Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for:

Infrared spectra of amorphous and crystalline urea ices

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We report here the calculated structures, in .cif fileformat, used in the DFT– B3LYP calculations.

Also, in Table S1 we report the main crystallographic parameters obtained and compared with experimental results.

Finally, in Figure S1, we present the IR spectra of three individual 2urea:8H_2O structures, and the corresponding average spectrum.

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H5     H    -0.70786   0.49536   0.52460   0.00000  Uiso   1.00
N6     N    -0.54217   0.41316   0.35161   0.00000  Uiso   1.00
H7     H    -0.46277   0.38123   0.29747   0.00000  Uiso   1.00
H8     H    -0.62025   0.34871   0.35614   0.00000  Uiso   1.00
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H1     H     0.26584   0.76584   0.27394   7.68386  Uani   1.00
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O1        5.63405   5.63405   0.89947   0.00000   0.00000   0.00000
N1        7.32126   7.32126   1.56283   0.00000  -0.09110  -0.09110
H1        9.53571   9.53571   3.98016   0.00000  -0.44249  -0.44249
H2       10.12321  10.12321   2.04630   0.00000  -0.29933  -0.29933
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C1     N1      1.358   2_565 S
N1     H1      1.019   .     S
N1     H2      1.016   1_554 S
H2     N1      1.016   1_556 S
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O2     O     0.65409   0.26880   0.10632   0.00000  Uiso   1.00
N3     N     0.50803   0.01307   0.09820   0.00000  Uiso   1.00
H4     H     0.54865  -0.01083  -0.03014   0.00000  Uiso   1.00
H5     H     0.38103  -0.03644   0.12109   0.00000  Uiso   1.00
N6     N     0.47003   0.21670   0.33710   0.00000  Uiso   1.00
H7     H     0.45223   0.33936   0.37780   0.00000  Uiso   1.00
H8     H     0.37159   0.13967   0.37721   0.00000  Uiso   1.00
C9     C     0.10379   0.51788   0.40264   0.00000  Uiso   1.00
O10    O     0.24570   0.48670   0.49465   0.00000  Uiso   1.00
N11    N    -0.06740   0.53515   0.47292   0.00000  Uiso   1.00
H12    H    -0.07763   0.51725   0.60561   0.00000  Uiso   1.00
H13    H    -0.16624   0.59877   0.40947   0.00000  Uiso   1.00
N14    N     0.11273   0.52641   0.22187   0.00000  Uiso   1.00
H15    H     0.23889   0.54757   0.17483   0.00000  Uiso   1.00
H16    H     0.00153   0.55378   0.14368   0.00000  Uiso   1.00
C17    C     0.45014   0.60296   0.94186   0.00000  Uiso   1.00
O18    O     0.33335   0.71052   0.91654   0.00000  Uiso   1.00
N19    N     0.55974   0.60721   1.10046   0.00000  Uiso   1.00
H20    H     0.52146   0.68986   1.20350   0.00000  Uiso   1.00
H21    H     0.61219   0.49495   1.13132   0.00000  Uiso   1.00
N22    N     0.48830   0.47489   0.81367   0.00000  Uiso   1.00
H23    H     0.39124   0.45216   0.71092   0.00000  Uiso   1.00
H24    H     0.57189   0.38276   0.85031   0.00000  Uiso   1.00
C25    C    -0.01106   0.89636   1.16539   0.00000  Uiso   1.00
O26    O     0.13868   0.96960   1.20603   0.00000  Uiso   1.00
N27    N    -0.15100   0.89387   1.28634   0.00000  Uiso   1.00
H28    H    -0.12888   0.97738   1.39674   0.00000  Uiso   1.00
H29    H    -0.28341   0.89569   1.23154   0.00000  Uiso   1.00
