707300377
N	-3.525440890407	-2.423754253888	1.231009598460
H	-3.249872251542	-1.711376913238	0.551428952768
H	-0.856315614634	-2.681703703779	-3.153448181544
H	-0.710751190658	-4.425917219983	-2.808466058717
H	-1.879219312145	-5.173895070657	0.008454180022
H	-3.017643030611	-4.269754737070	2.091374637056
C	-4.364060710041	-1.991102509115	2.252642008962
C	-4.722485617881	-0.494681281757	2.104667153036
C	-3.597249744346	0.431058977822	2.397722381914
C	-3.408160595465	1.728579275219	1.944686353106
O	-4.735400881865	-2.685484654797	3.188953485543
N	-5.865646678350	-0.021863286979	1.724957436211
O	-6.756719177949	-1.038122384545	1.368929617381
C	-8.034358249376	-0.453657782812	1.050016368507
N	-2.537743301825	-0.101035276942	3.123755710604
C	-1.556464566279	0.748429362642	3.213682843546
S	-1.840074083182	2.310229871942	2.444362997872
N	-0.310095709876	0.381835850838	3.825513275253
H	-0.509419496751	-0.062203257991	4.734661417832
H	0.311775708839	1.190038857481	3.968388820190
H	-8.457652988156	0.064498957964	1.934857884105
H	-8.677751243042	-1.305277467425	0.762576323663
H	-7.937377270384	0.259065010885	0.204668961922
H	-1.327010933414	-0.787768970632	-0.704686480658
H	-1.221155183422	0.992436822552	-0.972587856551
H	-0.826573721609	-0.155888529914	-2.311743136943
H	-4.082607314144	2.342748129918	1.336950585413
Mg	0.906537151605	-0.980089370572	2.429955337892