Electronic Supplementary Material (ESI) for RSC Advances.

L-Cysteine Electrooxidation in Alkaline and Acidic Media: A Combined Spectroelectrochemical and Computational Study

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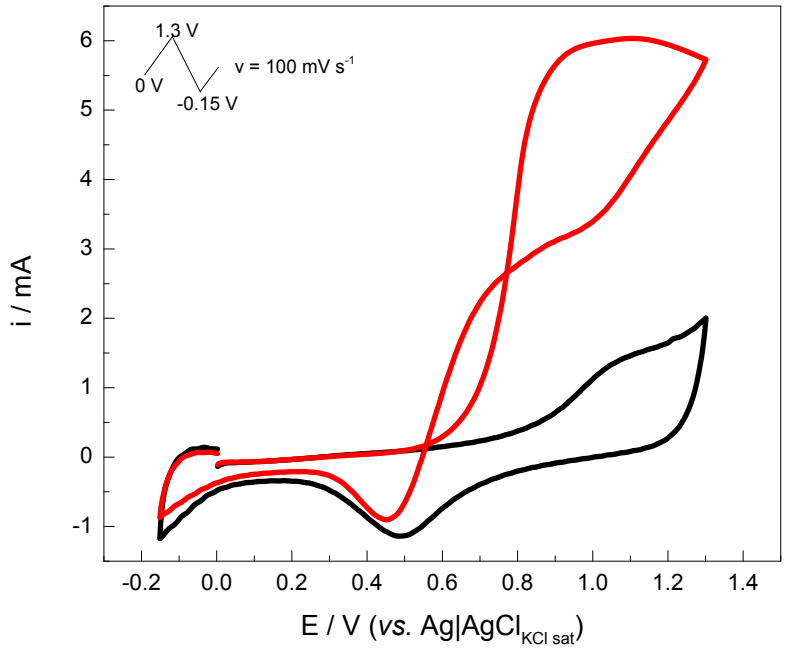
Surface Cleanness Process Efficiency

The process of cleaning the electrode, as shown in the experimental section, was verified by a cyclic voltammetry. For this, the electrode used for spectroelectrochemical measurements was cleaned in piranha solution and then placed into an electrochemical cell containing just the supporting electrolyte, H_2SO_4 0.50 mol L^{-1}, and the scan was registered (S.F. 1). Just after this, some crystals of L-Cys were added to the system and the procedure was repeated.



S.F.1. Cyclic voltammetry to verify the cleanness efficiency. Black line in absence and red line in the presence of L-Cys, perturbation program inserted.

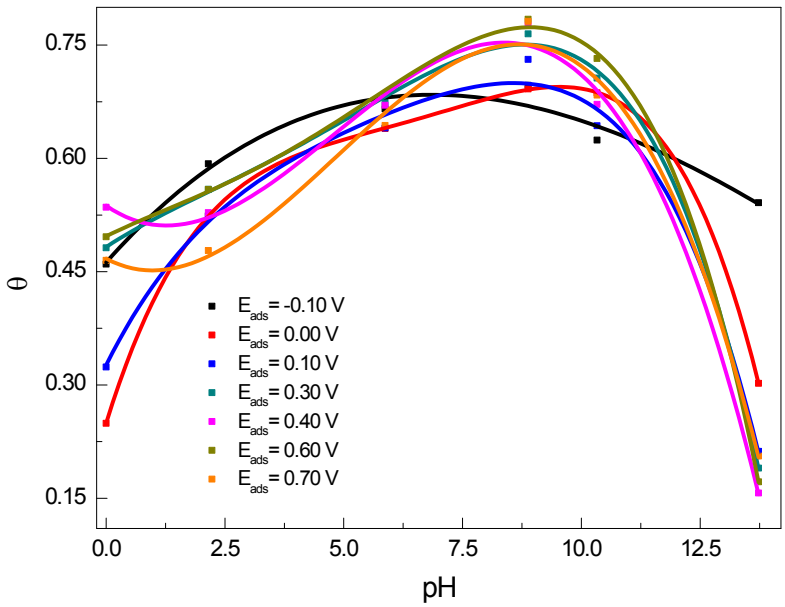
As could be seen, in absence of L-Cys a cyclic voltamogram with the predicted shape for Pt electrode in sulfuric acid media is observed, with a H_{UPD} region between -0.15 and 0.00 V, a oxide formation at potentials more positives than 0.90 V and reduction of it in the back scan around 0.50 V. In presence of L-Cys, even diluted, it

could be notice that the oxidation starts earlier, around 0.60 V, and the current increases at more positive potentials and almost did not reached a limit. A cross-over was observed at 0.80 V, but even with the positive current in a large region of the reverse scan, it was possible to observe the reduction of oxide in the same region as in the blank, just as the H_{UPD}, but with lower intensity, suggesting that some L-Cys is still adsorbed onto the electrode.

The cleanness could be verified, since the difference was very expressive between both situations and the shape of the blank experiment was in agreement with the expected for Pt electrodes.

Surface Coverage

To analyze the way in which the L-cys covers the electrode surface, some electrochemical measurements were performed. For this, the working electrode was inserted in solutions at the same pH conditions as for the IRRAS measurements. Then the electrode was submitted to a potential polarization that varied from -0.10 to 0.70 V (E_{ads}) and the coverage degree was estimated by the difference of charge of the H_{UPD} region before and after the modification with L-Cys, in a free amino acid solution.



S.F. 2. Coverage degree of Pt electrode in function of pH for different applied potentials. Lines does not present any physical meaning, just a guide for the tendency at each potential.

Spectroelectrochemical measurements

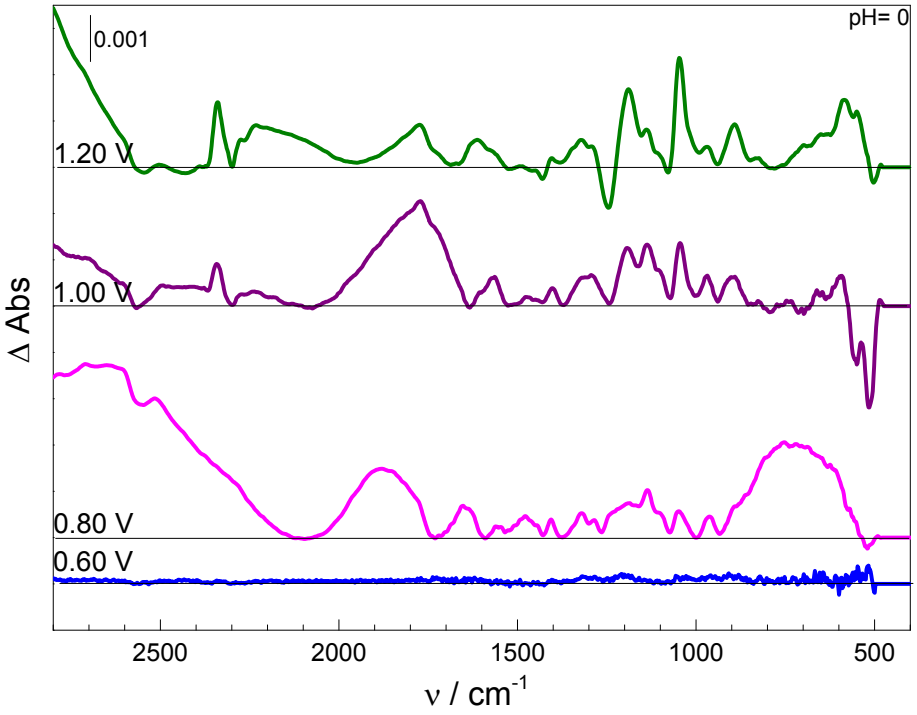
Because of the low intensity of the adsorption spectrum at pH 3 in Figure 3, it could be necessary a better comparison between spectra at pH 3 and 7. The type of signal observed (single/large band or multiplet) and the region observed at each condition are showed in S.T. 1. The small degree of variation at each pH condition corroborates the idea of similar spectra suggest in the text.

S.T. 1. Correspondence between the wavenumber observed in adsorption spectra at pH 3 and 7 (Figure 3).

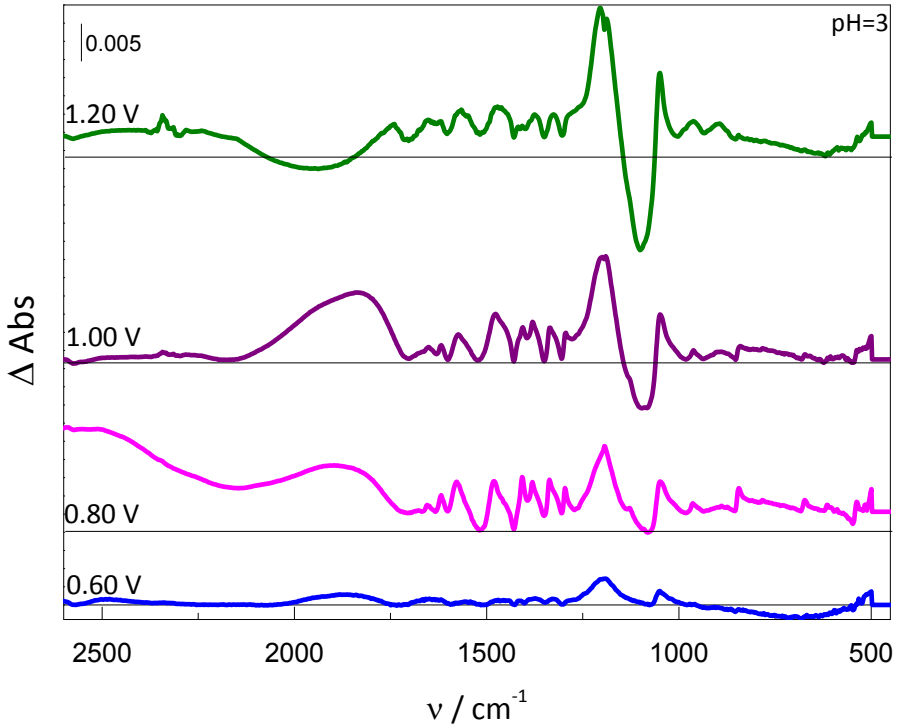
	large band	single band	single band	single band	single band	multiplet	single band	single band
pH 7	1898-1656	1609	1555	1551	1443	1401-1259	1172	1016
pH 3	2141-1692	1652	1616	1558	1486	1425-1299	1197	1049

