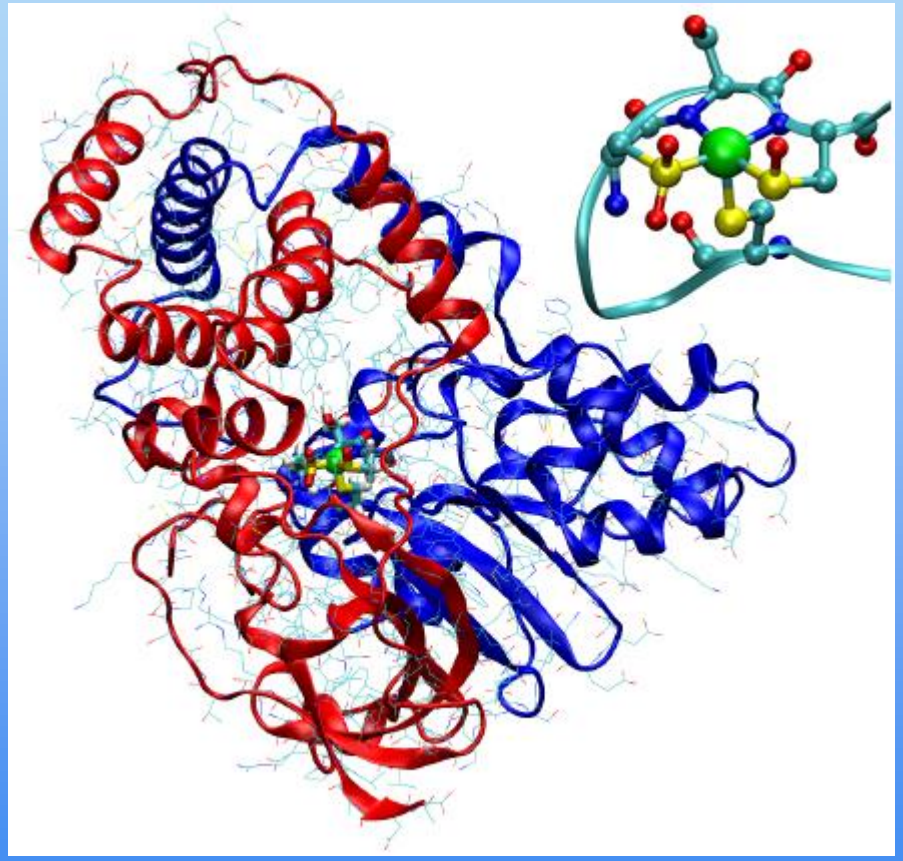
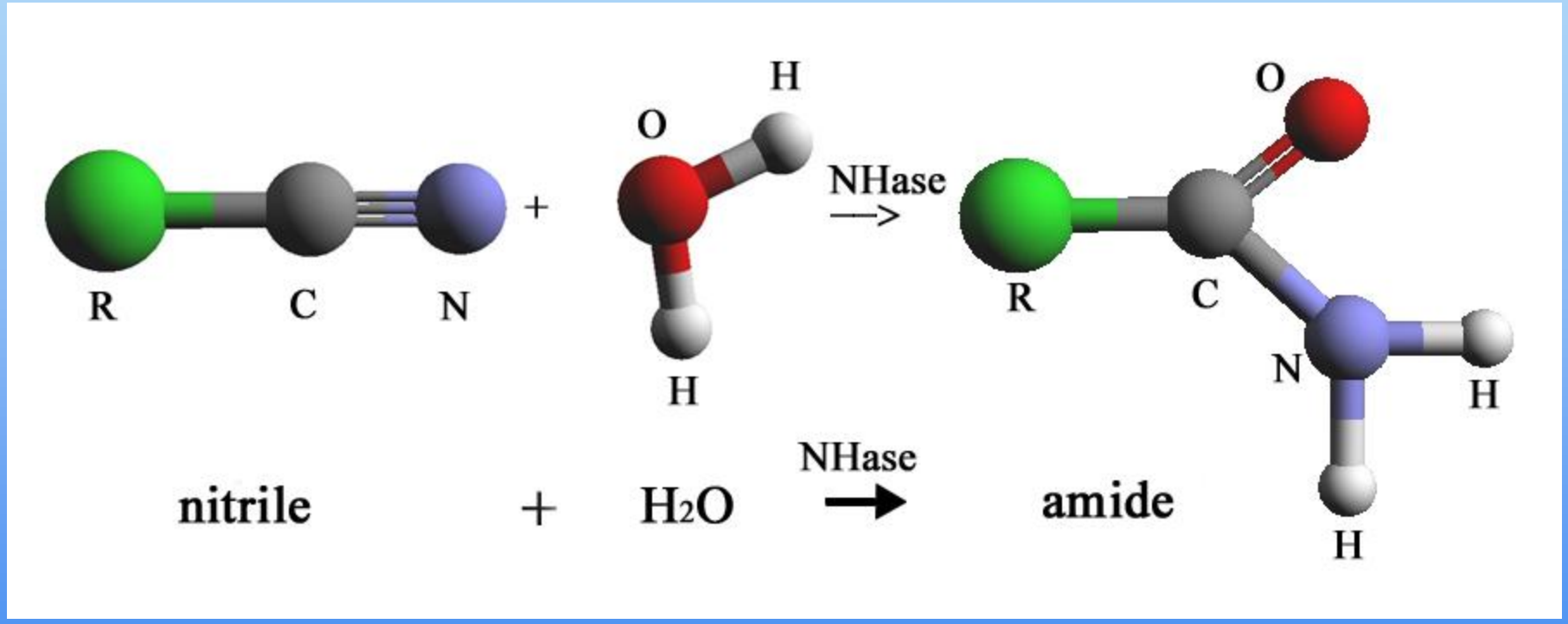
Nitryle hydration ex computational experiments



mgr Adrian Jasiński

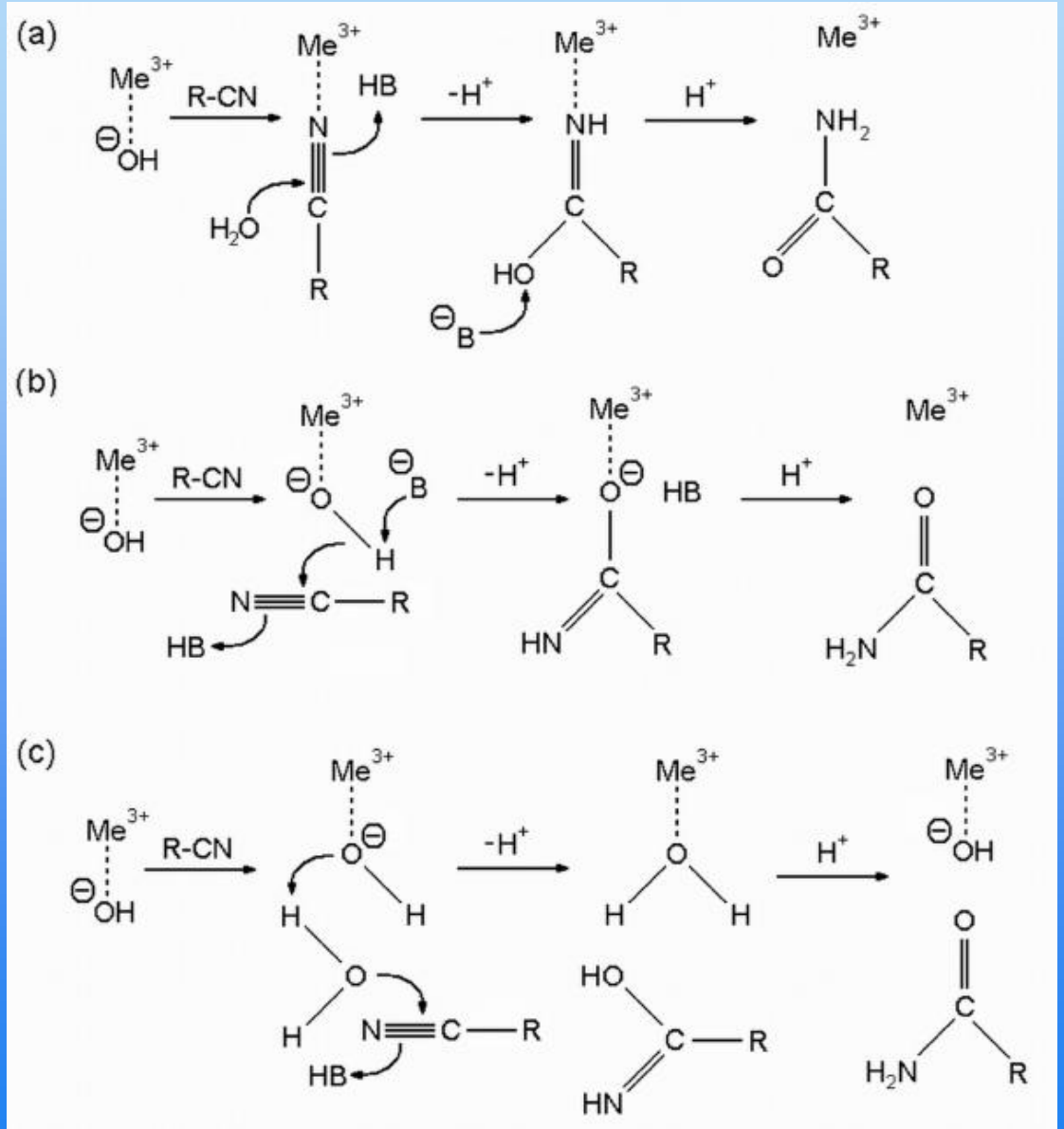
Theoretical Molecular Biophysics Group

Reaction



catalytic mechanism based on 2AHJ crystal structure

(Huang W., Jia J., Cummings J., Nelson M., Schneider G., Lindqvist Y., (1997), Structure, 5, 691-699.)



