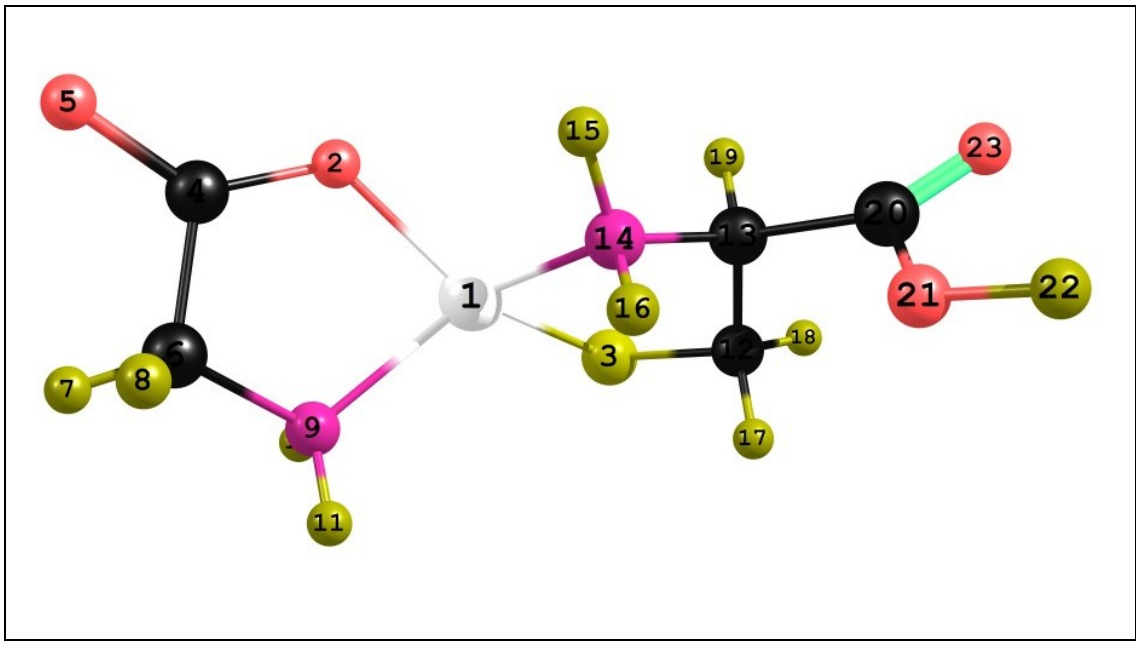
ANEXO A

A – 1

Coordenadas cartesianas do complexo [Zn(Cis)(Gli)] (sem água de hidratação)

N° átomo	massa at.		Coordenadas (Angstroms) X	Y	Z
1	30	0	0.734570	0.524138	-0.139064
2	8	0	2.010118	-0.600752	-1.050948
3	16	0	-0.729034	2.308992	-0.296508
4	6	0	3.099964	-0.979210	-0.406734
5	8	0	4.004698	-1.712015	-0.835710
6	6	0	3.191247	-0.485510	1.056684
7	1	0	4.229087	-0.249542	1.282998
8	1	0	2.887130	-1.308278	1.704972
9	7	0	2.277042	0.678640	1.312806
10	1	0	2.753259	1.556146	1.115524
11	1	0	1.968326	0.715753	2.279922
12	6	0	-2.197067	1.203219	0.191559
13	6	0	-2.067135	-0.224220	-0.384024
14	7	0	-0.816366	-0.880987	0.103415
15	1	0	-0.549139	-1.666937	-0.484799

16	1	0	-0.961431	-1.227005	1.049631
17	1	0	-2.277636	1.162045	1.276910
18	1	0	-3.086509	1.674119	-0.214940
19	1	0	-2.008875	-0.147905	-1.467585
20	6	0	-3.302280	-1.030638	-0.048353
21	8	0	-3.185718	-1.641318	1.191325
22	1	0	-4.003489	-2.119869	1.427546
23	8	0	-4.316144	-1.113658	-0.732478

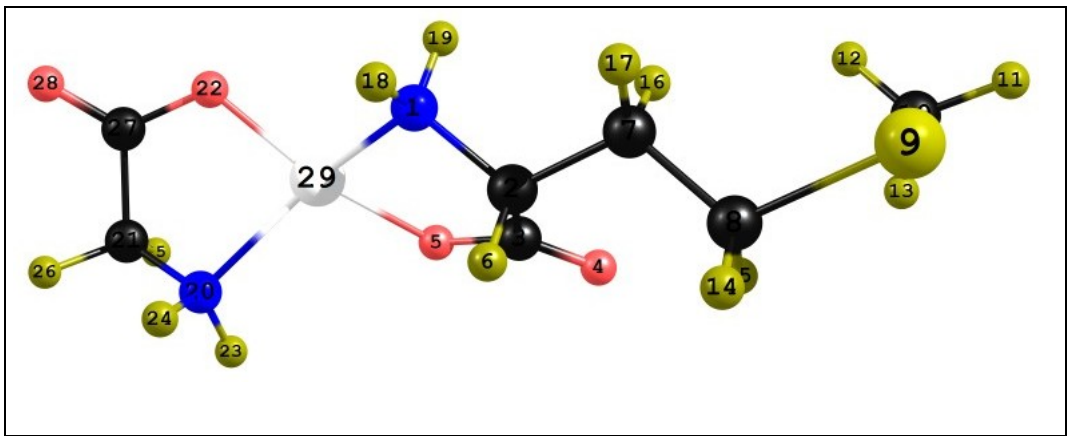


A – 2

Coordenadas cartesianas do complexo [Zn(Gli)(Met)] (sem água de hidratação)

N° átomo	massa at.		Coordenadas (Angstroms) X	Y	Z
1	7	0	0.008355	-1.086621	0.050000
2	6	0	-1.104135	-0.135502	0.417293
3	6	0	-0.849733	1.232060	-0.285918
4	8	0	-1.806348	1.979246	-0.551033
5	8	0	0.426738	1.504813	-0.505046
6	1	0	-0.994127	0.047246	1.491752
7	6	0	-2.496807	-0.728792	0.139542
8	6	0	-3.625979	0.000394	0.869611
9	16	0	-5.333767	-0.765800	0.534149
10	6	0	-5.697244	0.018179	-1.151346
11	1	0	-6.714082	-0.269608	-1.402594
12	1	0	-5.013611	-0.355814	-1.907373
13	1	0	-5.626705	1.098962	-1.072586
14	1	0	-3.507618	-0.068087	1.950922
15	1	0	-3.663675	1.044560	0.578675
16	1	0	-2.679771	-0.703648	-0.937455
17	1	0	-2.501999	-1.778684	0.446215
18	1	0	0.084830	-1.850746	0.715626
19	1	0	-0.170431	-1.502167	-0.863645
20	7	0	3.096164	0.914597	1.195560

21	6	0	4.427124	0.579727	0.577029
22	8	0	3.148191	-1.014050	-0.712465
23	1	0	2.965636	1.915835	1.307411
24	1	0	3.012481	0.479949	2.110507
25	1	0	4.691888	1.387820	-0.105927
26	1	0	5.214765	0.491711	1.321399
27	6	0	4.355684	-0.729129	-0.241745
28	8	0	5.392904	-1.379784	-0.428635
29	30	0	1.705524	0.112541	-0.175587

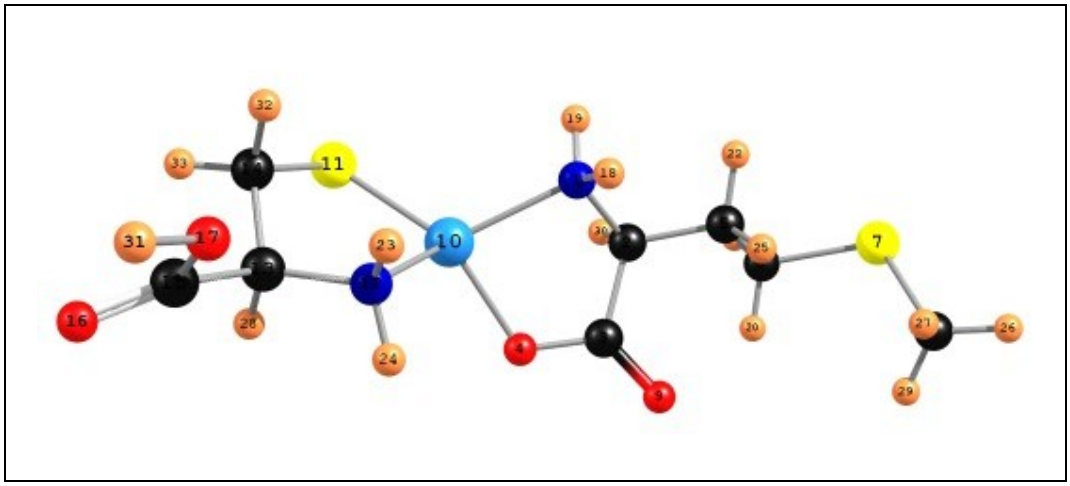


A – 3

Coordenadas cartesianas do complexo [Zn(Cis)(Met)] (sem água de hidratação)

			Coordenadas (Angstroms)		
N° átomo	massa at.		X	Y	Z
1	7	0	-0.779556	0.651920	-0.983821
2	6	0	-1.913490	0.549075	0.013610
3	6	0	-1.510515	-0.504364	1.086339
4	8	0	-0.222246	-0.495315	1.371645
5	6	0	-3.264847	0.269765	-0.661136
6	6	0	-4.461317	0.546954	0.250705
7	16	0	-6.125156	0.166772	-0.588906
8	6	0	-6.177457	-1.708399	-0.324522
9	8	0	-2.372750	-1.241783	1.597471
10	30	0	0.946319	0.541378	0.219107
11	16	0	2.497804	2.253762	0.129840
12	7	0	2.383410	-0.952746	-0.106750
13	6	0	3.709200	-0.343688	0.215967
14	6	0	3.850267	1.045452	-0.444405
15	6	0	4.860601	-1.231908	-0.200534
16	8	0	5.934637	-1.337131	0.380828
17	8	0	4.585000	-1.894194	-1.386883
18	1	0	-0.826087	-0.134173	-1.630127
19	1	0	-0.849350	1.507201	-1.529495
20	1	0	-4.403094	-0.048314	1.155834
21	1	0	-4.524083	1.602074	0.514918

22	1	0	-3.354855	0.890613	-1.557263
23	1	0	2.412881	-1.353948	-1.041613
24	1	0	2.134557	-1.690375	0.548725
25	1	0	-3.286057	-0.774336	-0.982860
26	1	0	-7.133171	-2.040521	-0.720023
27	1	0	-5.368474	-2.196024	-0.860118
28	1	0	3.768131	-0.213626	1.294218
29	1	0	-6.118538	-1.928360	0.737081
30	1	0	-1.945265	1.518699	0.520434
31	1	0	5.348699	-2.427329	-1.679912
32	1	0	3.814326	0.949263	-1.528663
33	1	0	4.799680	1.485098	-0.155930

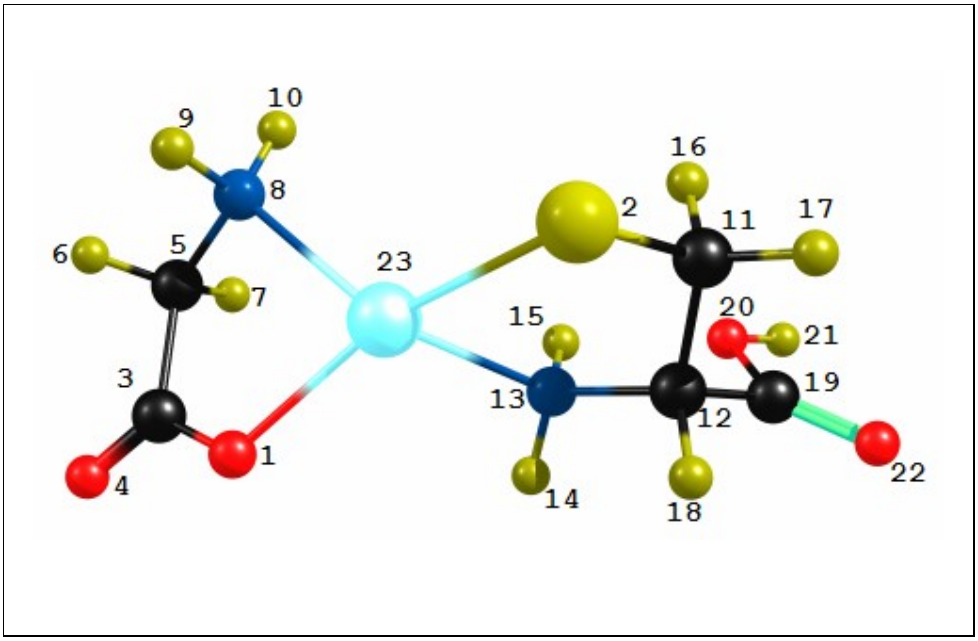


A – 4

Coordenadas cartesianas do complexo [Cd(Cis)(Gli)] (sem água de hidratação)

			Coordenadas (Angstroms)		
N° átomo	massa at.		X	Y	Z
1	8	0	2.283515	-0.448711	-1.151964
2	16	0	-1.105183	2.307731	-0.174187
3	6	0	3.264787	-0.986412	-0.451189
4	8	0	4.183092	-1.694848	-0.876550
5	6	0	3.225443	-0.760637	1.104127
6	1	0	4.257244	-0.656933	1.447885
7	1	0	2.803382	-1.666528	1.552496
8	7	0	2.356005	0.398992	1.531377
9	1	0	2.874331	1.282765	1.444316
10	1	0	2.053237	0.308462	2.508068
11	6	0	-2.444085	1.038645	0.315493
12	6	0	-2.334255	-0.301069	-0.451786
13	7	0	-1.058197	-1.021826	-0.096520
14	1	0	-0.845297	-1.742297	-0.798242
15	1	0	-1.214839	-1.492096	0.805489
16	1	0	-2.407259	0.839505	1.390344
17	1	0	-3.405390	1.495265	0.071989
18	1	0	-2.351009	-0.100572	-1.523380
19	6	0	-3.549506	-1.140339	-0.082506
20	8	0	-3.276099	-1.849880	1.083967
21	1	0	-4.092988	-2.347846	1.363227

22	8	0	-4.635166	-1.161754	-0.637578
23	48	0	0.698121	0.534517	-0.113897

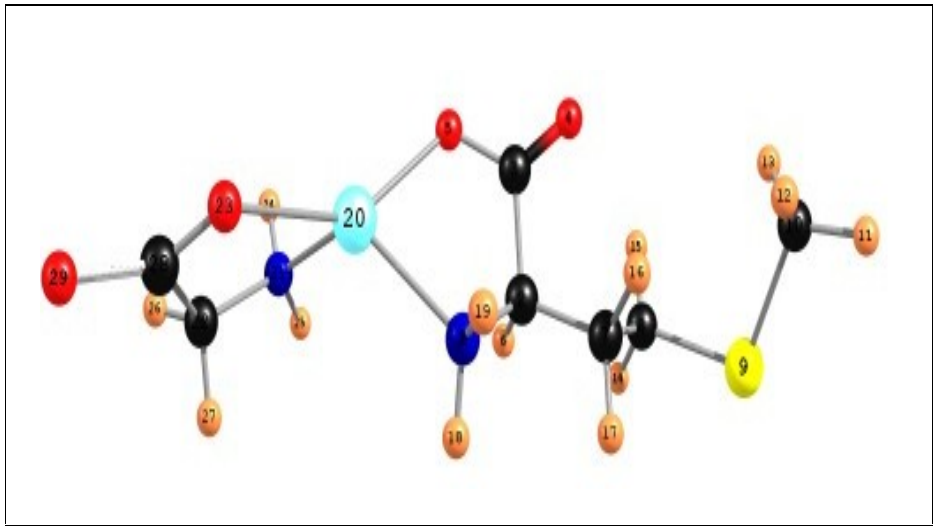


A – 5

Coordenadas cartesianas do complexo [Cd(Gli)(Met)] (sem água de hidratação).

			Coordenadas (Angstroms)		
N° átomo	massa at.		X	Y	Z
1	7	0	-0.280016	-1.080572	-0.352232
2	6	0	-1.408018	-0.313934	0.328990
3	6	0	-1.251740	1.225231	0.031128
4	8	0	-2.272146	1.898297	-0.178036
5	8	0	-0.016086	1.689103	0.068816
6	1	0	-1.253226	-0.457304	1.406424
7	6	0	-2.796012	-0.834939	-0.081139
8	6	0	-3.895955	-0.325615	0.862456
9	16	0	-5.616942	-0.947738	0.344466
10	6	0	-5.957407	0.288351	-1.061853
11	1	0	-6.952478	0.047808	-1.437875
12	1	0	-5.217086	0.169478	-1.853176
13	1	0	-5.935258	1.301834	-0.661012
14	1	0	-3.754888	-0.701807	1.879363
15	1	0	-3.892975	0.763021	0.852296
16	1	0	-3.007606	-0.486720	-1.098044
17	1	0	-2.800564	-1.931407	-0.075761
18	1	0	-0.223961	-2.039464	0.013232
19	1	0	-0.477211	-1.146942	-1.361735
20	48	0	1.576397	0.293649	-0.107145
21	7	0	3.144971	0.270661	1.606660

22	6	0	4.254367	-0.612307	1.075525
23	8	0	3.327202	-0.223399	-1.178588
24	1	0	3.473768	1.242110	1.686600
25	1	0	2.836901	-0.031953	2.538072
26	1	0	5.227929	-0.348383	1.493646
27	1	0	4.018811	-1.640886	1.369288
28	6	0	4.393690	-0.596546	-0.489826
29	8	0	5.470231	-0.986854	-0.948753

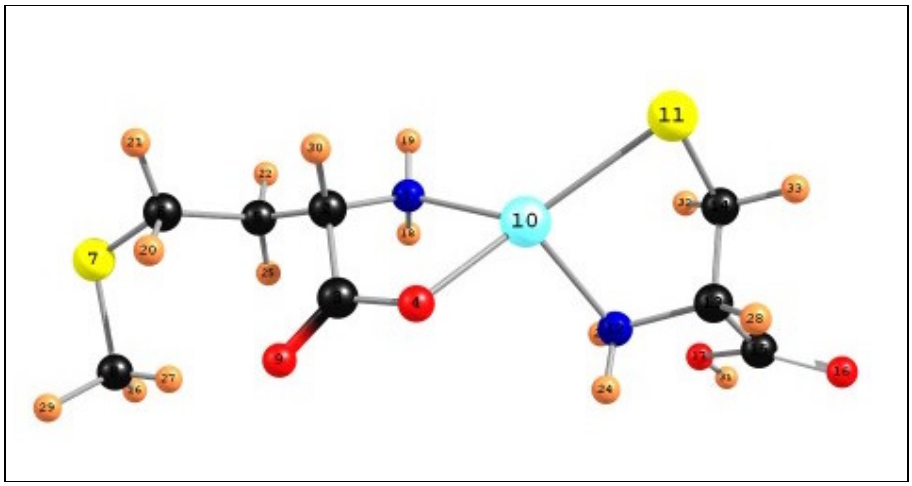


A – 6

Coordenadas cartesianas do complexo [Cd(Cis)(Met)] (sem água de hidratação).