Oxidation Spectra

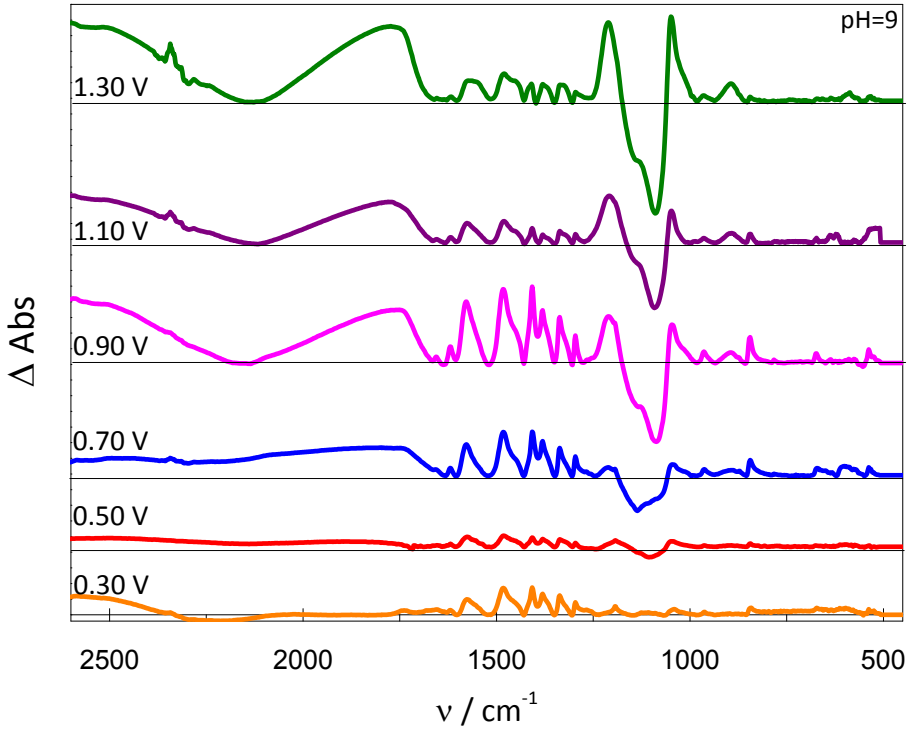
The following data presented in here are related to the oxidation spectra of L-Cys and L-Cys_2 for pH values different from 7.



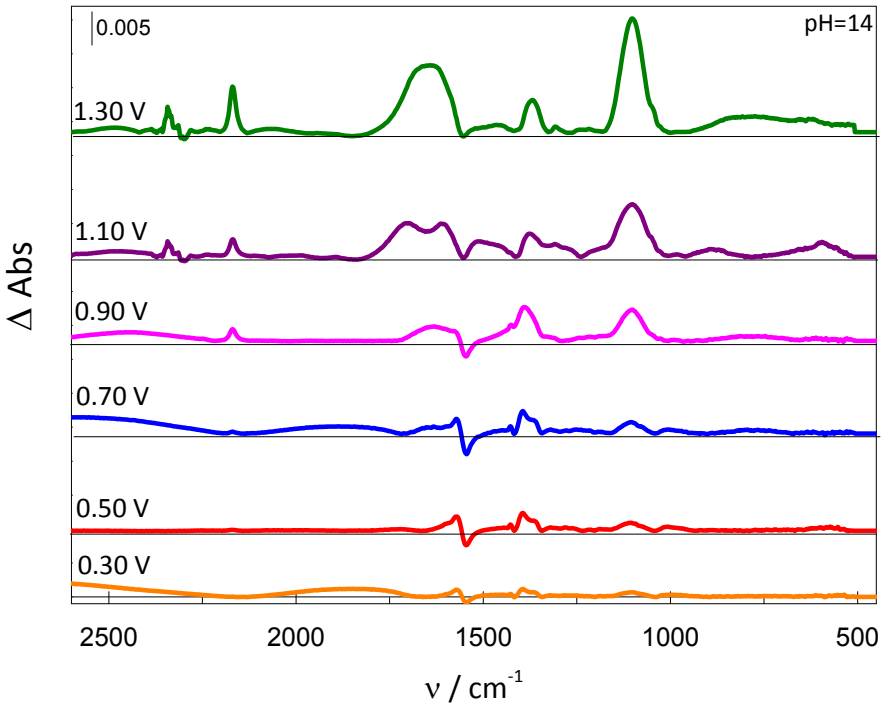
S.F.3. Oxidation spectra of L-Cys 0.10 mol L^{-1} in H_2SO_4 0.50 mol L^{-1}. Applied potentials showed.



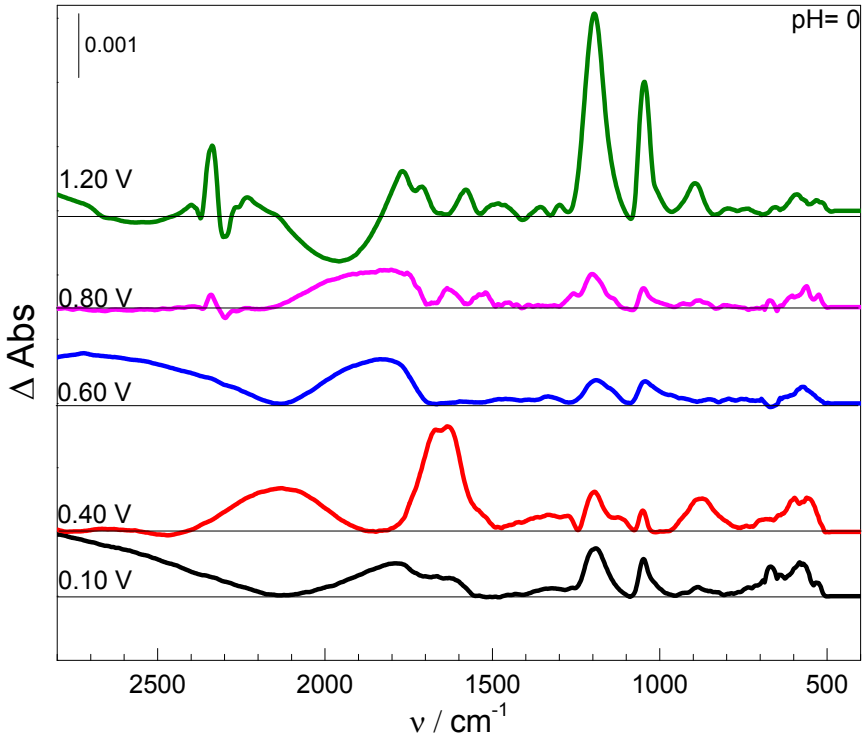
S.F.4. Oxidation spectra of cys 0.10 mol L^{-1} in Na_2SO_4 0.50 mol L^{-1}, pH (in the figure) adjusted by H_2SO_4. Applied potentials showed.



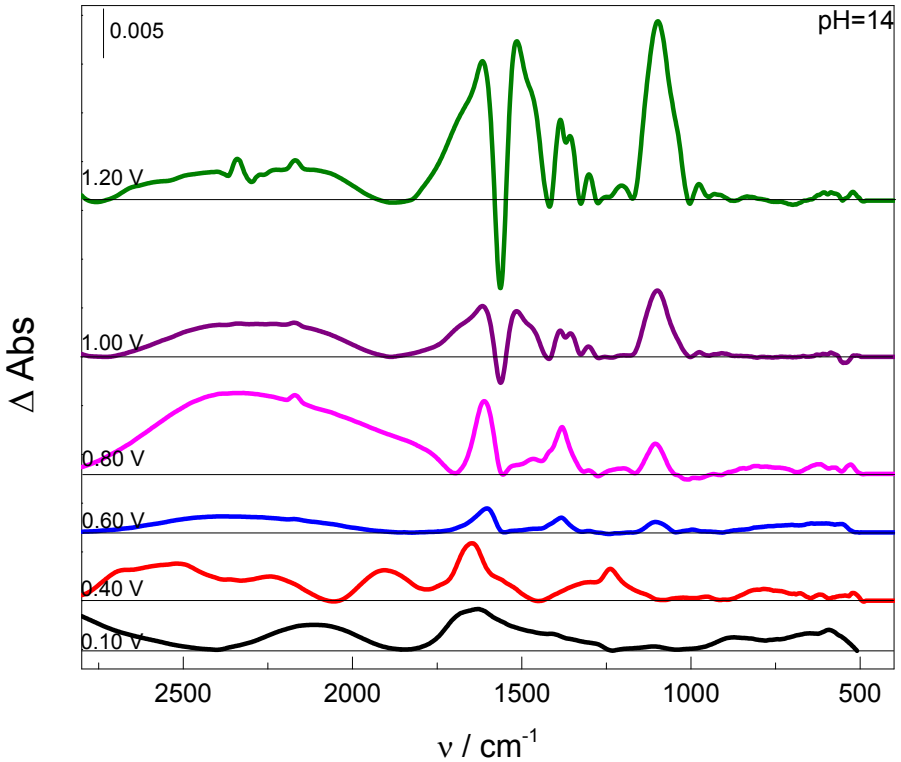
S.F.5. Oxidation spectra of cys 0.10 mol L^{-1} in Na_2SO_4 0.50 mol L^{-1}, pH showed in the figure (adjusted by NaOH addition). Applied potentials also inserted.



