Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information

Synthesis of CxNy-rich polycyclic oligomers from primeval monomers in aqueous media†

Nieves Lavado,*[a] Juan García de la Concepción,[b,a] Pedro Cintas[a] and Reyes Babiano*[a]

[a.] *Departamento de Química Orgánica e Inorgánica, Facultad de Ciencias, and IACYS-Unidad de Química Verde y Desarrollo Sostenible, Universidad de Extremadura, E-06006 Badajoz, Spain*
[b.] *Departamento de Astrofísica, Centro de Astrobiología (INTA-CSIC), 28850 Torrejón de Ardoz, Madrid, Spain.*

CONTENTS

1. ELEMENTAL MICROANALYSES DATA

Table S1.1. Elemental microanalyses and reaction mass efficiencies (RME) for oligomeric solids obtained for cyanamide-glyoxal mixtures in water

	Elemental analysis				Cyanamide		Glyoxal		RME					
	%C	%H	%N	%O	g	mmol	mL	mmol	g	% total	% C	% H	% N	% O
2:1	32.9	3.92	42.1	21.1	2.0	47.6	2.72	23.7869	0.0899	2.7	2.59	2.45	2.84	6.02
3:1 (1)*	32.04	4.1	45.99	17.9	3.0	71.4	2.72	23.7869	0.4138	9.4	9.28	8.84	9.52	23.48
3:1 (2) *	31.8	3.94	44.6	19.7	3.0	71.4	2.72	23.7869	0.0054	0.1	0.12	0.11	0.12	0.34
3:1 (3) *	31.7	4.18	43.8	20.3	3.0	71.4	2.72	23.7869	0.1967	4.5	4.37	4.29	4.31	12.69
4:1 (1) *	31.6	4.03	47.7	16.7	4.0	95.1	2.72	23.7869	0.7492	13.9	13.81	12.59	13.41	39.66
4:1 (2) *	31.5	4.03	46	18.5	4.0	95.1	2.72	23.7869	0.0256	0.5	0.47	0.43	0.44	1.50
4:1 (3) *	30.5	4.04	44.7	20.8	4.0	95.1	2.72	23.7869	0.1386	2.6	2.47	2.33	2.32	9.14
5:1 (1) *	31.5	4.03	50.2	14.3	5.0	118.9	2.72	23.7869	0.4166	6.5	6.56	5.83	6.28	18.88
5:1 (2) *	31.4	3.96	49.6	15.0	5.0	118.9	2.72	23.7869	0.1251	2.0	1.96	1.72	1.86	5.98
5:1 (3) *	30.1	4.01	45.9	20.0	5.0	118.9	2.72	23.7869	0.2398	3.8	3.61	3.34	3.30	15.22
6:1 (1) *	31.3	3.97	52.6	12.1	6.0	142.7	2.72	23.7869	0.5711	7.7	7.82	6.75	7.51	22.00
6:1 (2) *	30.3	4.11	49.9	15.7	6.0	142.7	2.72	23.7869	0.2763	3.7	3.66	3.38	3.45	13.77

(*) Numbering in parenthesis denote first, second, or third crop, respectively.

2. MASS SPECTROMETRY DATA

Mass spectra data		Global reaction stoichiometry[b]			2:1		3:1		4:1		5:1		6:1	
m/z (calcd)	**Formula[a]**	**C:G**	**H_2O**	**NH_3**	**Intensity**	**Error**	**Intensity**	**Error**	**Intensity**	**Error**	**Intensity**	**Error**	**Intensity**	**Error**
68.0249	$C_2H_2N_3$	2:0		-1			17.1	0.000	11.7	-0.003	8.3	-0.002	11.0	0.000
82.0405	$C_3H_4N_3$	1:1	-4	1	16.0	-0.002	9.6	-0.003	8.0	-0.003	5.2	0.000	5.0	-0.024
85.0514	$C_2H_5N_4$	2:0			51.8	0.000	50.0	-0.002	46.4	-0.001	37.6	-0.001	36.3	0.000
94.0504	$C_2H_8NO_3$	0:1	-1	1	41.8	0.009	22.0	0.009	21.3	0.010	5.7	0.009	12.8	0.011
99.0671	$C_3H_7N_4$	1:1	-4	2	19.3	-0.004	29.1	-0.001	19.8	0.001	17.1	-0.001	15.1	0.002
100.0511	$C_3H_5N_3O$	1:1	-3	1	36.0	0.000	22.0	-0.002	16.8	-0.001	7.4	0.000	7.7	0.001
107.0358	$C_4H_3N_4$	2:1	-4				13.1	-0.001	12.8	-0.003	5.1	-0.004	5.9	0.003
110.0467	$C_3H_4N_5$	3:0		-1	26.4	-0.002	62.3	-0.002	61.2	-0.001	44.2	-0.001	55.4	0.000
118.0617	$C_3H_8N_3O_2$	1:1	-2	1	34.7	-0.002	14.1	-0.002	13.6	-0.004	2.6	-0.001	9.9	0.000
124.0623	$C_4H_6N_5$	2:1	-4	1	46.2	0.000	87.7	-0.001	50.2	-0.002	35.1	-0.001	20.3	0.000
125.0463	$C_4H_5N_4O$	2:1	-3		41.5	-0.002	31.1	0.000	21.7	-0.001	12.0	-0.002	8.9	-0.001
127.0732	$C_3H_7N_6$	3:0			66.8	-0.002	**100**	-0.001	73.8	0.000	61.1	-0.001	45.9	0.001
142.0729	$C_4H_8N_5O$	2:1	-3	1	26.1	0.008	17.9	-0.001	18.5	0.001	6.3	0.001	5.8	-0.001
143.0569	$C_4H_7N_4O_2$	2:1	-2				14.8	-0.001	7.7	0.001	2.3	0.006	6.5	0.004
149.0576	$C_5H_5N_6$	3:1	-4		47.1	-0.002	75.3	-0.001	72.0	-0.001	65.8	-0.001	78.4	0.000
152.0685	$C_4H_6N_7$	4:0		-1	35.9	-0.001	91.5	-0.001	**100**	-0.002	**100**	-0.001	**100**	0.001
165.0413	$C_6H_5N_4O_2$	2:2	-6		21.5	-0.004	12.8	0.000	11.4	-0.001	6.3	0.005	4.6	-0.005
166.0841	$C_5H_8N_7$	3:1	-4	1			80.5	0.000	45.2	0.000	21.3	-0.001	22.8	0.001
167.0681	$C_5H_7N_6O$	3:1	-3		51.7	-0.003	36.1	-0.002	22.2	-0.006	7.8	-0.007	12.2	-0.001
169.095	$C_4H_9N_8$	4:0											7.1	-0.001
176.0671	$C_5H_{10}N_3O_4$	1:2	-4	1			10.1	-0.001						
177.0511	$C_5H_9N_2O_5$	1:2	-3		37.5	0.000	13.4	-0.001	12.7	-0.004	7.1	-0.012	10.8	-0.010
182.0678	$C_6H_8N_5O_2$	2:2	-6	1			9.5	0.000			2.8	-0.001		
188.0685	$C_7H_6N_7$	3:2	-8	1	80.8	0.001	72.2	0.002	44.4	0.002	9.9	0.003	6.0	0.002
191.0794	$C_6H_7N_8$	4:1	-4		33.4	0.000	29.6	0.000	61.6	-0.002	38.2	-0.001	36.6	0.002
201.0624	$C_6H_9N_4O_4$	2:2	-4				9.5	-0.001	7.0	-0.003				
206.079	$C_7H_8N_7O$	3:2	-7	1	22.0	-0.002	9.5	-0.004	8.7	-0.002	3.2	-0.004		
207.063	$C_7H_7N_6O_2$	3:2	-6				11.1	0.000	12.3	-0.008				
208.1059	$C_6H_{10}N_9$	4:1	-4	1			37.1	-0.005	36.5	-0.002	18.8	-0.001	19.3	0.001
209.0899	$C_6H_9N_8O$	4:1	-3		64.6	-0.003	62.6	-0.001	29.3	-0.004	12.0	-0.003	14.4	0.004
211.0368	$C_9H_3N_6O$	3:3	-11		22.5	0.005	18.5	0.002	17.1	0.003	4.6	0.004	6.4	0.005
224.0896	$C_7H_{10}N_7O_2$	3:2	-6	1			34.2	0.003	65.6	0.001	18.6	-0.001	16.8	0.004

Mass spectra data		Global reaction stoichiometry[b]			2:1		3:1		4:1		5:1		6:1	
m/z (calcd)	Formula[a]	C:G	H_2O	NH_3	Intensity	Error	Intensity	Error	Intensity	Error	Intensity	Error	Intensity	Error
225.0736	$C_7H_9N_6O_3$	3:2	-5				22.6	-0.001	30.7	-0.001	4.9	-0.003	7.5	0.003
230.0903	$C_8H_8N_9$	4:2	-8	1	25.8	-0.005	9.6	-0.001	10.1	-0.002	5.3	0.003		
231.0743	$C_8H_7N_8O$	4:2	-7				34.0	0.000	37.3	0.001	11.0	-0.001	6.8	0.001
232.1046	$C_7H_{14}N_5O_4$	1:3	-8	3	**100**	-0.002	40.4	-0.002	26.4	-0.002	5.2	-0.001	41.0	0.001
233.1012	$C_7H_9N_{10}$	5:1	-4		26.3	-0.006	17.0	-0.005	13.4	0.000	16.8	-0.001	14.9	-0.001
249.0848	$C_8H_9N_8O_2$	4:2	-6		25.6	0.001	46.0	0.000	34.2	0.000	13.2	0.000	10.2	0.003
251.1117	$C_7H_{11}N_{10}O$	5:1	-3				30.5	-0.002	14.8	-0.005	13.4	0.000	13.4	0.002
253.0586	$C_{10}H_5N_8O$	4:3	-11				6.3	-0.004	8.4	-0.007				
255.0855	$C_9H_7N_{10}$	5:2	-8		17.9	0.002	7.1	-0.002					5.2	-0.002
265.0685	$C_9H_9N_6O_4$	3:3	-8				8.2	0.011	9.1	0.007	6.6	0.010	7.0	0.008
268.1383	$C_7H_{14}N_{11}O$	5:1	-3	1					10.8	0.000	3.8	-0.003	6.9	0.002
269.1223	$C_7H_{13}N_{10}O_2$	5:1	-2		33.0	0.000	60.4	-0.002			3.6	-0.001		
271.0692	$C_{10}H_7N_8O_2$	4:3	-10						11.4	0.005				
273.0961	$C_9H_9N_{10}O$	5:2	-7				29.8	0.001	24.3	-0.003	6.8	-0.004	5.9	-0.005
275.123	$C_8H_{11}N_{12}$	6:1	-4		15.9	0.004			11.3	0.001	17.6	-0.001	23.7	0.003
277.0699	$C_{11}H_5N_{10}$	5:3	-12		17.6	0.000			7.1	0.007				
285.106	$C_8H_{13}N_8O_4$	4:2	-4				7.9	0.001	10.1	0.006	2.7	0.004		
288.0957	$C_{10}H_{10}N_9O_2$	4:3	-10	1			12.1	0.003	11.3	0.006				
289.0798	$C_{10}H_9N_8O_3$	4:3	-9		16.0	-0.016	8.5	-0.003	11.1	0.009			4.5	0.009
290.1226	$C_9H_{12}N_{11}O$	5:2	-7	1			6.9	-0.001	10.1	-0.003	3.8	0.001	4.6	0.003
291.1066	$C_9H_{11}N_{10}O_2$	5:2	-6		20.5	0.001	25.1	-0.003	24.4	-0.001	4.3	0.004	4.1	0.002
301.0897	$C_9H_{13}N_6O_6$	3:3	-6						7.6	0.003	2.7	0.007		
306.1063	$C_{10}H_{12}N_9O_3$	4:3	-9	1					9.8	0.002				
307.0903	$C_{10}H_{11}N_8O_4$	4:3	-8		22.6	0.002	16.9	0.007	8.4	-0.006	3.9	0.003		
311.1441	$C_8H_{15}N_{12}O_2$	6:1	-2				29.3	0.000	15.8	-0.006	15.3	-0.003	16.1	0.001
315.1179	$C_{10}H_{11}N_{12}O$	6:2	-7				6.6	0.003	12.2	0.002	2.6	-0.001		
325.1009	$C_{10}H_{13}N_8O_5$	4:3	-7		24.0	-0.008	8.5	-0.003			3.4	-0.010		
330.1175	$C_{11}H_{12}N_{11}O_2$	5:3	-10	1	19.5	-0.003	9.0	0.003			2.2	0.000		
331.1016	$C_{11}H_{11}N_{10}O_3$	5:3	-9		31.7	-0.006	19.6	-0.002	7.3	-0.004	2.9	-0.004		
333.1284	$C_{10}H_{13}N_{12}O_2$	6:2	-6		19.8	0.007	44.6	-0.001	95.2	0.001	21.6	-0.001	19.1	0.003
337.1022	$C_{12}H_9N_{12}O$	6:3	-11				8.1	0.007						
340.1006	$C_{11}H_{14}N_7O_6$	3:4	-10	1	16.8	-0.001								
341.0846	$C_{11}H_{13}N_6O_7$	3:4	-9						7.8	0.009				
348.1281	$C_{11}H_{14}N_{11}O_3$	5:3	-9	1	21.6	-0.006	6.8	0.005	14.4	0.004				