			Coordenadas (Angstroms)		
N° átomo	massa at.		X	Y	Z
1	7	0	-1.006577	-0.703381	1.199675
2	6	0	-2.195672	-0.712413	0.241799
3	6	0	-1.881569	0.299134	-0.920535
4	8	0	-0.705472	0.131381	-1.487137
5	6	0	-3.517243	-0.365846	0.937142
6	6	0	-4.724271	-0.691654	0.037757
7	16	0	-6.268321	0.287558	0.565724
8	6	0	-5.792481	1.960123	-0.245994
9	8	0	-2.723970	1.161156	-1.232091
10	48	0	0.842860	-0.674963	-0.236817
11	16	0	2.859379	-2.186371	-0.053521
12	7	0	2.353668	1.109056	-0.097303
13	6	0	3.745492	0.563682	-0.294494
14	6	0	3.953351	-0.732032	0.526168
15	6	0	4.791936	1.569517	0.166267
16	8	0	5.921765	1.716196	-0.268471
17	8	0	4.298168	2.273453	1.260791
18	1	0	-1.056383	0.141549	1.786737
19	1	0	-1.037648	-1.520232	1.822582
20	1	0	-4.510275	-0.416507	-0.993613
21	1	0	-5.001316	-1.746145	0.099313
22	1	0	-3.613174	-0.912911	1.882373
23	1	0	2.350001	1.621496	0.795339
24	1	0	2.115900	1.772715	-0.845679
25	1	0	-3.511932	0.706666	1.154345
26	1	0	-5.939495	2.744744	0.495874
27	1	0	-4.747167	1.895021	-0.555696
28	1	0	3.903021	0.344730	-1.351004

29	1	0	-6.440428	2.117807	-1.107880
30	1	0	-2.224705	-1.721007	-0.186771
31	1	0	5.005409	2.886331	1.603462
32	1	0	3.775152	-0.519282	1.584058
33	1	0	4.987969	-1.056025	0.398521

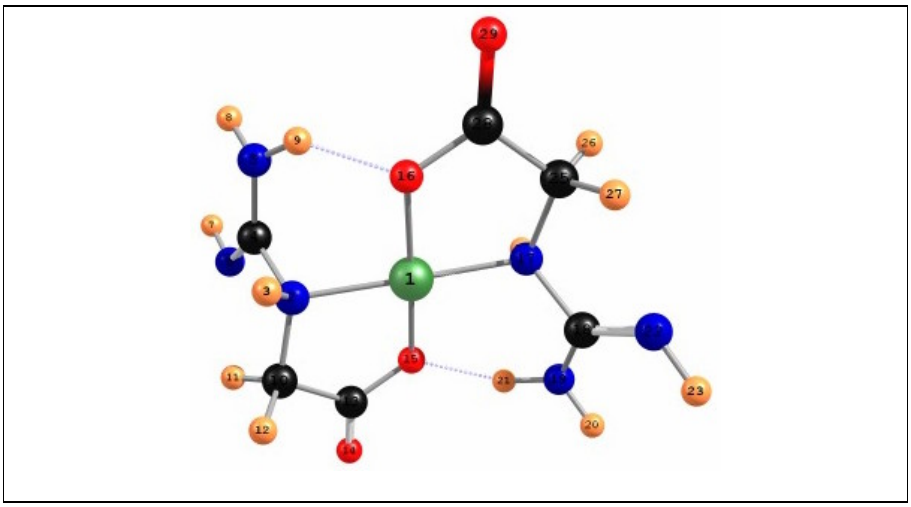


A – 7

Coordenadas cartesianas do complexo [Ni(Gaa)$_2$] (sem água de hidratação).

			Coordenadas Cartesianas		
Núm. Átomo		**massa at.**	**X**	**Y**	**Z**
1	28	0	0.013306	0.038879	0.054327
2	7	0	-1.806116	0.385335	0.696600
3	1	0	-1.673244	0.829436	1.604035
4	6	0	-2.521209	1.355794	-0.170468
5	7	0	-1.958920	2.597638	-0.094514
6	7	0	-3.547116	0.929497	-0.808126
7	1	0	-3.994602	1.606451	-1.425309
8	1	0	-2.376529	3.360064	-0.597743
9	1	0	-0.991238	2.688377	0.220012
10	6	0	-2.507950	-0.938369	0.852269
11	1	0	-3.523590	-0.843722	0.479725
12	1	0	-2.525774	-1.201193	1.909490
13	6	0	-1.784787	-2.028426	0.077289
14	8	0	-2.251838	-3.160989	-0.063483
15	8	0	-0.585267	-1.641921	-0.394896
16	8	0	0.553278	1.753080	0.453363
17	7	0	1.848220	-0.282572	-0.590014
18	6	0	2.487644	-1.509591	-0.045151
19	7	0	1.886398	-2.640792	-0.519827
20	1	0	2.275383	-3.533417	-0.268335
21	1	0	0.884552	-2.601859	-0.726306
22	7	0	3.502570	-1.354342	0.721889
23	1	0	3.886115	-2.210493	1.120540
24	1	0	1.716714	-0.439157	-1.589213
25	6	0	2.659750	0.969732	-0.370902
26	1	0	3.219289	1.221915	-1.269321
27	1	0	3.377135	0.738375	0.415988

28	6	0	1.782235	2.129569	0.052401
29	8	0	2.181808	3.297457	0.053840

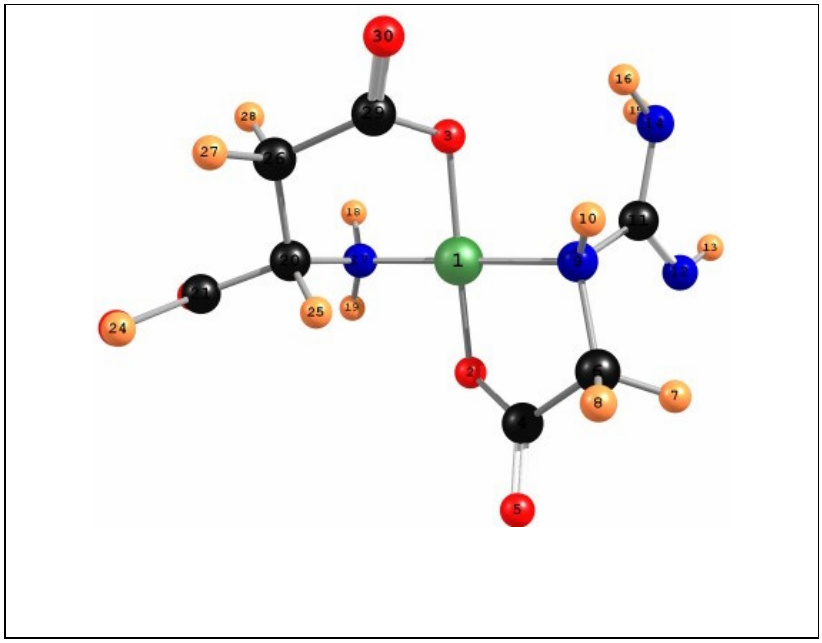


A – 8

Coordenadas cartesianas do complexo [Ni(Asp)(Gaa)] (sem água de hidratação).

			Coordenadas Cartesianas		
Núm.	**Átomo**	**massa at.**	**X**	**Y**	**Z**
1	28	0	-0.370130	0.034932	-0.305727
2	8	0	-0.566713	1.852786	-0.504400
3	8	0	-0.208605	-1.809421	-0.252342
4	6	0	-1.282425	2.251678	0.538441
5	8	0	-1.197790	3.428164	0.847382
6	6	0	-2.176752	1.230739	1.244908
7	1	0	-3.231811	1.594200	1.186157
8	1	0	-1.958513	1.240023	2.341295
9	7	0	-1.978262	-0.127879	0.636287
10	1	0	-1.956021	-0.802748	1.373122
11	6	0	-3.043668	-0.570985	-0.327499
12	7	0	-3.862530	0.311522	-0.810086
13	1	0	-4.550808	0.019852	-1.455126
14	7	0	-3.282869	-1.989186	-0.548831
15	1	0	-3.251451	-2.196825	-1.523900
16	1	0	-2.670035	-2.595922	-0.045526
17	7	0	1.244362	0.203336	-1.229461
18	1	0	1.417476	-0.500517	-1.915246
19	1	0	1.440637	1.095327	-1.631694
20	6	0	2.122678	-0.018292	-0.012786
21	6	0	3.529091	0.529073	-0.217934
22	8	0	4.041504	0.799787	-1.284192
23	8	0	4.359763	0.771187	0.812392
24	1	0	3.948770	0.552593	1.639912
25	1	0	1.607478	0.540353	0.838430
26	6	0	2.206390	-1.506729	0.356856
27	1	0	2.795506	-1.625124	1.286005

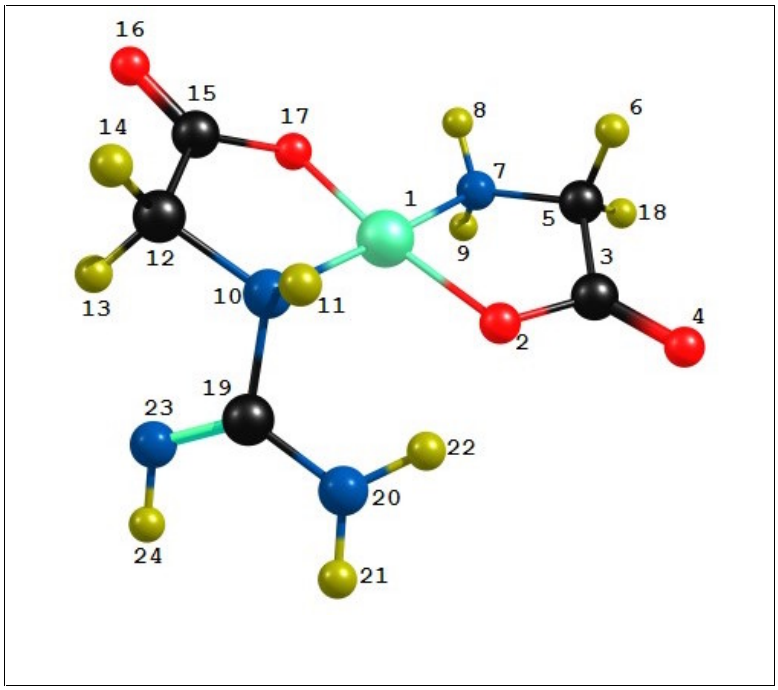
28	1	0	2.736321	-2.089200	-0.423310
29	6	0	0.811025	-2.115692	0.550659
30	8	0	0.595986	-3.016682	1.351037



A – 9

Coordenadas cartesianas do complexo [Ni(Gaa)(Gli)] (sem água de hidratação).

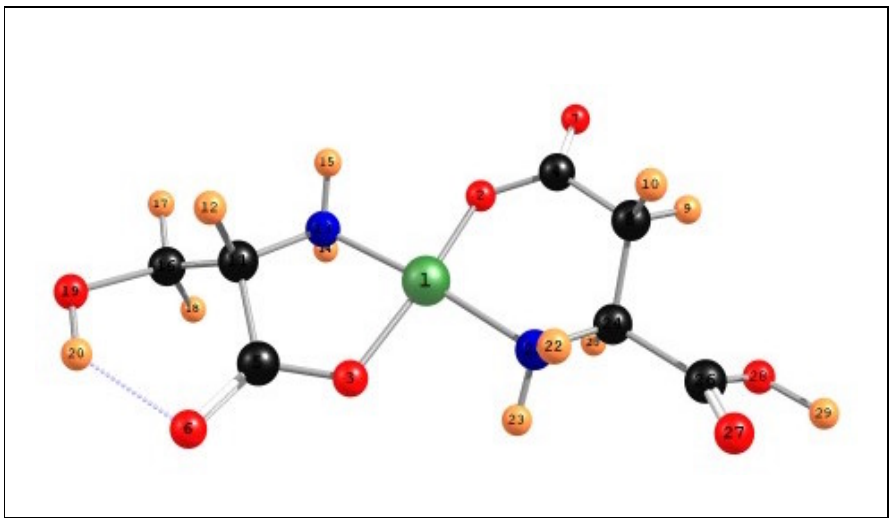
			Coordenadas Cartesianas		
Núm.	**Átomo**	**massa at.**	**X**	**Y**	**Z**
1	28	0	0.197993	-0.415258	0.096407
2	8	0	1.613080	0.713078	-0.295267
3	6	0	2.846914	0.184715	-0.232326
4	8	0	3.899186	0.799990	-0.429993
5	6	0	2.819261	-1.320456	0.067444
6	1	0	2.891927	-1.862819	-0.880526
7	7	0	1.510544	-1.661107	0.712246
8	1	0	1.157953	-2.589951	0.478022
9	1	0	1.569358	-1.600465	1.730509
10	7	0	-1.153607	0.796589	-0.588369
11	1	0	-0.816621	1.033910	-1.525074
12	6	0	-2.460570	0.046684	-0.668767
13	1	0	-3.175534	0.578882	-0.035034
14	1	0	-2.830068	0.053949	-1.697211
15	6	0	-2.304925	-1.389446	-0.176109
16	8	0	-3.234550	-2.200570	-0.251677
17	8	0	-1.095886	-1.659364	0.347826
18	1	0	3.674275	-1.600204	0.686791
19	6	0	-1.214430	2.060374	0.184292
20	7	0	-0.070593	2.793809	0.038378
21	1	0	-0.014966	3.702153	0.470404
22	1	0	0.800504	2.320040	-0.218922
23	7	0	-2.298491	2.314336	0.822837
24	1	0	-2.287752	3.170050	1.381669



A – 10

Coordenadas cartesianas do complexo [Ni(Asp)(Ser)] (sem água de hidratação).

			Coordenadas Cartesianas		
Núm.	**Átomo**	**massa at.**	**X**	**Y**	**Z**
1	28	0	0.051800	-0.593533	-0.234770
2	8	0	-0.979034	0.724281	-1.059033
3	7	0	-1.593283	-1.226361	0.524651
4	8	0	1.179178	-1.894879	0.503671
5	7	0	1.826124	-0.143972	-0.860262
6	6	0	2.653914	0.880866	-0.109108
7	6	0	1.889652	2.107611	0.299552
8	6	0	3.010793	-0.179698	0.973681
9	6	0	2.346411	-1.286757	0.111140
10	8	0	3.296641	-2.168468	-0.437333
11	8	0	2.155013	3.250845	-0.063985
12	8	0	0.846279	1.815731	1.147445
13	6	0	-2.711388	-0.779572	-0.373194
14	6	0	-2.288245	0.599473	-0.922686
15	8	0	-3.141524	1.473651	-1.170841
16	6	0	-4.038746	-0.694791	0.367771
17	8	0	-3.895684	0.234510	1.482160
18	1	0	0.286602	2.601648	1.296996
19	1	0	-1.732442	-0.781917	1.434502
20	1	0	-1.571370	-2.233784	0.657799
21	1	0	2.006514	-0.215545	-1.857498
22	1	0	4.074390	-0.325626	1.129196
23	1	0	-2.773626	-1.480524	-1.208156
24	1	0	2.491913	-0.041371	1.916350
25	1	0	3.506500	1.204314	-0.699023
26	1	0	2.847294	-3.005471	-0.660488
27	1	0	-3.944714	1.142273	1.127156
28	1	0	-4.818213	-0.368569	-0.319787
29	1	0	-4.314451	-1.652339	0.806211

