Electronic supplementary materials *Mendeleev Commun.*, 2023, **33**, 353–356

Concerning virial-based estimations of strength of bonding intermolecular interactions in molecular crystals and supramolecular complexes

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Acetic acid

Structure was retrieved from: R. Boese, D. Bläser, R. Latz and A. Bäumen, *Acta Cryst.*, 1999, **C55**, IUC9900001.

Parameters for the optimized crystal structure

Space group: $Pna2_1$

Unit cell parameters: 13.14307 3.91055 5.72820 90 90 90

Atom X Y Z (fractional coordinates):

O 0.37217 -0.10742 0.00603

H 0.31829 -0.03958 -0.11009

O 0.24504 -0.37624 0.18100

C 0.33461 -0.29105 0.17653

C 0.41072 -0.38492 0.35781

H 0.37404 -0.52051 0.50025

H 0.46877 -0.54738 0.27878

H 0.44913 -0.15584 0.42098

Cartesian coordinates for the molecular cluster (optimized central molecule):

Atom X Y Z (Cartesian coordinates)

O 0.145376 1.296697 0.517293

H -0.535719 2.028605 0.520423

O -1.629368 0.061667 0.056252

C -0.429443 0.136508 0.265601

C 0.511337 -1.012000 0.259483

H -0.036509 -1.945939 0.172622

H 1.182050 -0.910281 -0.595494

H 1.134365 -1.000372 1.154455

O -0.099251 -0.215031 -3.076881

H -0.774668 0.531971 -3.066691

O -1.848537 -1.471510 -3.589438

C -0.655384 -1.371024 -3.336901

C 0.296446 -2.514123 -3.305637

H -0.234085 -3.449618 -3.456220

H 1.037326 -2.379274 -4.095323

H 0.837171 -2.520681 -2.359044

O -0.252439 -5.484812 -0.836747

H -0.927857 -4.737820 -0.826542

O -2.001722 -6.741297 -1.349307

C -0.808561 -6.640805 -1.096791

C 0.143277 -7.783919 -1.065515

H -0.387270 -8.719405 -1.216088

H 0.884141 -7.649058 -1.855192

H 0.683962 -7.790605 -0.118989

O 0.256453 6.577572 -1.720834

H -0.418966 7.324564 -1.710629

O -1.492830 5.321086 -2.233394

C -0.299669 5.421577 -1.980878

C 0.652169 4.278465 -1.949603

H 0.121621 3.342978 -2.100175

H 1.393033 4.413325 -2.739278

H 1.192854 4.271778 -1.003076

O -0.049918 -3.962003 2.759429

H -0.725336 -3.215010 2.769634

O -1.799201 -5.218488 2.246868

C -0.606039 -5.117996 2.499384

C 0.345799 -6.261109 2.530660

H -0.184749 -7.196596 2.380087

H 1.086663 -6.126248 1.740983

H 0.886484 -6.267796 3.477186

O 0.458974 8.100381 1.875342

H -0.216444 8.847373 1.885547

O -1.290309 6.843896 1.362781

C -0.097148 6.944387 1.615298

C 0.854691 5.801274 1.646573

H 0.324143 4.865787 1.496001

H 1.595554 5.936134 0.856896

H 1.395375 5.794588 2.593099

O 0.305789 2.830594 4.115473

H -0.369629 3.577586 4.125678

O -1.443494 1.574108 3.602912

C -0.250325 1.674606 3.855437

C 0.701522 0.531459 3.886715

H 0.170955 -0.403998 3.736130

H 1.442351 0.666353 3.096966

H 1.242192 0.524781 4.833229

O 3.375294 2.596341 -3.549440

H 4.086288 3.073205 -4.079893

O 5.070971 2.008718 -2.252968

C 3.879188 1.955317 -2.525522

C 2.871807 1.187821 -1.744642

H 3.358739 0.622097 -0.955773

H 2.155159 1.885933 -1.309014

H 2.311718 0.528679 -2.408159

O 3.222109 -2.673445 -1.309309

H 3.933103 -2.196582 -1.839762

O 4.917786 -3.261069 -0.012837

C 3.725995 -3.314448 -0.285380

C 2.718617 -4.081950 0.495526

H 3.205526 -4.647720 1.284268

H 2.001966 -3.383868 0.931129

H 2.158579 -4.741048 -0.167982

O 3.577815 4.119151 0.046735

H 4.288809 4.596014 -0.483718

O 5.273493 3.531527 1.343207

C 4.081701 3.478148 1.0706640

C 3.074324 2.710646 1.8515710

H 3.561233 2.144876 2.640312

H 2.357673 3.408728 2.287172

H 2.514286 2.051548 1.188062

O 3.424630 -1.150635 2.286866

H 4.135624 -0.673773 1.756413

O 5.120308 -1.738260 3.583338

C 3.928516 -1.791639 3.310795

C 2.921139 -2.559141 4.091702

H 3.408048 -3.124911 4.880443

H 2.204488 -1.861059 4.527303

H 2.361101 -3.218239 3.428193

O -6.717370 -0.354566 -3.857703

H -7.420266 0.185811 -4.335427

O -8.357770 -0.792329 -2.436816

C -7.199114 -0.951294 -2.797016

C -6.209254 -1.808514 -2.090594

H -6.684882 -2.331045 -1.265956

H -5.402587 -1.178862 -1.711803

H -5.761357 -2.512891 -2.791692

O -6.514849 1.168243 -0.261528

H -7.217745 1.708620 -0.739252

O -8.155248 0.730481 1.159359

C -6.996592 0.571515 0.799159

C -6.006733 -0.285705 1.505580

H -6.482361 -0.808236 2.330218

H -5.200066 0.343947 1.884373

H -5.558836 -0.990082 0.804481

O 6.403360 -0.943971 -4.347022

H 5.700464 -0.403594 -4.824746

O 4.762961 -1.381734 -2.926136

C 5.921616 -1.540699 -3.286335

C 6.911476 -2.397919 -2.579913

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H 7.718143 -1.768267 -2.201122

H 7.359374 -3.102296 -3.281011

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H 5.902985 1.119215 -1.228572

O 4.965482 0.141076 0.670040

C 6.124138 -0.017890 0.309840

C 7.113998 -0.875110 1.016261

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H 7.920664 -0.245458 1.395053

H 7.561895 -1.579487 0.315164

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H -2.388848 4.008766 -2.321819

O -1.540526 1.918941 -2.916271

C -2.697812 2.125019 -2.576097

C -3.743211 1.071625 -2.470337

H -3.311222 0.092899 -2.656806

H -4.525665 1.274915 -3.203204

H -4.210462 1.110217 -1.486221

O -3.280508 -1.944495 -0.039168

H -2.542042 -1.261059 -0.081710

O -1.693711 -3.350846 -0.676140

C -2.850997 -3.144769 -0.335963

C -3.896396 -4.198162 -0.230206

H -3.464407 -5.176888 -0.416675

H -4.678850 -3.994872 -0.963073

H -4.363647 -4.159570 0.753910

O -2.924798 4.848097 1.316883

H -2.186327 5.531576 1.274356

O -1.338009 3.441735 0.679904

C -2.495290 3.647832 1.020078

C -3.540690 2.594435 1.125836

H -3.108701 1.615709 0.939369

H -4.323144 2.797725 0.392971

H -4.007940 2.633027 2.109954

O -3.077984 -0.421689 3.557011

H -2.339512 0.261789 3.514488

O -1.491190 -1.828036 2.920036

C -2.648476 -1.621959 3.260209

C -3.693875 -2.675353 3.365970

H -3.261886 -3.654078 3.179500

H -4.476329 -2.472062 2.633102

H -4.161125 -2.636761 4.350085

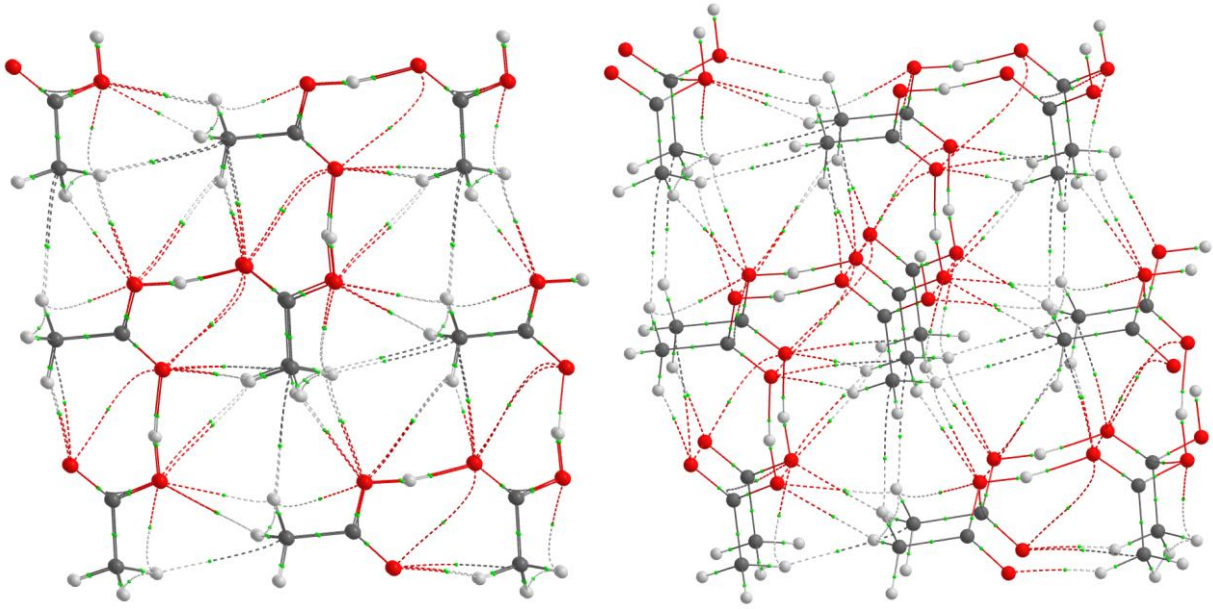

Figure S1. Atomic connectivity graph for the molecular cluster of acetic acid.

Aminomethane

Structure was retrieved from: M. Atoji and W. N. Lipscomb, *Acta Cryst.*, 1953, **6**, 770.

Parameters for the optimized crystal structure

Space group: Pcab

Unit cell parameters: 5.66946 6.00779 13.58275 90 90 90

Atom X Y Z (fractional coordinates):

C 0.227901 0.002166 0.107616

N 0.285467 0.059943 0.208636

H 0.260622 0.225516 0.220512

H 0.458914 0.028394 0.223208

H 0.332148 0.090296 0.051725

H 0.254066 -0.176162 0.096238

H 0.041887 0.037307 0.093435

Cartesian coordinates for the molecular cluster (optimized central molecule):

Atom X Y Z (Cartesian coordinates)