Mass spectra data		Global reaction stoichiometry[b]			2:1		3:1		4:1		5:1		6:1	
m/z (calcd)	**Formula[a]**	**C:G**	**H_2O**	**NH_3**	**Intensity**	**Error**	**Intensity**	**Error**	**Intensity**	**Error**	**Intensity**	**Error**	**Intensity**	**Error**
349.1121	$C_{11}H_{13}N_{10}O_4$	5:3	-8		44.2	0.001	36.3	0.006	41.1	0.008	12.6	0.009	11.9	0.008
351.139	$C_{10}H_{15}N_{12}O_3$	6:2	-5				13.1	-0.005	23.4	0.002	6.8	0.001	10.7	0.007
355.1128	$C_{12}H_{11}N_{12}O_2$	6:3	-10				15.5	-0.003						
357.1397	$C_{11}H_{13}N_{14}O$	7:2	-7				8.4	0.001					4.3	-0.004
365.1044	$C_9H_{21}N_2O_{13}$	1:4	-3		79.5	-0.003	26.2	-0.005	15.8	-0.004			9.4	-0.002
366.1387	$C_{11}H_{16}N_{11}O_4$	5:3	-8	1			15.3	0.006						
367.1227	$C_{11}H_{15}N_{10}O_5$	5:3	-7		32.5	0.003	13.7	-0.004	12.1	0.006			5.9	-0.003
373.1234	$C_{12}H_{13}N_{12}O_3$	6:3	-9		17.0	-0.005	14.9	-0.004	9.4	0.000				
375.1502	$C_{11}H_{15}N_{14}O_2$	7:2	-6				9.7	0.005			5.1	-0.002		
391.1339	$C_{12}H_{15}N_{12}O_4$	6:3	-8				19.2	0.001	24.0	-0.001	4.9	0.004	5.8	0.006
407.1176	$C_{13}H_{15}N_{10}O_6$	5:4	-10								2.6	0.013	4.0	0.001
415.1452	$C_{13}H_{15}N_{14}O_3$	7:3	-9				26.0	0.000	10.1	0.002	3.5	0.002		
433.1557	$C_{13}H_{17}N_{14}O_4$	7:3	-8				10.7	-0.001	7.5	0.000	2.7	-0.005		
451.1663	$C_{13}H_{19}N_{14}O_5$	7:3	-7				9.4	0.001	9.5	-0.002	4.0	-0.003		
457.167	$C_{14}H_{17}N_{16}O_3$	8:3	-9				10.0	-0.002			3.1	-0.005		
475.1775	$C_{14}H_{19}N_{16}O_4$	8:3	-8								4.3	0.004		

[a]Formulas correspond to M+H compositions. [b]The cyanamide:glyoxal ratio denotes the proportion that generates the corresponding formula, often involving dehydration steps (elimination of water referred to glyoxal hydrate) as well as occasional addition or removal of ammonia.

3. ^{13}C NMR SPECTRA

^{13}C NMR spectra of cyanamide-glyoxal reactions

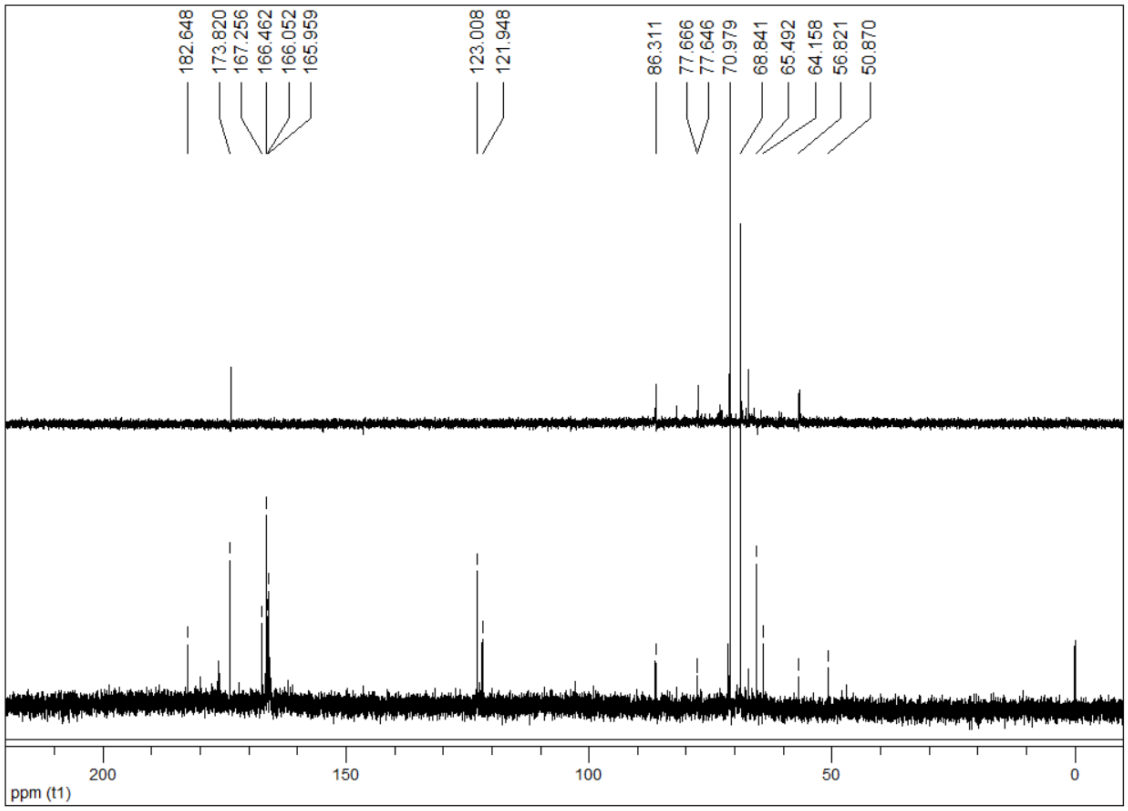

Fig. S3.1. ^{13}C NMR spectra (top: DEPT experiment) of cyanamide-glyoxal reactions at 100ºC (2:1 molar ratio) recorded in D_2O solution at 500 MHz.

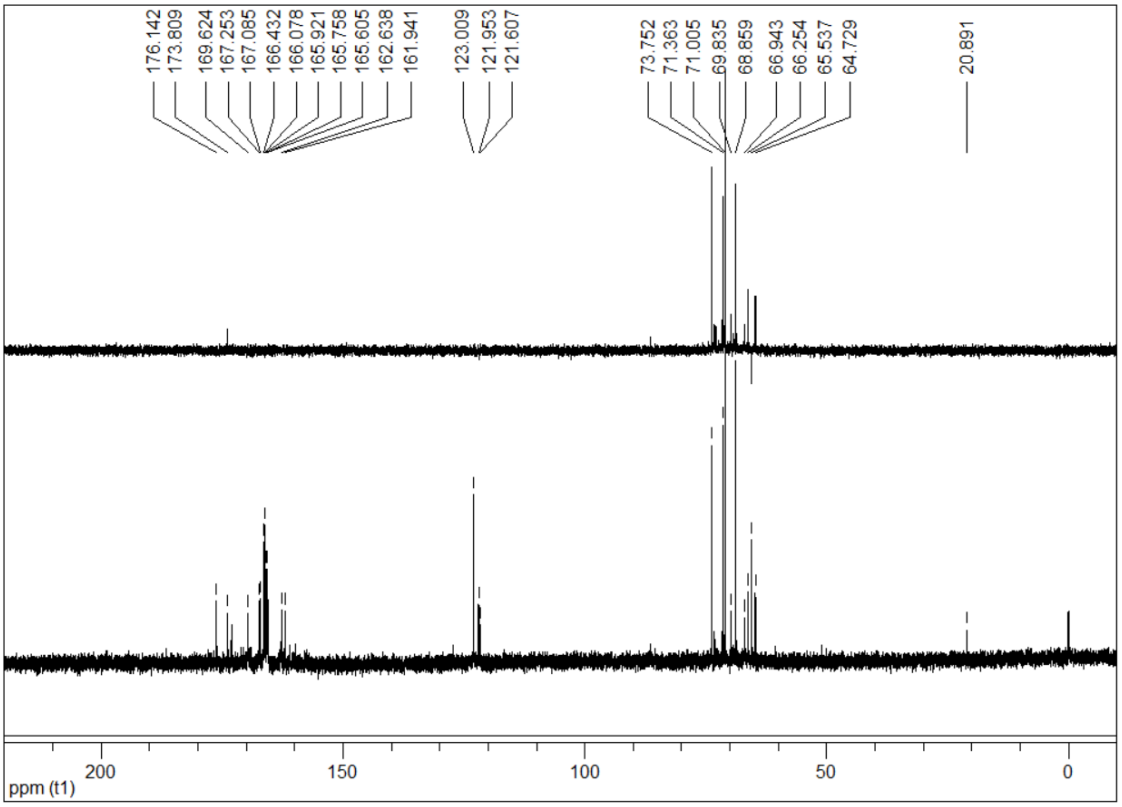

Fig. S3.2. ^{13}C NMR spectra (top: DEPT experiment) of cyanamide-glyoxal reactions (4:1 molar ratio) at 100ºC recorded in D_2O solution at 500 MHz.

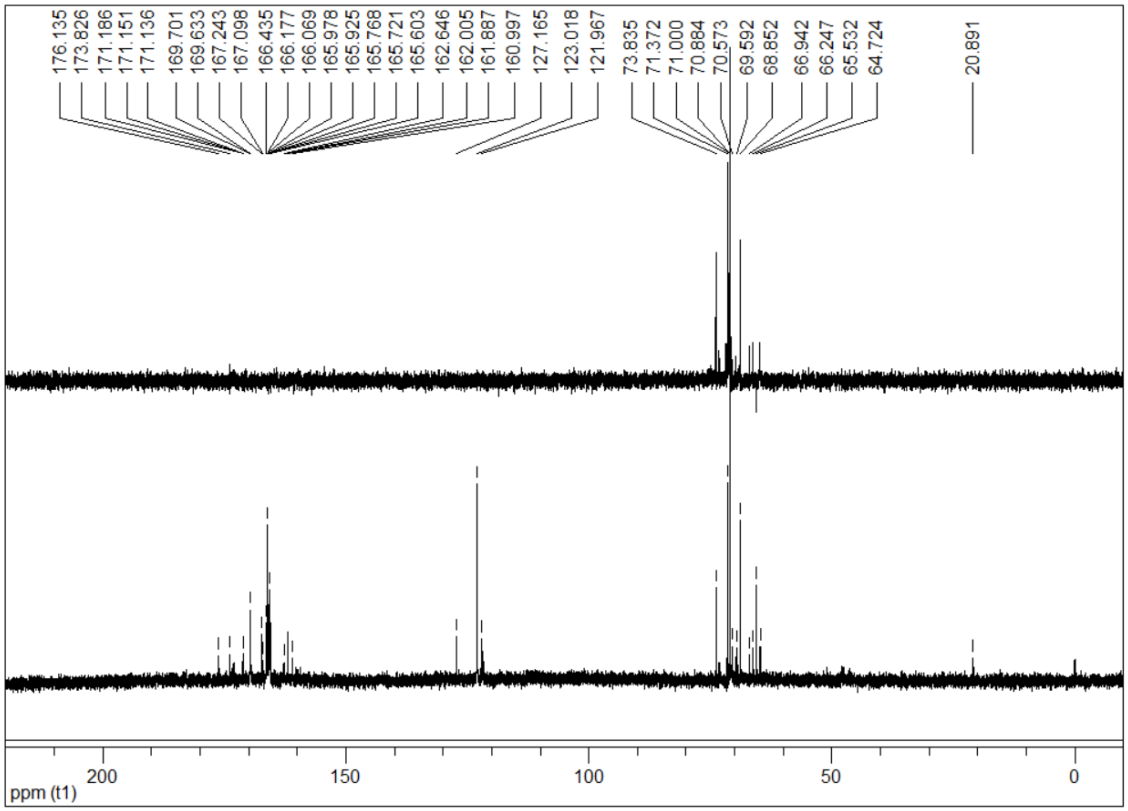

Fig. S3.3. ^{13}C NMR spectra (top: DEPT experiment) of cyanamide-glyoxal reactions (6:1 molar ratio) at 100ºC recorded in D_2O solution at 500 MHz.