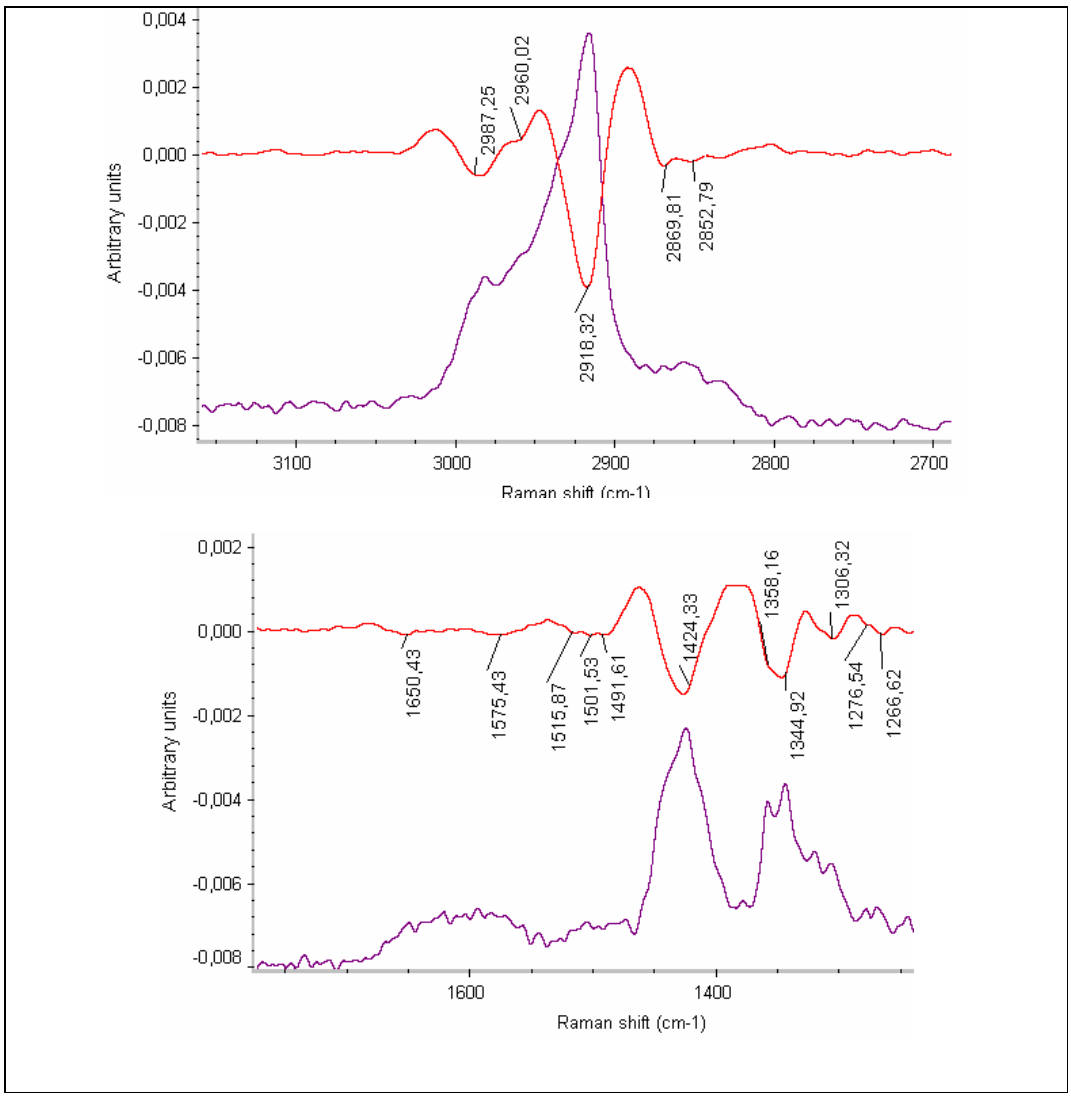


ANEXO B

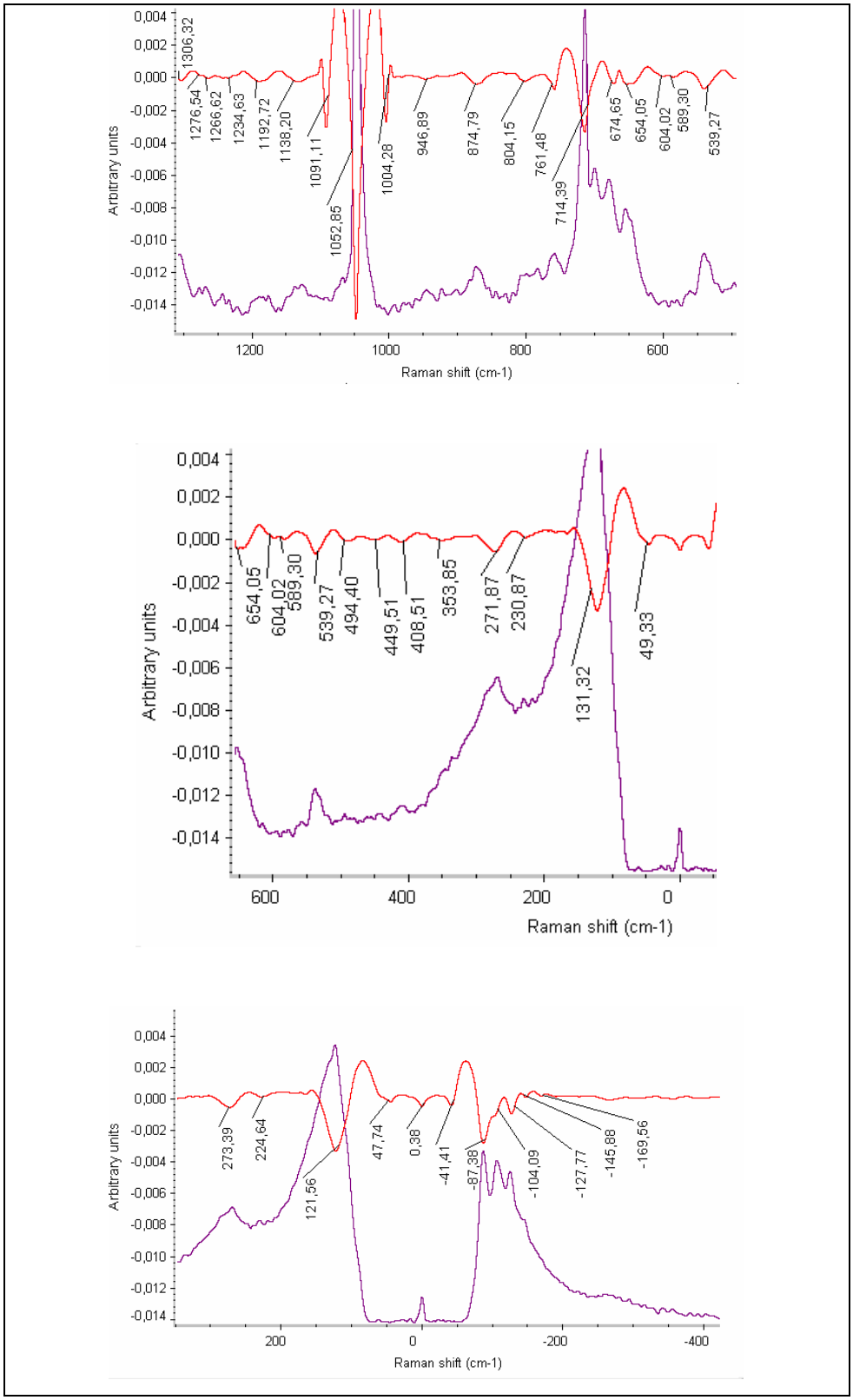
Segundas derivadas dos espectros infravermelho e Raman.

B – 1

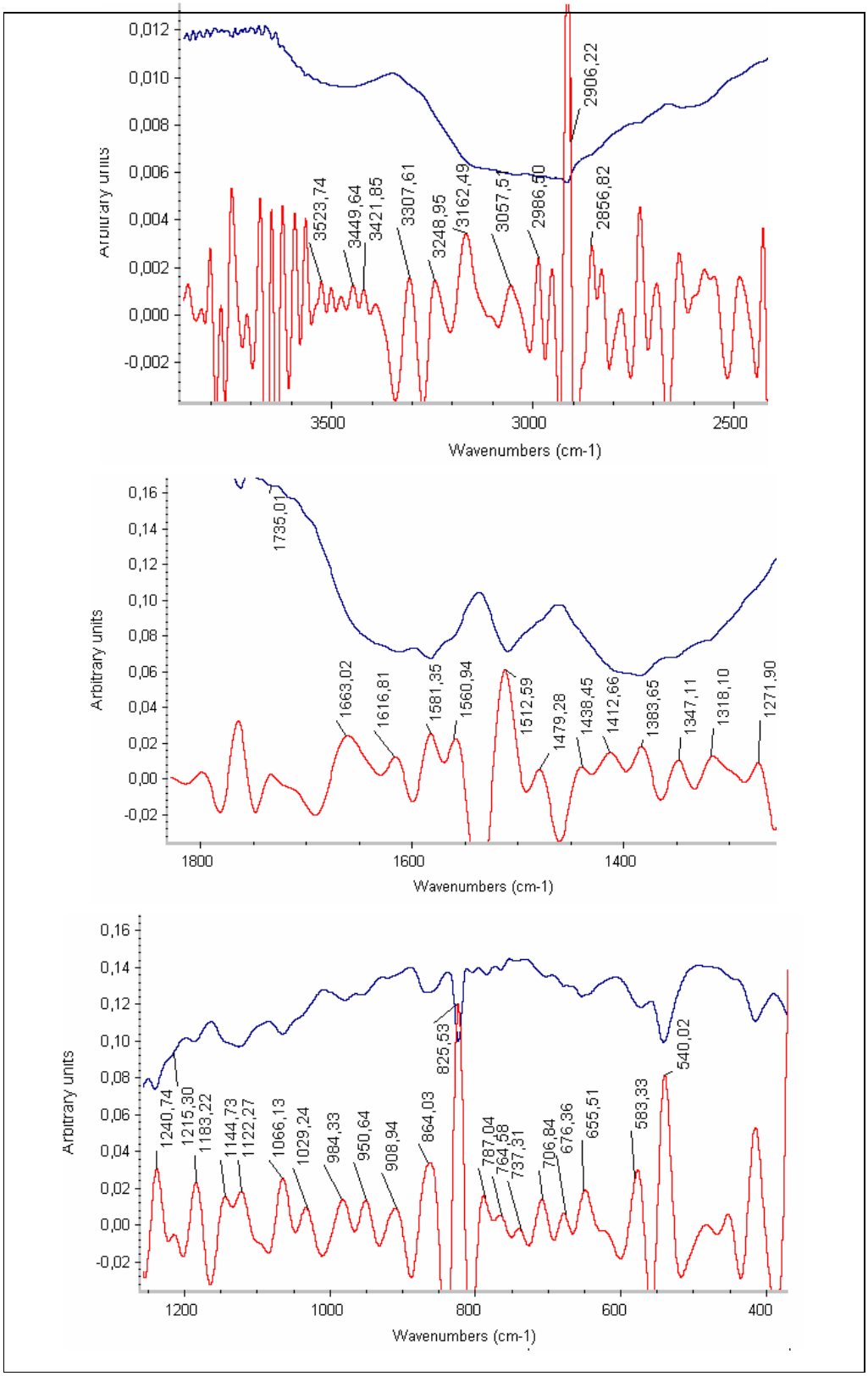
[Zn(Cis)(Met)]. H_2O



Espectro Raman e a segunda derivada espectral nas regiões entre 3100 – 2700 e 1650 – 1350 cm^{-1}.



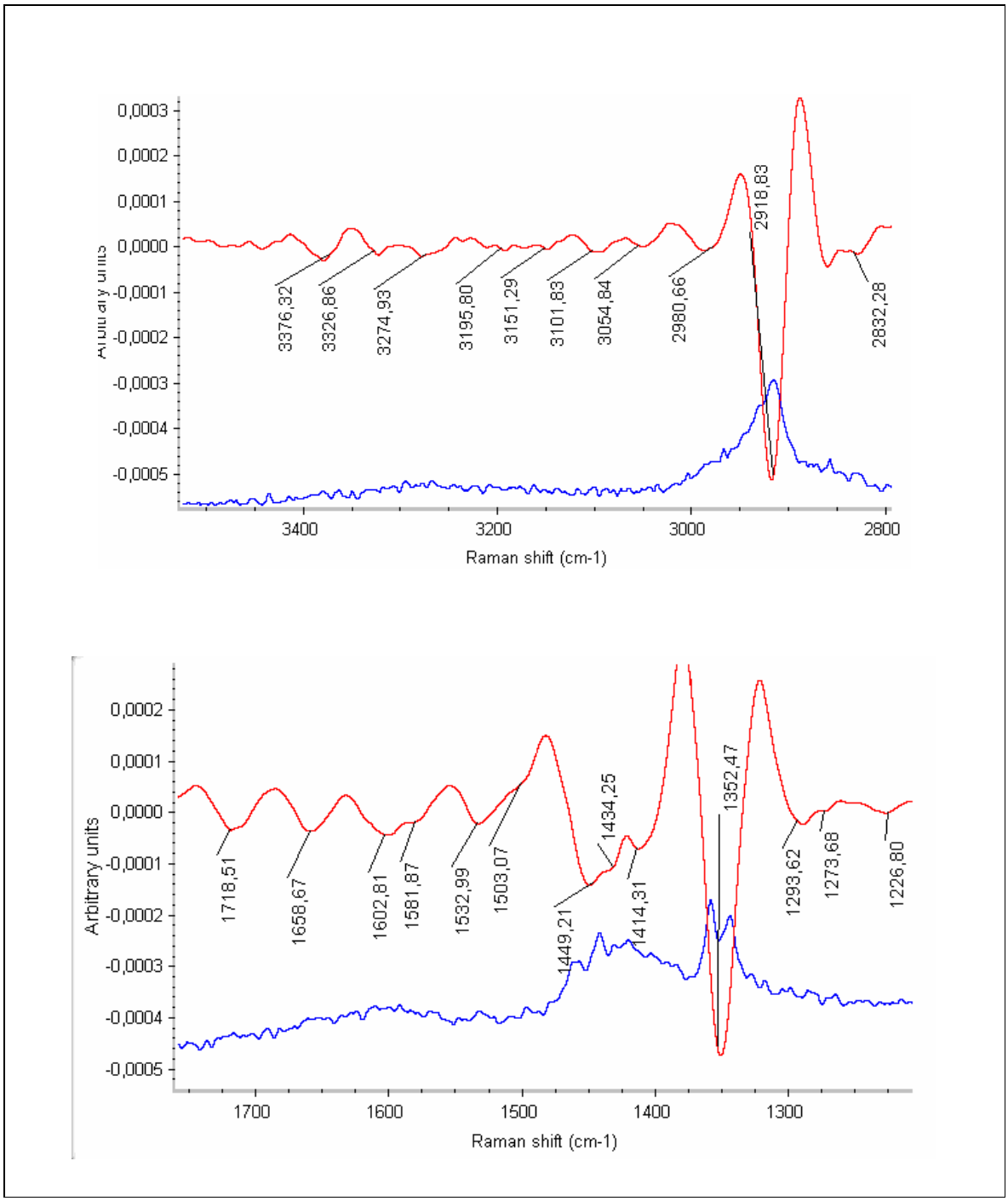
Espectro Raman e a segunda derivada espectral nas regiões entre 1200 – -400 cm^{-1}.



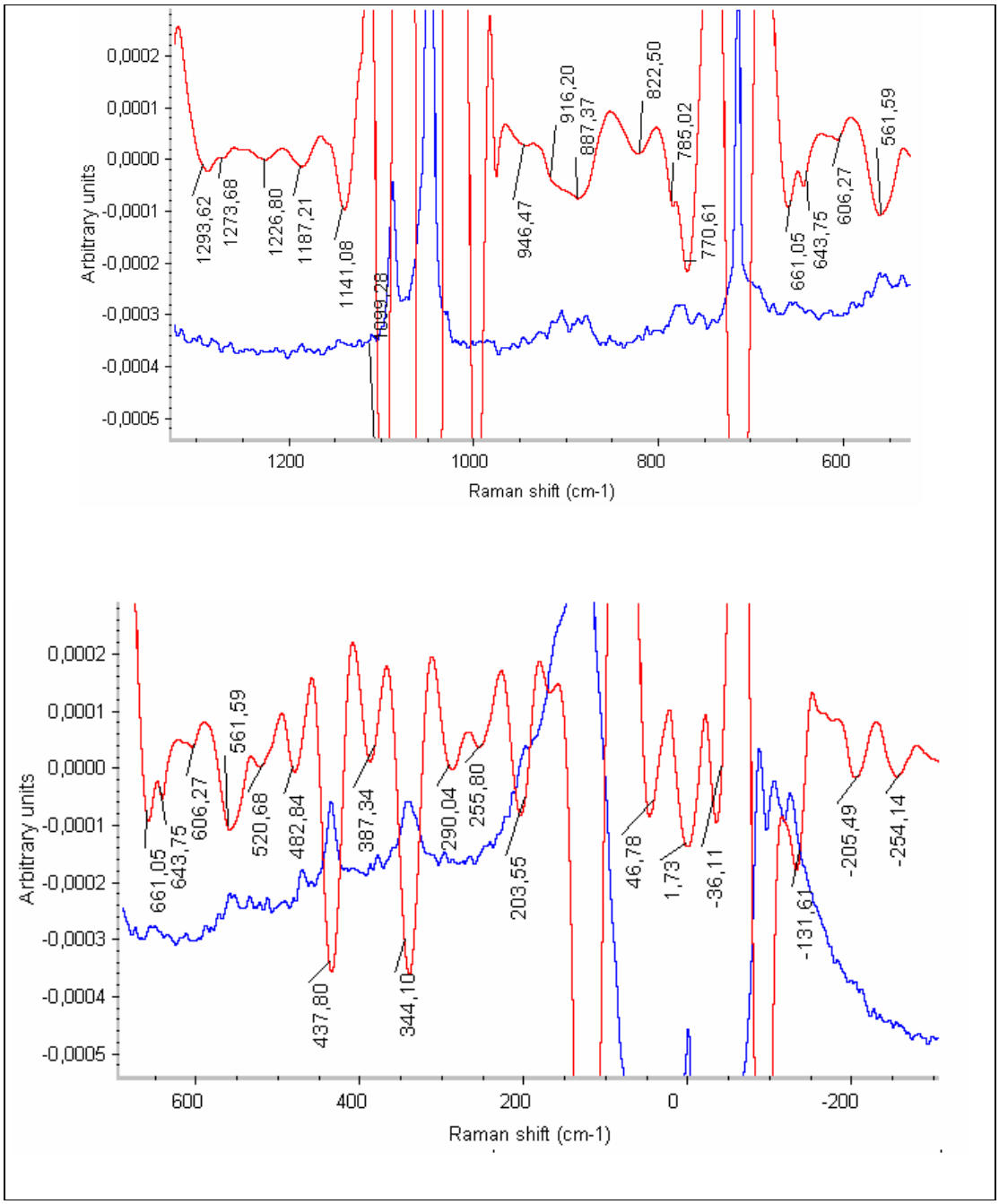
Espectro infravermelho e a segunda derivada espectral nas regiões entre 3500 – 400 cm^{-1}.

