

Supporting Information

Molecular Interaction of Pinic Acid with Sulfuric Acid - Exploring the Thermodynamic Landscape of Cluster Growth

Jonas Elm[†], Theo Kurtén[‡], Merete Bilde[¶] and Kurt V. Mikkelsen[†]

[†]*Department of Chemistry, H. C. Ørsted Institute, University of Copenhagen, DK-2100 Copenhagen Ø, Denmark*

[‡]*Department of Chemistry, University of Helsinki, FI-00014 Helsinki, Finland*

[¶]*Department of Chemistry, Aarhus University, Langelandsgade 140, DK-8000 Århus C, Denmark*

E-mail: elm@chem.ku.dk

**Identified vacuum structures optimized at the
M06-2X/6-31+G(d) level of theory:**

pinic acid

C -0.24753200 0.49319200 -0.17243000
C -1.47811200 -0.29802800 -0.74167700
C -0.67469800 -1.59993900 -0.60099400
C 0.60882100 -0.74423000 -0.58006600
H -1.65196200 -0.01653500 -1.78594900
H -0.77721800 -2.34497700 -1.39326700
H -0.87707200 -2.07289600 0.36527200
H 0.97268300 -0.59749200 -1.60465200
C -0.34610800 0.68543600 1.34063300
H 0.61283200 1.02129100 1.75001200
H -1.09961400 1.44848500 1.56992000
H -0.63815600 -0.23402400 1.86011900
C 0.08505200 1.80614900 -0.86268000
H -0.70141700 2.54795900 -0.68164500
H 1.02929300 2.21359400 -0.48028500
H 0.18490500 1.66986000 -1.94538800
C -2.75754700 -0.16902000 0.02845200
O -3.36532500 1.01371700 -0.21516600
O -3.20014000 -0.97171600 0.81438400
H -4.16287500 1.05034800 0.34216800
C 1.77619500 -1.17608000 0.30525900
H 1.45593200 -1.32708200 1.33885200
H 2.19398300 -2.11449000 -0.07701300
C 2.85744000 -0.12577200 0.30500800
O 3.16096300 0.58297700 1.23438200
O 3.45463900 -0.02055100 -0.90233400
H 4.11652400 0.69028800 -0.83730000

(1pa₁₋₀)(1sa) cluster

S 4.32474300 -0.35117400 -0.34976600
O 5.46572500 -0.91138900 -1.01610600
O 3.58721300 0.76650400 -0.90954400
O 3.33286100 -1.51550900 -0.01735500
H 2.44050200 -1.12599200 0.27129400
O 4.76957500 0.17374000 1.10248300
H 5.44269100 -0.42764200 1.47071500
C -1.94572700 0.80910300 -0.12883400
C -0.85310300 0.94263300 0.99838000
C -1.61237500 -0.09869500 1.82996100
C -2.86185600 0.16707900 0.96264700
H -0.88952900 1.94939300 1.42610700
H -1.68971300 0.08080400 2.90494500
H -1.20064000 -1.09967400 1.66350000
H -3.48088400 0.95591800 1.40703900
C -1.53859100 -0.17437200 -1.22312100
H -2.39934000 -0.39805800 -1.86410900

H -0.75932600 0.26313800 -1.85861500
 H -1.15183600 -1.11789500 -0.82195600
 C -2.39573700 2.13021800 -0.73125400
 H -1.56241700 2.60541500 -1.26270400
 H -3.22181100 1.97522700 -1.43093700
 H -2.74010700 2.81884000 0.04846200
 C 0.54653500 0.64294400 0.57158000
 O 1.12852800 1.65726200 -0.04055500
 O 1.07685200 -0.45414000 0.72481600
 H 2.02801700 1.40314600 -0.36025800
 C -3.73262400 -1.03149500 0.63272100
 H -3.14963700 -1.84529800 0.18347700
 H -4.17026600 -1.45176300 1.54760100
 C -4.86284400 -0.70580500 -0.30934300
 O -5.08738900 0.37617300 -0.79627300
 O -5.62641200 -1.78634500 -0.56795400
 H -6.32928000 -1.50680200 -1.18083300

(1pa₀₋₁)(1sa) cluster

S 4.32850700 -0.38928500 -0.13078800
 O 3.82105800 0.59426700 -1.06879300
 O 5.49283800 -1.17656300 -0.41735800
 O 4.58080000 0.45795500 1.21093700
 H 5.10374300 -0.07568800 1.83721600
 O 3.17302700 -1.36403700 0.28044900
 H 2.30050400 -0.85155200 0.31729500
 C -2.26179400 -0.46685900 0.07485500
 C -3.63586700 -0.15608000 0.77150900
 C -3.14070200 1.26578000 1.06816400
 C -1.69646600 0.76830400 0.84741200
 H -3.73991400 -0.77076800 1.67174700
 H -3.38979900 1.69196100 2.04285300
 H -3.46764800 1.95512800 0.28231700
 H -1.26151600 0.42079100 1.79188700
 C -2.31993500 -0.25209500 -1.43562300
 H -1.30993000 -0.26282100 -1.86338100
 H -2.88619900 -1.06217400 -1.91015400
 H -2.80148300 0.69321400 -1.70956300
 C -1.67001600 -1.82814800 0.40312600
 H -2.32569400 -2.62329100 0.02849300
 H -0.68202900 -1.94651300 -0.05258500
 H -1.55910500 -1.95839600 1.48543300
 C -4.85549100 -0.31321600 -0.08520600
 O -5.22389500 -1.60894300 -0.19214800
 O -5.43388100 0.57237100 -0.66809400
 H -5.99146900 -1.64498100 -0.79018600
 C -0.73229700 1.72245900 0.16769000
 H -1.11995600 2.08832500 -0.78989100
 H -0.57938600 2.61802400 0.78591300
 C 0.62691700 1.12793100 -0.08201700
 O 0.97708700 0.04722400 0.38145000