Calculation methods

- **PM3**, or **Parameterized Model number 3**, is a semi-empirical method for the quantum calculation of molecular electronic structure in computational chemistry.

  Stewart, J. J. P., *J. Comput. Chem.* ***10***, 209 (1989),
  Stewart, J. J. P., *J. Comput. Chem.* ***10***, 221 (1989)

- **BLYP** and **B3LYP –** DFT methods (density functional theory methods)

Calculation programs

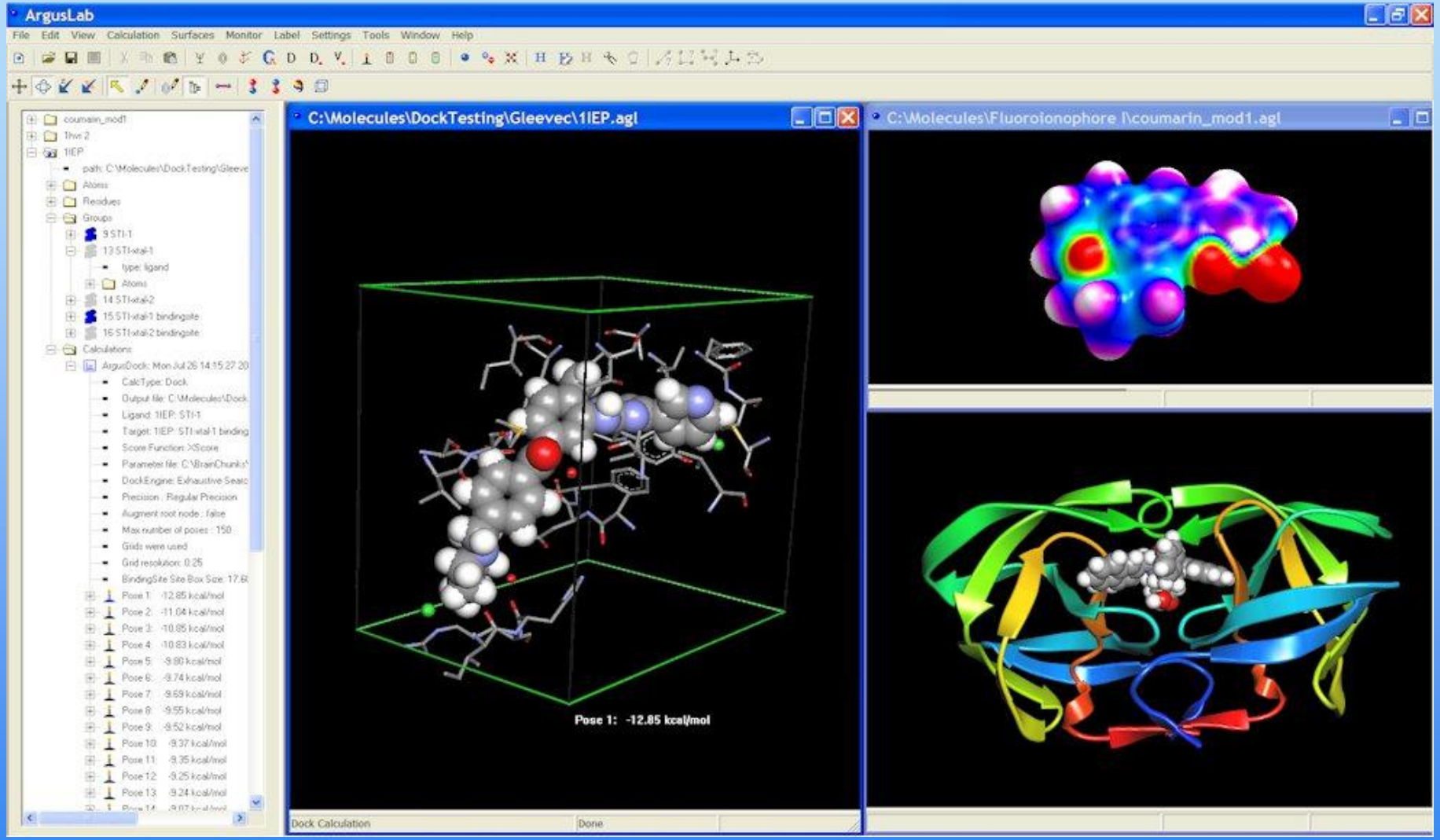
- **ArgusLab**

  Mark A. Thompson
  Planaria Software LLC, Seattle, WA
  http://www.arguslab.com

- **Gaussian**

  www.gaussian.com

Arguslab


ArgusLab
File Edit View Calculation Surfaces Monitor Label Settings Tools Window Help
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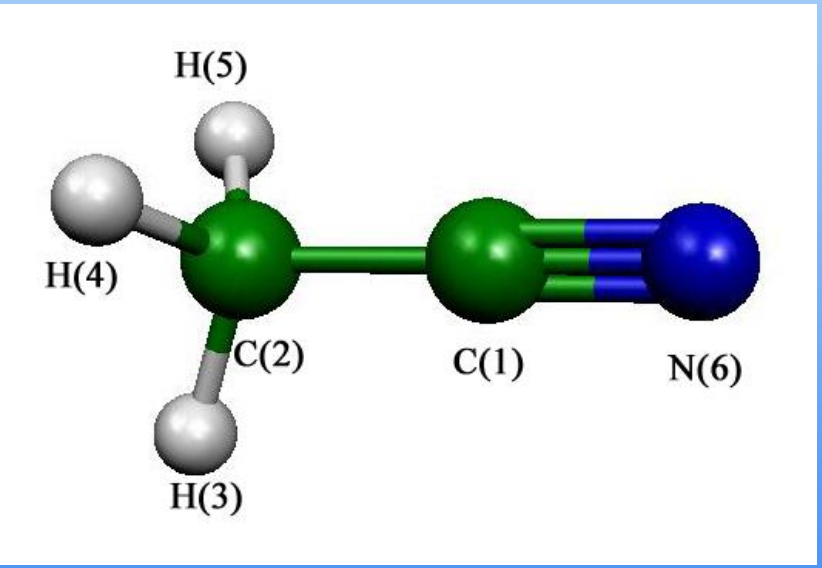
C:\Molecules\Fluoroionophore I\coumarin_mod1.agl
Pose 1: -12.85 kcal/mol
Dock Calculation
Done

Calculation results

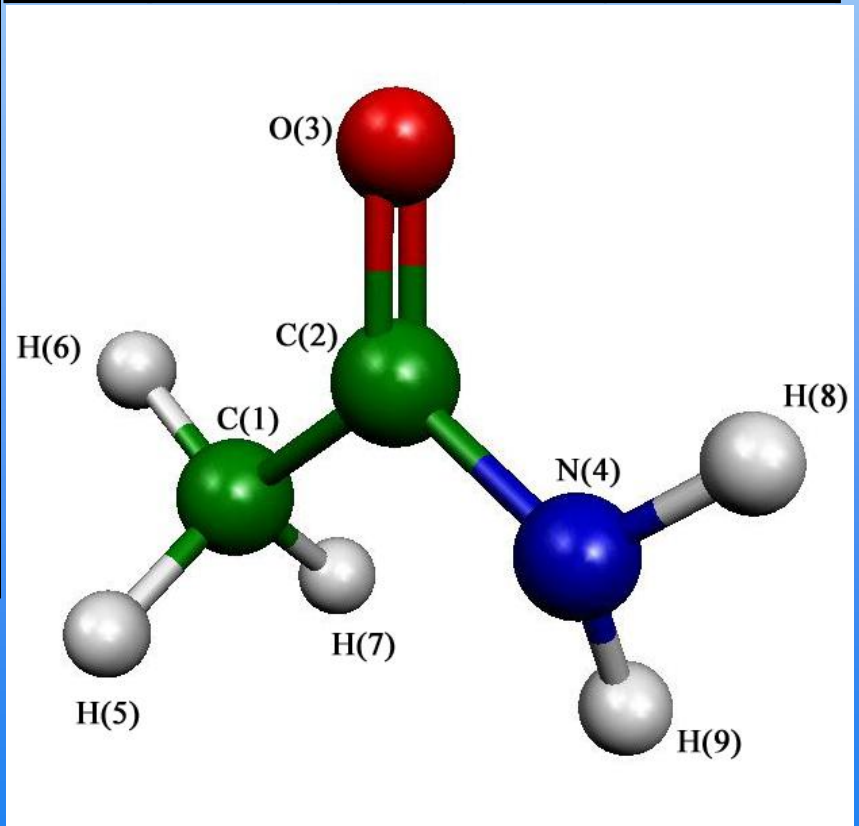
nitrile



	Definition	PM3	BLYP	B3LYP
length (Å)	R(1,2)	1.44	1.468	1.46
	R(1,6)	1.16	1.173	1.16
	R(2,3)	1.098	1.101	1.094
	R(2,4)	1.098	1.101	1.094
	R(2,5)	1.098	1.101	1.094
bonds (º)	A(2,1,6)	180	180	180
	A(1,2,3)	110.4	110.4	110.3
	A(1,2,4)	110.4	110.5	110.3
	A(1,2,5)	110.4	110.4	110.3
	A(3,2,4)	108.5	108.4	108.6
	A(3,2,5)	108.5	108.6	108.7
	A(4,2,5)	108.5	108.4	108.6
Torsia (º)	D(6,1,2,3)	-154.3	-140.6	-141.7
	D(6,1,2,4)	-34.3	-20.6	-21.7
	D(6,1,2,5)	85.8	99.2	98.2