C 0.317592 0.009733 -0.168267

N -1.068189 0.318389 0.131751

H -1.264782 1.302172 -0.041216

H -1.287601 0.133183 1.109263

H 1.053106 0.552273 0.442179

H 0.499284 -1.059030 -0.028475

H 0.520774 0.237633 -1.216937

C 0.571361 0.018598 -5.798152

N -0.819308 0.344471 -5.534351

H -0.988030 1.337699 -5.677096

H -1.060165 0.146102 -4.562384

H 1.294493 0.554960 -5.169381

H 0.734070 -1.051391 -5.648670

H 0.809935 0.238906 -6.841416

C 0.392510 -6.023542 -0.168153

N -0.998158 -5.697669 0.095649

H -1.166879 -4.704440 -0.047094

H -1.239020 -5.896033 1.067614

H 1.115643 -5.487180 0.460617

H 0.555220 -7.093531 -0.018671

H 0.631085 -5.803235 -1.211416

C 0.221263 5.990635 -0.101791

N -1.169404 6.316507 0.162009

H -1.338127 7.309736 0.019265

H -1.410271 6.118144 1.133977

H 0.944396 6.526998 0.526979

H 0.383972 4.920646 0.047691

H 0.459838 6.210943 -1.145054

C 0.042413 -0.051505 5.528208

N -1.348256 0.274369 5.792009

H -1.516978 1.267596 5.649264

H -1.589118 0.076004 6.763975

H 0.765546 0.484857 6.156977

H 0.205122 -1.121493 5.677690

H 0.280988 0.168803 4.484944

C -3.423834 -0.079017 -3.147461

N -2.063607 -0.408938 -2.759248

H -1.881753 -1.400414 -2.897906

H -1.914506 -0.222733 -1.766673

H -4.202108 -0.622690 -2.595491

H -3.600383 0.989135 -3.000588

H -3.564017 -0.286287 -4.211059

C -3.688311 -0.114082 2.515720

N -2.328095 -0.443985 2.903916

H -2.146216 -1.435462 2.765263

H -2.178962 -0.257788 3.896490

H -4.466582 -0.657747 3.067682

H -3.864860 0.954082 2.662600

H -3.828489 -0.321333 1.452120

C 3.257966 -2.980691 0.235354

N 4.638746 -2.612414 -0.024616

H 4.779114 -1.616415 0.129121

H 4.885011 -2.793083 -0.998672

H 2.519731 -2.458205 -0.387559

H 3.125799 -4.053156 0.074040

H 3.013379 -2.778799 1.280951

C 3.172348 3.026407 0.268537

N 4.553122 3.394677 0.008568

H 4.693490 4.390673 0.162302

H 4.799387 3.214005 -0.965491

H 2.434123 3.548854 -0.354385

H 3.040177 1.953932 0.107220

H 2.927755 3.228290 1.314132

C 3.347768 0.014366 -2.579788

N 4.738436 -0.311507 -2.843590

H 4.907158 -1.304735 -2.700844

H 4.979298 -0.113143 -3.815555

H 2.624635 -0.521996 -3.208558

H 3.185058 1.084354 -2.729270

H 3.109193 -0.205942 -1.536525

C 3.083294 -0.020685 3.083392

N 4.473962 -0.346559 2.819591

H 4.642684 -1.339786 2.962336

H 4.714824 -0.148194 1.847625

H 2.360161 -0.557048 2.454622

H 2.920584 1.049303 2.933910

H 2.844719 -0.240993 4.126656

C -3.513629 -3.074067 -0.332321

N -2.163293 -2.709834 0.059728

H -2.009819 -1.712055 -0.067938

H -2.008782 -2.902664 1.050192

H -4.306996 -2.558928 0.225500

H -3.659641 -4.148375 -0.197279

H -3.659831 -2.859143 -1.393583

C -3.599254 2.933023 -0.299136

N -2.248943 3.297247 0.092903

H -2.095420 4.294992 -0.034778

H -2.094375 3.104440 1.083396

H -4.392620 3.448168 0.258675

H -3.745267 1.858714 -0.164091

H -3.745452 3.147938 -1.360404

C 7.078489 0.076932 0.432701

N 5.718269 0.406840 0.044489

H 5.536406 1.398326 0.183146

H 5.569152 0.220635 -0.948069

H 7.856763 0.620602 -0.119269

H 7.255038 -0.991223 0.285828

H 7.218672 0.284200 1.496299

C -6.488094 -0.112937 -0.202042

N -7.848313 0.216972 -0.590254

H -8.030176 1.208458 -0.451596

H -7.997430 0.030766 -1.582812

H -5.709820 0.430733 -0.754011

H -6.311544 -1.181092 -0.348915

H -6.347911 0.094331 0.861556

C 0.482304 -3.028496 -2.983295

N -0.898468 -3.396765 -2.723328

H -1.038836 -4.392761 -2.877062

H -1.144731 -3.216093 -1.749268

H 1.220533 -3.550936 -2.360379

H 0.614477 -1.956020 -2.821980

H 0.726899 -3.230378 -4.028892

C 0.396683 2.978593 -2.950116

N -0.984094 2.610325 -2.690148

H -1.124453 1.614326 -2.843879

H -1.230360 2.790988 -1.716088

H 1.134908 2.456147 -2.327193

H 0.528854 4.051068 -2.788799

H 0.641275 2.776710 -3.995711

C 0.217833 -3.063546 2.679884

N -1.162942 -3.431816 2.939851

H -1.303310 -4.427812 2.786117

H -1.409207 -3.251144 3.913910

H 0.956057 -3.585993 3.302805

H 0.350004 -1.991071 2.841199

H 0.462425 -3.265429 1.634288

C 0.132210 2.943535 2.713062

N -1.248567 2.575270 2.973032

H -1.388943 1.579277 2.819303

H -1.494826 2.755951 3.947091

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H 0.264380 4.016017 2.874381

H 0.376801 2.741659 1.667469

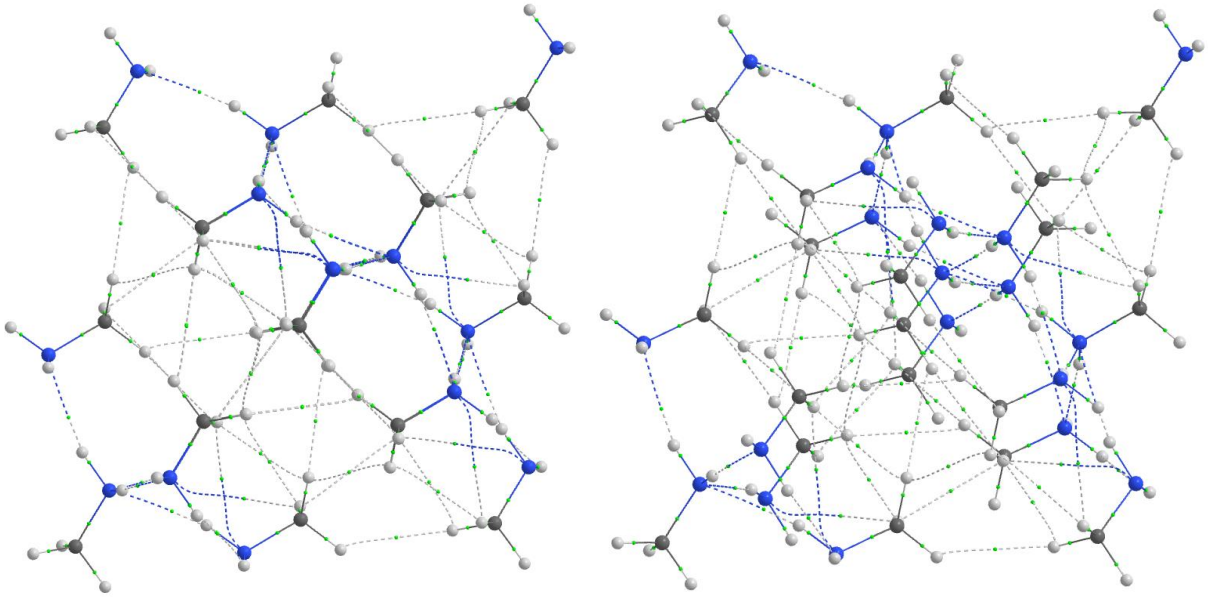

Figure S2. Atomic connectivity graph for the molecular cluster of aminomethane.

Butane

Structure was retrieved from: R. Boese, H. Weiss and D. Bläser, *Angew. Chem. Int. Ed.*, 1999, **38**(7), 988.

Parameters for the optimized crystal structure

Space group: $P2_1/c$

Unit cell parameters: 5.54835 5.90864 8.09094 90 121.259 90

Atom X Y Z (fractional coordinates):

C 0.22230 0.24018 0.42391

H 0.12508 0.31975 0.49699

H 0.05343 0.17272 0.28625

H 0.32907 0.37245 0.39123

C 0.42640 0.05495 0.54688

H 0.58539 0.12401 0.68767

H 0.31366 -0.07510 0.57713

Cartesian coordinates for the molecular cluster (optimized central molecule):

Atom X Y Z (Cartesian coordinates)

C -1.220641 1.419792 -0.525853

H -2.062967 1.894758 -0.018136

H -1.585674 1.019409 -1.475093

H -0.489416 2.198057 -0.758355

C -0.603446 0.326500 0.325841

H -0.307940 0.737484 1.297279

H -1.356392 -0.440166 0.540303

C 1.220641 -1.419792 0.525853

H 2.062967 -1.894758 0.018136

H 1.585674 -1.019409 1.475093

H 0.489416 -2.198057 0.758355

C 0.603446 -0.326500 -0.325841

H 0.307940 -0.737484 -1.297279

H 1.356392 0.440166 -0.540303

C -2.571176 1.419137 -7.442622

H -3.417412 1.889288 -6.937174

H -2.930162 1.020540 -8.394727

H -1.841572 2.200673 -7.668648

C -1.955046 0.324680 -6.592117

H -1.664019 0.732731 -5.618364

H -2.707571 -0.443739 -6.382898

C -0.128549 -1.419137 -6.390091

H 0.717687 -1.889288 -6.895538

H 0.230438 -1.020540 -5.437985

H -0.858152 -2.200673 -6.164064

C -0.744679 -0.324680 -7.240595

H -1.035706 -0.732731 -8.214349

H 0.007846 0.443739 -7.449815

C -6.769663 1.419137 -0.526265

H -7.615899 1.889288 -0.020818

H -7.128649 1.020540 -1.478371

H -6.040059 2.200673 -0.752292

C -6.153533 0.324680 0.324239

H -5.862506 0.732731 1.297993

H -6.906058 -0.443739 0.533459

C -4.327035 -1.419137 0.526266

H -3.480799 -1.889288 0.020818

H -3.968049 -1.020540 1.478371

H -5.056639 -2.200673 0.752292

C -4.943166 -0.324680 -0.324239

H -5.234193 -0.732731 -1.297992

H -4.190641 0.443739 -0.533458

C -6.769663 7.327778 -0.526265

H -7.615899 7.797928 -0.020818

H -7.128649 6.929181 -1.478371

H -6.040059 8.109314 -0.752292

C -6.153533 6.233320 0.324239

H -5.862506 6.641371 1.297993

H -6.906058 5.464902 0.533459

C -4.327035 4.489503 0.526266

H -3.480799 4.019353 0.020818

H -3.968049 4.888100 1.478371

H -5.056639 3.707967 0.752292

C -4.943166 5.583961 -0.324239

H -5.234193 5.175910 -1.297992

H -4.190641 6.352379 -0.533458

C -1.221313 -4.489503 -0.526265

H -2.067549 -4.019353 -0.020818

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H 0.314157 -6.641371 -1.297992

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H -0.491710 8.109314 -0.752292

C -0.605184 6.233320 0.324239

H -0.314157 6.641371 1.297992

H -1.357709 5.464902 0.533458

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H 2.067549 4.019353 0.020818

H 1.580300 4.888100 1.478371

H 0.491710 3.707967 0.752292

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H 0.314156 5.175910 -1.297993

H 1.357708 6.352379 -0.533459

C 4.327035 -4.489503 -0.526266

H 3.480799 -4.019353 -0.020818

H 3.968049 -4.888100 -1.478371

H 5.056639 -3.707967 -0.752292

C 4.943166 -5.583961 0.324239

H 5.234193 -5.175910 1.297992

H 4.190641 -6.352379 0.533458

C 6.769663 -7.327778 0.526265

H 7.615899 -7.797928 0.020818

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H 6.040059 -8.109314 0.752292

