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SUPPORTING INFORMATION

Possible interstellar formation of Glycine through a concerted mechanism: A computational study on the reaction of CH_2=NH, CO_2 and H_2

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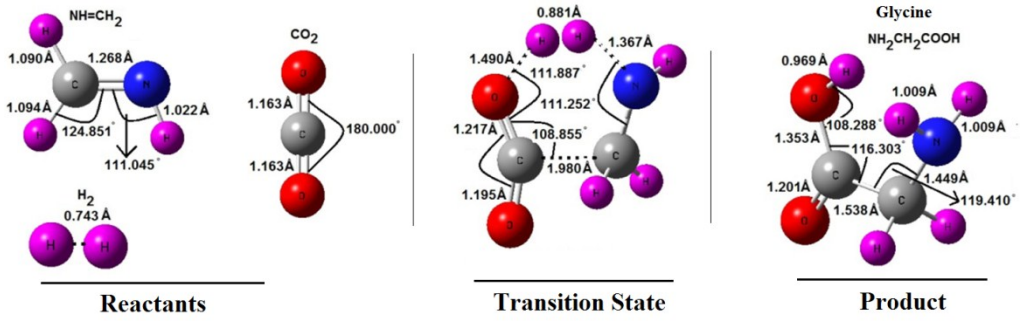


Figure S1: B3LYP/6-31G(3df,2pd) optimized geometries of the reactants, transition state and product.

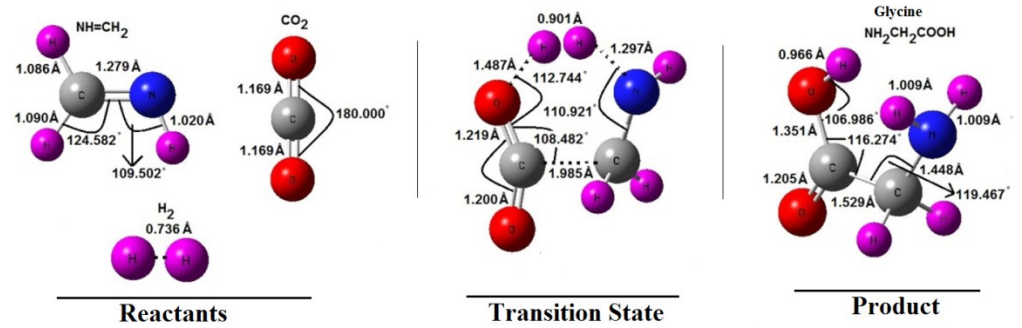


Figure S2: MP2/6-31G(3df,2pd) optimized geometries of the reactants, transition state and product.

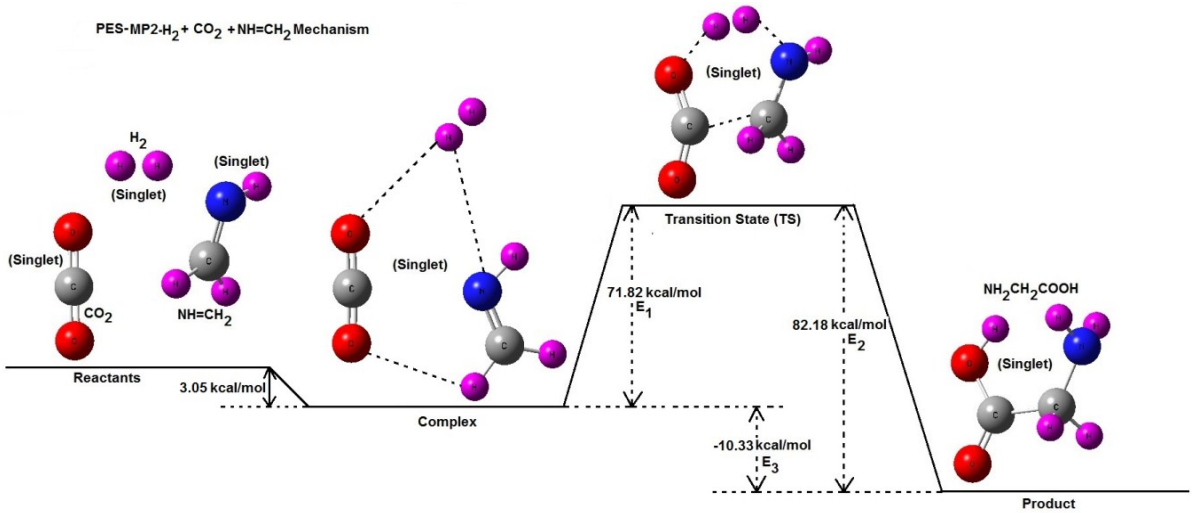
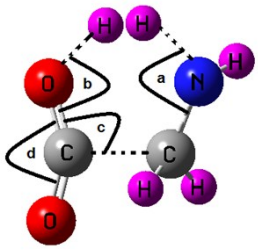


