Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

Computational Studies on the Possible Formation of Glycine via Open Shell Gas-Phase Chemistry in the Interstellar Medium

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In this work, We do not propose a three/four body collision. Instead, We are proposing a sequence of two body collisions as illustrated below with an example:

We deal with three bodies as part of this work. Yet, clearly three body collisions are highly improbable in low density gas-phase interstellar chemistry. In this context, we state explicitly that, we do not propose that the pre-reactant complexes are formed via a three-body collision. Instead, they are formed in a sequential order involving two body collisions. The exact sequence is insignificant because all of them lead to the same pre-reactant complex, and no barrier is encountered in the process as shown below. Once this pre-reactant complex is formed, further molecular reorganization occurring lead to the TS, which results in the product complexes. However, regardless of which sequence of two-body collision happen, the pre-reactant complex is always stabilized significantly.

We demonstrate details of the energetics for all possible sequences of two-body collisions resulting in the same stabilized pre-reactant complex. The same level of theory used in the figures corresponding to Path 3 (Figures 9 and 11 in the main text) are used here too. All energies are provided in kcal/mol.

Points to note are that: the barrierless formation of the pre-reactant complex is always exothermic via this sequential 2-body reaction, and the sequential 2-body reaction paves the way for what looks like a three/four body reaction.

Such a sequential arrangement of 2 body reactions effectively leading to a 3 (or even 4 body in some cases) has been espoused previously by our research group (and others) in the context of metal-ion mediated interstellar chemistry. A prominent reference includes (kindly see the SI of this paper too): Thripati and Ramabhadran, *J. Phys. Chem. A.* 2021, 125, 3457-3472.

1a. ***HCOOH + OH + H_2O → HO-CO + $2H_2O$***

a. $HCOOH + OH \longrightarrow HCOO + H_2O$ ΔE = 8.1

$HCOO + H_2O \rightarrow HO\text{-}CO + H_2O$ ΔE = 10.0 (Isomerization with one water)

$HCOOH + OH + H_2O \rightarrow HO\text{-}CO + 2H_2O$ **ΔE = 18.1**

1b. ***HCOOH + OH + H_2O+ H_2O → HO-CO + $3H_2O$***

a. $HCOOH + OH \longrightarrow HCOO + H_2O$ ΔE = 8.1

$HCOO + H_2O \rightarrow HCOO\_H_2O$ ΔE = 2.9

$HCOO\_H_2O + H_2O \rightarrow HO\text{-}CO + 2H_2O$ ΔE = 7.1 (Isomerization with two water)

$HCOOH + OH + H_2O + H_2O \rightarrow HO\text{-}CO + 3H_2O$ **ΔE = 18.1**

2. ***HOCO radical + CH_2NH + H_2 → NH_2CH_2COOH + H radical***

a. $HOCO + CH_2NH \longrightarrow HOCO\_CH_2NH$ ΔE = 13.1

$HOCO\_CH_2NH + H_2 \rightarrow NH_2CH_2COOH + H$ ΔE = 3.2

$HOCO + CH_2NH + H_2 \longrightarrow NH_2CH_2COOH + H$ **ΔE = 16.3**

b. $HOCO + H_2 \longrightarrow HOCO\_H_2$ ΔE = 0.4

$HOCO\_H_2 + CH_2NH \rightarrow NH_2CH_2COOH + H$ ΔE = 15.9

$HOCO + H_2 + CH_2NH \longrightarrow NH_2CH_2COOH + H$ **ΔE = 16.3**

c. $CH_2NH + H_2 \longrightarrow CH_2NH\_H_2$ ΔE = 0.7

$CH_2NH\_H_2 + HOCO \rightarrow NH_2CH_2COOH + H$ ΔE = 17.1

$CH_2NH + H_2 + HOCO \longrightarrow NH_2CH_2COOH + H$ **ΔE = 16.3**

3. *HOCO radical + CH_2NH + NH_3 → NH_2CH_2COOH + NH_2 radical*

a. $HOCO + CH_2NH \longrightarrow HOCO\_CH_2NH$ ΔE = 13.1

$HOCO\_CH_2NH + NH_3 \rightarrow NH_2CH_2COOH + NH_2$ ΔE = 10.2

$HOCO + CH_2NH + NH_3 \longrightarrow NH_2CH_2COOH + NH_2$ **ΔE = 23.4**

b. $HOCO + NH_3 \longrightarrow HOCO\_NH_3$ ΔE = 15.2

$HOCO\_NH_3 + CH_2NH \rightarrow NH_2CH_2COOH + NH_2$ ΔE = 8.1

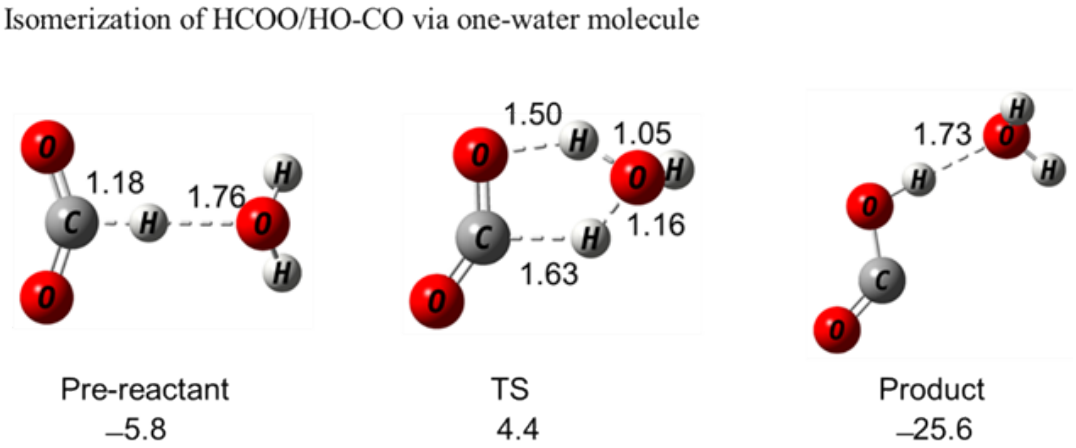
$HOCO + NH_3 + CH_2NH \longrightarrow NH_2CH_2COOH + NH_2$ **ΔE = 23.4**

c. $CH_2NH + NH_3 \longrightarrow CH_2NH\_NH_3$ ΔE = 4.4

$CH_2NH\_NH_3 + HOCO \rightarrow NH_2CH_2COOH + NH_2$ ΔE = 19.0

$CH_2NH + NH_3 + HOCO \longrightarrow NH_2CH_2COOH + NH_2$ **ΔE = 23.4**

Isomerization of HCOO/HO-CO via one-water molecule



Figure_SI_1: This a valid alternative mechanism for Figure 7(iii), reaction with one water molecule but the energy barrier is not nil.

Energy barrier calculations method used in this work:

Table_SI_1: Energy barrier = Transition State – (Infinity Separated Reactants)

The following method has been used for the main text.

Transition States	Infinity Separated Reactants
$COCH_2NH_2\_H_2O\_$ TS-III (Figure 3)	$COCH_2NH_2$ and H_2O
$CH_2COOH_NH_3$_TS-III (Figure 6)	CH_2COOH and NH_3
$NHCH_2COOH_H_2$_TS-V (Figure 11)	$NHCH_2COOH$ and H_2
$NHCH_2COOH_NH_3$_TS-VI (Figure 11)	$NHCH_2COOH$ and NH_3
$NH_2CHCOOH_H_2$_VII (Figure 12)	$NH_2CHCOOH$ and H_2
$NH_2CHCOOH_NH_3$_VIII (Figure 12)	$NH_2CHCOOH$ and NH_3
HCO_CH_2NH_TS-I	HCO and CH_2NH
$NHCH_2CHO_NH_2CH_2CO$_TS-II	HCO and CH_2NH
$NHCH_2CHO_NH_2CH_2CO$_PR_TS	HCO, CH_2NH and 2H2O

CH_3_CO_2_TS-I	CH_3 and CO_2
CH_3COO_CH_2COOH_TS-II	CH_3 and CO_2
CH_3COO_CH_2COOH_PR_TS	CH_3 and CO_2 and 2H2O
HCOOH_OH_TS-I	HCOOH and OH
HCOO_HOCO_TS-II	HCOO
HCOO_HOCO-PR-TS-I	HCOO, $2H_2O$
HOCO_CH_2NH_TS-III	HOCO and CH_2NH
$NHCH_2COOH$_$NH_2CHCOOH$_TS-IV	HOCO and CH_2NH
$NHCH_2COOH$_$NH_2CHCOOH$- PR-TS-II	HOCO and CH_2NH, and $2H_2O$

Table_SI_2: Energy barrier = Transition State - Infinity Separated Reactants

The following method used for the supporting information.

Transition States	Infinity Separated Reactants
$COCH_2NH_2$_H_2O_ TS-III	HCO and CH_2NH and H_2O
CH_2COOH_NH_3_TS-III	CH_3 and CO_2 and NH_3
$NHCH_2COOH$_H_2_TS-V	HOCO and CH_2NH and H_2
$NHCH_2COOH$_NH_3_TS-VI	HOCO and CH_2NH and NH_3
$NH_2CHCOOH$_H_2_VII	HOCO and CH_2NH and H_2
$NH_2CHCOOH$_NH_3_VIII	HOCO and CH_2NH and NH_3

Comparing the energy barriers with different DFT methods on representative TSs.

To validate our computational technique for obtaining the energy barriers, we have carried out single-point-energy calculations on representative TSs, and the energy values are shown in Table 1. This is in addition to the validation of the TS geometries themselves (presented in the SI). Overall, we observe, the same qualitative trend (UB2-PLYP(D3-BJ), UM06-2x, and UωB97X-D) in the electronic energy barrier heights was noticed with respect to the B3-LYP(D3-BJ) method, and the energy values can be seen in Table 1. The analysis of energy values in Table 1 clearly indicates that our method (B3-LYP(D3-BJ)) is acceptable with respect to the other three DFT methods used in the paper.

Table_SI_3. Comparing the energy barriers with different DFT methods on representative TSs at the UCCSD(T)(FC)/aug-cc-pVTZ//UB3-LYP(D3-BJ)/aug-cc-pVTZ, UCCSD(T)(FC)/aug-cc-pVTZ//B2-PLYP(D3-BJ)//aug-cc-pVTZ, UCCSD(T)(FC)/aug-cc-pVTZ//UM06-2x/aug-cc-pVTZ, and UCCSD(T)(FC)/aug-cc-pVTZ//UωB97X-D/aug-cc-pVTZ levels of theories. Where $\Delta E^{\neq} = E_{TS}-E_{\text{Infinity separated reactants}}$. The energy values (included zero-point corrections) are provided in kcal/mol.