	Definition	PM3	BLYP	B3LYP
length (Å)	R(1,2)	1.504	1.537	1.523
	R(1,5)	1.098	1.103	1.095
	R(1,6)	1.098	1.096	1.089
	R(1,7)	1.098	1.103	1.095
	R(2,3)	1.223	1.234	1.221
	R(2,4)	1.422	1.382	1.369
	R(4,8)	0.996	1.016	1.008
	R(4,9)	0.995	1.015	1.006
Bonds (°)	A(2,1,5)	110.9	111.2	110.9
	A(2,1,6)	111.5	108.5	108.5
	A(2,1,7)	111.3	111.1	110.9
	A(5,1,6)	107.5	109.1	109.2
	A(5,1,7)	107.8	107.6	107.7
	A(6,1,7)	107.5	109.1	109.2
	A(1,2,3)	124.6	123.2	123.1
	A(1,2,4)	117.8	114.6	114.7
	A(3,2,4)	117.5	122	122.1
	A(2,4,8)	115.4	118	118.0
	A(2,4,9)	114	123	122.7
	A(8,4,9)	112.9	118.9	119.1

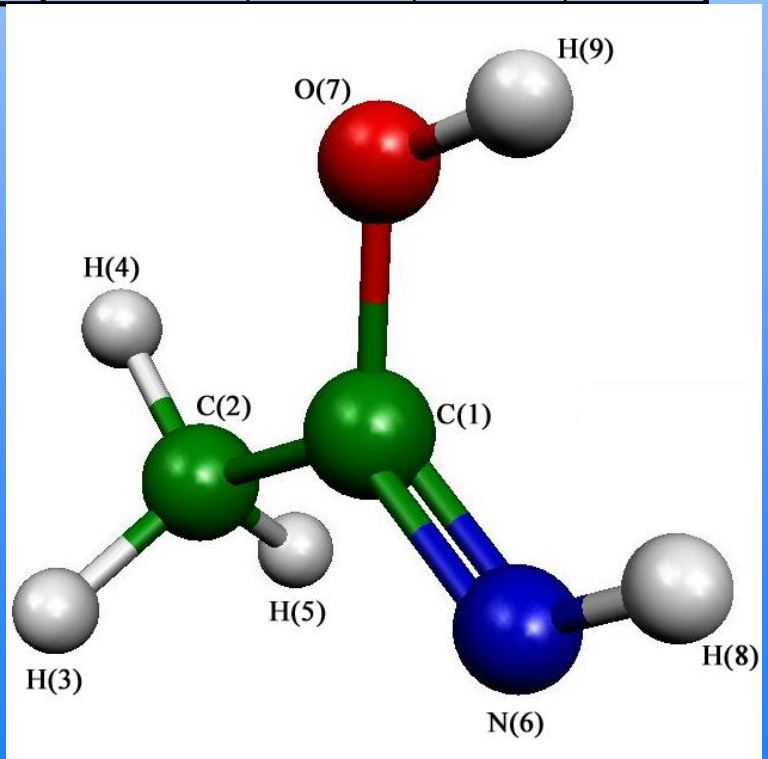
(°)	D(5,1,2,3)	-116.8	-120	-120
	D(5,1,2,4)	59	59.9	59.9
	D(6,1,2,3)	3	0	0
	D(6,1,2,4)	180	180	180
	D(7,1,2,3)	120	120	120
	D(7,1,2,4)	-60	-59.9	-59.9
	D(1,2,4,8)	164.9	-180	-180
	D(1,2,4,9)	31.8	0	0
	D(3,2,4,8)	-18	0	0
	D(3,2,4,9)	180	180	180



amide

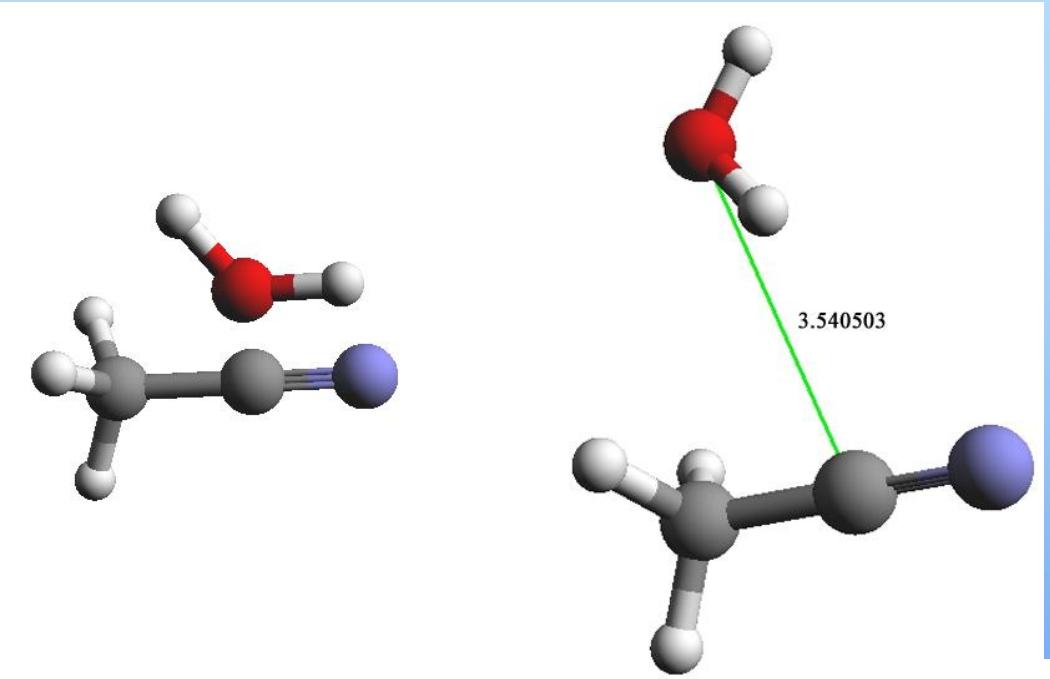
	Definicja	PM3	BLYP	B3LYP
length (Å)	R(1,2)	1.497	1.519	1.508
	R(1,6)	1.293	1.283	1.270
	R(1,7)	1.37	1.386	1.368
	R(2,3)	1.098	1.099	1.092
	R(2,4)	1.098	1.097	1.090
	R(2,5)	1.098	1.099	1.092
	R(6,8)	0.990	1.034	1.024
	R(7,9)	0.949	0.980	0.969
bonds (°)	A(2,1,6)	122.4	121.5	121.6
	A(2,1,7)	112.5	110.6	110.9
	A(6,1,7)	124.9	127.7	127.3
	A(1,2,3)	110.7	109.7	109.6
	A(1,2,4)	112.4	111	111
	A(1,2,5)	110.7	109.7	109.6
	A(3,2,4)	107.7	109.3	109.4
	A(3,2,5)	107.4	107.4	107.5
	A(4,2,5)	107.7	109.3	109.4
	A(1,6,8)	117.8	111.9	112.3
	A(1,7,9)	110.7	107.9	108.9

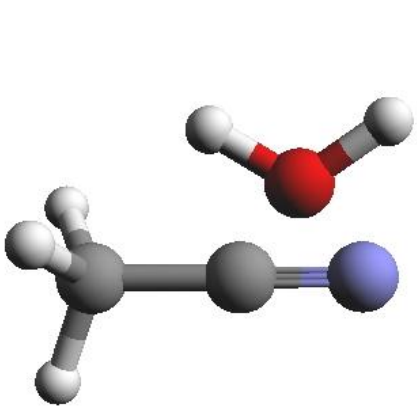
(°)	D(6,1,2,3)	59.4	58.8	58.8
	D(6,1,2,4)	180	180	180
	D(6,1,2,5)	-59.4	-58.8	-58.8
	D(7,1,2,3)	-120.5	-121.1	-121.1
	D(7,1,2,4)	0	0	0
	D(7,1,2,5)	120.5	121.1	121.1
	D(2,1,6,8)	180	-180	180
	D(7,1,6,8)	0	0	0
	D(2,1,7,9)	-180	180	180
	D(6,1,7,9)	0	0	0