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C33    C     0.00867   0.28111   0.80073   0.00000  Uiso   1.00
O34    O    -0.07232   0.41724   0.82161   0.00000  Uiso   1.00
N35    N     0.00266   0.18085   0.63659   0.00000  Uiso   1.00
H36    H    -0.03767   0.24347   0.53173   0.00000  Uiso   1.00
H37    H     0.11378   0.10469   0.61287   0.00000  Uiso   1.00
N38    N     0.10802   0.21836   0.93653   0.00000  Uiso   1.00
H39    H     0.09571   0.27667   1.06195   0.00000  Uiso   1.00
H40    H     0.14597   0.09744   0.92659   0.00000  Uiso   1.00
C41    C     0.48110   0.91042   0.61177   0.00000  Uiso   1.00
O42    O     0.32562   0.96742   0.58418   0.00000  Uiso   1.00
N43    N     0.52678   0.74796   0.55009   0.00000  Uiso   1.00
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H45    H     0.62993   0.69713   0.62225   0.00000  Uiso   1.00
N46    N     0.62244   1.00487   0.70553   0.00000  Uiso   1.00
H47    H     0.60465   1.12962   0.71672   0.00000  Uiso   1.00
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C9	N14	1.371	.	S
N11	H12	1.028	.	S
N11	H13	1.014	.	S
N14	H15	1.011	.	S
N14	H16	1.013	.	S
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N19	H20	1.015	.	S
N19	H21	1.031	.	S
N22	H23	1.018	.	S
N22	H24	1.015	.	S
C25	O26	1.237	.	D
C25	N27	1.389	.	S
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N27	H28	1.016	.	S
N27	H29	1.023	.	S
N30	H31	1.022	.	S
N30	H32	1.018	.	S
C33	O34	1.248	.	D
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C33	N38	1.365	.	S
N35	H36	1.015	.	S
N35	H37	1.024	.	S
N38	H39	1.014	.	S
N38	H40	1.013	.	S
C41	O42	1.233	.	D
C41	N43	1.391	.	S
C41	N46	1.386	.	S
N43	H44	1.026	.	S
N43	H45	1.016	.	S
N46	H47	1.012	.	S
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N3     N     0.66243   0.30508   0.48106   0.00000  Uiso   1.00
H4     H     0.76794   0.28625   0.55930   0.00000  Uiso   1.00
H5     H     0.69051   0.33744   0.36096   0.00000  Uiso   1.00
N6     N     0.39904   0.44415   0.44413   0.00000  Uiso   1.00
H7     H     0.28081   0.46959   0.49357   0.00000  Uiso   1.00
H8     H     0.38753   0.39743   0.32577   0.00000  Uiso   1.00
C9     C     0.22402   0.69486   0.92165   0.00000  Uiso   1.00
O10    O     0.22340   0.85370   0.85870   0.00000  Uiso   1.00
N11    N     0.27821   0.67459   1.08852   0.00000  Uiso   1.00
H12    H     0.24802   0.78019   1.16012   0.00000  Uiso   1.00
H13    H     0.24416   0.54616   1.13973   0.00000  Uiso   1.00
N14    N     0.18099   0.53827   0.83791   0.00000  Uiso   1.00
H15    H     0.14163   0.54532   0.71656   0.00000  Uiso   1.00
H16    H     0.19535   0.41255   0.88990   0.00000  Uiso   1.00
C17    C     0.68854   0.82735   0.59763   0.00000  Uiso   1.00
O18    O     0.76035   0.68740   0.63776   0.00000  Uiso   1.00
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H21    H     0.53778   1.02860   0.68598   0.00000  Uiso   1.00
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O26    O     0.23355   0.27258   0.13736   0.00000  Uiso   1.00
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H29    H    -0.09051  -0.05186   0.13067   0.00000  Uiso   1.00
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H34    H     0.22813   0.90729   0.64632   0.00000  Uiso   1.00
O35    O     0.23381   0.93050   0.52524   0.00000  Uiso   1.00
H36    H     0.66118   0.42304   0.84459   0.00000  Uiso   1.00