B – 2

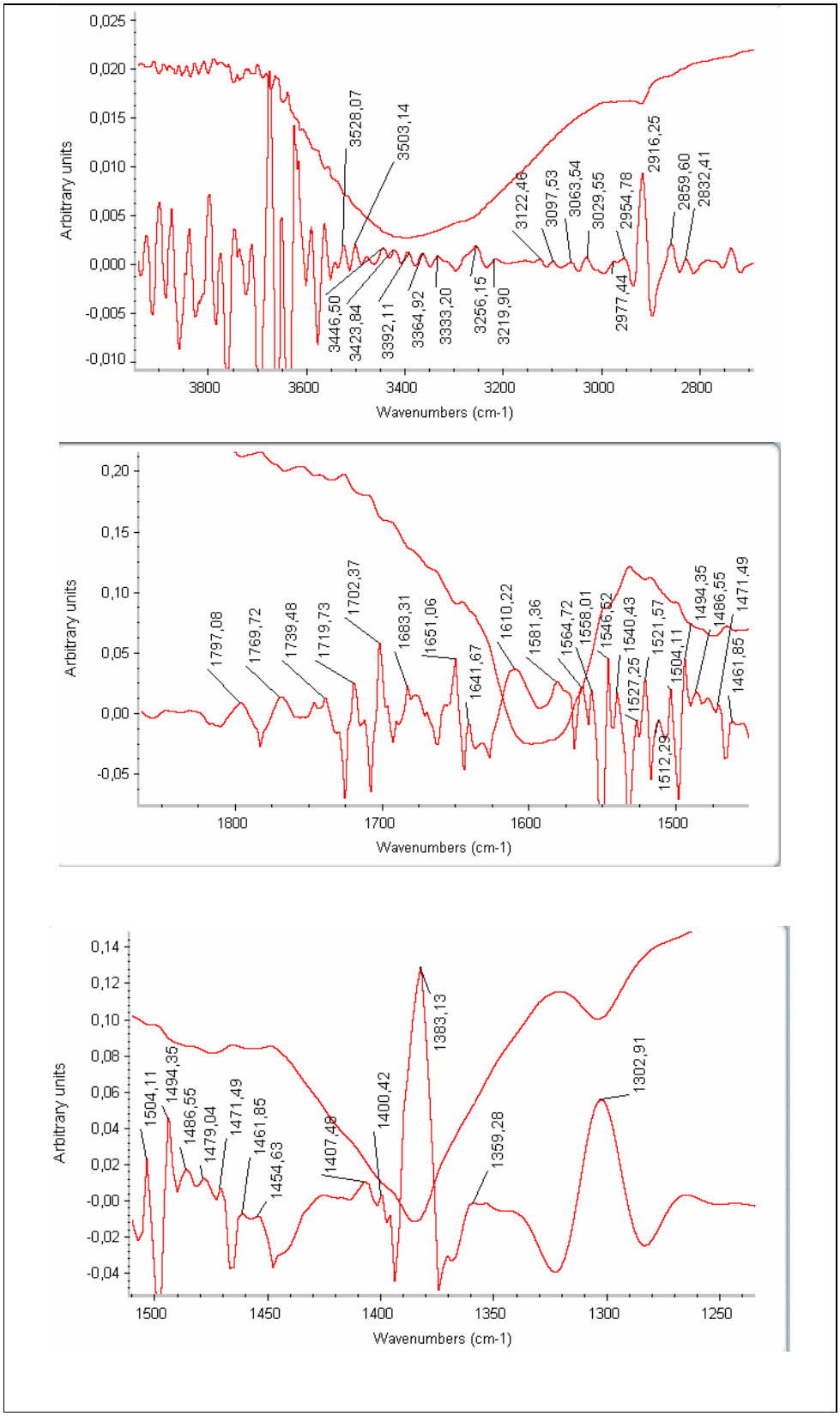
[Zn(Gli)(Met)]. H_2O



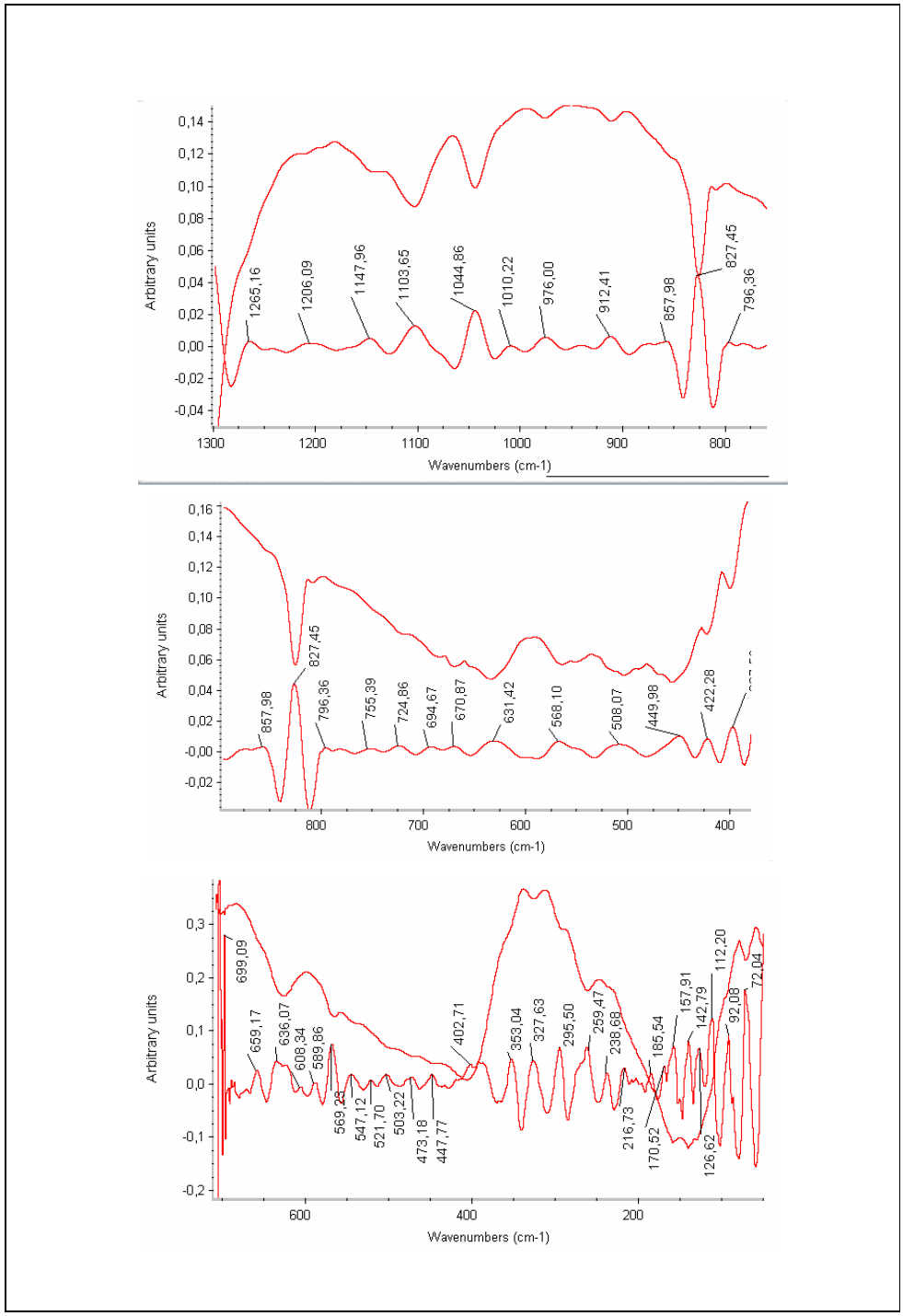
Espectro Raman e a segunda derivada espectral nas regiões entre 3400 – 1300 cm^{-1}.



Espectro Raman e a segunda derivada espectral nas regiões entre 1300 – - 200 cm^{-1}.



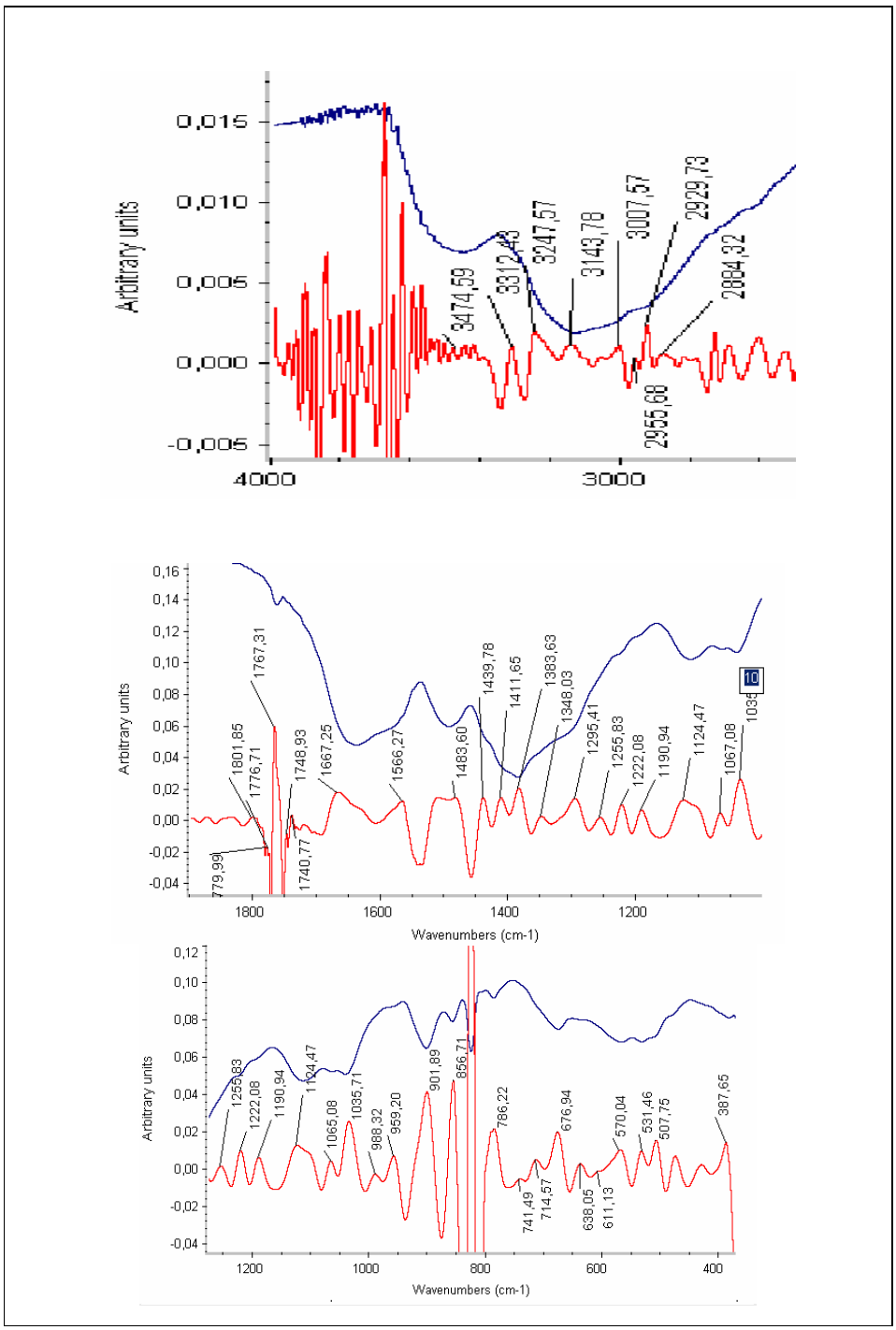
Espectros infravermelho e a segunda derivada espectral nas regiões entre 3600 – 1250 cm^{-1}



Espectro infravermelho e a segunda derivada espectral nas regiões entre 1300 – 70 cm^{-1}.

B – 3

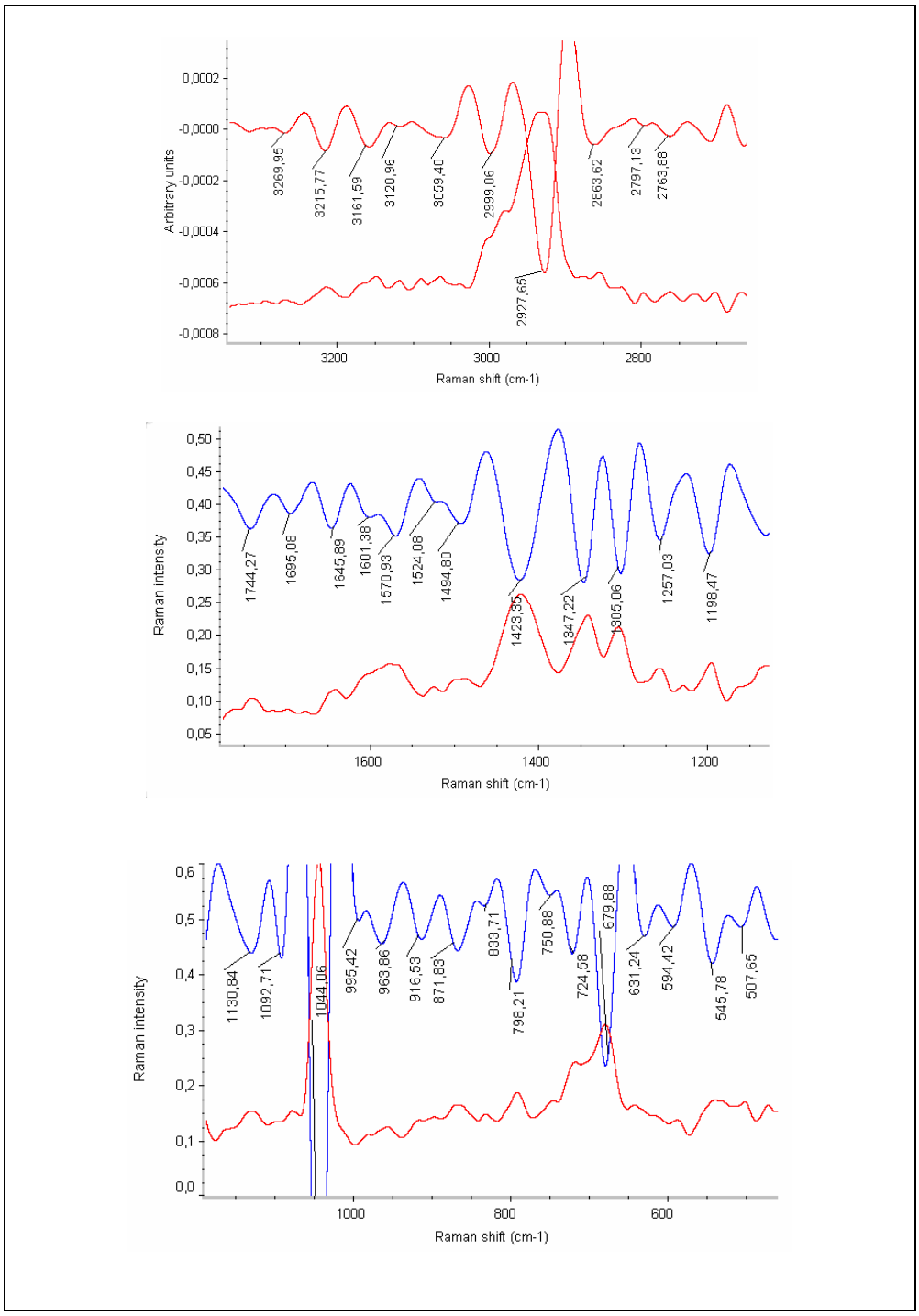
[Zn(Cis)(Gli)]. H_2O



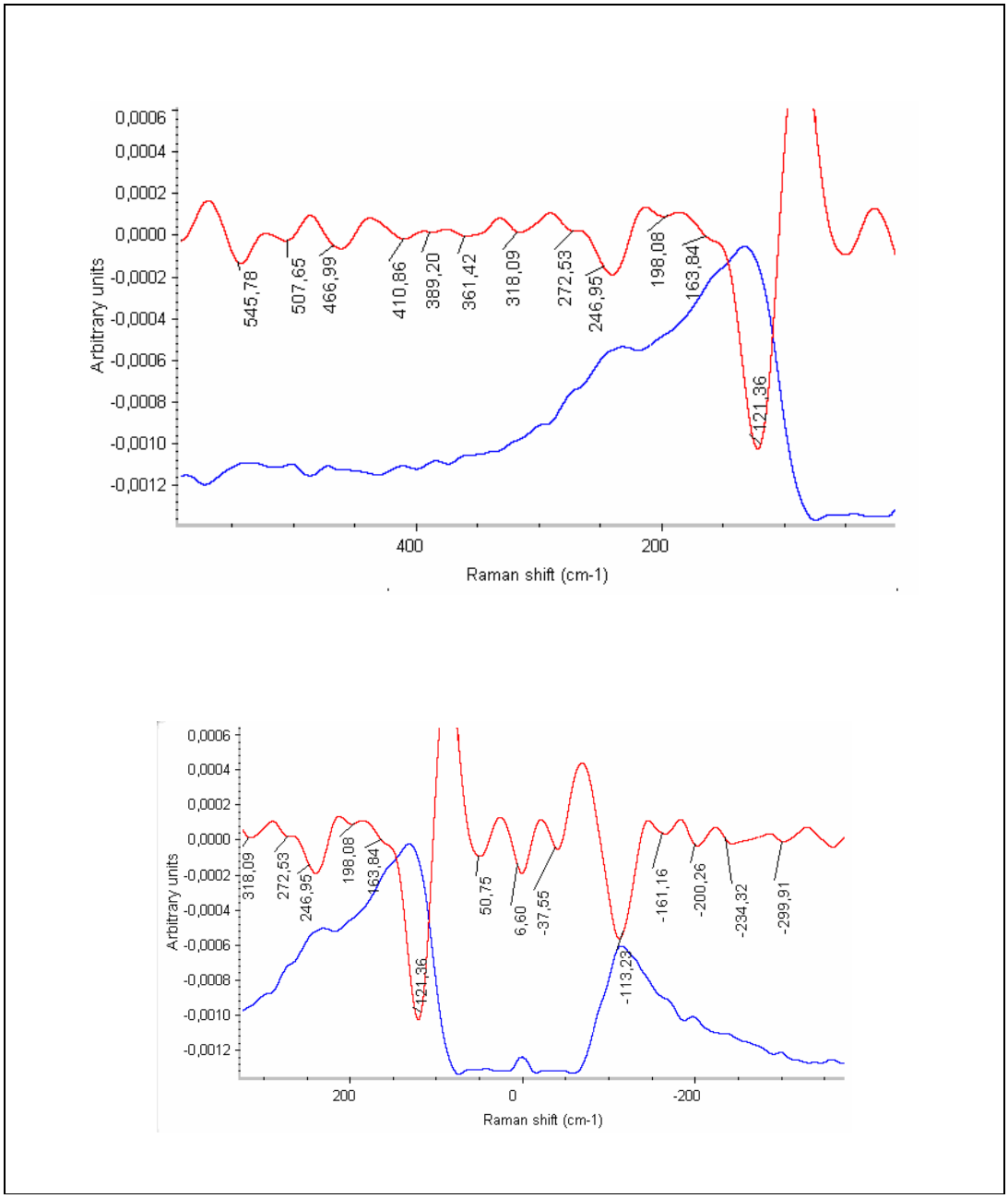
Espectro infravermelho e a segunda derivada espectral nas regiões entre 1300 – 70 cm^{-1}.

B – 4

[Cd(Cis)(Met)]. H_2O



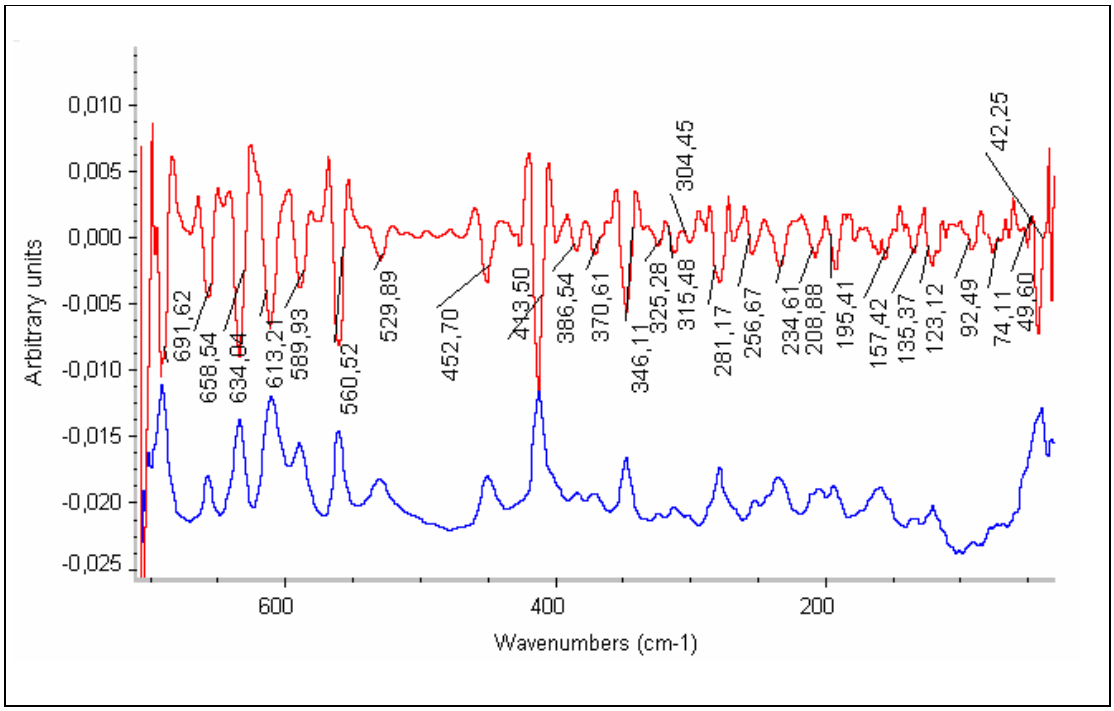
Espectros Raman e segunda derivada espectral nas regiões entre 3300 – 500 cm^{-1}.



Espectros Raman e segunda derivada espectral nas regiões entre 550 – -300 cm^{-1}.