O 1.39813800 1.88729100 -0.83361600
H 2.28630900 1.47232100 -0.95684700

(1pa₂₋₀)(2sa) cluster

S -5.02540700 1.44888600 0.15702800
O -4.55848400 0.49827400 1.16366400
O -5.90617000 2.51519900 0.50883800
O -3.74077300 2.08069600 -0.52875300
H -2.98620500 1.44698600 -0.50061600
O -5.71178200 0.63575500 -1.01284900
H -5.16279500 -0.15409200 -1.23246000
S -2.56437800 -1.42661400 -0.42161700
O -3.72683500 -1.27790300 -1.27235600
O -1.57205000 -2.43546000 -0.72845800
O -1.87288700 -0.01397100 -0.37024600
H -0.89662100 -0.09355900 0.01519300
O -3.00188900 -1.68677900 1.06703200
H -3.66992800 -0.99231100 1.31440900
C 3.73790100 -0.71093700 0.03806000
C 2.64162000 -0.90471100 1.15675900
C 3.03384600 0.45594200 1.74667200
C 4.36933000 0.36731500 0.97747300
H 2.91634500 -1.75064700 1.79397300
H 3.07512800 0.53295700 2.83552400
H 2.38733900 1.24892500 1.35632400
H 5.13907600 -0.11371100 1.59275700
C 3.16390800 -0.12169100 -1.24748900
H 3.97915100 0.18747600 -1.91176100
H 2.57294800 -0.87492700 -1.78255500
H 2.51845200 0.74507300 -1.06585400
C 4.56239600 -1.95300100 -0.25760300
H 3.92875100 -2.73128800 -0.69993100
H 5.37548200 -1.71903900 -0.95054500
H 5.00657000 -2.35503900 0.65957300
C 1.25160800 -1.10463600 0.65887700
O 0.99722200 -2.34276000 0.29561600
O 0.44396800 -0.17810300 0.54846700
H 0.08616600 -2.43842500 -0.07280300
C 4.91454600 1.66302500 0.40546500
H 4.17250000 2.17053600 -0.22418700
H 5.15248600 2.36973300 1.21089300
C 6.15840200 1.46928400 -0.42300700
O 6.67707500 0.40880500 -0.67736800
O 6.64733500 2.64077000 -0.87306500
H 7.44253000 2.44527600 -1.39994300

(1pa₁₋₁)(2sa) cluster

S -6.34466200 -0.57071700 -0.57729600
O -7.42436000 -1.01703300 -1.41020100

O -5.48076800 -1.50726900 0.11797200
O -5.46995400 0.42835900 -1.40704200
H -4.60827200 0.61668800 -0.90698600
O -6.93276900 0.35298000 0.59841100
H -7.68032700 0.87508600 0.25333300
S 6.31898500 -0.73055100 -0.32229500
O 5.76757000 -0.03608400 -1.47123600
O 7.34821200 -1.71998000 -0.45899700
O 6.84867900 0.45520300 0.62315600
H 7.41245600 0.08052400 1.32489100
O 5.15274800 -1.35648900 0.51667400
H 4.34267400 -0.75243600 0.46658200
C -0.10924200 0.00402400 0.74251400
C -1.36717400 0.70529800 1.37882200
C -0.80056600 2.06527100 0.95257600
C 0.58671400 1.40248900 0.81264000
H -1.35893200 0.55595400 2.46308000
H -0.90127300 2.89203400 1.65954200
H -1.21256600 2.36996100 -0.01511400
H 1.14214400 1.46985300 1.75550000
C -0.36539900 -0.46510600 -0.68731200
H 0.57927900 -0.74663000 -1.16805000
H -1.00934000 -1.35252400 -0.68749000
H -0.85081000 0.29960800 -1.30408100
C 0.47842800 -1.11870400 1.58227100
H -0.25329900 -1.92799700 1.69113400
H 1.38193200 -1.52529200 1.11810400
H 0.74472000 -0.76192700 2.58339100
C -2.68975900 0.26934100 0.83649100
O -3.11300500 -0.86387900 1.36375200
O -3.28802200 0.87579500 -0.04748200
H -3.96623500 -1.14447600 0.95172100
C 1.46464700 1.88260600 -0.32772300
H 0.95161500 1.82005200 -1.29496000
H 1.71978800 2.94292000 -0.19727200
C 2.75948200 1.12655800 -0.45208400
O 3.10677400 0.26510400 0.34928900
O 3.47429100 1.48620000 -1.49821700
H 4.31933700 0.97500600 -1.53766900

(1pa₀₋₂)(2sa) cluster

S 4.61787300 -1.66725500 0.29461400
O 5.30102400 -2.85219400 0.70107700
O 4.20801600 -0.66322100 1.27421000
O 5.51266300 -0.95934300 -0.80064300
H 5.10068700 -0.10178600 -1.06064600
O 3.31673500 -2.09867200 -0.50660500
H 2.65559700 -1.36848000 -0.50843800
S 2.65249700 1.54200200 -0.41665400
O 3.83443300 1.21436600 -1.18436700
O 1.84877200 2.68793600 -0.78397000

O 1.75153500 0.24810700 -0.42845900
 H 0.78131900 0.47851400 -0.12518000
 O 3.01637500 1.73226600 1.10131900
 H 3.55100600 0.94415200 1.38952300
 C -3.50067600 -0.58515200 -0.05925400
 C -4.83188900 -0.94579600 0.69297300
 C -4.76237300 0.40126200 1.42443500
 C -3.26347900 0.47697600 1.06360300
 H -4.66266700 -1.80202000 1.35436000
 H -5.03278500 0.41341700 2.48267700
 H -5.35582500 1.15437100 0.89504900
 H -2.65400000 0.02411600 1.85469500
 C -3.76156900 0.04096500 -1.42709100
 H -2.83966000 0.47966600 -1.82857300
 H -4.09581300 -0.72574100 -2.13582800
 H -4.53128100 0.82020000 -1.39502400
 C -2.50317300 -1.72744300 -0.17107400
 H -2.93785900 -2.54722400 -0.75529900
 H -1.58257600 -1.40014800 -0.66457900
 H -2.23745400 -2.11715800 0.81785300
 C -6.02453600 -1.21365400 -0.17498600
 O -5.98408800 -2.45597000 -0.70371500
 O -6.90320000 -0.42779300 -0.43579800
 H -6.76350300 -2.55355600 -1.27928300
 C -2.70884800 1.84739200 0.72057100
 H -3.28176600 2.33584800 -0.07690800
 H -2.77600600 2.52114800 1.58559000
 C -1.27022500 1.82645700 0.29123200
 O -0.59380400 0.79746300 0.30331700
 O -0.81355000 2.99841300 -0.08794700
 H 0.13798400 2.95182900 -0.34716000