C 6.153533 -6.233320 -0.324239

H 5.862506 -6.641371 -1.297993

H 6.906058 -5.464902 -0.533459

C 4.327035 1.419137 -0.526266

H 3.480799 1.889288 -0.020818

H 3.968049 1.020540 -1.478371

H 5.056639 2.200673 -0.752292

C 4.943166 0.324680 0.324239

H 5.234193 0.732731 1.297992

H 4.190641 -0.443739 0.533458

C 6.769663 -1.419137 0.526265

H 7.615899 -1.889288 0.020818

H 7.128649 -1.020540 1.478371

H 6.040059 -2.200673 0.752292

C 6.153533 -0.324680 -0.324239

H 5.862506 -0.732731 -1.297993

H 6.906058 0.443739 -0.533459

C 0.128549 1.419137 6.390091

H -0.717687 1.889288 6.895538

H -0.230438 1.020540 5.437985

H 0.858152 2.200673 6.164064

C 0.744679 0.324680 7.240595

H 1.035706 0.732731 8.214349

H -0.007846 -0.443739 7.449815

C 2.571176 -1.419137 7.442622

H 3.417412 -1.889288 6.937174

H 2.930162 -1.020540 8.394727

H 1.841572 -2.200673 7.668648

C 1.955046 -0.324680 6.592117

H 1.664019 -0.732731 5.618364

H 2.707571 0.443739 6.382898

C -2.227792 -1.535183 -2.931912

H -1.381556 -1.065032 -3.437360

H -1.868806 -1.933780 -1.979807

H -2.957396 -0.753647 -2.705886

C -2.843922 -2.629640 -3.782417

H -3.134949 -2.221590 -4.756171

H -2.091397 -3.398059 -3.991637

C -4.670420 -4.373458 -3.984444

H -5.516656 -4.843608 -3.478996

H -5.029406 -3.974861 -4.936549

H -3.940816 -5.154993 -4.210470

C -4.054290 -3.279000 -3.133939

H -3.763262 -3.687051 -2.160185

H -4.806815 -2.510581 -2.924719

C -2.227792 4.373458 -2.931912

H -1.381556 4.843608 -3.437360

H -1.868806 3.974861 -1.979807

H -2.957396 5.154993 -2.705886

C -2.843922 3.279000 -3.782417

H -3.134949 3.687051 -4.756171

H -2.091397 2.510581 -3.991637

C -4.670420 1.535183 -3.984444

H -5.516656 1.065032 -3.478996

H -5.029406 1.933780 -4.936549

H -3.940816 0.753647 -4.210470

C -4.054290 2.629640 -3.133939

H -3.763262 2.221590 -2.160185

H -4.806815 3.398059 -2.924719

C 3.320558 -1.535183 -2.931912

H 4.166794 -1.065032 -3.437360

H 3.679544 -1.933780 -1.979807

H 2.590954 -0.753647 -2.705886

C 2.704428 -2.629640 -3.782417

H 2.413400 -2.221590 -4.756171

H 3.456953 -3.398059 -3.991637

C 0.877930 -4.373458 -3.984444

H 0.031694 -4.843608 -3.478996

H 0.518944 -3.974861 -4.936549

H 1.607534 -5.154993 -4.210470

C 1.494060 -3.279000 -3.133939

H 1.785087 -3.687051 -2.160185

H 0.741535 -2.510581 -2.924719

C -0.877929 -1.535183 3.984444

H -0.031693 -1.065032 3.478997

H -0.518943 -1.933780 4.936550

H -1.607533 -0.753647 4.210471

C -1.494059 -2.629640 3.133940

H -1.785087 -2.221590 2.160186

H -0.741534 -3.398059 2.924720

C -3.320557 -4.373458 2.931913

H -4.166793 -4.843608 3.437360

H -3.679543 -3.974861 1.979807

H -2.590953 -5.154993 2.705886

C -2.704427 -3.279000 3.782417

H -2.413399 -3.687051 4.756171

H -3.456952 -2.510581 3.991637

C 3.320557 4.373458 -2.931913

H 4.166793 4.843608 -3.437360

H 3.679543 3.974861 -1.979807

H 2.590953 5.154993 -2.705886

C 2.704427 3.279000 -3.782417

H 2.413399 3.687051 -4.756171

H 3.456952 2.510581 -3.991637

C 0.877929 1.535183 -3.984444

H 0.031693 1.065032 -3.478997

H 0.518943 1.933780 -4.936550

H 1.607533 0.753647 -4.210471

C 1.494059 2.629640 -3.133940

H 1.785087 2.221590 -2.160186

H 0.741534 3.398059 -2.924720

C -0.877930 4.373458 3.984444

H -0.031694 4.843608 3.478996

H -0.518944 3.974861 4.936549

H -1.607534 5.154993 4.210470

C -1.494060 3.279000 3.133939

H -1.785087 3.687051 2.160185

H -0.741535 2.510581 2.924719

C -3.320558 1.535183 2.931912

H -4.166794 1.065032 3.437360

H -3.679544 1.933780 1.979807

H -2.590954 0.753647 2.705886

C -2.704428 2.629640 3.782417

H -2.413400 2.221590 4.756171

H -3.456953 3.398059 3.991637

C 4.670420 -1.535183 3.984444

H 5.516656 -1.065032 3.478996

H 5.029406 -1.933780 4.936549

H 3.940816 -0.753647 4.210470

C 4.054290 -2.629640 3.133939

H 3.763262 -2.221590 2.160185

H 4.806815 -3.398059 2.924719

C 2.227792 -4.373458 2.931912

H 1.381556 -4.843608 3.437360

H 1.868806 -3.974861 1.979807

H 2.957396 -5.154993 2.705886

C 2.843922 -3.279000 3.782417

H 3.134949 -3.687051 4.756171

H 2.091397 -2.510581 3.991637

C 4.670420 4.373458 3.984444

H 5.516656 4.843608 3.478996

H 5.029406 3.974861 4.936549

H 3.940816 5.154993 4.210470

C 4.054290 3.279000 3.133939

H 3.763262 3.687051 2.160185

H 4.806815 2.510581 2.924719

C 2.227792 1.535183 2.931912

H 1.381556 1.065032 3.437360

H 1.868806 1.933780 1.979807

H 2.957396 0.753647 2.705886

C 2.843922 2.629640 3.782417

H 3.134949 2.221590 4.756171

H 2.091397 3.398059 3.991637

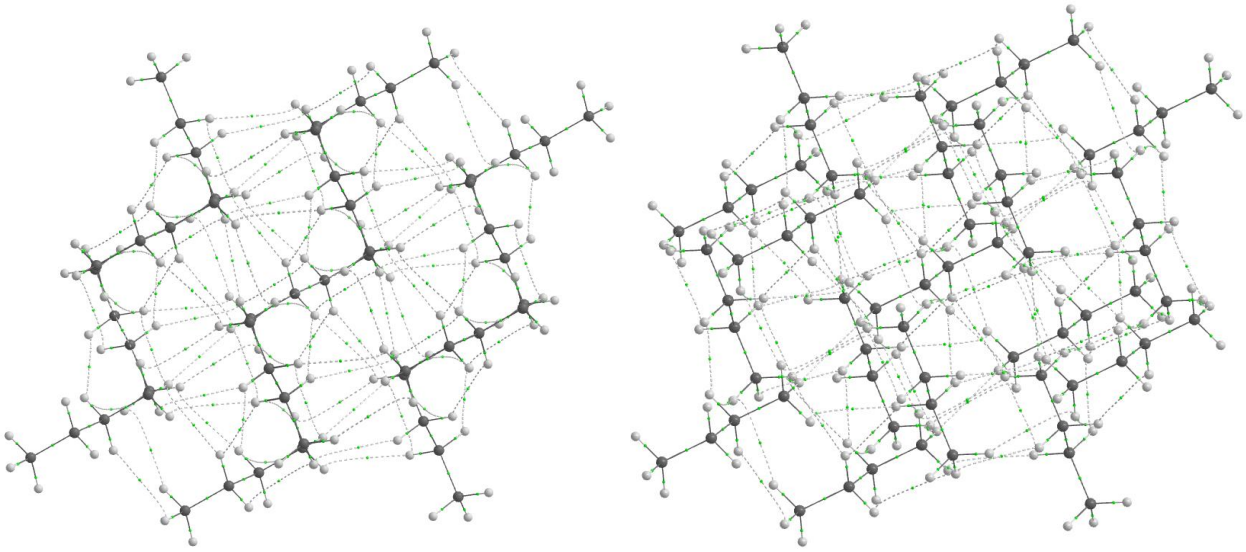

Figure S3. Atomic connectivity graph for the molecular cluster of butane.

Ethane

Structure was retrieved from: G. J. H. Nes and A. Vos, *Acta Cryst.*, 1979, **B35**, 2593.

Parameters for the optimized crystal structure

Space group: $P2_1/n$

Unit cell parameters: 4.15238 5.50878 5.78146 90 90.478 90

Atom X Y Z (fractional coordinates):

C -0.042359 0.097423 -0.087723

H 0.057347 0.056060 -0.257440

H 0.051638 0.274247 -0.034835

H -0.302685 0.115834 -0.109202

Cartesian coordinates for the molecular cluster (optimized central molecule):

Atom X Y Z (Cartesian coordinates)

C -0.160585 0.54012 -0.507102

H 0.266093 0.30875 -1.485584

H 0.237850 1.50821 -0.195787

H -1.238087 0.65647 -0.639360

C 0.160585 -0.54012 0.507102

H -0.266093 -0.30875 1.485584

H -0.237850 -1.50821 0.195787

H 1.238087 -0.65647 0.639360

C -4.324033 0.53668 -0.507149

H -3.901824 0.30882 -1.488326

H -3.936275 1.51076 -0.201390

H -5.403968 0.63810 -0.631325

C -3.980721 -0.53668 0.507149

H -4.402930 -0.30882 1.488326

H -4.368479 -1.51076 0.201390

H -2.900786 -0.63810 0.631325

C -0.171656 -4.97209 -0.507149

H 0.250553 -5.19995 -1.488326

H 0.216102 -3.99801 -0.201390

H -1.251591 -4.87067 -0.631325

C 0.171656 -6.04545 0.507149

H -0.250553 -5.81759 1.488326

H -0.216102 -7.01954 0.201390

H 1.251591 -6.14688 0.631325

C -0.123386 0.53668 -6.288404

H 0.298823 0.30882 -7.269581

H 0.264372 1.51076 -5.982645

H -1.203321 0.63810 -6.412580

C 0.219926 -0.53668 -5.274106

H -0.202283 -0.30882 -4.292929

H -0.167832 -1.51076 -5.579865

H 1.299861 -0.63810 -5.149930

C -0.219926 0.53668 5.274106

H 0.202283 0.30882 4.292929

H 0.167832 1.51076 5.579865

H -1.299861 0.63810 5.149930

C 0.123386 -0.53668 6.288404

H -0.298823 -0.30882 7.269581

H -0.264372 -1.51076 5.982645

H 1.203321 -0.63810 6.412580

C -0.171656 6.04545 -0.507149

H 0.250553 5.81759 -1.488326

H 0.216102 7.01954 -0.201390

H -1.251591 6.14688 -0.631325

C 0.171656 4.97209 0.507149

H -0.250553 5.19995 1.488326

H -0.216102 3.99801 0.201390

H 1.251591 4.87067 0.631325

C 3.980721 0.53668 -0.507149

H 4.402930 0.30882 -1.488326

H 4.368479 1.51076 -0.201390

H 2.900786 0.63810 -0.631325

C 4.324033 -0.53668 0.507149

H 3.901824 -0.30882 1.488326

H 3.936275 -1.51076 0.201390

H 5.403968 -0.63810 0.631325

C -1.880397 -2.21770 -2.383478

H -2.302606 -2.44556 -1.402301

H -2.268155 -1.24362 -2.689237

H -0.800462 -2.11628 -2.259303

C -2.223710 -3.29107 -3.397777

H -1.801501 -3.06321 -4.378954

H -1.835952 -4.26515 -3.092018

H -3.303644 -3.39249 -3.521952

C -1.928667 -2.21770 3.397777

H -2.350876 -2.44556 4.378954

H -2.316425 -1.24362 3.092018

H -0.848732 -2.11628 3.521952

C -2.271979 -3.29107 2.383478

H -1.849770 -3.06321 1.402301

H -1.884221 -4.26515 2.689237

H -3.351914 -3.39249 2.259303

C -1.880397 3.29107 -2.383478

H -2.302606 3.06321 -1.402301

H -2.268155 4.26515 -2.689237

H -0.800462 3.39249 -2.259303

C -2.223710 2.21770 -3.397777

H -1.801501 2.44556 -4.378954

H -1.835952 1.24362 -3.092018

H -3.303644 2.11628 -3.521952

C -1.928667 3.29107 3.397777

H -2.350876 3.06321 4.378954

H -2.316425 4.26515 3.092018

H -0.848732 3.39249 3.521952

C -2.271979 2.21770 2.383478

H -1.849770 2.44556 1.402301

H -1.884221 1.24362 2.689237

H -3.351914 2.11628 2.259303

C 2.271979 -2.21770 -2.383478

H 1.849770 -2.44556 -1.402301

H 1.884221 -1.24362 -2.689237

H 3.351914 -2.11628 -2.259303

C 1.928667 -3.29107 -3.397777

H 2.350876 -3.06321 -4.378954

H 2.316425 -4.26515 -3.092018

H 0.848732 -3.39249 -3.521952

C 2.223710 -2.21770 3.397777

H 1.801501 -2.44556 4.378954

H 1.835952 -1.24362 3.092018

H 3.303644 -2.11628 3.521952

C 1.880397 -3.29107 2.383478

H 2.302606 -3.06321 1.402301

H 2.268155 -4.26515 2.689237

H 0.800462 -3.39249 2.259303

C 2.271979 3.29107 -2.383478

H 1.849770 3.06321 -1.402301

H 1.884221 4.26515 -2.689237

H 3.351914 3.39249 -2.259303

C 1.928667 2.21770 -3.397777

H 2.350876 2.44556 -4.378954

H 2.316425 1.24362 -3.092018

H 0.848732 2.11628 -3.521952

C 2.223710 3.29107 3.397777

H 1.801501 3.06321 4.378954

H 1.835952 4.26515 3.092018

H 3.303644 3.39249 3.521952

C 1.880397 2.21770 2.383478

H 2.302606 2.44556 1.402301

H 2.268155 1.24362 2.689237

H 0.800462 2.11628 2.259303

C -4.324033 -4.97209 -0.507149

H -3.901824 -5.19995 -1.488326

H -3.936275 -3.99801 -0.201390

H -5.403968 -4.87067 -0.631325

C -3.980721 -6.04545 0.507149

H -4.402930 -5.81759 1.488326

H -4.368479 -7.01954 0.201390

H -2.900786 -6.14688 0.631325

C 3.980721 6.04545 -0.507149

H 4.402930 5.81759 -1.488326

H 4.368479 7.01954 -0.201390

H 2.900786 6.14688 -0.631325

C 4.324033 4.97209 0.507149

H 3.901824 5.19995 1.488326

H 3.936275 3.99801 0.201390

H 5.403968 4.87067 0.631325

C -4.372303 0.53668 5.274106

H -3.950094 0.30882 4.292929

H -3.984545 1.51076 5.579865

H -5.452238 0.63810 5.149930

C -4.028990 -0.53668 6.288404

H -4.451199 -0.30882 7.269581

H -4.416748 -1.51076 5.982645

H -2.949056 -0.63810 6.412580

C -4.324033 6.04545 -0.507149

H -3.901824 5.81759 -1.488326

H -3.936275 7.01954 -0.201390

H -5.403968 6.14688 -0.631325

C -3.980721 4.97209 0.507149

H -4.402930 5.19995 1.488326

H -4.368479 3.99801 0.201390

H -2.900786 4.87067 0.631325

C 3.980721 -4.97209 -0.507149

H 4.402930 -5.19995 -1.488326

H 4.368479 -3.99801 -0.201390

H 2.900786 -4.87067 -0.631325

C 4.324033 -6.04545 0.507149

H 3.901824 -5.81759 1.488326

H 3.936275 -7.01954 0.201390

H 5.403968 -6.14688 0.631325

C 4.028990 0.53668 -6.288404

H 4.451199 0.30882 -7.269581

H 4.416748 1.51076 -5.982645

H 2.949056 0.63810 -6.412580

C 4.372303 -0.53668 -5.274106

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H 3.984545 -1.51076 -5.579865

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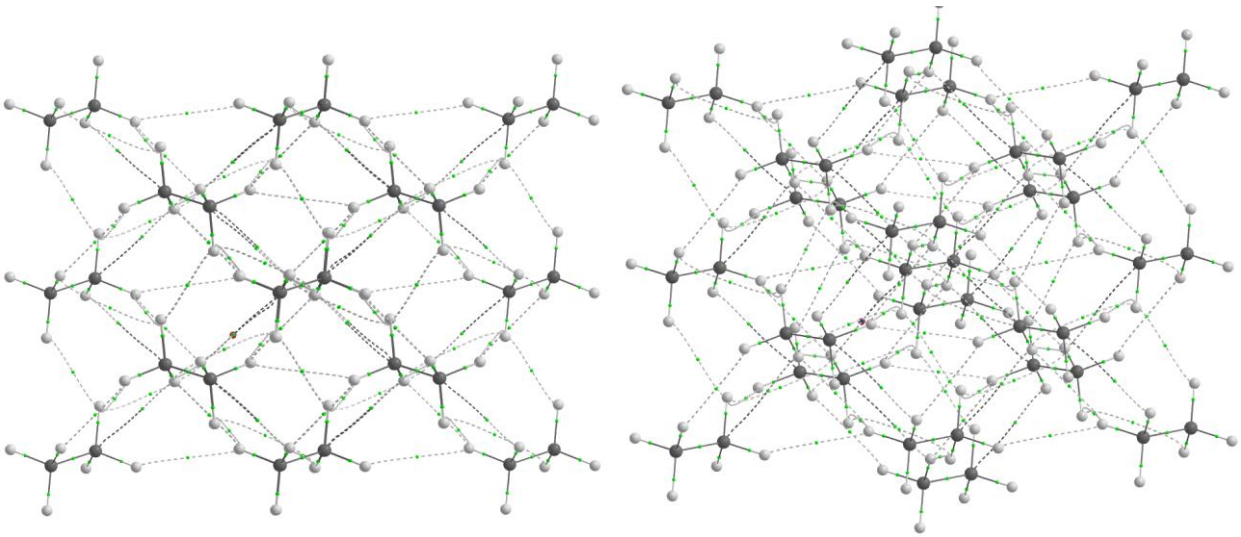

Figure S4. Atomic connectivity graph for the molecular cluster of ethane.