^{13}C NMR spectra of cyanamide

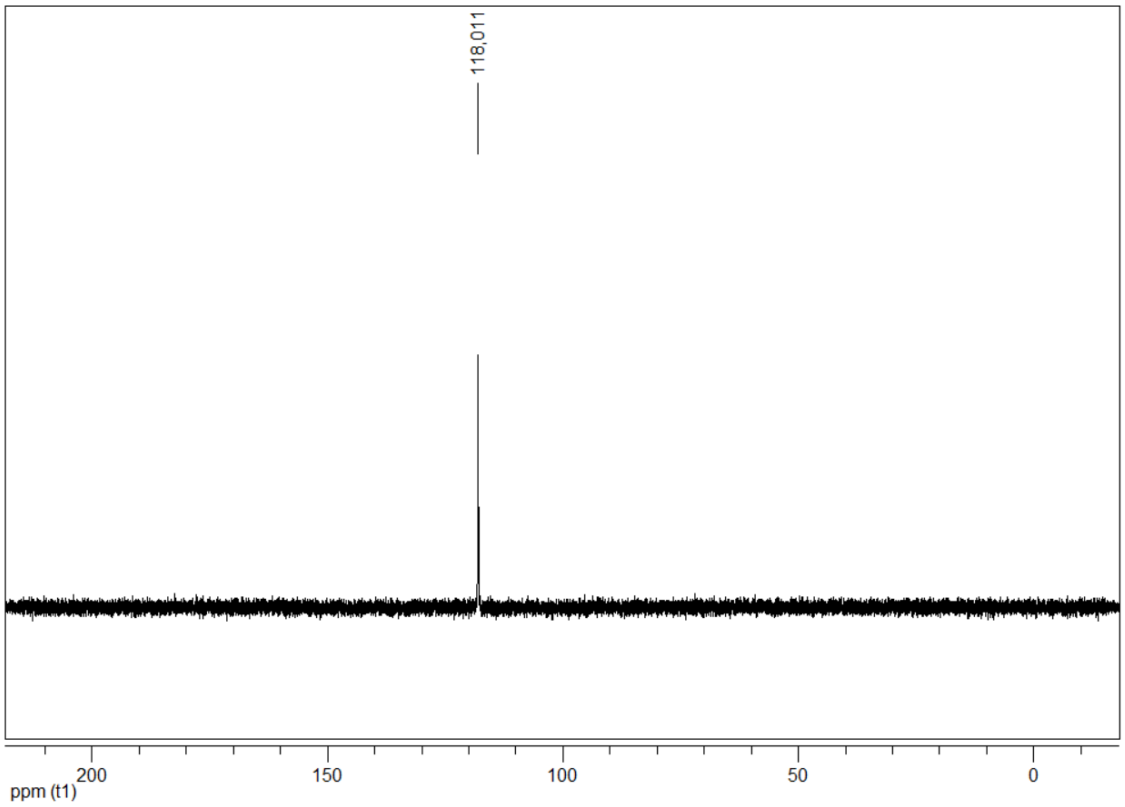

Fig. S3.4. ^{13}C NMR spectra of cyanamide recorder in D_2O solution at 500 MHz (after 0 hours).

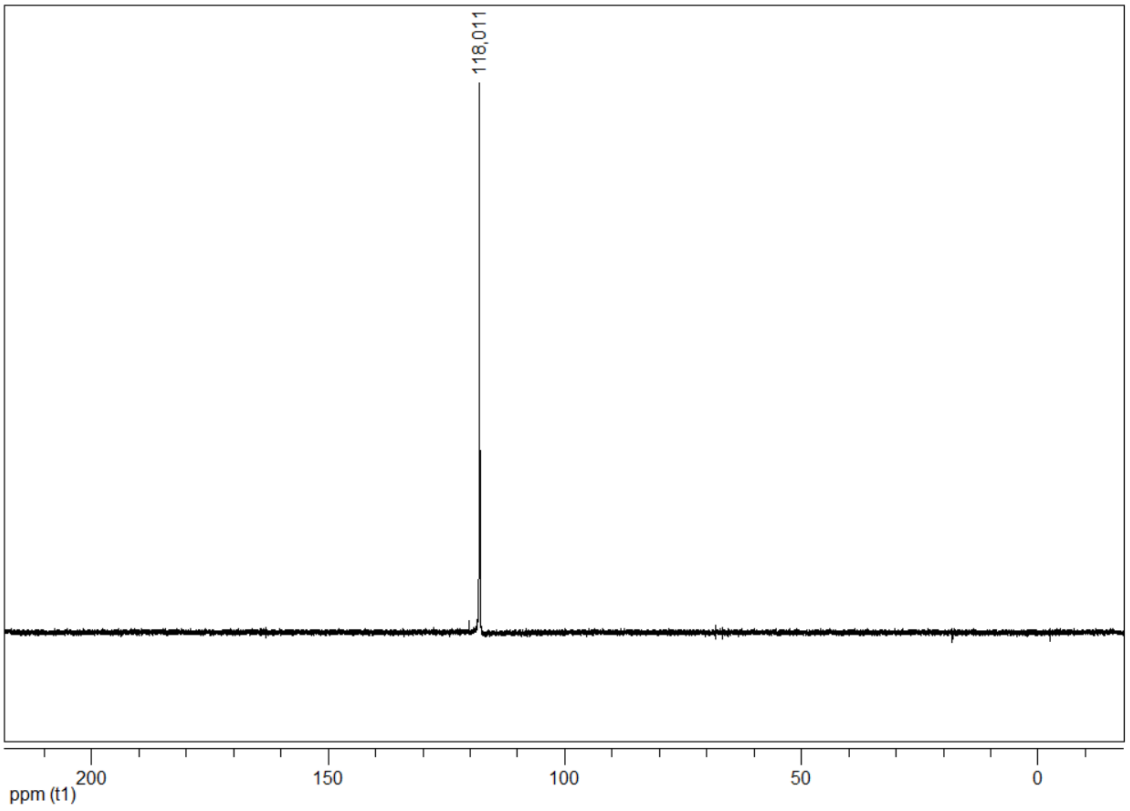

Fig. S3.5. ^{13}C NMR spectra of cyanamide recorder in D_2O solution at 500 MHz (after 20 days).

4. UV-VIS SPECTROPHOTOMETRY

UV-Vis spectra of cyanamide and dicyandiamide at pH 2.8

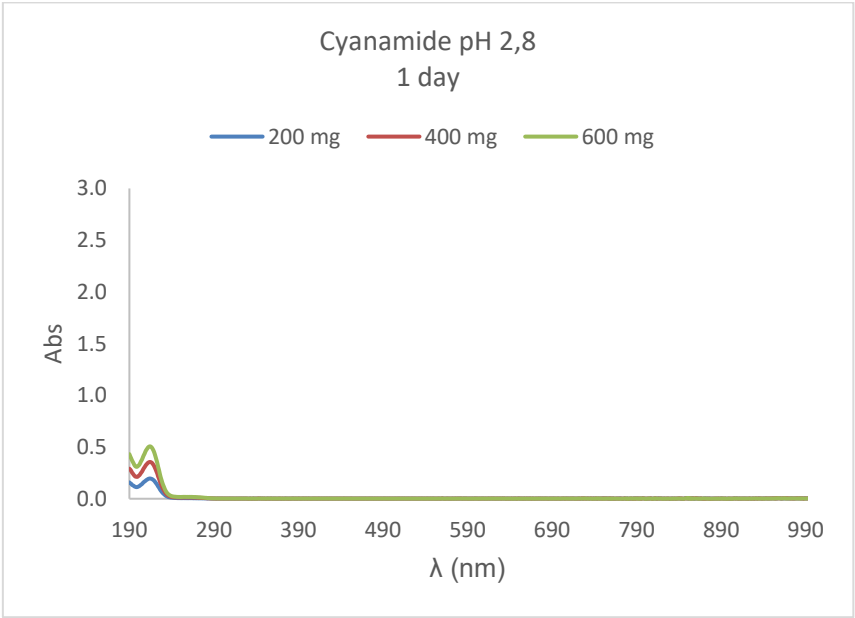

Fig. S4.1. UV-Vis spectra of cyanamide at pH 2.8 after 1 day.

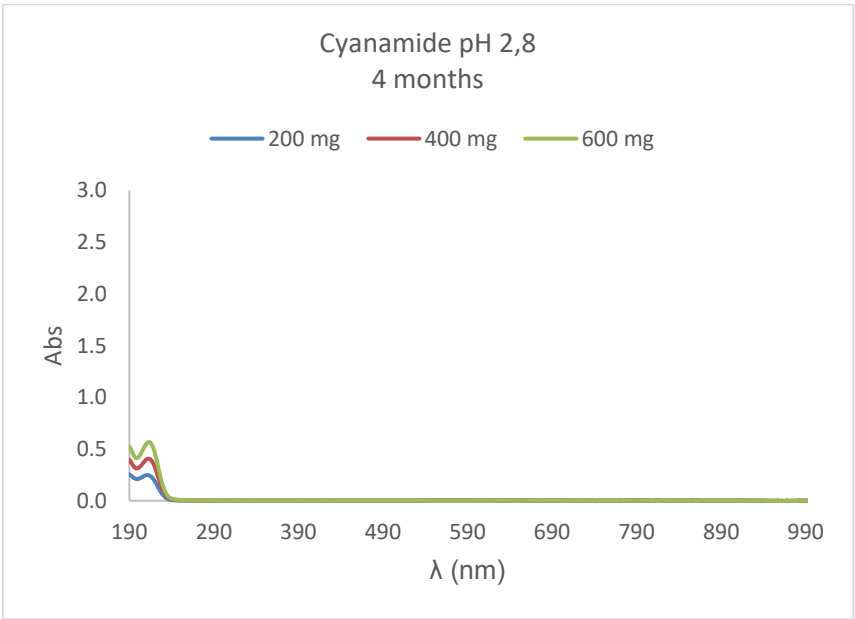

Fig. S4.2. UV-Vis spectra of cyanamide at pH 2.8 after 4 months.

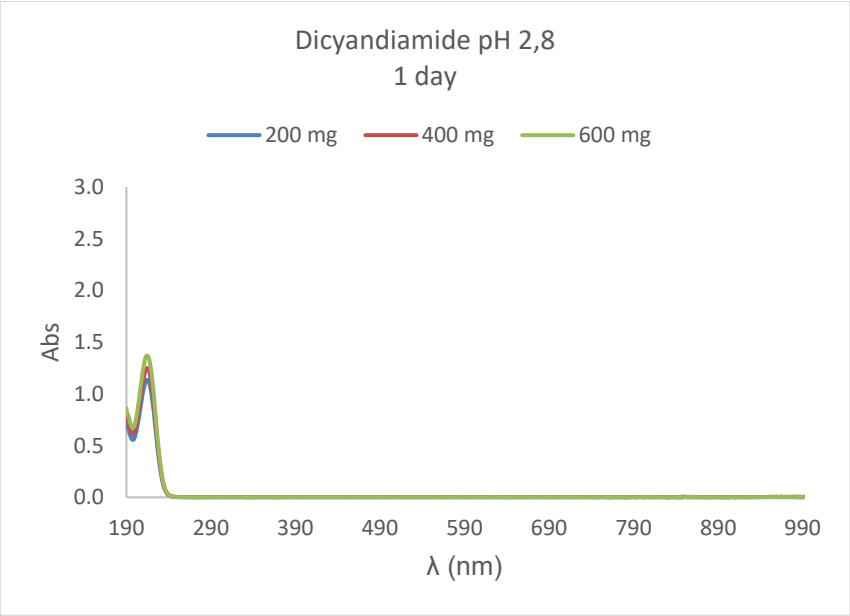

Fig. S4.3. UV-Vis spectra of dicyanamide at pH 2.8 after 1 day.

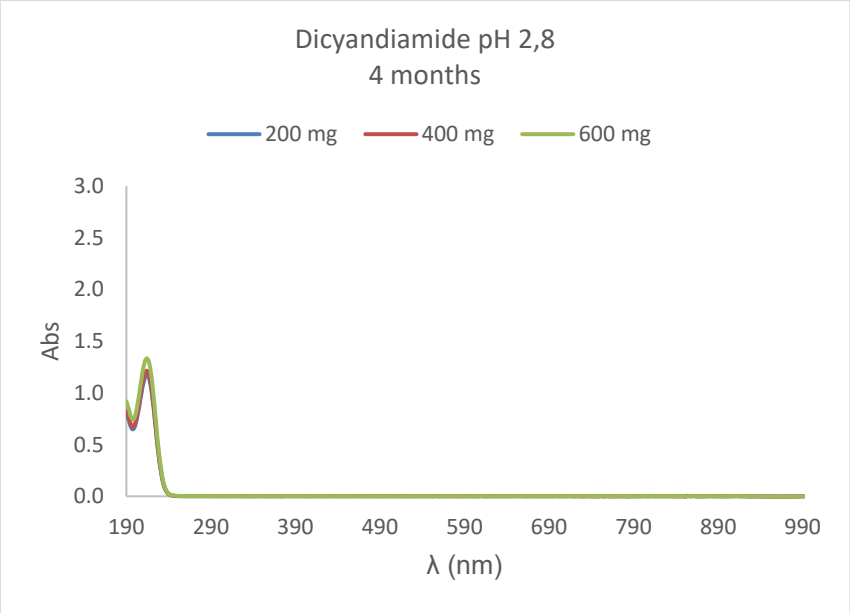

Fig. S4.4. UV-Vis spectra of dicyanamide at pH 2.8 after 4 months.

UV-Vis spectra of aqueous cyanamide-glyoxal solutions

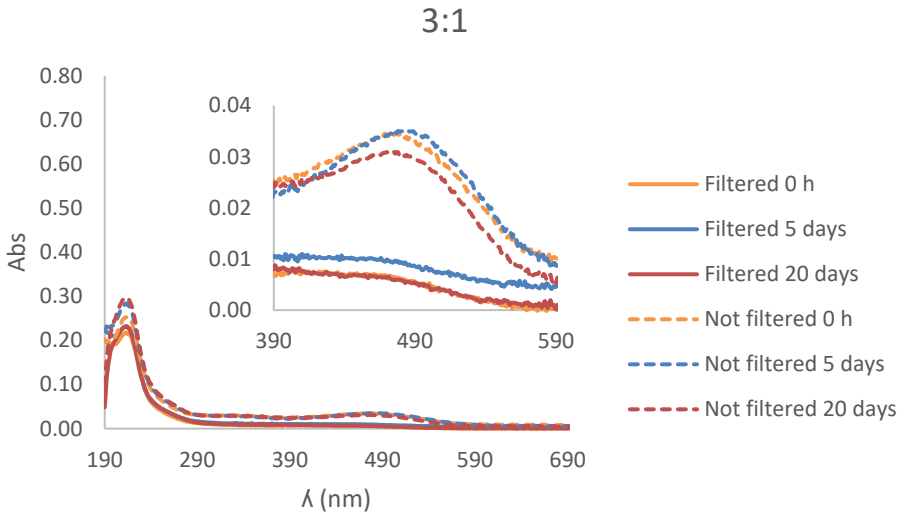

Fig. S4.5. UV-Vis spectra of aqueous cyanamide-glyoxal (3:1 molar ratio) solutions (5 mg·L^{-1}), both filtered (0.2-µm nylon membrane) and non-filtered at different reactions times.