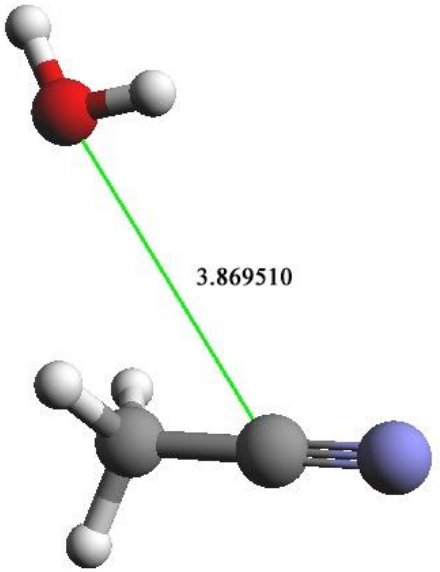


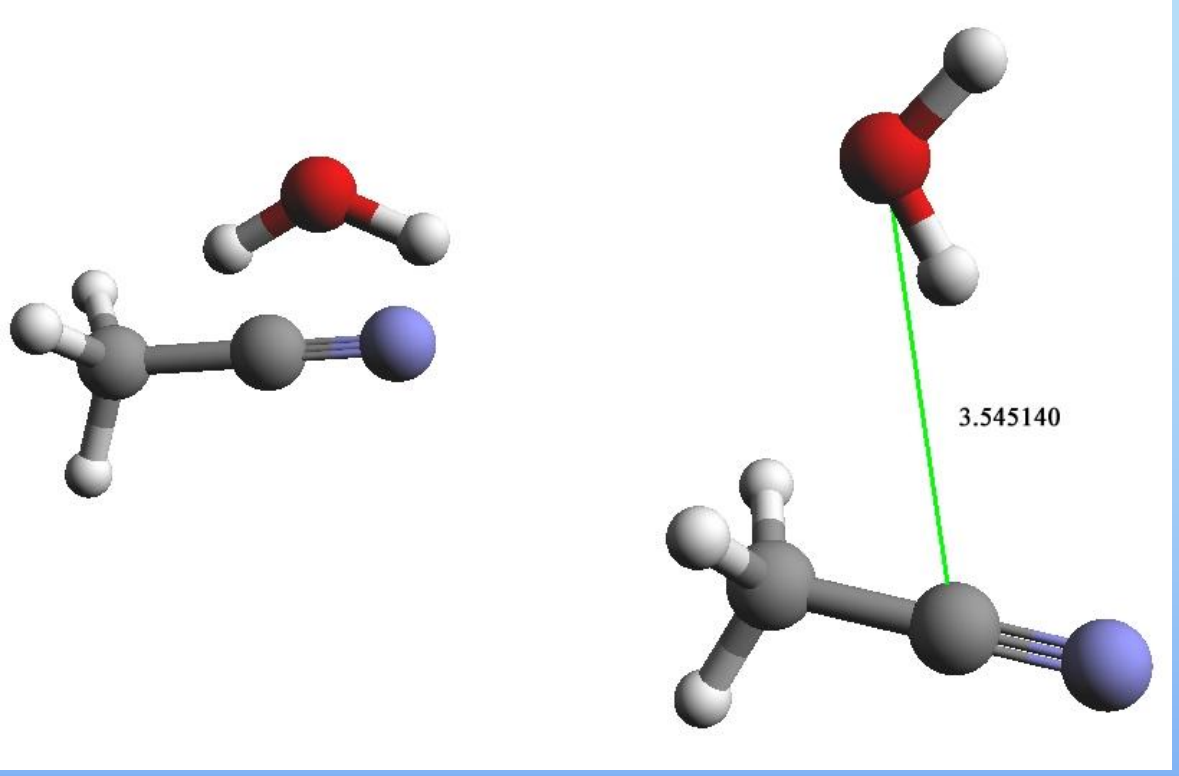
imid

Nitrile +H_2O





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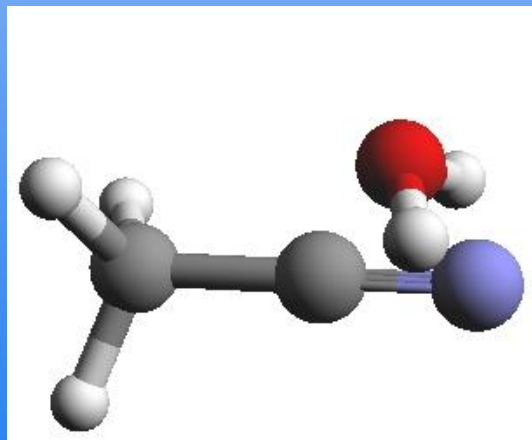

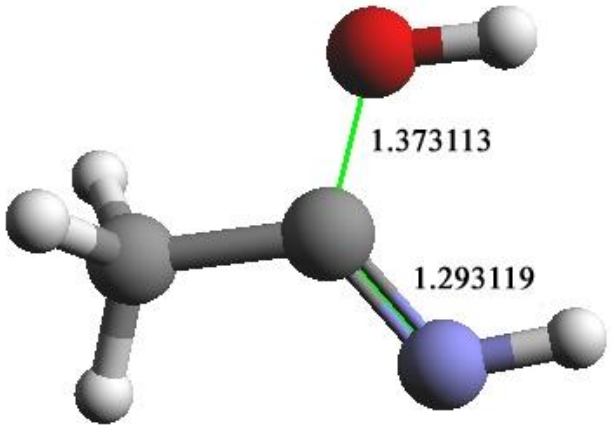
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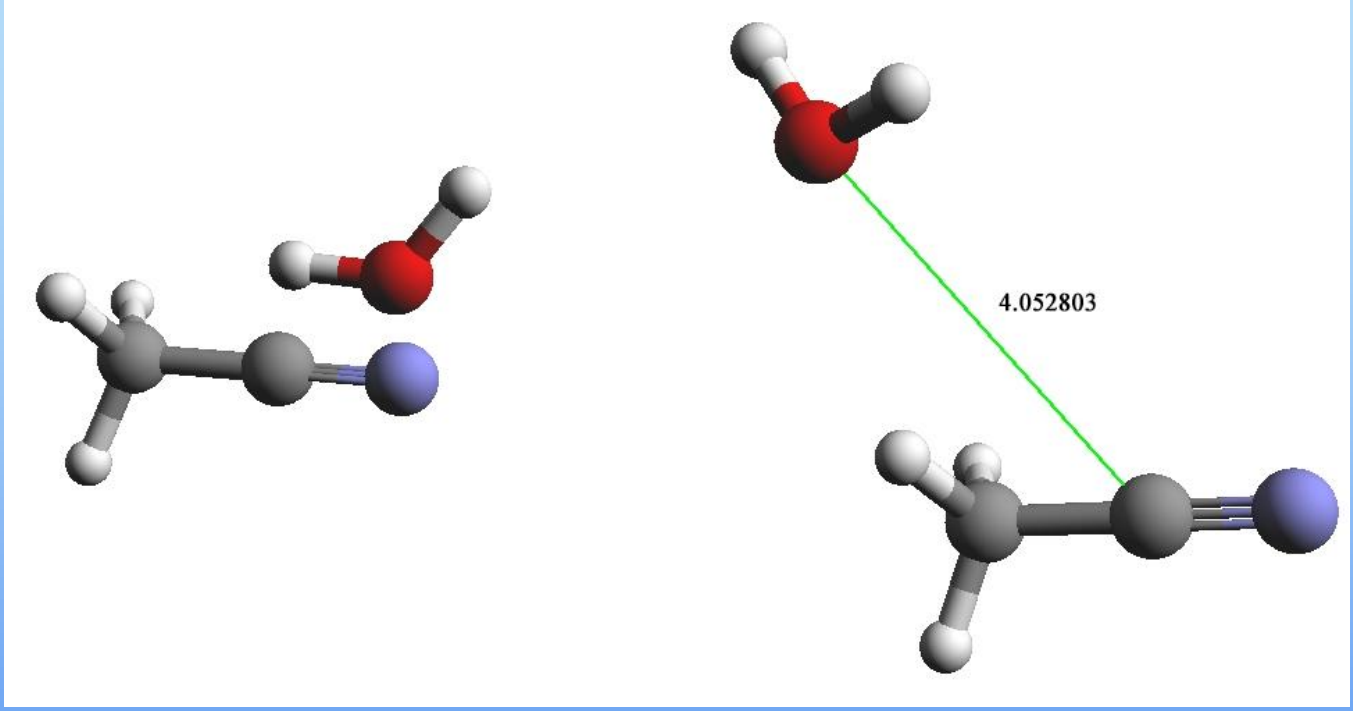
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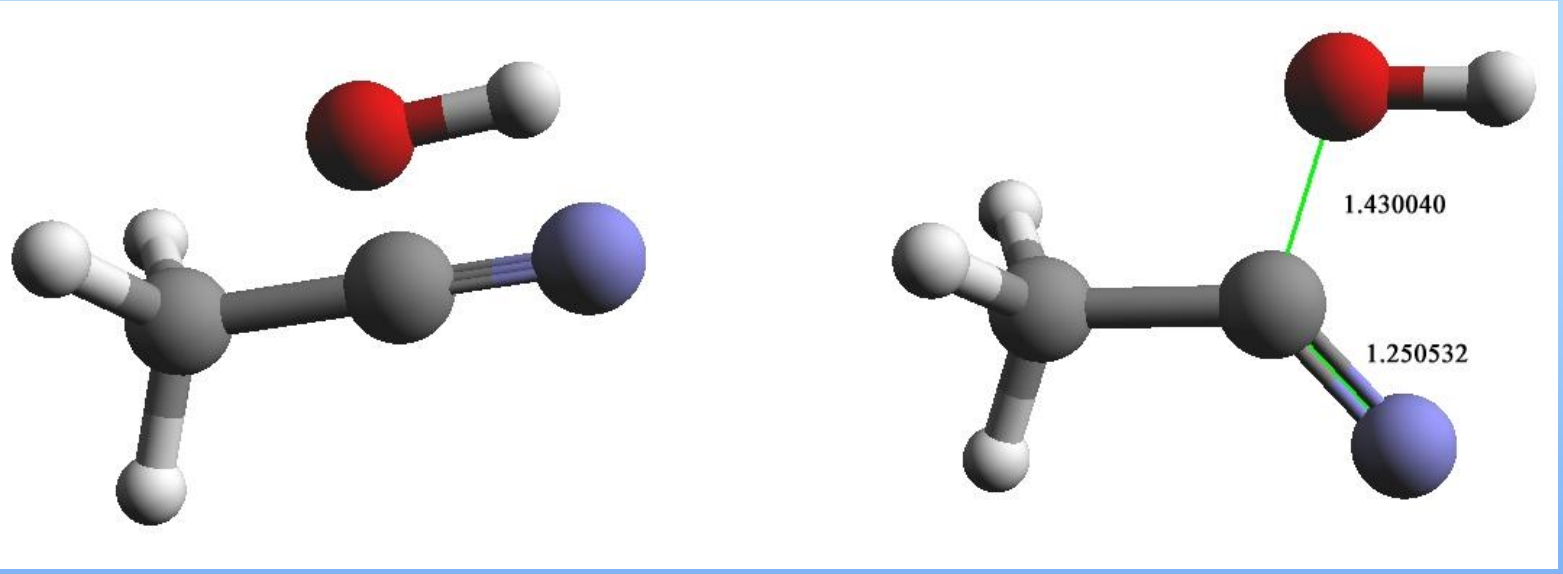
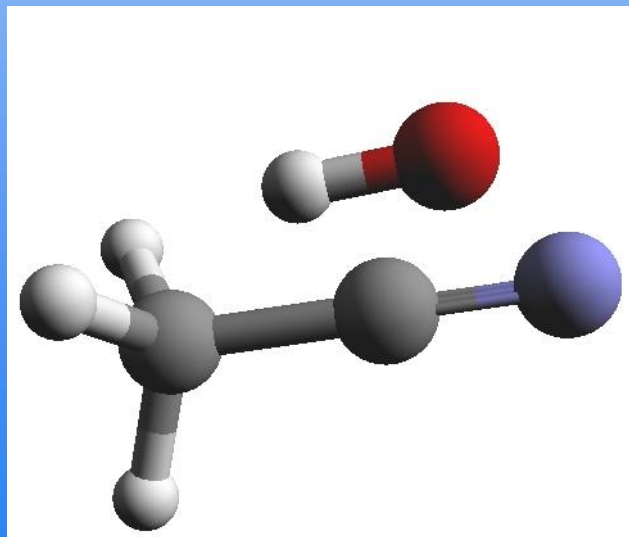
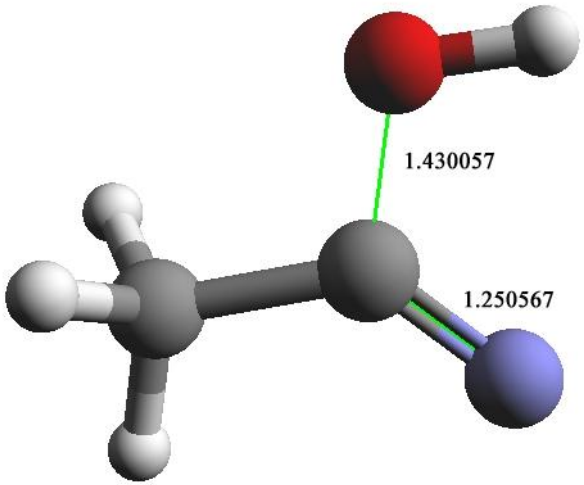
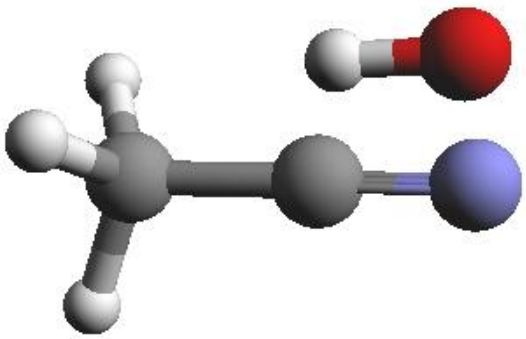
nitrile + OH^-