	B3-LYP $\Delta E^{\neq}$	B2-PLYP $\Delta E^{\neq}$	M06-2x $\Delta E^{\neq}$	ωB97X-D $\Delta E^{\neq}$
Glycine Precursor 1				
HCO_CH_2NH_TS-I	7.5	7.7	7.7	7.4
NHCH_2CHO_NH_2CH_2CO_TS-II	22.5	22.6	22.4	22.6
NHCH_2CHO_NH_2CH_2CO_PR_TS	1.3	1.3	0.59	1.3
COCH_2NH_2_H_2O_ TS-III	16.0	16.1	16.3	16.2
Glycine Precursor 2				
CH_3_CO_2_TS-I	21.2	20.6	20.6	21.4
CH_3COO_CH_2COOH_TS-II	46.5	45.8	46.1	46.9
CH_3COO_CH_2COOH_PR_TS	35.2	35.2	34.9	35.6
CH_2COOH_NH_3_TS-III	61.9	61.4	61.5	62.7
Glycine Path-3				
HCOOH_OH_TS-I	1.5	1.4	1.4	1.6
HCOO_HOCO_TS-II	20.6	18.9	18.6	18.8
HCOO_HOCO-PR-TS-I	11.2	12.7	13.0	12.9

HOCO_CH_2NH_TS-III	0.14	0.52	0.35	0.42
NHCH$_2$COOH_NH$_2$CHCOOH_TS-IV	9.0	9.3	9.3	9.3
NHCH$_2$COOH_NH$_2$CHCOOH- PR-TS-II	12.8	12.4	12.2	12.6
NHCH$_2$COOH_H_2_TS-V	19.7	19.4	19.7	19.4
NHCH$_2$COOH_NH_3_TS-VI	9.7	9.3	9.3	9.3
NH$_2$CHCOOH_H_2_VII	24.7	25.0	25.3	24.7
NH$_2$CHCOOH_NH_3_VIII	11.7	12.0	12.2	12.0

Effect of temperature on the transition states energy barriers:

To check if there is a prominent temperature effect on TSs, we have performed calculations at different temperatures, using the UB3-LYP(D3-BJ)/aug-cc-pVTZ method to optimize. The thermal corrections have been taken from optimized TSs geometries with various temperature conditions and added to the electronic energy values. The TSs energy barriers are shown in Table 2 with various temperatures.

Upon glancing at Table 2, it becomes clear that for all the pathways, the temperature effect is minimal. What is especially satisfying is that pathway 3 leading to glycine is feasible in the ISM, regardless of the temperature range. With regards to the first pathway, a barrier of ~ 7 kcal/mol is involved in the first step. We reckon this should be feasible only at temperatures higher than 200 K. The second pathway is definitely not feasible for the generation of interstellar glycine. Moreover, once glycine is formed, we also reckon that alanine and serine should be readily formed at all the temperature ranges studied.

Table_SI_4: Relative electronic energies computed at T = 20K, 50K, 100K, 200K, 298.15K, 400K, and 500K ($\Delta_{rel}E_{20}$, $\Delta_{rel}E_{50}$, $\Delta_{rel}E_{100}$, $\Delta_{rel}E_{200}$, $\Delta_{rel}E_{298.15}$, $\Delta_{rel}E_{400}$, and $\Delta_{rel}E_{500}$, respectively) for the TSs shown in the energy profile of Figure 1-15. The UB3-LYP(D3-BJ)/aug-cc-pVTZ level of theory used. Where $\Delta E^{\neq} = E_{TS}$-E $_{\text{Infinity separated reactants}}$.

	$\Delta E^{\neq}$						
	20K	50K	100K	200K	298.15K	400K	500K
Glycine Precursor 1							

HCO_CH_2NH_TS-I	7.4	7.2	7.1	6.9	7.0	7.3	7.6
NHCH$_2$CHO_NH$_2$CH$_2$CO_TS-II	22.4	22.2	22.0	21.7	21.6	21.7	22.0
NHCH$_2$CHO_NH$_2$CH$_2$CO_PR_TS	1.0	0.5	0.06	0.62	0.45	0.22	1.22
COCH$_2$NH$_2$_H_2O_ TS-III	15.8	15.4	15.0	14.4	14.3	14.6	15.1
Glycine Precursor 2							
CH_3_CO_2_TS-I	21.1	20.9	20.7	20.4	19.5	20.3	20.4
CH_3COO_CH_2COOH_TS-II	46.4	46.2	45.9	45.4	44.4	45.1	45.2
CH_3COO_CH_2COOH_PR_TS	34.9	34.4	33.8	33.0	32.1	33.2	33.9
CH_2COOH_NH_3_TS-III	61.7	61.3	60.8	60.1	59.0	59.8	60.1
Glycine Path-3							
HCOOH_OH_TS-I	1.8	1.9	2.2	2.4	2.4	2.3	2.1
HCOO_HOCO_TS-II	18.2	18.2	18.2	18.3	18.3	18.4	18.3
HCOO_HOCO-PR-TS-I	13.8	14.1	14.6	15.0	15.0	14.7	14.2
HOCO_CH_2NH_TS-III	0.30	0.13	0.07	0.18	0.09	0.11	0.38
NHCH$_2$COOH_NH$_2$CHCOOH_TS-IV	9.2	9.0	8.8	8.5	8.6	8.8	9.2
NHCH$_2$COOH_NH$_2$CHCOOH- PR-TS-II	12.9	13.4	14.0	14.6	14.5	13.9	12.9
NHCH$_2$COOH_H_2_TS-V	19.6	19.9	20.3	20.8	20.9	20.7	20.3
NHCH$_2$COOH_NH_3_TS-VI	9.6	9.9	10.2	10.4	10.2	9.6	8.9
NH$_2$CHCOOH_H_2_TS_VII	24.6	24.9	25.3	25.6	25.6	25.3	24.9
NH$_2$CHCOOH_NH_3_TS_VIII	11.7	12.0	12.2	12.3	12.1	11.5	10.7

Comparing the TSs energy barriers in the gas-phase and implicit CPCM model.

Whereas the liquids do not exist in the ISM, it shall be an instructive idea to compare the barriers in the gas-phase so that one could make a rough comparison of the interstellar reactions vis-à-vis, how these reactions could happen terrestrially. To calculate the electronic energy barrier in the gas-phase, UB3-LYP(D3-BJ)/aug-cc-pVTZ level of theory used and in the solution phase (UB3-LYP(D3-BJ)(CPCM))/aug-cc-pVTZ level of theory used. Table 3 clearly indicates that all the paths the TSs electronic energy barriers are of similar magnitude in the gas-phase and in the

solution phase with the CPCM[74] model. Hence it is interesting that, our conclusions that we draw for interstellar reactions may be extended to terrestrial chemistry too, insofar as the implicit solvent model is reliable, noting the limitation that the continuum modeling could miss out on capturing some weak local interactions.

Table_SI_5. Comparing the energy barriers in the gas-phase and CPCM model. The TSs optimized by using UB3-LYP(D3-BJ)/aug-cc-pVTZ level of theory for the gas-phase and (UB3-LYP(D3-BJ)(CPCM))/aug-cc-pVTZ level of theory for the solution phase. Where $\Delta E^{\neq} = E_{TS}$-E $_{\text{Infinity separated reactants}}$, the energy values (included zero-point corrections) are provided in kcal/mol.

	Gas-Phase ($\Delta E^{\neq}$)	CPCM($\Delta E^{\neq}$)
Glycine Precursor 1		
HCO_CH_2NH_TS-I	4.0	4.6
$NHCH_2CHO$_NH_2CH_2CO_TS-II	20.7	21.4
$NHCH_2CHO$_NH_2CH_2CO_PR_TS	8.7	4.4
$COCH_2NH_2$_H_2O_ TS-III	15.5	17.9
Glycine Precursor 2	Gas-Phase($\Delta E^{\neq}$)	CPCM($\Delta E^{\neq}$)
CH_3_CO_2_TS-I	16.1	14.0
CH_3COO_CH_2COOH_TS-II	43.6	39.7
CH_3COO_CH_2COOH_PR_TS	20.4	19.8
CH_2COOH_NH_3_TS-III	38.2	27.6
Glycine Path-3	Gas-Phase($\Delta E^{\neq}$)	CPCM($\Delta E^{\neq}$)
HCOOH_OH_TS-I	6.6	4.1
HCOO_HOCO_TS-II	21.1	22.0
HCOO_HOCO-PR-TS-I	15.3	Unable to locate TS
HOCO_CH_2NH_TS-III	4.8	2.3
$NHCH_2COOH$_$NH_2CHCOOH$_TS-IV	7.2	8.3
$NHCH_2COOH$_$NH_2CHCOOH$- PR-TS-II	20.0	15.1
$NHCH_2COOH$_H_2_TS-V	12.0	10.2
$NHCH_2COOH$_NH_3_TS-VI	14.3	11.5
$NH_2CHCOOH$_H_2_VII	15.1	13.7
$NH_2CHCOOH$_NH_3_VIII	16.0	13.8

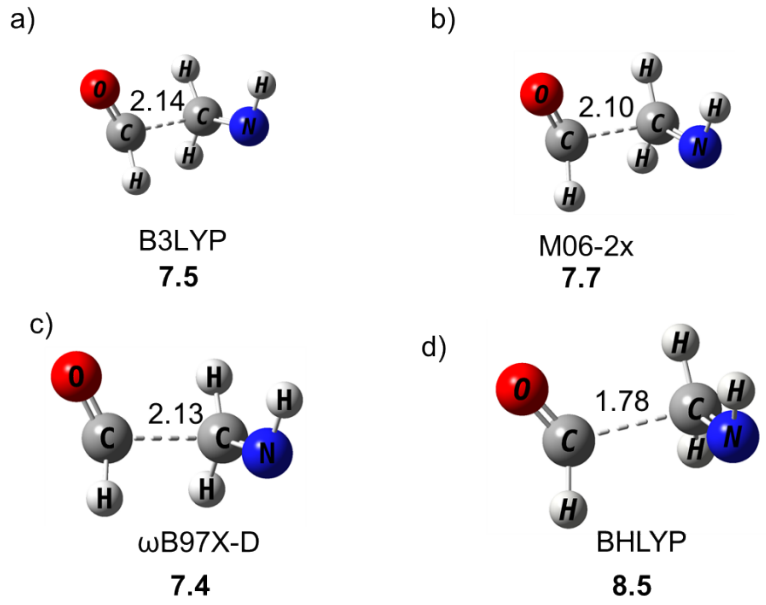


Figure SI_2: Optimized TSs of HCO/CH_2NH (UB3LYP). The geometry being calibrated with two different DFT methods. Throughout, the aug-cc-pVTZ basis set was used for the optimization. All the resulting optimized geometries are similar. The UCCSD(T)(FC)/aug-cc-pVTZ level of theory is used for the single-point energy calculation. The electronic energy barriers (including zero-point corrections) are given below the structure and the values given in kcal/mol.

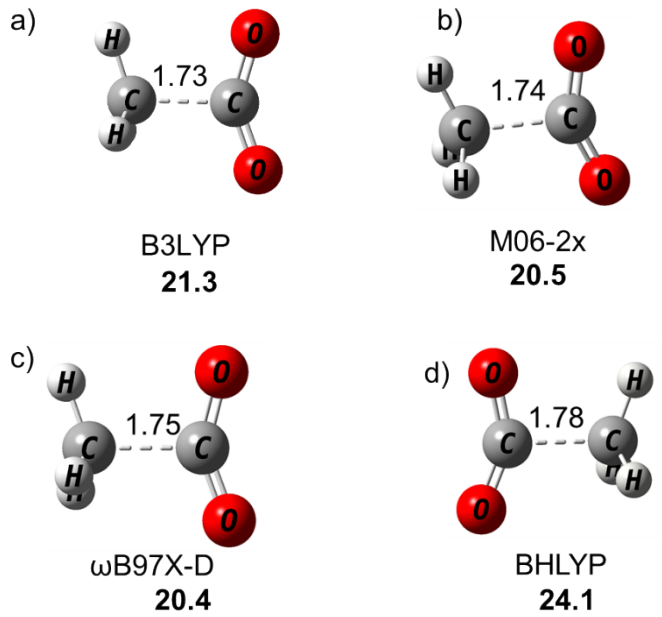


Figure SI_3: Optimized TSs of CH_3/CO_2 (UB3LYP). The geometry being calibrated with two different DFT methods. Throughout, the aug-cc-pVTZ basis set was used for the optimization. All the resulting optimized geometries are similar. The UCCSD(T)(FC)/aug-cc-pVTZ level of

theory is used for the single-point energy calculation. The electronic energy barriers (including zero-point corrections) are given below the structure and the values given in kcal/mol.