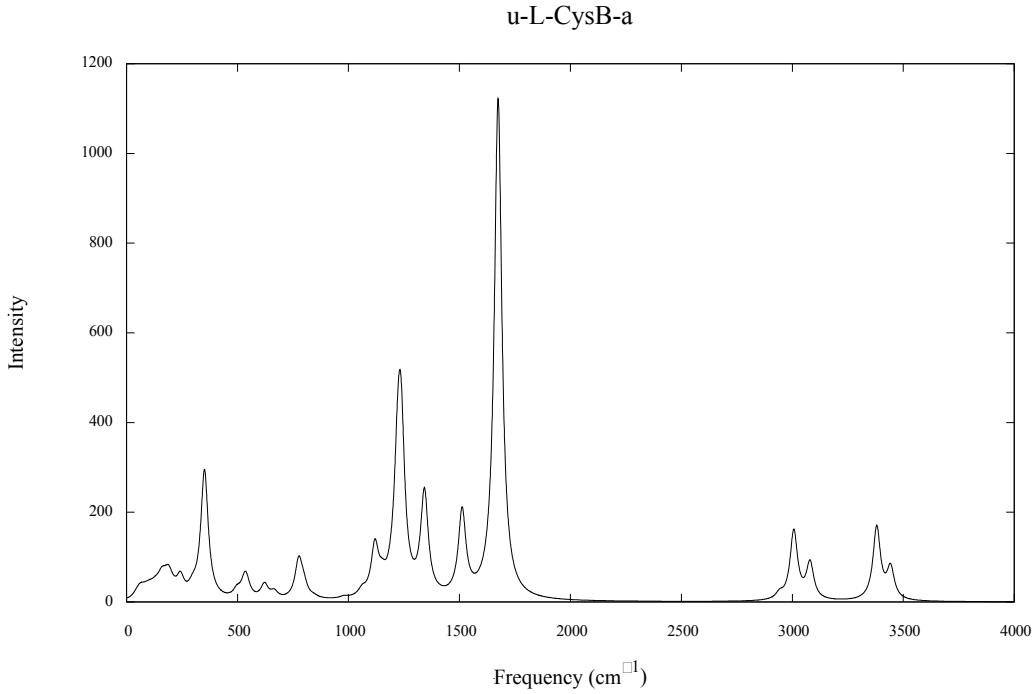
S.F.6. Oxidation spectra of cys 0.10 mol L^{-1} in NaOH 0.50 mol L^{-1}, pH showed in the figure. Applied potentials also inserted.



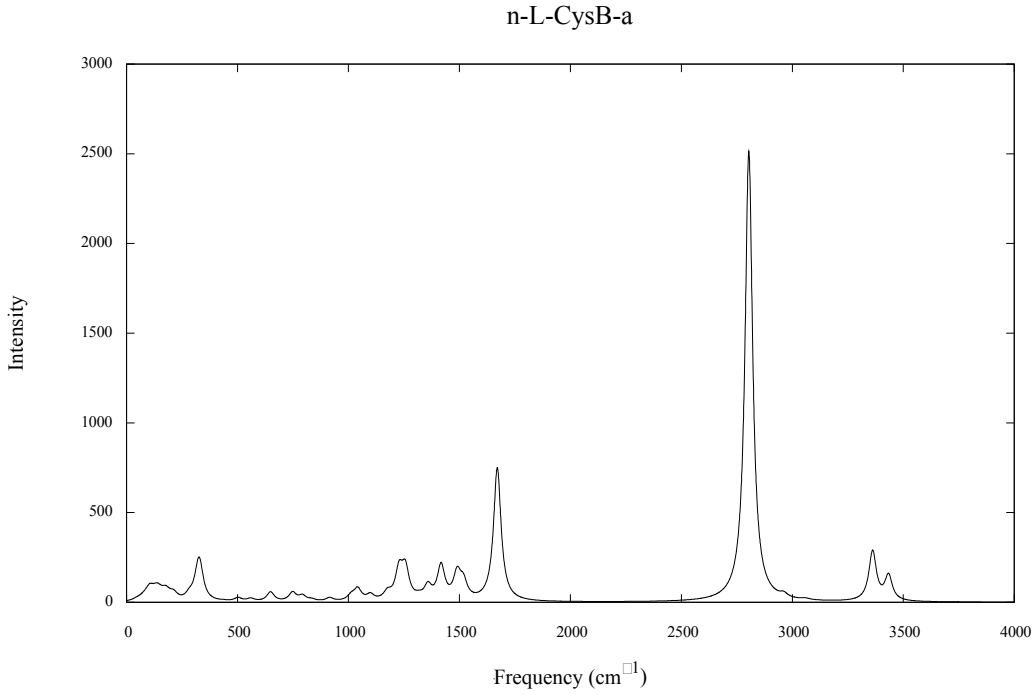
S.F.7. Oxidation spectra of L-Cys_2 sat. in H_2SO_4 0.50 mol L^{-1}, pH showed in the figure. Applied potentials also inserted.



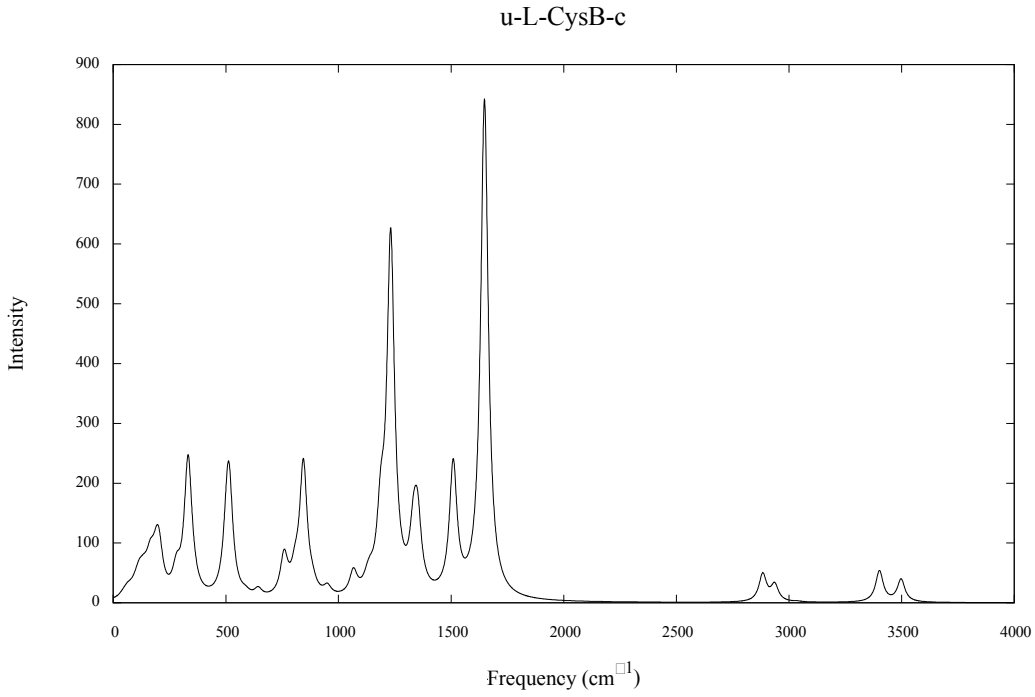
S.F.8. Oxidation spectra of cys_2 sat. in NaOH 0.50 mol L^{-1}, pH showed in the figure. Applied potentials also inserted.



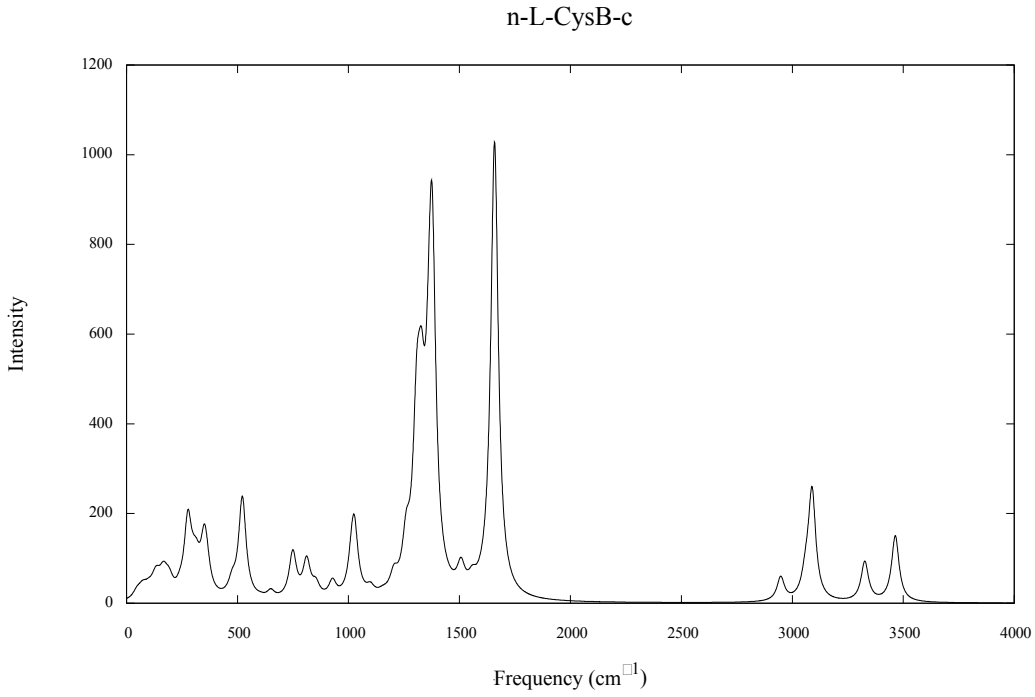
S.F.9. Computed infrared spectrum for u-L-CysB-a.



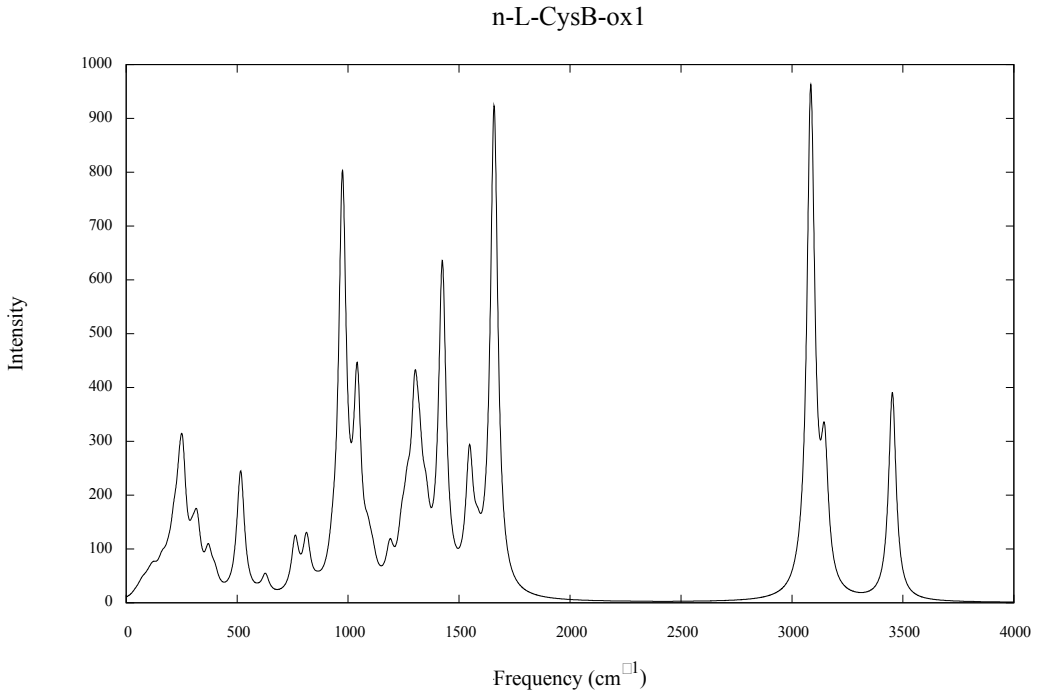
S.F.10. Computed infrared spectrum for n-L-CysB-a.