B – 5

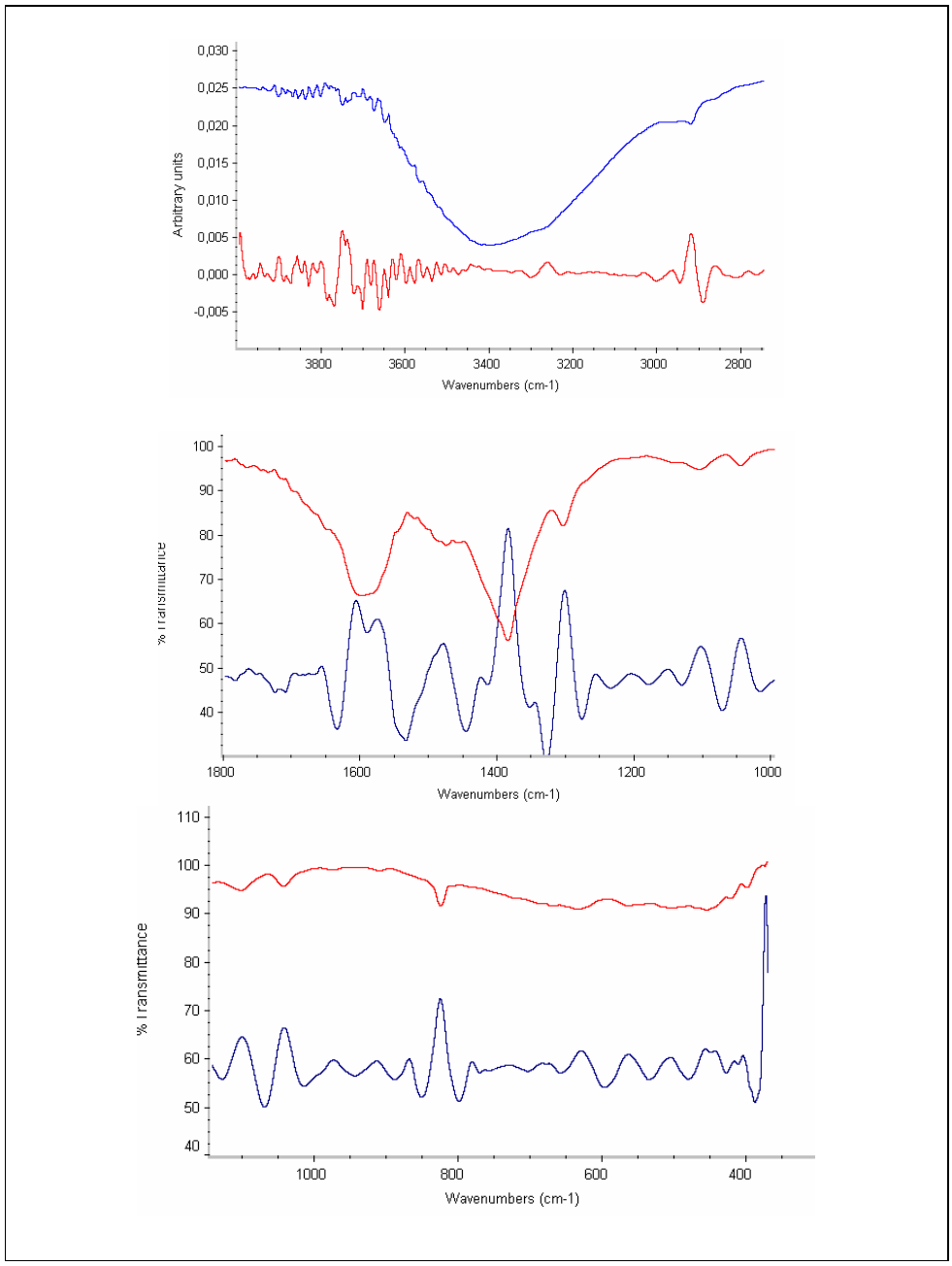
[Cd(Gli)(Met)]. H_2O



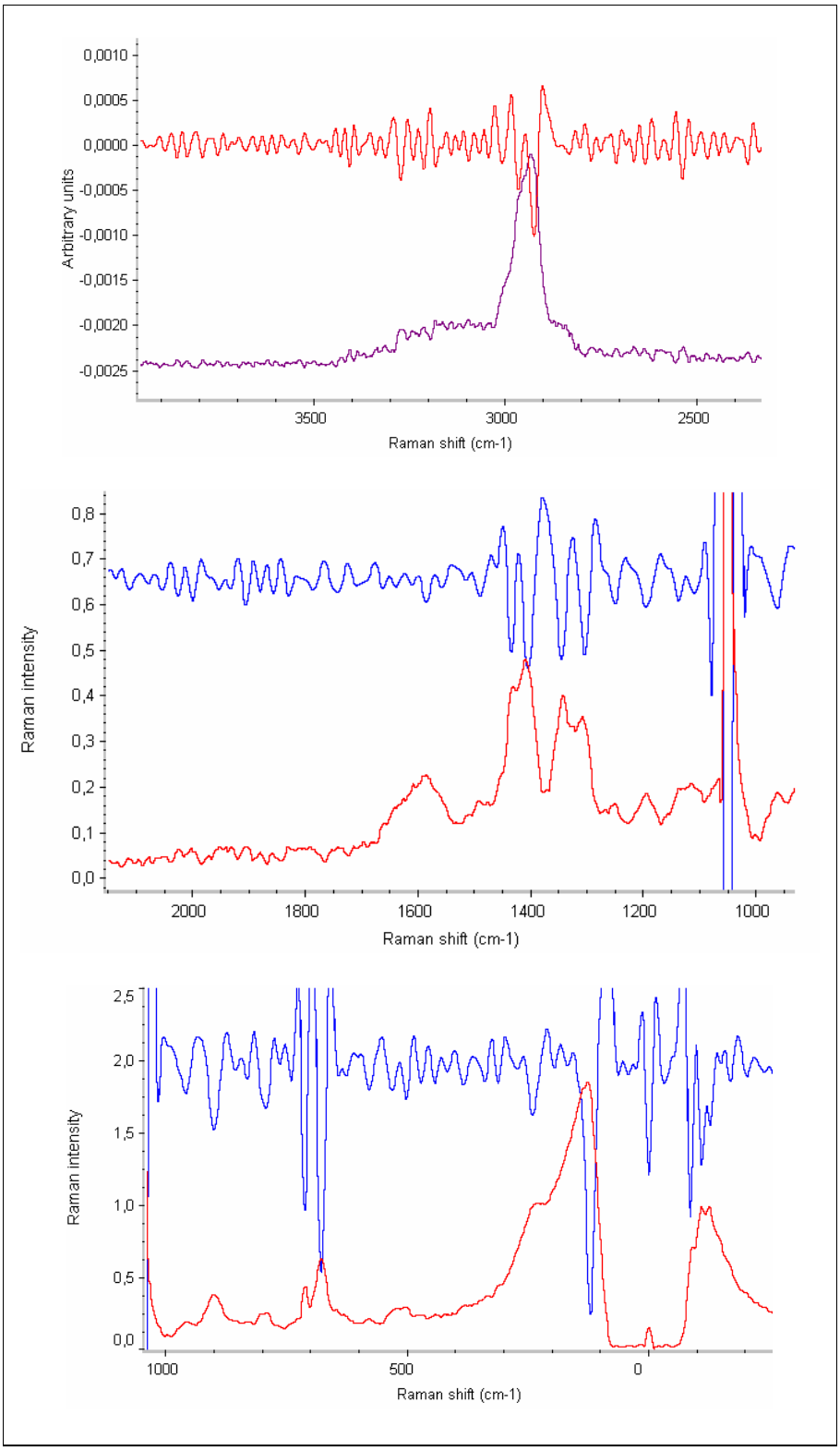
Espectro IV e segunda derivada espectral na região entre 700 e 50 cm^{-1}.

B – 6

[Cd(Cis)(Gli)]. H_2O



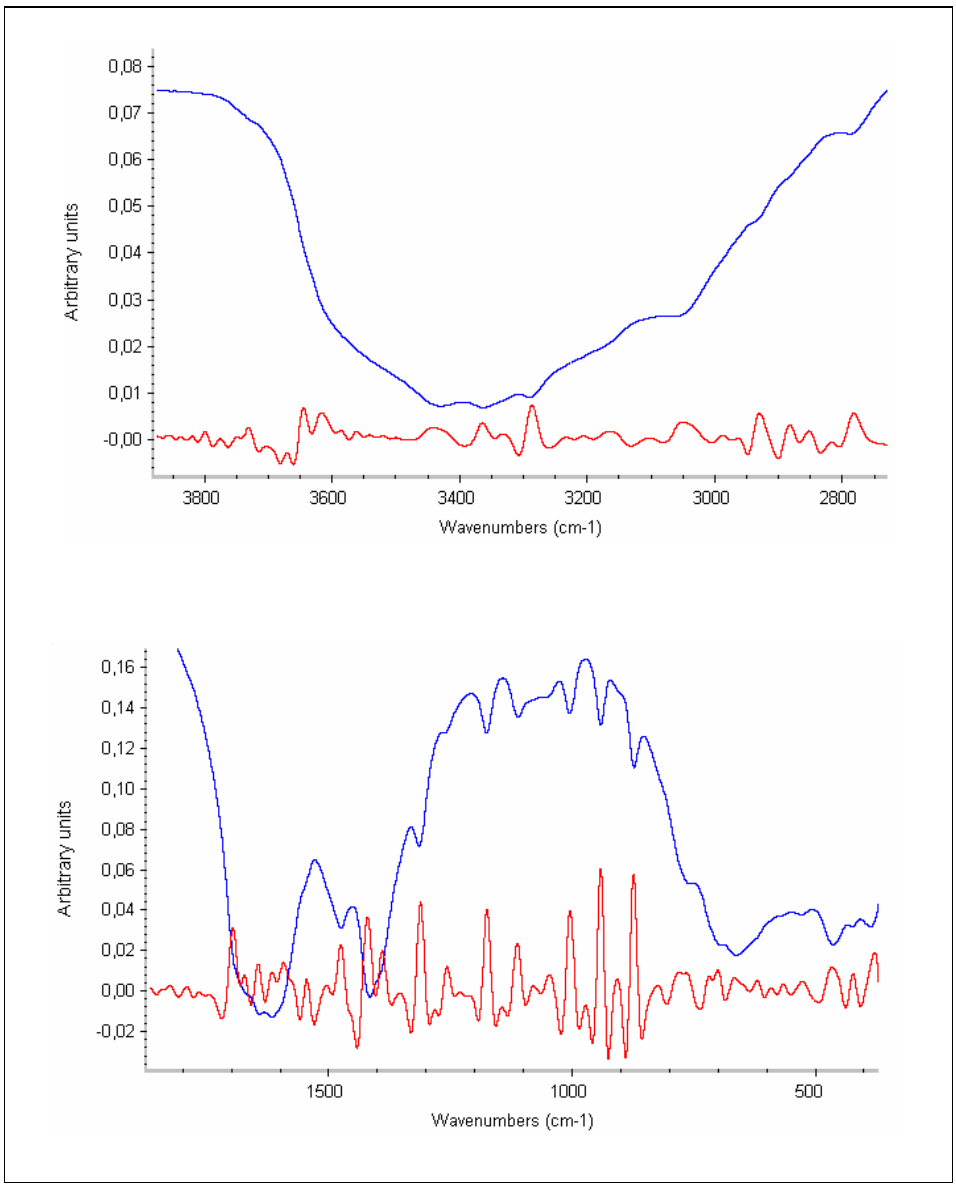
Espectros infravermelho e segunda derivada espectral nas regiões entre 3800 – 400 cm^{-1}.



Espectros Raman e segunda derivada espectral nas regiões entre 3800 – 0 cm^{-1}.

B – 7

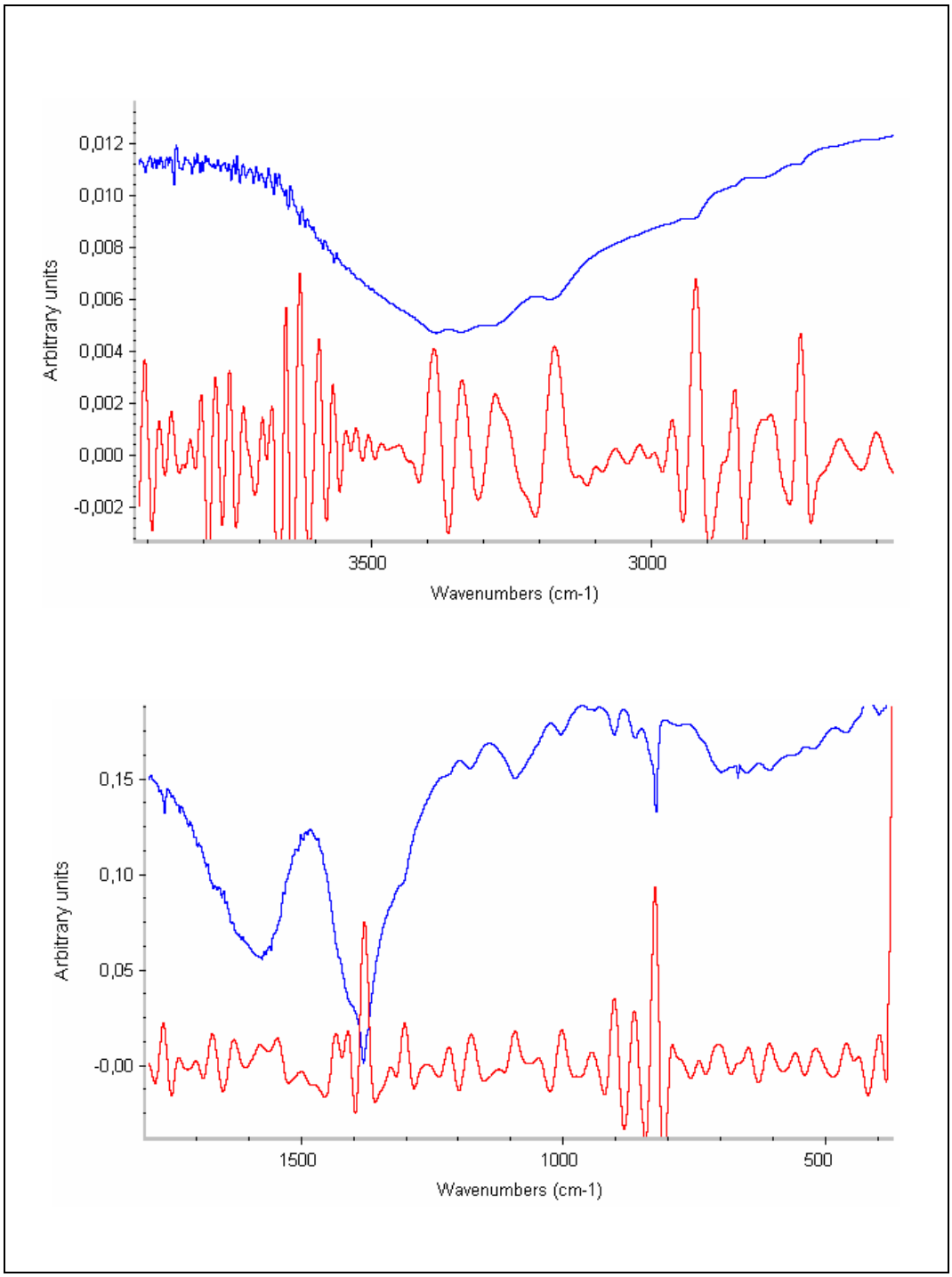
$[Ni(Gaa)_2]. 2H_2O$



Espectro infravermelho e segunda derivada espectral nas regiões entre 3800 – 400 cm^{-1}.

B – 8

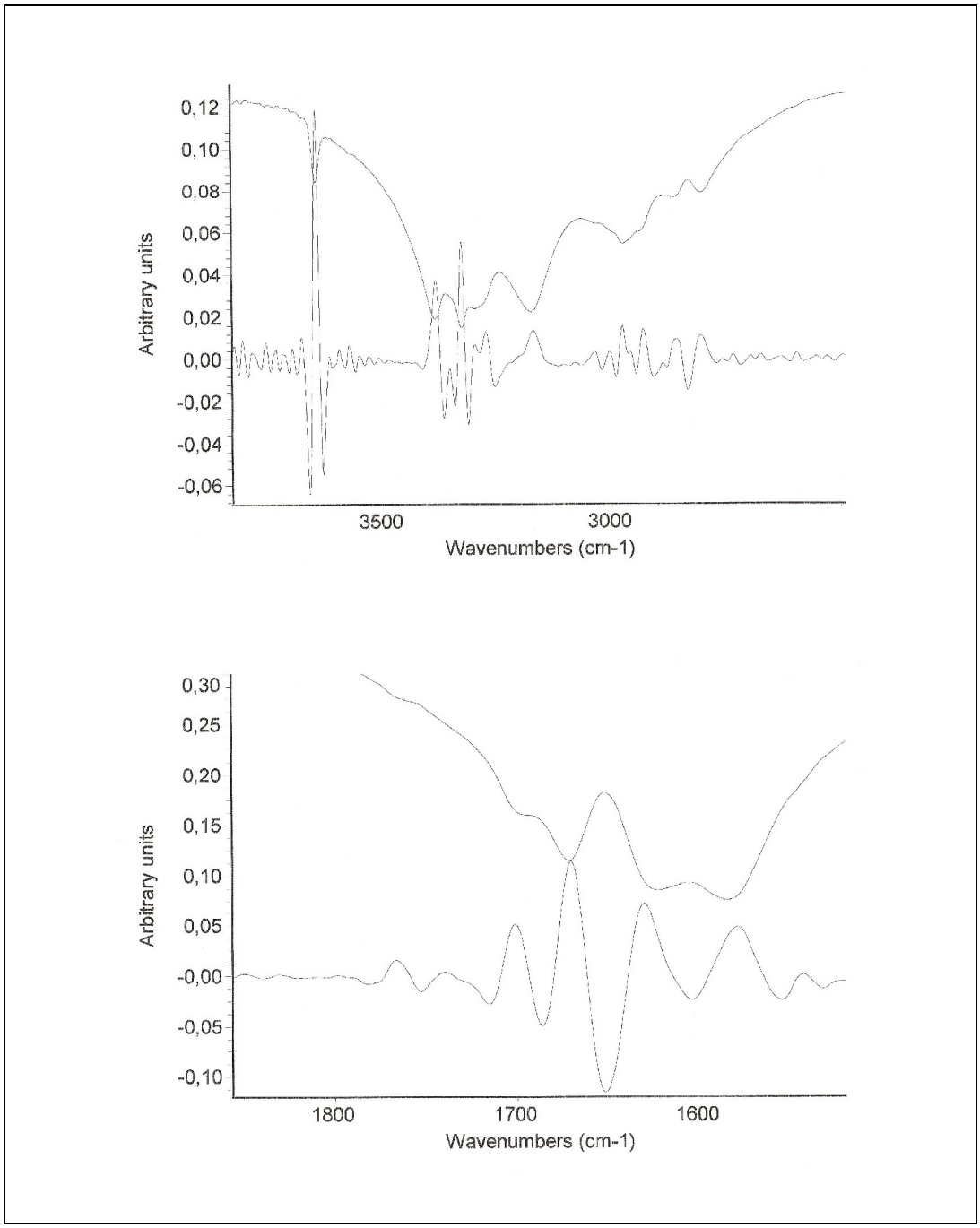
[Ni(Asp)(Gaa)]. $2H_2O$



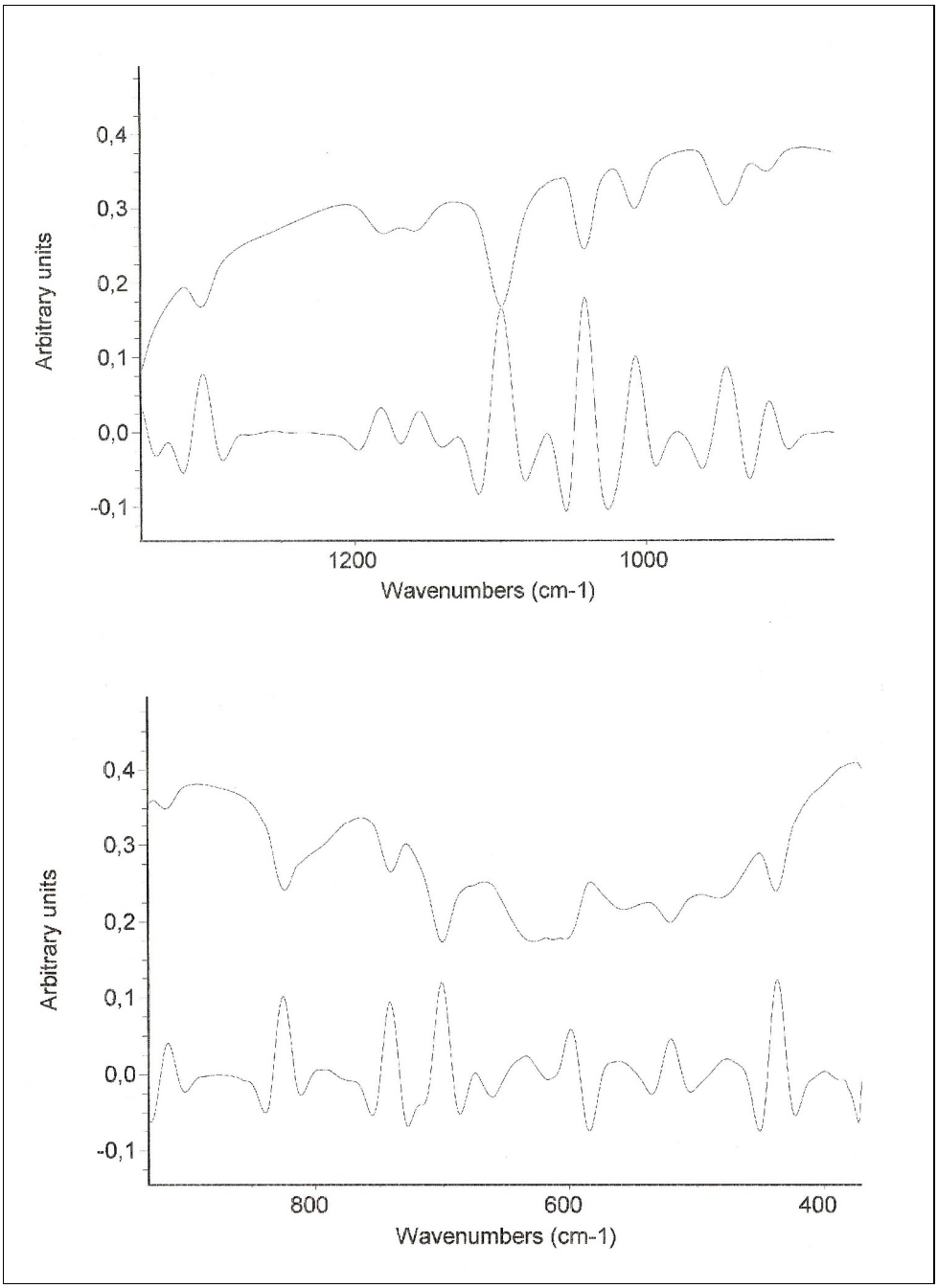
Espectro infravermelho e segunda derivada espectral nas regiões entre 3800 – 400 cm^{-1}.