H37    H     0.69528   0.33044   1.01262   0.00000  Uiso   1.00
O38    O     0.74615   0.43189   0.93998   0.00000  Uiso   1.00
H39    H     0.90151   0.30311   0.80614   0.00000  Uiso   1.00
H40    H     0.85548   0.10760   0.74275   0.00000  Uiso   1.00
O41    O     0.94023   0.21743   0.72536   0.00000  Uiso   1.00
H42    H     1.11171   0.70950   0.47783   0.00000  Uiso   1.00
H43    H     0.93068   0.60665   0.53169   0.00000  Uiso   1.00
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H45    H     0.52968   0.71897   0.08341   0.00000  Uiso   1.00
H46    H     0.70404   0.65115   0.01766   0.00000  Uiso   1.00
O47    O     0.65757   0.76033   0.06654   0.00000  Uiso   1.00
H48    H     0.59295   0.02526   0.08294   0.00000  Uiso   1.00
H49    H     0.44985   0.16371   0.11030   0.00000  Uiso   1.00
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N3     H5      1.012   .     S
N6     H7      1.016   .     S
N6     H8      1.018   .     S
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N11    H12     1.017   .     S
N11    H13     1.023   .     S
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N14    H16     1.015   .     S
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C17    N19     1.384   .     S
C17    N22     1.384   .     S
N19    H20     1.020   .     S
N19    H21     1.017   .     S
N22    H23     1.016   .     S
N22    H24     1.017   .     S
C25    O26     1.264   .     D
C25    N27     1.357   .     S
C25    N30     1.371   .     S
N27    H28     1.025   .     S
N27    H29     1.015   .     S
N30    H31     1.021   .     S
N30    H32     1.017   .     S
H33    O35     0.970   .     S
H34    O35     0.988   .     S
H36    O38     0.990   .     S
H37    O38     0.981   .     S
H39    O41     0.980   .     S
H40    O41     0.975   .     S
H42    O44     0.985   .     S
H43    O44     0.990   .     S
H45    O47     0.985   .     S
H46    O47     0.993   .     S
H48    O50     0.970   .     S
H49    O50     0.980   .     S
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N3     N     0.30222   0.69215   1.06022   0.00000  Uiso   1.00
H4     H     0.34062   0.82171   1.09043   0.00000  Uiso   1.00
H5     H     0.32938   0.60196   1.14642   0.00000  Uiso   1.00
N6     N     0.11332   0.49438   0.90430   0.00000  Uiso   1.00
H7     H     0.04372   0.45519   0.79711   0.00000  Uiso   1.00
H8     H     0.17536   0.38912   0.96829   0.00000  Uiso   1.00
C9     C     0.12895   0.21223   0.21239   0.00000  Uiso   1.00
O10    O     0.27357   0.26939   0.15266   0.00000  Uiso   1.00
N11    N     0.02392   0.09401   0.11942   0.00000  Uiso   1.00
H12    H     0.07267   0.03158   0.00459   0.00000  Uiso   1.00
H13    H    -0.10613   0.06649   0.15876   0.00000  Uiso   1.00
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H15    H     0.10188   0.39247   0.43082   0.00000  Uiso   1.00
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H17    H     0.65000   0.97044   0.91762   0.00000  Uiso   1.00
H18    H     0.84088   0.83180   0.90514   0.00000  Uiso   1.00
O19    O     0.71892   0.86299   0.96658   0.00000  Uiso   1.00
H20    H     0.88205   0.51516   0.05516   0.00000  Uiso   1.00
H21    H     0.69931   0.65111   0.10635   0.00000  Uiso   1.00
O22    O     0.78188   0.54379   0.14163   0.00000  Uiso   1.00
H23    H     0.38375  -0.08589   0.53693   0.00000  Uiso   1.00
