

Electronic Supplementary Information to

DFT study of vibrational circular dichroism spectra

of D-lactic acid-water complexes

by Joanna Sadlej, Jan Cz. Dobrowolski, Joanna E. Rode, Michał H. Jamróz

Cartesian coordinates for the complex structures optimized at the B3LYP/aug-cc-pVDZ level:

Complex 1a

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.531640249437
H	1.025135916128	0.000000000000	-0.390306895465
H	-0.535485039460	-0.878602311635	-0.383575506978
H	-0.517164618472	0.901036494909	-0.351270793604
O	-1.321421171533	0.115699139095	2.026331984757
C	0.658913011902	-1.244480158917	2.107938417390
H	0.599019756661	0.857785423959	1.887695549214
O	0.065995981225	-1.999539516011	2.871516654376
H	-1.456200470288	-0.613561188910	2.652484849152
O	1.919318733565	-1.417252951643	1.718933935872
H	2.272279586818	-2.238706198453	2.150248912455
H	1.354235907283	-3.449902183766	3.388313754974
O	2.298489152751	-3.631880027127	3.220917040588
H	2.355424281071	-4.552656460356	2.939365238007

Complex 1b

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.533273254748
H	1.019305848669	0.000000000000	-0.402035875566
H	-0.542609011254	-0.879019728662	-0.371837514181
H	-0.525910020120	0.898781118170	-0.342953250478
O	-1.333176953144	0.124965469930	1.957135523689
C	0.697352464292	-1.239655148223	2.084610515329
H	0.611630684656	0.853495871303	1.887870969974
O	0.218064819386	-2.069315148551	2.833811404890
H	-1.496008039289	-0.255461243531	2.839198726447
O	1.979277480927	-1.319587726920	1.662335173943

H	2.367172345351	-2.115635981716	2.061492227265
H	-2.292499557585	-1.578977711566	5.039259415315
O	-2.250185992535	-1.518952147303	4.078632695631
H	-1.467030550805	-2.029496030588	3.809265047076

Complex 1c

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.533490783458
H	1.027483267422	0.000000000000	-0.384696607305
H	-0.529429106563	-0.882585493425	-0.382666854570
H	-0.518140101040	0.897865994442	-0.355891774945
C	0.632380403457	-1.263360908045	2.093289827171
H	0.584964320179	0.858391076211	1.899448801239
O	-1.320921724313	0.109631289148	2.052732529537
O	0.013074711882	-2.098929252155	2.719610906945
O	1.946178990704	-1.365307028088	1.813101129898
H	-1.530047098200	-0.732788448426	2.489407662367
H	2.262858625102	-2.202677594691	2.190769924321
H	-2.483275531382	1.328753797148	1.109511105654
O	-2.841164905733	1.963276460183	0.464662344353
H	-3.545050886246	2.430358683317	0.927531780670

Complex 1d

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.535884527567
H	1.023434507644	0.000000000000	-0.394242417495
H	-0.547369242558	-0.870728293505	-0.385540987384
H	-0.507534628964	0.909708253646	-0.341417348945
C	0.599014912074	-1.283909675653	2.082814993552
H	0.621949282007	0.837185032289	1.890661755728
O	-1.309842421612	0.161004629348	2.050674364284
H	-1.566224441495	-0.675543383934	2.469056230997
O	-0.030124892359	-2.130936332779	2.677802376712
O	1.928631867350	-1.412920365408	1.828057243857
H	2.206725100321	-2.271389174075	2.188326685303
H	3.139689937158	0.200492596969	1.234580371498
O	3.316771089175	1.071253061431	0.851356280174
H	4.223934438991	1.282295610266	1.099199289383

Complex 2a

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.523320108322
H	1.026860010416	0.000000000000	-0.382157202261
H	-0.523992076831	-0.886114397579	-0.380332570893

H	-0.520623504897	0.896210371493	-0.358103956731
O	-1.345871357348	0.055828243094	1.975287993660
C	0.772776328084	-1.183831229823	2.101755675340
H	0.554233658185	0.890834361532	1.881260017303
O	1.800297633192	-1.625401418360	1.610054262768
H	-1.377479147543	-0.240666900238	2.894133918556
O	0.238842056654	-1.645765803756	3.240482708155
H	0.817094112190	-2.376509168778	3.585000995785
H	2.433786306886	-3.077969674183	2.781617375515
O	2.121198212374	-3.540174430958	3.584681381974
H	2.859901641621	-3.544819044720	4.204774294604