Figure S3: MP2/6-31G(3df,2pd) PES for the CH_2=NH + CO_2 + H_2 → Glycine, reaction. All the energies are in kcal/mol and the diagram is not to scale.(Colour Code: Pink=Hydrogen, Grey=Carbon, Blue=Nitrogen, Red=Oxygen)

Table S1: Results of effect of various basissets (with B3LYP method) on the potential energy surface of the CH_2=NH + CO_2 + H_2 → Glycine reaction. Where $\mathbf{\Delta E_1} = E_{TS} - E_{REACTANTS}$, $\mathbf{\Delta E_2} = E_{TS} - E_{PRODUCT}$ and $\mathbf{\Delta E_3} = E_{REACTANTS} - E_{PRODUCT}$. All the energies are ZPE corrected and are in kcal/mol.

Basissets	ΔE_1	ΔE_2	ΔE_3
6-31G	62.0	86.4	24.4
6-31G*	69.8	76.5	6.7
6-31++G(d,p)	69.0	85.3	16.3
6-31++G(2df,2p)	70.8	80.2	9.4
6-31++G(3df,2pd)	70.4	80.1	9.7
6-31++G(3df,3pd)	70.3	80.1	9.8
aug-cc-pvdz	67.0	80.6	13.6
aug-cc-pvtz	71.3	79.8	8.5

Table S2: Effect of various methods on the geometry of the transition state for the reaction, CH_2=NH + CO_2 + H_2 → Glycine. Some important geometric data are shown [Basisset used is 6-31++G(3df,2pd)] .



Methods	Bond length	Bond angles
X3LYP	H-H = O.880 Å	a = 111.334º
	N-H = 1.366 Å	b = 111.940º
	O-H = 1.490 Å	c = 108.819º
	C-C = 1.979 Å	d = 144.866º
B3PW91	H-H = 0.877 Å	a = 111.640º
	N-H = 1.367 Å	b = 112.315º
	O-H = 1.506 Å	c = 108.531º
	C-C = 1.981 Å	d = 145.674º
HF	H-H = 0.866 Å	a = 112.611º
	N-H = 1.394 Å	b = 110.478º
	O-H = 1.419 Å	c = 108.567º
	C-C = 1.957 Å	d = 145.622º
O3LYP	H-H = 0.878 Å	a = 111.337º
	N-H = 1.352 Å	b = 112.300º
	O-H = 1.525 Å	c = 118.587º
	C-C = 1.983 Å	d = 145.134º
MP2=full	H-H = 0.904 Å	a = 111.039º
	N-H = 1.285 Å	b = 113.148º
	O-H = 1.493 Å	c = 108.234º
	C-C = 1.982 Å	d = 146.184º
	H-H = 0.891 Å	a = 110.910º