H24    H     0.25408   0.10432   0.51288   0.00000  Uiso   1.00
O25    O     0.31872   0.03211   0.59649   0.00000  Uiso   1.00
H26    H     0.31294   0.64023   0.44518   0.00000  Uiso   1.00
H27    H     0.52257   0.53758   0.40375   0.00000  Uiso   1.00
O28    O     0.43996   0.65835   0.40414   0.00000  Uiso   1.00
H29    H     0.51620   0.25467   0.25060   0.00000  Uiso   1.00
H30    H     0.69140   0.35767   0.22228   0.00000  Uiso   1.00
O31    O     0.64431   0.27395   0.29400   0.00000  Uiso   1.00
H32    H     0.45869   0.13601   0.74798   0.00000  Uiso   1.00
H33    H     0.46443   0.23490   0.93230   0.00000  Uiso   1.00
O34    O     0.54630   0.17866   0.83781   0.00000  Uiso   1.00
H35    H     0.08207   0.71693   0.64064   0.00000  Uiso   1.00
H36    H    -0.03113   0.71942   0.47092   0.00000  Uiso   1.00
O37    O     0.07355   0.65059   0.52616   0.00000  Uiso   1.00
H38    H     0.79550   0.19994   0.75970   0.00000  Uiso   1.00
H39    H     1.00803   0.09919   0.71975   0.00000  Uiso   1.00
O40    O     0.91758   0.21035   0.70566   0.00000  Uiso   1.00
loop_
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_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry_2
_ccdc_geom_bond_type
C1     O2      1.266   .     D
C1     N3      1.356   .     S
C1     N6      1.371   .     S
N3     H4      1.010   .     S
N3     H5      1.017   .     S
N6     H7      1.018   .     S
N6     H8      1.022   .     S
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C9	O10	1.265	.	D
C9	N11	1.353	.	S
C9	N14	1.379	.	S
N11	H12	1.017	.	S
N11	H13	1.017	.	S
N14	H15	1.023	.	S
N14	H16	1.020	.	S
H17	O19	0.982	.	S
H18	O19	0.970	.	S
H20	O22	0.974	.	S
H21	O22	0.972	.	S
H23	O25	0.975	.	S
H24	O25	0.978	.	S
H26	O28	0.979	.	S
H27	O28	0.975	.	S
H29	O31	0.977	.	S
H30	O31	0.984	.	S
H32	O34	0.991	.	S
H33	O34	0.967	.	S
H35	O37	0.992	.	S
H36	O37	0.964	.	S
H38	O40	0.976	.	S
H39	O40	0.967	.	S

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data_Urea-amorphous-6(CH4N2O)-4(H2O)
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loop_
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_cell_length_c                    8.3070
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_cell_angle_gamma                 85.0385
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C1     C     0.51590   0.36573   0.50096   0.00000  Uiso   1.00
O2     O     0.45024   0.33156   0.63418   0.00000  Uiso   1.00
N3     N     0.66799   0.29524   0.46062   0.00000  Uiso   1.00
H4     H     0.74068   0.27362   0.55555   0.00000  Uiso   1.00
H5     H     0.72478   0.34180   0.36268   0.00000  Uiso   1.00
N6     N     0.43928   0.46833   0.39118   0.00000  Uiso   1.00
H7     H     0.31788   0.49177   0.40727   0.00000  Uiso   1.00
H8     H     0.48217   0.46595   0.27534   0.00000  Uiso   1.00
C9     C     0.79189   0.71648   0.07968   0.00000  Uiso   1.00
O10    O     0.80350   0.87317   0.04191   0.00000  Uiso   1.00
N11    N     0.73180   0.59724  -0.01984   0.00000  Uiso   1.00
H12    H     0.68708   0.64395  -0.12659   0.00000  Uiso   1.00
H13    H     0.67410   0.49613   0.02583   0.00000  Uiso   1.00
N14    N     0.83590   0.65841   0.22990   0.00000  Uiso   1.00
H15    H     0.89407   0.74458   0.29447   0.00000  Uiso   1.00
H16    H     0.88053   0.53160   0.24143   0.00000  Uiso   1.00
