Electronic Supplementary Information

Radical formation of amino acid precursors in interstellar regions? Ser, Cys and Asp.

Daniel J. Knowles, Tianfang Wang and John H. Bowie*

Department of Chemistry, The University of Adelaide, South Australia, 5005.

* Corresponding author. e-mail: john.bowie@adelaide.edu.au

Tables S1-S4 contain data concerning the geometries [B3LYP/6-31+G(d) level of theory] and single point energies [calculated at CCSD(T)/aug-cc-pVDZ] of all minima and transition states shown in the appropriate Figures in the text. Relative energies with zero-point corrections are recorded in kJ mol^{-1} units in all tables.

Table S1 Energy and geometry data of minima and transition state for the interconversion of doublet $NH_2CH_2^{\cdot}$ and $CH_3NH^{\cdot}$ Relative energies in kJ mol^{-1} with respect to A (0 kJ mol^{-1})

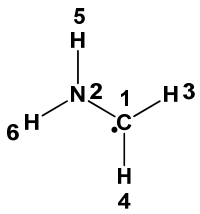
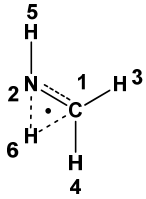
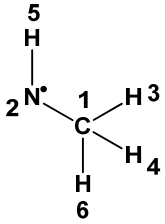
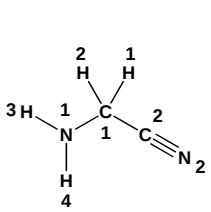
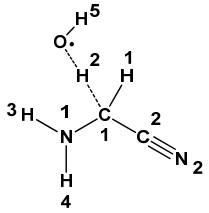
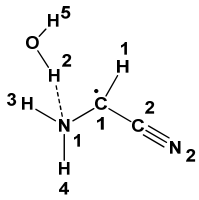
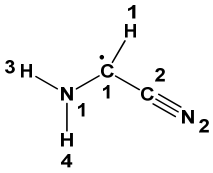
			
	A	**TS A/B**	**B**
State	^{2}A	^{2}A	^{2}A
Symmetry	C_1	C_1	C_1
Energy (Hartrees)	-94.91061	-94.84318	-94.90351
ΔE^o_r (kJ mol^{-1})	0	177	19
ΔG^o (kJ mol^{-1})	0	177	18
Bond Length (Å)			
C^1N^2	1.399	1.450	1.444
C^1H^3	1.085	1.089	1.104
C^1H^4	1.085	1.085	1.104
C^1H^6	-	1.290	1.094
N^2H^5	1.014	1.026	1.030
N^2H^6	1.014	-	-
Bond Angle (^{o})			
$C^1N^2H^5$	115.4	107.2	106.9
$C^1N^2H^6$	115.4	56.5	-
$H^3C^1H^4$	118.1	118.3	106.0
$H^5N^2H^6$	110.9	103.1	-
$H^3C^1N^2$	116.1	121.4	111.4
$H^4C^1N^2$	116.1	114.7	111.5
$H^6C^1N^2$	-	53.9	-
Dihedral Angle (^{o})			
$H^6N^2C^1H^5$	-	94.6	-
$H^5N^2C^1H^3$	-41.4	-15.2	-59.3
$H^5N^2C^1H^4$	172.9	-168.7	59.1
$H^6N^2C^1H^3$	-172.9	-109.8	-
$H^6N^2C^1H^4$	41.4	96.6	-
$H^5N^2C^1H^6$	-	94.6	179.9

Table S2 Energy and geometry data of minima and transition state for the reaction between NH_2CH_2CN and $HO^{\cdot}$. Relative energies in kJ mol^{-1} with respect to [A+B] (0 kJ mol^{-1})

	 **A**	 **TS [A+B]/C**	 **C**	 **D**
State	^{1}A	^{2}A	^{2}A	^{2}A
Symmetry	C_1	C_1	C_1	C_1
Energy (Hartrees)	-187.58000	-263.15176	-263.208618	-186.951365
ΔE (kJ mol^{-1})	0 [A+B]	11	-138	-128 [D+E]
ΔG (kJ mol^{-1})	0 [A+B]	41	-114	-130 [D+E]
Bond Length (Å)				
C^1N^1	1.460	1.436	1.391	1.383
C^1H^1	1.095	1.094	1.083	1.083
C^1H^2	1.095	1.144	-	-
N^1H^3	1.018	1.015	1.016	1.012
N^1H^4	1.018	1.015	1.015	1.013
C^2N^2	1.162	1.163	1.176	1.176
C^1C^2	1.483	1.475	1.391	1.391
OH^2	-	1.597	0.975	-
OH^5	-	0.982	0.969	-
N^1H^2	-	-	2.108	-
Bond Angle (°)				
$C^1N^1H^3$	111.1	114.1	115.3	117.1
$C^1N^1H^4$	111.1	114.0	116.1	117.7
$H^1C^1N^1$	108.9	110.0	117.5	117.5
$H^2C^1N^1$	108.9	108.9	-	-
$N^1C^1C^2$	115.5	116.1	121.6	121.8
$C^1C^2N^2$	177.6	178.2	179.3	179.2
$H^1C^1C^2$	108.2	109.6	120.5	120.3
$H^2C^1C^2$	108.2	106.8	-	-
OH^2C^1	-	174.4	-	-
H^5OH^2	-	102.7	106.3	-
$H^2N^1C^1$	-	-	114.1	-
OH^2N^1	-	-	149.1	-
Dihedral Angle (°)				
$H^3N^1C^1H^1$	-62.2	38.1	29.8	-25.4
$H^4N^1C^1H^1$	178.2	166.7	163.9	-167.3
$H^3N^1C^1C^2$	59.8	-87.0	-157.9	161.4
$H^4N^1C^1C^2$	-59.8	41.5	-23.8	19.5
$H^1C^1C^2N^2$	122.3	-171.1	-109.9	98.7
$H^2C^1C^2N^2$	-122.3	75.8	-	-
$OH^2C^1C^2$	-	31.1	-	-
$H^5OH^2C^1$	-	-18.4	-	-
$OH^2N^1C^1$	-	-	123.1	-
$H^5OH^2N^1$	-	-	-177.7	-