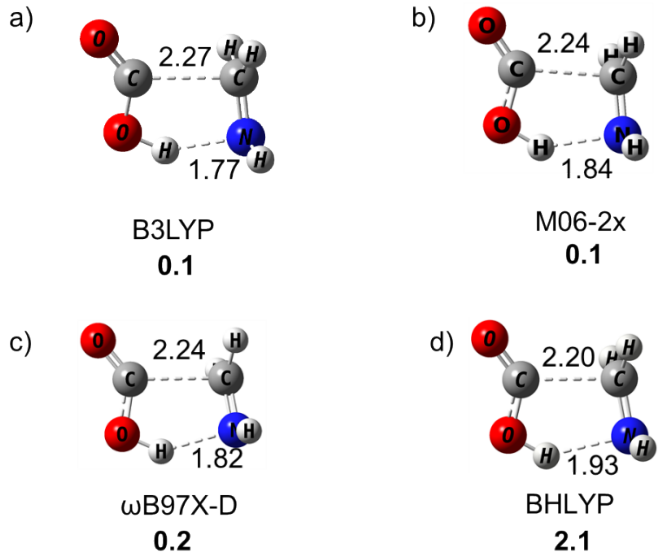


Figure SI_4: Optimized TSs of COOH radical/CH_2NH (UB3LYP). The geometry being calibrated with two different DFT methods. Throughout, the aug-cc-pVTZ basis set was used for the optimization. All the resulting optimized geometries are similar. The UCCSD(T)(FC)/aug-cc-pVTZ level of theory is used for the single point energy calculation. The electronic energy barriers (including zero-point corrections) are given below the structure and the values given in kcal/mol.

Table_SI_6. The computed TSs electronic energies, Gibbs free energies and enthalpies.

Glycine Precursor 1	**ΔE+ZPE**	**ΔE+ΔG**	**ΔE+ΔH**
HCO_CH_2NH_TS-I	7.5	17.1	6.5
$NHCH_2CHO$_NH_2CH_2CO_TS-II	22.5	32.8	21.0
$NHCH_2CHO$_NH_2CH_2CO_PR_TS	**13.4**	**29.6**	**⁻ 2.2**
$COCH_2NH_2$_H_2O_ TS-III	16.0	35.9	13.1
Glycine Precursor 2	**ΔE+ZPE**	**ΔE+ΔG**	**ΔE+ΔH**
CH_3_CO_2_TS-I	21.2	25.5	19.7
CH_3COO_CH_2COOH_TS-II	46.5	51.8	44.6
CH_3COO_CH_2COOH_PR_TS	**19.2**	**58.4**	**31.1**
CH_2COOH_NH_3_TS-III	61.9	76.9	58.6

Glycine Path-3	**ΔE+ZPE**	**ΔE+ΔG**	**ΔE+ΔH**
HCOOH_OH_TS-I	− 1.5	7.0	− 2.8
HCOO_HOCO_TS-II	20.6	18.4	18.3
HCOO_HOCO-PR-TS-I	− 11.2	4.6	− 16.2
HOCO_CH_2NH_TS-III	0.1	10.9	− 0.9
$NHCH_2COOH$_$NH_2CHCOOH$_TS-IV	9.0	20.1	7.7
$NHCH_2COOH$_$NH_2CHCOOH$- PR-TS-II	− 12.8	16.8	− 16.6
$NHCH_2COOH$_H_2_TS-V	− 19.7	− 2.4	− 22.3
$NHCH_2COOH$_NH_3_TS-VI	− 9.7	9.8	− 11.7
$NH_2CHCOOH$_H_2_VII	− 24.7	− 7.4	− 27.1
$NH_2CHCOOH$_NH_3_VIII	− 11.7	7.3	− 13.5

Table_SI_7. TSs energy barriers without ZPE and ZPE

	Without ZPE	**With ZPE**
Glycine Precursor 1		
HCO_CH_2NH_Pre-reactant	3.8	2.6
HCO_CH_2NH_TS-I	5.3	7.5
$HCOCH_2NH$_Int-I	15.4	12.1
$NHCH_2CHO$_NH_2CH_2CO_TS-II	21.0	22.5
$COCH_2NH_2$_Int-II	26.9	21.9
$COCH_2NH_2$_H_2O_Int-III	33.9	26.8
$COCH_2NH_2$_H_2O_TS-III	9.9	16.0
Product (O-Protonated Glycine)	35.8	25.9
$NHCH_2CHO$_NH_2CH_2CO_PR_Reactant	30.9	23.0
$NHCH_2CHO$_NH_2CH_2CO_PR_TS	2.6	1.3
$COCH_2NH_2$_PR_Product	45.0	35.6
Glycine Precursor 2		
CH_3_CO_2_Pre-reactant	1.1	0.2
CH_3_CO_2_TS-I	17.7	21.2
CH_3_CO_2_Int-I	11.2	15.9
CH_3COO_CH_2COOH_TS-II	44.8	46.5
CH_2COOH_Int-II	11.0	15.2
CH_2COOH_NH_3_Int-III	5.0	1.7
CH_2COOH_NH_3_TS-III	53.6	61.9
Product (O-Protonated Glycine)	9.8	19.5
CH_3COO_CH_2COOH_Pre-Reactant	12.3	3.6

$CH_3COO\_CH_2COOH\_PR\_TS$	30.5	35.2
$CH_3COO\_CH_2COOH\_PR\_Product$	13.5	4.1

Table_SI_8. TSs energy barriers without ZPE and ZPE

	Without ZPE	**With ZPE**
Glycine Path-3		
HCOOH_OH Pre-Reactant	10.4	8.2
HCOOH_OH TS-I	1.6	1.5
$HCOO\_H_2O\_Int\text{-}I$	10.9	9.0
HCOO_TS-II	21.5	0.9
HOCO_Int-III	16.5	3.1
HCOO_PR-PR-I	18.1	12.0
HCOO_PR_TS-I	15.7	11.2
HOCO_PR Product-I	35.7	28.0
$HOCO\_CH_2NH\_Int\text{-}IV$	12.8	11.2

HOCO_CH_2NH TS-III	1.4	0.14
$NHCH_2COOH$_Int-V	24.1	21.5
$NHCH_2COOH$_$NH_2CHCOOH$ TS-IV	8.4	9.0
$NH_2CHCOOH$_Int-VI	44.8	41.2
$NHCH_2COOH$ PR_ Reactant-II	59.1	52.3
$NHCH_2COOH$_$NH_2CHCOOH$ PR_TS-II	16.7	12.8
$NH_2CHCOOH$_PR_Pd-II	40.9	33.2
$NHCH_2COOH$_H_2_Int-VII	37.7	34.1
$NHCH_2COOH$_H_2_TS-V	23.6	19.7
NH_2CH_2COOH_H_Int-VIII	35.8	29.9
$NHCH_2COOH$_NH_3 Int-IX	29.3	25.6
$NHCH_2COOH$_NH_3 TS-VI	11.4	9.7
NH_2CH_2COOH_NH_2_Int-X	23.9	20.1
$NH_2CHCOOH$_H_2_Int-XI	57.5	53.1
$NH_2CHCOOH$_H_2 TS-VII	29.2	24.7
NH_2CH_2COOH_H_Int-XII	35.8	29.9
$NH_2CHCOOH$_NH_3_Int-XIII	51.9	46.8
$NH_2CHCOOH$_NH_3_TS-VIII	14.2	11.7
NH_2CH_2COOH_NH_2_Int-XIV	21.9	18.5

Table_SI_9. The imaginary frequencies of the TSs in different levels of theory in computed aug-cc-pVTZ basis-set using harmonic analysis.

	UB3-LYP	UB2-PLYP	UM06-2x	UωB97X-D
Glycine Precursor 1				
HCO_CH_2NH_TS-I	*i*385.08 cm^{-1}	*i*521.11 cm^{-1}	*i*429.89 cm^{-1}	*i*471.96 cm^{-1}
$NHCH_2CHO$_NH_2CH_2CO_TS-II	*i*1968.32 cm^{-1}	*i*2175.92 cm^{-1}	*i*2119.86 cm^{-1}	*i*2123.79 cm^{-1}
$NHCH_2CHO$_NH_2CH_2CO_PR_TS	*i*1170.66 cm^{-1}	*i*1121.39 cm^{-1}	*i*1401.44 cm^{-1}	*i*1228.74 cm^{-1}
$COCH_2NH_2$_H_2O_ TS-III	*i*1695.55 cm^{-1}	*i*1701.28 cm^{-1}	*i*1544.76 cm^{-1}	*i*1723.92 cm^{-1}
Glycine Precursor 2				
CH_3_CO_2_TS-I	*i*108.70 cm^{-1}	*i*649.06 cm^{-1}	*i*312.07 cm^{-1}	*i*253.82 cm^{-1}
CH_3COO_CH_2COOH_TS-II	*i*2022.58cm^{-1}	*i*2022.87 cm^{-1}	*i*1959.54 cm^{-1}	*i*2025.76 cm^{-1}
CH_3COO_CH_2COOH_PR_TS	*i*1349.55 cm^{-1}	*i*520.47cm^{-1}	*i*1291.2 cm^{-1}	*i*1315.06 cm^{-1}
CH_2COOH_NH_3_TS-III	*i*531.97 cm^{-1}	*i*587.60cm^{-1}	*i*627.54 cm^{-1}	*i*602.57 cm^{-1}
Glycine Path-3				
Path-3	B3-LYP	B2-PLYP	M06-2x	ωB97X-D
HCOOH_OH_TS-I	*i*1383.44 cm^{-1}	*i*1547.9258 cm^{-1}	*i*1445.15 cm^{-1}	*i*1496.16 cm^{-1}
HCOO_HOCO_TS-II	*i*1833.63 cm^{-1}	*i*1798.2241 cm^{-1}	*i*1722.05 cm^{-1}	*i*2123.79 cm^{-1}
HCOO_HOCO-PR-TS-I	*i*641.05 cm^{-1}	*i*613.4172 cm^{-1}	*i*346.08 cm^{-1}	*i*634.056 cm^{-1}
HOCO_CH_2NH_TS-III	*i*215.89 cm^{-1}	*i*267.5005 cm^{-1}	*i*259.213 cm^{-1}	*i*250.671 cm^{-1}
$NHCH_2COOH$_$NH_2CHCOOH$_TS-IV	*i*1925.00 cm^{-1}	*i*1957.365 cm^{-1}	*i*1872.09 cm^{-1}	*i*1941.09 cm^{-1}
$NHCH_2COOH$_$NH_2CHCOOH$- PR-TS-II	*i*1146.10 cm^{-1}	*i*1138.2513 cm^{-1}	*i*1140.47 cm^{-1}	*i*1171.28 cm^{-1}
$NHCH_2COOH$_H_2_TS-V	*i*1336.06 cm^{-1}	*i*1533.2631 cm^{-1}	*i*1830.31 cm^{-1}	*i*1511.64 cm^{-1}
$NHCH_2COOH$_NH_3_TS-VI	*i*1693.51 cm^{-1}	*i*1659.2477 cm^{-1}	*i*1704.51 cm^{-1}	*i*1842.82 cm^{-1}
$NH_2CHCOOH$_H_2_VII	*i*617.60 cm^{-1}	*i*1213.8028 cm^{-1}	*i*1577.15 cm^{-1}	*i*1080.53 cm^{-1}
$NH_2CHCOOH$_NH_3_VIII	*i*357.73 cm^{-1}	*i*897.3583 cm^{-1}	*i*1160.19 cm^{-1}	*i*918.16 cm^{-1}

Note: NP- Not Performed Calculation

Table_SI_10. The <S**2> values of the TSs in different levels of theory in computed aug-cc-pVTZ basis-set.