(1pa_{bridged})(2sa) cluster

C -3.16610000 -1.08803100 -0.67230000
 C -2.31185100 -1.90240000 0.37382300
 C -3.78211100 -0.27301400 0.51693600
 C -2.99417700 -1.14668500 1.52903400
 C -4.21304300 -1.97894500 -1.33316900
 C -2.39516700 -0.31294200 -1.73238400
 C -3.63826000 1.26074300 0.55475100
 C -2.24003800 1.82011200 0.62356600
 C -0.82636400 -1.72751500 0.25543400
 O -0.32134200 -2.40004700 -0.77068100
 O -1.60798700 1.49909300 1.73574000
 H -4.16035600 1.62040700 1.45035500
 H -4.12270300 1.70258600 -0.32000100
 O -1.74924300 2.52172400 -0.25377500
 O -0.14379300 -1.03449400 1.00077100
 H -1.99586500 -0.99975100 -2.48651000
 H -3.73858200 -2.69618500 -2.01242600
 H -4.91825500 -1.37137200 -1.91302900

H -4.78547900 -2.54231100 -0.58669700
 H -3.05877400 0.39762100 -2.23879100
 H -2.51148800 -2.97764900 0.31916600
 H -3.63114600 -1.78123100 2.14928100
 H -4.86100100 -0.45658900 0.57623700
 H -2.29271000 -0.61012300 2.16797500
 H -1.55427400 0.25609800 -1.32823100
 H 0.64196500 -2.22023900 -0.85719500
 H -0.64894800 1.71747100 1.65828300
 S 1.39890400 1.97914900 -0.31529700
 S 3.21851600 -1.34490100 0.14091900
 O 1.01632200 1.77641800 1.07181300
 O 4.30862300 -0.24198400 -0.08721600
 O 2.24245800 -1.29922200 -0.97364300
 O 2.81906100 2.02118500 -0.61396400
 O 0.71803000 3.26333300 -0.87614800
 O 0.71370700 0.88432300 -1.22808900
 O 2.46541600 -0.79814600 1.40376500
 O 3.88742300 -2.58355100 0.38833800
 H 1.46420300 -0.86128300 1.28325800
 H 1.27807200 0.06112800 -1.24460300
 H -0.26179200 3.19002900 -0.65296900
 H 3.89168100 0.64642200 -0.24349000

(1pa₃₋₀)(3sa) cluster

S 7.74503200 0.52783200 -0.24430600
 O 9.10498500 0.18064200 -0.53015500
 O 6.65055000 0.06434300 -1.07786600
 O 7.46855000 0.14089700 1.25555100
 H 6.50465900 0.27931900 1.45944400
 O 7.57361900 2.12035800 -0.24542500
 H 8.36279200 2.53816500 0.14726000
 S 3.77073800 0.36292700 0.51280900
 O 4.85440900 0.79019300 1.37717300
 O 2.42771000 0.83139500 0.79136000
 O 4.06105200 0.77550600 -0.97558000
 H 5.01131300 0.57583200 -1.19509400
 O 3.82132600 -1.20521100 0.51165200
 H 3.02159100 -1.56185500 0.03023000
 S 0.26291700 -1.21077900 -0.53031500
 O 1.59187200 -1.69795100 -0.86571900
 O -0.25943400 -1.54984900 0.78651200
 O 0.22079000 0.35809000 -0.72445100
 H 0.97291500 0.75654300 -0.21591400
 O -0.71752700 -1.66352900 -1.63460600
 H -1.68526700 -1.63295400 -1.28139700
 C -5.62271800 0.07122300 0.80583100
 C -5.08997000 -1.39564300 0.58168300
 C -6.03127600 -1.53125200 -0.62164700
 C -6.84621400 -0.33859600 -0.07597200
 H -5.37656700 -2.02290300 1.43134800

H -6.54506000 -2.48705600 -0.74785000
 H -5.50825800 -1.28067100 -1.55050500
 H -7.64922500 -0.68873700 0.58360700
 C -4.73315300 1.12161100 0.14583500
 H -5.23951000 2.09393400 0.14669500
 H -3.79806600 1.23741100 0.70700500
 H -4.47298900 0.86813600 -0.88792900
 C -5.89377000 0.42837700 2.25817200
 H -4.95713200 0.42718000 2.82857800
 H -6.35490400 1.41702100 2.33317900
 H -6.57508500 -0.29588900 2.71832600
 C -3.61869000 -1.51307800 0.36309000
 O -2.92307500 -1.49988500 1.48243400
 O -3.10956900 -1.55664500 -0.75620200
 H -1.95292200 -1.52139800 1.29656400
 C -7.41708600 0.62633000 -1.09887800
 H -6.64235000 1.00339600 -1.77813700
 H -8.14974300 0.11799700 -1.73921500
 C -8.09948600 1.81700900 -0.47604000
 O -8.20682500 2.03027800 0.70767000
 O -8.59519400 2.65440800 -1.40850700
 H -9.01691300 3.39662200 -0.94035900

(1pa₂₋₁)(3sa) cluster

S -7.99253700 -0.41789300 -0.76601500
 O -7.13869700 -1.51487900 -1.18297900
 O -9.15775300 -0.04058400 -1.51129900
 O -8.42391900 -0.81787400 0.72846700
 H -9.16220800 -0.25003300 1.01710900
 O -7.11822500 0.86556400 -0.54881700
 H -6.21601300 0.59412300 -0.18598700
 S 6.93236700 -1.62505400 0.00393200
 O 6.54637300 -0.58862400 0.95911800
 O 7.78036400 -2.70378800 0.39521500
 O 5.59424300 -2.24045400 -0.58841600
 H 4.86614000 -1.57737200 -0.55640100
 O 7.60488900 -0.92577300 -1.24486900
 H 7.07354400 -0.13793200 -1.50818200
 S 4.56893200 1.31311300 -0.65702000
 O 5.66399100 1.03491700 -1.56189400
 O 3.60534000 2.34290600 -0.98470400
 O 3.81790100 -0.05620200 -0.44634800
 H 2.89682900 0.10490500 0.02071400
 O 5.11194800 1.66788700 0.77602700
 H 5.75864800 0.95956600 1.04142700
 C -1.69435500 1.00927200 0.47399400
 C -0.47036600 1.24941400 1.43819000
 C -0.85616500 -0.01892700 2.21036900
 C -2.26645800 0.07652400 1.58983000
 H -0.62950100 2.16940400 2.00902900
 H -0.77378300 0.01685000 3.29890200

