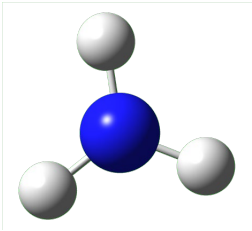
S.0 Supplemental Information

Table S1. Gaussian09 Input Data for the optimization and frequency of the NH_3 species, showing a Gaussview 5 model of the structure.

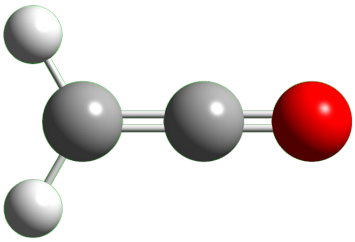


```
0 1
 N          -0.19230770  -0.68047336   0.00000000
 H          -1.50887582   0.34023668   0.00000000
 H           0.93195271   0.44378698   0.00000000
 H          -0.13313610  -2.11538458   0.00000000
```

APFD/6-31g(d)

opt=calcfc freq apfd/6-31g(d) pressure=0 temperature=15

Table S2. Gaussian09 Input Data for the optimization and frequency of the CH_2CO species (Ketene), showing a Gaussview 5 model of the structure.



```
0 1
 O          -0.41420121   2.14497038   0.00000000
 C          -0.44378701   0.54733727   0.00000000
 C          -0.44378701  -1.09467454   0.00000000
 H          -1.86390542  -2.18934908  -0.00000000
 H           0.84319531  -2.23372778   0.00000000
```

APFD/6-31g(d)

opt=calcfc freq apfd/6-31g(d) pressure=0 temperature=15

Table S3. Gaussian09 Input Data for the frequency of the first transition state species, showing a Gaussview 5 model of the structure.

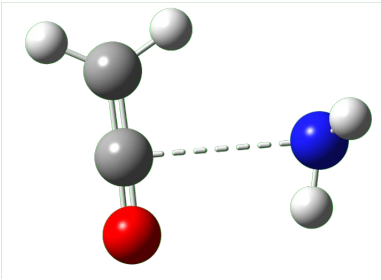
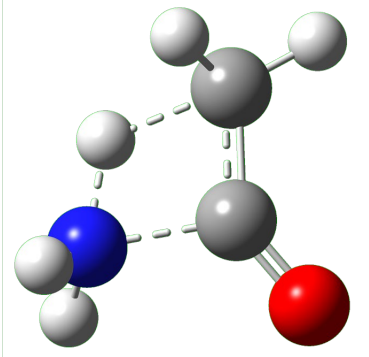

0 1 C 1.08607700 -1.15370400 -0.00004900 H 2.07000500 -1.57163800 -0.00004500 H 0.21642500 -1.77162200 -0.00036700 C 0.91926700 0.13142400 0.00007900 N -1.99147300 -0.11887200 -0.00004900 H -2.45130600 -0.44259900 0.83164400 H -1.87583400 0.87836800 0.00071800 O 0.80023300 1.28928300 -0.00003700 H -2.45291400 -0.44098600 -0.83148900
APFD/6-31g(d)
freq apfd/6-31g(d) pressure=0 temperature=15

Table S4. Gaussian09 Input Data for the frequency of the second transition state species, showing a Gaussview 5 model of the structure.



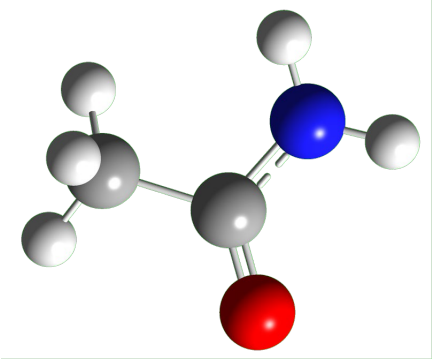
0 1

C	0.31813700	-0.07879500	0.08508300
C	0.26994800	1.34157300	-0.06615900
H	1.20020100	1.85001900	-0.31503100
H	-0.30318900	1.85601300	0.71066900
O	1.10213800	-0.98500800	0.01455200
N	-1.28005700	-0.36041700	-0.03167900
H	-1.45556300	-1.09082400	-0.72107000
H	-1.06457000	0.80206900	-0.52243600
H	-1.76210000	-0.59096400	0.83966600

APFD/6-31g(d)

freq apfd/6-31g(d) pressure=0 temperature=15

Table S5. Gaussian09 Input Data for the optimization and frequency of the CH_3CONH_2 product species, showing a Gaussview 5 model of the structure.



0 1

C	-0.07396450	-0.81360946	0.00000000
C	1.67159772	-1.27218933	0.00000000
N	-1.98224862	-1.27218933	0.00000000
O	-0.05917160	1.18343194	0.00000000
H	-3.53550314	-0.66568046	0.00000000
H	-2.85502973	-2.54437866	0.00000000
H	2.64792913	-0.35502958	0.00000000
H	3.18047354	-1.80473370	0.00000000
H	1.73076932	-2.79585795	0.00000000

APFD/6-31g(d)

```
# opt=calcfc freq apfd/6-31g(d) pressure=0 temperature=15
```

Table S6: Thermodynamic Properties of Components in Proposed Reaction Mechanism

	Reactant Ammonia (NH_3)	**Reactant Ketene (CH_2CO)**	**Intermediate**	**Transition State**	**Product Acetamide (CH_3CONH_2)**
ΔE (kJ/mol)	-148221.41	-400226.01	-548482.79	-548339.79	-548644.64
ΔG (kJ/mol)	-148222.80	-400227.97	-548485.15	-548342.08	-548646.93
ΔH (kJ/mol)	-148221.28	-400225.88	-548482.67	-548339.67	-548644.51

Table S7: Sum of Thermodynamic Properties of Reaction Pathway

	Sum of Reactants	**Intermediate**	**Transition State**	**Product**
ΔE (kJ/mol)	-548447.42	-548482.79	-548339.79	-548644.64
ΔG (kJ/mol)	-548450.77	-548485.15	-548342.08	-548646.93
ΔH (kJ/mol)	-548447.16	-548482.67	-548339.67	-548644.51

Table S8: Summary of Differences in Thermodynamic Properties of Reaction Mechanism

	Reactants Ammonia and Ketene (NH_3 and CH_2CO)	**Intermediate**	**Transition State**	**Product Acetamide (CH_3CONH_2)**
ΔE (kJ/mol)	0	-35.38	107.62	-197.22
ΔG (kJ/mol)	0	-34.38	108.70	-196.15
ΔH (kJ/mol)	0	-35.51	107.50	-197.36