	UB3-LYP <S**2>	UB2-PLYP <S**2>	UM06-2x <S**2>	UωB97X-D <S**2>
Glycine Precursor 1				
HCO_CH_2NH_TS-I	0.7666	0.8181	0.7695	0.7729
$NHCH_2CHO$_NH_2CH_2CO_TS-II	0.7643	0.784	0.7661	0.7664
$NHCH_2CHO$_NH_2CH_2CO_PR_TS	0.7578	0.7723	0.7603	0.7599
$COCH_2NH_2$_H_2O_ TS-III	0.7534	0.7566	0.7543	0.7537

Glycine Precursor 2				
CH_3_CO_2_TS-I	0.7559	0.7601	0.7581	0.7573
CH_3COO_CH_2COOH_TS-II	0.7592	0.773	0.7608	0.7601
CH_3COO_CH_2COOH_PR_TS	0.758	0.7668	0.7587	0.7578
CH_2COOH_NH_3_TS-III	0.7539	0.7576	0.7542	0.7542
Glycine Path-3				
HCOOH_OH_TS-I	0.7568	0.7629	0.7598	0.7573
HCOO_HOCO_TS-II	0.754	0.7622	0.7556	0.7549
HCOO_HOCO-PR-TS-I	0.7528	0.7571	0.7539	0.7533
HOCO_CH_2NH_TS-III	0.7644	0.8037	0.7669	0.7697
$NHCH_2COOH$_$NH_2CHCOOH$_TS-IV	0.7585	0.7715	0.7588	0.7591
$NHCH_2COOH$_$NH_2CHCOOH$- PR-TS-II	0.7544	0.7603	0.7549	0.7551
$NHCH_2COOH$_H_2_TS-V	0.7586	0.7695	0.76	0.7588
$NHCH_2COOH$_NH_3_TS-VI	0.7582	0.7705	0.7606	0.7595
$NH_2CHCOOH$_H_2_VII	0.7555	0.7634	0.759	0.7571
$NH_2CHCOOH$_NH_3_VIII	0.7569	0.7648	0.7606	0.7591

Table_SI_11. The electronic energies for all investigated compounds (in Hartrees)

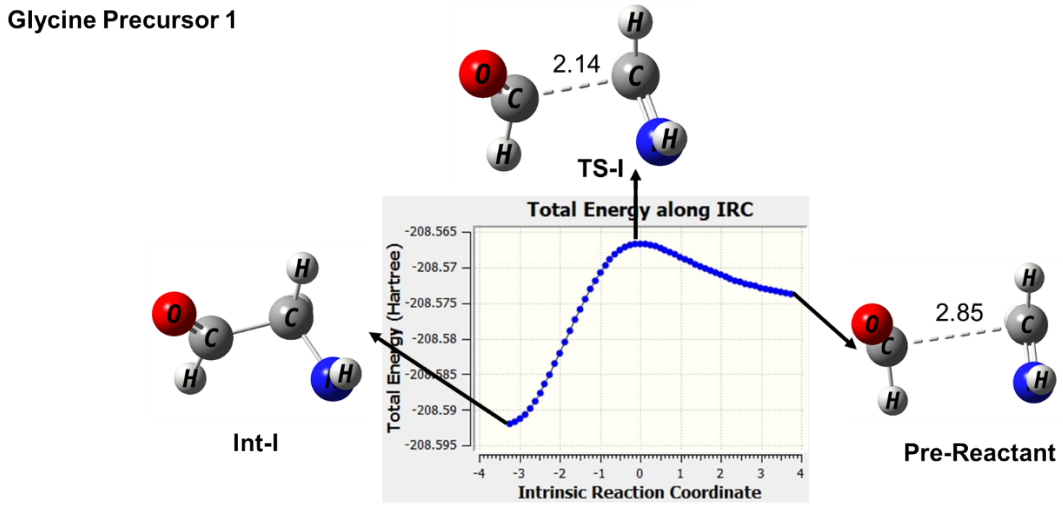
	Zero-point correction (B3-LYP(D3-BJ))	UCCSD(T)	UCCSD(T)+ Zero-point correction
Glycine Precursor 1			
HCO_CH_2NH_Pre-reactant	0.054676	-208.1787908	-208.1241148
HCO_CH_2NH_TS-I	0.056308	-208.1641038	-208.1077958
$HCOCH_2NH$_Int-I	0.058084	-208.1972577	-208.1391737
$NHCH_2CHO$_NH_2CH_2CO_TS-II	0.055094	-208.1389887	-208.0838947
$COCH_2NH_2$_Int-II	0.060667	-208.2155074	-208.1548404
$COCH_2NH_2$_H_2O_Int-III	0.08519	-284.5689343	-284.4837443
$COCH_2NH_2$_H_2O_TS-III	0.083821	-284.4991237	-284.4153027
Product (O-Protonated Glycine)	0.089726	-284.5719939	-284.4822679
$NHCH_2CHO$_NH_2CH_2CO_PR_Reactant	0.107775	-360.9064967	-360.7987217
$NHCH_2CHO$_NH_2CH_2CO_PR_TS	0.101668	-360.8614704	-360.7598024
$COCH_2NH_2$_PR_Product	0.110188	-360.9289479	-360.8187599
Glycine Precursor 2			
CH_3_CO_2_Pre-reactant	0.042078	-228.1059817	-228.0639037
CH_3_CO_2_TS-I	0.045304	-228.0757276	-228.0304236
CH_3_CO_2_Int-I	0.047427	-228.0862	-228.038773
CH_3COO_CH_2COOH_TS-II	0.042525	-228.0326334	-227.9901084
CH_2COOH_Int-II	0.046549	-228.0864435	-228.0398945

$CH_2COOH_NH_3$_Int-III	0.084773	-284.5926142	-284.5078412
$CH_2COOH_NH_3$_TS-III	0.087222	-284.4991237	-284.4119017
Product (O-Protonated Glycine)	0.089483	-284.5689671	-284.4794841
$CH_3COO_CH_2COOH$_Pre-Reactant	0.096148	-380.8083558	-380.7122078
$CH_3COO_CH_2COOH$_PR_TS	0.08991	-380.7400885	-380.6501785
$CH_3COO_CH_2COOH$_PR_Product	0.097336	-380.8103664	-380.7130304

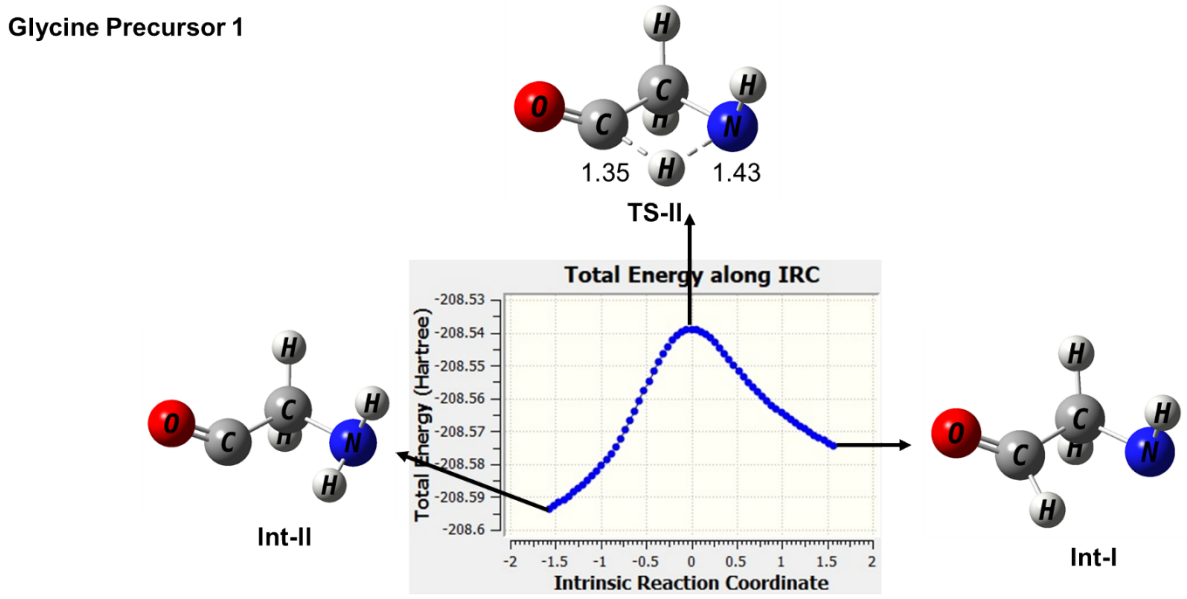
Table_SI_12. The electronic energies for all investigated compounds (in Hartrees)

	Zero-point correction (B3-LYP(D3-BJ))	UCCSD(T)	UCCSD(T)+ Zero-point correction
Glycine Path-3			
HCOOH_OH Pre-Reactant	0.045219	-265.1731921	-265.1279731
HCOOH_OH TS-I	0.041888	-265.1591386	-265.1172506
HCOO_H_2O_Int-I	0.044766	-265.1739461	-265.1291801
HCOO_Int-II	0.015809	-188.8254476	-188.8096386
HCOO_TS-II	0.014357	-188.7911252	-188.7767682
HOCO_Int-III	0.020899	-188.8517475	-188.8308485
HCOO_PR-PR-I	0.068053	-341.5389623	-341.4709093
HCOO_PR_TS-I	0.065457	-341.535172	-341.469715
HOCO_PR Product-I	0.070605	-341.5670242	-341.4964192
HOCO_CH_2NH_Int-IV	0.063187	-283.3524557	-283.2892687
HOCO_CH_2NH TS-III	0.063263	-283.3343689	-283.2711059
$NHCH_2COOH$_Int-V	0.064804	-283.3704589	-283.3056549
$NHCH_2COOH\_NH_2CHCOOH$ TS-IV	0.061578	-283.3184916	-283.2569136
$NH_2CHCOOH$_Int-VI	0.066409	-283.4035227	-283.3371137
$NHCH_2COOH$ PR_ Reactant-II	0.115317	-436.1109081	-435.9955911
$NHCH_2COOH\_NH_2CHCOOH$ PR_TS-II	0.109269	-436.0432461	-435.9339771
$NH_2CHCOOH$_PR_Pd-II	0.113951	-436.0818359	-435.9678849
$NHCH_2COOH_H_2$_Int-VII	0.076438	-284.5458601	-284.4694221
$NHCH_2COOH_H_2$_TS-V	0.076896	-284.5234278	-284.4465318
NH_2CH_2COOH_H_Int-VIII	0.080132	-284.5429577	-284.4628257
$NHCH_2COOH\_NH_3$ Int-IX	0.100608	-339.8592269	-339.7586189
$NHCH_2COOH\_NH_3$ TS-VI	0.09765	-339.8308222	-339.7331722
$NH_2CH_2COOH_NH_2$_Int-X	0.100906	-339.850688	-339.749782
$NH_2CHCOOH_H_2$_Int-XI	0.077654	-284.5774216	-284.4997676
$NH_2CHCOOH\_H_2$ TS-VII	0.077918	-284.5323601	-284.4544421
NH_2CH_2COOH_H_Int-XII	0.080132	-284.5429577	-284.4628257
$NH_2CHCOOH_NH_3$_Int-XIII	0.103028	-339.8953652	-339.7923372
$NH_2CHCOOH_NH_3$_TS-VIII	0.098772	-339.8352572	-339.7364852
$NH_2CH_2COOH_NH_2$_Int-XIV	0.100183	-339.8474789	-339.7472959

IRCs for the glycine precursors 1, glycine precursor 2, glycine path 3.
The ub3lyp/aug-cc-pvtz irc=(calcfc,maxpoints=30, stepsize=5) level of theory used.