H -0.29903300 -0.88451800 1.83753600
 H -2.93084100 0.66610000 2.23206300
 C -1.29859600 0.25373900 -0.79242100
 H -2.19445600 -0.07855600 -1.33033500
 H -0.73708300 0.90996100 -1.46821200
 H -0.67784700 -0.62539100 -0.58610700
 C -2.48524600 2.26145500 0.13153100
 H -1.85974800 2.96080000 -0.43594700
 H -3.36446100 2.01287600 -0.47016800
 H -2.83054200 2.76905600 1.03873900
 C 0.86431600 1.31425000 0.77619400
 O 1.13180400 2.49058300 0.25151000
 O 1.61141600 0.33757400 0.68902800
 H 2.00607400 2.49707300 -0.20792400
 C -2.94584600 -1.22833600 1.21809000
 H -2.31209300 -1.85744800 0.58309700
 H -3.14826500 -1.82434700 2.11857800
 C -4.26227400 -1.03893700 0.51251300
 O -4.81831300 0.05085800 0.42514600
 O -4.74876400 -2.15543200 0.01244200
 H -5.61639700 -1.99192500 -0.43304100

(1pa₁₋₂)(3sa) cluster

S 7.77725200 -0.82733600 0.58016800
 O 6.67860100 -1.77614500 0.57696100
 O 8.87917100 -0.95091900 1.49024800
 O 8.32900500 -0.87866300 -0.92745700
 H 9.19506000 -0.43283600 -0.96998100
 O 7.20827200 0.62728000 0.70084100
 H 6.32310400 0.68345300 0.21280600
 S -6.77136100 -1.23488200 -0.77277300
 O -5.49423300 -1.82944200 -0.38425400
 O -7.65326300 -1.90628300 -1.67180600
 O -7.59092700 -0.92053800 0.54422700
 H -6.99425600 -0.53776400 1.22983800
 O -6.45937600 0.20038100 -1.37170600
 H -5.63401800 0.56831100 -0.97298900
 S -4.18074900 0.30715900 1.38064500
 O -5.48297100 0.19431400 1.99929700
 O -4.16057200 0.93188900 0.04338300
 O -3.21224800 1.04417000 2.31585700
 H -2.36981000 1.37377900 1.79519900
 O -3.48936900 -1.10597100 1.26966300
 H -4.06662400 -1.66350800 0.68692300
 C 1.57152100 0.19464700 -0.52246400
 C 2.78831500 0.17902500 -1.51946000
 C 2.48898700 1.64408600 -1.87058900
 C 1.06098800 1.42647600 -1.33147900
 H 2.58477100 -0.51089100 -2.34474800
 H 2.59508300 1.94485000 -2.91509200
 H 3.07486900 2.31897500 -1.23898600

H 0.40973100 1.07501200 -2.14167400
 C 2.00588200 0.54259500 0.90074600
 H 1.13338100 0.75961900 1.52573800
 H 2.53635500 -0.30614400 1.34830600
 H 2.67625300 1.40861800 0.93497100
 C 0.68647900 -1.04150800 -0.53228500
 H 1.22547000 -1.90509000 -0.12633400
 H -0.20675100 -0.88257600 0.08518800
 H 0.36217600 -1.28889600 -1.54902500
 C 4.11315900 -0.15722100 -0.91218600
 O 4.27534000 -1.45159300 -0.71796900
 O 4.93413800 0.69280700 -0.58282900
 H 5.13812100 -1.63421200 -0.27070700
 C 0.37109100 2.58581600 -0.60649700
 H 0.96390900 2.92542100 0.24554200
 H 0.22854500 3.41551100 -1.30670100
 C -0.97001700 2.13755800 -0.10610300
 O -1.17064700 1.83224400 1.07012800
 O -1.88426000 2.04900000 -1.04726700
 H -2.72935800 1.68019800 -0.69355400

(1pa₀₋₃)(3sa) cluster

S -6.97902300 -1.33749400 -0.73114100
 O -8.26618800 -1.64815900 -1.28002400
 O -6.43513600 0.00597700 -0.76850200
 O -6.95829200 -1.87406800 0.74897200
 H -6.14576500 -1.54137100 1.21618000
 O -5.85745900 -2.22114000 -1.45250000
 H -6.22260300 -3.10076000 -1.66328800
 S -3.90857700 0.30278100 1.17600200
 O -3.05614100 -0.05938900 0.05400400
 O -4.71470400 -0.74901800 1.76464200
 O -3.07340200 0.94105200 2.32434700
 H -2.36151800 1.52887400 1.93940000
 O -4.81882200 1.52857500 0.77677500
 H -5.51087100 1.20843100 0.14477800
 S -0.37567500 1.92942300 -0.02311300
 O 0.59437700 2.85157200 -0.57561900
 O -1.35748200 2.42363500 0.92774600
 O -1.11600900 1.29584700 -1.26084000
 H -1.89017400 0.76262200 -0.93892200
 O 0.34605400 0.73116100 0.66833400
 H 1.20755000 0.51096300 0.16779500
 C 5.52569500 -0.73162400 0.34643300
 C 6.70583700 -1.69857200 -0.02877500
 C 6.47363900 -1.37893900 -1.51170300
 C 5.06761300 -0.85976800 -1.14270500
 H 6.44107500 -2.72759400 0.23597900
 H 6.54046100 -2.20798200 -2.21992000
 H 7.14223000 -0.57545200 -1.83876700
 H 4.32640900 -1.66384900 -1.21634700

C 6.01677800 0.66950700 0.70252300
 H 5.17510300 1.37212000 0.74191700
 H 6.48626600 0.66428900 1.69330000
 H 6.75322000 1.05367700 -0.01181900
 C 4.58196700 -1.25971100 1.41549000
 H 5.11869800 -1.38194600 2.36378500
 H 3.74578100 -0.57177600 1.57587700
 H 4.16811600 -2.23279900 1.12871900
 C 8.04210700 -1.36074400 0.56109900
 O 8.12859600 -1.75130900 1.85173400
 O 8.93519800 -0.76819100 0.00468500
 H 9.00052500 -1.47111500 2.18258900
 C 4.56481000 0.36515200 -1.88608000
 H 5.29338900 1.18299700 -1.87162500
 H 4.39893900 0.12898800 -2.94658100
 C 3.26385600 0.89486000 -1.34946500
 O 2.53461300 0.23786600 -0.61152600
 O 2.98601800 2.11584000 -1.75715600
 H 2.12199000 2.42336200 -1.39248300

