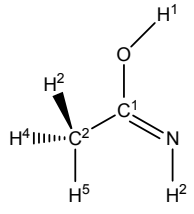
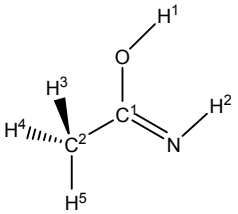
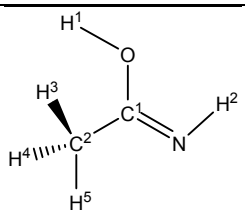
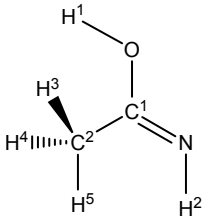
Electronic Supplementary Material for PCCP

TABLE S1: Theoretical geometrical parameters of the four acetimidic acid stereoisomers. Bond lengths given in Å, angles in degrees.

				
Parameters	(s-Z)-(E)	(s-Z)-(Z)	(s-E)-(Z)	(s-E)-(E)
r(OH^1)	0.97	0.96	0.96	0.96
r(C^1O)	1.36	1.37	1.37	1.36
r(C^1C^2)	1.50	1.50	1.50	1.51
r(C^1N)	1.27	1.27	1.26	1.26
r(C^2H)	1.08	1.08	1.08	1.09
r(H^1N)	2.26	2.45	3.08	3.04
r(H^2N)		1.02	1.02	1.01
r(H^3O)	2.63	2.63	2.73	2.71
α(C^1NH^2)	111.8	113.2	111.1	111.0
α(C^1OH^1)	106.6	109.5	111.0	110.0
Θ($C^2C^1OH^1$)	180	180	0	0
Θ($C^2C^1N^1H^2$)	0	180	180	0
Θ($H^5C^2C^1O$)	180	180	180	180
Dipolar moment (debey)	1.6	1.6	3.1	4.4
Energy (Hartree)	-209.2765	-209.2716	-209.2706	-209.2662
$E_{relative}$ (kJ mol^{-1})[a]	0	13	15	27

[a] $E_{relative}$: relative energy, the (s-Z)-(E) conformer is chosen as the reference.