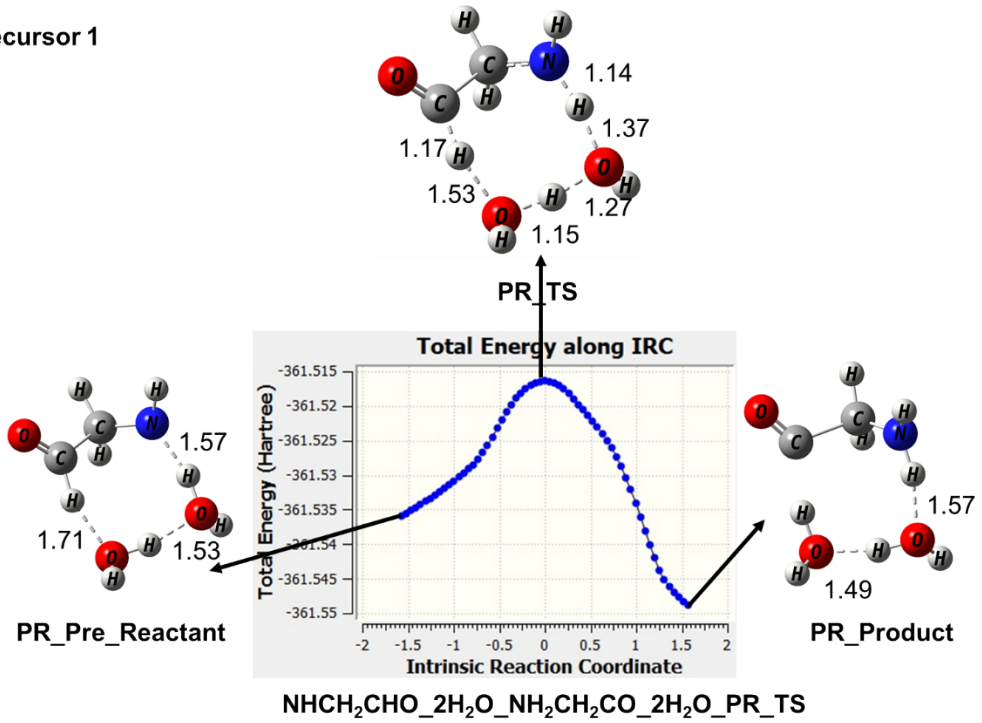


HCO_CH_2NH_TS-I



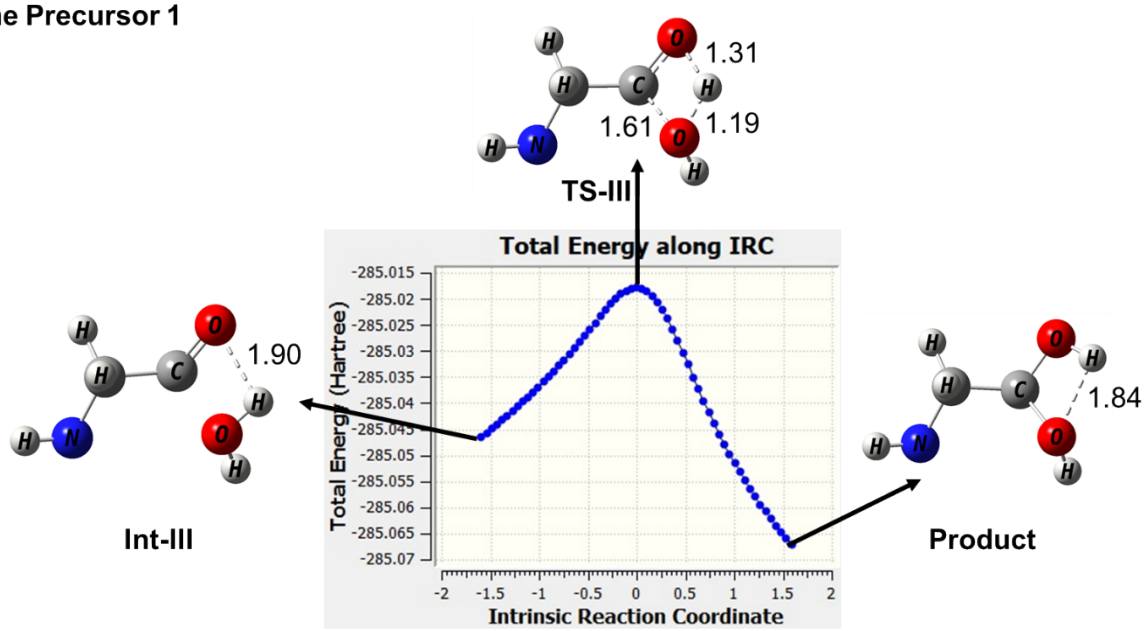
$NHCH_2CHO$_NH_2CH_2CO_TS-II

Glycine Precursor 1



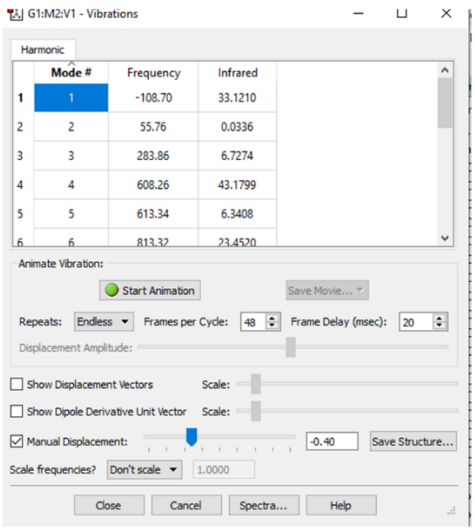
$NHCH_2CHO\_2H_2O\_NH_2CH_2CO\_2H_2O\_PR\_TS$

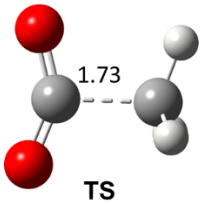
Glycine Precursor 1



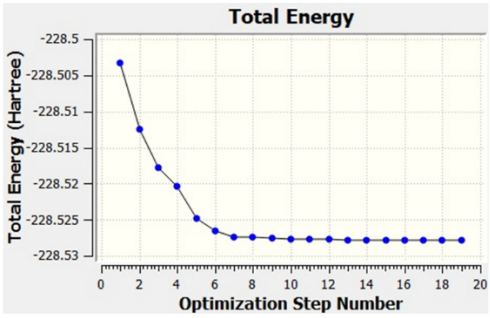
$COCH_2NH_2\_H2O\_TS\text{-}III$

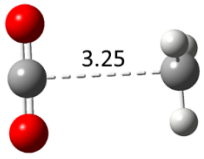
Glycine Precursor 2 **$CH_3\_CO_2\_TS\text{-}I$**





TS

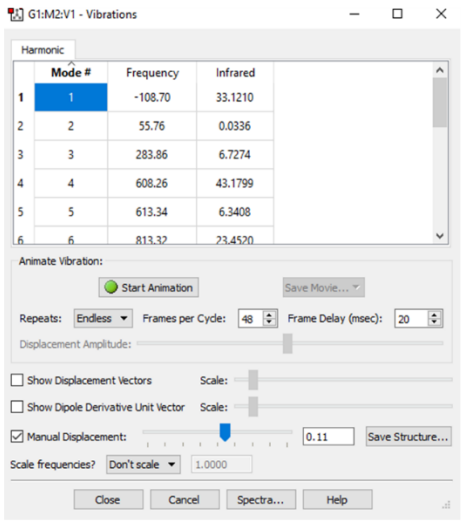


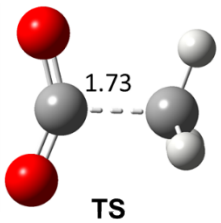


Pre-Reactant

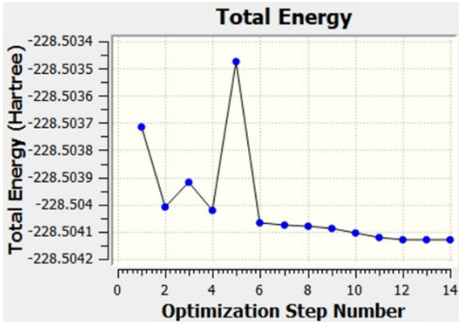
The IRC calculation doesn't work,
So, slightly moved the structure
in the direction of imaginary vibration
and optimized

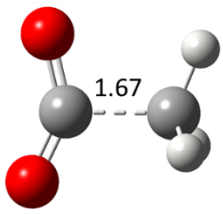
Glycine Precursor 2 **$CH_3\_CO_2\_TS\text{-}I$**