(1pa_{bridged})(3sa) cluster

S -1.56143900 2.68092200 -0.09127000
 O -0.75100400 1.94768900 1.05264700
 O -0.84186400 3.91790400 -0.31506900
 O -1.38198800 1.72429000 -1.32627600
 O -2.97554800 2.69952900 0.21706400
 S -0.79442300 -2.54083600 -0.43533100
 O 0.02173700 -3.40612900 -1.44962800
 O -2.15719700 -3.31498200 -0.59313000
 O -0.25915000 -2.70990800 0.90699800
 O -0.92672400 -1.17254200 -0.91241400
 C 3.61544100 0.88659700 0.70298200
 C 3.42652600 1.56446100 -0.70560900
 C 3.72371500 0.21262000 -1.37334500
 C 4.38002900 -0.24309000 -0.05194800
 H 4.20060700 2.32113300 -0.86780900
 H 4.35132200 0.22212200 -2.26729700
 H 2.79640200 -0.32077700 -1.59291500
 H 5.44269700 0.03027300 -0.06887300
 C 2.28683600 0.44456400 1.31357400
 H 2.45975000 -0.19754800 2.18335800
 H 1.72053000 1.32036100 1.65019300
 H 1.65145500 -0.10169100 0.60427300
 C 4.42386500 1.68632300 1.71202400
 H 3.86678500 2.57242100 2.03667200
 H 4.64234600 1.08004300 2.59972100
 H 5.37566500 2.01983200 1.28405500
 C 2.07753600 2.17285500 -0.91953200
 O 1.93363900 3.33938900 -0.31306100
 O 1.18184000 1.61069600 -1.53883500
 H 1.00677400 3.66717800 -0.38629100

C 4.32224100 -1.70382500 0.42331600
 H 4.99184300 -2.29720000 -0.20972300
 H 4.67387000 -1.77499600 1.45689800
 C 2.96417100 -2.34418700 0.31830200
 O 2.40807500 -2.52742800 -0.75913400
 O 2.43740100 -2.69367900 1.47739800
 H 1.49216000 -2.94568800 1.35604200
 H -0.38660900 1.66441800 -1.53073500
 H -1.21046500 1.09587500 1.27059900
 H 0.99155100 -3.18446900 -1.29206500
 H -2.88868700 -2.88499800 -0.07914300
 S -3.65341800 -0.41358100 0.51938800
 O -3.42800800 -0.05971300 -0.99744400
 O -4.79995700 0.59881800 0.87094600
 H -2.46451300 -0.11422700 -1.21704400
 H -4.43890600 1.51067600 0.74456300
 O -4.18569700 -1.75479800 0.63054000
 O -2.45658600 -0.11972800 1.28969100

(1pa₃₋₁)(4sa) cluster

S -10.01513700 -1.17988600 -0.79281800
 O -9.22400400 -2.28667800 -0.28740300
 O -11.02163300 -1.36758500 -1.79692100
 O -10.69308600 -0.56038600 0.52471900
 H -11.40725900 0.04984700 0.26348200
 O -9.05883600 -0.03383900 -1.27088500
 H -8.23853800 -0.01035200 -0.67916900
 S 5.90659500 -0.11495500 0.60209000
 O 4.83462700 0.53139100 1.33076700
 O 6.84794000 -0.94272100 1.33221300
 O 5.33241800 -1.03258400 -0.53476900
 H 4.60132000 -0.54992600 -1.01220500
 O 6.66165700 1.03533000 -0.15533100
 H 7.47542300 0.66292700 -0.59175400
 S 2.35533500 1.19847400 -0.78944200
 O 3.49512600 0.65086100 -1.50500600
 O 1.37626700 1.97777900 -1.51948900
 O 1.66719900 0.00032100 -0.06446100
 H 0.75557400 0.29537500 0.28653900
 O 2.85884400 2.13578600 0.37361400
 H 3.61975100 1.70026700 0.83858100
 C -3.93980000 1.11696700 0.14518400
 C -2.79813000 1.83638900 0.95906300
 C -3.18847600 1.01297000 2.19294100
 C -4.55402100 0.73172400 1.53010700
 H -3.03236800 2.90098900 1.05683500
 H -3.18488900 1.52563300 3.15756800
 H -2.57154100 0.11099000 2.26421500
 H -5.28458700 1.49844500 1.81447800
 C -3.42662200 -0.08949900 -0.63672000
 H -4.27029600 -0.68284600 -1.00890300

H -2.84766300 0.23820000 -1.50823000
 H -2.78491400 -0.74215000 -0.03469800
 C -4.74670000 2.03912000 -0.75446600
 H -4.09719200 2.47374300 -1.52369100
 H -5.55616200 1.49406800 -1.24850500
 H -5.19210300 2.85889700 -0.18000900
 C -1.42120200 1.68782400 0.39953000
 O -1.16474200 2.53822900 -0.57586800
 O -0.63421000 0.82265400 0.77581900
 H -0.26385200 2.38762600 -0.94999700
 C -5.14951600 -0.64559700 1.75515600
 H -4.45066200 -1.44345500 1.47497300
 H -5.36192700 -0.80392800 2.82078400
 C -6.43036700 -0.88823500 1.00438700
 O -6.96243500 -0.03663400 0.29953700
 O -6.91330800 -2.10003100 1.18317900
 H -7.75473100 -2.22070600 0.67821000
 S 9.66902500 -1.23533700 -0.44063100
 O 10.21161800 -0.27642400 0.72141500
 O 8.91998200 -2.36852700 0.35325000
 H 10.99591300 -0.67662400 1.14135200
 H 8.08883900 -1.99784600 0.75505200
 O 8.70244000 -0.41028900 -1.14252800
 O 10.76885800 -1.84813700 -1.12350200