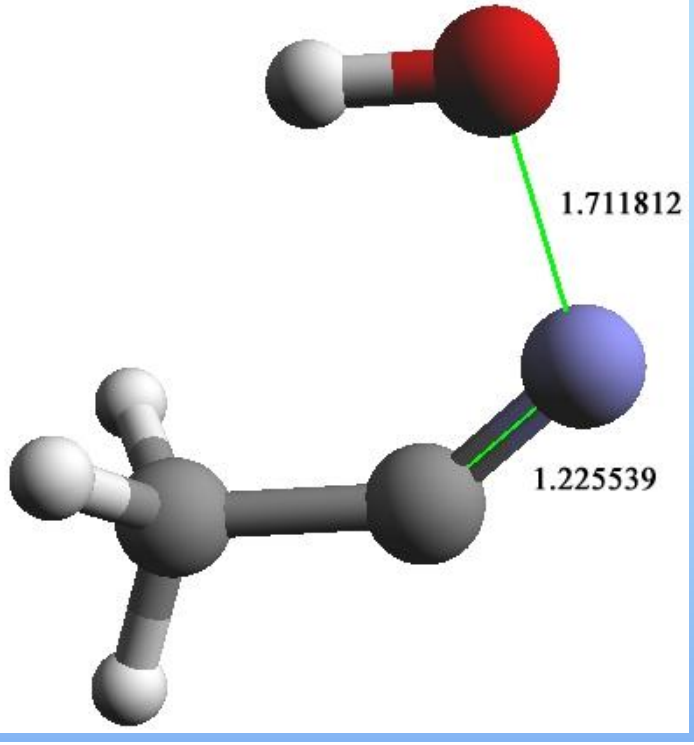
mechanism (c)







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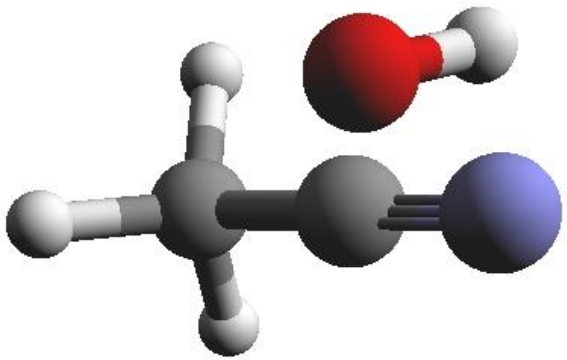