B – 9

[Ni(Gaa)(Gli)].2H_2O



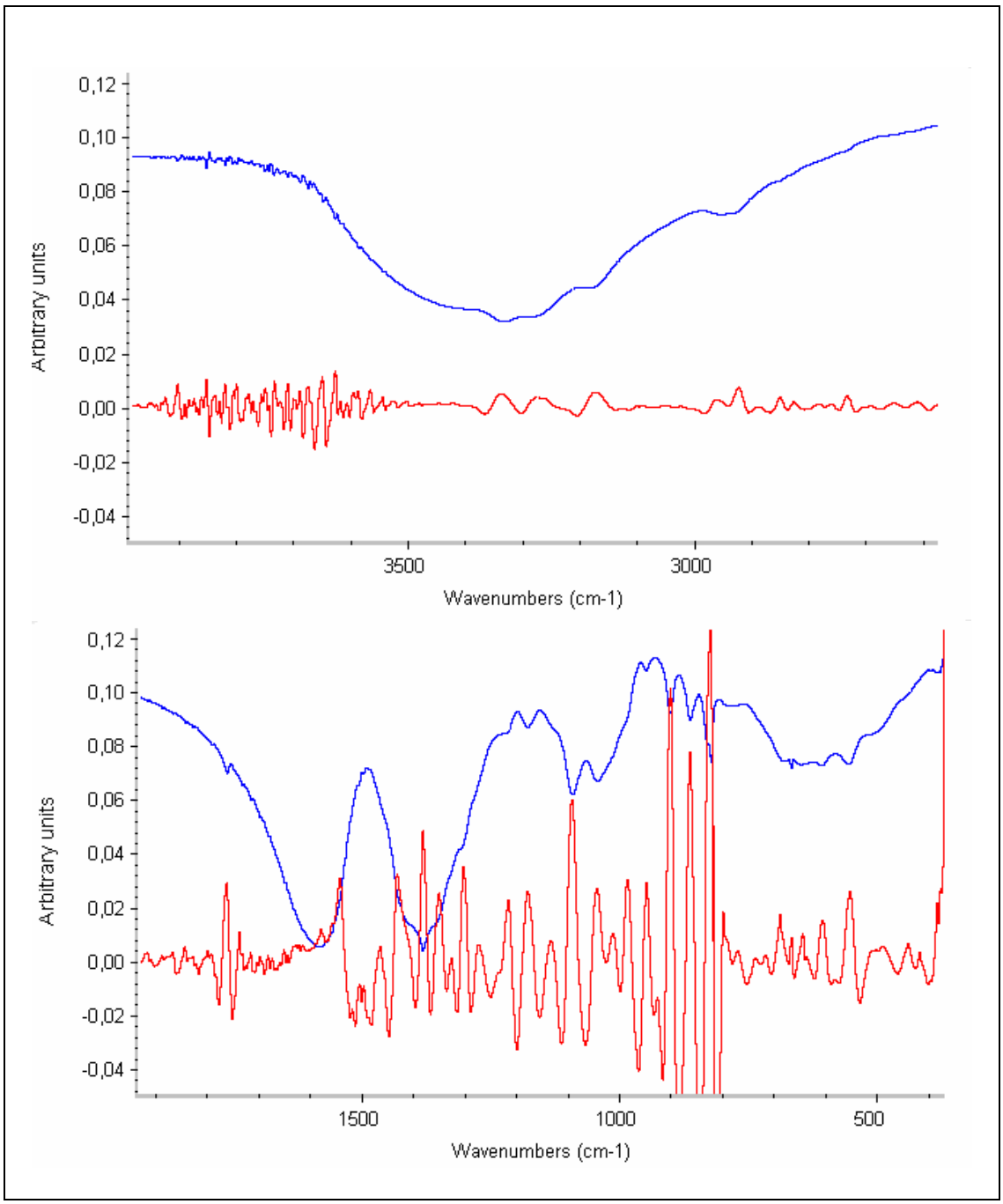
Espectro infravermelho e segunda derivada espectral nas regiões entre 3800 – 1400 cm^{-1}.



Espectro infravermelho e segunda derivada espectral nas regiões entre 1300 – 400 cm^{-1}.

B – 10

[Ni(Asp)(Ser)].2H_2O



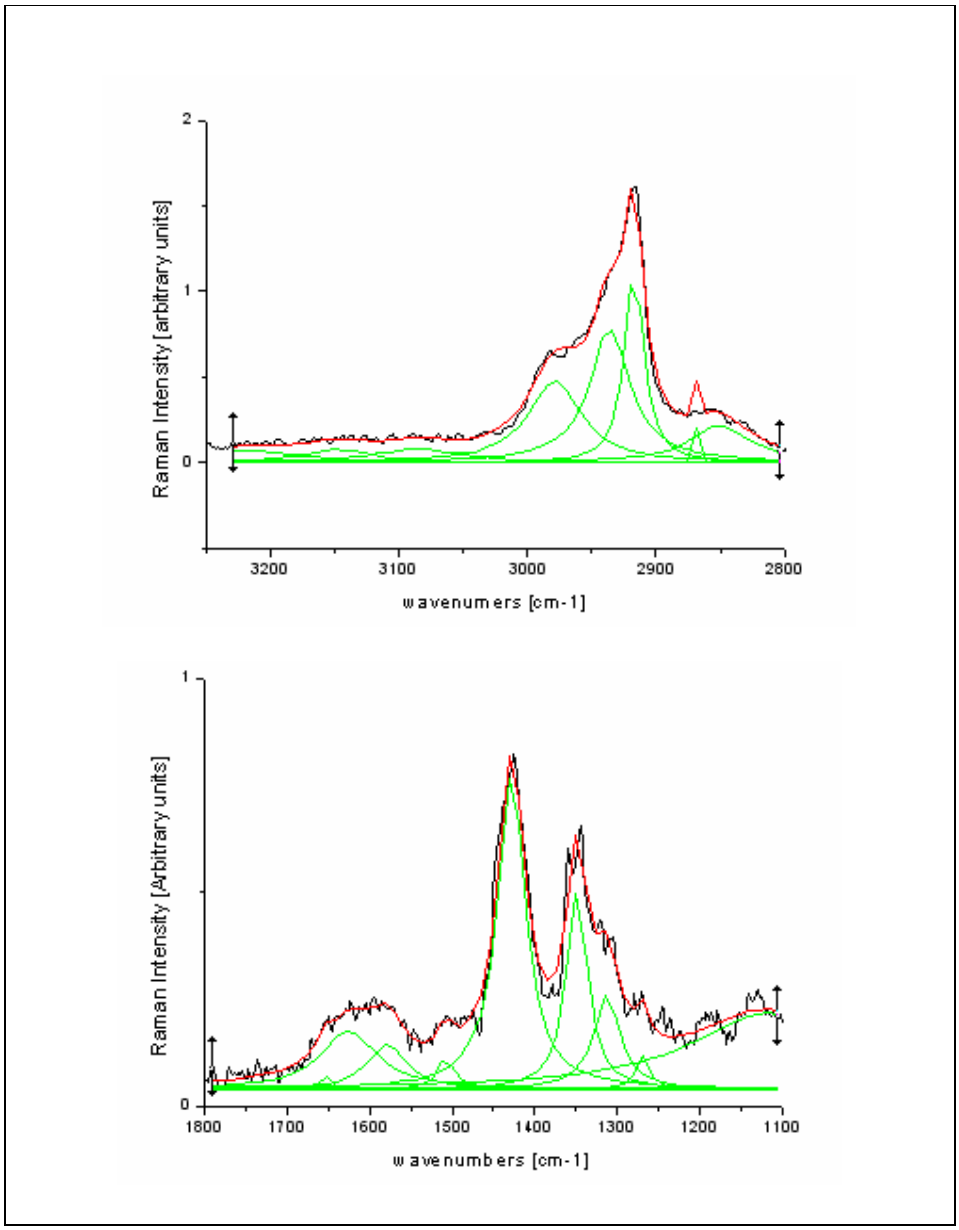
Espectro infravermelho e segunda derivada espectral nas regiões entre 3800 – 400 cm^{-1}.

ANEXO C

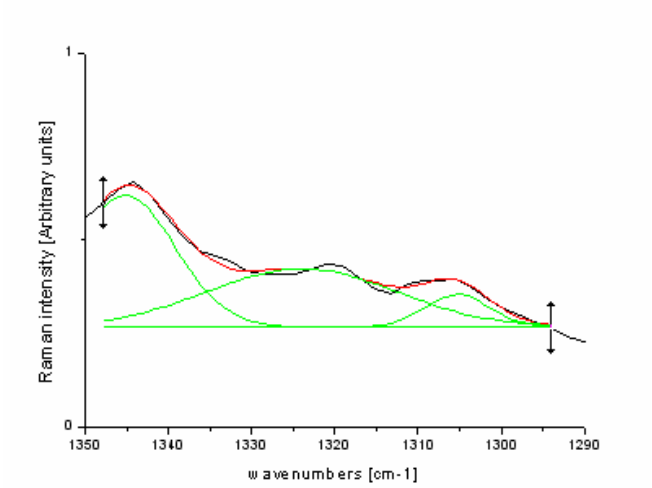
ANÁLISE DE DECONVOLUÇÃO DE BANDAS (ADB) NO ESPECTRO INFRAVERMELHO E/OU RAMAN.

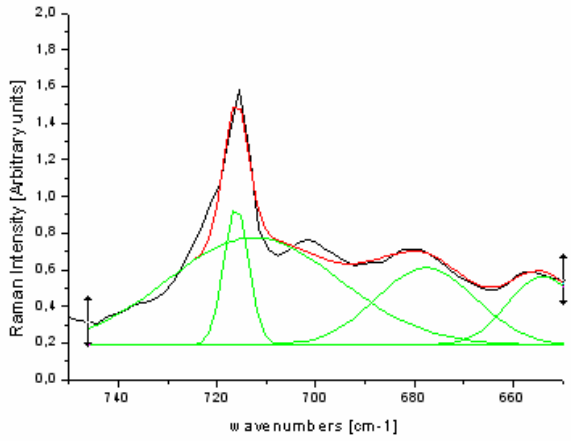
C – 1

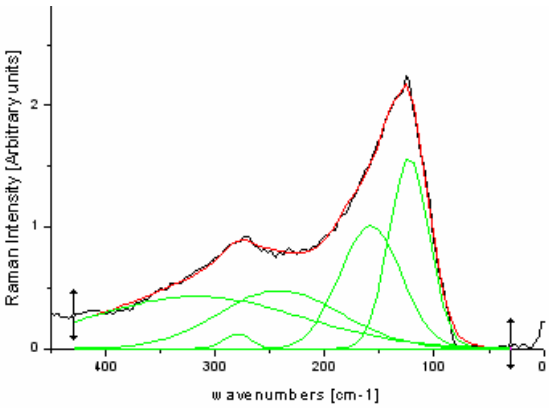
[Zn(Cis)(Met)]. H_2O



ADB no espectro Raman nas regiões entre 3200 – 2800 e 1880 – 1100 cm^{-1}.



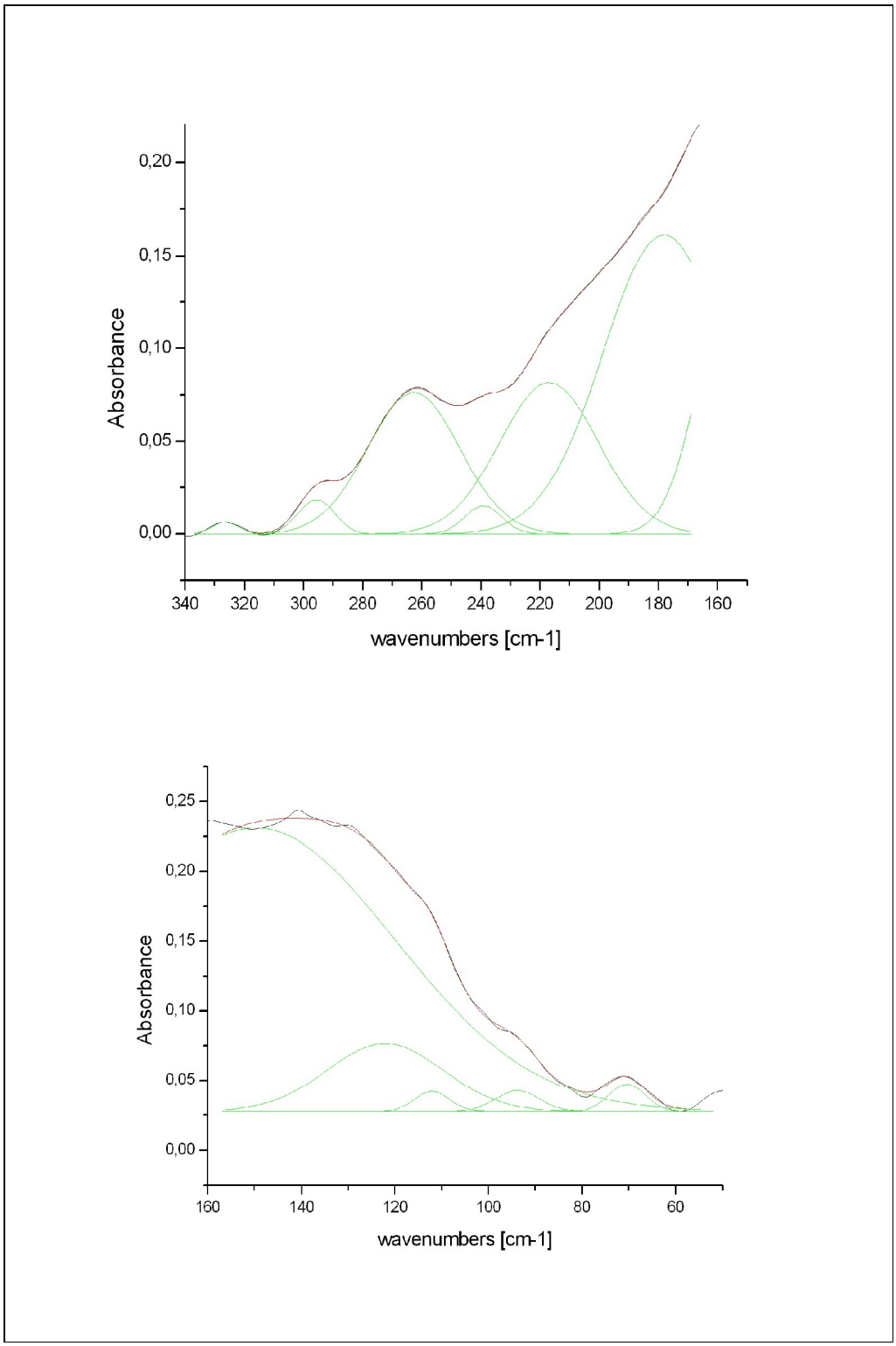




ADB no espectro Raman nas regiões entre 1350 – 1290, 740 – 650 e 500 – 0 cm^{-1}.

C – 2

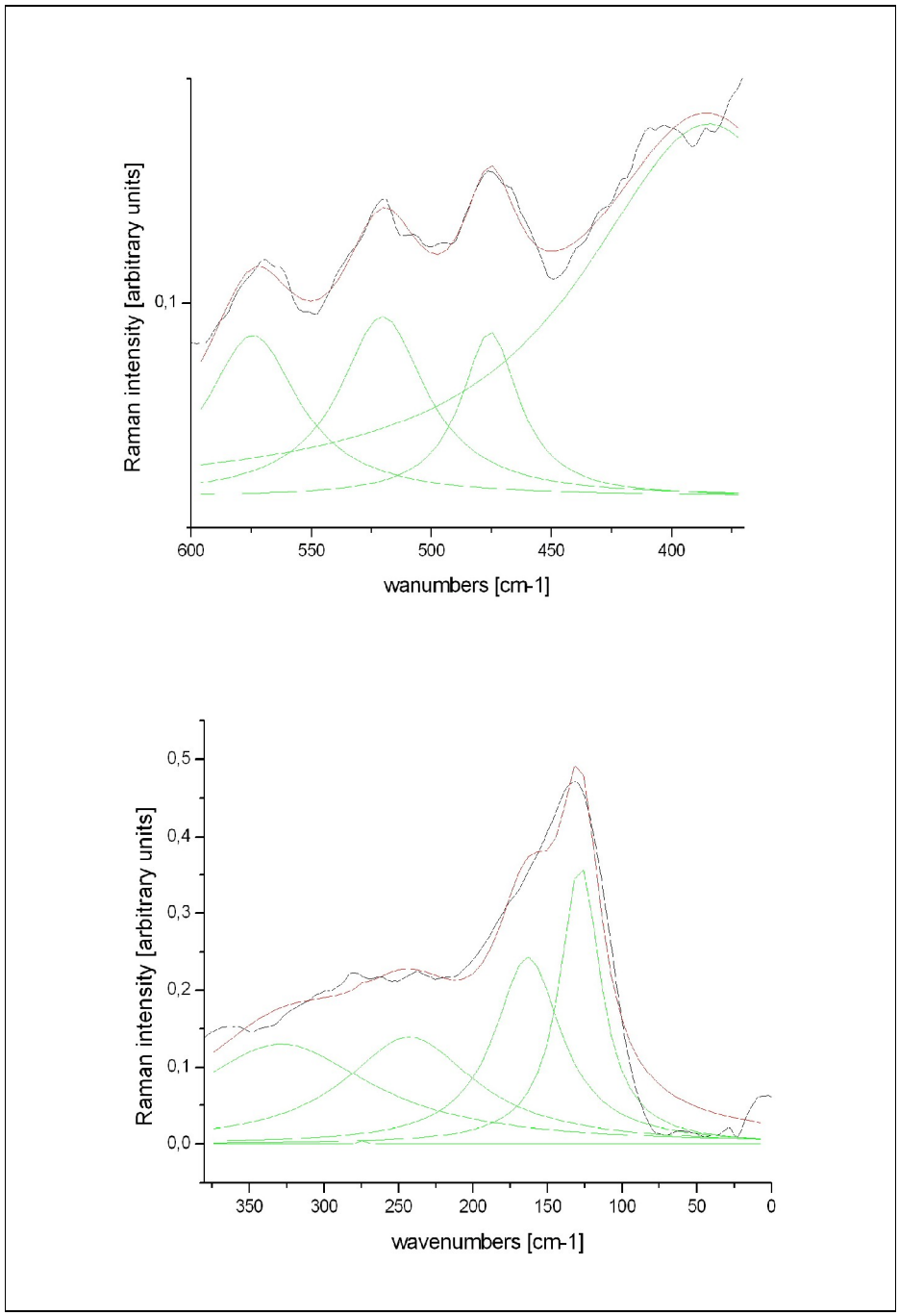
[Zn(Gli)(Met)]. H_2O



ADB no espectro infravermelho na região entre 340 – 50 cm^{-1}.