S.F.11. Computed infrared spectrum for u-L-CysB-c.

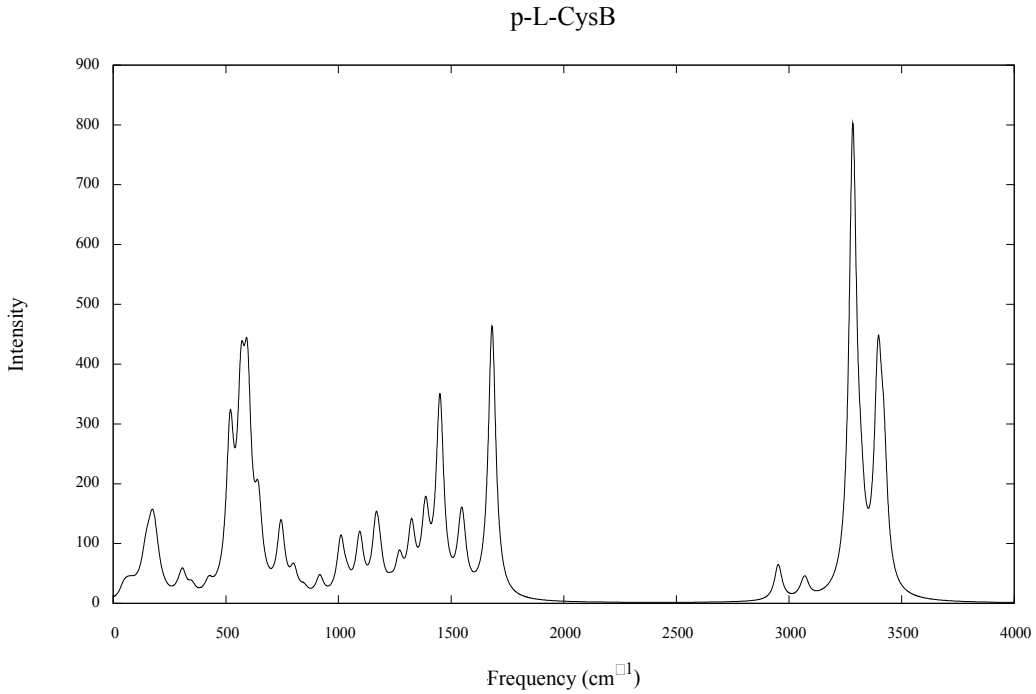


S.F.12. Computed infrared spectrum for n-L-CysB-c.

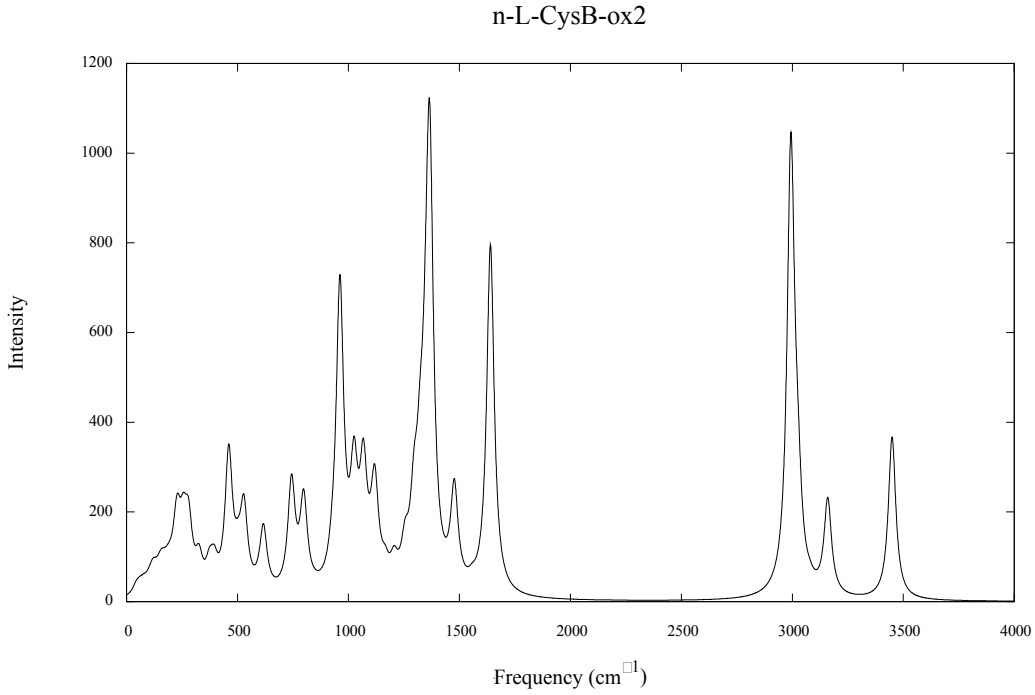


S.F.13

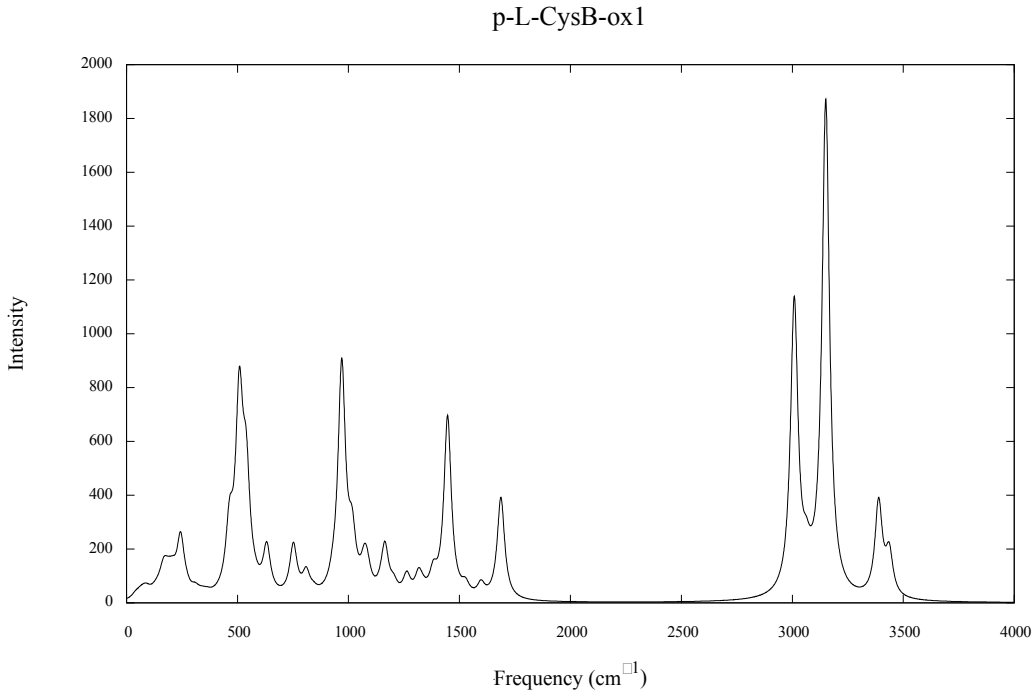
. Computed infrared spectrum for n-L-CysB-ox1.



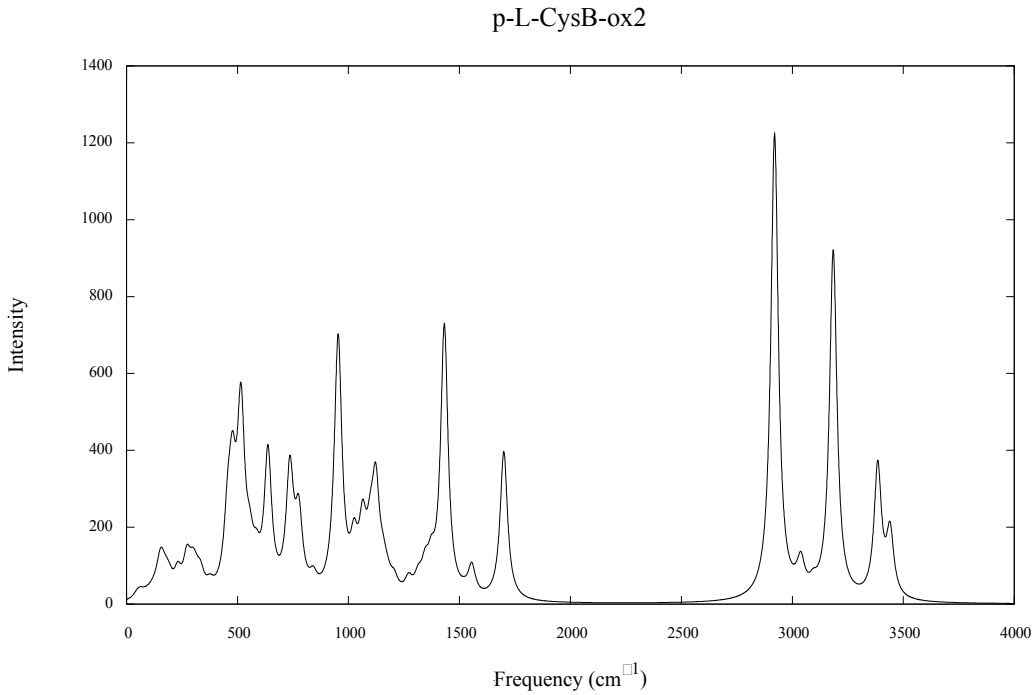
S.F.14. Computed infrared spectrum for p-L-CysB.



