Supplementary Information

The role of tautomers in the UV absorption of urocanic acid

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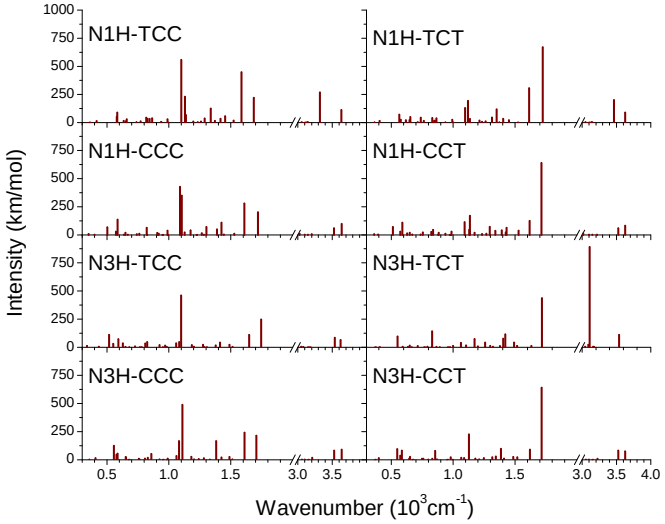
IR spectra of *cis* isomers of urocanic acid



IR spectra (fundamental frequencies) of the *trans* tautomers of urocanic acid computed at B3LYP/TZVP level. wavenumbers above 1000 cm^{-1} were multiplied by a factor 0.97.

Cartesian geometries (Angstrom)

Optimized at B3LYP/TZVP

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16
N1H-TTC
      n         0.059104        -1.333098        -2.171376
      c         0.035511        -2.654612        -2.485868
      n         0.119149        -3.416187        -1.415749
      c         0.199035        -2.551170        -0.364109
      c         0.164963        -1.234981        -0.792203
      c         0.225973        -0.020684        -0.038833
      c         0.209576         1.238047        -0.513598
      c         0.280864         2.379916         0.404944
      o         0.346968         2.330650         1.612850
      o         0.265027         3.562164        -0.272406
      h        -0.043945        -3.006999        -3.502511
      h         0.003586        -0.565999        -2.821584
      h         0.278851        -2.902144         0.652838
      h         0.294397        -0.146539         1.037315
      h         0.148304         1.471585        -1.569538
      h         0.314591         4.266302         0.392498
 16
N1H-TTT
      n         0.070629        -1.328595        -2.168061
      c         0.060877        -2.654072        -2.467022
      n         0.133514        -3.402167        -1.386750
      c         0.191407        -2.523847        -0.344564
      c         0.154722        -1.213365        -0.789062
      c         0.194402         0.012489        -0.050018
      c         0.177395         1.260469        -0.554613
      c         0.222625         2.478607         0.256622
      o         0.259613         2.248144         1.599081
      o         0.227845         3.600290        -0.201368
      h        -0.000751        -3.018785        -3.480655
      h         0.019829        -0.570185        -2.828794
      h         0.258256        -2.862525         0.677521
      h         0.244636        -0.107136         1.026353
      h         0.134446         1.460295        -1.618564
      h         0.292032         3.117103         2.026926
 16
N1H-CTT
      n         0.015663        -1.251304        -2.092191
      c         0.069570        -2.534329        -2.530456
      n         0.161631        -3.385741        -1.529462
      c         0.165536        -2.623025        -0.399760
      c         0.074654        -1.275182        -0.704984
      c         0.040258        -0.074071         0.082367
      c         0.057854        -0.009293         1.425296
      c         0.022376         1.242251         2.184600
      o        -0.012849         2.363516         1.406228
      o         0.022772         1.306026         3.393738
      h         0.038963        -2.794731        -3.576723
      h        -0.059718        -0.426194        -2.665927
      h         0.236585        -3.072730         0.577637
      h        -0.004455         0.862052        -0.466485
      h         0.095781        -0.896767         2.043500
      h        -0.037913         3.117470         2.014504
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 16
N1H-CTC
      n          0.011960        -1.274904        -2.105590
      c          0.087130        -2.559491        -2.534140
      n          0.187444        -3.402567        -1.526295
      c          0.175483        -2.631970        -0.402563
      c          0.066109        -1.287520        -0.717994
      c          0.008827        -0.080419         0.055242
      c          0.033014         0.018393         1.394984
      c         -0.033203         1.337782         2.034535
      o         -0.107591         2.408263         1.471184
      o         -0.001852         1.235058         3.390913
      h          0.065252        -2.828130        -3.578617
      h         -0.071776        -0.453650        -2.683886
      h          0.247610        -3.073268         0.578666
      h         -0.061887         0.853363        -0.498156
      h          0.098706        -0.845345         2.043410
      h         -0.048799         2.137741         3.742240
 16
N3H-TTC
      n          0.049499        -1.260294        -2.157664
      c          0.124778        -2.504856        -2.538362
      n          0.221933        -3.356588        -1.469108
      c          0.206111        -2.586091        -0.334954
      c          0.098464        -1.282945        -0.773620
      c          0.041250        -0.092994         0.040770