C – 3

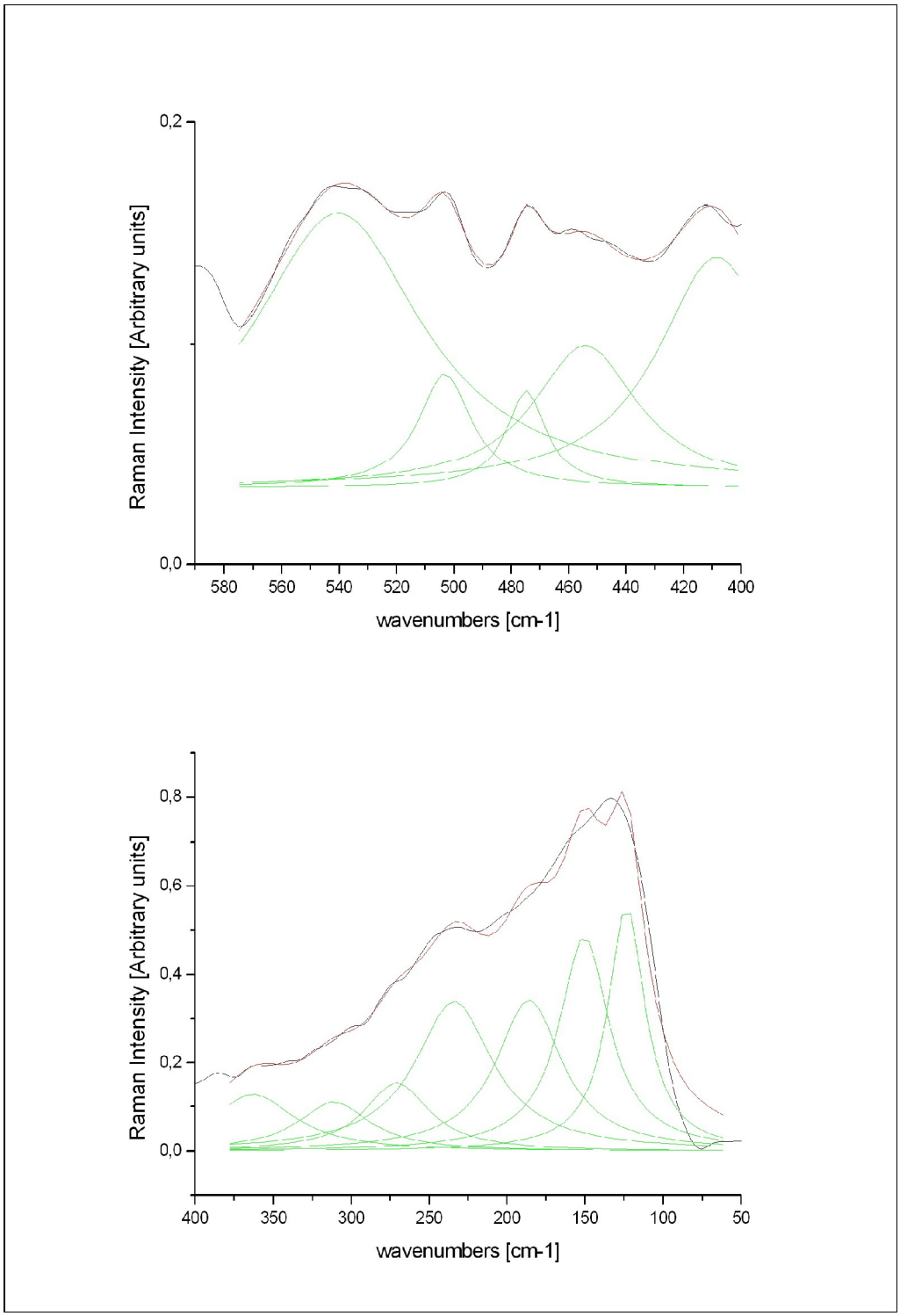
[Zn(Cis)(Gli)]. H_2O



ADB no espectro Raman na região metal –ligante entre 600 – 0 cm^{-1}.

C – 4

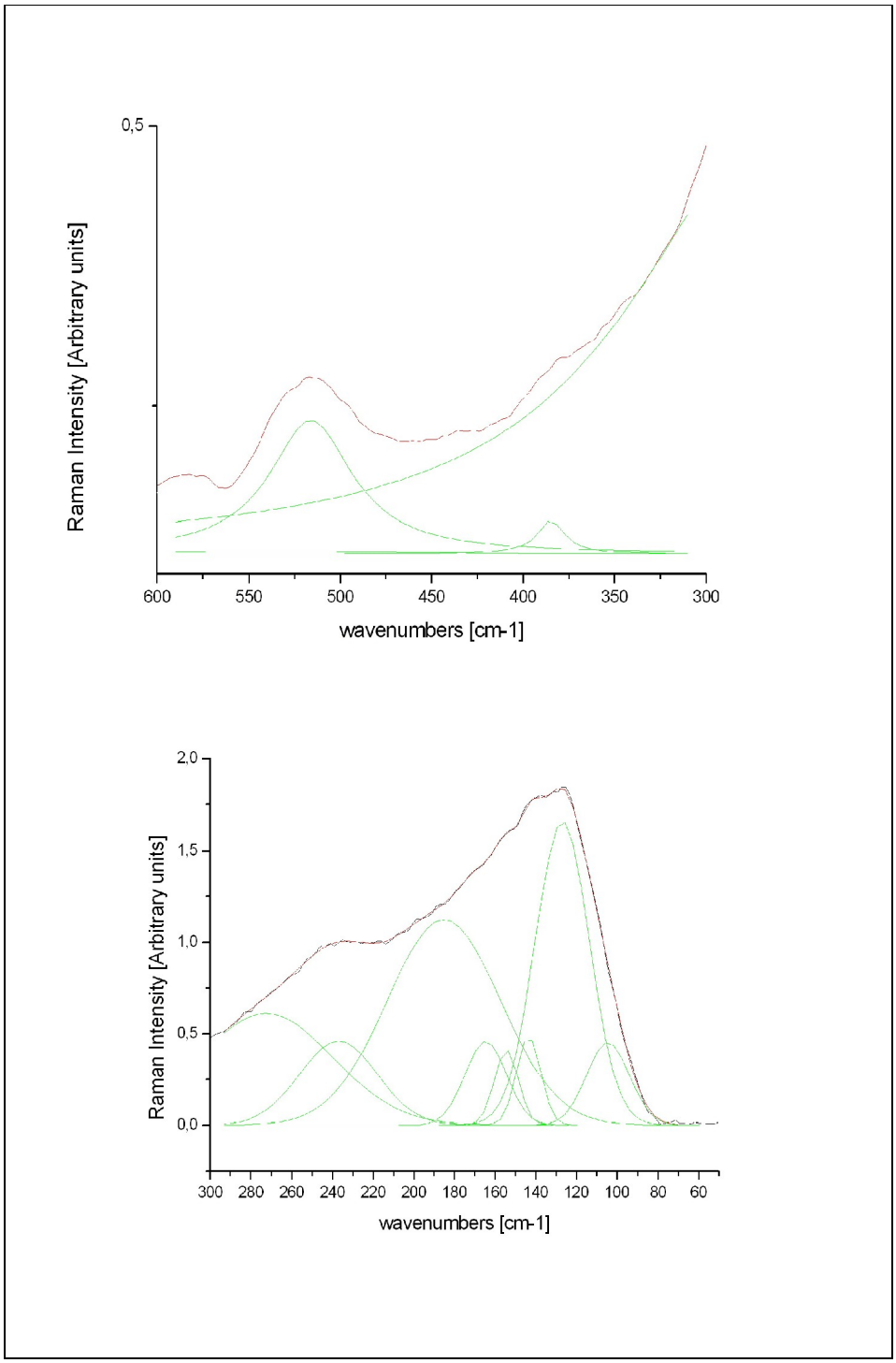
[Cd(Cis)(Met)]. H_2O



ADB no espectro Raman na região metal – ligante entre 580 – 50 cm^{-1}.

C – 5

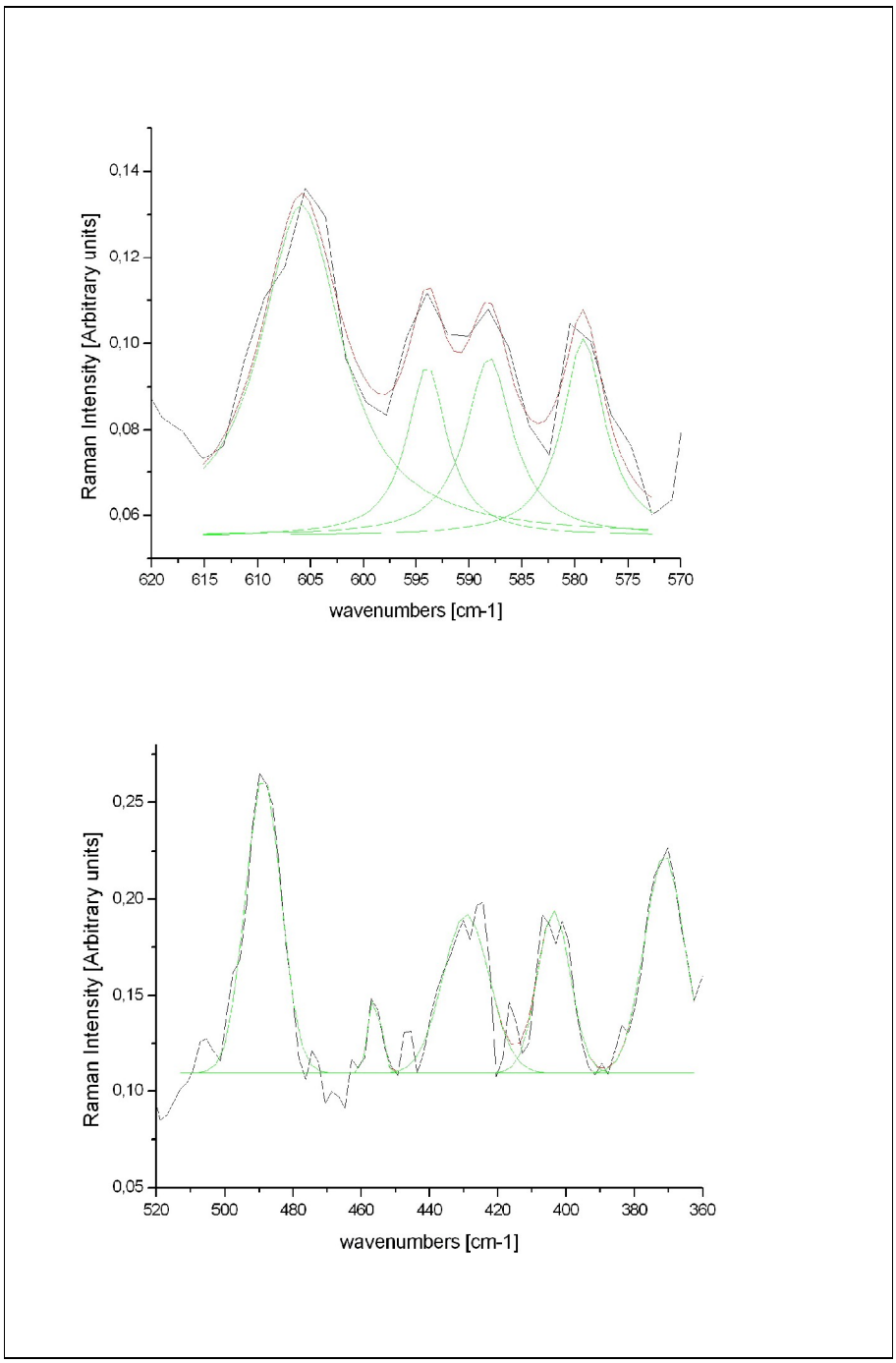
[Cd(Cis)(Gli)]. H_2O



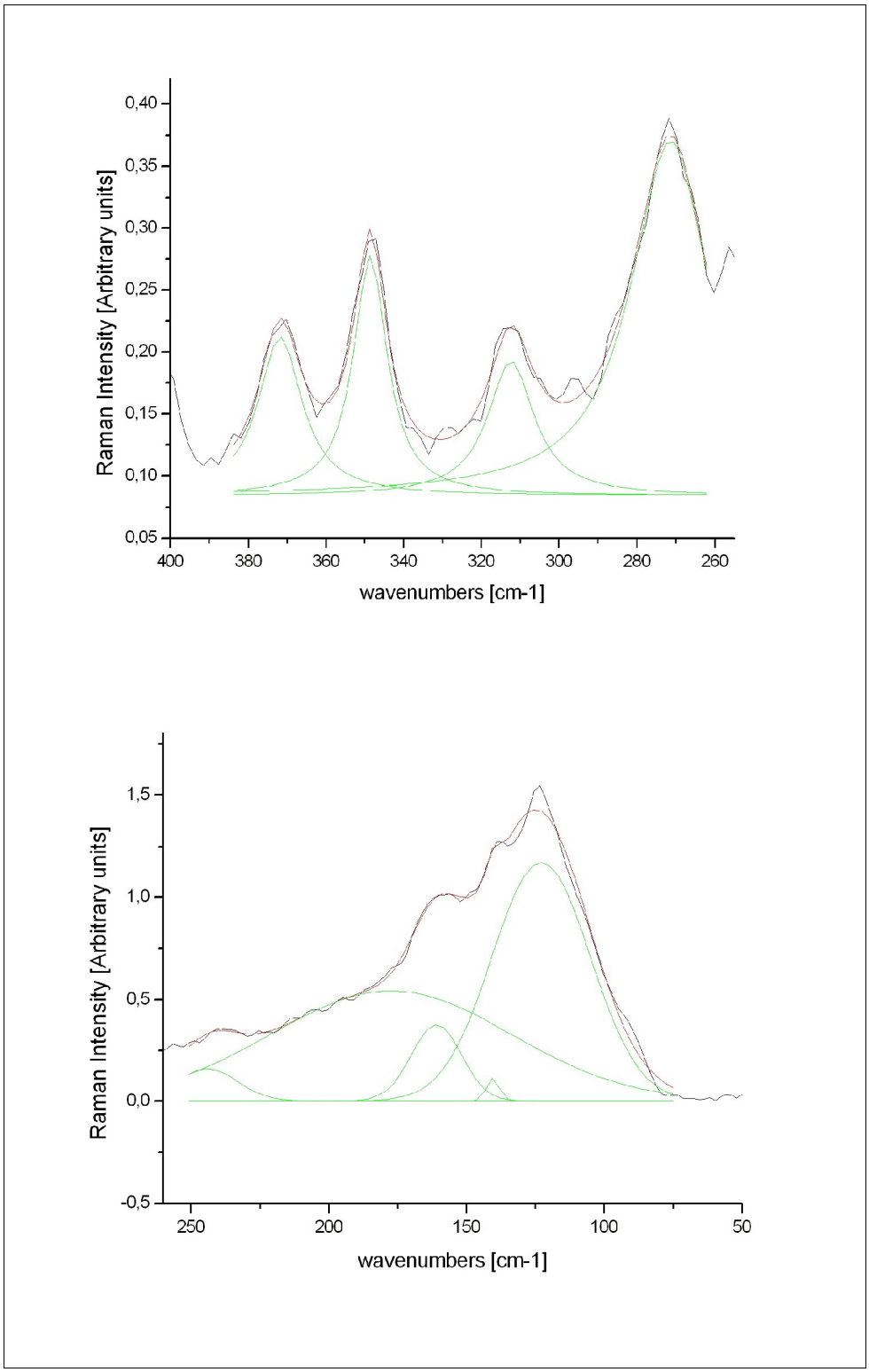
ADB no espectro Raman na região metal – ligante entre 600 – 50 cm^{-1}.

C – 6

[Cd(Gli)(Met)]. H_2O



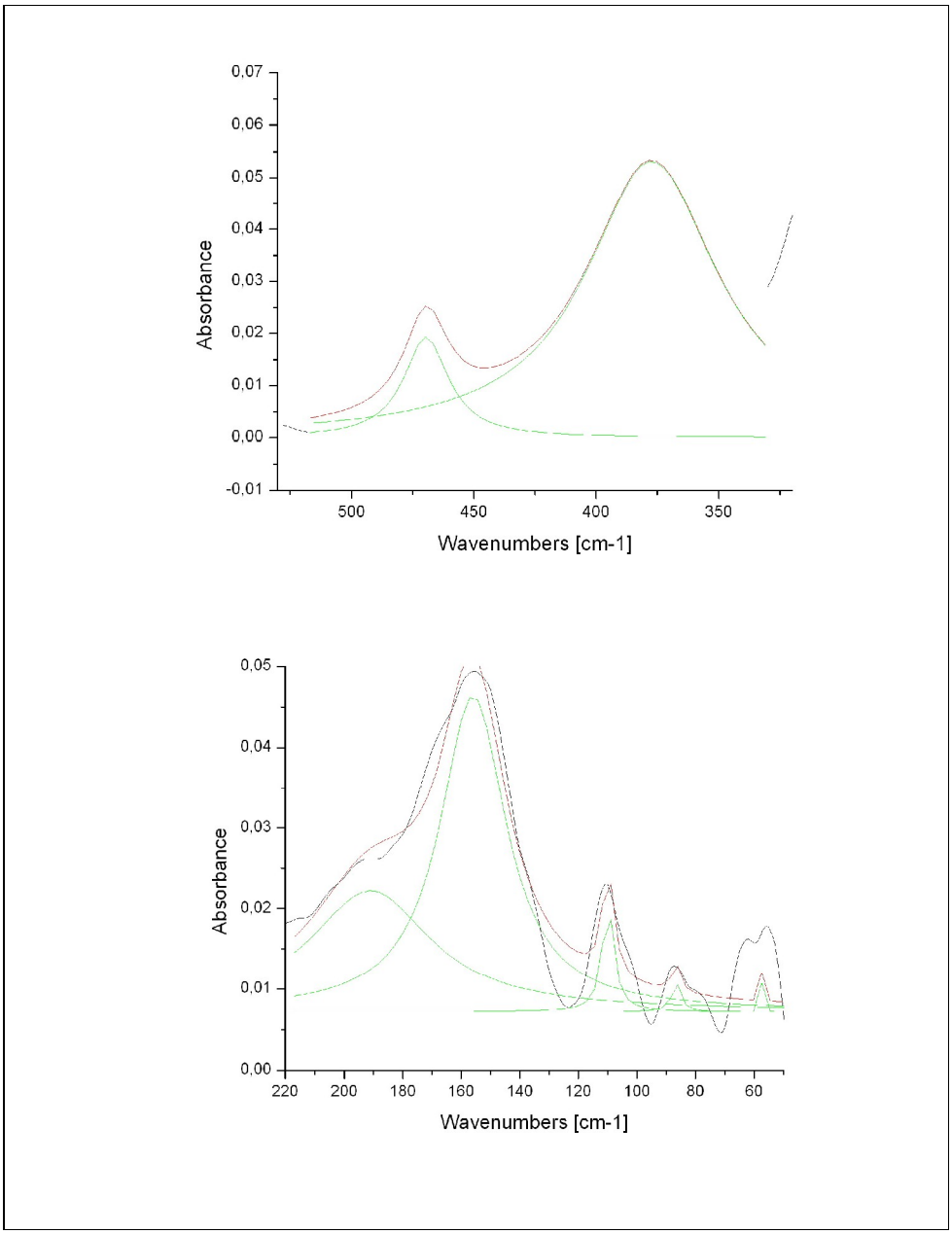
ADB no espectro Raman na região metal- ligante entre 600 – 360 cm^{-1}.