(1pa₂₋₂)(4sa) cluster

S 5.86869900 -1.52925400 0.50112100
 O 4.70238800 -2.34835800 0.75530800
 O 6.97571800 -1.53977200 1.43277300
 O 6.35507300 -1.90985800 -0.94494000
 H 7.14384600 -1.34434500 -1.16287500
 O 5.42864500 -0.02056300 0.36641700
 H 4.49905900 0.04068000 -0.09476500
 S -8.46845500 -1.12426800 -0.56171000
 O -7.17368700 -1.67473500 -0.16553200
 O -9.37110200 -1.87786500 -1.36987800
 O -9.24985500 -0.70262400 0.74817600
 H -8.63889400 -0.24443100 1.37201200
 O -8.18671000 0.25593400 -1.29140600
 H -7.34542100 0.65486400 -0.96247600
 S -5.81799000 0.61660000 1.34551000
 O -7.10660800 0.57754500 2.00045500
 O -5.82227000 1.10516600 -0.04669400
 O -4.82502900 1.43610000 2.18457400
 H -3.98663400 1.67992500 1.62340000
 O -5.13622400 -0.80586500 1.36376700
 H -5.73163300 -1.41704100 0.85651300
 C -0.23298100 -0.05183900 -0.57228800
 C 0.95775300 -0.31812900 -1.56599300
 C 0.78675800 1.10522200 -2.11702300
 C -0.64613100 1.09379500 -1.54647800

H 0.67424100 -1.09407800 -2.28453800
 H 0.90279100 1.24569300 -3.19361800
 H 1.43969400 1.80711300 -1.58926200
 H -1.33736100 0.68851200 -2.29602000
 C 0.26092000 0.45422900 0.78305100
 H -0.57487700 0.83894800 1.37641400
 H 0.72027000 -0.36759000 1.34510000
 H 1.00640400 1.25188700 0.68786100
 C -1.22569600 -1.18951600 -0.39721800
 H -0.75927800 -2.03378000 0.12296400
 H -2.08577700 -0.86180600 0.19994000
 H -1.59581600 -1.54649800 -1.36439800
 C 2.25464100 -0.69479000 -0.92940800
 O 2.28982200 -1.94711200 -0.52845400
 O 3.17000700 0.11041400 -0.75739000
 H 3.13996500 -2.16062200 -0.07296800
 C -1.22805600 2.39476400 -0.98635700
 H -0.59078300 2.80619900 -0.20048200
 H -1.32780300 3.12646300 -1.79455200
 C -2.58497800 2.11917100 -0.40711600
 O -2.77535000 1.98635500 0.80164600
 O -3.52625700 1.97302900 -1.31430100
 H -4.38424500 1.70995800 -0.90178700
 S 8.82948700 0.85600300 0.04926300
 O 9.31238300 -0.05216900 1.25031800
 H 8.61681900 -0.71786400 1.46288200
 O 7.64727400 1.71009900 0.67772000
 H 6.79093700 1.23231700 0.58722900
 O 8.24009400 -0.00523300 -0.97379000
 O 9.89959500 1.74485600 -0.26758700

(1pa₁₋₃)(4sa) cluster

S 9.41706400 -1.48177300 -0.31821300
 O 10.53527600 -2.02849300 -1.02731900
 O 8.63081200 -0.39007200 -0.86366000
 O 8.46823800 -2.67993200 0.05749900
 H 7.62892200 -2.32509900 0.45612600
 O 9.89056900 -0.93350000 1.11007600
 H 10.57687100 -1.52095100 1.47829900
 S 5.66582800 -0.21084900 0.56841600
 O 4.55813100 0.34918600 1.31614500
 O 6.42167200 -1.30091400 1.15472300
 O 5.18467300 -0.73498500 -0.83101000
 H 4.57878600 -0.06224400 -1.24932200
 O 6.61240200 0.99820500 0.23748900
 H 7.44576300 0.65514700 -0.18621100
 S 2.42139300 1.73222800 -0.84011500
 O 1.56697200 2.74378500 -1.42721700
 O 3.63642300 1.33880800 -1.53187500
 O 2.77713000 2.26435300 0.60043100
 H 3.46005700 1.67024900 1.00893400

O 1.61540300 0.41705600 -0.58742600
 H 0.68650500 0.65683300 -0.25355600
 C -3.73778300 -0.08982100 0.42413900
 C -4.95024300 -0.30651300 1.40344300
 C -4.71272700 1.09606200 1.97775500
 C -3.28633800 1.05406800 1.38902500
 H -4.71214800 -1.10828700 2.10979600
 H -4.81464000 1.21877000 3.05846900
 H -5.34757400 1.83188000 1.47325300
 H -2.58110600 0.64002400 2.11900000
 C -4.18317000 0.42347700 -0.94333500
 H -3.31665600 0.76738400 -1.52098500
 H -4.65897400 -0.38197600 -1.51499800
 H -4.89845800 1.25069000 -0.87262300
 C -2.81662100 -1.28997200 0.27509800
 H -3.36166200 -2.12873800 -0.17379400
 H -1.96080900 -1.04938900 -0.36314200
 H -2.43054400 -1.61365800 1.24790900
 C -6.26185400 -0.60459600 0.75082600
 O -6.36334300 -1.85775500 0.35001800
 O -7.12777100 0.24454600 0.56281100
 H -7.22404200 -2.00993500 -0.11131000
 C -2.73135900 2.35044100 0.82832400
 H -3.40043200 2.79776000 0.08403600
 H -2.62853700 3.10164300 1.62331100
 C -1.37591200 2.19624600 0.19429900
 O -0.72581300 1.15769600 0.26259500
 O -0.96270700 3.28187400 -0.42651100
 H -0.06331700 3.14972300 -0.81173000
 S -9.93826100 -1.23602300 -0.68010400
 O -10.34830300 -1.53455200 0.84411300
 O -9.45247400 0.25238200 -0.62902100
 H -11.21985500 -1.13861000 1.02935800
 H -8.54388900 0.28918500 -0.18283200
 O -8.80014200 -2.10806900 -0.90578300
 O -11.10897200 -1.29513300 -1.50672200

(1pa_{bridged})(4sa) cluster

S 0.54404600 -3.65475900 -0.32851100
 O 0.41001900 -2.96790400 1.08584300
 O -0.61105500 -4.52276300 -0.44687200
 O 0.42942700 -2.47467900 -1.34684800
 O 1.87298900 -4.21446400 -0.47815200
 S 3.31742300 2.15017600 0.45795800
 O 3.77382700 2.62820500 -0.97859500
 O 4.69972800 1.77921100 1.07862700
 O 2.78252300 3.27315900 1.20089600
 O 2.48753300 0.96321000 0.32755400
 S 0.04796000 3.54982900 -0.69525400
 O 0.40975700 4.49221500 0.51743000
 O -1.17174300 4.08755000 -1.26220700