CBS-QB3	N-H = 1.343 Å	b = 111.813º
	O-H = 1.489 Å	c = 108.681º
	C-C = 1.981 Å	d = 114.584º
G3B3	H-H = 0.881 Å	a = 109.682º
	N-H = 1.374 Å	b = 110.968º
	O-H = 1.500 Å	c = 110.082º
	C-C = 1.942 Å	d = 142.944º
G3MP2B3	H-H = 0.881 Å	a = 109.682º
	N-H = 1.374 Å	b = 110.968º
	O-H = 1.500 Å	c = 110.080º
	C-C = 1.942 Å	d = 142.944º

Table S3: Effect of various Basissets on the geometry of the transition state. Some important geometric data are shown (Method used is B3LYP).

Basissets	Bond length	Bond angles
6-31G	H-H = O.882 Å	a = 110.552º
	N-H = 1.361 Å	b = 111.346º
	O-H = 1.557 Å	c = 110.468º
	C-C = 1.961 Å	d = 142.490º
6-31G(d)	H-H = O.881 Å	a = 109.682º
	N-H = 1.374 Å	b = 110.968º
	O-H = 1.500 Å	c = 110.082º
	C-C = 1.942 Å	d = 142.944º
6-31+G(d)	H-H = 0.875 Å	a = 110.274º
	N-H = 1.378 Å	b = 111.352º
	O-H = 1.517 Å	c = 110.062º
	C-C = 1.946 Å	d = 143.080º
6-31++G(d)	H-H = 0.877 Å	a = 110.324º
	N-H = 1.375 Å	b = 111.415º
	O-H = 1.516 Å	c = 110.000º
	C-C = 1.948 Å	d = 143.158º
6-31++G(d,p)	H-H = 0.877 Å	a = 111.142º
	N-H = 1.365 Å	b = 111.733º
	O-H = 1.514 Å	c = 109.279º
	C-C = 1.974 Å	d = 144.127º
6-31++G(2df,2p)	H-H = 0.882 Å	a = 111.266º
	N-H = 1.357 Å	b = 111.934º
	O-H = 1.498 Å	c = 108.949º
	C-C = 1.976 Å	d = 144.519º
6-31++G(2df,2pd)	H-H = 0.882 Å	a = 111.317º
	N-H = 1.360 Å	b = 111.954º
	O-H = 1.493 Å	c = 108.824º
	C-C = 1.983 Å	d = 144.726º
6-31++G(3df,2pd)	H-H = 0.881 Å	a = 111.252º
	N-H = 1.367 Å	b = 111.887º
	O-H = 1.490 Å	c = 108.885º
	C-C = 1.980 Å	d = 144.701º
6-31++G(3df,3pd)	H-H = 0.880 Å	a = 111.286º
	N-H = 1.368 Å	b = 111.877º

	O-H = 1.489 Å	c = 108.838º
	C-C = 1.981 Å	d = 144.726º
aug-cc-pvdz	H-H = 0.890 Å	a = 111.651º
	N-H = 1.365 Å	b = 112.087º
	O-H = 1.514 Å	c = 109.056º
	C-C = 1.981 Å	d = 144.570º
aug-cc-pvtz	H-H = 0.885 Å	a = 111.509º
	N-H = 1.357 Å	b = 111.921º
	O-H =1.486 Å	c = 108.710º
	C-C = 1.987 Å	d = 144.630º

Cartesian Coordinates of stationary points

[From B3LYP/6-31++G(3df,2pd) optimized geometries]

vdW-Complex

C	-2.203213	-0.336688	0.001473
N	-1.280195	0.551229	-0.010608
H	-1.611679	1.525427	-0.022085
H	-3.278983	-0.131151	0.000174
H	-1.907027	-1.383933	0.014057
H	0.595324	3.116494	0.039220
H	0.277356	3.788759	0.052167
C	1.234283	-0.378808	-0.000894
O	0.826328	-1.496510	0.012374
O	1.761166	0.686357	-0.013968