ADB no espectro Raman na região metal – ligante entre 400 – 50 cm^{-1}.

C – 7

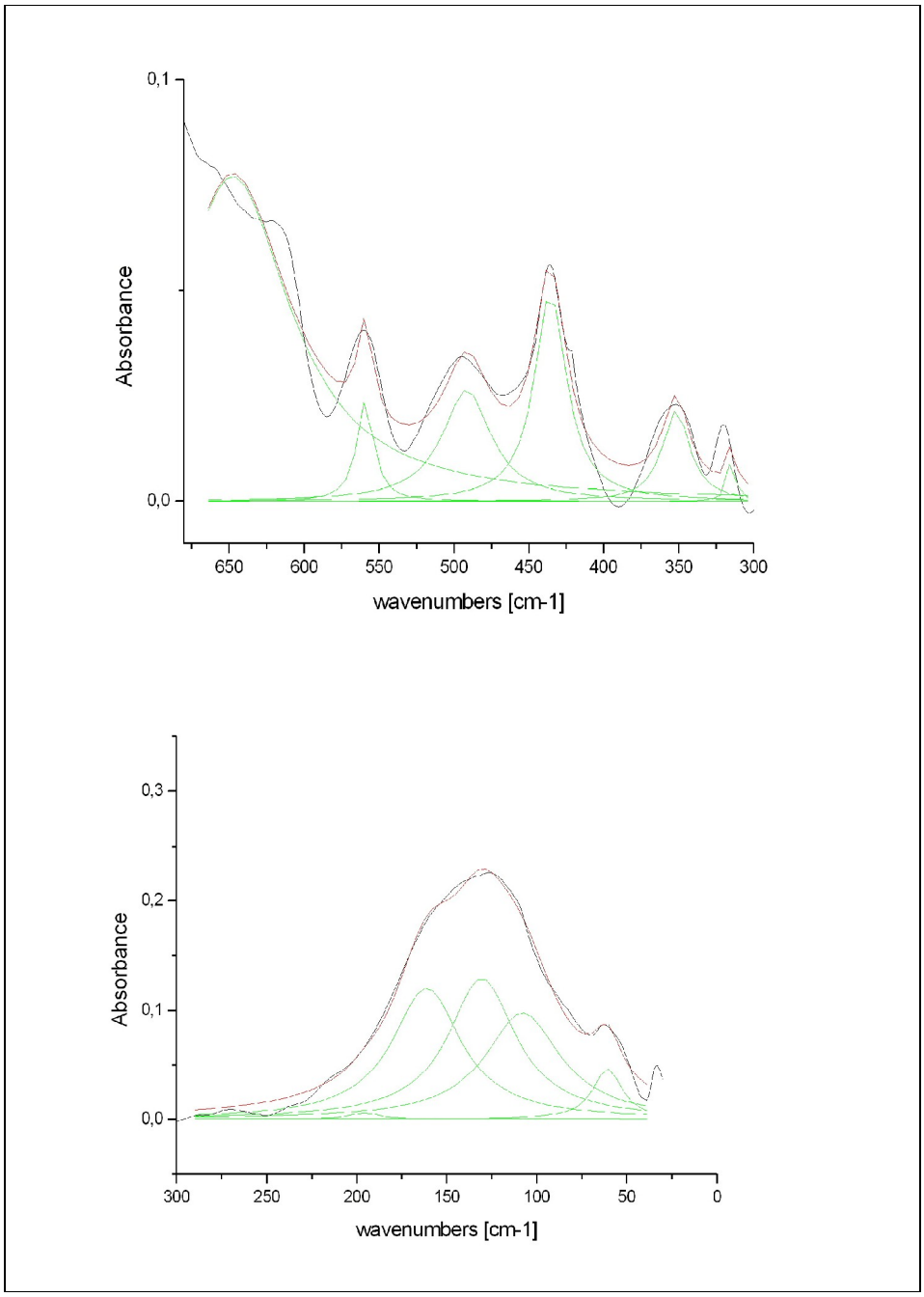
[Ni(Gaa$_2$)]. 2 H_2O



ADB no espectro infravermelho na região metal – ligante entre 500 0 50 cm^{-1}.

C – 8

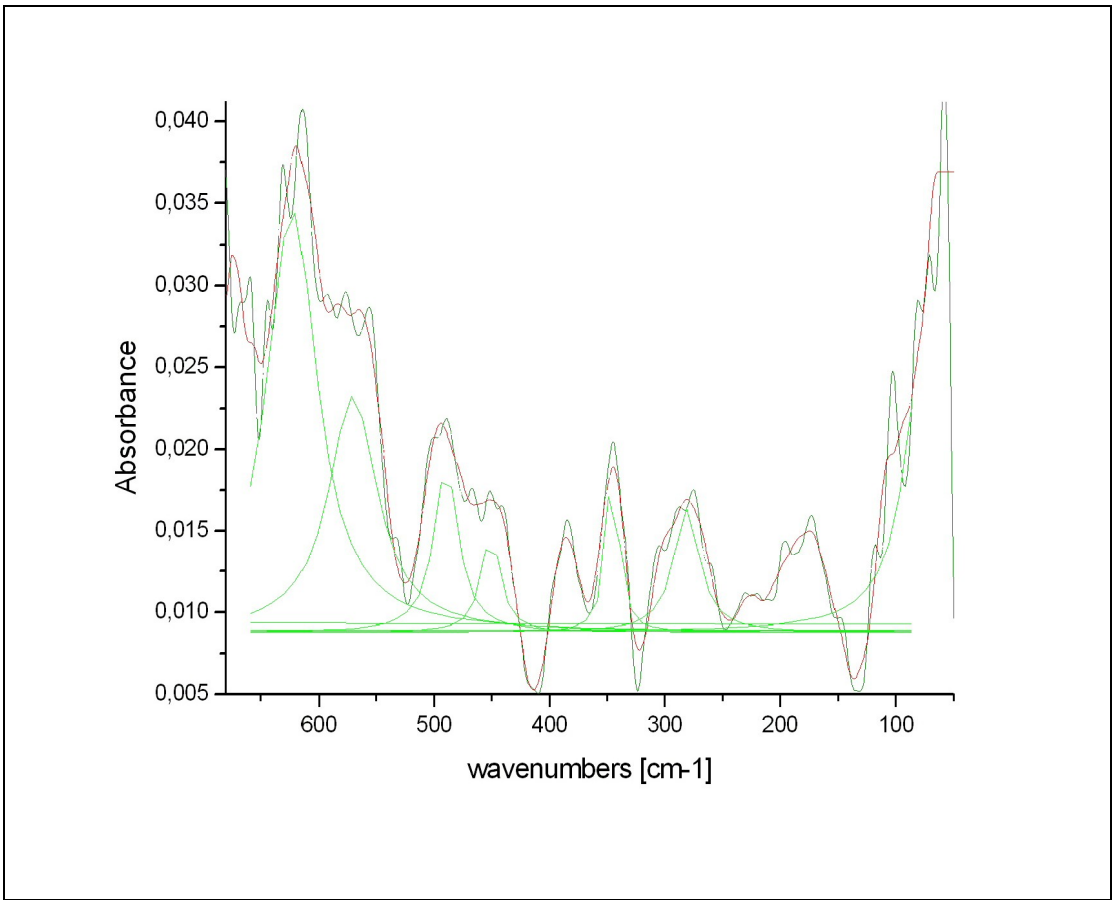
[Ni(Asp)(Gaa)]. 2 H_2O



ADB no infravermelho na região metal – ligante entre 650 – 50 cm^{-1}.

C – 9

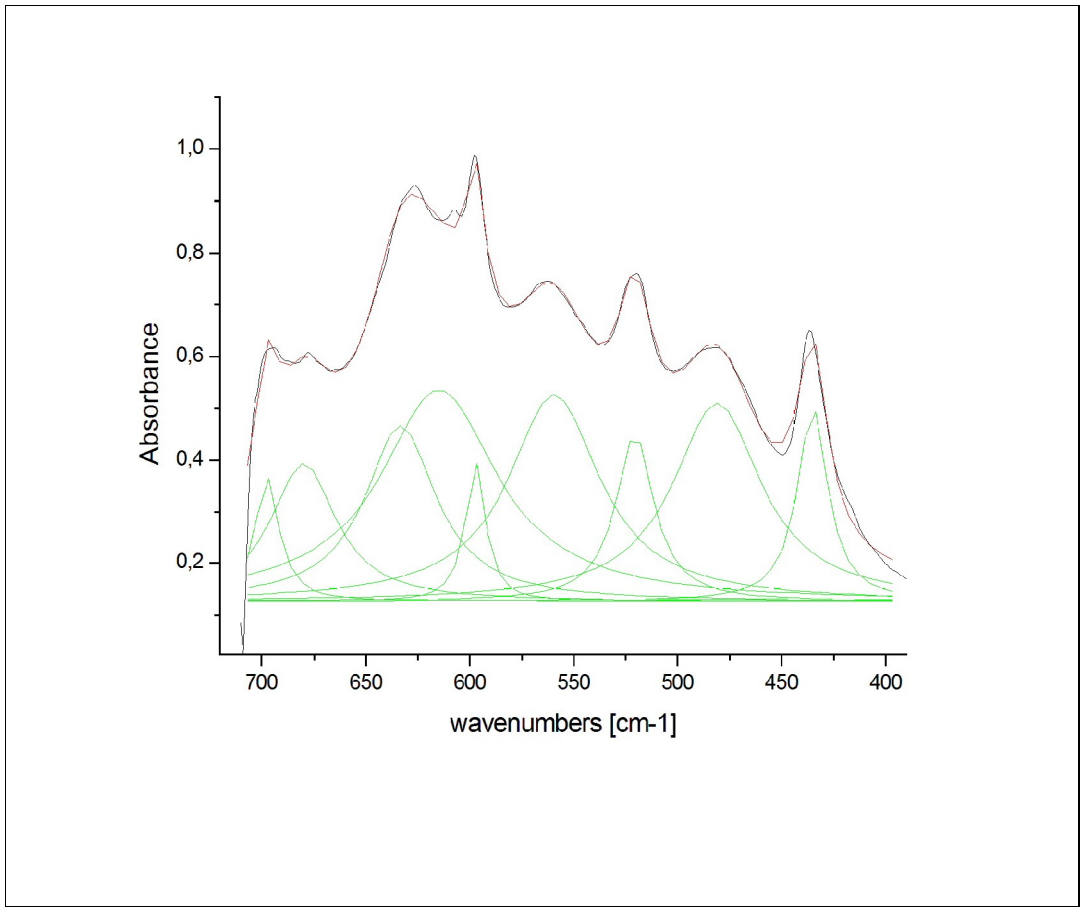
[Ni(Asp)(Ser)]. 2 H_2O



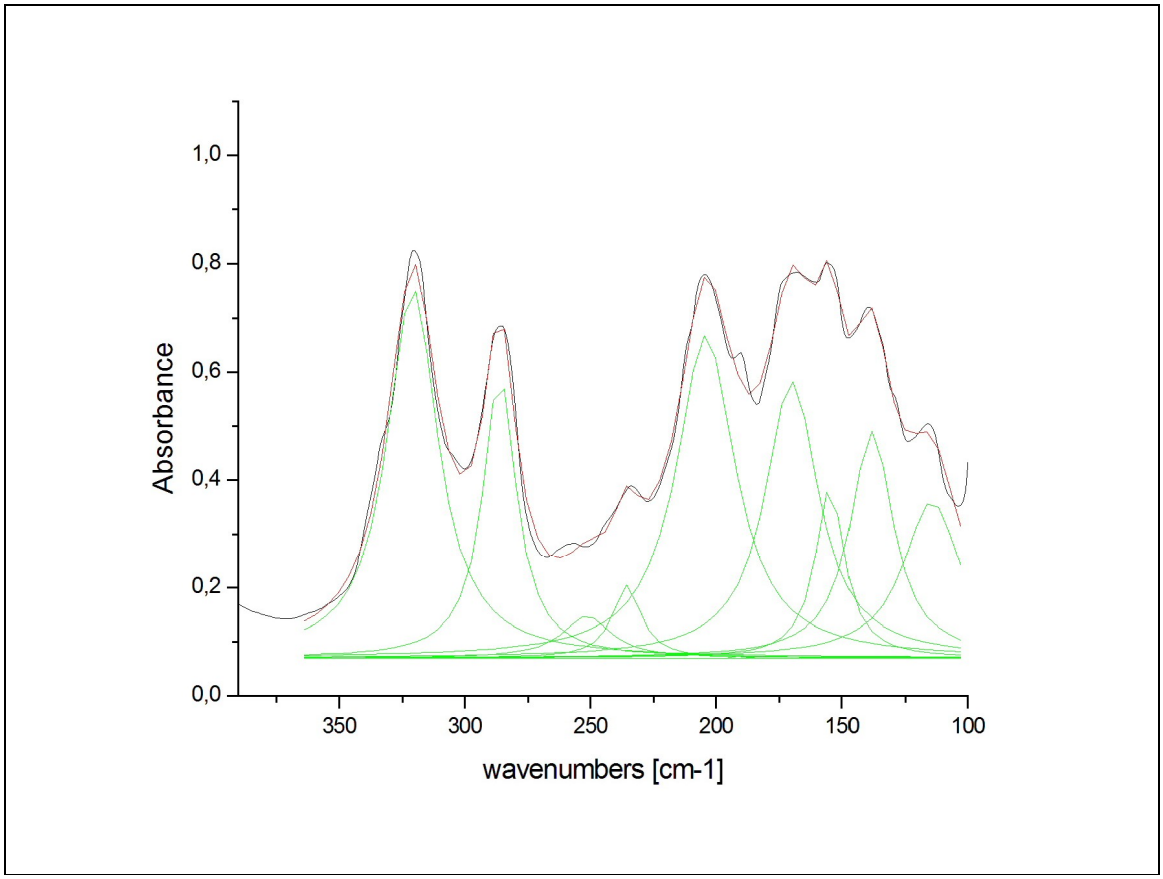
ADB no espectro infravermelho na região metal – ligante entre 650 – 50 cm^{-1}.

C – 10

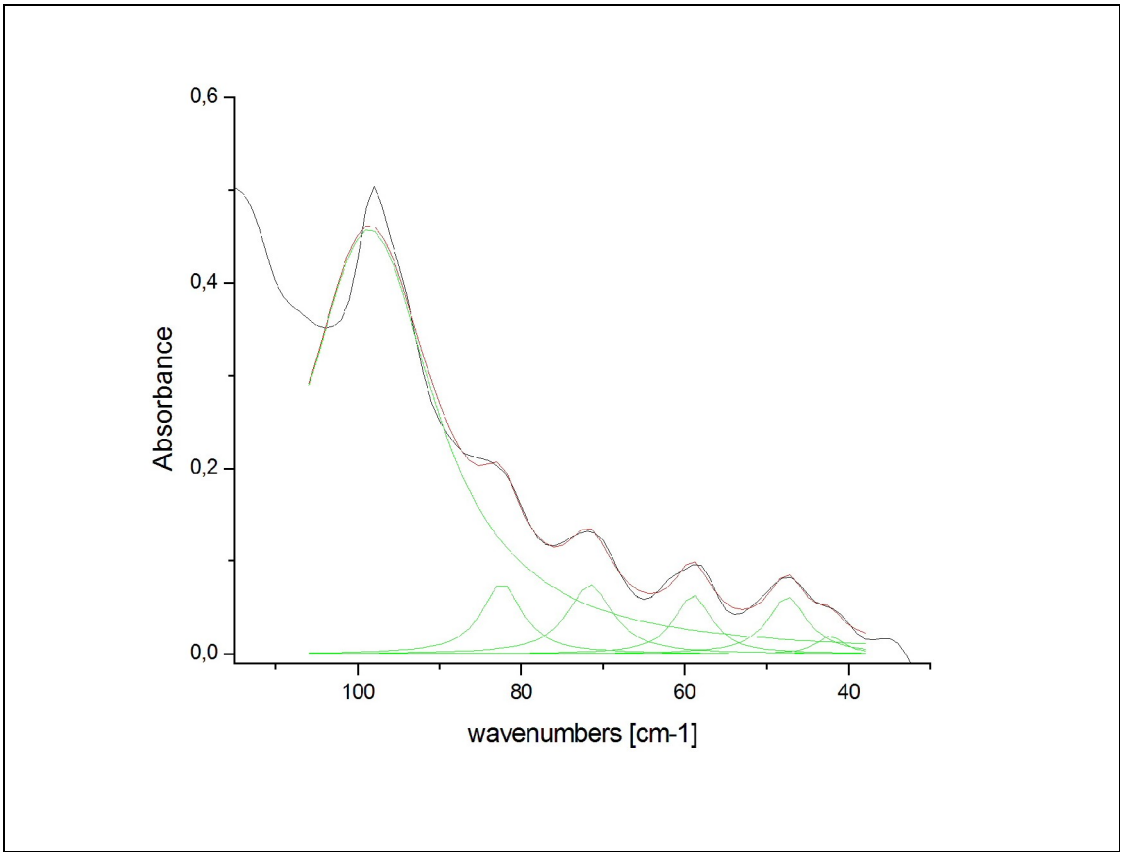
[Ni(Gaa)(Gli)].2H_2O



ADB no espectro infravermelho na região metal-ligante, entre 700 – 400 cm^{-1} para o complexo [Ni(Gaa)(Gli)].2H_2O.



ADB no espectro infravermelho na região metal-ligante, entre 375 – 100 cm^{-1} para o complexo $[Ni(Gaa)(Gli)].2H_2O$.



ADB no espectro infravermelho na região metal-ligante, entre 100 – 40 cm^{-1} para o complexo [Ni(Gaa)(Gli)].2H_2O.