Ethene

Structure was retrieved from: G. J. H. Nes and A. Vos, *Acta Cryst.*, 1979, **B35**, 2593.

Parameters for the optimized crystal structure

Space group: $P2_1/n$

Unit cell parameters: 4.49827 6.44789 3.97306 90 92.557 90

Atom X Y Z (fractional coordinates):

C -0.120397 0.054985 -0.041450

H -0.201835 0.175124 0.122056

H -0.246390 0.029198 -0.276721

Cartesian coordinates for the molecular cluster (optimized central molecule):

Atom X Y Z (Cartesian coordinates)

C -0.527634 0.359901 -0.174363

H -0.932188 1.134593 0.469167

H -1.031909 0.203471 -1.121404

C 0.527634 -0.359901 0.174363

H 0.932188 -1.134593 -0.469167

H 1.031909 -0.203471 1.121404

C -4.855220 0.354537 -4.133623

H -5.250536 1.129181 -3.484651

H -5.380262 0.188266 -5.067438

C -3.786760 -0.354537 -3.804585

H -3.391444 -1.129181 -4.453557

H -3.261718 -0.188266 -2.870770

C -5.032498 0.354537 -0.164519

H -5.427814 1.129181 0.484453

H -5.557540 0.188266 -1.098334

C -3.964038 -0.354537 0.164519

H -3.568722 -1.129181 -0.484453

H -3.438996 -0.188266 1.098334

C -0.356952 0.354537 -4.133623

H -0.752270 1.129180 -3.484652

H -0.881994 0.188266 -5.067438

C 0.711510 -0.354540 -3.804585

H 1.106824 -1.129181 -4.453557

H 1.236544 -0.188261 -2.870773

C -0.711510 0.354540 3.804585

H -1.106824 1.129181 4.453557

H -1.236544 0.188261 2.870773

C 0.356952 -0.354537 4.133623

H 0.752270 -1.129180 3.484652

H 0.881994 -0.188266 5.067438

C 3.964038 0.354537 -0.164519

H 3.568722 1.129181 0.484453

H 3.438996 0.188266 -1.098334

C 5.032498 -0.354537 0.164519

H 5.427814 -1.129181 -0.484453

H 5.557540 -0.188266 1.098334

C 3.786760 0.354537 3.804585

H 3.391444 1.129181 4.453557

H 3.261718 0.188266 2.870770

C 4.855220 -0.354537 4.133623

H 5.250536 -1.129181 3.484651

H 5.380262 -0.188266 5.067438

C -1.626264 -2.869410 -1.820034

H -1.230948 -2.094767 -2.469007

H -1.101223 -3.035682 -0.886217

C -2.694725 -3.578484 -2.149071

H -3.090041 -4.353128 -1.500099

H -3.219767 -3.412212 -3.082886

C -1.803542 -2.869409 2.149071

H -1.408224 -2.094766 1.500099

H -1.278501 -3.035681 3.082886

C -2.872003 -3.578484 1.820033

H -3.267319 -4.353128 2.469005

H -3.397045 -3.412212 0.886218

C -1.626262 3.578484 -1.820035

H -1.230949 4.353128 -2.469005

H -1.101214 3.412214 -0.886217

C -2.694725 2.869409 -2.149071

H -3.090042 2.094766 -1.500098

H -3.219767 3.035681 -3.082886

C -1.803543 3.578484 2.149071

H -1.408228 4.353128 1.500099

H -1.278501 3.412212 3.082886

C -2.872003 2.869409 1.820032

H -3.267320 2.094765 2.469005

H -3.397045 3.035681 0.886218

C 2.872003 -2.869409 -1.820032

H 3.267320 -2.094765 -2.469005

H 3.397045 -3.035681 -0.886218

C 1.803543 -3.578484 -2.149071

H 1.408228 -4.353128 -1.500099

H 1.278501 -3.412212 -3.082886

C 2.694725 -2.869409 2.149071

H 3.090042 -2.094766 1.500098

H 3.219767 -3.035681 3.082886

C 1.626262 -3.578484 1.820035

H 1.230949 -4.353128 2.469005

H 1.101214 -3.412214 0.886217

C 2.872003 3.578484 -1.820033

H 3.267319 4.353128 -2.469005

H 3.397045 3.412212 -0.886218

C 1.803542 2.869409 -2.149071

H 1.408224 2.094766 -1.500099

H 1.278501 3.035681 -3.082886

C 2.694725 3.578484 2.149071

H 3.090041 4.353128 1.500099

H 3.219767 3.412212 3.082886

C 1.626264 2.869410 1.820034

H 1.230948 2.094767 2.469007

H 1.101223 3.035682 0.886217

C -5.209776 0.354537 3.804585

H -5.605092 1.129181 4.453557

H -5.734818 0.188266 2.870770

C -4.141316 -0.354537 4.133623

H -3.746000 -1.129181 3.484651

H -3.616274 -0.188266 5.067438

C 4.141316 0.354537 -4.133623

H 3.746000 1.129181 -3.484651

H 3.616274 0.188266 -5.067438

C 5.209776 -0.354537 -3.804585

H 5.605092 -1.129181 -4.453557

H 5.734818 -0.188266 -2.870770

C -0.534230 -6.093356 -0.164519

H -0.929545 -5.318712 0.484452

H -1.059272 -6.259628 -1.098334

C 0.534230 -6.802431 0.164519

H 0.929546 -7.577074 -0.484453

H 1.059272 -6.636159 1.098334

C -0.534230 6.802431 -0.164519

H -0.929546 7.577074 0.484453

H -1.059272 6.636159 -1.098334

C 0.534230 6.093356 0.164519

H 0.929545 5.318712 -0.484452

H 1.059272 6.259628 1.098334

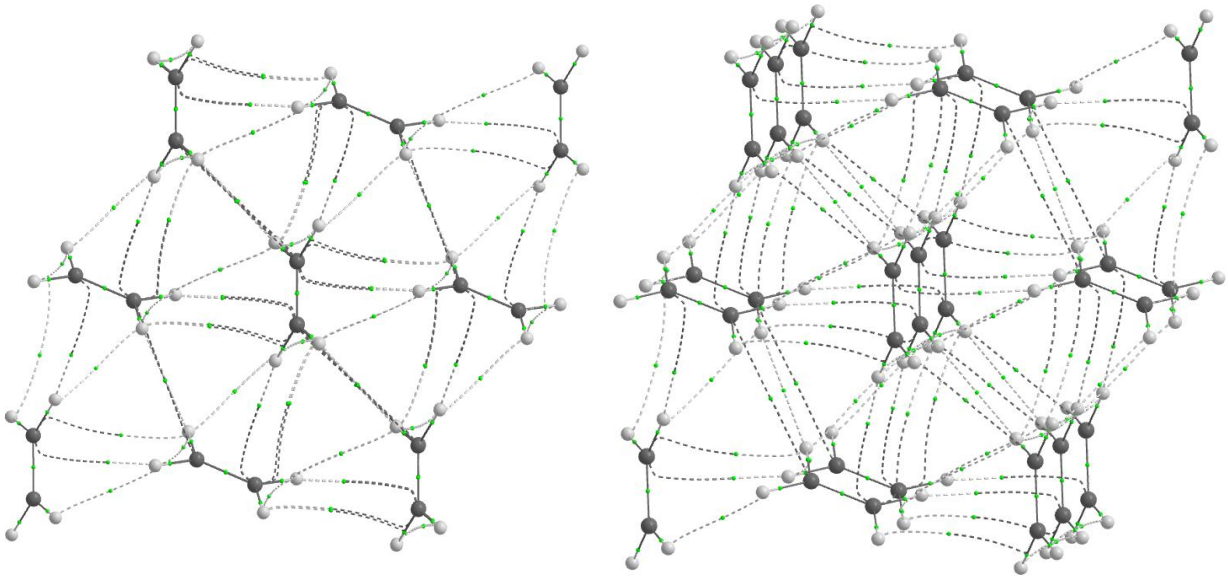

Figure S5. Atomic connectivity graph for the molecular cluster of ethene.

Formic acid

Structure was retrieved from: I. Nahringbauer, *Acta Cryst.*, 1978, **B34**, 315.

Parameters for the optimized crystal structure

Space group: $Pna2_1$

Unit cell parameters: 10.39583 3.60093 5.32204 90 90 90

Atom X Y Z (fractional coordinates):

C 0.161767 0.378430 0.165489

O 0.090511 0.205761 0.003363

O 0.278187 0.414518 0.144753

H 0.145051 0.102688 -0.139196

H 0.107587 0.492748 0.323849

Cartesian coordinates for the molecular cluster (optimized central molecule):

Atom X Y Z (Cartesian coordinates)