C17    C     0.08889   0.72011   0.51937   0.00000  Uiso   1.00
O18    O     0.10646   0.57141   0.44991   0.00000  Uiso   1.00
N19    N    -0.04171   0.76948   0.61839   0.00000  Uiso   1.00
H20    H    -0.12629   0.68370   0.63626   0.00000  Uiso   1.00
H21    H    -0.03479   0.86302   0.70562   0.00000  Uiso   1.00
N22    N     0.19161   0.84534   0.48859   0.00000  Uiso   1.00
H23    H     0.30590   0.80291   0.45391   0.00000  Uiso   1.00
H24    H     0.18334   0.95588   0.56091   0.00000  Uiso   1.00
C25    C     0.20693   0.69479   0.95493   0.00000  Uiso   1.00
O26    O     0.22255   0.82105   0.86458   0.00000  Uiso   1.00
N27    N     0.25518   0.69429   1.11102   0.00000  Uiso   1.00
H28    H     0.29081   0.80914   1.15435   0.00000  Uiso   1.00
H29    H     0.20948   0.61124   1.19120   0.00000  Uiso   1.00
N30    N     0.13857   0.54695   0.90462   0.00000  Uiso   1.00
H31    H     0.12248   0.53311   0.78521   0.00000  Uiso   1.00
H32    H     0.15179   0.43650   0.97101   0.00000  Uiso   1.00
C33    C     0.59010   0.83732   0.63561   0.00000  Uiso   1.00
O34    O     0.63441   0.68461   0.67614   0.00000  Uiso   1.00
N35    N     0.57355   0.97681   0.74194   0.00000  Uiso   1.00
H36    H     0.61713   0.95842   0.85272   0.00000  Uiso   1.00
H37    H     0.54814   1.10233   0.70551   0.00000  Uiso   1.00
N38    N     0.55073   0.86985   0.47909   0.00000  Uiso   1.00
H39    H     0.58680   0.77138   0.39859   0.00000  Uiso   1.00
H40    H     0.54820   0.99296   0.43435   0.00000  Uiso   1.00
C41    C     0.10842   0.20896   0.19980   0.00000  Uiso   1.00
O42    O     0.21598   0.30677   0.16446   0.00000  Uiso   1.00
N43    N     0.07697   0.07113   0.10520   0.00000  Uiso   1.00
H44    H     0.15145   0.03230   0.00941   0.00000  Uiso   1.00
H45    H    -0.02341   0.00597   0.11793   0.00000  Uiso   1.00
N46    N     0.00998   0.24216   0.33712   0.00000  Uiso   1.00
H47    H     0.04273   0.33639   0.41510   0.00000  Uiso   1.00
H48    H    -0.03512   0.13707   0.38883   0.00000  Uiso   1.00
H49    H     1.00029   0.23543   0.73518   0.00000  Uiso   1.00
H50    H     0.86448   0.36959   0.80751   0.00000  Uiso   1.00
O51    O     0.89136   0.28587   0.71958   0.00000  Uiso   1.00
H52    H     0.44942   0.11798   0.12362   0.00000  Uiso   1.00
H53    H     0.59809  -0.01185   0.11957   0.00000  Uiso   1.00
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O54    O     0.49086   0.00823   0.16784   0.00000  Uiso   1.00
H55    H     0.39310   0.35808   1.02109   0.00000  Uiso   1.00
H56    H     0.49237   0.36113   0.86128   0.00000  Uiso   1.00
O57    O     0.50153   0.34000   0.97609   0.00000  Uiso   1.00
H58    H     0.25284   0.04649   0.77723   0.00000  Uiso   1.00
H59    H     0.28696   0.21696   0.68275   0.00000  Uiso   1.00
O60    O     0.20245   0.14383   0.71860   0.00000  Uiso   1.00
loop_
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_geom_bond_atom_site_label_2
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_geom_bond_site_symmetry_2
_ccdc_geom_bond_type
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C1     N3      1.373   .     S
C1     N6      1.362   .     S
N3     H4      1.026   .     S
N3     H5      1.014   .     S
N6     H7      1.027   .     S
N6     H8      1.013   .     S
C9     O10     1.255   .     D
