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Supplementary Material

The Structure of Uric Acid Dihydrate Crystals Revisited *via* First-Principle Methods

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Symmetry, lattice parameters (in Å and degrees) and fractional coordinates of the asymmetric unit of the five UAD models.

P1

7.15912628 6.40788014 17.34829179 89.616527 90.323171 90.064310
O 3.924157381882E-02 5.383854332051E-02 9.389091446816E-02
O -2.519579603709E-03 -4.694925813605E-01 3.855711657905E-01
O -4.719034181406E-01 4.695490835375E-01 4.114531810721E-01
O -4.974383296210E-01 5.038962035092E-04 1.094350032991E-01
O -2.303753780653E-02 -4.941423187779E-02 -1.021003370187E-01
O 9.202911808175E-03 4.561876504320E-01 -4.095265784612E-01
O 4.685323177757E-01 -4.912241003198E-01 -3.874624394756E-01
O -4.837554630292E-01 1.386833680092E-03 -1.011137512940E-01
N 1.505356133938E-01 2.588322459359E-01 -2.545438110685E-03
N -1.343057553973E-01 -2.562755474700E-01 4.779258577058E-01
N -3.740396225792E-01 2.447915743265E-01 -4.945787827550E-01
N 3.866328196597E-01 -2.332735546576E-01 1.936019117363E-02
N -1.257912560349E-01 -2.493537098257E-01 -2.255662151743E-03
N 1.285214000884E-01 2.521518736874E-01 4.955380468520E-01
N 3.590142612628E-01 -2.568567067221E-01 -4.791055692146E-01
N -3.602807430475E-01 2.409296107891E-01 -1.492377836371E-02
N 1.911223764813E-01 3.536528823635E-01 1.263997151347E-01
N -1.580478133496E-01 -1.579802266677E-01 3.560486551514E-01
N -3.219203452032E-01 1.717284656817E-01 3.753013672525E-01
N 3.523534943876E-01 -3.132669654739E-01 1.424171460176E-01
N -1.748511720099E-01 -3.540938743768E-01 -1.298611079151E-01
N 1.503339387609E-01 1.500726032862E-01 -3.749574890929E-01
N 3.093835079434E-01 -1.843066797668E-01 -3.566681115082E-01
N -3.356565045810E-01 3.100228430212E-01 -1.393533275086E-01
C 2.765539018637E-01 -4.707970251058E-01 1.007732355153E-01
C -2.409012086956E-01 -9.165503216278E-03 3.989306969710E-01
C -2.577167791049E-01 4.716916269562E-01 -1.009977892108E-01
C 2.376401314286E-01 -2.501696731407E-02 -3.992000182361E-01
C 1.228749159215E-01 2.143836461577E-01 7.415470258350E-02
C -8.940138552081E-02 -3.111549164738E-01 4.048944353518E-01
C -3.935986103140E-01 3.041320896038E-01 4.293057974420E-01
C 4.226563325410E-01 -1.645024989913E-01 9.190418310651E-02
C -1.037165325787E-01 -2.092593383931E-01 -7.987911525504E-02
C 9.158727045647E-02 2.947322377202E-01 -4.282254006463E-01
C 3.876873599204E-01 -3.275238839944E-01 -4.061141475423E-01
C -4.020024577499E-01 1.671785316561E-01 -8.615555072563E-02
H 9.648096104741E-02 1.516429456208E-01 -4.039994929686E-02
H -9.599781430414E-02 -3.433521757750E-01 -4.750157029999E-01
H -4.289879295397E-01 3.466901222895E-01 -4.546575154118E-01
H 4.277982481717E-01 -1.529026222454E-01 -2.935074843649E-02
H -7.037584549011E-02 -1.377953722099E-01 3.371048605118E-02
H 8.309363366700E-02 3.616779026833E-01 4.554881466744E-01
H 4.078220797260E-01 -3.351091685010E-01 4.740735598760E-01
H -3.981682181587E-01 1.659544083341E-01 3.513747279992E-02
H 1.641258285365E-01 3.235609638290E-01 1.852404901062E-01