 , **[B]**, **State $^2\Sigma$, Symmetry** $C_{\infty v}$**, Energy** -75.57593 **Hartree,** OH 0.967 Å

 , **[E]**, **State $^1A_1$, Symmetry** C_{2v}**, Energy** -76.25314 **Hartree,** OH 0.959 Å**,** HOH 104.5°

Table S3 Energy and geometry data of minima and transition state for the interconversion of doublet $^{\cdot}CH_2SH$ and $CH_3S^{\cdot}$. Relative energies in kJ mol^{-1} with respect to A (0 kJ mol^{-1})

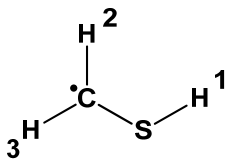
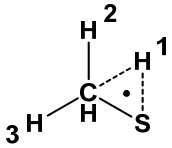
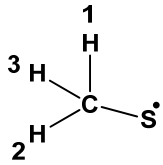
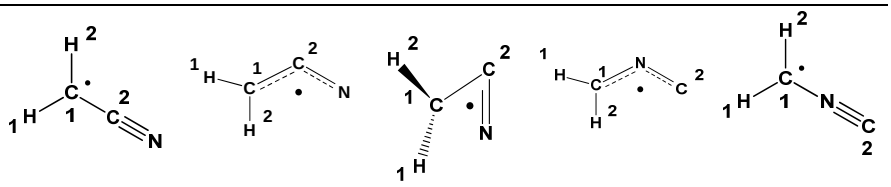
			
	A	**TS A/B**	**B**
State	^2A	^2A	^2A
Symmetry	C_1	C_1	C_1
Energy (Hartrees)	-437.38893	-437.34623	-437.40532
ΔE (kJ mol^{-1})	0	50	-43
ΔG (kJ mol^{-1})	0	114	-41
Bond Length(Å)			
CS	1.731	1.793	1.810
CH^1	-	1.492	1.092
CH^3	1.081	1.081	1.092
CH^2	1.081	1.081	1.092
SH^1	1.341	1.451	-
Bond Angle(°)			
H^1SC	97.8	53.6	-
H^2CS	121.7	119.4	111.7
H^3CS	116.7	119.4	106.8
H^3CH^2	120.8	120.4	107.8
SCH^1	-	51.6	111.7
H^3CH^1	-	111.0	110.6
H^2CH^1	-	111.0	107.8
Dihedral Angle(°)			
H^1SCH^2	-15.4	94.5	-
H^1SCH^3	179.1	-94.5	-

Table S4 Energy and geometry data of minima and transition states for the interconversion of $^{\cdot}CH_2CN$ and $^{\cdot}CH_2NC$. Relative energies in kJ mol^{-1} with respect to A (0 kJ mol^{-1})



	A	TS A/B	B	TS B/C	C
State	^2A	^2A	^2A	^2A	^2A
Symmetry	C_1	C_1	C_1	C_1	C_1
Energy (Hartrees)	-131.76223	-131.67871	-131.68230	-131.67920	-131.72525
ΔE (kJ mol^{-1})	0	219	210	218	97
ΔG (kJ mol^{-1})	0	214	211	213	96
Bond Length (Å)					
C^1C^2	1.38	1.498	1.498	1.787	-
C^2N	1.178	1.197	-	1.223	1.198
C^1N	-	-	1.635	1.461	1.336
C^1H^1	1.083	1.085	1.085	1.083	1.083
C^1H^2	1.083	1.085	1.085	1.083	1.083
Bond Angle (°)					
C^1C^2N	-	94.1	73.1	-	-
C^1NC^2	-	-	-	82.9	-
H^2C^1N	-	-	-	-	118.9
H^2C^1N	-	-	-	-	118.9
$C^2C^1H^2$	120.2	118.9	120.2	-	-
$C^2C^1H^1$	120.2	118.9	120.2	-	-
$H^1C^1H^2$	119.5	120.7	118.2	120.4	122.1
H^1C^1N	-	-	-	118.5	-
H^2C^1N	-	-	-	118.5	-
Dihedral Angle (°)					
$H^2C^1C^2N$	-78.0	83.4	96.8	-	-
$H^2C^1C^2N$	101.9	-83.4	96.8	-	-
$H^1C^1NC^2$	-	-	-	-98.7	87.3
$H^2C^1NC^2$	-	-	-	98.7	-92.7