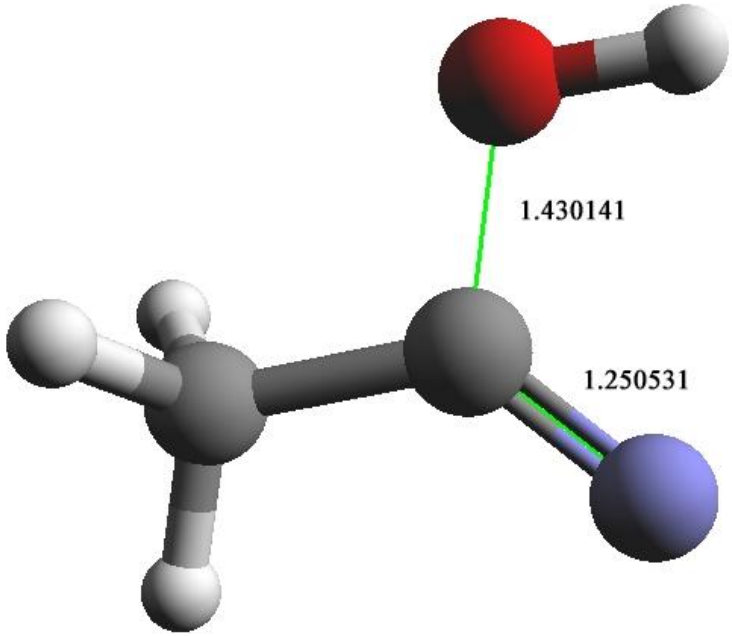
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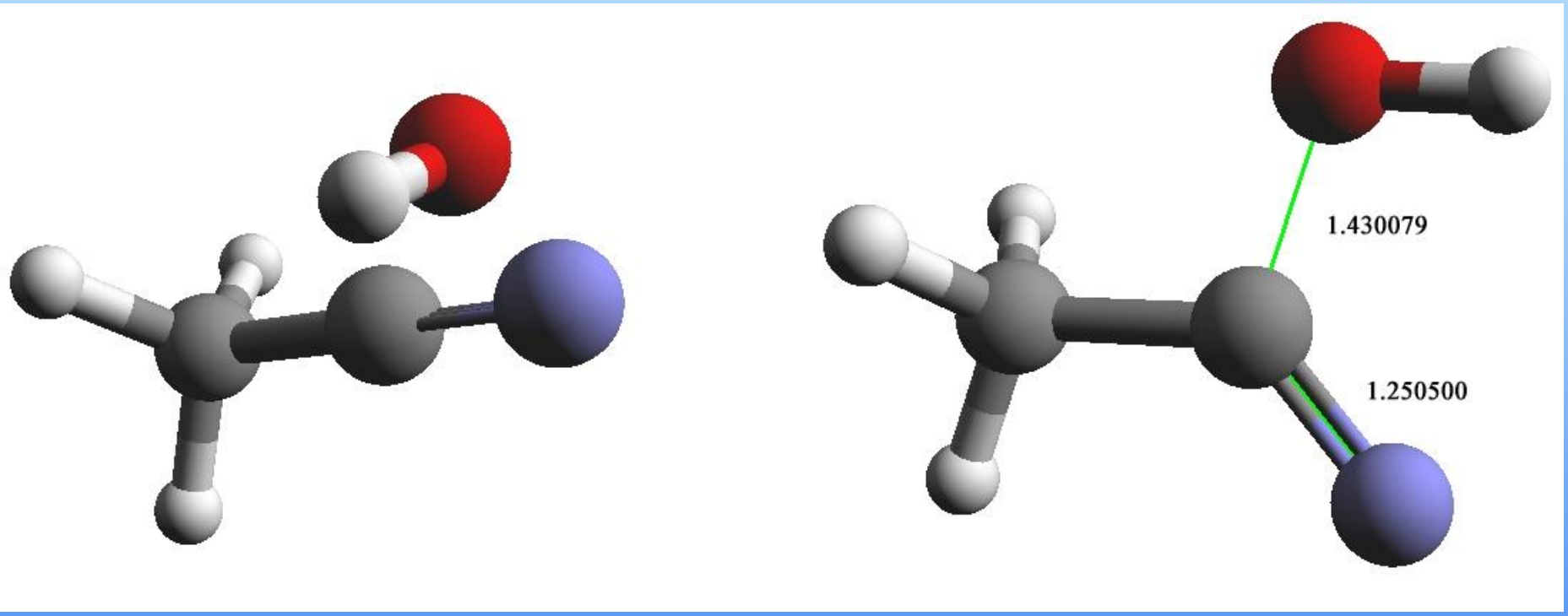
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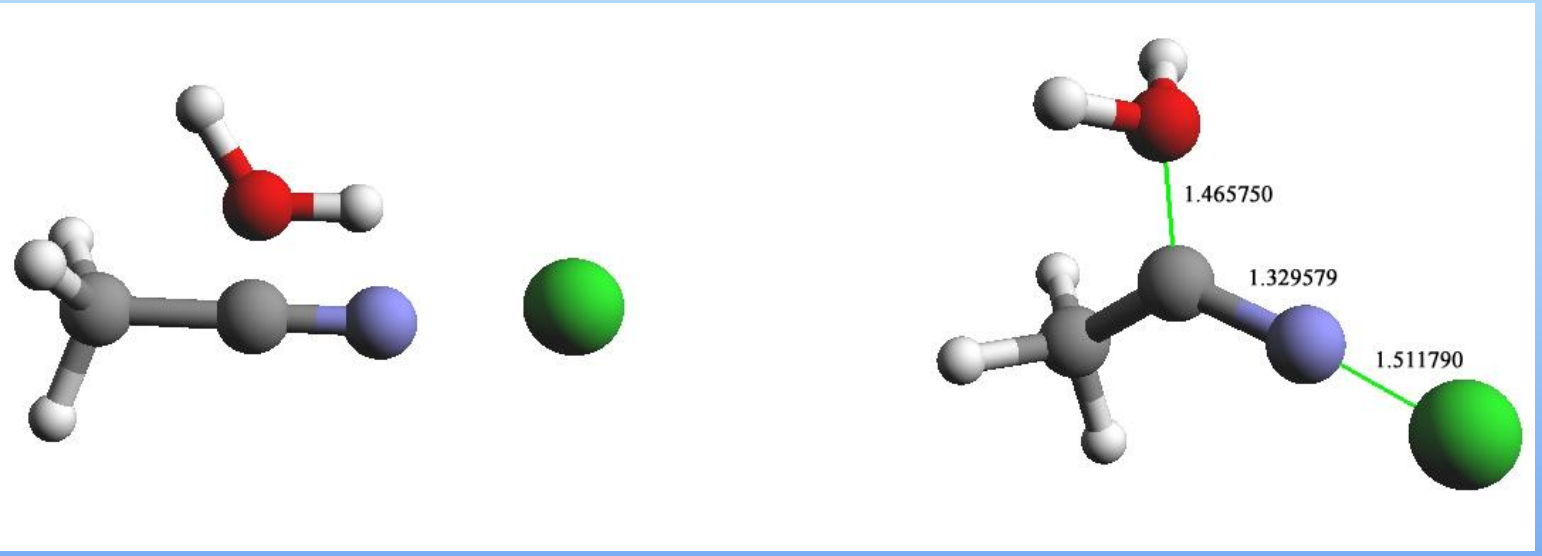
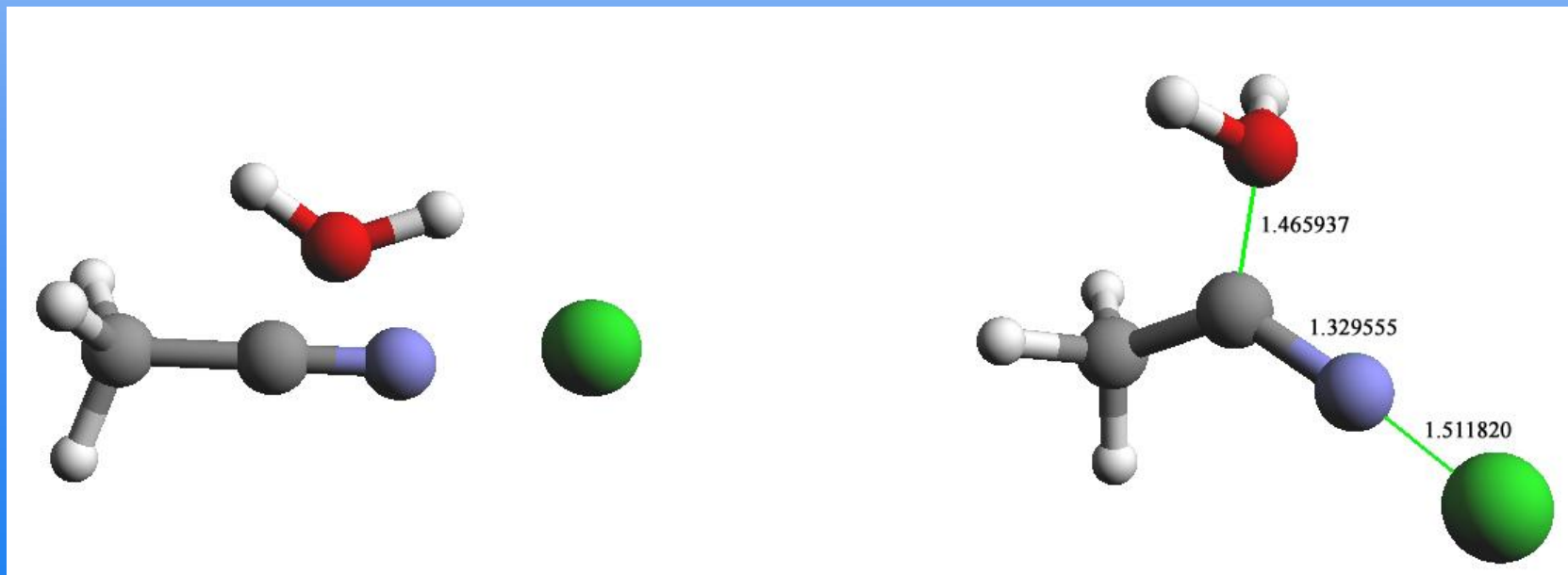
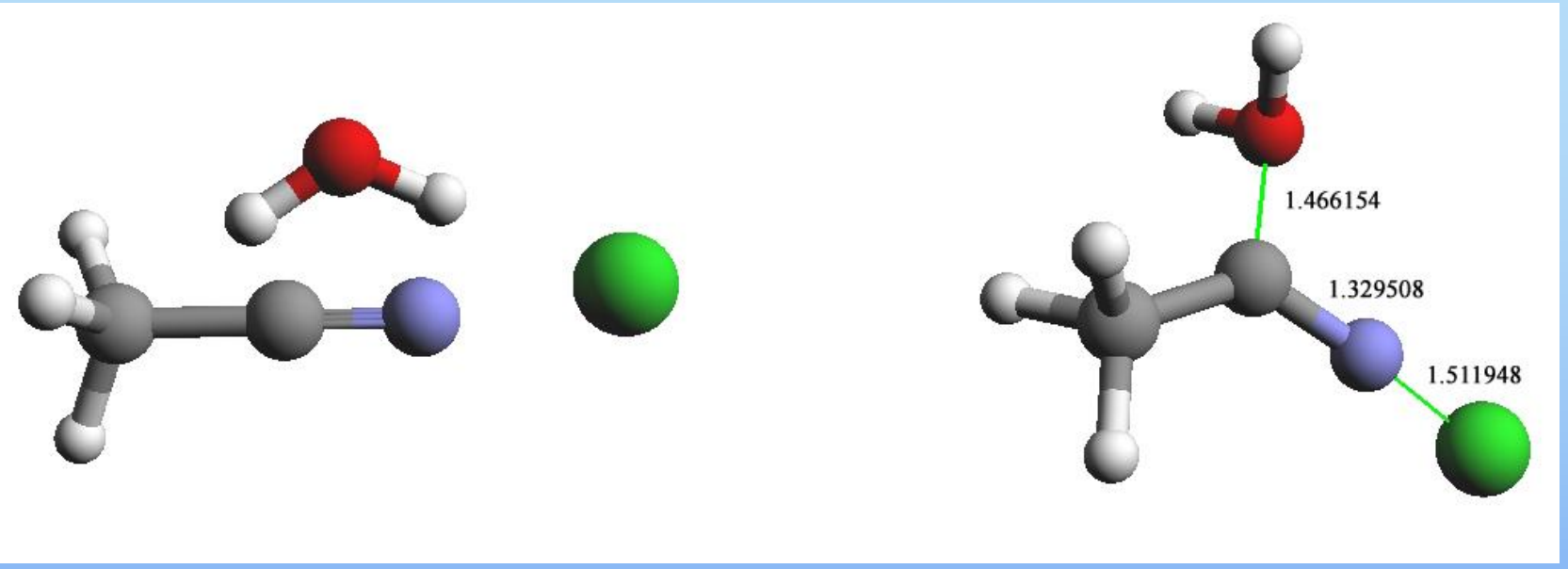
1.250500

nitrile + metal ion

mechanism (a)