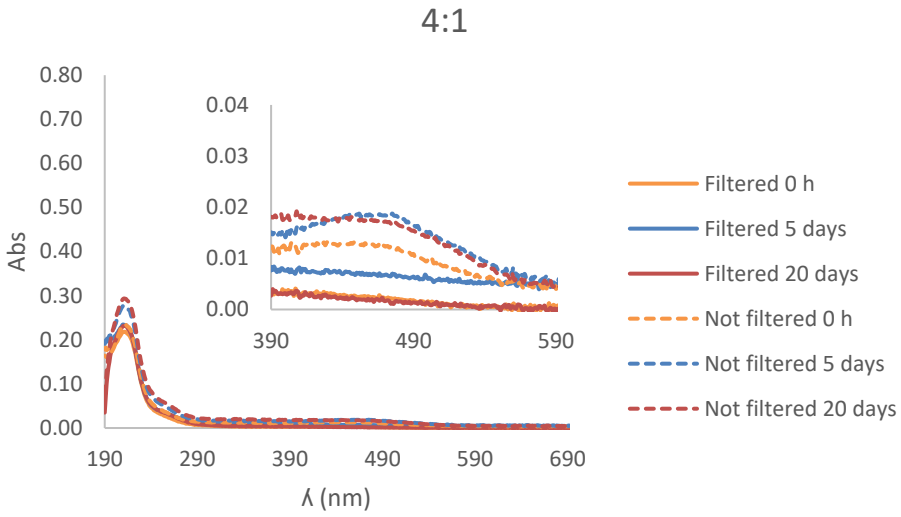

Fig. S4.6. UV-Vis spectra of aqueous cyanamide-glyoxal (4:1 molar ratio) solutions (5 mg·L^{-1}), both filtered (0.2-µm nylon membrane) and non-filtered at different reactions times.

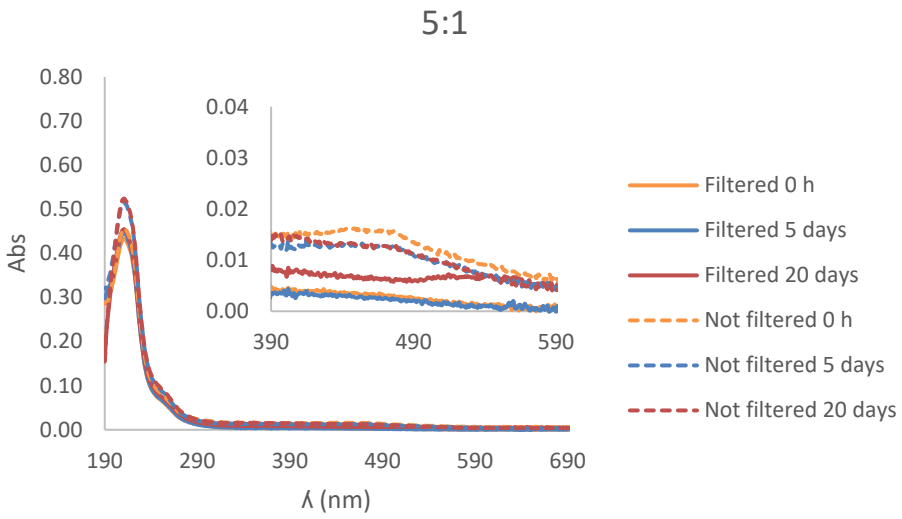

Fig. S4.7. UV-Vis spectra of aqueous cyanamide-glyoxal (5:1 molar ratio) solutions (5 mg·L^{-1}), both filtered (0.2-µm nylon membrane) and non-filtered at different reactions times.

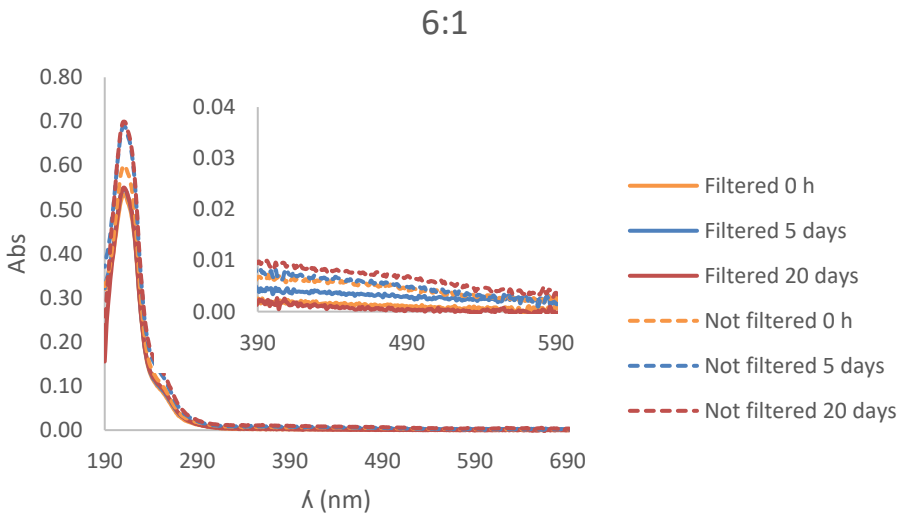

Fig. S4.8. UV-Vis spectra of aqueous cyanamide-glyoxal (6:1 molar ratio) solutions (5 mg·L^{-1}), both filtered (0.2-µm nylon membrane) and non-filtered at different reactions times.

5. FT-IR SPECTRA

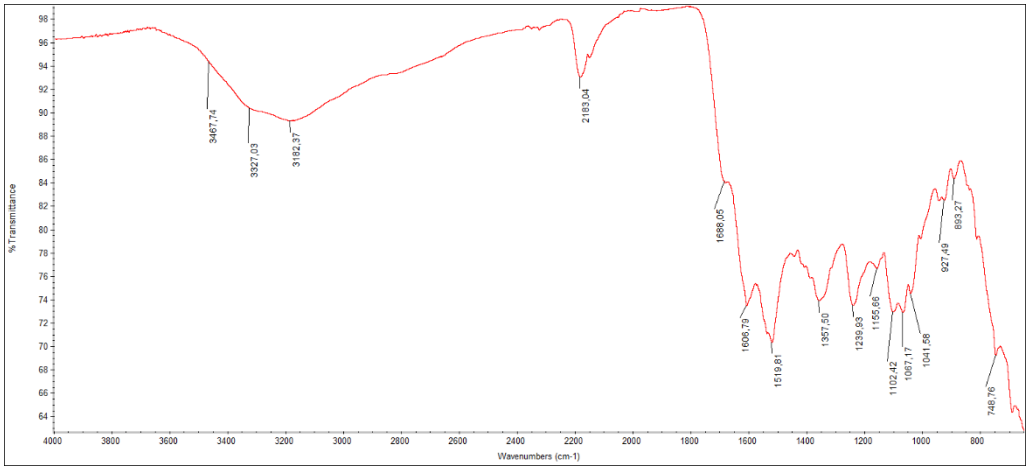

Fig. S5.1. FT-IR spectrum (ATR mode) of the solid (first crop) isolated from cyanamide-glyoxal reaction (2:1 molar ratio).

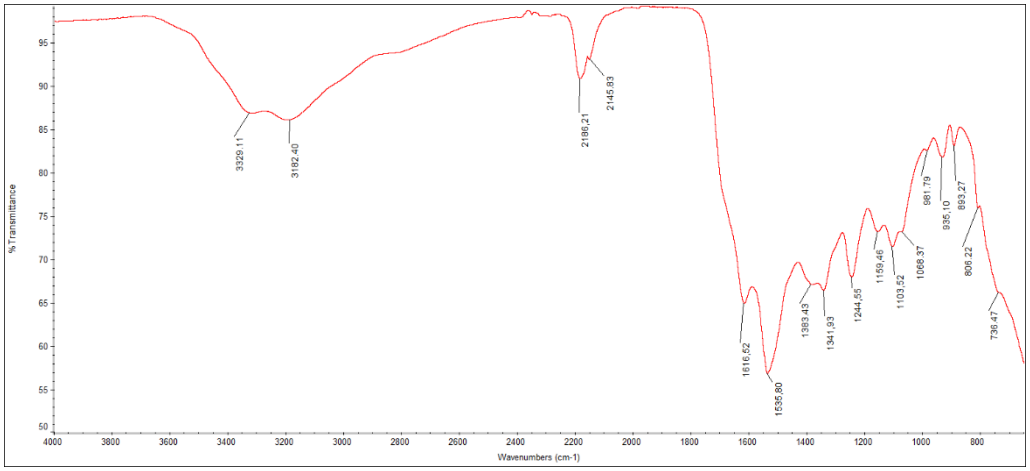

Fig. S5.2. FT-IR spectrum (ATR mode) of the solid (first crop) isolated from cyanamide-glyoxal reaction (3:1 molar ratio).

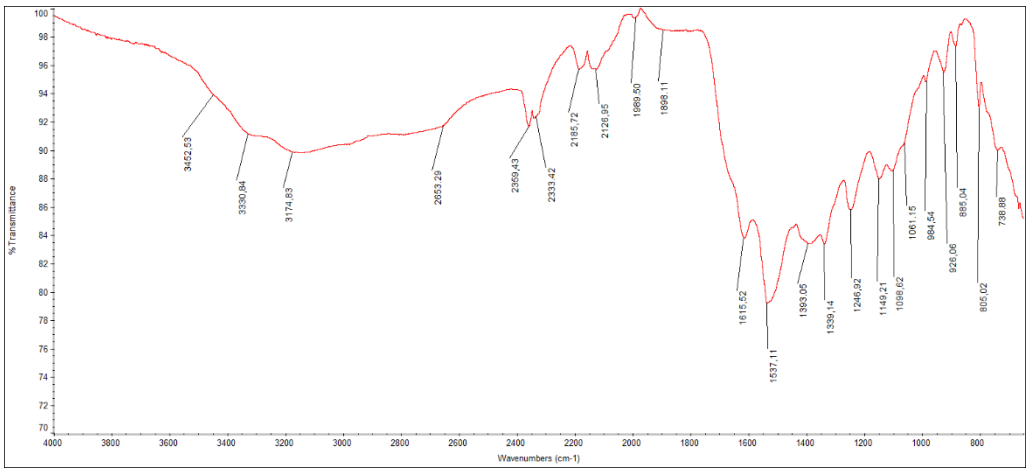

Fig. S5.3. FT-IR spectrum (ATR mode) of the solid (first crop) isolated from cyanamide-glyoxal reaction (4:1 molar ratio).

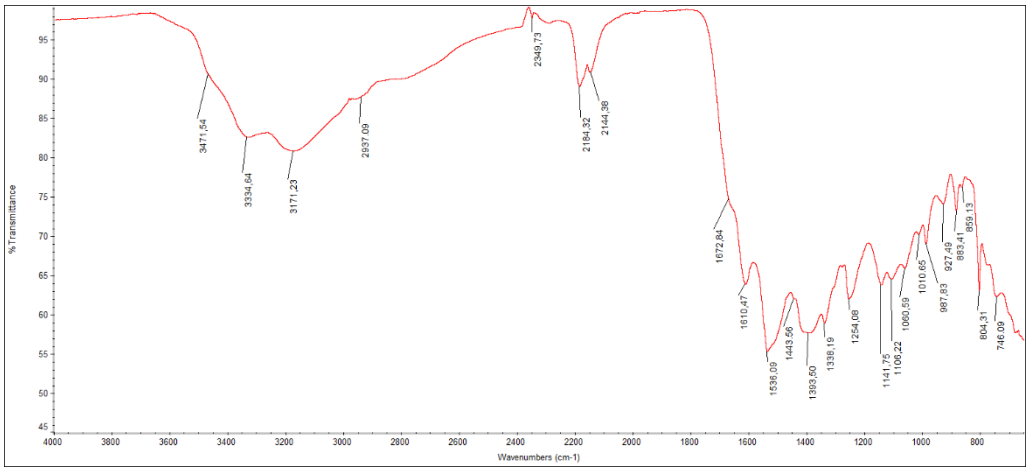

Fig. S5.4. FT-IR spectrum (ATR mode) of the solid (first crop) isolated from cyanamide-glyoxal reaction (5:1 molar ratio).

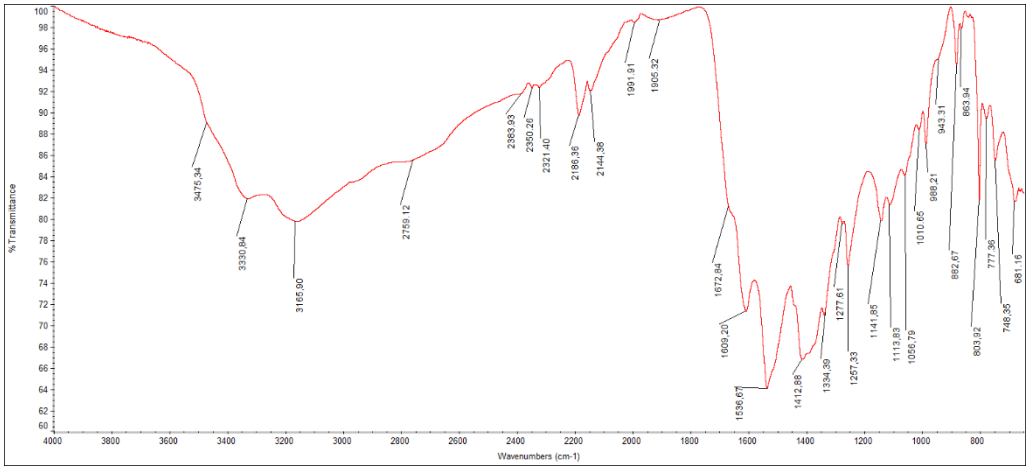

Fig. S5.5. FT-IR spectrum (ATR mode) of the solid (first crop) isolated from cyanamide-glyoxal reaction (6:1 molar ratio).