Complex 2b

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.534728021864
H	1.026041840180	0.000000000000	-0.392728226760
H	-0.527626182150	-0.878705838694	-0.394580730952
H	-0.514115315695	0.901708909427	-0.354427290805
O	-1.300016247854	0.018634628035	2.090579957303
C	0.849426921181	-1.160160595433	2.060249685524
H	0.503228149998	0.902309544150	1.902435543752
O	1.985457877449	-1.073194028976	2.459170938097
H	-1.841074104269	-0.687537104632	1.687508909052
O	0.205788056972	-2.371858501734	2.006814714213
H	0.832256154718	-3.032552058154	2.345052656602
H	-3.011937984394	-2.718969630278	1.866112189228
O	-2.516345268953	-2.376799115641	1.111630209457
H	-1.608442128541	-2.687559634309	1.260087433056

Complex 2c

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.521072632729
H	1.029390771810	0.000000000000	-0.374777850983
H	-0.517417132983	-0.889375906407	-0.381358055750
H	-0.515336330209	0.898166060339	-0.359385559088
C	0.785873021769	-1.173520816341	2.101601873461
H	0.521816114721	0.904605332293	1.885460533939
O	-1.358663384345	0.019534093315	1.974780572708
O	1.774294128713	-1.664030722516	1.611138855962
O	0.277353441855	-1.579376258657	3.297310275761
H	-1.377896330921	-0.199638385556	2.915903765841
H	0.849840617864	-2.290703817563	3.628137713615
H	-2.064285519073	1.785461581546	1.608008371951
O	-2.125249226535	2.737052078156	1.413304114870

H	-3.053739035003	2.899034453468	1.213344642556
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Complex 2d

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.525434723338
H	1.022254192141	0.000000000000	-0.392417805589
H	-0.538516376464	-0.877372542498	-0.380252805513
H	-0.515246827541	0.903691819077	-0.346201481684
C	0.715699388194	-1.222166172190	2.098598144707
H	0.597839859937	0.861085146883	1.882222572388
O	-1.345412584718	0.116414176807	1.964315606162
H	-1.390441902564	-0.033596130228	2.916663275638
O	1.776550280545	-1.663307558975	1.703433103357
O	0.073141798648	-1.756497442803	3.161598402657
H	0.616282165253	-2.493792235773	3.486443715681
H	3.026369919786	-0.896124775164	0.430821568839
O	3.498575026964	-0.351086576901	-0.221238794841
H	4.397556904518	-0.696634718909	-0.241054194023

Cartesian coordinates for the complex structures optimized at the B3LYP/aug-cc-pVTZ level:

Complex 1a

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.528379153476
H	1.016343518420	0.000000000000	-0.390343337704
H	-0.531542654851	-0.872136123652	-0.381304438310
H	-0.514213470301	0.893462060868	-0.350254234800
O	-1.317997804448	0.100931299387	2.022798555148
C	0.671338305424	-1.238335928901	2.098990908898
H	0.587080470765	0.856896644131	1.881558733691
O	0.085064368494	-2.007225943050	2.841737455323
H	-1.453542044276	-0.639530567854	2.630619938433
O	1.934784764874	-1.384133753289	1.723697763203
H	2.299945341419	-2.202208249045	2.144310926747
H	1.397151986486	-3.455811638544	3.364026872715
O	2.341823086032	-3.620961714375	3.201377400080
H	2.420168569279	-4.534130808605	2.910248706301

Complex 2a

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.520646439781
H	1.018421990021	0.000000000000	-0.381473969570

H	-0.521390894763	-0.878621184683	-0.378518716133
H	-0.516791085167	0.889082227411	-0.356822836369
O	-1.340004687795	0.052267843258	1.976770942744
C	0.781946401282	-1.179736882546	2.088863424499
H	0.549415349724	0.885758607038	1.873743210662
O	1.844391721983	-1.556901025713	1.637529705478
H	-1.383308325763	-0.324574774614	2.862032034545
O	0.205688922538	-1.715185529220	3.168422288949
H	0.785918307699	-2.440805080626	3.511688254925
H	2.477915466551	-3.059813164884	2.773464560376
O	2.137294650011	-3.566608602305	3.532809585452
H	2.836815293500	-3.587491632082	4.192284533632