      c         -0.061141         1.155552        -0.437002
      c         -0.111989         2.304548         0.475100
      o         -0.080700         2.273835         1.686337
      o         -0.202759         3.477168        -0.212322
      h          0.114896        -2.857980        -3.557623
      h          0.291922        -4.360735        -1.507421
      h          0.269899        -3.007670         0.653591
      h          0.084940        -0.229392         1.117327
      h         -0.107646         1.348144        -1.499920
      h         -0.232754         4.185556         0.448766
 16
N3H-TTT
      n          0.147539        -1.281078        -2.185706
      c          0.149003        -2.543882        -2.510699
      n          0.199369        -3.351277        -1.404842
      c          0.231521        -2.531688        -0.306325
      c          0.199073        -1.245027        -0.802447
      c          0.216514        -0.020189        -0.037368
      c          0.200344         1.212011        -0.568225
      c          0.223966         2.444461         0.223915
      o          0.232145         2.238541         1.574699
      o          0.236187         3.561082        -0.245151
      h          0.115048        -2.940755        -3.513443
      h          0.211514        -4.358455        -1.397550
      h          0.274365        -2.913532         0.699439
      h          0.246747        -0.128581         1.041489
      h          0.174111         1.357606        -1.639953
      h          0.252451         3.117447         1.982098
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 16
N3H-CTT
      n         0.070443        -1.225323        -2.100591
      c         0.123997        -2.457158        -2.528158
      n         0.200809        -3.344680        -1.487988
      c         0.194438        -2.619073        -0.327282
      c         0.112033        -1.297249        -0.717405
      c         0.068602        -0.089009         0.076348
      c         0.065417        -0.016017         1.416697
      c         0.017905         1.235948         2.176707
      o         0.001432         2.357175         1.403302
      o        -0.005869         1.295753         3.387222
      h         0.111706        -2.773855        -3.559101
      h         0.254801        -4.348431        -1.558999
      h         0.249708        -3.087280         0.640321
      h         0.033141         0.826402        -0.503295
      h         0.091841        -0.898602         2.043941
      h        -0.035276         3.109309         2.013060
 16
N3H-CTC
      n         0.038615        -1.255930        -2.123078
      c         0.111615        -2.493125        -2.531076
      n         0.223741        -3.361686        -1.477833
      c         0.219752        -2.617078        -0.329373
      c         0.102221        -1.303762        -0.739563
      c         0.046145        -0.085244         0.035449
      c         0.029381         0.016623         1.373026
      c        -0.022108         1.330636         2.026443
      o        -0.034603         2.412305         1.483554
      o        -0.056417         1.205257         3.384723
      h         0.090076        -2.827171        -3.556421
      h         0.301098        -4.364828        -1.533642
      h         0.303510        -3.067283         0.644676
      h         0.012125         0.827913        -0.550246
      h         0.048096        -0.848075         2.024712
      h        -0.088406         2.104748         3.745476
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Optimized at MP2/TZVP

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16
N1H-TTC
      n         0.004141        -1.313154        -2.148075
      c         0.071043        -2.628134        -2.497070
      n         0.253754        -3.409448        -1.445584
      c         0.289929        -2.556859        -0.377657
      c         0.103871        -1.240350        -0.775729
      c         0.183887        -0.025528        -0.015542
      c         0.260671         1.220546        -0.516017
      c         0.304899         2.375893         0.394334
      o         0.309678         2.336512         1.606335
      o         0.339820         3.542800        -0.305016
      h        -0.018413        -2.958674        -3.518845
      h        -0.216128        -0.548219        -2.767540
      h         0.427407        -2.917202         0.629254
      h         0.178255        -0.138798         1.064184
      h         0.288225         1.430753        -1.577502
      h         0.369700         4.247715         0.361106
 16
N1H-TTT
      n        -0.014257        -1.311306        -2.146348
      c         0.052521        -2.631725        -2.473355