C 0.347892 -0.025677 0.165928

O -0.779840 0.619922 0.032649

O 0.418568 -1.242412 0.124445

H -1.525545 -0.040474 -0.080249

H 1.214351 0.627617 0.308655

C -6.049470 -0.752040 -0.306451

O -7.180447 -0.128689 -0.416649

O -5.931746 -1.966414 -0.379154

H -7.942493 -0.788728 -0.552672

H -5.196667 -0.084878 -0.149504

C -1.933662 -0.067195 2.997361

O -3.064640 0.556156 2.887162

O -1.815938 -1.281569 2.924658

H -3.826685 -0.103882 2.751139

H -1.080859 0.599967 3.154308

C -3.795475 -0.750746 -3.114690

O -4.926453 -0.127396 -3.224889

O -3.677752 -1.965120 -3.187394

H -5.688499 -0.787434 -3.360911

H -2.942673 -0.083584 -2.957743

C 4.436141 0.618944 3.492933

O 3.305163 1.242295 3.382733

O 4.553865 -0.595430 3.420230

H 2.543117 0.582257 3.246711

H 5.288943 1.286106 3.649880

C 2.574327 -0.064607 -2.619119

O 1.443350 0.558743 -2.729318

O 2.692051 -1.278981 -2.691821

H 0.681304 -0.101295 -2.865340

H 3.427130 0.602555 -2.462171

C 6.690136 0.620238 0.684693

O 5.559157 1.243589 0.574494

O 6.807859 -0.594136 0.611991

H 4.797112 0.583550 0.438471

H 7.542938 1.287400 0.841640

C -4.934053 -2.229522 2.896831

O -5.916024 -3.075383 2.905553

O -5.059783 -1.043457 2.629830

H -6.792121 -2.610873 2.678507

H -3.967952 -2.679485 3.144201

C -2.680058 -2.228228 0.088591

O -3.662029 -3.074089 0.097313

O -2.805788 -1.042163 -0.178410

H -4.538127 -2.609580 -0.129733

H -1.713958 -2.678192 0.335961

C 1.435750 -1.543383 3.392402

O 0.453779 -2.389244 3.401125

O 1.310019 -0.357318 3.125402

H -0.422318 -1.924734 3.174079

H 2.401850 -1.993346 3.639773

C -0.426064 -2.226935 -2.719649

O -1.408035 -3.072796 -2.710926

O -0.551794 -1.040869 -2.986650

H -2.284132 -2.608286 -2.937973

H 0.540037 -2.676898 -2.472278

C 3.689744 -1.542089 0.584162

O 2.707774 -2.387950 0.592886

O 3.564014 -0.356024 0.317162

H 1.831676 -1.923440 0.365839

H 4.655845 -1.992053 0.831533

C 5.943738 -1.540796 -2.224077

O 4.961768 -2.386656 -2.215353

O 5.818009 -0.354730 -2.491078

H 4.085671 -1.922147 -2.442400

H 6.909839 -1.990759 -1.976707

C -0.781418 5.088463 0.493210

O -1.134006 5.712261 -0.586781

O -0.826378 3.873996 0.623195

H -1.431400 5.052490 -1.301710

H -0.443960 5.755330 1.292222

C 1.472577 5.089757 -2.315030

O 1.119988 5.713555 -3.395020

O 1.427616 3.875289 -2.185045

H 0.822595 5.053784 -4.109950

H 1.810035 5.756624 -1.516017

C 0.264162 -5.220931 1.327681

O -0.088426 -4.597132 0.247690

O 0.219202 -6.435398 1.457666

H -0.385820 -5.256904 -0.467240

H 0.601620 -4.554063 2.126693

C 2.518156 -5.219637 -1.480559

O 2.165568 -4.595839 -2.560550

O 2.473196 -6.434104 -1.350574

H 1.868175 -5.255610 -3.275480

H 2.855615 -4.552770 -0.681547

C -3.781809 2.926136 0.392680

O -3.985391 2.080722 -0.568389

O -4.070224 4.112108 0.328367

H -4.396836 2.545499 -1.374343

H -3.331053 2.475878 1.282115

C 0.333999 3.610981 3.696491

O 0.130418 2.765568 2.735423

O 0.045584 4.796953 3.632178

H -0.281027 3.230344 1.929469

H 0.784755 3.160723 4.585926

C -1.527815 2.927429 -2.415560

O -1.731396 2.082016 -3.376629

O -1.816229 4.113401 -2.479873

H -2.142842 2.546793 -4.182582

H -1.077059 2.477171 -1.526124

C 2.587993 3.612275 0.888251

O 2.384413 2.766862 -0.072817

O 2.299579 4.798247 0.823938

H 1.972967 3.231638 -0.878770

H 3.038749 3.162017 1.777687

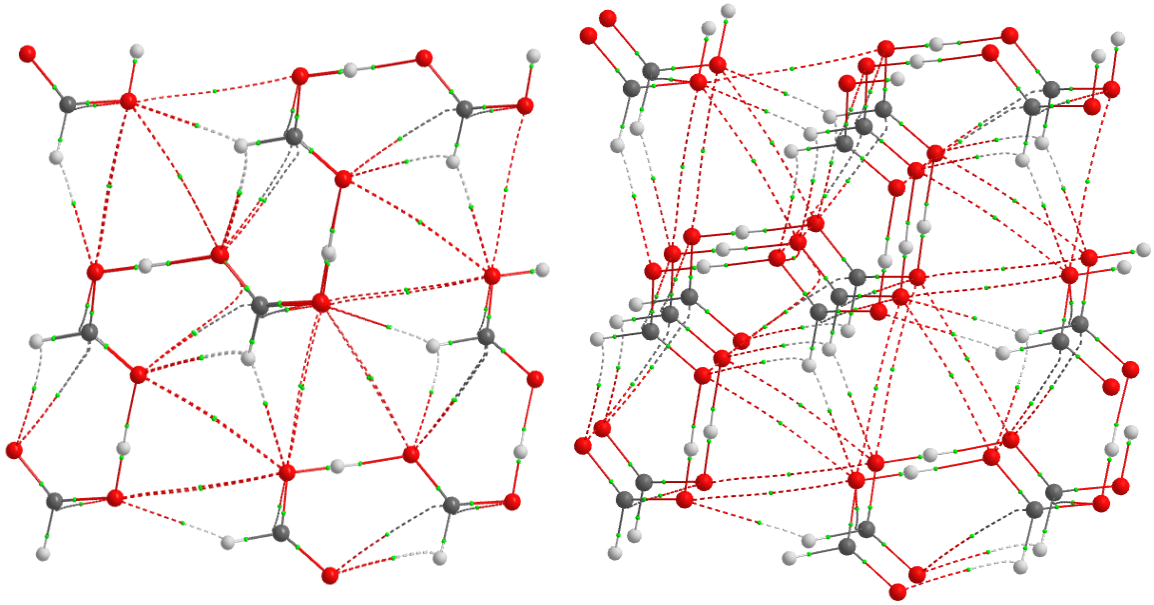

Figure S6. Atomic connectivity graph for the molecular cluster of formic acid.

Formaldehyde

Structure was retrieved from: T. Thakur, M. Kirchner, D. Bläser, R. Boese and G. Desiraju, *Phys. Chem. Chem. Phys.*, 2011, **13**, 14076.

Parameters for the optimized crystal structure

Space group: P-42_1c

Unit cell parameters: 8.12138 8.12138 4.60071 90 90 90

Atom X Y Z (fractional coordinates):

O 0.23587 0.05430 0.36996

C 0.24670 0.00965 0.62007

H 0.34269 -0.07723 0.69000

H 0.16446 0.05812 0.78957

Cartesian coordinates for the molecular cluster (optimized central molecule):

Atom X Y Z (Cartesian coordinates)

O -0.918851 -0.043429 0.494076

C 0.235449 0.068096 0.150655

H 0.579345 0.941265 -0.422953

H 0.994177 -0.677159 0.431624

O -5.543755 0.098666 0.394750

C -4.385631 0.209775 0.063533

H -4.034890 1.075292 -0.516942

H -3.627653 -0.527316 0.365747

O 3.654081 -0.129421 0.512427

C 4.812205 -0.018312 0.181210

H 5.162947 0.847205 -0.399265

H 5.570184 -0.755403 0.483424

O -5.616255 -3.562723 -1.035216

C -4.473908 -3.730879 -0.674566

H -4.181446 -4.612346 -0.085863

H -3.672854 -3.032449 -0.956835

O -1.017337 -3.676767 -0.976377

C 0.125010 -3.844923 -0.615728

H 0.417473 -4.726389 -0.027024

H 0.926064 -3.146493 -0.897996

O 3.581581 -3.790810 -0.917539

C 4.723929 -3.958966 -0.556889

H 5.016391 -4.840433 0.031814

H 5.524983 -3.260536 -0.839158

O -5.432176 4.470122 0.146458

C -4.289829 4.301966 0.507108

H -3.997367 3.420500 1.095812

H -3.488774 5.000397 0.224840

O -0.833258 4.356079 0.205297

C 0.309089 4.187923 0.565946

H 0.601552 3.306456 1.154650

H 1.110144 4.886354 0.283678

O 3.765660 4.242035 0.264135

C 4.908008 4.073879 0.624785

H 5.200470 3.192413 1.213488

H 5.709063 4.772310 0.342516

O -4.342783 -1.047448 -2.135811

C -5.499807 -1.364824 -2.290301

H -5.824730 -1.941583 -3.168289

H -6.281259 -1.053091 -1.582259

O 0.256135 -1.161491 -2.076973

C -0.900889 -1.478868 -2.231462

H -1.225811 -2.055627 -3.109451

H -1.682341 -1.167134 -1.523421

O 4.855054 -1.275535 -2.018134

C 3.698029 -1.592911 -2.172624

H 3.373107 -2.169670 -3.050613

H 2.916577 -1.281178 -1.464582

O -4.425055 -2.475930 1.525951

C -5.568500 -2.101507 1.651009

H -5.886783 -1.508798 2.520768

H -6.346082 -2.374580 0.923021

O 0.173863 -2.589974 1.584789

C -0.969583 -2.215551 1.709847

H -1.287864 -1.622841 2.579606

H -1.747164 -2.488623 0.981859

O 4.772782 -2.704017 1.643628

C 3.629336 -2.329594 1.768685

H 3.311053 -1.736885 2.638445

H 2.851754 -2.602667 1.040697

O -1.976996 0.828423 -3.544275

C -3.123330 0.822586 -3.930520

H -3.451132 0.161908 -4.746081

H -3.894107 1.445399 -3.453890

O 2.621922 0.714380 -3.485437

C 1.475588 0.708543 -3.871682

H 1.147787 0.047865 -4.687243

H 0.704811 1.331356 -3.395051

O -2.109019 -0.350437 4.490008

C -3.255353 -0.356274 4.103763

H -3.583156 -1.016952 3.288202

H -4.026130 0.266539 4.580393

O 2.489899 -0.464481 4.548846

C 1.343565 -0.470317 4.162601

H 1.015763 -1.130995 3.347040

H 0.572787 0.152496 4.639232

O 2.539018 -3.401028 -4.982191

C 1.384881 -3.338145 -4.625379

H 1.069479 -2.661516 -3.818047

H 0.596625 -3.922297 -5.121955

O 2.406994 -4.579888 3.052092

C 1.252858 -4.517005 3.408904

H 0.937456 -3.840377 4.216237

H 0.464602 -5.101157 2.912328

O 2.723097 4.631818 -3.800517

C 1.568961 4.694701 -3.443705

H 1.253559 5.371330 -2.636372

H 0.780705 4.110550 -3.940281

O 2.591074 3.452958 4.233766

C 1.436937 3.515841 4.590578

H 1.121535 4.192470 5.397911

H 0.648681 2.931690 4.094002

O -3.233373 1.479817 2.357954

C -2.073489 1.822727 2.338420

H -1.723220 2.625804 1.673988

H -1.313752 1.317095 2.951858

O 1.365545 1.365773 2.416792

C 2.525429 1.708684 2.397259

H 2.875697 2.511760 1.732827

H 3.285166 1.203051 3.010696

O -3.143640 2.974928 -1.757907

C -2.003053 2.574971 -1.708941

H -1.710116 1.755944 -1.036280

H -1.203757 3.041943 -2.302432

O 1.455278 2.860885 -1.699069

C 2.595865 2.460927 -1.650103

H 2.888802 1.641901 -0.977442

H 3.395161 2.927899 -2.243594

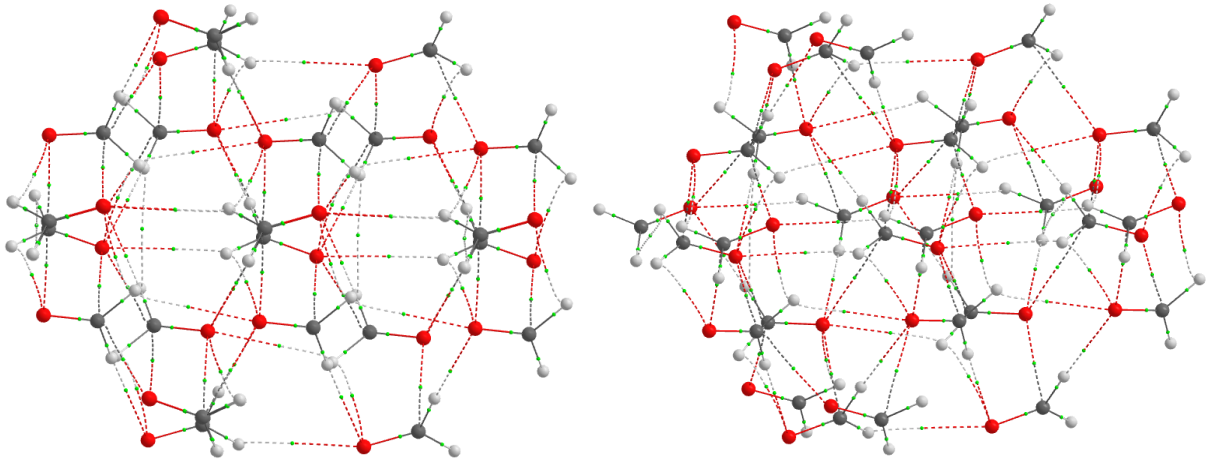

Figure S7. Atomic connectivity graph for the molecular cluster of formaldehyde.

Formamide

Structure was retrieved from: T. Ottersen, *Acta Chem. Scand. A*, 1975, **29**, 939.

Parameters for the optimized crystal structure

Space group: $P2_1/c$

Unit cell parameters: 3.61203 8.97549 8.38678 90 125.285 90

Atom X Y Z (fractional coordinates):

C -0.40671 0.05167 0.25833

H -0.64069 0.13031 -0.01138

H -0.66696 0.25472 0.14682

H -0.36821 0.08631 0.39284

N -0.58859 0.15311 0.11957

O -0.27755 -0.07334 0.24734

Cartesian coordinates for the molecular cluster (optimized central molecule):

Atom X Y Z (Cartesian coordinates)