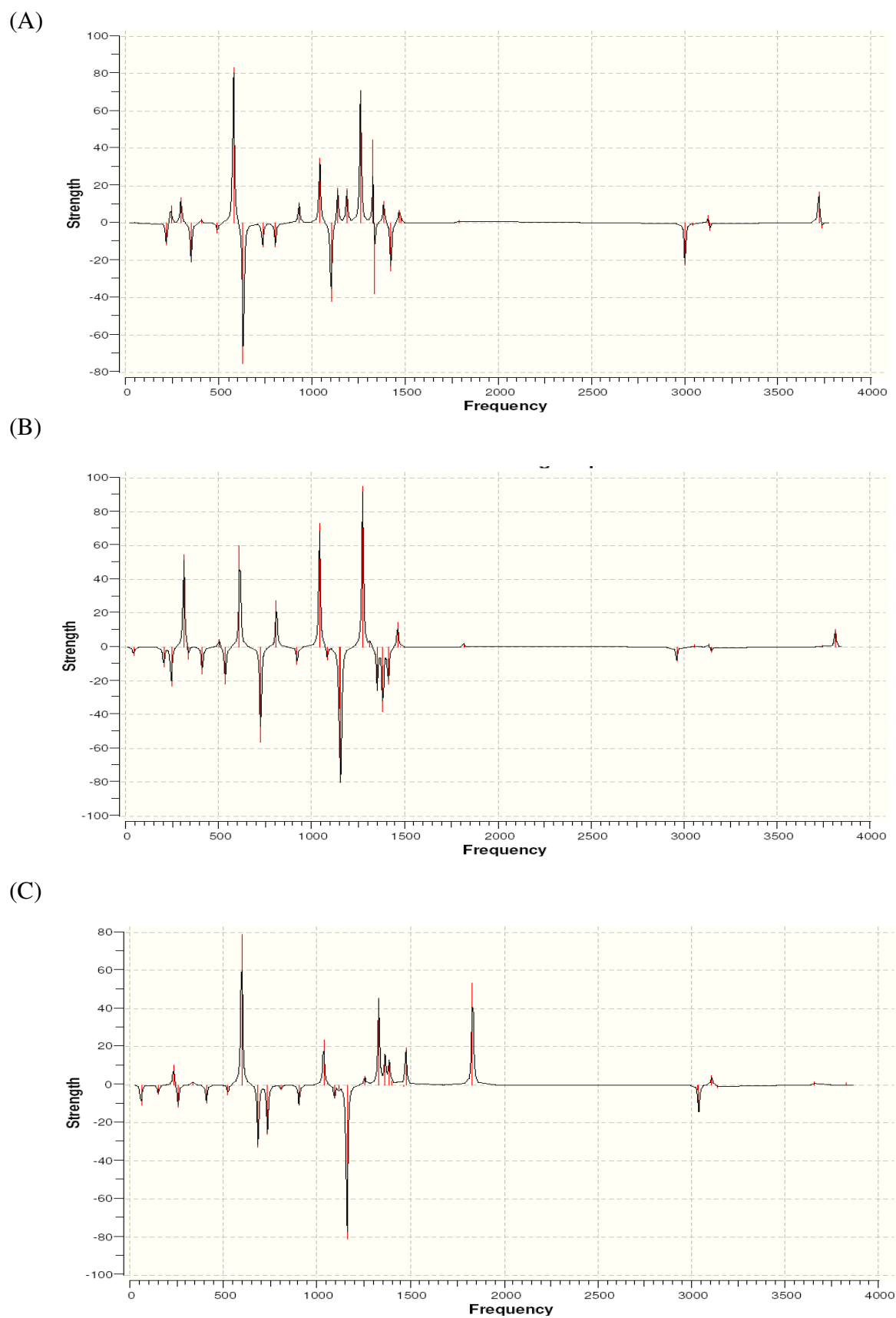