TS

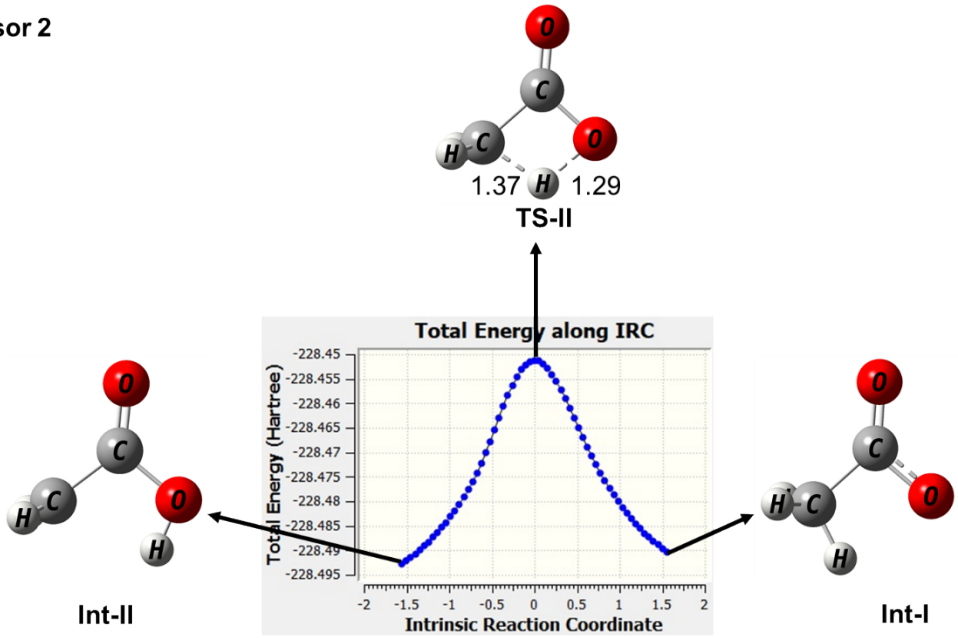




Int-I

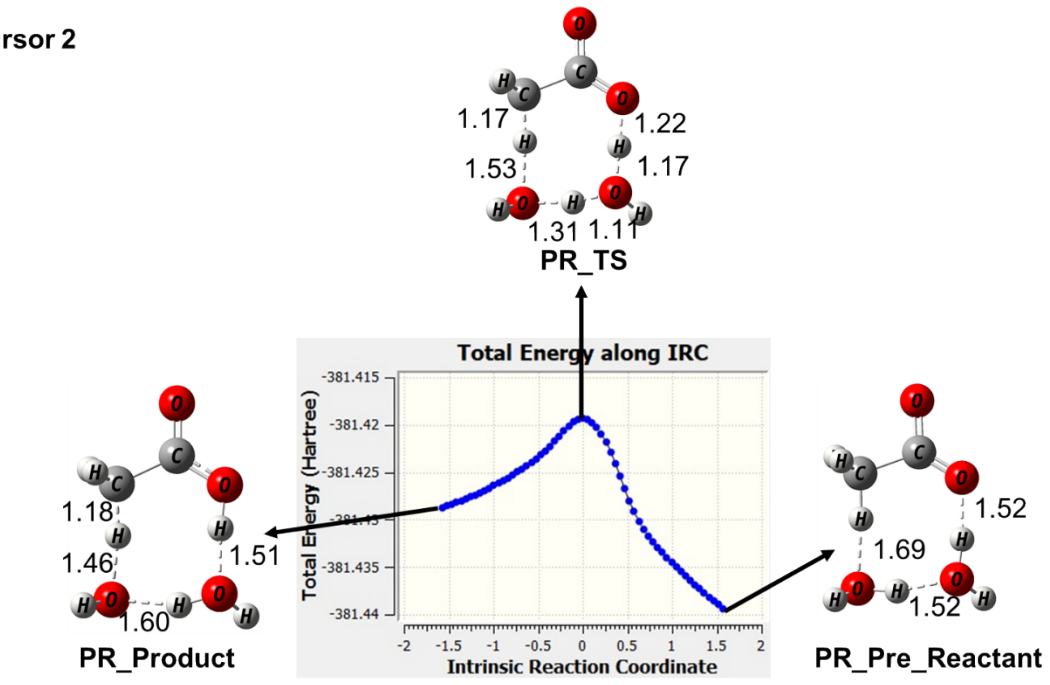
The IRC calculation doesn't work,
So, slightly moved the structure
in the direction of imaginary vibration
and optimized