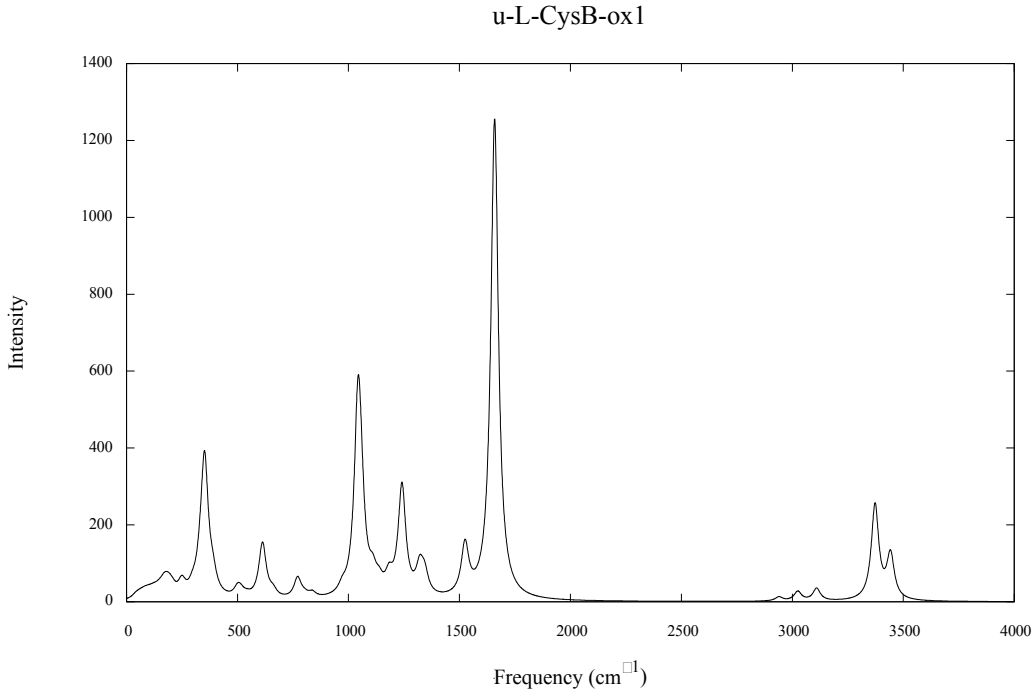
S.F.15. Computed infrared spectrum for n-L-CysB-ox2.



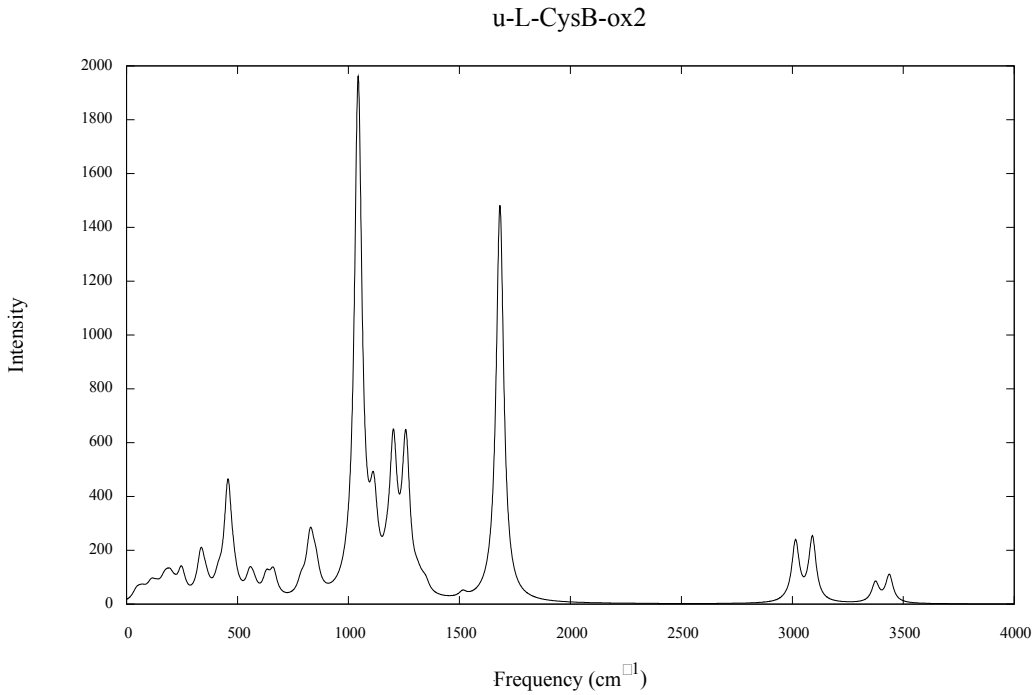
S.F.16. Computed infrared spectrum for p-L-CysB-ox1.



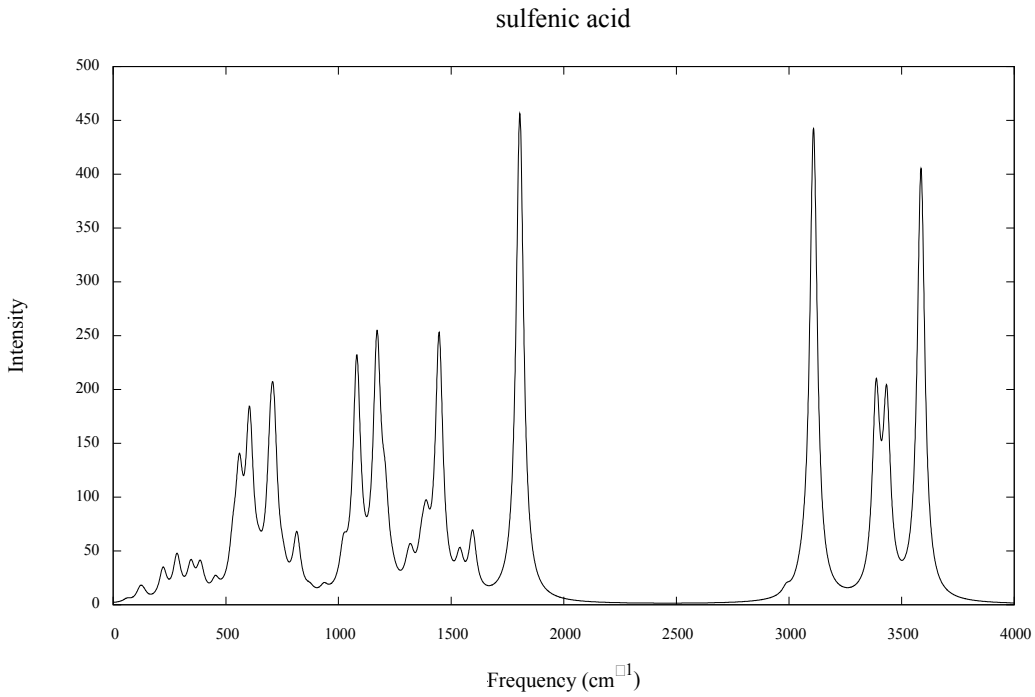
S.F.17. Computed infrared spectrum for p-L-CysB-ox2.



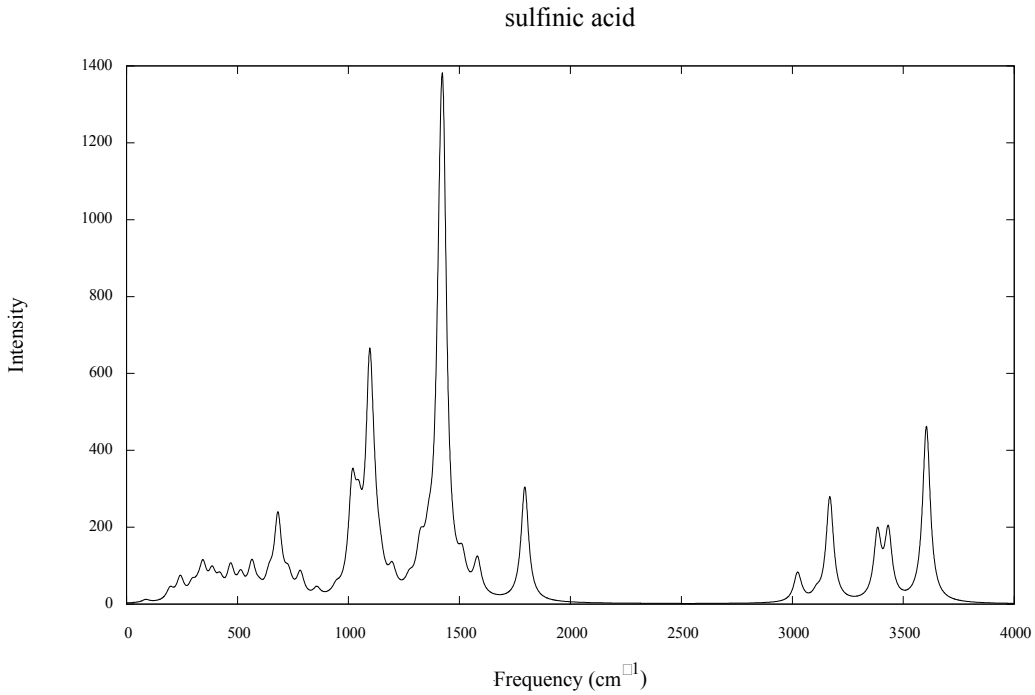
S.F.18. Computed infrared spectrum for u-L-CysB-ox1.