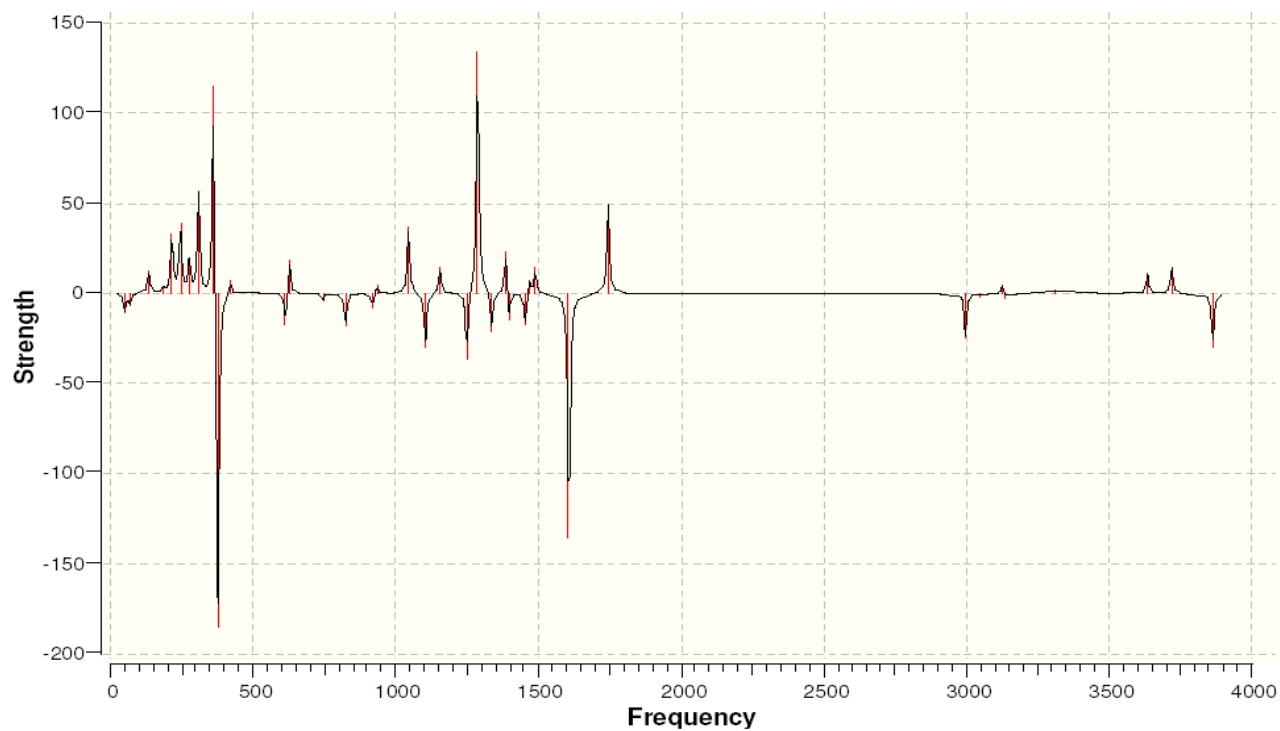