Glycine Precursor 2



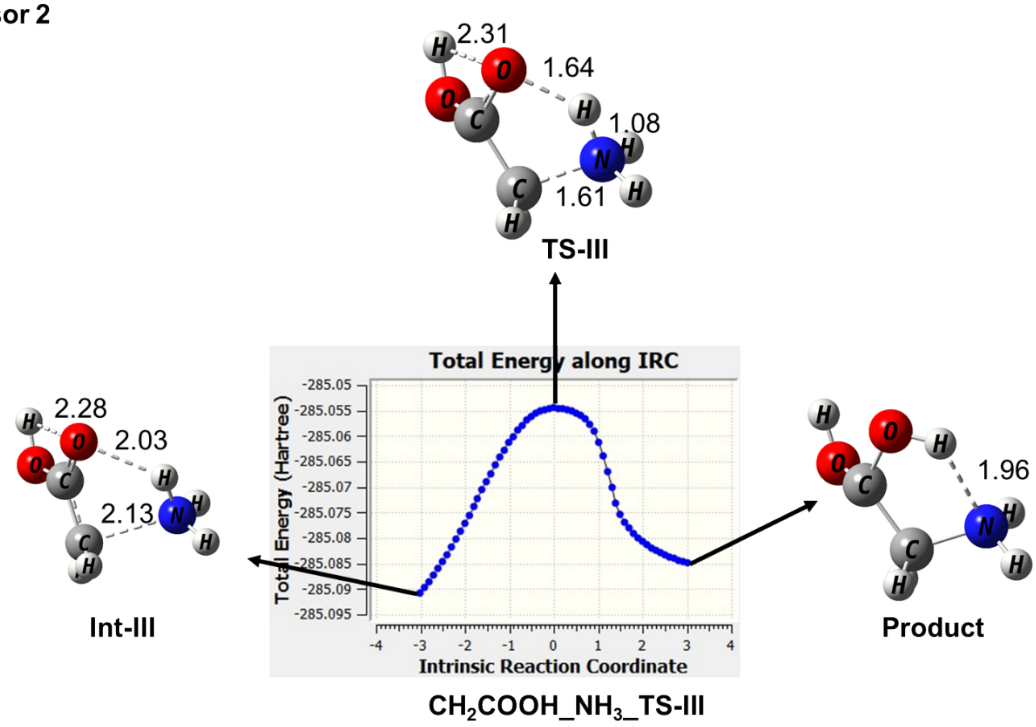
$CH_3COO\_CH_2COOH\_TS\text{-}II$

Glycine Precursor 2

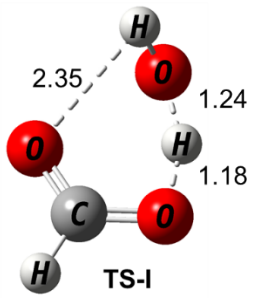


$CH_3COO\_CH_2COOH\_PR\_TS$

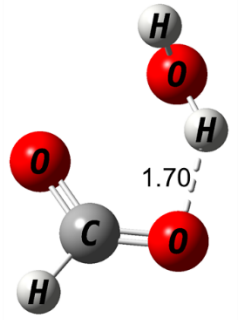
Glycine Precursor 2



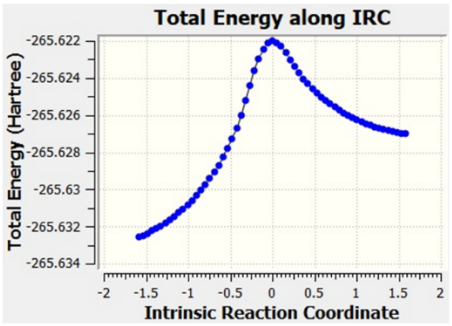
Glycine Path 3

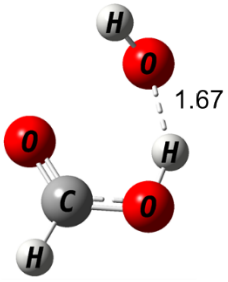


TS-I



Pre-Reactant

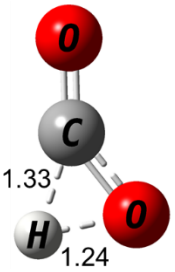




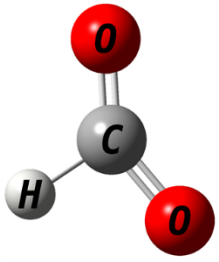
Int-I

HCOOH_OH_TS-I

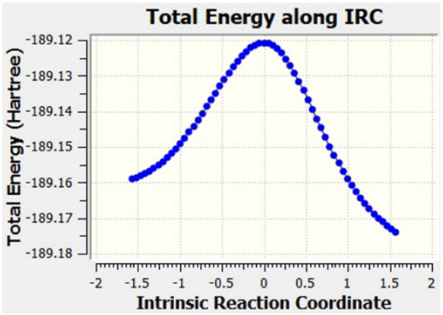
Glycine Path 3



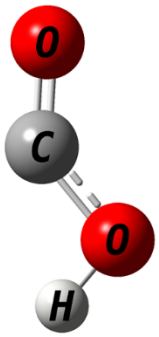
TS-II



Int-II

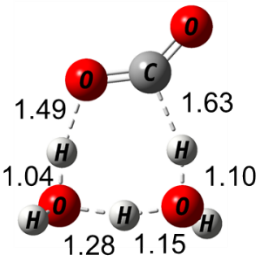


HCOO_HOCO_TS-II

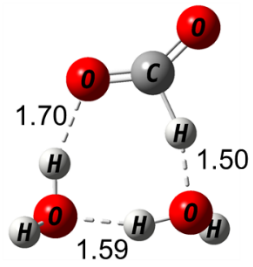


Int-III

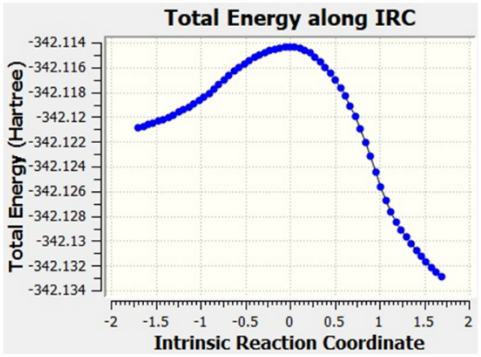
Glycine Path 3



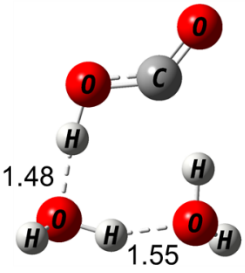
PR_TS-I



PR-PR-I

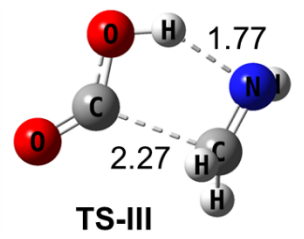


HCOO_HOCO-PR-TS-I



PR Product-I

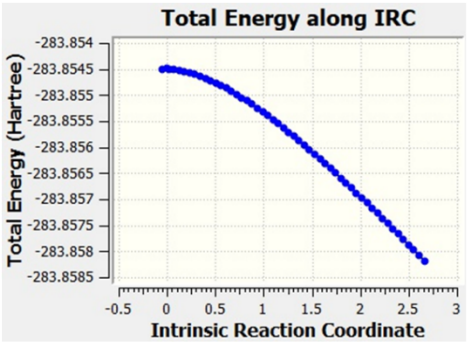
Glycine Path 3

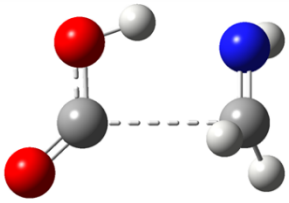


TS-III

Optimized TS as an Initial Step

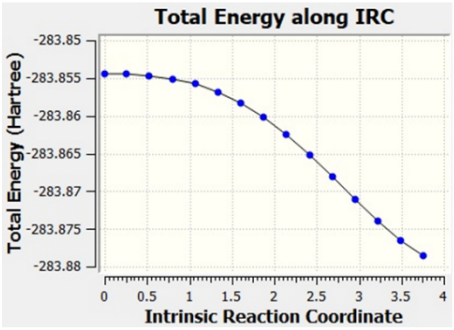
IRC Forward

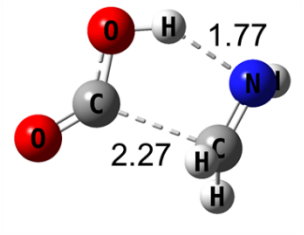




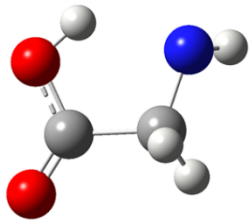
Int-IV

IRC Reverse





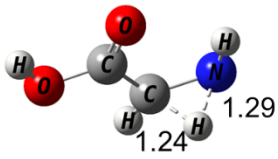
Optimized TS as an Initial Step



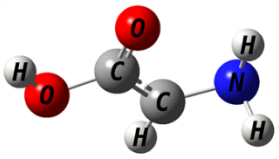
Int-V

$HOCO\_CH_2NH\_TS\text{-}III$

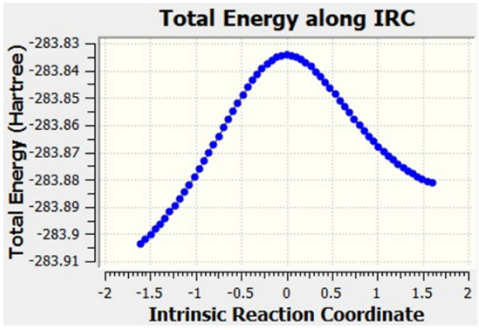
Glycine Path 3

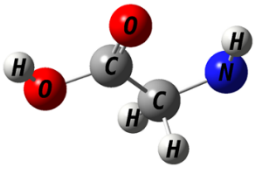


TS-IV



Int-V

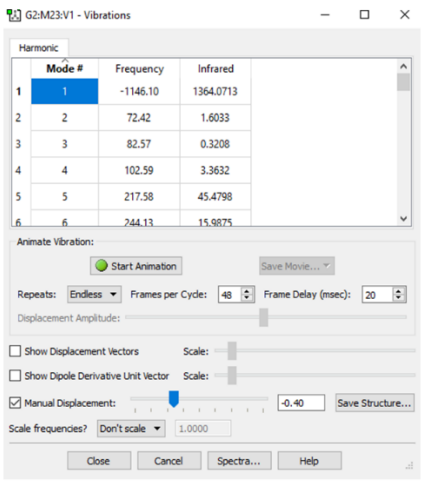




Int-VI

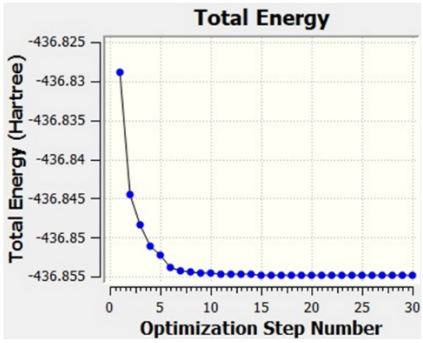
$NHCH_2COOH\_NH_2CHCOOH\_TS\text{-}IV$

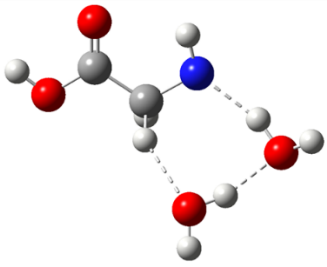
Glycine Path 3



The IRC calculation doesn't work,
So, slightly moved the structure
in the direction of imaginary vibration
and optimized

PR_TS-II

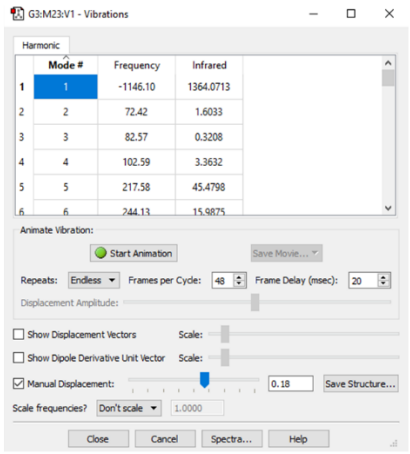




PR_ Reactant-II

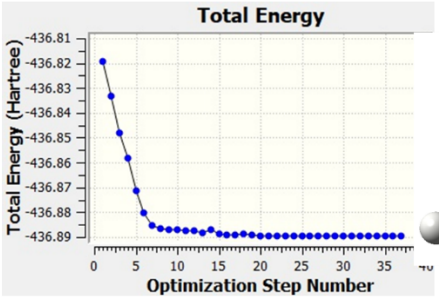
$NHCH_2COOH\_NH_2CHCOOH$- PR-TS-II

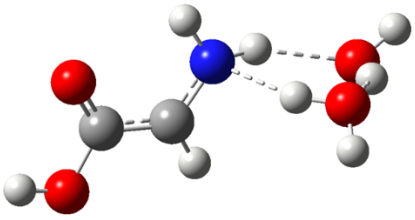
Glycine Path 3



The IRC calculation doesn't work,
So, slightly moved the structure
in the direction of imaginary vibration
and optimized

PR_TS-II

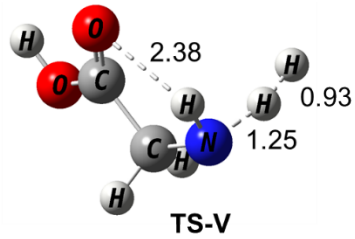




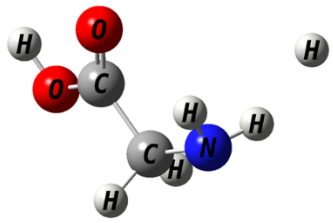
PR_Pd-II

$NHCH_2COOH\_NH_2CHCOOH$- PR-TS-II

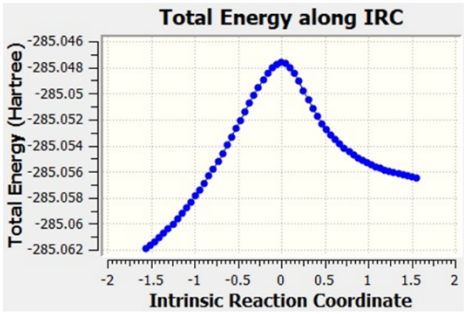
Glycine Path 3

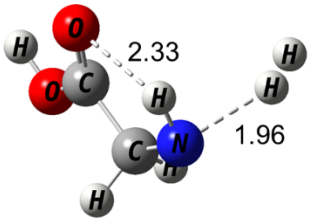


TS-V



Int-VII

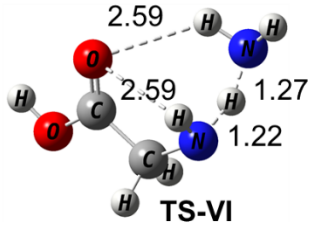




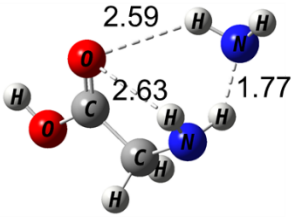
Int-VIII

$NHCH_2COOH\_H_2\_TS\text{-}V$

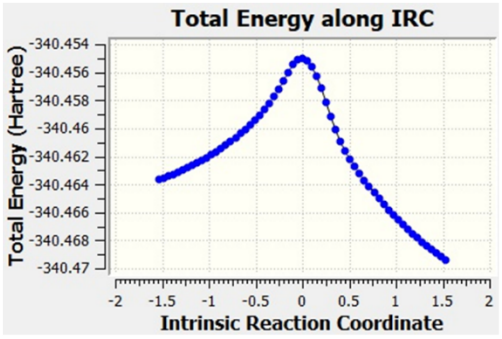
Glycine Path 3

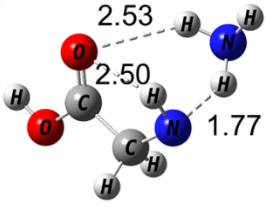


TS-VI



Int-IX

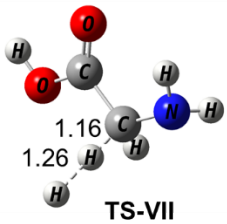




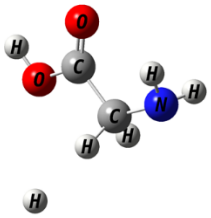
Int-X

$NHCH_2COOH\_NH_3\_TS\text{-}VI$

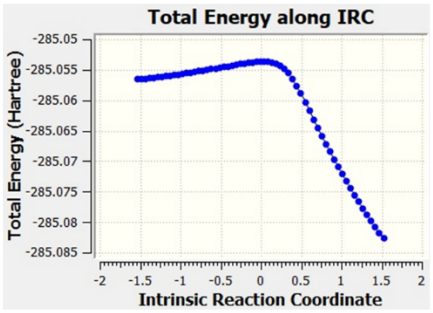
Glycine Path 3

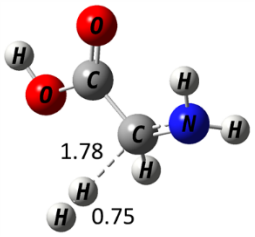


TS-VII



Int-XI

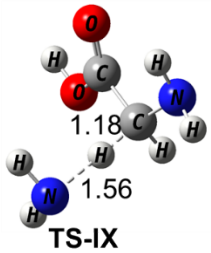




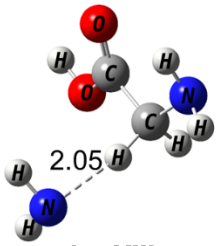
Int-XII

$NH_2CHCOOH\_H_2\_VII$

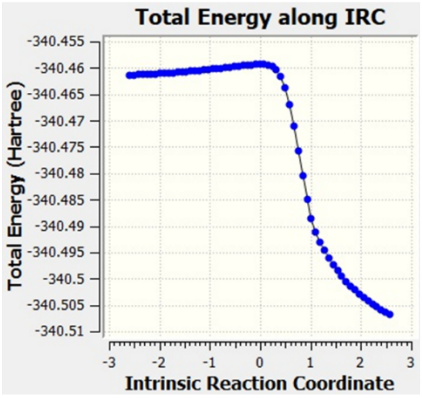
Glycine Path 3

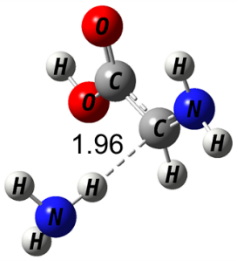


TS-IX
TS-VIII



Int-XIII





Int-XIV

$NH_2CHCOOH\_NH_3\_VIII$

Cartesian Coordinates of TSs and Magnitude of Imaginary Frequencies

The order of paths in which the coordinates are presented here is the same as that given in the main text. The same level of theory as described in the main text is used.