6. THERMOGRAVIMETRIC ANALYSIS

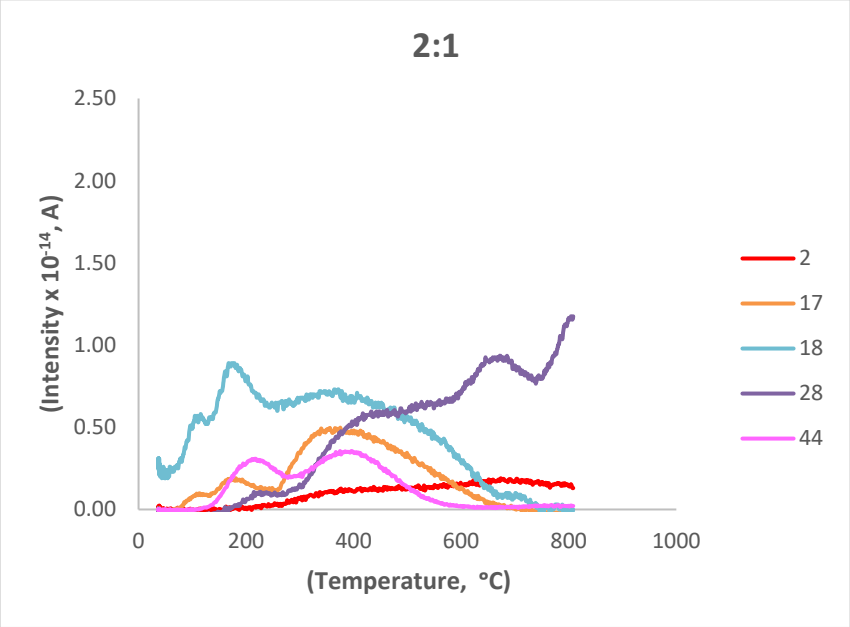

Fig. S6.1. Thermogravimetric analysis of the solid phase (first crop) isolated from cyanamide-glyoxal reaction (2:1 molar ratio). Curves in color denote the masses of gases released upon heating: H_2 (2), NH_3 (17), H_2O (18), CO (28) and CO_2 (44). The Y-axis corresponds to ion current intensity (in Amp) (quadrupole mass spectra analysis).

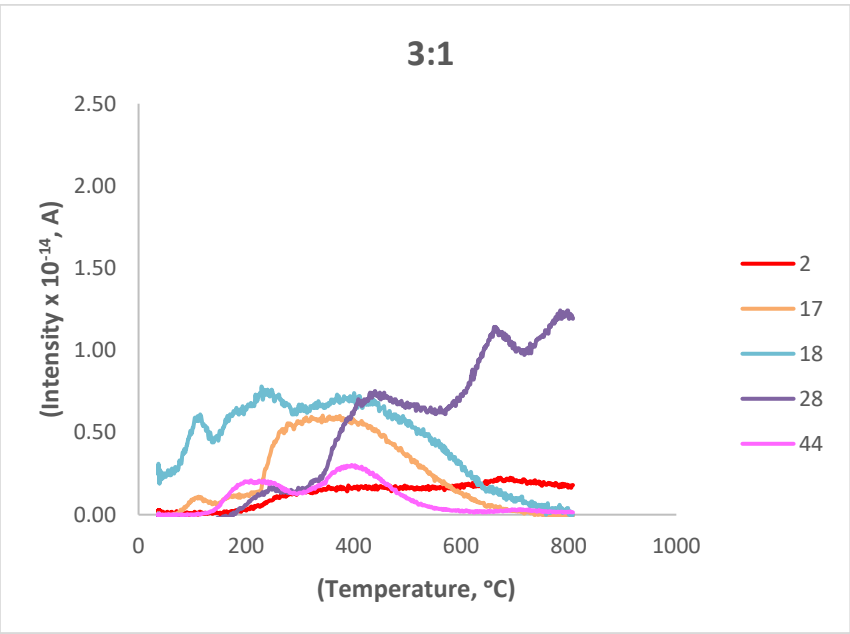

Fig. S6.2. Thermogravimetric analysis of the solid phase (first crop) isolated from cyanamide-glyoxal reaction (3:1 molar ratio). Curves in color denote the masses of gases released upon heating: H_2 (2), NH_3 (17), H_2O (18), CO (28) and CO_2 (44). The Y-axis corresponds to ion current intensity (in Amp) (quadrupole mass spectra analysis).

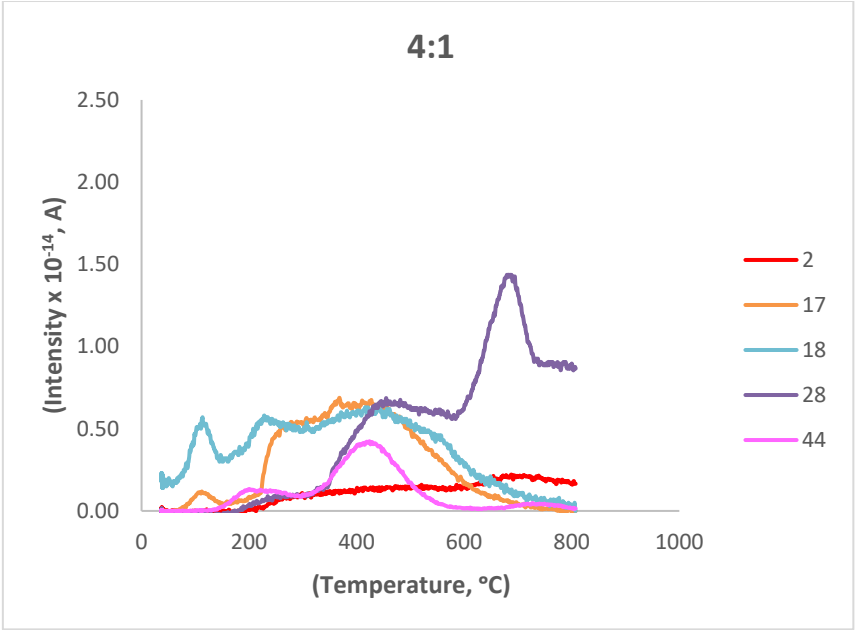

Fig. S6.3. Thermogravimetric analysis of the solid phase (first crop) isolated from cyanamide-glyoxal reaction (4:1 molar ratio). Curves in color denote the masses of gases released upon heating: H_2 (2), NH_3 (17), H_2O (18), CO (28) and CO_2 (44). The Y-axis corresponds to ion current intensity (in Amp) (quadrupole mass spectra analysis).

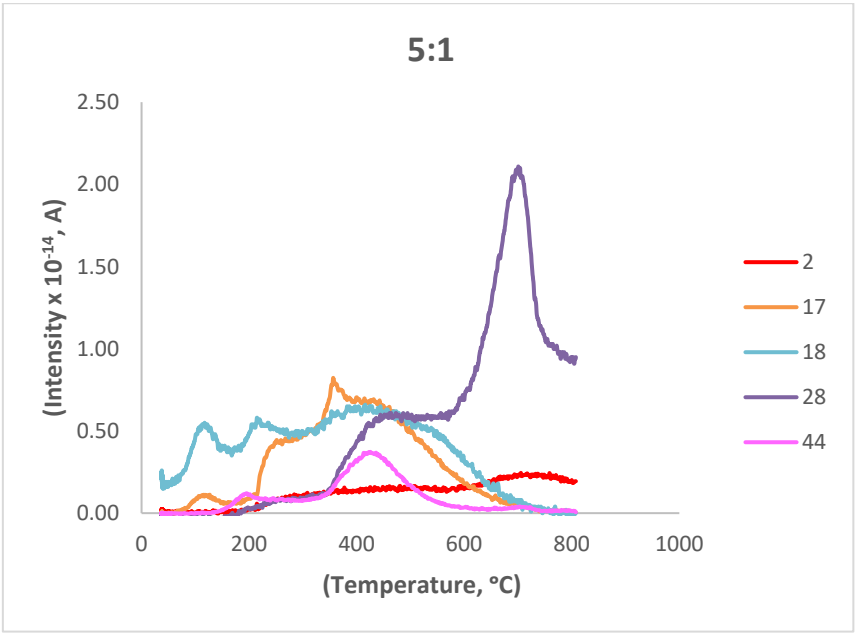

Fig. S6.4. Thermogravimetric analysis of the solid phase (first crop) isolated from cyanamide-glyoxal reaction (5:1 molar ratio). Curves in color denote the masses of gases released upon heating: H_2 (2), NH_3 (17), H_2O (18), CO (28) and CO_2 (44). The Y-axis corresponds to ion current intensity (in Amp) (quadrupole mass spectra analysis).

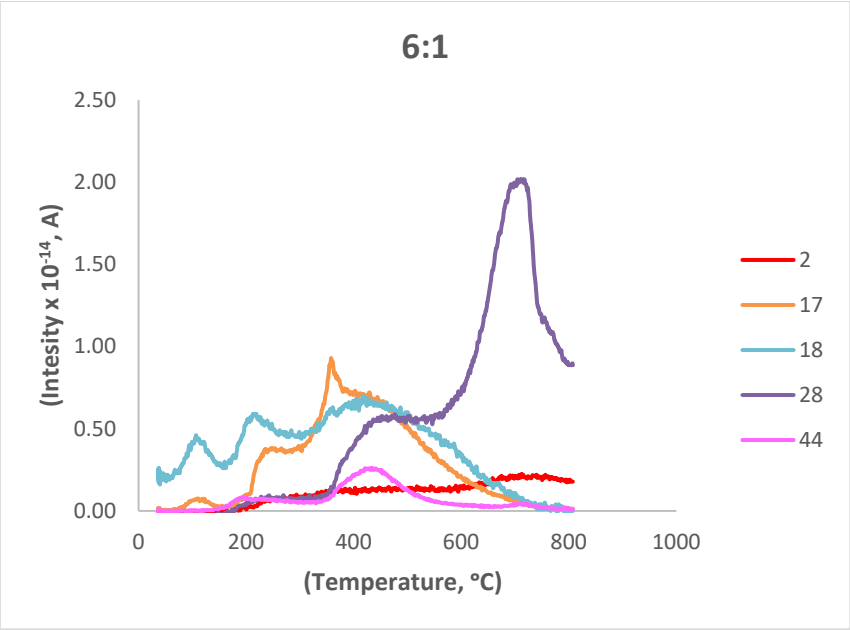

Fig. S6.5. Thermogravimetric analysis of the solid phase (first crop) isolated from cyanamide-glyoxal reaction (6:1 molar ratio). Curves in color denote the masses of gases released upon heating: H_2 (2), NH_3 (17), H_2O (18), CO (28) and CO_2 (44). The Y-axis corresponds to ion current intensity (in Amp) (quadrupole mass spectra analysis).

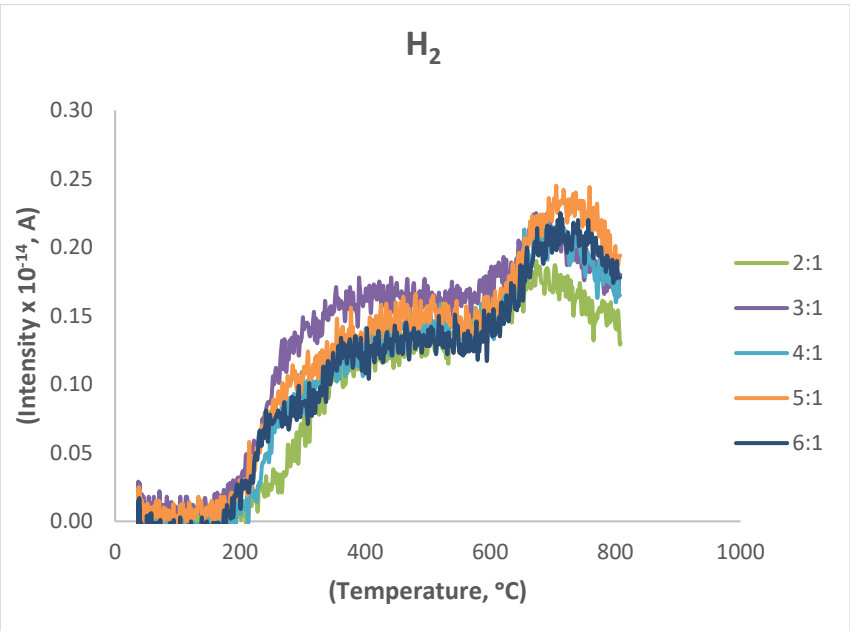

Fig. S6.6. Thermogravimetric analysis of insoluble solids isolated from cyanamide-glyoxal reactions at different starting molar ratios (2:1 to 6:1). Plot shows the profiles observed for H_2 (2). The Y-axis corresponds to ion current intensity (in Amp) (quadrupole mass spectra analysis).