O 1.21183900 3.37883900 -1.54438500
 O -0.22556700 2.15962300 -0.03657200
 H -1.12366200 2.17864700 0.43634200
 C -4.62142800 -0.90988600 0.81571700
 C -4.34505400 -1.43018400 -0.64400100
 C -4.36892500 0.02192800 -1.14236800
 C -5.13972000 0.39887800 0.14241200
 H -5.19037200 -2.02927900 -0.99720800
 H -4.84606800 0.22446400 -2.10328200
 H -3.35105100 0.42625100 -1.16034500
 H -6.21303900 0.26922400 -0.03836100
 C -3.33361000 -0.74372300 1.61926400
 H -3.51504100 -0.15562300 2.52513500
 H -2.96033100 -1.72683800 1.92969300
 H -2.54263500 -0.24117200 1.05690800
 C -5.64812600 -1.69916800 1.61192900
 H -5.26038500 -2.69305000 1.86262700
 H -5.88557400 -1.18279500 2.55036500
 H -6.57917000 -1.82747000 1.04883300
 C -3.07970400 -2.20970000 -0.80753600
 O -3.17675900 -3.45427400 -0.37867400
 O -2.04424800 -1.71541900 -1.24134900
 H -2.30249300 -3.91150500 -0.42618300
 C -4.94832100 1.77414100 0.81836600
 H -5.75701900 2.44684000 0.52325600
 H -4.96054200 1.66471300 1.90694100
 C -3.64684300 2.41090500 0.41938400
 O -2.59266900 2.22552600 1.01859400
 O -3.73974800 3.14958000 -0.66958500
 H -2.86202900 3.53344200 -0.90893700
 H -0.53656500 -2.16078200 -1.37185700
 H 1.25597600 -2.49476900 1.30908700
 H 1.26800600 4.19031000 0.91057800
 H 2.97067500 2.98346100 -1.43640000
 H 4.90832200 0.81845300 0.91043000
 S 3.82631100 -1.72562600 0.28480800
 O 3.05322100 -1.28328100 -1.01794400
 O 4.35996600 -3.11112000 -0.20165500
 H 2.59910100 -0.42527500 -0.82927200
 H 3.57820200 -3.70398100 -0.35919500
 O 4.98041100 -0.87793600 0.51501500
 O 2.88108000 -1.88732300 1.37860800

pinic acid dimer (2pa)

C 3.00102000 0.65825500 0.91764100
 C 2.83743000 1.74536500 -0.20677000
 C 3.35280200 0.73924100 -1.25040700
 C 3.85617300 -0.16337100 -0.10002500
 H 3.50665500 2.59399100 -0.02700000
 H 4.10729400 1.10087200 -1.95308300
 H 2.52496400 0.30194700 -1.80947500

H 4.91417800 0.05267100 0.09522000
 C 1.67754500 0.00615800 1.29923800
 H 1.84214400 -0.89535200 1.89942300
 H 1.07083200 0.70333600 1.88710300
 H 1.09190400 -0.27978200 0.41691100
 C 3.73992200 1.12268000 2.16359500
 H 3.13150600 1.83821900 2.72871000
 H 3.96260600 0.27178000 2.81949600
 H 4.68737500 1.60919200 1.90553000
 C 1.44088900 2.26066200 -0.41345900
 O 0.98496900 2.97803400 0.60476800
 O 0.76911100 2.00591200 -1.40220800
 H 0.02029000 3.16125300 0.46673200
 C 3.74803400 -1.69764900 -0.17577700
 H 4.41451400 -2.04383300 -0.97601100
 H 4.08750200 -2.14360300 0.76368800
 C 2.37680700 -2.26150900 -0.46702500
 O 1.76081300 -2.98137500 0.30589100
 O 1.90186200 -1.90193700 -1.64884700
 H 0.93659800 -2.12871200 -1.69614800
 C -3.00100300 -0.65822800 0.91765400
 C -2.83744000 -1.74535900 -0.20673800
 C -3.35276500 -0.73922500 -1.25039100
 C -3.85616100 0.16338800 -0.10002200
 H -3.50669000 -2.59396300 -0.02695800
 H -4.10724200 -1.10084500 -1.95308700
 H -2.52490800 -0.30193400 -1.80943600
 H -4.91416700 -0.05266200 0.09521600
 C -1.67750700 -0.00616500 1.29923300
 H -1.84207200 0.89534700 1.89942200
 H -1.07080100 -0.70336200 1.88708400
 H -1.09187200 0.27976100 0.41689700
 C -3.73990400 -1.12262800 2.16361800
 H -3.13149400 -1.83816500 2.72873900
 H -3.96257400 -0.27171500 2.81950600
 H -4.68736500 -1.60913100 1.90556500
 C -1.44091600 -2.26070800 -0.41340700
 O -0.98498800 -2.97797700 0.60488800
 O -0.76912800 -2.00601200 -1.40216500
 H -0.02030400 -3.16119500 0.46687600
 C -3.74804100 1.69766300 -0.17580600
 H -4.41453700 2.04381400 -0.97604100
 H -4.08749700 2.14364300 0.76365200
 C -2.37682900 2.26152300 -0.46711400
 O -1.76082900 2.98144000 0.30575100
 O -1.90188000 1.90182600 -1.64889600
 H -0.93661400 2.12859300 -1.69621300