H -1.311820781190E-01 -1.615166404689E-01 2.963432827242E-01
H -3.380190336311E-01 2.117594392526E-01 3.171860716933E-01
H 3.625682703201E-01 -2.987072834196E-01 2.021307392906E-01
H -1.607268146367E-01 -3.275576696771E-01 -1.888332153873E-01
H 1.239126334822E-01 1.781331467251E-01 -3.165767150109E-01
H 3.237851455766E-01 -2.010635608620E-01 -2.967258449174E-01
H -3.662509211613E-01 2.912332302960E-01 -1.984980175220E-01
O 8.649999230447E-02 2.696037171701E-01 2.697682630016E-01
O -4.877774386739E-02 -2.047826378236E-01 2.134960407055E-01
O -3.934268877862E-01 2.797158129574E-01 2.235429179651E-01
O 4.179390949772E-01 -2.462171792857E-01 2.951886371014E-01
O -1.120749340624E-01 -2.780742060668E-01 -2.862222749858E-01
O 6.131067869921E-02 2.222504848820E-01 -2.250326803436E-01
O 4.023860654534E-01 -2.670296197718E-01 -2.116170581456E-01
O -4.649051706110E-01 2.258697586321E-01 -2.769904927533E-01
H 1.539048905341E-01 1.896559425960E-01 3.090735310294E-01
H -1.179425141966E-01 -2.873037193932E-01 1.756309398816E-01
H -3.177848693059E-01 3.630881384137E-01 1.887183055452E-01
H 3.425052552068E-01 -1.611496340957E-01 3.292282313690E-01
H -1.851498897926E-01 -1.910997804643E-01 -3.211790414234E-01
H 1.387442809002E-01 3.004955602340E-01 -1.890307647692E-01
H 3.367920800055E-01 -3.536582271272E-01 -1.741221798874E-01
H -3.936134429203E-01 1.503972734373E-01 -3.157662928310E-01
H 4.290614138753E-02 3.911561069401E-01 2.981892634161E-01
H -8.947804285794E-03 -8.126095634543E-02 1.849475234919E-01
H -4.368977501725E-01 1.628167355012E-01 1.923552192463E-01
H 4.591019639389E-01 -3.658236570747E-01 3.257029033304E-01
H -6.826326539586E-02 -3.938520684113E-01 -3.173070141251E-01
H 2.082280297237E-02 1.009700764341E-01 -1.953833657476E-01
H 4.483747164633E-01 -1.475495741744E-01 -1.824439087454E-01
H 4.951375150111E-01 3.517368859750E-01 -3.045745985985E-01
C -2.720672049551E-01 4.326041805764E-01 -2.317047456320E-02
C -2.066566535218E-01 -4.254257479197E-01 3.187693450065E-02
O -2.157743876814E-01 -4.458364667900E-01 1.030140186484E-01
C 2.973611540463E-01 -4.252818340957E-01 2.359764589881E-02
C 2.324674252275E-01 4.378819554129E-01 -3.379435371024E-02
O 2.410756349901E-01 4.608552523416E-01 -1.048453009746E-01
C 2.669462311720E-01 -6.682352689819E-02 -4.758320150427E-01
C 2.129267749438E-01 7.367658781249E-02 4.659777466584E-01
O 2.353727164607E-01 5.047769894866E-02 3.955570564980E-01
C -2.284707125027E-01 -6.732135786825E-02 4.752937543781E-01
C -2.963798750843E-01 5.988263356780E-02 -4.658241246454E-01
O -2.903100731856E-01 2.113978834913E-02 -3.95554320075E-01

P2₁/c(a)