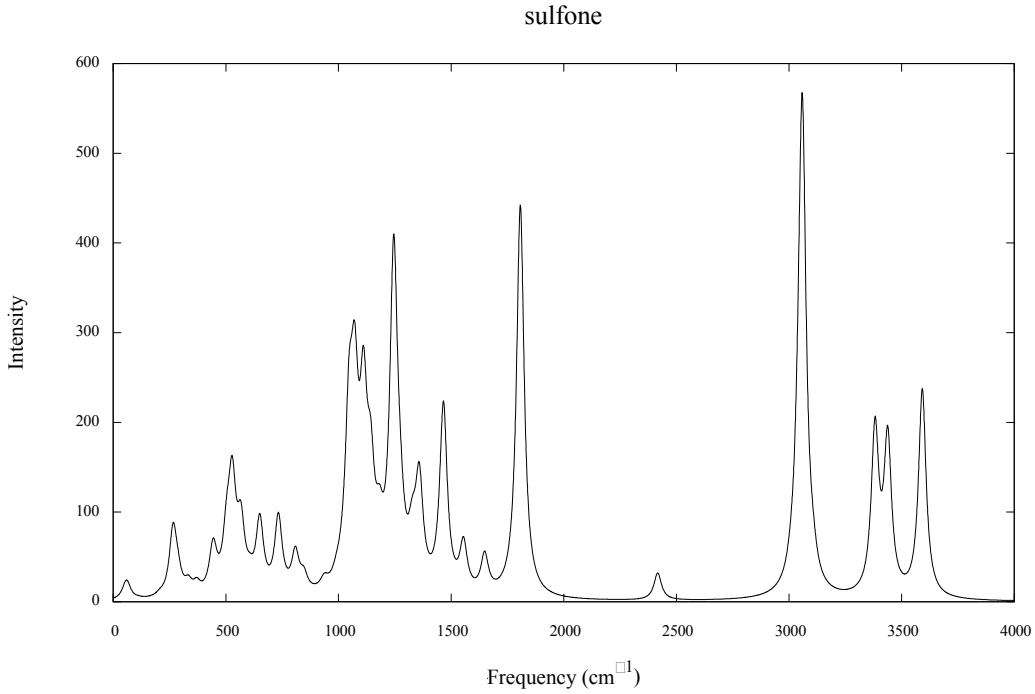
S.F.19. Computed infrared spectrum for u-L-CysB-ox2.



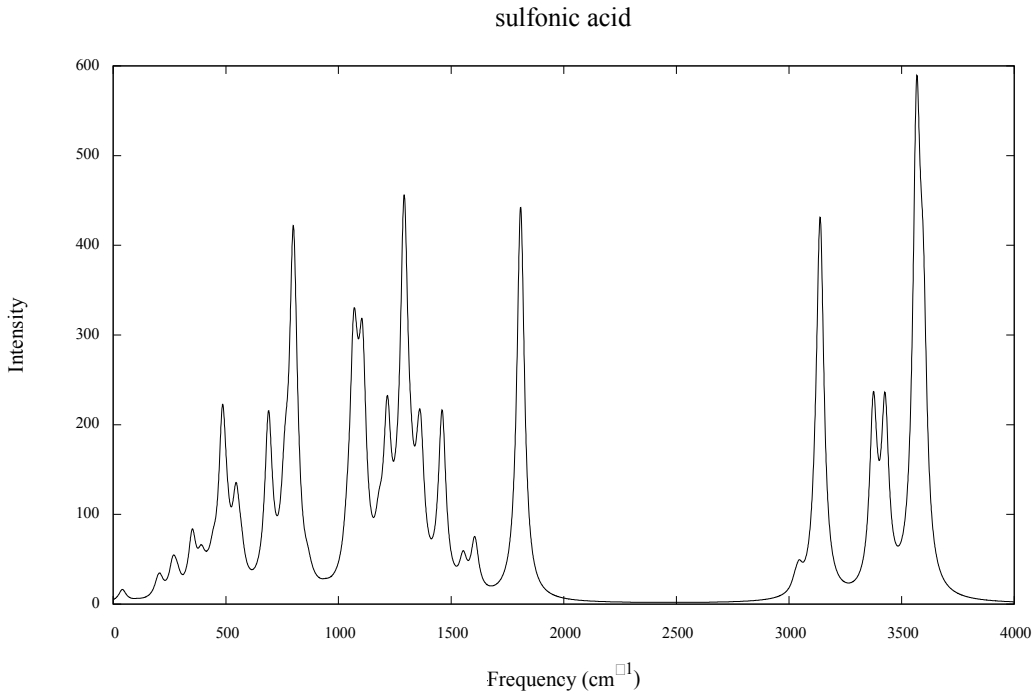
S.F.20. Computed infrared spectrum for sulfenic acid.



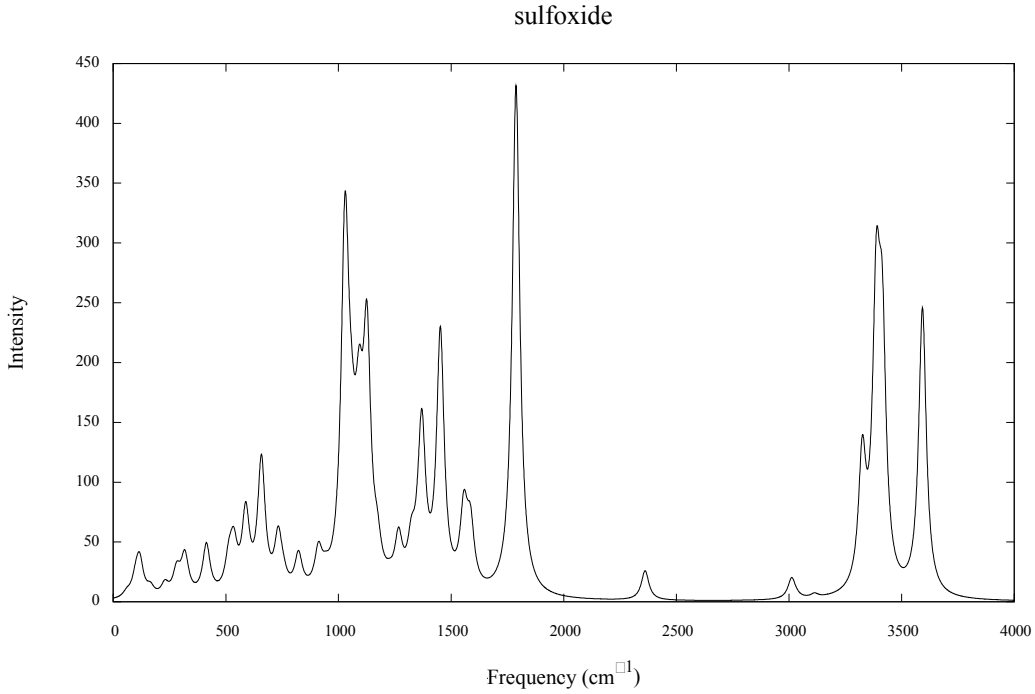
S.F.21. Computed infrared spectrum for sulfinic acid.



S.F.22. Computed infrared spectrum for sulfone.



S.F.23. Computed infrared spectrum for sulfonic acid.



S.F.24. Computed infrared spectrum for sulfoxide.

################# n-L-CysB-a ######################

>>>>>>>>>>>>>>>> n-L-CysB-a.xyz <<<<<<<<<<<<<<<<

33

n-L-CysB-a Energy: -3109.3580346

Pt	-2.53339	-0.95124	2.72548
Pt	0.04995	-0.48934	2.97520
Pt	2.60742	-0.58417	3.23348
Pt	-3.68721	-1.66667	0.21836
Pt	-1.15433	-1.64960	0.58427
Pt	1.62671	-1.69626	1.00468
Pt	4.13169	-1.59841	0.21709
Pt	-2.87956	-1.59362	-2.26536
Pt	-0.27035	-1.68122	-1.85615
Pt	2.31688	-1.95966	-1.61451
Pt	-2.69907	0.70879	0.74965
Pt	0.05098	0.78466	0.71242
Pt	3.07905	0.64446	1.01288
Pt	-1.63365	0.60413	-1.90192
Pt	1.37637	0.47001	-1.52629
Pt	-1.32627	3.05522	1.38360
Pt	1.47630	2.99223	1.38497
Pt	0.04382	2.83007	-1.04293
Pt	2.84217	2.73758	-0.99053
Pt	-2.74593	2.88285	-1.00261
O	-2.67259	-4.66129	1.85530
H	0.34655	-5.60818	0.36253
H	-1.79574	-6.16898	-0.20808
H	0.29846	-4.32113	-0.88428
C	-0.20857	-4.71212	0.02457