(2pa)(1sa) cluster

C -3.01144900 -2.12383100 0.79456400
 C -2.44386500 -2.92145000 -0.43037600

C -3.21404000 -1.98281300 -1.37309000
 C -4.13542200 -1.65445200 -0.17705600
 H -2.84888700 -3.94013700 -0.42360500
 H -3.67597700 -2.42291500 -2.25981000
 H -2.59295700 -1.13700900 -1.67663400
 H -4.92960200 -2.41214700 -0.13876800
 C -2.06412000 -1.00507400 1.22418000
 H -2.55045100 -0.33873600 1.94456800
 H -1.17875400 -1.43115900 1.71146400
 H -1.71584600 -0.39526300 0.38295000
 C -3.44747100 -2.94932200 1.99378200
 H -2.57795400 -3.39492000 2.49014000
 H -3.97045800 -2.32116600 2.72555900
 H -4.12199000 -3.75973600 1.69504300
 C -0.95190900 -3.00042900 -0.52872900
 O -0.41895800 -3.74638000 0.42490600
 O -0.29072300 -2.40912900 -1.37260700
 H 0.57420600 -3.69051300 0.38373300
 C -4.84343700 -0.30422600 -0.00516200
 H -5.62579700 -0.22750200 -0.77010000
 H -5.32185200 -0.26383900 0.97774700
 C -3.99506400 0.93383000 -0.13095300
 O -3.79798100 1.69989800 0.80467700
 O -3.52154400 1.13021000 -1.34839700
 H -2.99979000 1.96879900 -1.39149200
 C 3.94027000 0.17069700 0.85278900
 C 3.99035300 1.26843500 -0.28401400
 C 4.23835600 0.15524800 -1.31585400
 C 4.64052600 -0.78721100 -0.16156800
 H 4.83799300 1.94170200 -0.13008200
 H 4.99414500 0.35292500 -2.07988700
 H 3.30390100 -0.13909800 -1.79460200
 H 5.72302900 -0.70658500 0.00177400
 C 2.51497700 -0.23274600 1.22698000
 H 2.52597400 -1.11549700 1.87487900
 H 2.02506000 0.58048700 1.77729200
 H 1.89565000 -0.45651600 0.35215100
 C 4.73638400 0.50987000 2.10403600
 H 4.26549200 1.33417300 2.65208600
 H 4.78483000 -0.35792000 2.77325200
 H 5.76122800 0.80673600 1.85572200
 C 2.72727300 2.05421700 -0.41656400
 O 2.68947800 3.14290800 0.33217700
 O 1.77664600 1.67596500 -1.09609800
 H 1.81647600 3.59472100 0.23817400
 C 4.33075600 -2.29027000 -0.20154800
 H 4.90745400 -2.73175800 -1.02479300
 H 4.65424100 -2.76747100 0.72795300
 C 2.88931100 -2.68120300 -0.41871200
 O 2.25874500 -3.36169200 0.37981600
 O 2.37876700 -2.23790700 -1.55291900
 H 1.39406400 -2.39978700 -1.56934200
 S -1.04820800 3.29458800 -0.07996800

O -1.84636400 3.39106800 1.25865200
O -0.56676900 1.79375500 -0.03670800
H 0.31017400 1.70557800 -0.54359400
H -2.67858700 2.82971800 1.16133200
O 0.09834400 4.17764000 0.01451800
O -1.96242200 3.44689000 -1.20300100

(2pa)(2sa) cluster

C 3.94962600 -2.30806200 0.33046400
C 2.69113400 -2.23893100 1.26231100
C 3.27993000 -0.99086000 1.93899400
C 4.66179300 -1.42698900 1.40222800
H 2.67300500 -3.11336400 1.92278100
H 3.16194000 -0.89476400 3.02058300
H 2.91277100 -0.08097200 1.45950600
H 5.12523300 -2.10668200 2.12845000
C 3.71439300 -1.59557600 -0.99920900
H 4.66135400 -1.43760000 -1.52579500
H 3.07099200 -2.20802400 -1.64098200
H 3.22860300 -0.62061300 -0.87728000
C 4.53730800 -3.69113800 0.10186200
H 3.86195500 -4.30056600 -0.50884200
H 5.49770500 -3.61985800 -0.42387600
H 4.70626000 -4.21379200 1.05006500
C 1.36394100 -2.17343600 0.57258100
O 0.70766700 -1.04562900 0.73209000
O 0.95868500 -3.11980600 -0.10200000
H -0.18270100 -1.07084900 0.29969200
C 5.74154300 -0.40591300 1.00299600
H 6.26837900 -0.08491100 1.90785000
H 6.46687500 -0.86842900 0.32666100
C 5.18692000 0.84488900 0.37682400
O 4.51550200 1.64397900 1.01761500
O 5.48143900 1.00221800 -0.90073900
H 4.95108600 1.74470000 -1.27419200
C -4.01501800 2.27374600 0.30147800
C -2.72375800 2.25099200 1.18935300
C -3.18597800 0.91360200 1.78642700
C -4.62110900 1.30901600 1.36307100
H -2.76645500 3.07219700 1.91443200
H -2.99760200 0.73305700 2.84676500
H -2.78929400 0.07593100 1.20475900
H -5.05403800 1.93504000 2.15345900
C -3.77213700 1.61976000 -1.05836200
H -4.72217200 1.39426800 -1.55462800
H -3.21063200 2.30521900 -1.70406000
H -3.20526200 0.68526100 -0.98302100
C -4.70595400 3.61738400 0.14006900
H -4.10345800 4.29070600 -0.47954100
H -5.68129200 3.49167700 -0.34657100
H -4.86909600 4.09954200 1.11042700

C -1.42028400 2.34012700 0.46162200
O -1.24145000 3.52903400 -0.08615300
O -0.62366800 1.41249800 0.35888400
H -0.39948400 3.56704300 -0.60170000
C -5.68884900 0.27246500 0.96860100
H -6.27474500 0.00440300 1.85284900
H -6.36366100 0.69421600 0.21765300
C -5.10064500 -0.99809600 0.42042500
O -5.03608000 -1.26534200 -0.77126600
O -4.64235800 -1.79315900 1.37383700
H -4.16607700 -2.56126900 0.97695600
S 2.24728400 2.75120700 -0.98988000
O 2.60710600 3.37416400 0.41121500
O 1.79690300 1.28742700 -0.64559700
S -2.25191400 -2.70818400 -0.92987600
O -1.08733400 -3.48531500 -1.59541700
O -3.13841300 -2.48338700 -2.20587600
H 3.38958600 2.86145400 0.76762700
H 0.86418300 1.29320700 -0.24331700
H -0.24087000 -3.34445800 -1.03237500
H -3.99395200 -2.09121900 -1.87649900
O 1.12139300 3.51740100 -1.48920000
O 3.44234400 2.63366200 -1.80091000
O -2.97543900 -3.53405400 0.02820800
O -1.77407200 -1.42329200 -0.41746000