C 0.087265 0.106759 -0.077976

H 1.265704 1.745046 -0.269737

H 2.033452 0.301100 0.418518

H 0.131415 -0.927944 0.288912

N 1.214366 0.774007 0.039651

O -0.960163 0.550385 -0.570157

C 1.842954 6.811789 -0.373255

H 3.004509 8.462444 -0.589250

H 3.787527 7.028417 0.112285

H 1.897138 5.783343 0.009826

N 2.963875 7.493012 -0.267968

O 0.790910 7.236709 -0.870657

C -0.018065 -0.382309 3.515135

H 1.143490 1.268347 3.299140

H 1.926509 -0.165680 4.000675

H 0.036119 -1.410755 3.898215

N 1.102857 0.298915 3.620421

O -1.070108 0.042612 3.017732

C 0.179085 0.561791 -3.644247

H 1.340640 2.212446 -3.860242

H 2.123658 0.778419 -3.158707

H 0.233269 -0.466656 -3.261167

N 1.300006 1.243014 -3.538961

O -0.872958 0.986711 -4.141650

C -1.681933 -6.632308 0.244143

H -0.520378 -4.981651 0.028148

H 0.262640 -6.415678 0.729684

H -1.627749 -7.660753 0.627224

N -0.561012 -5.951084 0.349430

O -2.733977 -6.207387 -0.253259

C -4.346019 0.788928 4.148985

H -4.142205 -1.220157 4.355313

H -2.765183 -0.353170 3.638484

H -3.798774 1.659490 3.761647

N -3.705711 -0.354642 4.031229

O -5.464433 0.933782 4.661755

C 4.335116 -1.489988 4.087522

H 4.538929 -3.499073 4.293850

H 5.915951 -2.632086 3.577021

H 4.882361 -0.619426 3.700183

N 4.975424 -2.633558 3.969766

O 3.216703 -1.345134 4.600292

C -4.247444 1.260978 0.569294

H -4.043631 -0.748107 0.775622

H -2.666608 0.118880 0.058794

H -3.700199 2.131540 0.181956

N -3.607136 0.117408 0.451538

O -5.365858 1.405832 1.082063

C 4.433690 -1.017939 0.507830

H 4.637504 -3.027023 0.714159

H 6.014526 -2.160036 -0.002669

H 4.980936 -0.147376 0.120493

N 5.073998 -2.161508 0.390074

O 3.315278 -0.873084 1.020600

C -4.148869 1.733027 -3.010397

H -3.945056 -0.276057 -2.804068

H -2.568033 0.590930 -3.520898

H -3.601624 2.603589 -3.397735

N -3.508561 0.589457 -3.128153

O -5.267283 1.877882 -2.497627

C 4.532265 -0.545889 -3.071860

H 4.736079 -2.554974 -2.865532

H 6.113101 -1.687986 -3.582361

H 5.079510 0.324673 -3.459199

N 5.172573 -1.689459 -3.189616

O 3.413853 -0.401035 -2.559090

C 0.027949 3.482021 2.180410

H -1.133606 1.831365 2.396405

H -1.916624 3.265393 1.694869

H -0.026235 4.510468 1.797330

N -1.092972 2.800798 2.075123

O 1.079993 3.057101 2.677812

C 0.126524 3.954071 -1.399281

H -1.035031 2.303415 -1.183286

H -1.818049 3.737442 -1.884821

H 0.072340 4.982517 -1.782361

N -0.994397 3.272848 -1.504567

O 1.178568 3.529150 -0.901878

C -1.734494 -3.240027 2.489109

H -2.896049 -4.890682 2.705104

H -3.679067 -3.456655 2.003569

H -1.788679 -2.211581 2.106028

N -2.855416 -3.921250 2.383823

O -0.682451 -3.664947 2.986512

C -1.635920 -2.767977 -1.090582

H -2.797474 -4.418633 -0.874587

H -3.580493 -2.984605 -1.576122

H -1.690104 -1.739531 -1.473662

N -2.756841 -3.449200 -1.195868

O -0.583876 -3.192897 -0.593179

C -1.537345 -2.295927 -4.670273

H -2.698900 -3.946583 -4.454278

H -3.481918 -2.512556 -5.155813

H -1.591529 -1.267482 -5.053354

N -2.658266 -2.977150 -4.775559

O -0.485301 -2.720847 -4.172870

C -4.325231 4.589701 1.608023

H -4.529044 6.598785 1.401695

H -5.906067 5.731798 2.118524

H -4.872476 3.719139 1.995361

N -4.965539 5.733271 1.725780

O -3.206818 4.444847 1.095254

C 4.355903 2.310785 1.546560

H 4.152090 4.319869 1.340232

H 2.775068 3.452882 2.057060

H 3.808658 1.440223 1.933898

N 3.715595 3.454354 1.664316

O 5.474317 2.165930 1.033791

C 4.454478 2.782834 -2.033131

H 4.250665 4.791919 -2.239459

H 2.873642 3.924932 -1.522630

H 3.907233 1.912272 -1.645792

N 3.814170 3.926404 -1.915375

O 5.572892 2.637980 -2.545901

C 2.593460 -4.411263 1.855260

H 2.389646 -2.402180 1.648931

H 1.012624 -3.269167 2.365759

H 2.046215 -5.281825 2.242598

N 1.953152 -3.267693 1.973015

O 3.711874 -4.556118 1.342490

C -5.989100 -1.660297 -1.662969

H -6.192913 0.348786 -1.869296

H -7.569936 -0.518201 -1.152468

H -6.536345 -2.530859 -1.275630

N -6.629408 -0.516727 -1.545213

O -4.870687 -1.805151 -2.175738

C 2.692035 -3.939213 -1.724432

H 2.488221 -1.930130 -1.930759

H 1.111199 -2.797117 -1.213931

H 2.144790 -4.809776 -1.337093

N 2.051727 -2.795644 -1.606676

O 3.810449 -4.084068 -2.237202

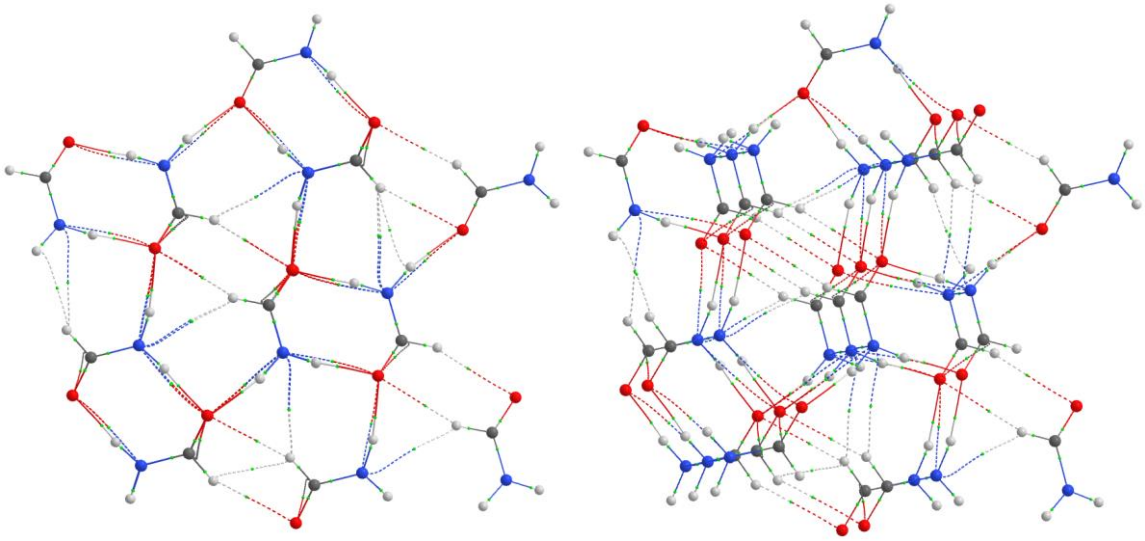

Figure S8. Atomic connectivity graph for the molecular cluster of formamide.

H2O2

Structure was retrieved from: W. Busing and H. Levy, *J. Chem. Phys.*, 1965, **42**, 3054.

Parameters for the optimized crystal structure

Space group: $P4_12_12$

Unit cell parameters: 4.05696 4.05696 7.72078 90 90 90

Atom X Y Z (fractional coordinates):

O 0.058509 0.175569 0.220334

H -0.060995 0.293640 0.127645

Cartesian coordinates for the molecular cluster (optimized central molecule):

Atom X Y Z (Cartesian coordinates)

O -0.707386 -0.054042 -0.626395

H -0.873836 -0.758687 0.046272

O 0.707387 0.054043 -0.626399

H 0.873840 0.758686 0.046269

O 4.823689 -1.564599 -0.644868

H 4.637828 -2.255686 0.036666

O 6.240093 -1.479157 -0.644868

H 6.425954 -0.788071 0.036666

O 2.057743 -0.803660 2.223840

H 1.871882 -1.494746 2.905373

O 3.474148 -0.718218 2.223840

H 3.660008 -0.027131 2.905373

O 2.057743 -0.803661 -3.513575

H 1.871882 -1.494747 -2.832042

O 3.474148 -0.718218 -3.513575

H 3.660008 -0.027132 -2.832042

O -3.474148 0.718218 2.223839

H -3.660009 0.027132 2.905373

O -2.057743 0.803660 2.223839

H -1.871883 1.494747 2.905373

O -3.474148 0.718217 -3.513576

H -3.660008 0.027131 -2.832042

O -2.057743 0.803660 -3.513576

H -1.871882 1.494746 -2.832042

O -6.240093 1.479157 -0.644868

H -6.425954 0.788070 0.036665

O -4.823689 1.564599 -0.644868

H -4.637828 2.255685 0.036665

O 2.328649 -4.882002 1.552219

H 2.134861 -5.570908 0.870685

O 1.155266 -4.084084 1.552219

H 1.349055 -3.395179 0.870685

O 4.376625 2.562207 1.552218

H 4.182836 1.873301 0.870684

O 3.203242 3.360125 1.552218

H 3.397030 4.049030 0.870684

O -0.437296 -4.121063 4.420926

H -0.631085 -4.809969 3.739393

O -1.610679 -3.323145 4.420926

H -1.416891 -2.634239 3.739392

O 1.610679 3.323146 4.420925

H 1.416891 2.634240 3.739392

O 0.437296 4.121064 4.420925

H 0.631085 4.809969 3.739392

O -0.437296 -4.121064 -1.316489

H -0.631085 -4.809969 -1.998022

O -1.610679 -3.323145 -1.316489

H -1.416891 -2.634240 -1.998023

O 1.610679 3.323146 -1.316490

H 1.416891 2.634239 -1.998023

O 0.437296 4.121063 -1.316490

H 0.631085 4.809969 -1.998023

O -3.203242 -3.360124 1.552218

H -3.397030 -4.049030 0.870685

O -4.376625 -2.562206 1.552218

H -4.182836 -1.873301 0.870685

O -1.155266 4.084085 1.552218

H -1.349055 3.395179 0.870684

O -2.328649 4.882003 1.552218

H -2.134861 5.570908 0.870684

O 3.540966 0.790197 -0.309178

H 4.008260 -0.080579 -0.313288

O 3.662477 1.231877 -1.652180

H 4.509421 1.741093 -1.648069

O 0.775020 1.551136 2.559530

H 1.242315 0.680361 2.555419

O 0.896531 1.992817 1.216528

H 1.743475 2.502033 1.220638

O 0.775021 1.551136 -3.177885

H 1.242315 0.680360 -3.181995

O 0.896531 1.992816 -4.520887

H 1.743475 2.502032 -4.516777

O -1.990925 2.312075 -0.309178

H -1.523630 1.441299 -0.313288

O -1.869414 2.753755 -1.652180

H -1.022470 3.262971 -1.648070

O 1.869414 -2.753756 -1.652179

H 1.022470 -3.262972 -1.648069

O 1.990925 -2.312075 -0.309177

H 1.523630 -1.441300 -0.313288

O -0.896531 -1.992817 1.216528

H -1.743475 -2.502033 1.220638

O -0.775021 -1.551136 2.559530

H -1.242315 -0.680360 2.555420

O -0.896531 -1.992817 -4.520887

H -1.743475 -2.502033 -4.516777

O -0.775021 -1.551137 -3.177885

H -1.242315 -0.680361 -3.181995

O -3.662477 -1.231878 -1.652180

H -4.509421 -1.741094 -1.648069

O -3.540966 -0.790197 -0.309178

H -4.008261 0.080579 -0.313288

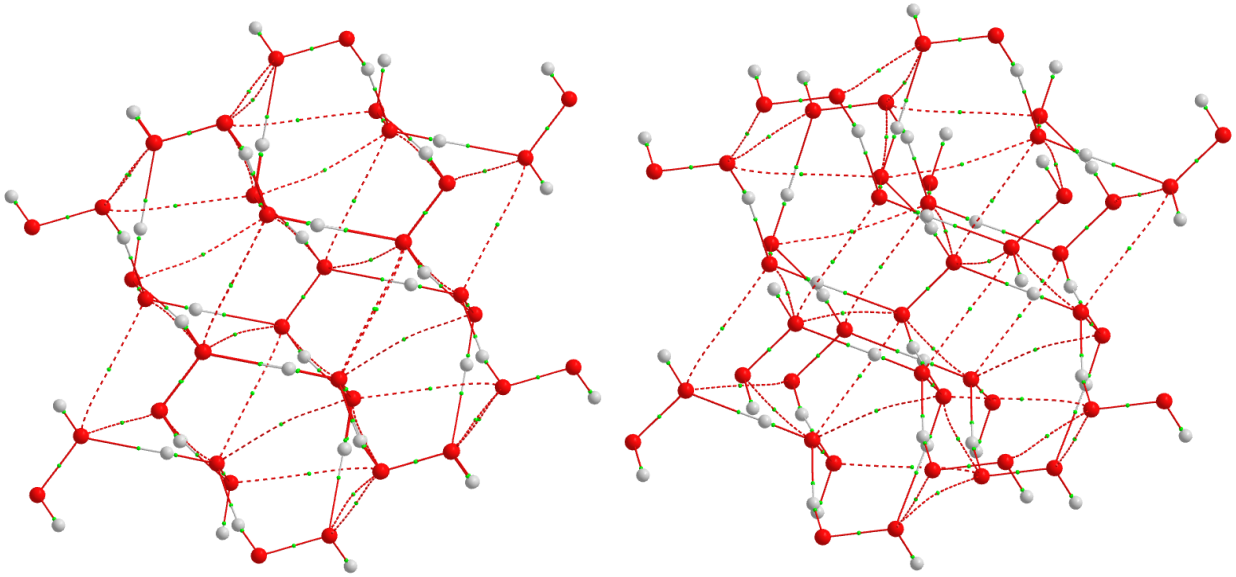

Figure S9. Atomic connectivity graph for the molecular cluster of H2O2.

Me2O

Structure was retrieved from: K. Vojinović, U. Losehand and N. Mitzel, *Dalton Trans.*, 2004, 2578.