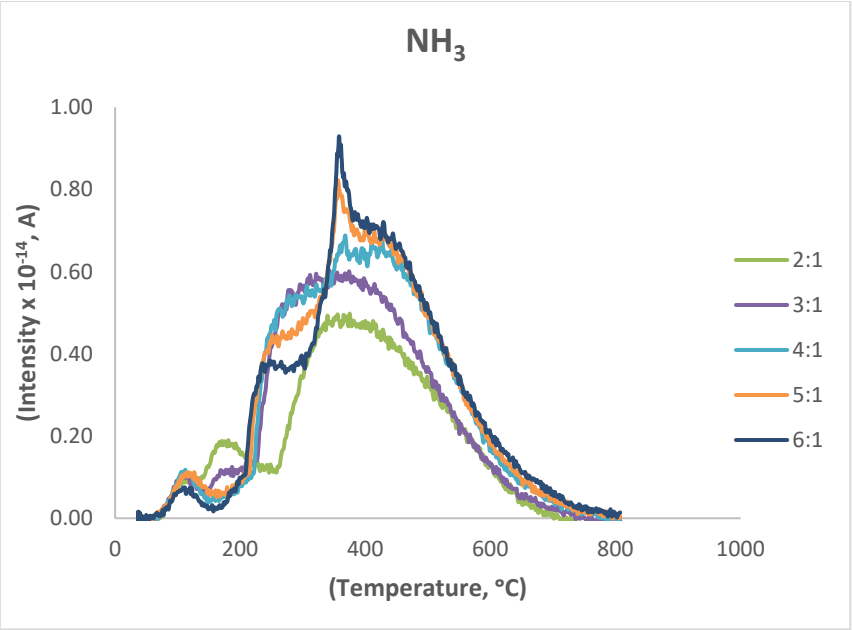

Fig. S6.7. Thermogravimetric analysis of insoluble solids isolated from cyanamide-glyoxal reactions at different starting molar ratios (2:1 to 6:1). Plot shows the profiles observed for NH_3 (17). The Y-axis corresponds to ion current intensity (in Amp) (quadrupole mass spectra analysis).

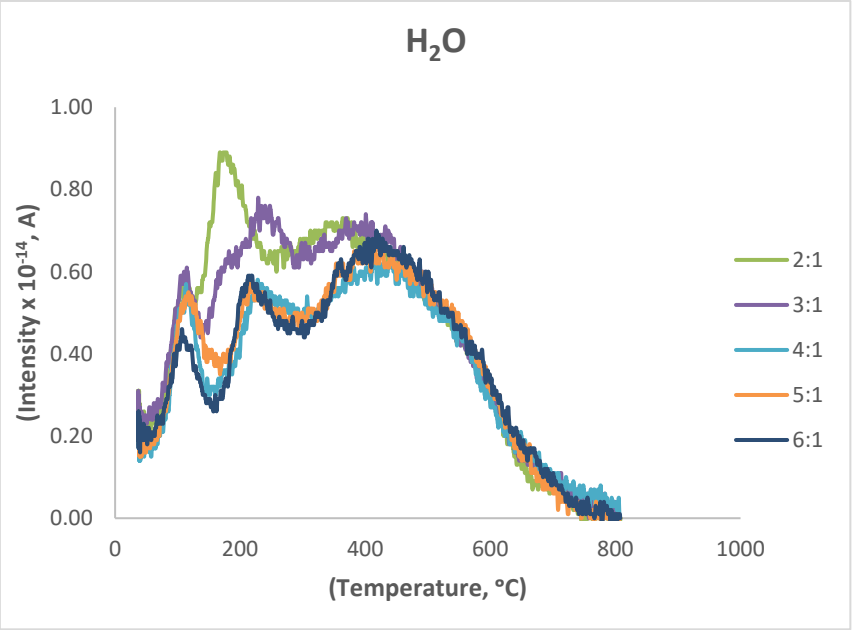

Fig. S6.8. Thermogravimetric analysis of insoluble solids isolated from cyanamide-glyoxal reactions at different starting molar ratios (2:1 to 6:1). Plot shows the profiles observed for H_2O (18). The Y-axis corresponds to ion current intensity (in Amp) (quadrupole mass spectra analysis).

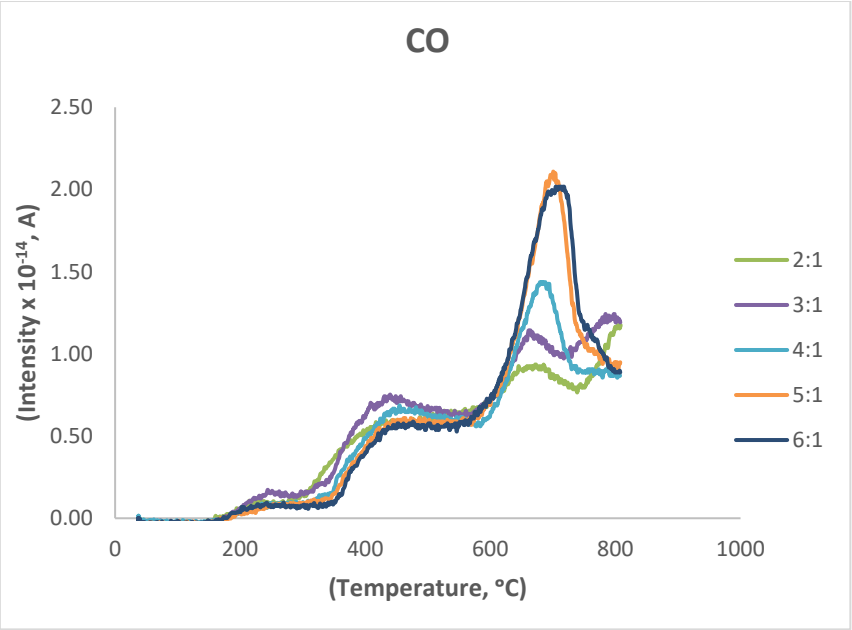

Fig. S6.9. Thermogravimetric analysis of insoluble solids isolated from cyanamide-glyoxal reactions at different starting molar ratios (2:1 to 6:1). Plot shows the profiles observed for CO (28). The Y-axis corresponds to ion current intensity (in Amp) (quadrupole mass spectra analysis).

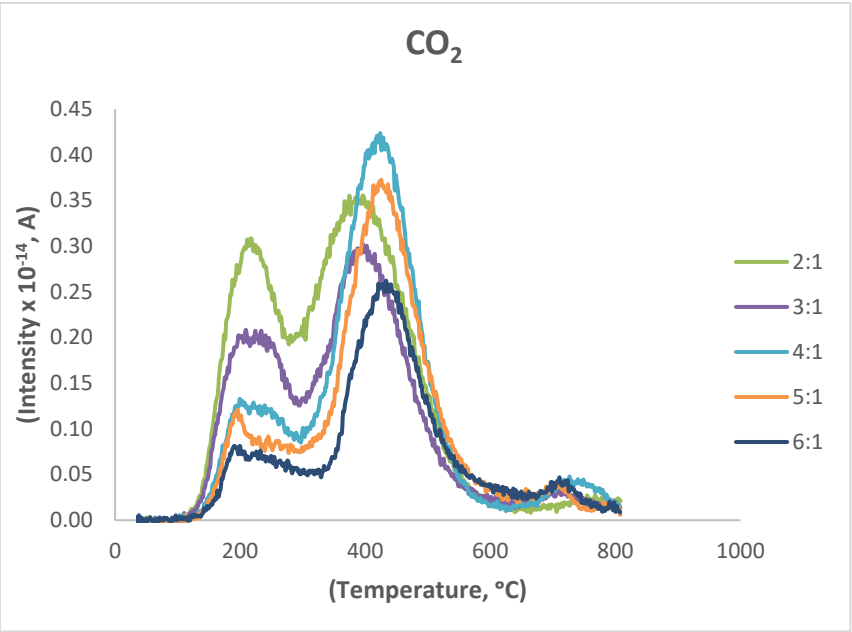

Fig. S6.10. Thermogravimetric analysis of insoluble solids isolated from cyanamide-glyoxal reactions at different starting molar ratios (2:1 to 6:1). Plot shows the profiles observed for CO_2 (44). The Y-axis corresponds to ion current intensity (in Amp) (quadrupole mass spectra analysis).

8. CARTESIAN COORDINATES FOR ALL OPTIMIZED STRUCTURES

CN

Zero-point correction= 0.034076 (Hartree/Particle)
Thermal correction to Energy= 0.037592
Thermal correction to Enthalpy= 0.038536
Thermal correction to Gibbs Free Energy= 0.010515
Sum of electronic and zero-point Energies= -148.762160
Sum of electronic and thermal Energies= -148.758644
Sum of electronic and thermal Enthalpies= -148.757700
Sum of electronic and thermal Free Energies= -148.785721

Zero imaginary frequencies

N -1.11096800 0.00000700 -0.08669100
C 0.21486800 -0.00001700 0.00098500
N 1.36989900 0.00000800 0.01254600
H -1.55085700 -0.84626500 0.25654800
H -1.55087300 0.84626000 0.25655300

CN-

Zero-point correction= 0.020922 (Hartree/Particle)
Thermal correction to Energy= 0.024123
Thermal correction to Enthalpy= 0.025067
Thermal correction to Gibbs Free Energy= -0.002046
Sum of electronic and zero-point Energies= -148.295776
Sum of electronic and thermal Energies= -148.292575
Sum of electronic and thermal Enthalpies= -148.291631
Sum of electronic and thermal Free Energies= -148.318745

Zero imaginary frequencies

C -0.11450000 -0.00142300 0.00000200
N 1.16421100 -0.13104000 -0.00000100
N -1.29660900 0.02096600 -0.00000100
H 1.61378500 0.77905300 -0.00000100

GLY-

Zero-point correction= 0.082239 (Hartree/Particle)
Thermal correction to Energy= 0.088937
Thermal correction to Enthalpy= 0.089881
Thermal correction to Gibbs Free Energy= 0.052054
Sum of electronic and zero-point Energies= -380.177981
Sum of electronic and thermal Energies= -380.171282
Sum of electronic and thermal Enthalpies= -380.170338
Sum of electronic and thermal Free Energies= -380.208165

Zero imaginary frequencies

C 0.64546600 -0.00539300 -0.32754000
H 0.56967700 0.01034400 -1.41691900
C -0.75046100 -0.15217800 0.28633100
H -0.60095800 -0.07807900 1.39039000
O -1.39104000 -1.24687600 -0.10917300
O -1.49957500 1.04289900 -0.09694400
O 1.46574000 -1.10412900 -0.00486500
O 1.20912700 1.19800500 0.15240500

H 1.34681500 -1.29635300 0.93439300
H 2.01133900 1.38169800 -0.34853500
H -0.97092700 1.80863800 0.15654100

W

Zero-point correction= 0.021296 (Hartree/Particle)
Thermal correction to Energy= 0.024131
Thermal correction to Enthalpy= 0.025076
Thermal correction to Gibbs Free Energy= 0.003650
Sum of electronic and zero-point Energies= -76.416151
Sum of electronic and thermal Energies= -76.413315
Sum of electronic and thermal Enthalpies= -76.412371
Sum of electronic and thermal Free Energies= -76.433797

Zero imaginary frequencies

O 0.00000000 0.00000000 0.11828300
H 0.00000000 0.75850400 -0.47313200
H 0.00000000 -0.75850400 -0.47313200

$C_{CN\text{-}CN}$-

Zero-point correction= 0.056141 (Hartree/Particle)
Thermal correction to Energy= 0.063787
Thermal correction to Enthalpy= 0.064731
Thermal correction to Gibbs Free Energy= 0.022716
Sum of electronic and zero-point Energies= -297.069833
Sum of electronic and thermal Energies= -297.062187
Sum of electronic and thermal Enthalpies= -297.061243
Sum of electronic and thermal Free Energies= -297.103258

Zero imaginary frequencies

C 1.71930200 0.19287500 -0.00217600
C -1.71119200 0.11179100 -0.01370700
N -1.25491800 -1.10322500 0.23469000
H -1.59676600 -1.50496900 1.09934900
H -0.21439800 -1.20470700 0.05953500
N -2.12065700 1.15989200 -0.29040900
N 1.46562500 -1.05425400 -0.23259400
N 1.88956800 1.31920900 0.29216800
H 1.90517700 -1.36967700 -1.09057100

$P_{CN\text{-}CN}$-

Zero-point correction= 0.059583 (Hartree/Particle)
Thermal correction to Energy= 0.065915
Thermal correction to Enthalpy= 0.066860
Thermal correction to Gibbs Free Energy= 0.029733
Sum of electronic and zero-point Energies= -297.039636
Sum of electronic and thermal Energies= -297.033303
Sum of electronic and thermal Enthalpies= -297.032359
Sum of electronic and thermal Free Energies= -297.069486

Zero imaginary frequencies

C 1.50978300 -0.27740900 0.00346900
C -0.86939900 0.29484700 0.00226900
N -2.02947200 -0.52860000 -0.10773700
H -2.84860400 0.02255800 0.11047800

H -1.99341000 -1.33739200 0.50254400
N -0.70860100 1.50427500 0.00900900
N 0.28143000 -0.73717700 0.06971300
N 2.57953400 0.17081800 -0.01547500
H 0.13947100 -1.65501200 -0.33600800

$C_{CN\text{-}GLY}$-

Zero-point correction= 0.119939 (Hartree/Particle)
Thermal correction to Energy= 0.130552
Thermal correction to Enthalpy= 0.131496
Thermal correction to Gibbs Free Energy= 0.083093
Sum of electronic and zero-point Energies= -528.970598
Sum of electronic and thermal Energies= -528.959985
Sum of electronic and thermal Enthalpies= -528.959041
Sum of electronic and thermal Free Energies= -529.007444