Transition State

C	-0.862934	-0.842765	-0.036846
H	-0.638687	-1.360943	-0.963695
H	-0.628966	-1.362549	0.886707
O	1.721333	-0.754475	0.014891
C	0.881010	0.094701	0.006462
O	0.682131	1.295036	0.013443
H	-0.768861	1.618030	-0.081691
N	-1.926940	-0.024242	-0.067513
H	-2.261122	0.169088	0.878724
H	-1.549954	1.269967	-0.291813

Methanimine (CH_2=NH)

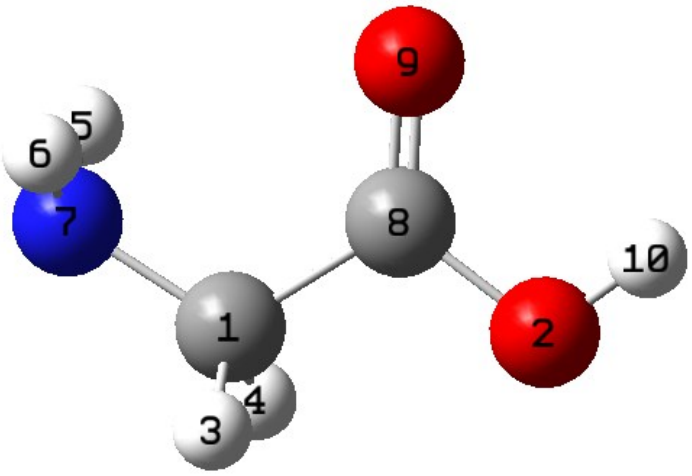
C	0.586885	0.028877	-0.000014
H	1.245720	-0.839259	0.000030
H	1.076099	1.007625	0.000028
N	-0.667824	-0.154020	0.000003
H	-1.168363	0.736515	0.000004

Product (Glycine)

C	0	0.745907	-0.750143	0.000094
O	0	-1.672056	-0.714322	-0.000069
H	0	0.764079	-1.412175	-0.869017
H	0	0.764093	-1.411864	0.869445
H	0	1.949029	0.692680	0.812616
H	0	1.949047	0.692359	-0.812971
N	0	1.931433	0.088161	-0.000058

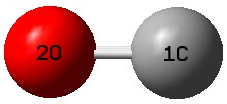
C	0	-0.634976	-0.097365	0.000002
O	0	-0.590688	1.257176	0.000038
H	0	-1.509914	1.564093	-0.000001

Optimized structure and Cartesian co-ordinates of the most stable structure of the glycine [B3LYP/6-31++G(3df,2pd)]:

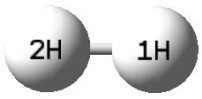


C	-0.728457	-0.727536	0.000185
O	1.650900	-0.667486	-0.000017
H	-0.686102	-1.387480	0.870798
H	-0.685992	-1.387893	-0.870104
H	-2.022536	0.621328	-0.809568
H	-2.022468	0.621978	0.808951
N	-1.975150	0.012175	-0.000066
C	0.543433	0.113333	0.000110
O	0.590811	1.318687	-0.000135
H	2.419598	-0.077555	-0.000166

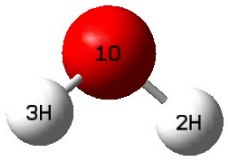
B3LYP/6-31++G(d,p) Optimized structures and the geometric parameters of the various stationary points (in the reaction 1 and 3 (for reaction 2, see the reference 35)