<u>Parameters for the optimized crystal structure</u>

Space group: $P4_2/n$

Unit cell parameters: 11.20288 11.20288 4.92168 90 90 90

Atom X Y Z (fractional coordinates):

O 0.49903 -0.27082 0.22660

C 0.57706 -0.27690 0.00327

C 0.42759 -0.37360 0.24647

H 0.63029 -0.19546 0.00253

H 0.63662 -0.35424 0.01940

H 0.48266 -0.45385 0.27207

H 0.52778 -0.28312 -0.18903

H 0.37216 -0.38581 0.06465

H 0.37021 -0.36382 0.42401

Cartesian coordinates for the molecular cluster (optimized central molecule):

Atom X Y Z (Cartesian coordinates)

O -0.177235 -0.834524 0.313823

C -0.962898 0.304318 0.067857

C 1.178656 -0.501493 0.483644

H -1.996080 -0.025680 -0.043858

H -0.899332 1.015519 0.900060

H 1.314425 0.177201 1.335521

H -0.650632 0.815742 -0.851986

H 1.586497 -0.009807 -0.408957

H 1.729964 -1.422382 0.675228

O -0.955829 2.688052 -3.034920

C -1.755654 3.821523 -3.263986

C 0.392988 3.035302 -2.845175

H -2.783681 3.480215 -3.385207

H -1.704416 4.518156 -2.418825

H 0.510536 3.700699 -1.980200

H -1.445916 4.352439 -4.173701

H 0.805693 3.545787 -3.725046

H 0.954344 2.118840 -2.661548

O 0.642111 -4.384376 3.622330

C -0.157714 -3.250905 3.393264

C 1.990928 -4.037126 3.812076

H -1.185741 -3.592213 3.272044

H -0.106476 -2.554272 4.238425

H 2.108476 -3.371729 4.677050

H 0.152024 -2.719989 2.483550

H 2.403633 -3.526641 2.932204

H 2.552284 -4.953588 3.995703

O -0.516517 -1.788831 -4.257877

C -1.296956 -1.502840 -5.391927

C -0.871825 -0.977668 -3.166243

H -0.979618 -2.175820 -6.188432

H -2.362461 -1.662427 -5.188332

H -1.922875 -1.129112 -2.888554

H -1.156039 -0.465664 -5.723288

H -0.730159 0.087243 -3.392055

H -0.242091 -1.255642 -2.320722

O 0.282453 -5.325046 -0.929251

C -0.497986 -5.039054 -2.063301

C -0.072855 -4.513882 0.162382

H -0.180648 -5.712034 -2.859807

H -1.563491 -5.198641 -1.859707

H -1.123904 -4.665327 0.440072

H -0.357069 -4.001878 -2.394663

H 0.068811 -3.448971 -0.063430

H 0.556879 -4.791855 1.007903

O 3.350149 1.415592 -1.781727

C 3.773721 2.709085 -2.134441

C 3.737210 0.463898 -2.741081

H 3.455200 3.387298 -1.342861

H 4.865001 2.754593 -2.230653

H 4.829166 0.434289 -2.848344

H 3.325521 3.031937 -3.083268

H 3.305006 0.684896 -3.725690

H 3.391173 -0.513768 -2.404674

O 4.149119 -2.120623 1.546899

C 4.572691 -0.827130 1.194185

C 4.536180 -3.072316 0.587545

H 4.254170 -0.148916 1.985764

H 5.663971 -0.781621 1.097971

H 5.628136 -3.101926 0.480282

H 4.124491 -0.504277 0.245356

H 4.103976 -2.851318 -0.397065

H 4.190143 -4.049982 0.923951

O 3.789462 -3.061292 -3.004683

C 4.232418 -2.615278 -4.262381

C 2.472395 -3.549072 -3.062149

H 5.259264 -2.268737 -4.146087

H 4.206955 -3.425990 -5.000160

H 2.395755 -4.395523 -3.756698

H 3.615396 -1.786167 -4.632856

H 1.769152 -2.773648 -3.392699

H 2.194738 -3.888248 -2.063848

O -4.723479 0.817205 3.159057

C -4.280523 1.263219 1.901358

C -6.040546 0.329425 3.101590

H -3.253677 1.609761 2.017653

H -4.305986 0.452507 1.163580

H -6.117186 -0.517026 2.407042

H -4.897544 2.092330 1.530884

H -6.743788 1.104849 2.771041

H -6.318203 -0.009751 4.099892

O 2.696766 3.859602 1.312107

C 3.496591 2.726132 1.541172

C 1.347949 3.512353 1.122360

H 4.524619 3.067440 1.662393

H 3.445352 2.029499 0.696012

H 1.230401 2.846956 0.257387

H 3.186852 2.195215 2.450888

H 0.935244 3.001867 2.002233

H 0.786593 4.428814 0.938734

O 3.495736 0.323388 4.640732

C 4.295561 -0.810083 4.869797

C 2.146919 -0.023862 4.450986

H 5.323589 -0.468775 4.991019

H 4.244322 -1.506716 4.024637

H 2.029371 -0.689258 3.586012

H 3.985822 -1.340999 5.779513

H 1.734214 -0.534347 5.330858

H 1.585563 0.892600 4.267359

O -4.794282 1.578418 -2.951843

C -4.013843 1.292426 -1.817793

C -4.438973 0.767254 -4.043476

H -4.331181 1.965406 -1.021287

H -2.948337 1.452012 -2.021387

H -3.387925 0.918699 -4.321165

H -4.154760 0.255250 -1.486431

H -4.580640 -0.297657 -3.817664

H -5.068707 1.045227 -4.888997

O -3.995312 -1.957797 0.376783

C -3.214872 -2.243788 1.510832

C -3.640003 -2.768960 -0.714851

H -3.532211 -1.570808 2.307339

H -2.149368 -2.084201 1.307238

H -2.588955 -2.617516 -0.992540

H -3.355790 -3.280964 1.842194

H -3.781670 -3.833871 -0.489039

H -4.269737 -2.490987 -1.560372

O -1.609213 5.132063 0.058912

C -2.032785 3.838570 0.411627

C -1.996273 6.083756 1.018267

H -1.714263 3.160356 -0.379953

H -3.124064 3.793061 0.507840

H -3.088228 6.113366 1.125530

H -1.584583 3.515718 1.360455

H -1.564069 5.862758 2.002876

H -1.650236 7.061422 0.681861

O -0.810243 1.595848 3.387538

C -1.233815 0.302355 3.740252

C -1.197303 2.547542 4.346892

H -0.915293 -0.375858 2.948673

H -2.325094 0.256847 3.836465

H -2.289258 2.577152 4.454156

H -0.785613 -0.020496 4.689080

H -0.765099 2.326544 5.331501

H -0.851267 3.525208 4.010485

O 7.263386 2.194235 -1.553246

C 6.820430 1.748221 -0.295547

C 8.580452 2.682015 -1.495779

H 5.793583 1.401680 -0.411841

H 6.845892 2.558933 0.442232

H 8.657092 3.528466 -0.801231

H 7.437451 0.919110 0.074927

H 9.283695 1.906591 -1.165229

H 8.858110 3.021192 -2.494080

O -8.301290 -0.685336 -0.876412

C -8.744246 -1.131350 0.381287

C -6.984224 -0.197556 -0.818944

H -9.771093 -1.477892 0.264993

H -8.718784 -0.320638 1.119066

H -6.907584 0.648894 -0.124396

H -8.127225 -1.960462 0.751762

H -6.280982 -0.972980 -0.488394

H -6.706567 0.141620 -1.817246

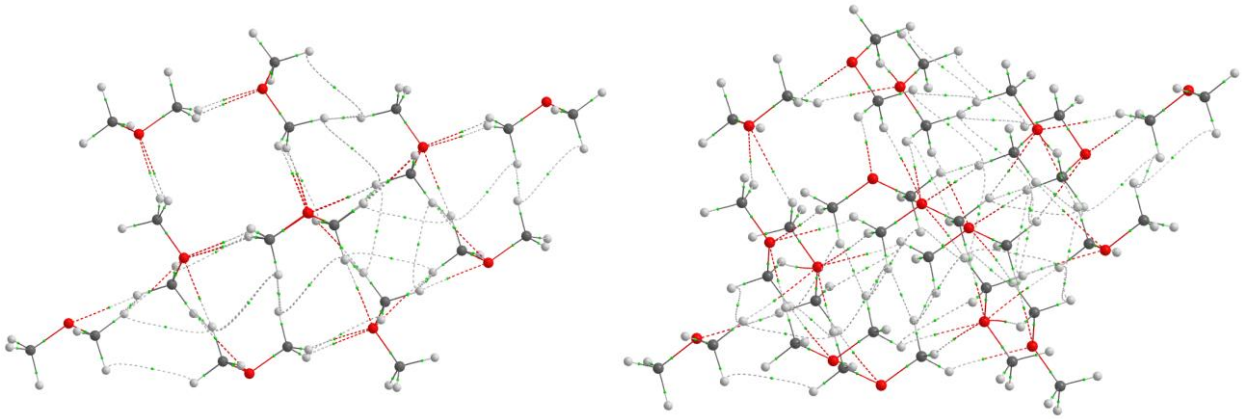

Figure S10. Atomic connectivity graph for the molecular cluster of Me2O.

MeOH

Structure was retrieved from: M. Kirchner, D. Das and R. Boese, *Cryst. Growth Des.*, 2008, **8(3)**, 763.

Parameters for the optimized crystal structure

Space group: $P2_12_12_1$

Unit cell parameters: 4.53981 5.00138 8.87817 90 90 90

Atom X Y Z (fractional coordinates):

O 0.23201 0.29644 -0.07479

H 0.41661 0.26220 -0.01937

C 0.25159 0.55014 -0.14467

H 0.25790 0.71222 -0.06193

H 0.05799 0.57695 -0.21583

H 0.44721 0.56417 -0.21622

Cartesian coordinates for the molecular cluster (optimized central molecule):

Atom X Y Z (Cartesian coordinates)

O 0.349394 -0.737916 0.925310

H -0.348672 -0.250639 1.412794

C 0.285533 -0.391624 -0.443515

H -0.650095 -0.721764 -0.905422

H 1.111477 -0.889112 -0.951637

H 0.396598 0.688166 -0.586409

O 2.393093 -4.694156 0.067185

H 1.688968 -4.208215 0.558929

C 2.339400 -4.315244 -1.295286

H 1.417631 -4.656690 -1.776216

H 3.188188 -4.767475 -1.809715

H 2.413376 -3.229533 -1.408800

O 2.328722 -0.727987 5.534267

H 1.624597 -0.242046 6.026010

C 2.275029 -0.349075 4.171797

H 1.353261 -0.690521 3.690866

H 3.123817 -0.801306 3.657368

H 2.349005 0.736636 4.058282

O -1.669330 -0.767740 -3.634654

H -2.373455 -0.281799 -3.142911

C -1.723022 -0.388828 -4.997124

H -2.644791 -0.730274 -5.478054

H -0.874234 -0.841059 -5.511553

H -1.649046 0.696883 -5.110639

O -1.733700 3.198429 1.832429

H -2.437826 3.684371 2.324172

C -1.787394 3.577342 0.469958

H -2.709162 3.235895 -0.010972

H -0.938605 3.125111 -0.044471

H -1.713417 4.663052 0.356444

O 2.975252 1.580411 -2.435198

H 2.896040 0.608021 -2.583262

C 4.016668 1.814873 -1.506078

H 3.768944 1.430066 -0.512047

H 4.173696 2.891711 -1.432936

H 4.954020 1.357192 -1.836268

O -4.092029 -2.808347 0.665474

H -4.171241 -3.780738 0.517410

C -3.050614 -2.573886 1.594595

H -3.298337 -2.958692 2.588625

H -2.893585 -1.497048 1.667736

H -2.113261 -3.031566 1.264404

O 0.911855 5.526704 -1.552576

H 0.832643 4.554313 -1.700641

C 1.953272 5.761165 -0.623456

H 1.705547 5.376359 0.370575

H 2.110300 6.838004 -0.550314

H 2.890623 5.303486 -0.953647

O -6.155426 1.137946 1.548096

H -6.234638 0.165554 1.400032

C -5.114010 1.372406 2.477217

H -5.361734 0.987601 3.471247

H -4.956982 2.449245 2.550358

H -4.176658 0.914727 2.147026

O 4.763183 -1.031175 1.745945

H 5.604201 -1.515755 1.568147

C 3.802570 -1.420172 0.782261

H 4.076334 -1.085169 -0.222907

H 2.846595 -0.969007 1.050871

H 3.672501 -2.506441 0.767136

O 2.764157 -1.051052 -2.838515

H 3.605176 -1.535631 -3.016314

C 1.803544 -1.440049 -3.802200

H 2.077308 -1.105046 -4.807368

H 0.847569 -0.988883 -3.533589

H 1.673475 -2.526317 -3.817325

O 2.699786 2.915118 2.628567

H 3.540805 2.430537 2.450768

C 1.739174 2.526120 1.664883

H 2.012938 2.861123 0.659715

H 0.783198 2.977286 1.933493

H 1.609105 1.439852 1.649758

O 0.700760 2.895241 -1.955893

H 1.541779 2.410661 -2.133693

C -0.259852 2.506243 -2.919578

H 0.013912 2.841247 -3.924746

H -1.215827 2.957409 -2.650967

H -0.389921 1.419975 -2.934703

O 0.489940 -3.375634 1.398100

H 0.432259 -2.404604 1.232220

C 0.462830 -3.600010 2.795133

H 1.358558 -3.208761 3.287203

H 0.412989 -4.675783 2.967812

H -0.418430 -3.141772 3.253965

O -1.509086 -3.395510 -3.186361

H -1.566766 -2.424481 -3.352240

C -1.536195 -3.619886 -1.789327

H -0.640467 -3.228637 -1.297257

H -1.586036 -4.695659 -1.616648

H -2.417455 -3.161648 -1.330495

O -1.573457 0.570659 2.280722

H -1.631138 1.541689 2.114842

C -1.600567 0.346283 3.677755

H -0.704838 0.737532 4.169824

H -1.650407 -0.729491 3.850433

H -2.481826 0.804520 4.136587

O -3.572483 0.550783 -2.303739

H -3.630163 1.521812 -2.469618

C -3.599592 0.326407 -0.906705

H -2.703864 0.717655 -0.414636

H -3.649433 -0.749367 -0.734027

H -4.480852 0.784644 -0.447873

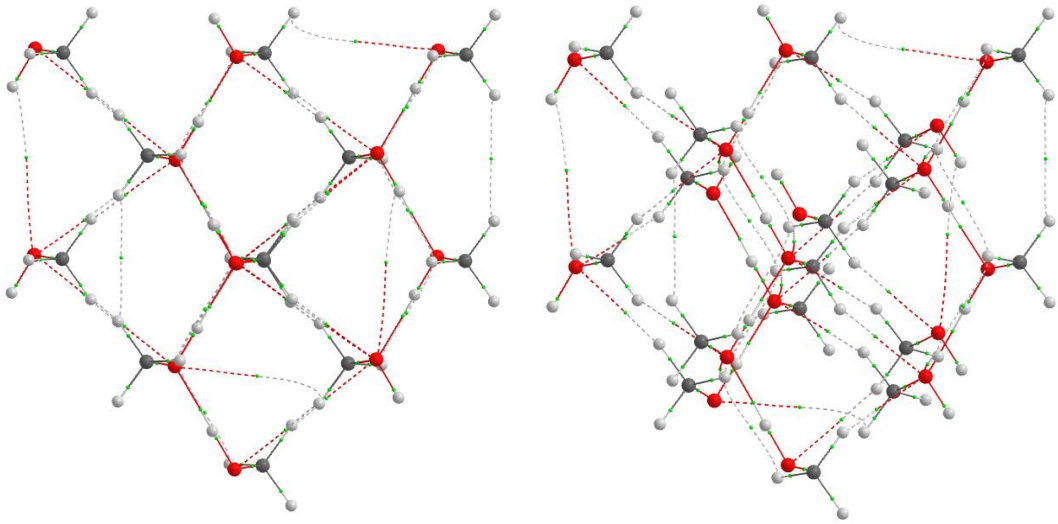

Figure S11. Atomic connectivity graph for the molecular cluster of MeOH.