C9     N11     1.361   .     S
C9     N14     1.388   .     S
N11    H12     1.036   .     S
N11    H13     1.020   .     S
N14    H15     1.012   .     S
N14    H16     1.016   .     S
C17    O18     1.257   .     D
C17    N19     1.369   .     S
C17    N22     1.366   .     S
N19    H20     1.018   .     S
N19    H21     1.014   .     S
N22    H23     1.018   .     S
N22    H24     1.021   .     S
C25    O26     1.247   .     D
C25    N27     1.375   .     S
C25    N30     1.377   .     S
N27    H28     1.015   .     S
N27    H29     1.017   .     S
N30    H31     1.011   .     S
N30    H32     1.018   .     S
C33    O34     1.251   .     D
C33    N35     1.363   .     S
C33    N38     1.378   .     S
N35    H36     1.013   .     S
N35    H37     1.019   .     S
N38    H39     1.014   .     S
N38    H40     1.017   .     S
C41    O42     1.254   .     D
C41    N43     1.352   .     S
C41    N46     1.389   .     S
N43    H44     1.016   .     S
N43    H45     1.022   .     S
N46    H47     1.021   .     S
N46    H48     1.014   .     S
H49    O51     0.980   .     S
H50    O51     0.967   .     S
H52    O54     0.966   .     S
H53    O54     0.973   .     S
H55    O57     0.971   .     S
H56    O57     0.976   .     S
H58    O60     0.974   .     S
H59    O60     0.984   .     S
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data_ Urea-amorphous-2(CH4N2O)-8(H2O)- 2
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_symmetry_cell_setting            triclinic
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_symmetry_equiv_pos_as_xyz
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_cell_length_c                    7.3761
_cell_angle_alpha                 100.2057
_cell_angle_beta                  90.3297
_cell_angle_gamma                 95.6338
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
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_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C1     C     0.40377   0.18296   0.83019   0.00000  Uiso   1.00
O2     O     0.28776   0.15923   0.69630   0.00000  Uiso   1.00
N3     N     0.37635   0.06411   0.96640   0.00000  Uiso   1.00
H4     H     0.24145  -0.00772   0.96250   0.00000  Uiso   1.00
H5     H     0.43237   0.12367   1.09696   0.00000  Uiso   1.00
N6     N     0.56309   0.31650   0.84402   0.00000  Uiso   1.00
H7     H     0.58699   0.39857   0.74163   0.00000  Uiso   1.00
H8     H     0.66484   0.33234   0.94741   0.00000  Uiso   1.00
C9     C    -0.07226   0.02944   0.39613   0.00000  Uiso   1.00
O10    O    -0.20665  -0.04539   0.28136   0.00000  Uiso   1.00
N11    N    -0.09849   0.05568   0.58169   0.00000  Uiso   1.00
H12    H    -0.21132  -0.02810   0.62793   0.00000  Uiso   1.00
H13    H     0.01955   0.09506   0.66677   0.00000  Uiso   1.00
N14    N     0.10146   0.09454   0.33596   0.00000  Uiso   1.00
H15    H     0.10171   0.13331   0.20915   0.00000  Uiso   1.00
H16    H     0.21001   0.15951   0.42561   0.00000  Uiso   1.00
H17    H     0.42596   0.63293   0.15689   0.00000  Uiso   1.00
H18    H     0.60546   0.74716   0.27684   0.00000  Uiso   1.00
O19    O     0.49739   0.64119   0.27287   0.00000  Uiso   1.00
H20    H     0.25521   0.87492   0.59289   0.00000  Uiso   1.00
H21    H     0.33065   0.70597   0.44192   0.00000  Uiso   1.00