      n         0.198013        -3.398550        -1.405264
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      c          0.213713        -2.529658        -0.350313
      c          0.047451        -1.217953        -0.773026
      c          0.138331         0.008639        -0.031363
      c          0.186763         1.245752        -0.560504
      c          0.259023         2.471646         0.243428
      o          0.122581         2.249023         1.578938
      o          0.420160         3.582046        -0.220873
      h         -0.011177        -2.977227        -3.492106
      h         -0.200818        -0.553228        -2.785027
      h          0.320907        -2.875603         0.665269
      h          0.142108        -0.097056         1.047613
      h          0.212276         1.423646        -1.628488
      h          0.229305         3.117330         1.997011
 16
N1H-CTT
      n         -0.019570        -1.257403        -2.089514
      c          0.077659        -2.544513        -2.521081
      n          0.265732        -3.383726        -1.514996
      c          0.272292        -2.600918        -0.394711
      c          0.059748        -1.266607        -0.712800
      c          0.060667        -0.055572         0.069354
      c         -0.168565        -0.011810         1.394033
      c         -0.113851         1.225959         2.182575
      o         -0.027462         2.350427         1.416925
      o         -0.147307         1.265216         3.395150
      h          0.012361        -2.812944        -3.562471
      h         -0.236794        -0.452852        -2.658682
      h          0.430811        -3.024053         0.583911
      h          0.233139         0.878427        -0.456611
      h         -0.360645        -0.907854         1.970013
      h          0.041439         3.084586         2.046528
 16
N1H-CTC
      n         -0.043685        -1.289004        -2.098058
      c          0.071677        -2.581157        -2.508778
      n          0.317543        -3.395882        -1.494852
      c          0.343198        -2.591490        -0.390487
      c          0.088127        -1.268932        -0.725683
      c          0.068023        -0.046734         0.035806
      c         -0.128831         0.024323         1.363247
      c         -0.080938         1.333029         2.036558
      o          0.026276         2.413964         1.495050
      o         -0.178340         1.191089         3.384514
      h         -0.021182        -2.871194        -3.542218
      h         -0.296890        -0.500084        -2.674410
      h          0.547794        -2.990098         0.589836
      h          0.206054         0.888447        -0.501567
      h         -0.294359        -0.854266         1.972616
      h         -0.148742         2.090409         3.747702
 16
N3H-TTC
      n          0.048200        -1.246589        -2.153933
      c          0.125288        -2.504159        -2.534749
      n          0.222096        -3.353277        -1.469017
      c          0.205837        -2.588027        -0.333753
      c          0.096605        -1.280955        -0.773818
      c          0.041874        -0.091569         0.043905
      c         -0.061637         1.153247        -0.447962
      c         -0.111927         2.301741         0.469774
      o         -0.079683         2.260458         1.683311
      o         -0.202496         3.473609        -0.216681
      h          0.116069        -2.856974        -3.552932
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      h         0.291758        -4.358329        -1.510392
      h         0.269223        -3.012700         0.653411
      h         0.085301        -0.221645         1.121346
      h        -0.107538         1.336197        -1.512512
      h        -0.230530         4.169140         0.459052
 16
N3H-TTT
      n         0.081229        -1.261018        -2.167443
      c         0.141677        -2.531694        -2.504778
      n         0.240939        -3.343987        -1.410787
      c         0.239454        -2.539590        -0.302732
      c         0.127532        -1.248064        -0.786945
      c         0.188361        -0.024962        -0.018455
      c         0.173979         1.199505        -0.571973
      c         0.218584         2.438853         0.211819
      o         0.066879         2.238824         1.553636
      o         0.369618         3.547402        -0.260978
      h         0.116614        -2.920062        -3.509713
      h         0.271739        -4.351861        -1.416589
      h         0.300883        -2.931680         0.697943
      h         0.215315        -0.120622         1.061577
      h         0.158778         1.323915        -1.646216