C -2.79368 -4.47180 0.64349

C -1.68803 -5.06976 -0.28907

O -3.78163 -3.88299 0.02509

S 0.04370 -3.47266 1.36745

N -2.01623 -4.73114 -1.70469

H -3.02056 -4.91395 -1.87764

H -1.88278 -3.68967 -1.89407

H -1.46149 -5.26666 -2.39246

################## n-L-CysB-c ########################

>>>>>>>>>>>>>>>> n-L-CysB-c.xyz <<<<<<<<<<<<<<<<<

33

n-L-CysB-c Energy: -3109.3909915

Pt -2.54629 -1.22692 2.43146

Pt 0.06541 -0.95596 2.71870

Pt 2.66005 -1.02401 2.77441

Pt -3.91109 -1.40613 -0.16159

Pt -1.35386 -1.87620 0.18852

Pt 1.39412 -1.87365 0.54259

Pt 4.02606 -1.62149 0.26792

Pt -2.70397 -1.50600 -2.47053

Pt -0.08174 -1.74370 -2.12864

Pt 2.57637 -1.84529 -1.90251

Pt -2.74892 0.72446 0.76139

Pt 0.02049 0.66805 0.75140

Pt 2.79495 0.62137 0.76335

Pt -1.36772 0.52963 -1.63902

Pt 1.40899 0.47749 -1.63218

Pt -1.32218 3.01663 1.39495

Pt 1.45064 2.96434 1.39736

Pt 0.06253 2.81858 -1.00428

Pt 2.83885 2.76730 -0.99745

Pt -2.71543 2.86852 -1.00069

O -2.52187 -3.08724 3.55536

H -0.06394 -3.46448 2.93066

H -1.38039 -5.54953 3.58392

H 0.67343 -5.02840 2.41881

C -0.18919 -4.34970 2.26864

C -2.72479 -4.08338 2.75744

C -1.50935 -5.04130 2.60749

O -3.76498 -4.37005 2.14200

S -0.04938 -3.78728 0.51728

N -1.90901 -6.07415 1.60409

H -2.94621 -5.93054 1.48190

H -1.46762 -5.91378 0.67819

H -1.71214 -7.04620 1.88898

################## n-L-CysB-ox1 ########################

>>>>>>>>>>>>>>>> n-L-CysB-ox1.xyz <<<<<<<<<<<<<<<<

34

temp.out Energy: -3184.4567194

Pt -2.58107 -1.22164 2.43864

Pt 0.03040 -0.93341 2.72302

Pt 2.63002 -0.98736 2.80140

Pt -3.95256 -1.38352 -0.17870

Pt -1.39521 -1.83405 0.17236

Pt 1.31206 -1.87129 0.51338

Pt 3.95298 -1.71446 0.44722

Pt -2.69112 -1.49066 -2.46156

Pt -0.04625 -1.73168 -2.15324

Pt 2.62011 -1.80775 -1.83839

Pt -2.75085 0.72844 0.76994

Pt 0.00259 0.68662 0.74221

Pt 2.79472 0.61787 0.77919

Pt -1.32483 0.53980 -1.67800

Pt 1.41037 0.50157 -1.66080

Pt -1.34420 3.00193 1.41643

Pt 1.43365 2.96193 1.42104

Pt 0.06694 2.84258 -1.00990

Pt 2.84705 2.75190 -0.99206

Pt -2.68216 2.88543 -1.00752

O -2.65558 -3.14694 3.43711

H -0.17249 -3.60096 2.96224

H -1.59105 -5.63568 3.44498

H 0.52896 -5.13345 2.28967

C -0.32153 -4.42571 2.23714

C -2.85751 -4.10568 2.59445

C -1.66651 -5.10278 2.47601

O -3.86553 -4.32576 1.90618

S -0.13667 -3.66189 0.56263

N -2.01839 -6.09578 1.41584

H -3.02786 -5.90620 1.19423

H -1.45322 -5.93284 0.54432

H -1.90476 -7.07872 1.70707

O -0.25198 -4.87040 -0.38263

################## n-L-CysB-ox2 ##########################

>>>>>>>>>>>>>>>> n-L-CysB-ox2.xyz <<<<<<<<<<<<<<<<<

35

temp.out Energy: -3259.5359326

Pt -2.55713 -1.27900 2.40527

Pt 0.03681 -1.20568 2.52900

Pt 2.64043 -1.20328 2.61841

Pt -3.98589 -1.43444 0.01022

Pt -1.32405 -1.80614 0.15517

Pt	1.31369	-1.90558	0.29925
Pt	4.02498	-1.61328	0.26510
Pt	-2.64408	-1.65301	-2.22367
Pt	0.00081	-1.76571	-2.15744
Pt	2.69396	-1.76235	-2.00936
Pt	-2.74891	0.72451	0.76140
Pt	0.02051	0.66800	0.75138
Pt	2.79500	0.62140	0.76330
Pt	-1.36770	0.52960	-1.63899
Pt	1.40900	0.47750	-1.63220
Pt	-1.32220	3.01660	1.39500
Pt	1.45060	2.96430	1.39741
Pt	0.06250	2.81860	-1.00430
Pt	2.83890	2.76730	-0.99750
Pt	-2.71540	2.86850	-1.00070
O	-1.81953	-3.24594	3.25476
H	0.83592	-3.79812	2.86244
H	-0.77064	-5.71635	3.32470
H	1.41399	-5.45306	2.44809
C	0.67284	-4.67004	2.19771
C	-1.94637	-4.20030	2.39735
C	-0.75264	-5.20426	2.34041
O	-2.93229	-4.45526	1.68284
S	1.28725	-4.15171	0.50536
N	-1.09556	-6.21160	1.29664
H	-2.12497	-6.09242	1.13365
H	-0.60859	-5.95348	0.39533
H	-0.87461	-7.18490	1.55441
O	2.69931	-4.66352	0.46751
O	0.33626	-4.80075	-0.49365

################## p-L-CysB-ox1 ##########################

>>>>>>>>>>>>>>>> p-L-CysB-ox1.xyz <<<<<<<<<<<<<<<<

35

temp.out Energy: -3184.8799058

Pt	-2.64531	-1.13976	2.53915
Pt	-0.00714	-0.94919	2.73368
Pt	2.59748	-1.07295	2.73503
Pt	-3.95393	-1.42597	0.00222
Pt	-1.37345	-1.83940	0.30651
Pt	1.37524	-1.86852	0.48551
Pt	3.97561	-1.67940	0.18088
Pt	-2.74102	-1.56971	-2.31722
Pt	-0.10365	-1.76147	-2.07179
Pt	2.55800	-1.84091	-2.01040
Pt	-2.74685	0.73932	0.80539
Pt	0.03375	0.68595	0.76259
Pt	2.79374	0.59053	0.74582
Pt	-1.40659	0.51460	-1.58798
Pt	1.37761	0.45227	-1.66181
Pt	-1.32063	3.01289	1.46255
Pt	1.44056	3.00533	1.33875
Pt	0.04604	2.79377	-0.99822
Pt	2.84725	2.72007	-1.02609
Pt	-2.71505	2.87491	-0.94950
O	-2.57535	-3.35085	3.43653
H	0.07087	-3.65622	3.01069
H	-1.30689	-5.66895	3.58506
H	0.79498	-5.14680	2.27454
C	-0.08421	-4.47322	2.27780
C	-2.53814	-4.23298	2.57708
C	-1.38370	-5.23076	2.57097
O	-3.35417	-4.36268	1.54717