O22    O     0.25662   0.72594   0.55626   0.00000  Uiso   1.00
H23    H     0.13943   0.68364   0.96226   0.00000  Uiso   1.00
H24    H     0.28378   0.55019   0.85269   0.00000  Uiso   1.00
O25    O     0.23290   0.58444   0.97446   0.00000  Uiso   1.00
H26    H     0.89872   0.88134   0.06196   0.00000  Uiso   1.00
H27    H     0.86923   0.79516  -0.14653   0.00000  Uiso   1.00
O28    O     0.96891   0.84548  -0.05272   0.00000  Uiso   1.00
H29    H     0.89108   0.40844   0.53884   0.00000  Uiso   1.00
H30    H     1.02167   0.60030   0.50859   0.00000  Uiso   1.00
O31    O     0.89282   0.52822   0.48064   0.00000  Uiso   1.00
H32    H     0.99997   0.42786   0.04805   0.00000  Uiso   1.00
H33    H     0.88786   0.43235   0.22904   0.00000  Uiso   1.00
O34    O     0.88761   0.36394   0.09954   0.00000  Uiso   1.00
H35    H     0.54131   0.85435   0.84945   0.00000  Uiso   1.00
H36    H     0.52677   0.72420   0.65710   0.00000  Uiso   1.00
O37    O     0.61791   0.77438   0.75812   0.00000  Uiso   1.00
H38    H     0.62591   0.16196   0.32161   0.00000  Uiso   1.00
H39    H     0.55205   0.37882   0.31647   0.00000  Uiso   1.00
O40    O     0.51367   0.23751   0.33163   0.00000  Uiso   1.00
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C1     N3      1.387   .     S
C1     N6      1.352   .     S
N3     H4      1.019   .     S
N3     H5      1.034   .     S
N6     H7      1.012   .     S
N6     H8      1.028   .     S
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C9	O10	1.269	.	D
C9	N11	1.365	.	S
C9	N14	1.361	.	S
N11	H12	1.021	.	S
N11	H13	1.024	.	S
N14	H15	1.013	.	S
N14	H16	1.018	.	S
H17	O19	0.980	.	S
H18	O19	0.981	.	S
H20	O22	0.979	.	S
H21	O22	0.990	.	S
H23	O25	0.991	.	S
H24	O25	0.967	.	S
H26	O28	0.987	.	S
H27	O28	0.975	.	S
H29	O31	0.967	.	S
H30	O31	0.987	.	S
H32	O34	0.973	.	S
H33	O34	0.982	.	S
H35	O37	0.980	.	S
H36	O37	0.971	.	S
H38	O40	0.974	.	S
H39	O40	0.976	.	S

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Urea-amorphous-2(CH4N2O)-8(H2O)- 3
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_cell_length_c                    6.9490
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_cell_angle_gamma                 91.5831
loop_
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_atom_site_type_symbol
_atom_site_fract_x
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_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C1     C     0.62459   0.05760   0.27578   0.00000  Uiso   1.00
O2     O     0.51661  -0.09062   0.28157   0.00000  Uiso   1.00
N3     N     0.62467   0.21145   0.42370   0.00000  Uiso   1.00
H4     H     0.49851   0.22689   0.50007   0.00000  Uiso   1.00
H5     H     0.70043   0.33643   0.40919   0.00000  Uiso   1.00
N6     N     0.75360   0.07110   0.13304   0.00000  Uiso   1.00
H7     H     0.74269  -0.02810   0.01208   0.00000  Uiso   1.00
H8     H     0.82265   0.19985   0.11875   0.00000  Uiso   1.00
C9     C     0.38336   0.74390   0.71211   0.00000  Uiso   1.00
O10    O     0.46908   0.62622   0.59042   0.00000  Uiso   1.00
N11    N     0.21425   0.68686   0.79797   0.00000  Uiso   1.00
H12    H     0.18762   0.54164   0.78836   0.00000  Uiso   1.00
H13    H     0.17492   0.76356   0.92474   0.00000  Uiso   1.00
N14    N     0.45070   0.92899   0.76244   0.00000  Uiso   1.00
H15    H     0.56943   0.97535   0.69501   0.00000  Uiso   1.00