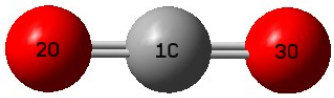
R(1,2) 1.1373



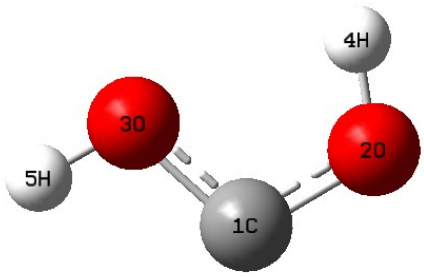
R(1,2) 0.7438



R(1,2)	0.9653
R(1,3)	0.9653
A(2,1,3)	105.7192

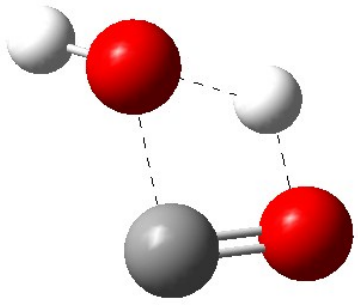


R(1,2)	1.1694
R(1,3)	1.1694
A(2,1,3)	180.0000



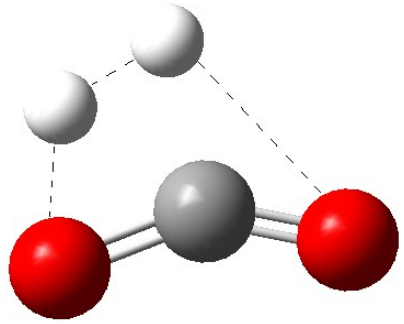
R(1,2)	1.3132
R(1,3)	1.3436
R(2,4)	0.9855
R(3,5)	0.9679
A(2,1,3)	107.2889
A(1,2,4)	112.1525
A(1,3,5)	107.9239
D(3,1,2,4)	-0.0236
D(2,1,3,5)	180.0107

Transition state for CO + H_2O → Dihydroxy Carbene in Cartesian coordinates

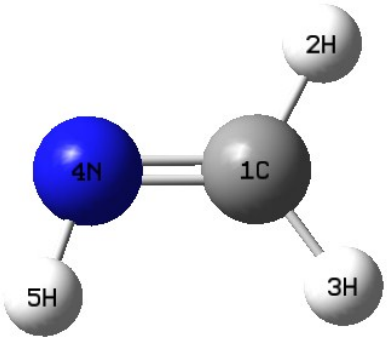


C	0.331554	0.724044	-0.009582
O	1.028719	-0.303161	0.024499
O	-1.053836	-0.138371	-0.092728
H	-0.038883	-0.895925	0.053308
H	-1.749501	0.083921	0.550012

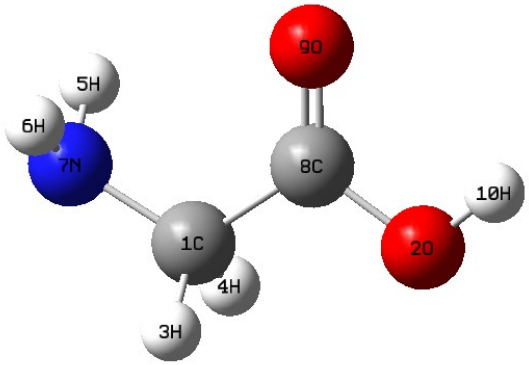
Transition state for $CO_2 + H_2 \rightarrow$ Dihydroxy Carbene in Cartesian co-ordinates



C	0.000000	0.154507	0.000000
O	-0.858268	-0.769092	0.000000
O	1.143441	0.438118	0.000000
H	-1.414272	0.426526	0.000000
H	-0.867110	1.294223	0.000000

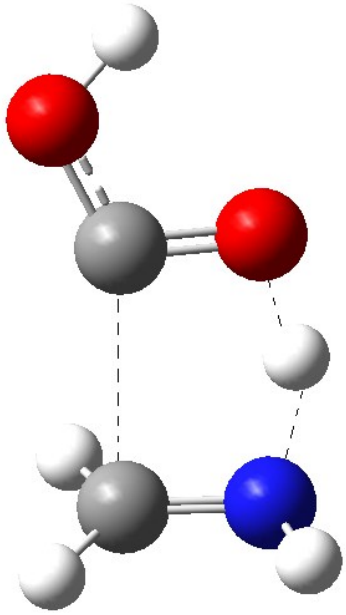


R(1,2)	1.093
R(1,3)	1.0985
R(1,4)	1.272
R(4,5)	1.0252
A(2,1,3)	116.1708
A(2,1,4)	118.8487
A(3,1,4)	124.9805
A(1,4,5)	110.9655
D(2,1,3,4)	180.0
D(2,1,4,5)	180.0
D(3,1,4,5)	0.0