7.01963440 6.47105226 17.28937571 90 91.692578 90
O 2.138123144175E-02 -4.911595024367E-01 3.963749865795E-01
O -4.825127560868E-01 6.481558733111E-02 9.833437469072E-02
N 1.303959661062E-01 2.618103715941E-01 4.842602198892E-01
N -3.609090830714E-01 2.511679789901E-01 -1.783421063802E-04
N 1.740460449398E-01 2.033292888347E-01 3.602219028014E-01
N -3.314677264110E-01 3.681375493996E-01 1.275848997003E-01
C 2.437536249775E-01 3.807584837680E-02 3.999900994503E-01
C 9.997939353989E-02 3.419959664433E-01 4.123437968862E-01
C -3.959029175661E-01 2.201049325712E-01 7.691639462042E-02

H 8.343184996945E-02 3.335339108803E-01 -4.668099797495E-01
H -4.114836997410E-01 1.375577851858E-01 -3.702853883206E-02
H 1.609567849906E-01 2.273901698841E-01 3.003598629204E-01
H -3.576958984714E-01 3.486521523761E-01 1.866516164175E-01
O 8.894104955518E-02 2.930855258551E-01 2.122235423293E-01
O -4.194168048156E-01 3.159672309288E-01 2.768172309394E-01
H 1.600379482459E-01 3.767980769879E-01 1.762569733922E-01
H -3.491112215726E-01 2.316887783443E-01 3.147330864415E-01
H 4.378255648617E-02 1.736146211438E-01 1.824627124341E-01
H -4.618145601501E-01 4.346098667741E-01 3.063501012553E-01
C -2.167404086436E-01 -6.983378918837E-02 -4.776483885289E-01
C -2.755531060919E-01 7.671042365621E-02 4.666142985259E-01
O -2.585076691400E-01 6.522715949598E-02 3.953911835232E-01

P2₁/c(b)

6.44857014 7.03190103 18.98049856 90 113.854682 90
O 5.166344617282E-02 1.908916656494E-02 -4.037562521045E-01
O -1.174048740474E-01 -1.817985119568E-02 -1.058834768743E-01
N -2.575142542011E-01 1.418553138501E-01 4.991299267177E-01
N -2.533589778910E-01 -1.274649504778E-01 -1.695137086074E-02
N -2.144471885928E-01 1.687302589714E-01 -3.727952576132E-01
N -4.661866004552E-01 -1.728779040619E-01 -1.404014449741E-01
C -4.190800110840E-01 2.565906103608E-01 -3.997574247073E-01
C -1.302337150606E-01 1.055906543055E-01 -4.240865838388E-01
C -2.631003943501E-01 -9.738100845175E-02 -8.898788091178E-02
H -1.881936911554E-01 9.167808663881E-02 4.626028963329E-01
H -1.217424476711E-01 -8.139740207247E-02 3.245250303959E-02
H -1.206872556326E-01 1.433948481361E-01 -3.139640800291E-01
H 4.829383892133E-01 -1.583125078272E-01 -2.001505237985E-01
O 2.425463764862E-02 8.296281597111E-02 -2.208823295680E-01
O 4.475490845633E-01 -8.412283470892E-02 -2.847150157171E-01
H 1.513551320655E-01 1.530025449826E-01 -1.836069666909E-01
H 4.911052273187E-01 -1.564449284138E-01 -3.204642940521E-01
H -6.357988148784E-02 4.160725815779E-02 -1.921558611515E-01
H 2.947917836192E-01 -3.898675726270E-02 -3.158492261075E-01
C -4.522401982474E-01 -2.842665976711E-01 4.770713789387E-01
C 4.708761970379E-01 -2.279996704708E-01 -4.66667207472E-01
O -4.289642739378E-01 -2.479689567089E-01 -3.957977794328E-01

To transform into $P2_1/n$ – for comparison with the other structures as mentioned in the paper, multiply by matrix (-1 0 0, 0 1 0, -1 0 -1)

