Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

The formation of carbamate ion in interstellar ice analogues

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Supplementary information

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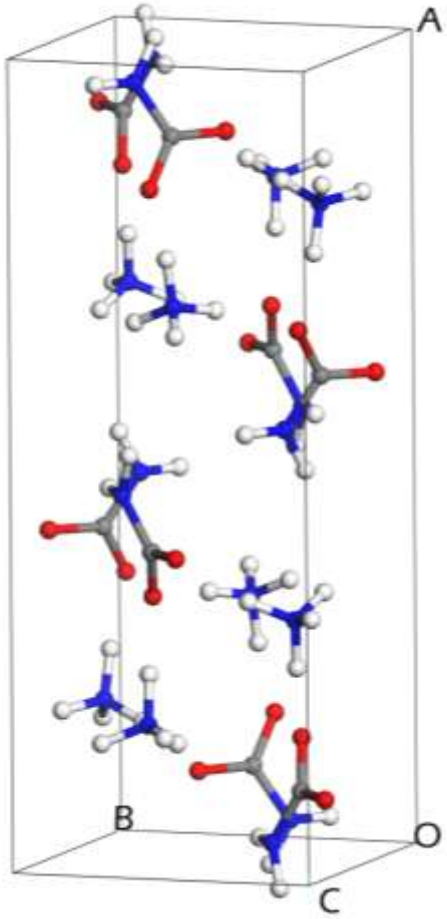
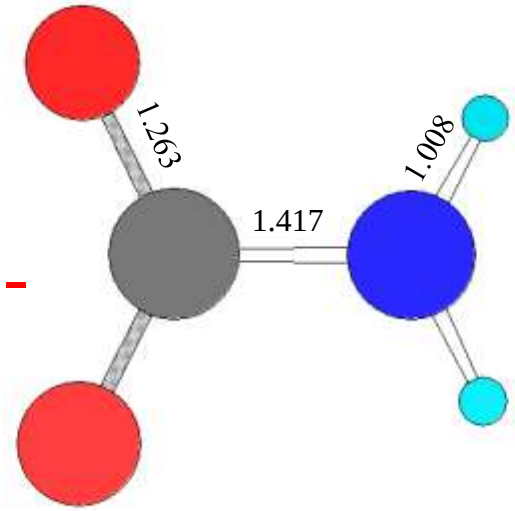
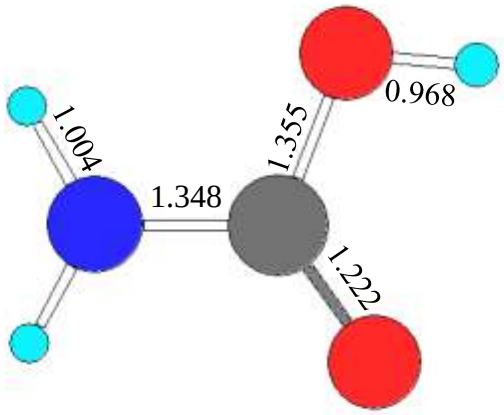


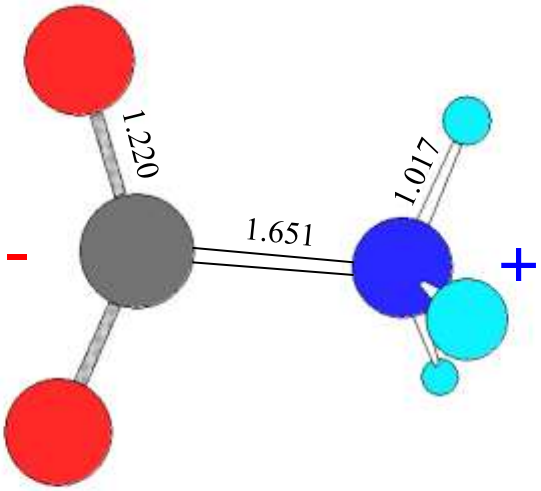
Figure S1.



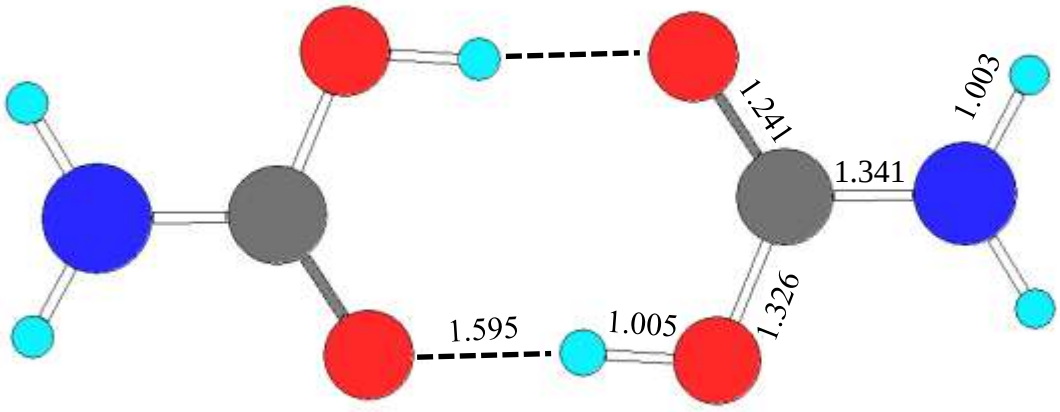
Carbamate anion



Neutral Carbamic Acid



Zwitterionic Carbamic Acid



Carbamic Acid Dimer

Figure S2.

Table S1. Calculated (this work) and experimental lattice parameters (a, b, c in Å and volume in $Å^3$), bond distances (Å) and angles (degrees) of crystalline Ammonium Carbamate.

Parameter	**Theoretical[a]**	**Experimental[b]**
a		17.121(6)
b		6.531(2)
c		6.742(3)
Volume		753.955
r(C-O)	1.290	1.289(5)
r(C-O)	1.280	1.279(5)
$r(N-H)_{carbamate}$	1.032	0.86(5)
$r(N-H)_{carbamate}$	1.017	0.82(6)
β(O-C-O)	123.4	123.5(3)
β(O-C-N)	118.5	118.7(3)
β(O-C-N)	117.9	117.9(3)
$\beta(H-N-H)_{carbamate}$	118.8	115(4)
β(H-N-C)	117.1	120(3)
β(H-N-C)	119.8	125(5)
$r(N-H)_{ammonium}$	1.062	0.99(5)
$r(N-H)_{ammonium}$	1.047	0.85(5)
$r(N-H)_{ammonium}$	1.055	0.91(5)
$r(N-H)_{ammonium}$	1.040	0.75(5)
$\beta(H-N-H)_{ammonium}$	111.4	121(4)
$\beta(H-N-H)_{ammonium}$	107.4	120(5)
$\beta(H-N-H)_{ammonium}$	108.7	108(5)
$\beta(H-N-H)_{ammonium}$	110.3	107(4)
$\beta(H-N-H)_{ammonium}$	111.7	94(5)
$r(O\bullet\bullet\bullet H)_{minimum}$	1.688	1.77(5)
$r(O\bullet\bullet\bullet H)_{maximum}$	1.910	2.19(5)

[a] PBE gradient-corrected functional (GGA). Cell parameters fixed to the experimental values.

[b] Ref. S1

References

S1. J. M. Adams and R. W. Small. *Acta Cryst.*, 1973, **B29**, 2317.