H16    H     0.37839   1.02704   0.85552   0.00000  Uiso   1.00
H17    H     0.14288   0.16137   0.47841   0.00000  Uiso   1.00
H18    H     0.16199   0.38360   0.47364   0.00000  Uiso   1.00
O19    O     0.19153   0.28425   0.55356   0.00000  Uiso   1.00
H20    H     0.42811   0.48684   1.29034   0.00000  Uiso   1.00
H21    H     0.47148   0.66592   1.19074   0.00000  Uiso   1.00
O22    O     0.42416   0.53006   1.16395   0.00000  Uiso   1.00
H23    H     1.02808   0.84339   0.35043   0.00000  Uiso   1.00
H24    H     1.26008   0.89206   0.33389   0.00000  Uiso   1.00
O25    O     1.12528   0.93638   0.31450   0.00000  Uiso   1.00
H26    H     0.56599   0.44779   0.74778   0.00000  Uiso   1.00
H27    H     0.52585   0.40479   0.95559   0.00000  Uiso   1.00
O28    O     0.61078   0.36818   0.84513   0.00000  Uiso   1.00
H29    H    -0.09687   0.54687   0.19149   0.00000  Uiso   1.00
H30    H    -0.17557   0.45070  -0.01724   0.00000  Uiso   1.00
O31    O    -0.05880   0.46592   0.07451   0.00000  Uiso   1.00
H32    H     0.15571   0.07978   0.12682   0.00000  Uiso   1.00
H33    H     0.14440   0.28117   0.05083   0.00000  Uiso   1.00
O34    O     0.19673   0.15161   0.02204   0.00000  Uiso   1.00
H35    H     1.01975   0.06862   0.81708   0.00000  Uiso   1.00
H36    H     0.85730   0.12578   0.67571   0.00000  Uiso   1.00
O37    O     0.90983   0.01492   0.72827   0.00000  Uiso   1.00
H38    H     0.91975   0.72152   0.57942   0.00000  Uiso   1.00
H39    H     0.71176   0.67399   0.48805   0.00000  Uiso   1.00
O40    O     0.85261   0.65419   0.46201   0.00000  Uiso   1.00
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_geom_bond_site_symmetry_2
_ccdc_geom_bond_type
C1     O2      1.254   .     D
C1     N3      1.381   .     S
C1     N6      1.355   .     S
N3     H4      1.021   .     S
N3     H5      1.016   .     S
N6     H7      1.013   .     S
N6     H8      1.018   .     S
```

C9	O10	1.264	.	D
C9	N11	1.381	.	S
C9	N14	1.351	.	S
N11	H12	1.016	.	S
N11	H13	1.015	.	S
N14	H15	1.010	.	S
N14	H16	1.023	.	S
H17	O19	0.982	.	S
H18	O19	0.965	.	S
H20	O22	0.966	.	S
H21	O22	0.982	.	S
H23	O25	0.972	.	S
H24	O25	0.980	.	S
H26	O28	0.976	.	S
H27	O28	0.985	.	S
H29	O31	0.972	.	S
H30	O31	0.990	.	S
H32	O34	0.981	.	S
H33	O34	0.977	.	S
H35	O37	0.981	.	S
H36	O37	0.968	.	S
H38	O40	0.975	.	S
H39	O40	0.985	.	S

Table S1. Crystal structural calculated and experimental parameters

Structure	a	b	c	α	β	γ	Volume Å^3	Density gm/cm^3
Urea-molecule optimized	10.00	10.00	10.00	90.00	90.00	90.00	1000.00	0.010
Urea-crystal-Optimized	5.45	5.45	4.71	90.00	90.00	90.00	140.08	1.423
Exp[1]	5.66	5.66	4.71	90.00	90.00	90.00	151.00	1.321
Exp[2]	5.56	5.56	4.68	90.00	90.00	90.00	144.67	1.380
Urea-amorphous-6(CH4N2O)-4(H2O)	8.44	7.64	8.31	91.22	87.62	85.04	532.79	1.35
Urea-amorphous-4(CH4N2O)-6(H2O)	7.51	7.28	8.06	88.89	90.26	96.31	438.01	1.32
Urea-amorphous-2(CH4N2O)-8(H2O)	6.95	7.24	8.11	97.69	90.52	81.77	400.51	1.09
Urea-amorphous-2(CH4N2O)-8(H2O)-2	7.04	6.63	7.37	100.20	90.32	95.63	337.93	1.29
Urea-amorphous-2(CH4N2O)-8(H2O)-3	6.75	6.96	6.94	97.74	92.07	91.58	323.69	1.35

1(Worsham, Levy et al. 1957) 2(Swaminathan, Craven et al. 1984)

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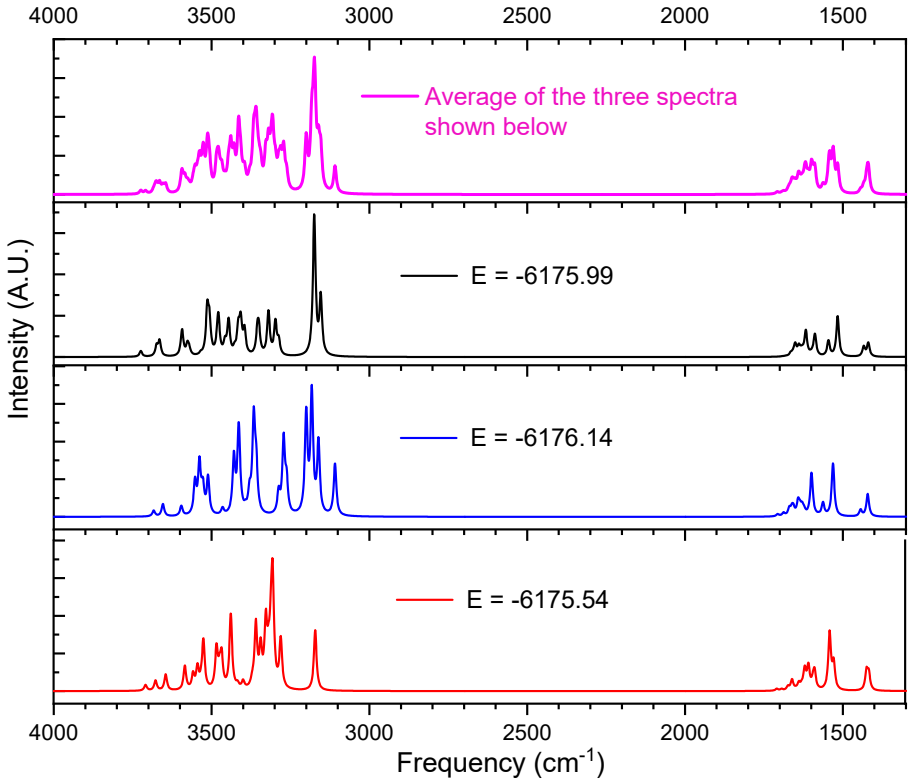

Figure S1. Calculated IR spectra of amorphous 2 urea: 8 H_2O structures.