

# Complex Ca(II) with Ceftriaxone: Synthesis, Structure, Spectral and Antibacterial Properties

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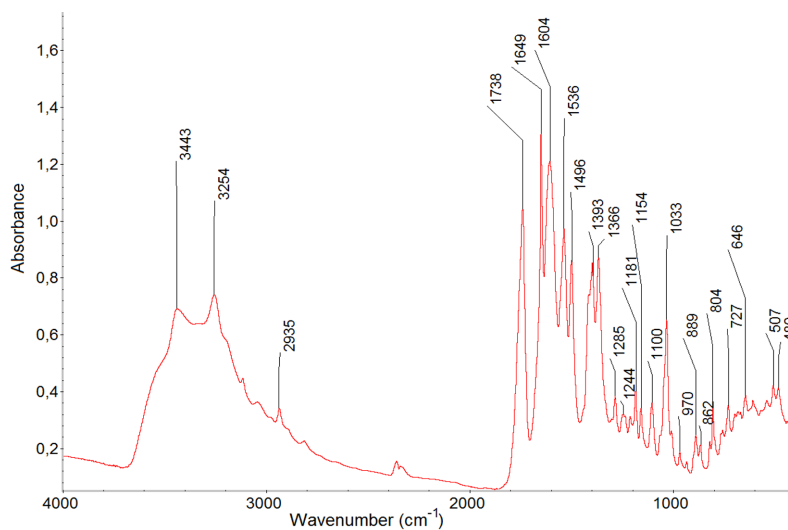


Fig. S1. IR spectra of Na<sub>2</sub>CefTria·3.5H<sub>2</sub>O

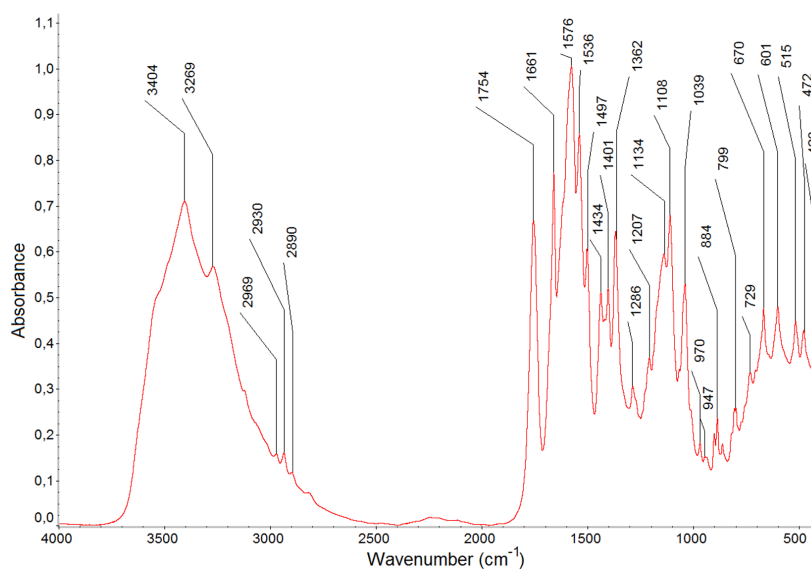


Fig. S2. IR spectra of [CaCefTria]·4H<sub>2</sub>O

**Optimized B3LYP/SBKJC(p, d) Atomic Coordinates**

The energies are in Hartree and the atomic coordinates are in Angstroms.

The favorable coordination of Ca(II) compound,  $E = -332.9171603951$

C	1.361535500358	0.851657540631	0.799433351624
C	2.481022570857	1.106060274523	-0.208215226905
C	1.202486706450	-0.152919641920	-1.708745156237
O	1.527698676289	0.958808656573	2.078421040054
O	3.406069930456	1.878677834171	0.025880536012
N	0.176549465910	0.401172455838	0.381465640816
N	0.071926616992	-0.011792794000	-0.946481653589
N	2.367587344906	0.355504076813	-1.385687247371
C	-1.320818413402	-0.137618680947	-1.386339192366
S	1.100416835493	-1.184631446479	-3.207550898561
C	1.408907912359	-2.873417497678	-2.439512924869
C	0.266001083881	-3.391879554464	-1.588064990288
H	2.355168761926	-2.830604356731	-1.875507759125
H	1.566640266310	-3.509330510392	-3.335619440488
C	0.381648219826	-3.423096027464	-0.229665023883
C	1.653832938261	-3.029709226630	0.573946419722
C	-0.971959616580	-3.829909772285	-2.362336763944
S	-2.605168936795	-3.716579857317	-1.495085472325
O	1.442579719322	-2.055706614069	1.388283538384
O	2.690667822759	-3.667899013344	0.365659222859
C	-2.025752241085	-4.402868655025	0.101422721949
N	-0.747292512637	-3.791993678294	0.565521188764
C	-1.264522832433	-3.370794359446	1.770205552190
O	-0.839000654636	-2.661810516816	2.689865573803
C	-2.688314032777	-3.878640154233	1.429558411340
N	-3.554012920387	-2.707368608794	1.270732433439
H	-3.481650414433	-2.208696019013	0.379387961817
H	-1.101621921475	-3.183333973580	-3.252913357519
H	-0.843222358601	-4.871791961766	-2.725901749742
H	-1.951248859139	-5.504557529487	0.047193666986
H	-3.140791746566	-4.632989578920	2.094296783036
C	-3.853549785266	-1.952143022108	2.392107099929
C	-4.022050387165	-0.437961077798	2.168649800007
C	-3.222264096542	0.445036837818	3.066229881591
C	-3.752261573294	1.445836246320	3.853667072270
O	-3.927092586201	-2.415838209926	3.527025381395
N	-4.842875239802	0.133447361958	1.345191540394
O	-5.569563105450	-0.805490398661	0.593392604736
C	-6.499612368054	-0.108364424968	-0.259386340857
N	-1.847164355148	0.250091050902	3.202402444574
C	-1.329775624396	1.101584777519	4.066840619141
S	-2.492257120855	2.211416824003	4.787738039843
N	0.055967307980	1.073833637503	4.325202965032
H	0.323943079843	1.538581267322	5.198170630646
H	0.623703594713	1.439278382336	3.516392304419
H	-7.218901320746	0.478002690792	0.347390647833
H	-7.028853231832	-0.903104407578	-0.817091776655
H	-5.960984101283	0.561386443755	-0.960674018547
H	-1.844177018183	-0.881597986623	-0.759595367675
H	-1.821406572171	0.843572592606	-1.273404915445
H	-1.348931983370	-0.461476204789	-2.436498388881
H	-4.806091477807	1.727678353228	3.957240913231
Ca	0.301019172853	-0.820300345642	2.501988945845