R(1,3)	1.0965
R(1,4)	1.0965
R(1,7)	1.4489
R(1,8)	1.5255
R(2,8)	1.3566
R(2,10)	0.9726
R(5,7)	1.0163
R(6,7)	1.0163
R(8,9)	1.2125
A(3,1,4)	105.6019
A(3,1,7)	109.8916
A(3,1,8)	107.5308
A(4,1,7)	109.8917
A(4,1,8)	107.532
A(7,1,8)	115.8688
A(8,2,10)	107.4783
A(1,7,5)	110.6883
A(1,7,6)	110.6881
A(5,7,6)	106.4526
A(1,8,2)	111.5141
A(1,8,9)	125.709
A(2,8,9)	122.7769
D(3,1,7,5)	-178.9936
D(3,1,7,6)	63.2173
D(4,1,7,5)	-63.203
D(4,1,7,6)	179.008
D(8,1,7,5)	58.9025
D(8,1,7,6)	-58.8865
D(3,1,8,2)	56.6567
D(3,1,8,9)	-123.3429
D(4,1,8,2)	-56.6458
D(4,1,8,9)	123.3546
D(7,1,8,2)	-179.9951
D(7,1,8,9)	0.0054
D(10,2,8,1)	-179.9986
D(10,2,8,9)	0.001

Transition state for CH_2=NH + Dihydroxy Carbene → Glycine in Cartesian co-ordinates



C	1.559382	0.831178	0.114655
H	1.255435	1.191327	1.091298
H	1.792364	1.589295	-0.633570
N	1.842668	-0.436990	-0.035242
H	2.193751	-0.645546	-0.969736
C	-0.789193	0.223403	-0.068325
O	-0.511287	-1.004661	0.121062
O	-2.091138	0.495747	-0.088378
H	0.669602	-1.007492	0.164719
H	-2.611566	-0.324829	0.054532

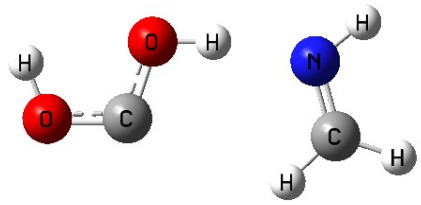
Pre-reaction complex for CO_2 + H_2 → Dihydroxy Carbene in Cartesian co-ordinates

C	0.377868	-0.000850	-0.000039
O	-0.791581	-0.005607	-0.000119
O	1.547023	0.003856	0.000047
H	-4.527355	0.012111	-0.002479
H	-3.783386	0.006997	0.003295

Pre-reaction complex for CO + H_2O → Dihydroxy Carbene in Cartesian coordinates

C	0.984844	0.102639	0.006397
O	2.109682	-0.050449	-0.004060
O	-2.325829	-0.127510	-0.000966
H	-2.795790	0.715065	-0.010819
H	-1.384095	0.092773	0.012644

Pre-reaction Complex for CH_2=NH + Dihydroxy Carbene → Glycine in Cartesian co-ordinates



C	2.293978	-0.713912	0.000111
H	1.500801	-1.462698	-0.000956
H	3.333583	-1.057367	0.001456
N	1.957264	0.515099	-0.000215
H	2.754434	1.154577	0.001053
C	-1.146396	-0.420505	-0.000513
O	-0.731561	0.832590	-0.000012
O	-2.471699	-0.427343	0.000271
H	0.275487	0.832108	-0.000749
H	-2.824561	0.492213	0.001044