      h         0.167049         3.116797         1.952105
 16
N3H-CTT
      n         0.280327        -1.220961        -2.101924
      c         0.320721        -2.476070        -2.501914
      n         0.157217        -3.342717        -1.459862
      c        -0.009258        -2.597690        -0.323542
      c         0.087059        -1.279760        -0.735984
      c         0.005093        -0.067015         0.052506
      c         0.229759        -0.008334         1.375843
      c         0.080871         1.213432         2.177060
      o        -0.071187         2.338744         1.427626
      o         0.091547         1.237104         3.391791
      h         0.462171        -2.812490        -3.515626
      h         0.114939        -4.348496        -1.521979
      h        -0.184016        -3.046311         0.639176
      h        -0.222236         0.839770        -0.495948
      h         0.486331        -0.888741         1.951898
      h        -0.202669         3.056161         2.066321
 16
N3H-CTC
      n         0.012485        -1.251641        -2.120851
      c         0.020813        -2.514615        -2.496847
      n         0.165552        -3.356744        -1.431983
      c         0.268070        -2.585904        -0.305328
      c         0.153057        -1.279054        -0.747376
      c         0.175248        -0.051776         0.020468
      c        -0.111637         0.035518         1.328905
      c        -0.015096         1.327438         2.027668
      o         0.226704         2.405042         1.527044
      o        -0.239774         1.173499         3.363083
      h        -0.072603        -2.874455        -3.508041
      h         0.239733        -4.361733        -1.472779
      h         0.417844        -3.010722         0.672226
      h         0.418126         0.853941        -0.525890
      h        -0.397358        -0.826955         1.917493
      h        -0.167992         2.063250         3.742947
 16
N1H-TCC
      n         0.176191        -1.554440        -2.205104
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      c         -0.054519         -2.873708         -2.400470
      n         -0.137277         -3.546561         -1.255802
      c          0.053490         -2.607947         -0.291233
      c          0.286948         -1.350352         -0.849978
      c          0.404491         -0.101188         -0.160922
      c          0.603510          1.170845         -0.582755
      c          0.650068          1.648050         -1.962941
      o          0.638537          0.986626         -2.992298
      o          0.732597          2.998973         -2.003574
      h         -0.154728         -3.303555         -3.383644
      h          0.325270         -0.811187         -2.884802
      h          0.042199         -2.860385          0.757880
      h          0.395808         -0.228223          0.917779
      h          0.663276          1.947505          0.166838
      h          0.782333          3.233556         -2.944032
 16
N1H-TCT
      n          0.145530         -1.570467         -2.209189
      c         -0.099934         -2.892287         -2.388712
      n         -0.156902         -3.552732         -1.238584
      c          0.070640         -2.605535         -0.287743
      c          0.299559         -1.355345         -0.860473
      c          0.440540         -0.108408         -0.163659
      c          0.607908          1.181692         -0.537444
      c          0.608331          1.822545         -1.854552
      o          0.809756          0.982360         -2.925679
      o          0.480672          3.016116         -2.023303
      h         -0.230482         -3.327394         -3.365988
      h          0.302115         -0.858372         -2.910114
      h          0.083957         -2.848130          0.763390
      h          0.457803         -0.262393          0.911769
      h          0.649685          1.918170          0.253933
      h          0.799942          1.568439         -3.699999
 16
N1H-CTT
      n         -0.144104         -1.332125         -2.116369
      c          0.222571         -2.526028         -2.652590
      n          0.764649         -3.320745         -1.743301
      c          0.716570         -2.614525         -0.575234
      c          0.126932         -1.370781         -0.761107
      c         -0.039740         -0.177137          0.037024
      c         -0.197032         -0.009819          1.365531
      c         -0.311275         -1.013964          2.437155
      o         -0.643805         -2.255542          2.006787
      o         -0.161057         -0.746206          3.612410
      h          0.076313         -2.764446         -3.693068