Pca2₁

17.31505421 6.43415992 7.06799356 90 90 90
O 3.359443546859E-01 -2.097766946491E-01 -2.820963082833E-02

O -3.678791924305E-01 2.662666589492E-01 9.701873438927E-03
N 2.428020146614E-01 6.991566265709E-03 -1.406611192165E-01
N -2.737618225976E-01 4.881707413750E-01 1.254987666961E-01
N 3.736636199649E-01 8.985899473507E-02 -1.734477657391E-01
N -3.956040489733E-01 -4.212304851021E-01 1.662966334891E-01
C 3.512187473662E-01 2.687044962334E-01 -2.581696816150E-01
C 3.187949287094E-01 -4.607173044901E-02 -1.099547306645E-01
C -3.476161881438E-01 4.274566887890E-01 9.179743653154E-02
H 2.019798784498E-01 -9.667972427595E-02 -9.099493559315E-02
H -2.274758329790E-01 4.028092389913E-01 8.036795766691E-02
H 4.318573369981E-01 5.318140028714E-02 -1.452181352946E-01
H -4.557240583104E-01 -4.298084155943E-01 1.547150135660E-01
O -4.823587371988E-01 -9.198237675593E-03 -6.781169422766E-02
O 4.532810920359E-01 -4.770219181799E-01 9.427162334285E-02
H -4.448295622101E-01 -8.689709720906E-02 -1.423212175139E-01
H 4.178884975501E-01 4.330606104258E-01 1.633409593788E-01
H -4.529800963085E-01 1.123259118967E-01 -2.653524863174E-02
H 4.230589286755E-01 -3.584512825339E-01 5.145363727159E-02
C 2.251878786232E-01 3.217311316963E-01 2.181397827221E-01
C 2.850375639574E-01 1.903188142691E-01 2.785752736793E-01
O 3.555601997349E-01 2.229726662950E-01 2.651652015409E-01

To transform into $P2_{ca}$ – for comparison with the other structures as mentioned in the paper, multiply by matrix
(0 1 0, 0 0 1, 1 0 0)

Pna2₁

7.00628700 17.50856229 6.50100496 90 90 90
O 4.723071073009E-01 3.583459742089E-01 2.545825943743E-02
O -6.412951453008E-03 -3.439278868564E-01 4.627680268671E-01
N 3.414674862367E-01 2.694347609483E-01 2.483785713320E-01
N -1.104735203794E-01 -2.483544065774E-01 2.529373478670E-01
N 3.131109123654E-01 3.914815458371E-01 3.284368615735E-01
N -1.521500158297E-01 -3.764572194629E-01 1.599954014176E-01
C 2.333110132011E-01 3.508250704099E-01 4.832797985318E-01
C 3.845443546575E-01 3.411195343229E-01 1.843242173559E-01
C -8.508936791189E-02 -3.245132153480E-01 3.008357006974E-01
H 3.826402677228E-01 2.218423599599E-01 1.697354540225E-01
H -6.091046525700E-02 -2.096669636175E-01 3.608111050441E-01
H 3.434395351375E-01 4.503821691009E-01 3.173540986286E-01
H -1.376331138393E-01 -4.344427748140E-01 1.906464080943E-01
O 4.433770924203E-01 -4.710460433393E-01 2.647538867656E-01
O -1.015350108969E-01 4.665326405021E-01 2.357013172169E-01
H 3.801025890794E-01 -4.315253074758E-01 1.830641478461E-01
H -1.914272833642E-01 4.359153960519E-01 3.133697712712E-01
H 4.845489957759E-01 -4.431479832454E-01 3.871068736324E-01
H -6.03602081865E-02 4.341089000511E-01 1.223607611012E-01
C -2.511613927490E-01 2.254503430882E-01 4.365048466704E-01
C -3.112172165107E-01 2.823008530746E-01 -4.267589990441E-01
O -2.971348622196E-01 3.521860026508E-01 -4.554438563288E-01

To transform into $Pn2_{1a}$ – for comparison with the other structures as mentioned in the paper, multiply by matrix
(1 0 0, 0 0 1, 0 1 0)