Zero imaginary frequencies

N -2.62035400 1.15525100 0.34633600
C -2.71568200 -0.12676600 0.31095200
N -2.67876800 -1.30605500 0.32117400
H -3.33809900 1.59593600 -0.22048100
C 1.92071500 -0.01990000 -0.18760300
H 2.22756900 -0.07592100 -1.23555500
C 0.40159800 -0.04900800 -0.11063200
H 0.09367400 -0.13086300 0.93994000
O -0.03735200 -1.17060200 -0.83230000
O -0.06137000 1.16035700 -0.65282800
O 2.49785500 -1.12195900 0.45093600
O 2.40860600 1.15659100 0.41840600
H -0.95169800 -1.36503400 -0.54404200
H 2.16952900 -1.14785000 1.35948200
H 1.78341400 1.86230300 0.20464700
H -0.99223200 1.29599800 -0.32657100

$P_{CN\text{-}GLY}$-

Zero-point correction= 0.122685 (Hartree/Particle)
Thermal correction to Energy= 0.132190
Thermal correction to Enthalpy= 0.133134
Thermal correction to Gibbs Free Energy= 0.088257
Sum of electronic and zero-point Energies= -528.963263
Sum of electronic and thermal Energies= -528.953758
Sum of electronic and thermal Enthalpies= -528.952814
Sum of electronic and thermal Free Energies= -528.997691

Zero imaginary frequencies

C 1.48173800 -0.34946800 -0.44013700
H 1.64420200 0.09144400 -1.45031800
C 0.49873200 0.58196700 0.27488300
H 0.34733700 0.25729500 1.30489900
O -0.76089300 0.57285800 -0.41160500
O 0.92914900 1.91159700 0.30647000
O 1.09971700 -1.62450400 -0.46125600
O 2.72799300 -0.15321400 0.29180800
H -0.66133800 -1.55465700 0.74387900
H 3.19228800 -0.99031400 0.18240000
H 1.33146700 2.12002400 -0.54706900
C -1.76691100 -0.20750500 0.06889700
N -2.97199000 0.29673000 -0.33431200
H -3.77233600 -0.13030600 0.10524100

H -3.01818200 1.29974700 -0.42970300
N -1.64408300 -1.28202800 0.74366500

$INT_{2CN-GLY}$-

Zero-point correction= 0.159613 (Hartree/Particle)
Thermal correction to Energy= 0.172846
Thermal correction to Enthalpy= 0.173790
Thermal correction to Gibbs Free Energy= 0.119447
Sum of electronic and zero-point Energies= -677.705028
Sum of electronic and thermal Energies= -677.691794
Sum of electronic and thermal Enthalpies= -677.690850
Sum of electronic and thermal Free Energies= -677.745194

Zero imaginary frequencies

C -1.85399500 0.70745300 -0.08014800
H -1.80139000 1.25543800 -1.02877600
C -1.20739400 -0.66194400 -0.24463800
H -1.29148600 -1.21527700 0.69266900
O 0.12479600 -0.49796100 -0.59989700
O -1.88175900 -1.42317500 -1.22067200
O -1.20296600 1.43412200 0.94047600
O -3.18804000 0.51904300 0.30288200
H 0.23041100 -0.90236400 2.07832500
H -3.65836400 1.35302400 0.19407100
H -1.83332300 -0.94320000 -2.05732200
C 1.21419600 -0.81463500 0.43941700
N 2.27182600 -1.44016600 -0.31058300
H 2.04062000 -2.42522000 -0.37484100
H 2.27322800 -1.07566000 -1.25823200
N 0.86695700 -1.48529700 1.54094200
H -0.24307600 1.29486400 0.86840100
N 1.65063900 0.64468000 0.73224200
C 2.05293200 1.37417600 -0.30543200
N 2.34156800 2.01169200 -1.22703300
H 2.31576600 0.65551400 1.49923100

2CN

Zero-point correction= 0.075136 (Hartree/Particle)
Thermal correction to Energy= 0.081399
Thermal correction to Enthalpy= 0.082344
Thermal correction to Gibbs Free Energy= 0.045256
Sum of electronic and zero-point Energies= -297.544096
Sum of electronic and thermal Energies= -297.537833
Sum of electronic and thermal Enthalpies= -297.536888
Sum of electronic and thermal Free Energies= -297.573976

Zero imaginary frequencies

N -0.68493500 1.34114100 -0.04405300
C -0.92222800 0.00065300 0.00814600
N -2.09079300 -0.50517000 -0.05542800
H 0.12357200 1.69759600 0.44574400
H -1.51583900 1.90337500 0.06403700
H -2.04359200 -1.51935300 -0.09450400
N 0.24527900 -0.78552500 0.08727100
H 0.13980800 -1.79156800 0.13938500
C 1.46973500 -0.29001100 -0.00218700
N 2.53202100 0.15614000 -0.07213500

CY

Zero-point correction= 0.109349 (Hartree/Particle)
Thermal correction to Energy= 0.117047
Thermal correction to Enthalpy= 0.117991
Thermal correction to Gibbs Free Energy= 0.077328
Sum of electronic and zero-point Energies= -453.033103
Sum of electronic and thermal Energies= -453.025405
Sum of electronic and thermal Enthalpies= -453.024461
Sum of electronic and thermal Free Energies= -453.065125

Zero imaginary frequencies

C 0.85527900 0.70479100 -0.34332800
C 0.92885600 -0.64159500 0.37491100
C -1.16585400 -0.13642500 0.05260200
H 1.43581000 0.74862900 -1.26114100
H 1.55497500 -0.56770400 1.26225000
O 1.47270000 -1.58354800 -0.52868800
H 1.50685700 -2.43655900 -0.08055600
O 1.19613000 1.72108700 0.54736800
H 1.26052100 2.55177800 0.06162600
O -0.52885100 0.80458700 -0.69991500
N -0.44357400 -0.94902600 0.73122000
N -2.50426100 -0.11680400 -0.05711100
H -3.02154900 -0.67914600 0.59965100
H -2.93128100 0.74617800 -0.35583400

$C_{CY\text{-}W\text{-}CN}$

Zero-point correction= 0.170058 (Hartree/Particle)
Thermal correction to Energy= 0.184781
Thermal correction to Enthalpy= 0.185725
Thermal correction to Gibbs Free Energy= 0.127793
Sum of electronic and zero-point Energies= -678.229980
Sum of electronic and thermal Energies= -678.215257
Sum of electronic and thermal Enthalpies= -678.214313
Sum of electronic and thermal Free Energies= -678.272245

Zero imaginary frequencies

C -1.97645600 0.49051900 0.22430600
C -1.40101500 -0.51828500 -0.79612900
C -0.15072600 -0.53874300 1.00920000
H -3.00047400 0.25657200 0.50306900
H -1.17068800 -0.00804600 -1.73085400
O -2.32295200 -1.52966200 -1.13550700
H -2.54180300 -2.02181300 -0.33392700
O -1.93584300 1.81816200 -0.17381000
H -1.03091600 2.02384100 -0.48030100
O -1.14479300 0.29636900 1.38535700
N -0.20040600 -1.04064800 -0.17393400
N 0.77083200 -0.78387200 1.95183700
H 1.62356600 -1.22947000 1.64618000
H 0.84251900 -0.12453100 2.71165200
N 2.87764700 0.89464300 -0.22110800
H 2.83811100 -0.11436300 -0.42133400
H 3.29353900 1.13876900 0.67017700
C 1.76370500 1.54313800 -0.50383900
N 0.81806200 2.13445000 -0.80950800
O 2.37919700 -1.84760100 -0.88778500
H 2.63797800 -2.45265700 -0.18439500
H 1.42730100 -1.65823600 -0.71854900

$INT_{CY\text{-}W\text{-}CN}$

Zero-point correction= 0.169104 (Hartree/Particle)
Thermal correction to Energy= 0.183505
Thermal correction to Enthalpy= 0.184449
Thermal correction to Gibbs Free Energy= 0.127446
Sum of electronic and zero-point Energies= -678.224175
Sum of electronic and thermal Energies= -678.209774
Sum of electronic and thermal Enthalpies= -678.208830
Sum of electronic and thermal Free Energies= -678.265833

Zero imaginary frequencies

C -1.97110100 0.45380300 0.14851400
C -1.32328200 -0.57172100 -0.81238000
C -0.13857900 -0.43677300 1.12704400
H -2.99789300 0.19118900 0.38540600
H -1.02091700 -0.08796700 -1.73732300
O -2.17435000 -1.62296900 -1.17014100
H -2.51227000 -2.04953200 -0.37154800
O -1.90350100 1.75535200 -0.25631400
H -0.95041300 1.95161400 -0.50526300
O -1.20124600 0.28830900 1.39432900
N -0.16288700 -1.00954200 -0.05935200
N 0.80741100 -0.55560600 2.02218800
H 1.65000100 -1.06548600 1.79588000
H 0.75256200 -0.01962100 2.87599100
N 2.80529100 0.87619600 -0.38972900
H 2.64999300 -0.83018500 -0.64021500
H 3.30708200 1.19518600 0.43273300
C 1.70748700 1.51476000 -0.55461100
N 0.68783500 2.05556400 -0.79292600
O 2.41445900 -1.78722100 -0.80049800
H 2.73403300 -2.26139900 -0.02549700
H 0.69422600 -1.41827000 -0.46185200

$P_{CY\text{-}W\text{-}CN}$

Zero-point correction= 0.173780 (Hartree/Particle)
Thermal correction to Energy= 0.187111
Thermal correction to Enthalpy= 0.188055
Thermal correction to Gibbs Free Energy= 0.134327
Sum of electronic and zero-point Energies= -678.218638
Sum of electronic and thermal Energies= -678.205307
Sum of electronic and thermal Enthalpies= -678.204363
Sum of electronic and thermal Free Energies= -678.258091

Zero imaginary frequencies

C 0.61008400 -1.04305300 1.00982700
C 1.07562200 -1.19691200 -0.44555100
O 0.52743000 0.37187700 1.17874800
N 0.55031000 -0.00502000 -1.10144000
O 2.47877400 -1.25812100 -0.54045500
H 0.67121000 -2.09591300 -0.90048200
O -0.61446300 -1.65061200 1.27706100
H 1.33350100 -1.42566100 1.72466900
C 0.62184400 1.01595000 -0.07998600
H -0.41818100 -0.16675100 -1.36461800
H 2.82210000 -0.38353000 -0.30270900
H -1.20613700 -1.59725300 0.49741100
N 1.88539000 1.68332700 -0.13577500
H 1.96268500 2.21031900 -0.99934600
H 1.96986500 2.32156400 0.64958400
N -0.49085800 1.96347600 -0.23468900

C -1.70956800 1.51781500 0.04806300
H -0.29586800 2.90708000 0.08398100
N -2.76579900 1.09496200 0.24657700
O -2.39151800 -1.71295800 -0.84210400
H -1.97935500 -1.89149500 -1.69490200
H -2.70278700 -0.79986900 -0.89641100

TS-isom$_{CN-W}$

Zero-point correction= 0.058409 (Hartree/Particle)
Thermal correction to Energy= 0.063389
Thermal correction to Enthalpy= 0.064333
Thermal correction to Gibbs Free Energy= 0.031192
Sum of electronic and zero-point Energies= -225.133484
Sum of electronic and thermal Energies= -225.128504
Sum of electronic and thermal Enthalpies= -225.127560
Sum of electronic and thermal Free Energies= -225.160701

One imaginary frequency: 282.76i cm^{-1}

N -0.96527000 -1.08229300 -0.11551000
C -0.89641300 0.19006400 0.00760700
N -0.63126500 1.34366500 0.01847000
H 1.02336300 -0.87429000 -0.09438400
H -1.33910200 -1.52535100 0.71815400
O 1.68935500 -0.12850300 -0.08790100
H 2.26910000 -0.22100400 0.68791700
H 1.08602700 0.67868100 0.02516500

TS-isom$_{GLY-CN}$

Zero-point correction= 0.126284 (Hartree/Particle)
Thermal correction to Energy= 0.136001
Thermal correction to Enthalpy= 0.136945
Thermal correction to Gibbs Free Energy= 0.091061
Sum of electronic and zero-point Energies= -529.380136
Sum of electronic and thermal Energies= -529.370420
Sum of electronic and thermal Enthalpies= -529.369476
Sum of electronic and thermal Free Energies= -529.415360

One imaginary frequency: 972.91i cm^{-1}

N -2.18635800 -1.22028500 -0.34647300
C -2.24465200 0.06793900 -0.30685300
N -2.12262800 1.23768800 -0.27855000
H -3.00914200 -1.66606700 0.04527700
C 1.22669600 0.75342900 0.21976000
H 2.16845400 0.80622700 0.76264400
C 0.93361800 -0.68127400 -0.28272000
H 0.38235800 -0.63326000 -1.22271000
O 0.12263500 -1.26830800 0.72397400
O 2.09381200 -1.40509100 -0.52142800
O 0.19083000 0.99571400 1.23062400
O 1.14250200 1.64125900 -0.81995200
H -0.85134900 -1.43612400 0.30728400
H -0.63668800 1.32576900 0.76449800
H 1.60749600 2.45601300 -0.59100200
H 2.64124000 -1.39743000 0.27514000
H -0.03167100 -0.12609900 1.34716200

TS$_{CN-CN-W}$

Zero-point correction= 0.091705 (Hartree/Particle)
Thermal correction to Energy= 0.101220
Thermal correction to Enthalpy= 0.102164
Thermal correction to Gibbs Free Energy= 0.057098
Sum of electronic and zero-point Energies= -373.901023
Sum of electronic and thermal Energies= -373.891508
Sum of electronic and thermal Enthalpies= -373.890564
Sum of electronic and thermal Free Energies= -373.935630