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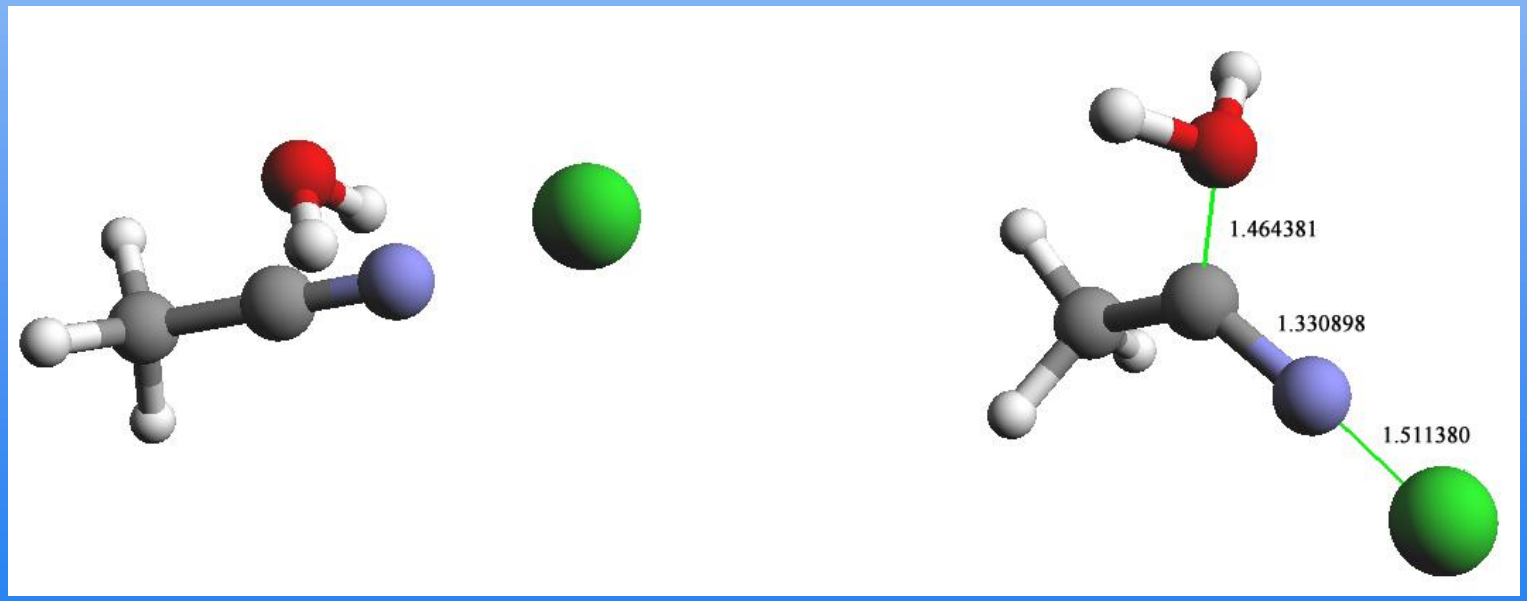
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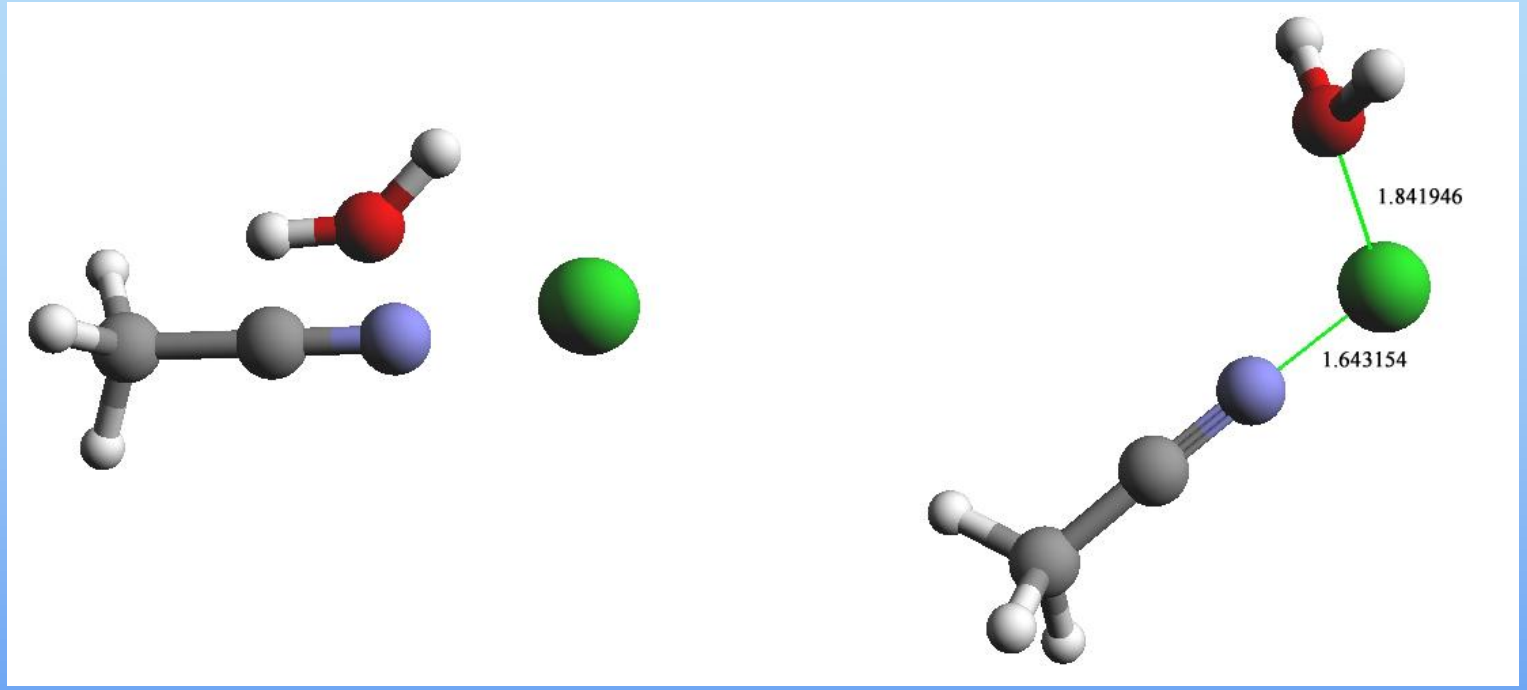
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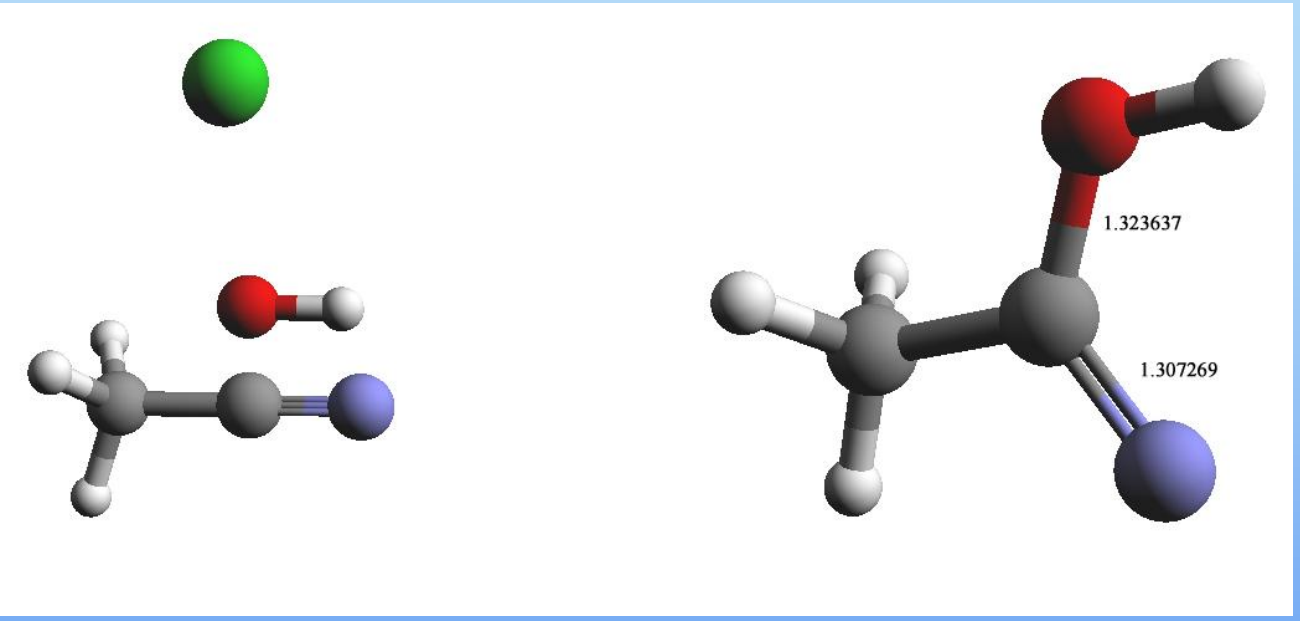
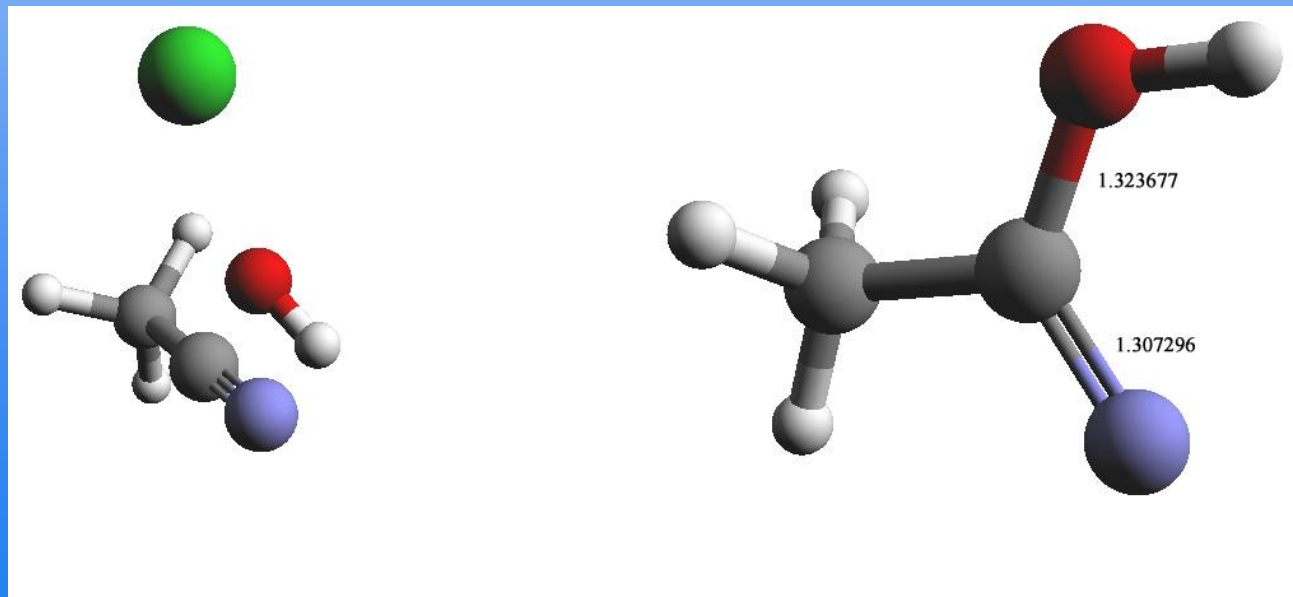
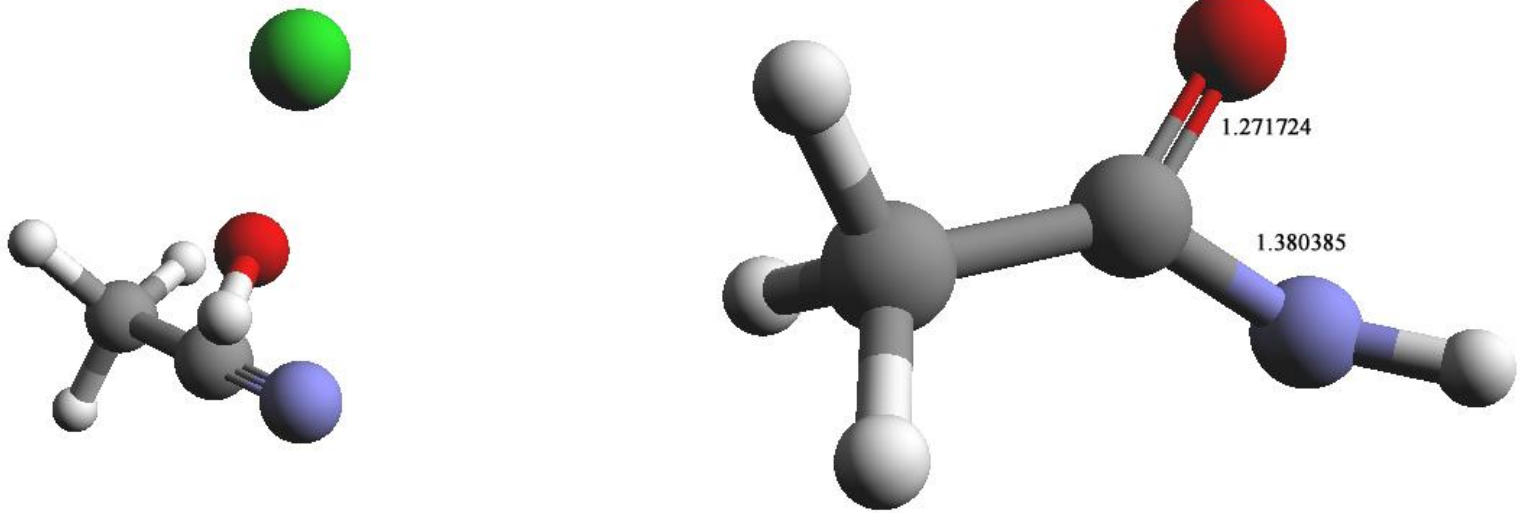
nitrile + metal ion