Glycine Precursors 1

$HCO\_CH_2NH\_TS\text{-}I$
Imaginary Frequency = 385.0862i

0 2

C	0.94989500	0.13064700	0.45201400
O	1.76164200	-0.16392100	-0.34440600
C	-1.05323100	0.60124400	-0.15596800
H	-0.75872100	0.92960100	-1.15344900
N	-1.55628000	-0.56657800	0.10921900
H	-1.48238800	-1.18406200	-0.69923500
H	0.84467500	-0.25068600	1.48708000
H	-1.18271700	1.39121100	0.58003400

$HCOCH_2NH\_TS\text{-}II$
Imaginary Frequency = 1968.3246i

0 2

C	-0.59082000	-0.09490500	-0.21501800
O	-1.72812100	-0.12883800	0.11436700
C	0.62007200	0.73526200	0.01136500
H	0.61277200	1.29099000	0.94837600
N	1.48370200	-0.50295100	-0.03293400
H	1.51229100	-0.88875500	0.91467400
H	0.26897400	-1.09325700	-0.51092200
H	0.86951000	1.40024300	-0.81460000

$HCOCH_2NH\_PR\_TS$
Imaginary Frequency = 1170.6700i

0 2

C	-1.29588800	0.50116100	0.04783400

C	-0.85697600	-1.05050400	0.57952600
H	-1.80322600	-1.58404900	0.62975700
N	0.08010600	-1.56843600	-0.27948000
H	-0.26953400	-2.02989400	-1.10701100
H	-0.44234000	-0.82995800	1.56333500
O	1.10815300	1.69501500	0.20159200
H	1.33614200	2.36959900	-0.44507100
H	-0.33676900	1.18469300	0.08492700
O	-2.38738200	0.70540700	-0.34162900
H	1.75332900	0.75815000	0.01156900
O	2.28435100	-0.38140600	-0.20569700
H	1.14577200	-1.14299000	-0.24664200
H	2.93208800	-0.60257500	0.46722000

$COCH_2NH_2\_H_2O\_TS\text{-}III$
Imaginary Frequency = 1695.5538i

0 2
C	0.89438500	-0.55256000	0.32596500
H	1.06156100	-1.62076600	0.13845900
N	1.94061800	0.33540200	-0.17098300
H	2.12859000	0.15381700	-1.14910500
C	-0.42386800	-0.24071600	-0.30528700
O	-1.50670300	-0.91548700	-0.12204300
H	2.80252900	0.19654700	0.33963700
H	0.81029800	-0.42174700	1.41057000
O	-1.03157900	1.16323900	0.21043900
H	-1.87455600	0.31901600	0.13982300
H	-1.02958600	1.80295500	-0.51374100

Glycine Precursors 2
$CH_3\_CO_2\_TS\text{-}I$
Imaginary Frequency = 108.7065i

0 2
C	-0.33852400	0.02810600	0.00001200
O	-0.51809700	1.23588900	0.00000200
O	-0.88860600	-1.04346600	0.00000200
C	1.38803700	-0.17086800	-0.00000200
H	1.85461200	0.80287100	0.00009900

H	1.55086500	-0.74271900	-0.90583200
H	1.55106800	-0.74296900	0.90563600

CH_3CO_2_TS-II
Imaginary Frequency = 2022.5880i

0 2

C	0.24408800	-0.06804700	-0.00000100
O	-0.17232400	1.21818100	0.00000100
O	1.36759100	-0.46877200	0.00000000
C	-1.11753200	-0.67730300	0.00000000
H	-1.48895800	-1.09980600	-0.92598300
H	-1.34357200	0.67645400	0.00000800
H	-1.48895000	-1.09983000	0.92597500

CH_3CO_2_PR_TS-III
Imaginary Frequency = 1349.5589i

0 2

C	1.26775400	-0.10319200	-0.00915000
O	0.65214000	-1.20572800	-0.00535000
O	2.49595700	0.02834900	-0.10532200
C	0.60736800	1.25460500	0.14544000
H	0.75630700	1.62202800	1.16002900
H	-2.02028800	-0.15449700	-0.00889000
H	1.00909900	1.97343000	-0.56466500
O	-1.75221600	-1.22878200	0.15543900
H	-0.57490200	-1.22508200	0.07694900
H	-2.13335200	-1.78135100	-0.53412200
O	-2.06527900	1.13910900	-0.22461400
H	-0.54413100	1.17658800	-0.05857300
H	-2.38828500	1.61682600	0.55031400

CH_2COOH_NH_3_TS-III
Imaginary Frequency = 531.9789i

0 2

C	0.61546600	-0.75020400	0.52693600
H	0.55568900	-1.79108700	0.22523100
C	-0.61995300	0.04508100	0.37459600

O	-0.42341200	1.30396000	0.18465800
O	-1.61367900	-0.61407600	-0.37168000
H	-2.18458100	0.08913200	-0.70541700
H	1.08219300	-0.63753300	1.50169900
N	1.64843200	0.03931900	-0.43918600
H	2.60188100	0.12048100	-0.10081700
H	1.08627200	0.96370500	-0.36743200
H	1.64317800	-0.30826500	-1.39198000

Glycine Path-3

HCOOH_OH_TS-I

Imaginary Frequency = 1383.4455i

0 2

C	-1.01075900	0.10573400	-0.00125800
O	-0.29551500	1.12786400	-0.01334500
O	-0.56887100	-1.08111300	0.02204800
H	0.59174100	-0.83133100	0.01236600
O	1.58714800	-0.09437500	-0.10156600
H	1.78960300	0.33193400	0.74389100
H	-2.09888600	0.24598000	-0.00580500

HCOO_TS-II

Imaginary Frequency = 1833.6259i

0 2

C	0.07887300	0.23756000	0.00003800
O	1.20281400	-0.10025300	-0.00003700
O	-1.13724900	-0.20640200	-0.00001500
H	-0.99776400	1.02788300	0.00018600

HCOO_PR_TS

Imaginary Frequency = 641.0529i

0 2

C	1.15579400	-0.08214900	-0.01129600
O	2.28399800	0.33514800	-0.02129100
O	0.55887300	-1.17897500	0.04035100
H	-0.93166100	-1.09533500	0.06354200
O	-1.91314800	-0.74931900	0.08194200

H	-0.01823300	1.06094500	-0.07376700
H	-2.38101300	-1.10990200	-0.67838200
O	-1.03476100	1.48242600	-0.09194500
H	-1.14583500	2.02982700	0.69719100
H	-1.61772500	0.49312700	-0.01326200

COOH_CH_2NH_TS-III
Imaginary Frequency = 215.8982i

0 2

C	-0.87312600	-0.05902600	-0.02434000
O	-1.88531600	-0.65953700	-0.11157900
C	1.25185300	-0.83461600	0.16487500
H	1.22955600	-1.67021000	-0.53237900
N	1.85099900	0.29473700	-0.06765000
H	2.20547600	0.33913500	-1.02120400
H	0.96130900	-1.06419600	1.18655000
O	-0.61610700	1.21146500	0.09349900
H	0.38568600	1.27853700	0.14200900

$NHCH_2COOH$_$NH_2CHCOOH$_TS-IV
Imaginary Frequency = 1925.00i

0 2

C	0.75234300	-0.66371300	0.01831900
H	0.73928100	-1.72414300	-0.19069000
N	2.01051000	-0.00048000	-0.11316600
H	1.51210200	-0.46988200	0.99036000
C	-0.50214700	0.09421400	-0.00184000
O	-0.56575800	1.30436500	0.01296700
O	-1.59160100	-0.71066100	-0.01997000
H	-2.37058400	-0.13591700	-0.01032400
H	1.80332800	1.00066000	-0.04003300

$NHCH_2COOH$_$NH_2CHCOOH$- PR-TS-II
Imaginary Frequency = 1146.10i

0 2

C	0.24115500	-0.19961500	-0.57600800
H	0.11712500	0.25057400	-1.55918800

N	-0.55376700	-1.27731500	-0.29326000
H	-0.55132200	0.86784700	0.12844200
C	1.58281000	-0.12055300	0.00187400
O	2.00849700	-0.82595800	0.89307100
O	2.32425600	0.89221100	-0.53460300
H	3.17028100	0.88891300	-0.06548800
H	-0.14084500	-1.81234400	0.46990200
O	-1.46582000	1.46071300	0.57523600
H	-2.25287700	0.75118100	0.30297800
H	-1.57604300	2.28436600	0.08455500
O	-2.90790200	-0.35470300	-0.18308300
H	-3.49592400	-0.80727700	0.42860000
H	-2.01006000	-0.93915200	-0.29715700

$NHCH_2COOH\_H_2\_TS\text{-}V$
Imaginary Frequency = 1336.06i

0 2

C	-0.64875800	-0.75050900	-0.18376600
H	-0.65029200	-1.52436800	0.58427200
N	-1.90143300	-0.02739400	-0.18086000
H	-1.71073500	0.92896500	-0.49026400
H	-0.55318900	-1.27989400	-1.13986900
C	0.59162400	0.10795800	-0.03389800
O	0.61056000	1.30855300	-0.10902700
O	1.69533900	-0.64225200	0.16558400
H	2.45235300	-0.04019200	0.22218700
H	-2.19544900	0.18424400	1.02514800
H	-2.13705100	0.44790200	1.91807200

$NHCH_2COOH\_NH_3\_TS\text{-}VI$
Imaginary Frequency = 1693.51i

0 2

C	0.12835800	1.10277800	-0.15089600
H	0.04035300	1.24019500	-1.23021100
N	-1.18052600	1.11360100	0.45342300
H	-1.11444200	0.72975500	1.39479600
H	0.70964200	1.95910100	0.21211800
C	0.96860900	-0.13696700	0.09931500

O	0.64593200	-1.07674000	0.77979400
O	2.15550800	-0.06264500	-0.53983200
H	2.64545800	-0.87475800	-0.34244300
N	-2.33750000	-0.77492800	-0.61320100
H	-1.87357400	0.32874300	-0.18055600
H	-1.64735300	-1.48223300	-0.35635200
H	-3.12721700	-0.95129600	0.01088900

$NH_2CHCOOH\_H_2\_VII$
Imaginary Frequency = 617.60i

0 2

C	0.72856300	-0.63464600	-0.09752900
N	1.91768500	0.15175300	-0.05332400
H	0.67051900	-1.34532300	0.82724100
C	-0.55636900	0.14724600	-0.02276800
O	-0.63280300	1.32638700	0.21399800
O	-1.63463600	-0.64542400	-0.20066900
H	-2.42296900	-0.09511000	-0.08359000
H	1.73872800	1.07153200	0.32831600
H	2.36616900	0.24290900	-0.95199200
H	0.61855700	-2.13562600	1.80778800
H	0.71154400	-1.32396100	-0.93934800

$NH_2CHCOOH\_NH_3\_VIII$
Imaginary Frequency = 357.73i

0 2

C	0.31375900	0.50395000	-0.59760000
H	0.33468400	0.35816600	-1.67702500
N	0.43179900	1.87502100	-0.22883300
C	-0.88962500	-0.13490700	0.01741700
O	-1.46043600	0.27028900	0.99923300
O	-1.23775900	-1.27617800	-0.61948900
H	-1.98131300	-1.65959000	-0.13171900
H	0.15735800	2.03298500	0.73180200
H	1.35048300	2.25376300	-0.40563300
N	2.39082800	-1.00933700	0.36970800
H	1.98656000	-1.18993400	1.29440100
H	2.21196800	-1.87828400	-0.14359000

H	1.22262600	-0.14403700	-0.21122100