One imaginary frequency: 333.89i cm^{-1}

C -1.59937900 -0.87021600 0.09203500
C 0.50354400 1.26662300 0.06085100
N -0.60764900 1.89171400 -0.09658300
H -0.68207800 2.55946500 -0.85717200
H -1.45293800 1.56430800 0.35659000
N 1.67277700 1.09294400 0.13405400
H 2.10106300 0.14505200 -0.11126600
O 2.12892900 -1.43604500 -0.40585500
H 2.60470400 -1.90190600 0.29092500
H 1.17356300 -1.46020500 -0.13831100
N -0.37481300 -0.85845700 0.52083000
N -2.67089500 -0.82064600 -0.37899000
H -0.33668000 -0.93567500 1.53358400

$TS_{GLY\text{-}CN\text{-}W}$

Zero-point correction= 0.151886 (Hartree/Particle)
Thermal correction to Energy= 0.164277
Thermal correction to Enthalpy= 0.165222
Thermal correction to Gibbs Free Energy= 0.113225
Sum of electronic and zero-point Energies= -605.796083
Sum of electronic and thermal Energies= -605.783691
Sum of electronic and thermal Enthalpies= -605.782747
Sum of electronic and thermal Free Energies= -605.834743

One imaginary frequency: 905.38i cm^{-1}

C -1.86088400 0.34620600 -0.17562400
H -2.00037700 0.54590400 -1.23909300
C -0.65580800 -0.56577100 0.02571200
H -0.54822200 -0.75931900 1.10361000
O 0.47999100 0.00724100 -0.50336100
O -0.86920500 -1.79158400 -0.65656300
O -1.66980400 1.59386200 0.43957300
O -2.96344000 -0.33853800 0.36469000
H -1.43611600 1.44546000 1.36602800
H -3.77201200 0.08281900 0.05215900
H -1.62492900 -2.23258000 -0.24940400
C 2.10865300 -0.48658500 0.17925200
N 1.86841100 -1.78702900 0.42923700
H 2.70149700 -2.32706600 0.61873100
H 1.16763300 -2.23558300 -0.14486100
N 2.88562200 0.41351900 0.26058000
H 2.19261500 1.60592100 -0.01646100
O 1.31228300 2.24232900 -0.26390100
H 1.46628900 2.66968600 -1.11781400
H 0.70502100 1.34974800 -0.42115100

TS-$anti_{CN\text{-}CN}$-

Zero-point correction= 0.058443 (Hartree/Particle)

Thermal correction to Energy= 0.064539
Thermal correction to Enthalpy= 0.065483
Thermal correction to Gibbs Free Energy= 0.028624
Sum of electronic and zero-point Energies= -297.039103
Sum of electronic and thermal Energies= -297.033007
Sum of electronic and thermal Enthalpies= -297.032063
Sum of electronic and thermal Free Energies= -297.068922

One imaginary frequency: 310.00i cm^{-1}

C 1.53386400 -0.30868800 0.00516300
C -0.95702200 0.35461000 0.00797000
N -2.02456900 -0.52951900 -0.11975900
H -2.89757300 -0.07398600 0.11241300
H -1.90207200 -1.37810900 0.41606100
N -0.72080700 1.52335600 0.01533500
N 0.35482900 -0.85221600 0.12289000
N 2.54788800 0.26561600 -0.03926000
H 0.23720600 -1.67410000 -0.46171800

TS-syn$_{CN-CN}$-

Zero-point correction= 0.058410 (Hartree/Particle)
Thermal correction to Energy= 0.064586
Thermal correction to Enthalpy= 0.065530
Thermal correction to Gibbs Free Energy= 0.028011
Sum of electronic and zero-point Energies= -297.037879
Sum of electronic and thermal Energies= -297.031704
Sum of electronic and thermal Enthalpies= -297.030759
Sum of electronic and thermal Free Energies= -297.068278

One imaginary frequency: 308.40i cm^{-1}

C 1.50434800 -0.28640600 0.01793700
C -1.17127500 -0.03555800 -0.02270600
N -0.87453400 1.29969400 0.22025700
H -1.52412300 1.90534600 -0.26362700
H 0.08161200 1.56236800 0.02114000
N -2.09240700 -0.73558400 -0.31446600
N 0.37215900 -0.81049100 0.40587800
N 2.47709700 0.28160900 -0.29280800
H 0.26787400 -1.78252500 0.13907800

TS-1-2$_{CN-GLY}$-

Zero-point correction= 0.119483 (Hartree/Particle)
Thermal correction to Energy= 0.129399
Thermal correction to Enthalpy= 0.130343
Thermal correction to Gibbs Free Energy= 0.084118
Sum of electronic and zero-point Energies= -528.933386
Sum of electronic and thermal Energies= -528.923469
Sum of electronic and thermal Enthalpies= -528.922525
Sum of electronic and thermal Free Energies= -528.968750

One imaginary frequency: 260.52i cm^{-1}

C 1.44258700 -0.37263000 -0.46459900
H 1.71783200 -0.06086000 -1.47524000
C 0.52414500 0.65924600 0.18654100
H 0.35610200 0.30033500 1.21944100
O -0.63716500 0.81432500 -0.48560000
O 1.20709900 1.91825900 0.25014600
O 0.79069200 -1.61618200 -0.55310000

O 2.59976000 -0.46356700 0.34178600
H 0.02263100 -1.60244900 0.05461300
H 3.27515800 -0.94751800 -0.14542700
H 2.03587300 1.77188100 0.72181400
C -1.97453300 -0.29735900 0.26170200
N -2.98718300 0.32117600 -0.40620600
H -3.89052600 0.14131700 0.01081500
H -2.81245600 1.29691000 -0.59144200
N -1.63294400 -1.18658300 0.96016600

TS-gem$_{CN-GLY}$-

Zero-point correction= 0.119842 (Hartree/Particle)
Thermal correction to Energy= 0.129830
Thermal correction to Enthalpy= 0.130774
Thermal correction to Gibbs Free Energy= 0.084087
Sum of electronic and zero-point Energies= -528.932226
Sum of electronic and thermal Energies= -528.922238
Sum of electronic and thermal Enthalpies= -528.921294
Sum of electronic and thermal Free Energies= -528.967981

One imaginary frequency: 251.39i cm^{-1}

C 1.79415700 -0.27138200 -0.25592500
H 1.94312400 -0.39234500 -1.33080000
C 0.39348700 0.26480400 0.01611100
H 0.31918000 0.46544200 1.10131200
O -0.56380900 -0.59479600 -0.40352500
O 0.31106800 1.53039900 -0.65437400
O 1.97289900 -1.54955600 0.30524100
O 2.72047300 0.64652900 0.27733800
H 1.68650100 -1.51373200 1.22720400
H 3.60200800 0.37876800 -0.00576600
H -0.55951000 1.86295100 -0.39306400
C -2.21413800 0.07684800 0.25038700
N -2.93429600 -0.99678200 -0.18959900
H -3.89680400 -0.75655900 -0.38684600
H -2.48536600 -1.48900000 -0.94721900
N -2.20501900 1.10567300 0.82878500

TS1$_{2CN-GLY}$-

Zero-point correction= 0.159015 (Hartree/Particle)
Thermal correction to Energy= 0.171607
Thermal correction to Enthalpy= 0.172551
Thermal correction to Gibbs Free Energy= 0.120057
Sum of electronic and zero-point Energies= -677.704327
Sum of electronic and thermal Energies= -677.691735
Sum of electronic and thermal Enthalpies= -677.690790
Sum of electronic and thermal Free Energies= -677.743284

One imaginary frequency: 302.33i cm^{-1}

C 1.73838800 0.67475700 -0.05279300
H 1.53084000 1.37412900 0.76775200
C 1.21225800 -0.70396800 0.33004400
H 1.40438500 -1.41275400 -0.47603300
O -0.16032000 -0.62120000 0.61682400
O 1.86639000 -1.19953700 1.46747900
O 1.14002000 1.12528800 -1.24486400
O 3.11598500 0.56035000 -0.27294200
H 0.02767600 -1.17993000 -1.87601900

H 3.48480000 1.44841000 -0.34257500
H 1.77214100 -0.55223900 2.17864300
C -1.15565100 -0.90248600 -0.39982000
N -2.33595700 -1.37305800 0.26464600
H -2.20159600 -2.36326000 0.44057200
H -2.41724100 -0.91806500 1.16835700
N -0.84655200 -1.54003600 -1.50928100
H 0.16332500 1.13289000 -1.12639300
N -1.57578500 0.75368100 -0.73411800
C -1.92593900 1.47996000 0.31061000
N -2.15337600 2.09123400 1.27268600
H -2.29357600 0.73927600 -1.45205300

$TS2_{2CN\text{-}GLY^-}$

Zero-point correction= 0.158760 (Hartree/Particle)
Thermal correction to Energy= 0.171686
Thermal correction to Enthalpy= 0.172630
Thermal correction to Gibbs Free Energy= 0.119397
Sum of electronic and zero-point Energies= -677.707041
Sum of electronic and thermal Energies= -677.694114
Sum of electronic and thermal Enthalpies= -677.693170
Sum of electronic and thermal Free Energies= -677.746403

One imaginary frequency: -221.81i cm^{-1}

C -2.03233900 0.51615000 -0.27719000
H -2.31267400 0.58563300 -1.33090300
C -1.06797800 -0.65051200 -0.06247900
H -0.90014300 -0.74393100 1.02302000
O 0.08771600 -0.46697700 -0.74515300
O -1.72393500 -1.86832400 -0.42638200
O -1.43146700 1.74656400 0.04743800
O -3.16594900 0.28237000 0.52572000
H 0.92333000 -1.56954100 1.87707400
H -3.83821500 0.93141700 0.29026600
H -1.76102100 -1.87798500 -1.39099700
C 1.52665700 -0.83102000 0.23517300
N 2.47639200 -0.93459800 -0.81493900
H 2.45510200 -1.88850500 -1.15539200
H 2.21617400 -0.32765400 -1.58487700
N 1.39694900 -1.86119300 1.02828300
H -0.95153900 1.63913000 0.87979200
N 1.57373500 0.49466600 0.89925700
C 1.72688400 1.57600700 0.14511100
N 1.83138900 2.52296400 -0.51049900
H 2.16947600 0.48576100 1.72063200

$TS1_{CY\text{-}W\text{-}CN}$

Zero-point correction= 0.162284 (Hartree/Particle)
Thermal correction to Energy= 0.175675
Thermal correction to Enthalpy= 0.176620
Thermal correction to Gibbs Free Energy= 0.121904
Sum of electronic and zero-point Energies= -678.221257
Sum of electronic and thermal Energies= -678.207866
Sum of electronic and thermal Enthalpies= -678.206921
Sum of electronic and thermal Free Energies= -678.261637

One imaginary frequency: 1237.52i cm^{-1}

C -1.91315400 0.56980800 0.11112000
C -1.27252600 -0.44416000 -0.86451800
C -0.24225900 -0.54748400 1.10929300
H -2.97542000 0.38846400 0.24816600
H -0.90298200 0.06853800 -1.75059400
O -2.18397700 -1.41035100 -1.32654700
H -2.54610300 -1.88337100 -0.56593600
O -1.72472700 1.89534300 -0.20834300
H -0.76159600 2.04607200 -0.38359600
O -1.25932200 0.27123400 1.37660600
N -0.18075500 -1.01773400 -0.10298600
N 0.59070700 -0.81974300 2.09823600
H 1.40855300 -1.37983900 1.91257600
H 0.52113900 -0.30497300 2.96192800
N 2.88842400 0.59632400 -0.31531500
H 2.54042000 -0.66456300 -0.62467200
H 3.45741000 0.76959400 0.50570700
C 1.89221600 1.41639400 -0.42120000
N 0.97430100 2.11843800 -0.60362500
O 2.06544200 -1.67429900 -0.91129200
H 2.43204500 -2.35738300 -0.33636300
H 0.95280500 -1.44630400 -0.55294800

$TS2_{CY\text{-}W\text{-}CN}$

Zero-point correction= 0.170453 (Hartree/Particle)
Thermal correction to Energy= 0.183677
Thermal correction to Enthalpy= 0.184622
Thermal correction to Gibbs Free Energy= 0.130914
Sum of electronic and zero-point Energies= -678.198071
Sum of electronic and thermal Energies= -678.184847
Sum of electronic and thermal Enthalpies= -678.183902
Sum of electronic and thermal Free Energies= -678.237610

One imaginary frequency: 412.73i cm^{-1}

C -1.74705700 -0.05669600 0.46265400
C -1.15248700 -0.67489000 -0.82114700
C 0.44087000 -0.58468700 0.84530800
H -2.54483100 -0.67904400 0.86045200
H -1.10576300 0.05843400 -1.62330200
O -1.92582600 -1.73360500 -1.31848100
H -2.02462900 -2.39903200 -0.62448800
O -2.23931400 1.22329700 0.33824000
H -1.59580300 1.78182800 -0.14331600
O -0.66630200 -0.11795600 1.43097700
N 0.16146800 -1.10020500 -0.38348600
N 1.35087600 -1.17114000 1.66353100
H 2.19376700 -1.46016600 1.18090800
H 1.54634700 -0.63370300 2.49952700
N 1.42994600 1.09897300 0.40555400
H 2.60380800 0.11956500 -0.73488300
H 1.76670500 1.50779200 1.27413200
C 0.69659100 1.92663900 -0.27517400
N -0.02172400 2.56608100 -0.94146500
O 2.94435400 -0.54654400 -1.36384100
H 3.45310300 -1.15775800 -0.82110200
H 0.93252800 -1.15761400 -1.04186900