      h         -0.637133         -0.592181         -2.593668
      h          1.110709         -3.017471          0.340166
      h         -0.017048          0.745464         -0.539609
      h         -0.220540          1.002176          1.747767
      h         -0.706223         -2.798814          2.808917
 16
N1H-CCC
      n          0.002645         -1.260081         -2.145845
      c          0.210903         -2.476453         -2.711128
      n          0.442901         -3.404542         -1.796621
      c          0.361930         -2.758920         -0.595606
      c          0.050144         -1.411453         -0.769810
      c         -0.018307         -0.230443          0.054188
      c         -0.237737         -0.063617          1.375786
      c         -0.432257         -1.123773          2.370930
      o         -0.234526         -2.313157          2.231639
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      o        -0.895408        -0.594469         3.538064
      h         0.185285        -2.632821        -3.777031
      h        -0.261443        -0.416573        -2.632630
      h         0.511402        -3.271169         0.335592
      h         0.058621         0.697392        -0.508914
      h        -0.286636         0.946779         1.757937
      h        -0.992175        -1.345170         4.144999
 16
N3H-TCC
      n        -0.251573        -1.333794        -2.122139
      c        -0.153623        -2.593546        -2.495888
      n         0.247152        -3.396184        -1.466737
      c         0.407689        -2.600166        -0.363124
      c         0.109222        -1.320756        -0.790096
      c         0.141577        -0.091815        -0.012101
      c         0.447551         1.113945        -0.512512
      c         0.962181         1.333309        -1.887279
      o         1.902057         0.763847        -2.393919
      o         0.291630         2.344608        -2.500644
      h        -0.371247        -2.980113        -3.477759
      h         0.381347        -4.394678        -1.506027
      h         0.734231        -2.987408         0.586739
      h        -0.144865        -0.159476         1.032381
      h         0.343711         2.000884         0.099906
      h         0.710581         2.443259        -3.370701
 16
N3H-TCT
      n         0.145395        -1.542299        -2.208051
      c         0.023697        -2.830644        -2.460088
      n         0.041465        -3.551713        -1.307266
      c         0.178688        -2.676029        -0.263576
      c         0.223770        -1.417962        -0.837960
      c         0.422354        -0.163119        -0.141735
      c         0.462700         1.107899        -0.592593
      c         0.483594         1.717141        -1.960939
      o         0.181457         0.988238        -3.039119
      o         0.747880         2.900393        -2.060654
      h        -0.073822        -3.279710        -3.433961
      h        -0.034014        -4.555065        -1.236261
      h         0.209662        -2.999006         0.762511
      h         0.469013        -0.274178         0.937755
      h         0.607943         1.876144         0.156775
      h         0.111672         0.022289        -2.827024
 16
N3H-CCT
      n         0.036174        -1.250023        -2.150391
      c         0.217910        -2.439529        -2.681952
      n         0.377761        -3.395619        -1.721258
      c         0.284662        -2.785185        -0.501229
      c         0.058502        -1.445967        -0.776751
      c        -0.011443        -0.255796         0.048616
      c        -0.162523        -0.030691         1.370085
      c        -0.263513        -0.955828         2.505051
      o        -0.579598        -2.241429         2.178662
      o        -0.112585        -0.613641         3.661009
      h         0.247141        -2.665140        -3.735055
      h         0.519624        -4.381947        -1.876853
      h         0.365249        -3.325928         0.421107
      h         0.044090         0.638384        -0.565021
      h        -0.135443         0.999289         1.700741
      h        -0.639152        -2.700892         3.031818
 16
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N3H-CCC

n	0.142475	-1.226197	-2.151702
c	0.301590	-2.419167	-2.682011
n	0.309593	-3.394110	-1.726270
c	0.140208	-2.795021	-0.509637
c	0.023694	-1.439618	-0.784352
c	-0.067402	-0.262286	0.050479
c	-0.272407	-0.077775	1.372012
c	-0.364635	-1.108395	2.407668
o	-0.368402	-2.316701	2.263038
o	-0.462939	-0.537108	3.640613
h	0.417352	-2.635242	-3.731283
h	0.394820	-4.386657	-1.884642
h	0.094646	-3.341832	0.412198
h	-0.022543	0.643501	-0.546316
h	-0.310071	0.939305	1.737360
h	-0.536235	-1.276901	4.263689