Fig. 1ESI. The calculated VCD spectra of the lactic acid conformers computed at the B3LYP/aug-cc-pVDZ level: (A) conformer I; (B) conformer II ; (C) conformer III

(A)



(B)

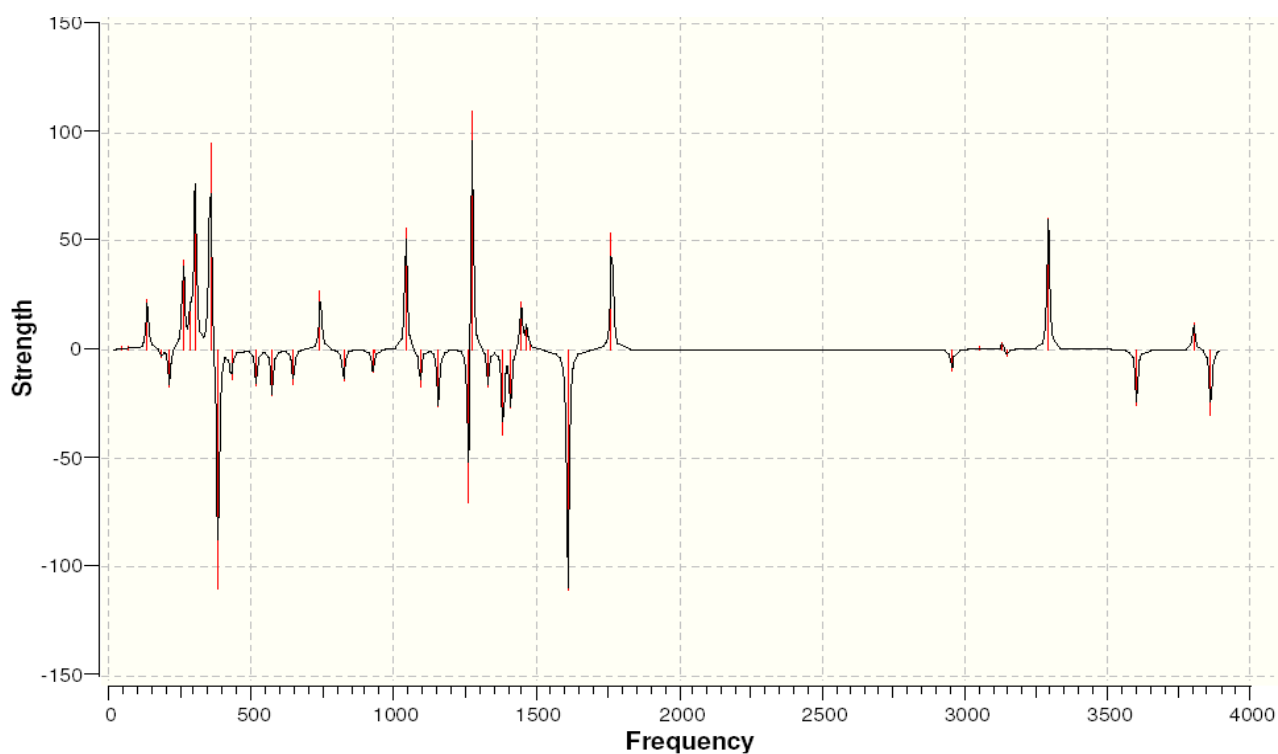
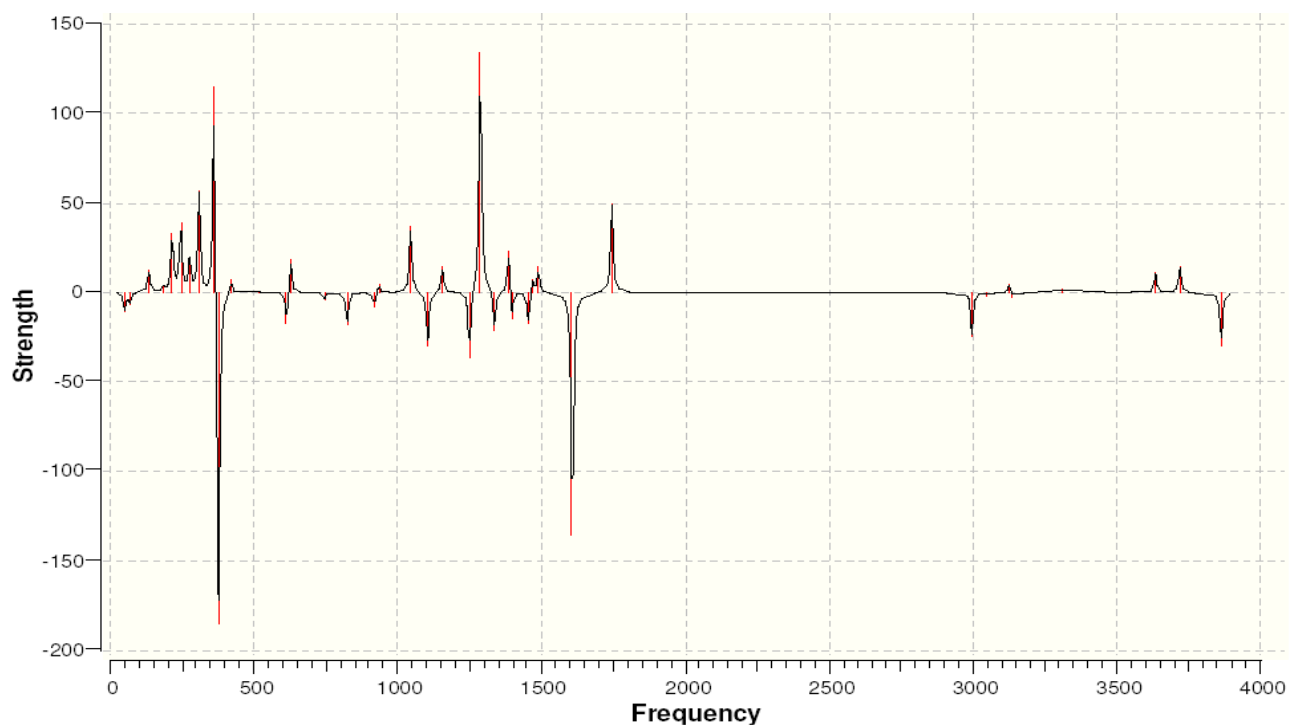