S -0.06440 -3.67591 0.59925

N -1.58563 -6.33955 1.58846

H -2.57778 -6.62279 1.50839

H -1.24094 -6.04389 0.63445

H -3.88496 -3.51699 1.41711

H -1.05224 -7.18255 1.86121

O -0.24913 -4.87746 -0.34499

################# p-L-CysB-ox2 ########################

>>>>>>>>>>>>>>>> p-L-CysB-ox2.xyz <<<<<<<<<<<<<<<<

36

temp.out Energy: -3259.9660322

Pt -2.57701 -1.23650 2.43106

Pt 0.02315 -1.22022 2.52369

Pt 2.63320 -1.25442 2.58329

Pt -3.99105 -1.46494 0.02635

Pt -1.30363 -1.78289 0.18048

Pt 1.35016 -1.90066 0.28337

Pt 4.06184 -1.56102 0.19460

Pt -2.62494 -1.66641 -2.19388

Pt 0.02501 -1.75796 -2.14417

Pt 2.71794 -1.72335 -2.05785

Pt -2.75490 0.72500 0.74950

Pt 0.01770 0.66740 0.74730

Pt 2.79230 0.61580 0.76580

Pt -1.36440 0.53680 -1.64250

Pt 1.41210 0.48400 -1.63160

Pt -1.32550 3.01170 1.40150

Pt 1.44820 2.95760 1.41050

Pt 0.06610 2.82480 -0.99570

Pt 2.84140 2.77080 -0.98320

Pt -2.71000 2.87930 -1.00040

O -1.74418 -3.57946 3.15433

H 0.96685 -3.99672 2.71266

H -0.60913 -5.95410 3.07703

H 1.57969 -5.60304 2.17016

C 0.81828 -4.82106 1.98758

C -1.71202 -4.37472 2.21817

C -0.59185 -5.41010 2.11078

O -2.60226 -4.46204 1.24051

S 1.34438 -4.15615 0.31730

N -0.85851 -6.39748 1.02574

H -1.85761 -6.65762 0.96713

H -0.55822 -5.96321 0.10410

H -3.20843 -3.66174 1.26004

H -0.32213 -7.26980 1.16589

O 2.75063 -4.65607 0.16463

O 0.33385 -4.72307 -0.67566

################## p-L-CysB ########################

>>>>>>>>>>>>>>>> p-L-CysB.xyz <<<<<<<<<<<<<<<<<

34

p-L-CysB Energy: -3109.8164265

Pt -2.59628 -1.22439 2.40361

Pt 0.03871 -1.02454 2.66430

Pt 2.64049 -1.08761 2.73480

Pt -3.88482 -1.43761 -0.13284

Pt -1.31817 -1.90274 0.18381

Pt 1.44124 -1.86142 0.46979

Pt 4.05955 -1.57644 0.17470

Pt -2.67216 -1.53240 -2.45112

Pt -0.04794 -1.73229 -2.14181

Pt 2.62538 -1.79102 -1.99849

Pt -2.75490 0.72500 0.74950

Pt 0.01770 0.66740 0.74730

Pt 2.79230 0.61580 0.76580

Pt -1.36440 0.53680 -1.64250

Pt 1.41210 0.48400 -1.63160

Pt -1.32550 3.01170 1.40150

Pt 1.44820 2.95760 1.41050

Pt 0.06610 2.82480 -0.99570

Pt 2.84140 2.77080 -0.98320

Pt -2.71000 2.87930 -1.00040

O -2.41583 -3.34922 3.38171

H 0.21375 -3.60019 2.82320

H -1.07117 -5.63017 3.53598

H 0.95435 -5.12315 2.20920

C 0.07239 -4.45718 2.12872

C -2.37756 -4.24876 2.53725

C -1.20574 -5.21643 2.51821

O -3.21970 -4.41513 1.53393

S 0.06998 -3.81333 0.39652

N -1.45680 -6.36038 1.59406

H -2.33552 -6.86209 1.81558

H -1.52381 -6.05201 0.60405

H -3.77873 -3.59088 1.41388

H -0.69568 -7.06057 1.64791

################## sulfenic_acid ########################

>>>>>>>>>>>>>>>> sulfenic_acid.xyz <<<<<<<<<<<<<<<<<

16

temp.out Energy: -796.5905979

O -2.77393 -3.17972 3.23595

H 0.13547 -3.60318 2.98951

H -1.36818 -5.35768 3.80034

H 0.72770 -5.16577 2.34142

C -0.10374 -4.43368 2.29450

C -2.60059 -4.15078 2.53109

C -1.41377 -5.10040 2.72464

O -3.37645 -4.52100 1.49823

S -0.18860 -3.62431 0.66000

N -1.58349 -6.37648 1.95884

H -2.52891 -6.78258 2.06156

H -1.40519 -6.18487 0.94045

H -4.12451 -3.88495 1.41086

H -0.90553 -7.09330 2.26950

O -0.94761 -4.86131 -0.26755

H -1.87450 -4.55456 -0.39487

################## sulfinic_acid ########################

>>>>>>>>>>>>>>>> sulfinic_acid.xyz <<<<<<<<<<<<<<<<<

17

temp.out Energy: -871.6753264

O -2.48785 -2.68862 3.55289

H -0.17411 -3.37341 2.88992

H -1.45654 -5.34734 3.84706

H 0.41760 -4.97302 2.28974

C -0.43733 -4.27293 2.30166

C -2.77189 -3.81022 3.18417

C -1.70997 -4.87620 2.87446

O -4.00723 -4.31288 3.08139

S -0.71334 -3.70341 0.55686

N -2.27798 -5.94140 1.99455

H -3.11872 -6.37612 2.41276

H -2.55908 -5.49004 1.09148

H -4.65884 -3.61822 3.33109

H -1.59644 -6.69359 1.79432

O -0.19487 -5.19850 -0.04783

H -0.07744 -5.08162 -1.01841

O -2.23138 -3.65791 0.42881

################ sulfone ######################

>>>>>>>>>>>>>>>> sulfone.xyz <<<<<<<<<<<<<<<<<

17

temp.out Energy: -871.6431262

O -2.34941 -2.82960 3.86911

H 0.07502 -3.50905 2.82091

H -1.22651 -5.28555 3.95315

H 0.42194 -5.11262 2.05583

C -0.35488 -4.34499 2.23821

C -2.62690 -3.84521 3.26789

C -1.57039 -4.92107 2.96477

O -3.83592 -4.20162 2.82398

S -0.83594 -3.67814 0.61073

N -2.14115 -6.09160 2.22869

H -3.10024 -6.31117 2.54957

H -2.17363 -5.87251 1.19749

H -4.49360 -3.51109 3.07230

H -1.56657 -6.94157 2.35550

O -1.54823 -4.79059 -0.09846

O -1.51320 -2.37331 0.77410

H 0.39386 -3.49210 -0.00300

################ sulfonic_acid ######################

>>>>>>>>>>>>>>>> sulfonic_acid.xyz <<<<<<<<<<<<<<<<<

18

temp.out Energy: -946.7570470

O -2.47744 -2.90945 4.01244

H 0.00309 -3.42043 3.07077

H -1.26996 -5.33702 3.98133

H 0.46993 -4.94807 2.22474

C -0.35010 -4.22722 2.40266

C -2.69124 -3.89498 3.33982

C -1.57922 -4.90451 3.00901

O -3.86647 -4.27119 2.82861

S -0.73897 -3.45898 0.80550

N -2.06413 -6.03243 2.15534

H -3.03552 -6.29860 2.39607

H -2.04062 -5.76106 1.14140

H -4.56306 -3.62638 3.09357

H -1.47541 -6.87618 2.26370

O -1.26450 -4.54223 -0.06988

O -1.51918 -2.23325 1.01212

O 0.71488 -2.97430 0.26856

H 1.16105 -3.72142 -0.19648

################## sulfoxide ########################

>>>>>>>>>>>>>>>> sulfoxide.xyz <<<<<<<<<<<<<<<<<

16

temp.out Energy: -796.5533887

O -3.52919 -3.24615 3.75308

H -0.82436 -3.31113 3.09842

H -1.55250 -5.40851 4.13671

H -0.25847 -4.66619 2.05699

C -1.15198 -4.14052 2.44666

C -3.38568 -4.44835 3.64181

C -2.06193 -5.09235 3.20235

O -4.30242 -5.37868 3.91558

S -1.94660 -3.42712 0.90721

N -2.32561 -6.34476 2.42644

H -3.05433 -6.92335 2.88482

H -2.65802 -6.14548 1.46427

H -5.13750 -4.94562 4.20892

H -1.47709 -6.93131 2.33838

O -0.82738 -2.78070 0.09765

H -2.59982 -2.43587 1.65241

################# u-L-CysB-a ######################

>>>>>>>>>>>>>>>> u-L-CysB-a.xyz <<<<<<<<<<<<<<<<

32

u-L-CysB-a Energy: -3108.9659300

Pt -2.58697 -1.14706 2.55842

Pt 0.01657 -1.23022 2.50564

Pt 2.60218 -1.31405 2.49975

Pt -4.01917 -1.44684 0.14693

Pt -1.39013 -1.86204 0.25694

Pt 1.34711 -1.94958 0.16111

Pt 4.02099 -1.56158 0.07298

Pt -2.62083 -1.61759 -2.13056

Pt 0.03177 -1.66815 -2.33024

Pt 2.71713 -1.70256 -2.17096

Pt -2.75488 0.72497 0.74959

Pt 0.01759 0.66733 0.74724

Pt 2.79226 0.61578 0.76580

Pt -1.36431 0.53677 -1.64251

Pt 1.41213 0.48407 -1.63159

Pt -1.32542 3.01179 1.40145

Pt 1.44821 2.95759 1.41052

Pt 0.06597 2.82480 -0.99569

Pt 2.84145 2.77080 -0.98319

Pt -2.71000 2.87930 -1.00041

O -2.94438 -5.25293 -1.04440

H -0.39338 -5.92652 -0.56315

H -0.93917 -5.61426 -2.77956

H 0.99192 -5.04980 -1.29418

C -0.06870 -4.95678 -0.98616

C -2.45376 -4.48165 -1.86984

C -0.94448 -4.66152 -2.19894

O -3.14653 -3.61987 -2.58216

S -0.08000 -3.84808 0.49596

N -0.37203 -3.62778 -3.09097

H 0.51687 -3.97393 -3.48360

H -1.00702 -3.50111 -3.89439

################## u-L-CysB-c ########################

>>>>>>>>>>>>>>>> u-L-CysB-c.xyz <<<<<<<<<<<<<<<<<

32

u-L-CysB-c Energy: -3108.9298590

Pt -2.53714 -1.27731 2.38528

Pt 0.06238 -0.98501 2.69275

Pt 2.66233 -1.03737 2.76310

Pt -3.89471 -1.41770 -0.18004

Pt -1.33741 -1.89188 0.13791

Pt 1.39562 -1.88927 0.53111

Pt 4.03300 -1.61843 0.27494

Pt -2.69391 -1.49819 -2.49826

Pt -0.06488 -1.73423 -2.17203

Pt 2.58745 -1.83686 -1.90212

Pt -2.74965 0.71555 0.75976

Pt 0.01725 0.67203 0.75147

Pt 2.79543 0.62218 0.76299

Pt -1.35860 0.52933 -1.64197

Pt 1.41328 0.48601 -1.63504

Pt -1.31862 3.00900 1.41058

Pt 1.45274 2.96155 1.40754

Pt 0.07460 2.82280 -0.99533

Pt 2.84409 2.77429 -0.98753

Pt -2.66210 2.81356 -0.99335

O -2.52250 -3.10998 3.45753

H -0.09857 -3.46402 2.89024

H -1.45654 -5.54812 3.46196

H 0.63779 -5.03149 2.38149

C -0.22010 -4.34673 2.22374

C -2.74211 -4.09955 2.61742

C -1.55373 -5.07202 2.45259

O -3.80662 -4.31131 2.02506

S -0.02855 -3.79185 0.47569

N -1.81954 -6.01995 1.38223

H -2.84016 -6.12753 1.30380

H -1.42260 -6.94173 1.59756

################## u-L-CysB-ox1 ##########################

>>>>>>>>>>>>>>>> u-L-CysB-ox1.xyz <<<<<<<<<<<<<<<<

33

temp.out Energy: -3184.0263213

Pt -2.73020 -0.97567 2.69016

Pt -0.15365 -1.13063 2.57938

Pt 2.44554 -1.34498 2.43220

Pt -3.87771 -1.57112 0.31628

Pt -1.29919 -1.83494 0.21144

Pt 1.41230 -1.93428 0.05742

Pt 4.00224 -1.51594 -0.12206

Pt -2.52841 -1.66062 -2.18305

Pt 0.20852 -1.70924 -2.40145

Pt 2.86045 -1.47792 -2.44557

Pt -2.75490 0.72500 0.74960

Pt 0.01760 0.66730 0.74720

Pt 2.79230 0.61580 0.76580

Pt -1.36430 0.53680 -1.64250

Pt 1.41210 0.48410 -1.63160

Pt -1.32540 3.01180 1.40150

Pt 1.44820 2.95760 1.41050

Pt 0.06600 2.82480 -0.99570

Pt 2.84150 2.77080 -0.98320

Pt -2.71000 2.87930 -1.00040

O -2.77704 -5.09423 -0.99187

H -0.33054 -5.83809 -0.45441

H -0.74413 -5.67125 -2.76703

H 1.13603 -5.07702 -1.19739

C 0.05744 -4.94658 -0.97871

C -2.28083 -4.47695 -1.93931

C -0.76485 -4.69400 -2.22902

O -2.92468 -3.72272 -2.79061

S 0.01734 -3.67289 0.38489

N -0.18785 -3.68431 -3.14290

H 0.69300 -4.03949 -3.54418

H -0.84313 -3.56931 -3.93274

O 0.09902 -4.51798 1.64419

################## u-L-CysB-ox2 ##########################

>>>>>>>>>>>>>>>> u-L-CysB-ox2.xyz <<<<<<<<<<<<<<<<

34

temp.out Energy: -3259.1080446

Pt -2.67730 -0.98056 2.72429

Pt -0.05694 -1.08890 2.64230

Pt 2.42052 -1.57171 2.16501

Pt -4.07127 -1.42594 0.23580

Pt -1.44870 -1.76982 0.49811

Pt 1.12511 -1.93822 -0.21344

Pt 3.89020 -1.60333 -0.05479

Pt -2.46816 -1.75000 -1.93240

Pt	0.05839	-1.53941	-2.65424
Pt	2.78426	-1.56942	-2.41403
Pt	-2.75490	0.72500	0.74960
Pt	0.01760	0.66730	0.74720
Pt	2.79230	0.61580	0.76580
Pt	-1.36430	0.53680	-1.64250
Pt	1.41210	0.48410	-1.63160
Pt	-1.32540	3.01180	1.40150
Pt	1.44820	2.95760	1.41050
Pt	0.06600	2.82480	-0.99570
Pt	2.84150	2.77080	-0.98320
Pt	-2.71000	2.87930	-1.00040
O	-2.48474	-5.82009	-1.74371
H	0.17138	-6.03782	-1.25353
H	-0.60053	-5.52391	-3.37057
H	1.41604	-4.96955	-2.00597
C	0.38059	-5.01169	-1.61281
C	-2.12726	-4.73147	-2.19446
C	-0.64728	-4.65081	-2.68114
O	-2.95041	-3.73440	-2.39760
S	0.46196	-4.09759	-0.00103
N	-0.28630	-3.47074	-3.50739
H	0.58294	-3.68676	-4.02114
H	-1.00664	-3.35243	-4.23643
O	-1.03865	-4.04333	0.45395
O	1.30307	-5.00977	0.85066