Mechanism (b)



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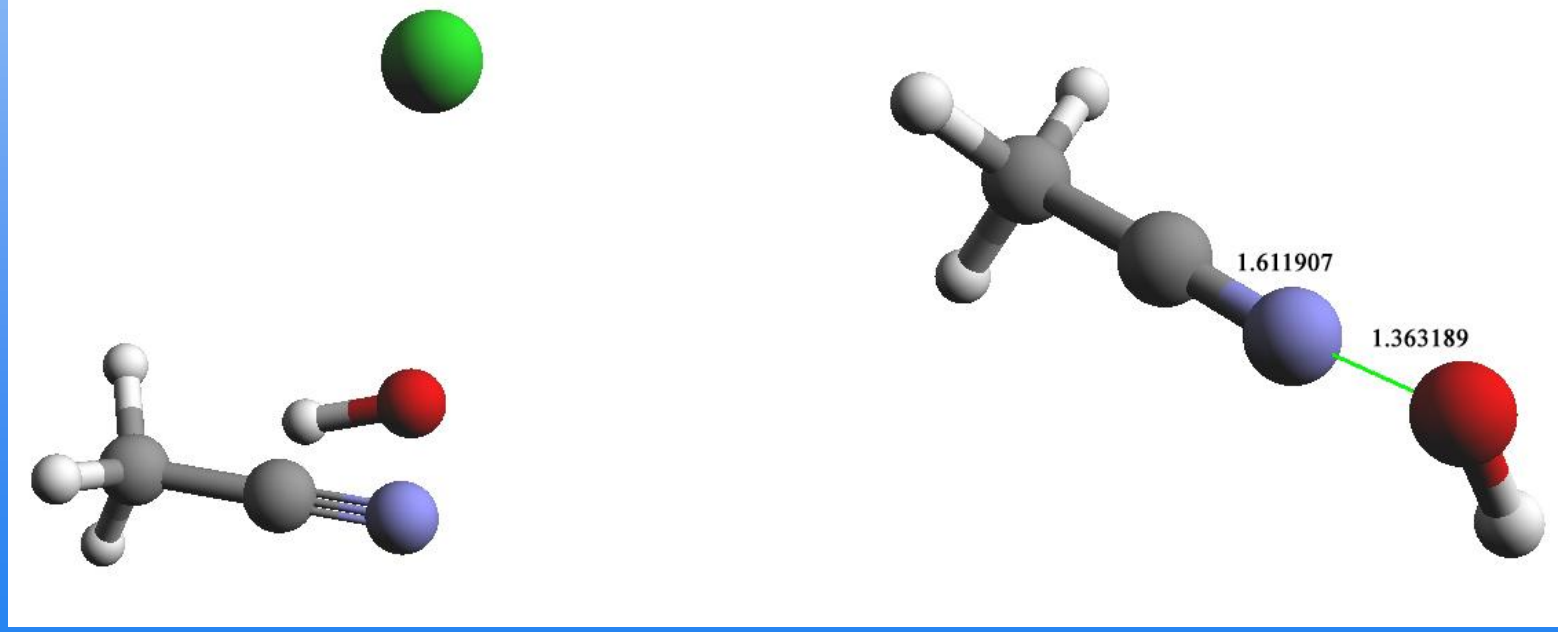
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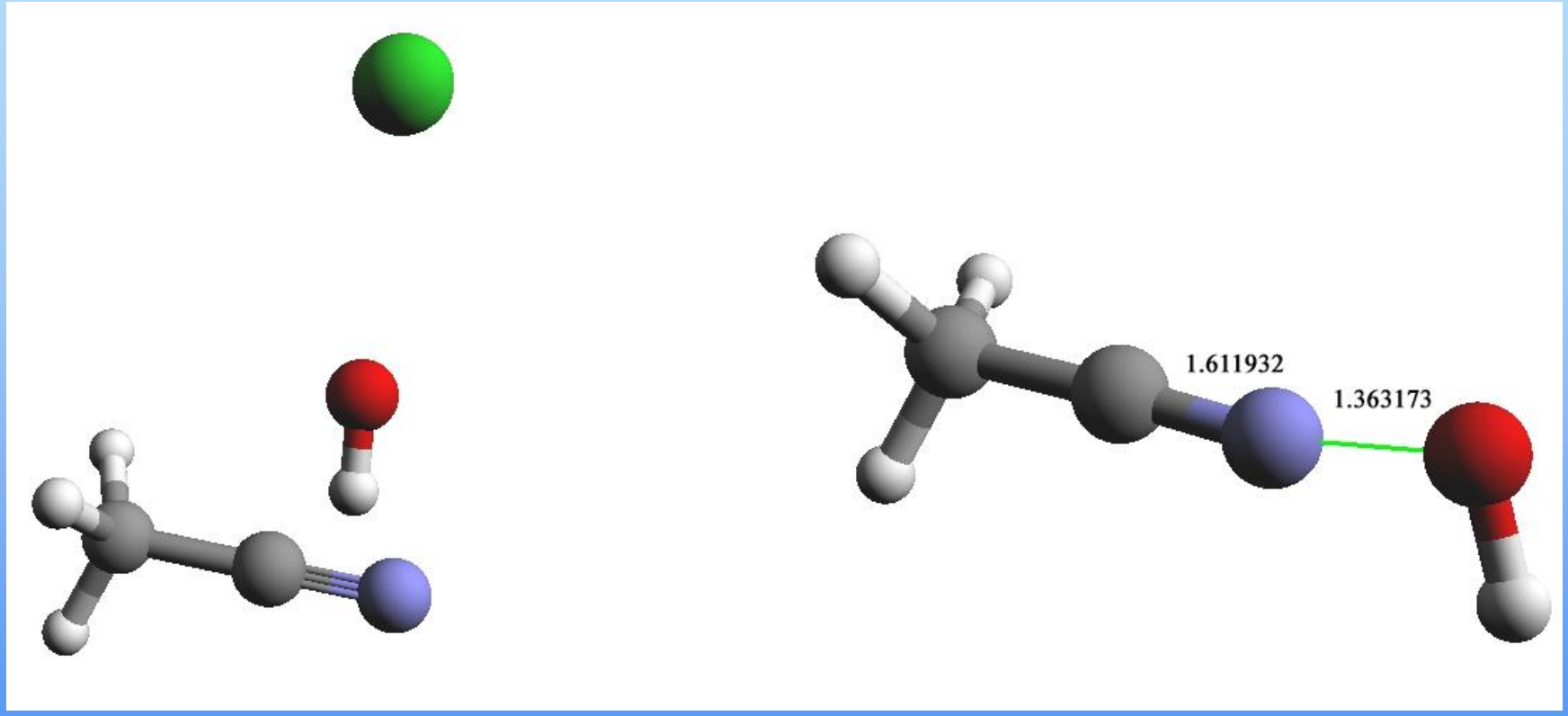
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Thank You
for
Your Attention