Fig. 2ESI. The calculated VCD spectra of the lactic acid conformer II (A) and its complex with water molecule (B) computed at the B3LYP/aug-cc-pVDZ level.

(A)



(B)

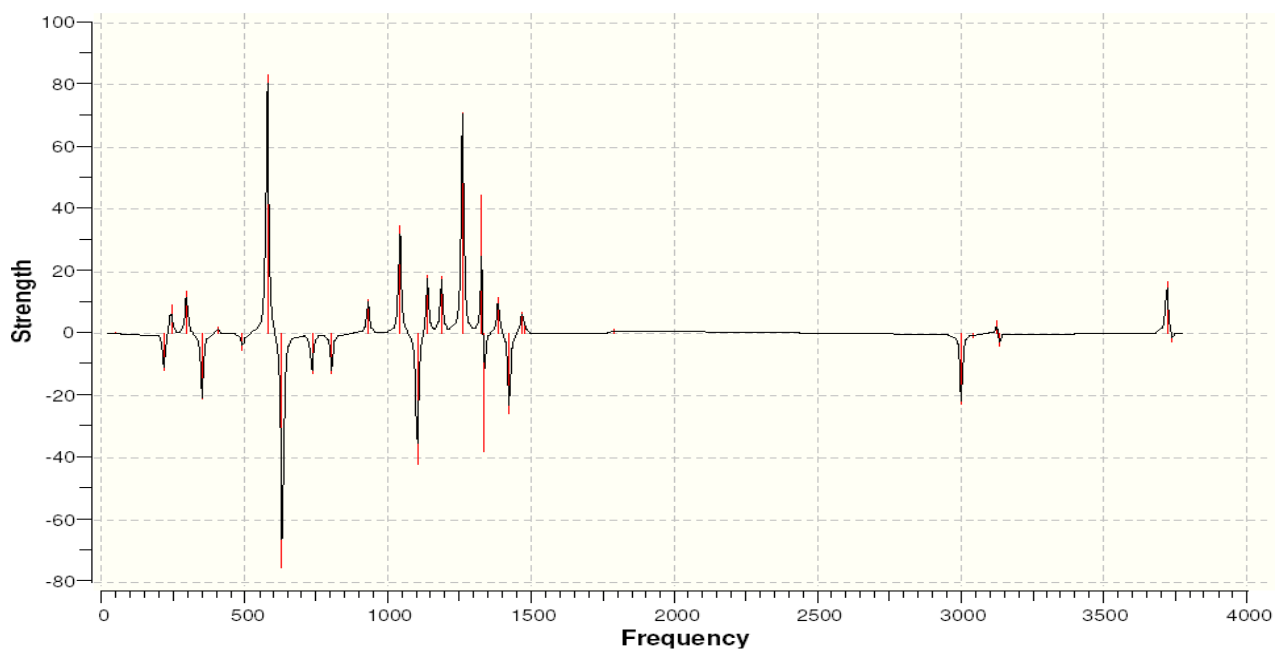


Fig. 3ESI. The calculated VCD spectra of the lactic acid complex with water molecule computed at the B3LYP/aug-cc-pVDZ level: (A) complex Ia (B) complex IIa