Methylhydrazine

Structure was retrieved from: M. Foulon, N. Lebrun, M. Muller, A. Amazzal, M. T. Cohen-Adad, *Acta Cryst.*, 1994, **B50**, 472.

Parameters for the optimized crystal structure

Space group: $P2_1/c$

Unit cell parameters: 9.94512 3.86136 7.58447 90 106.619 90

Atom X Y Z (fractional coordinates):

N 0.18988 -0.44065 0.03924

N 0.11600 -0.20695 -0.10022

C 0.33595 -0.45168 0.04452

H 0.18013 -0.36413 0.16435

H 0.12928 0.04299 -0.05201

H 0.01241 -0.26337 -0.12900

H 0.34692 -0.57039 -0.08146

H 0.38597 -0.19529 0.05826

H 0.39335 -0.60983 0.16125

Cartesian coordinates for the molecular cluster (optimized central molecule):

Atom X Y Z (Cartesian coordinates)

N -0.596335 -0.459128 0.824610

N -1.638917 -0.141366 -0.093005

C 0.688145 -0.303553 0.184967

H -0.660823 0.153347 1.641088

H -1.766703 0.876829 -0.140112

H -2.497204 -0.532704 0.278970

H 0.805808 -1.059616 -0.595196

H 0.830775 0.683075 -0.278548

H 1.478778 -0.447042 0.925528

N 0.566802 -3.924180 2.082132

N -0.443248 -3.602736 1.130878

C 1.871376 -3.746321 1.493162

H 0.468859 -3.327159 2.908999

H -0.587567 -2.586355 1.097832

H -1.309026 -4.020341 1.453135

H 2.028701 -4.490054 0.707845

H 2.022345 -2.752198 1.048502

H 2.634003 -3.891873 2.261749

N -1.763474 2.996364 -0.431102

N -2.773524 3.317808 -1.382355

C -0.458900 3.174223 -1.020071

H -1.861417 3.593386 0.395765

H -2.917843 4.334190 -1.415401

H -3.639302 2.900203 -1.060098

H -0.301575 2.430491 -1.805388

H -0.307931 4.168347 -1.464732

H 0.303727 3.028671 -0.251485

N -3.722605 -4.316130 -0.952651

N -3.257140 -3.020243 -0.588740

C -5.001475 -4.570323 -0.335961

H -3.802974 -4.383592 -1.971831

H -3.695250 -2.306904 -1.183852

H -2.259888 -2.993096 -0.769201

H -4.882174 -4.648128 0.747702

H -5.749905 -3.790088 -0.535669

H -5.395570 -5.519255 -0.707080

N -4.887743 -0.855858 -2.209268

N -4.422278 0.440029 -1.845356

C -6.166614 -1.110051 -1.592578

H -4.968112 -0.923320 -3.228447

H -4.860389 1.153368 -2.440469

H -3.425026 0.467177 -2.025817

H -6.047312 -1.187856 -0.508915

H -6.915043 -0.329815 -1.792285

H -6.560708 -2.058983 -1.963697

N 5.715440 -0.174017 1.702266

N 6.180905 1.121869 2.066176

C 4.436570 -0.428210 2.318956

H 5.635071 -0.241480 0.683086

H 5.742794 1.835209 1.471065

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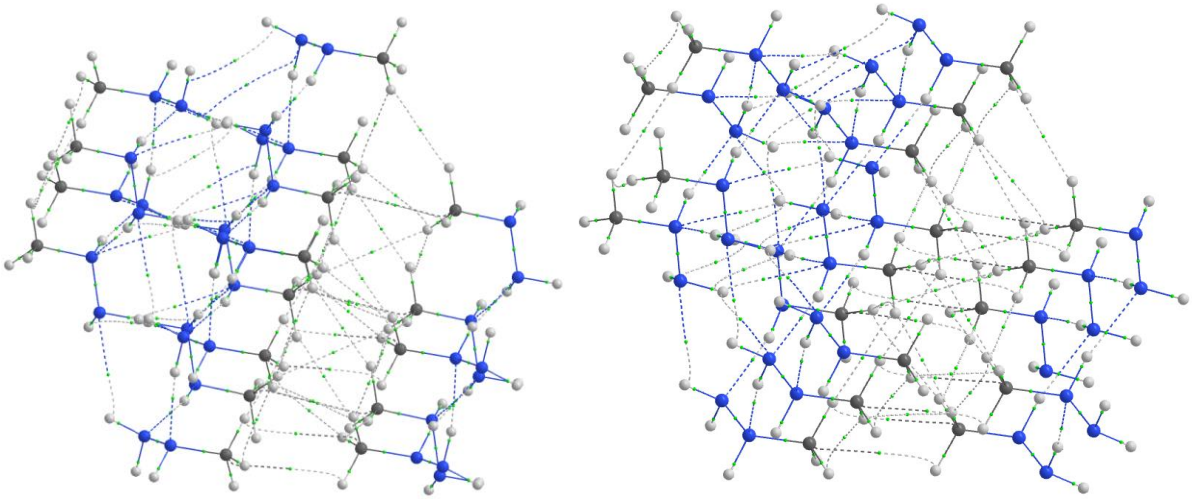

Figure S12. Atomic connectivity graph for the molecular cluster of methylhydrazine.

Propane

Structure was retrieved from: R. Boese, H. Weiss and D. Bläser, *Angew. Chem. Int. Ed.*, 1999, **38**(7), 988.

Parameters for the optimized crystal structure

Space group: $P2_1/n$

Unit cell parameters: 4.12146 12.57412 6.90752 90 91.258 90

Atom X Y Z (fractional coordinates):

C 0.21796 -0.05298 0.22032

H -0.04354 -0.05481 0.19060

H 0.33744 -0.07740 0.08774

H 0.28581 0.02948 0.24956

C 0.31158 -0.12560 0.38794

H 0.18783 -0.09994 0.51867

H 0.57118 -0.11721 0.42109

C 0.23473 -0.24156 0.34659

H -0.02563 -0.25382 0.32225

H 0.35675 -0.26858 0.21651

H 0.31313 -0.29300 0.46601

Cartesian coordinates for the molecular cluster (optimized central molecule):

Atom X Y Z (Cartesian coordinates)

C -0.950154 -0.097199 0.131702

H -0.941046 -0.263320 1.211996

H -0.720456 -1.053849 -0.345337

H -1.967811 0.178688 -0.151171

C 0.053818 0.967237 -0.271774

H -0.193165 1.913347 0.222143

H -0.034167 1.163109 -1.344970

C 1.484117 0.575647 0.052754

H 1.624954 0.437029 1.128276

H 1.749144 -0.367294 -0.433418

H 2.196451 1.332043 -0.281990

C -0.943756 0.083856 4.250296

H -0.936005 -0.074300 5.331711

H -0.710645 -0.875177 3.780001

H -1.961650 0.354667 3.963679

C 0.057790 1.148229 3.840800

H -0.191858 2.096547 4.328927

H -0.030304 1.336874 2.766457

C 1.489011 0.762381 4.167458

H 1.630434 0.630674 5.243669

H 1.756068 -0.182497 3.686396

H 2.198777 1.518825 3.827529

C -1.494656 -6.984734 0.290289

H -1.486906 -7.142890 1.371704

H -1.261545 -7.943766 -0.180006

H -2.512550 -6.713922 0.003672

C -0.493110 -5.920361 -0.119205

H -0.742758 -4.972042 0.368920

H -0.581204 -5.731715 -1.193549

C 0.938111 -6.306208 0.207451

H 1.079534 -6.437916 1.283663

H 1.205168 -7.251087 -0.273611

H 1.647876 -5.549764 -0.132477

C -0.400990 6.783354 -0.024350

H -0.393240 6.625198 1.057065

H -0.167879 5.824322 -0.494644

H -1.418884 7.054166 -0.310967

C 0.600556 7.847727 -0.433845

H 0.350908 8.796046 0.054281

H 0.512462 8.036373 -1.508188

C 2.031777 7.461880 -0.107188

H 2.173200 7.330172 0.969023

H 2.298834 6.517001 -0.588250

H 2.741542 8.218323 -0.447116

C -0.951890 -0.285235 -3.984357

H -0.944140 -0.443391 -2.902941

H -0.718779 -1.244268 -4.454651

H -1.969785 -0.014424 -4.270974

C 0.049656 0.779138 -4.393851

H -0.199993 1.727456 -3.905726

H -0.038438 0.967783 -5.468195

C 1.480876 0.393290 -4.067195

H 1.622299 0.261582 -2.990983

H 1.747934 -0.551588 -4.548255

H 2.190642 1.149734 -4.407122

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H 5.393899 0.137705 2.911928

H 5.734854 0.893630 4.465093

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C 6.174759 -1.225689 4.407399

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H 6.052522 -1.397639 5.481201

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H 7.816504 -0.963279 3.012791

H 8.060893 -0.179480 4.571015

H 8.230377 -1.929395 4.431455

C -7.178885 0.978143 3.961012

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H 5.777062 -2.307492 -0.199707

H 6.048455 -1.582185 1.363875

C 7.646511 -1.255137 -0.029114

H 7.812437 -1.147825 -1.104535

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H 8.226310 -2.113941 0.314129

C -7.182952 0.793598 -0.156314

H -7.144826 0.948112 -1.237611

H -6.803871 1.704037 0.315553

H -8.232273 0.686874 0.124991

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H -6.757595 -1.312540 -0.231921

H -6.486202 -0.587233 1.331662

C -4.888147 -0.260184 -0.061327

H -4.722221 -0.152873 -1.136748

H -4.477832 0.630927 0.421475

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C 5.347638 -0.385900 -4.241427

H 5.385765 -0.231386 -5.322724

H 5.726720 0.524539 -3.769560

H 4.298317 -0.492624 -3.960122

C 6.166625 -1.594780 -3.827254

H 5.772995 -2.492038 -4.317033

H 6.044388 -1.766731 -2.753451

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H -5.657711 -4.383172 2.416468

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H -2.201457 4.894874 2.306677

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H -2.752357 -2.173716 -1.653330

H -1.501352 -3.403560 -1.837007

C -3.520792 -4.197121 -1.714129

H -3.271144 -5.145440 -2.202256

H -3.432698 -4.385767 -0.639786

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H -4.546603 3.204478 -3.274317

H -4.672237 4.017649 -1.717044

H -5.114945 2.316327 -1.858177

C 3.719950 -3.842490 2.282985

H 3.681824 -3.997005 3.364283

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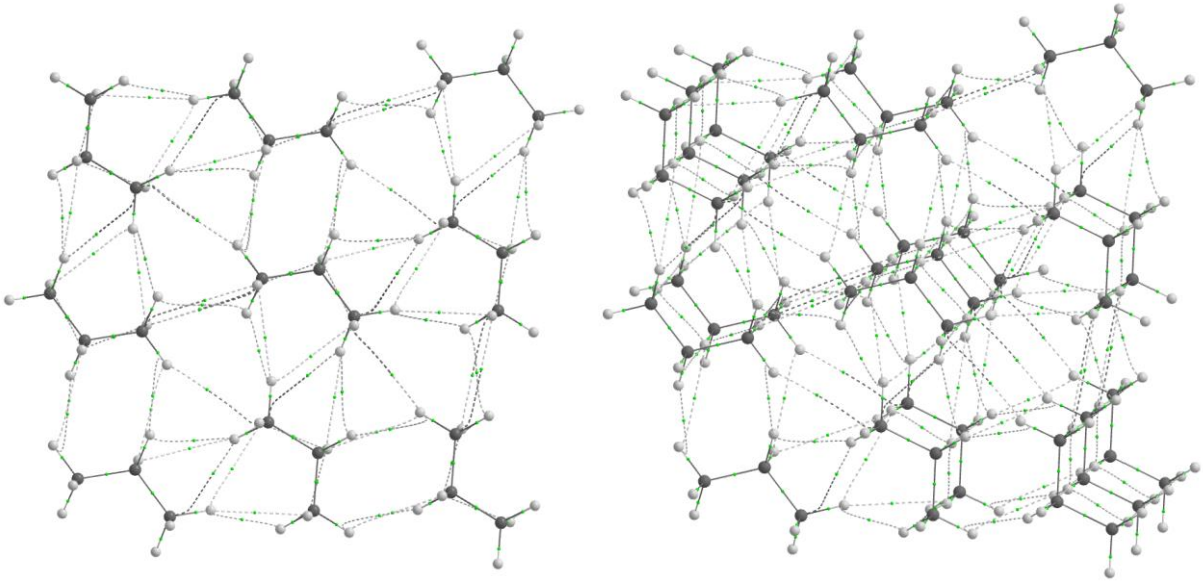

Figure S13. Atomic connectivity graph for the molecular cluster of propane.