Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information

Polyureas from Diamines and Carbon Dioxide: Synthesis, Structures and Properties

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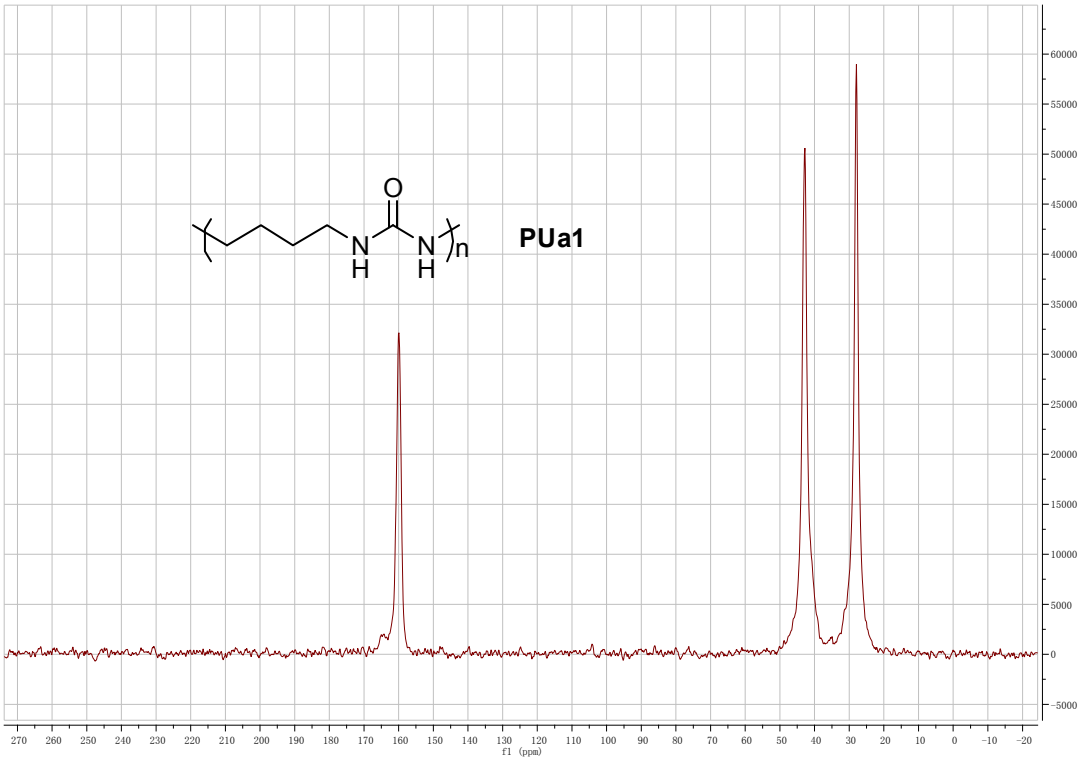
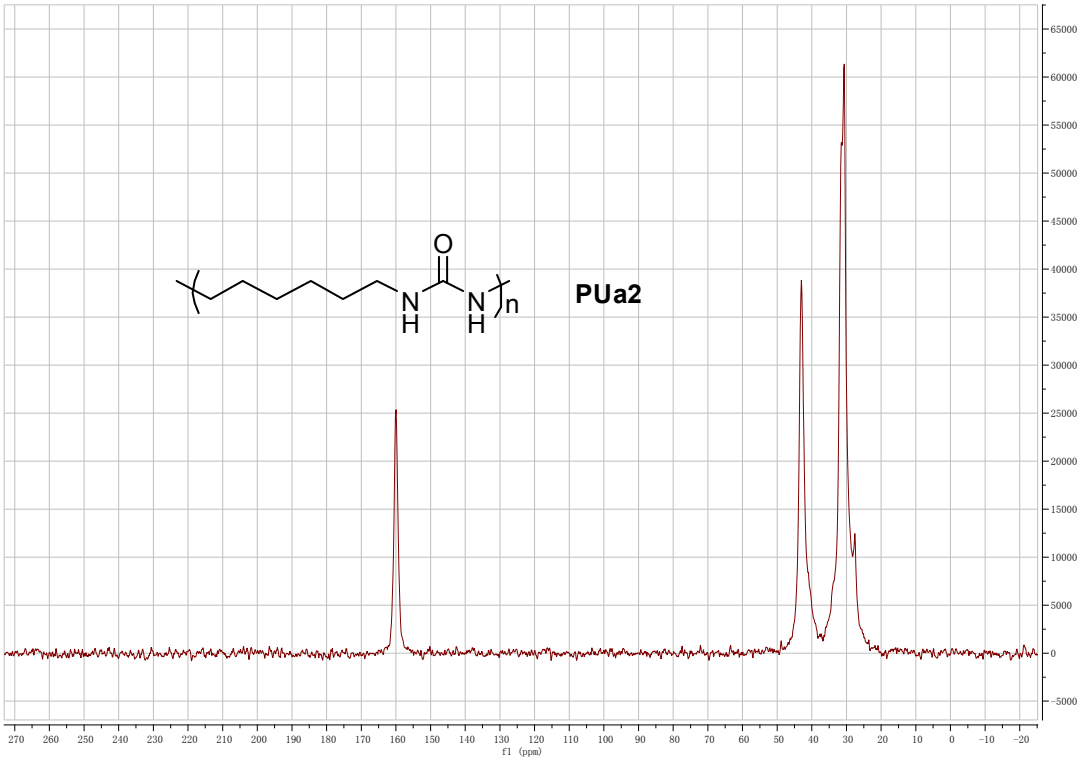
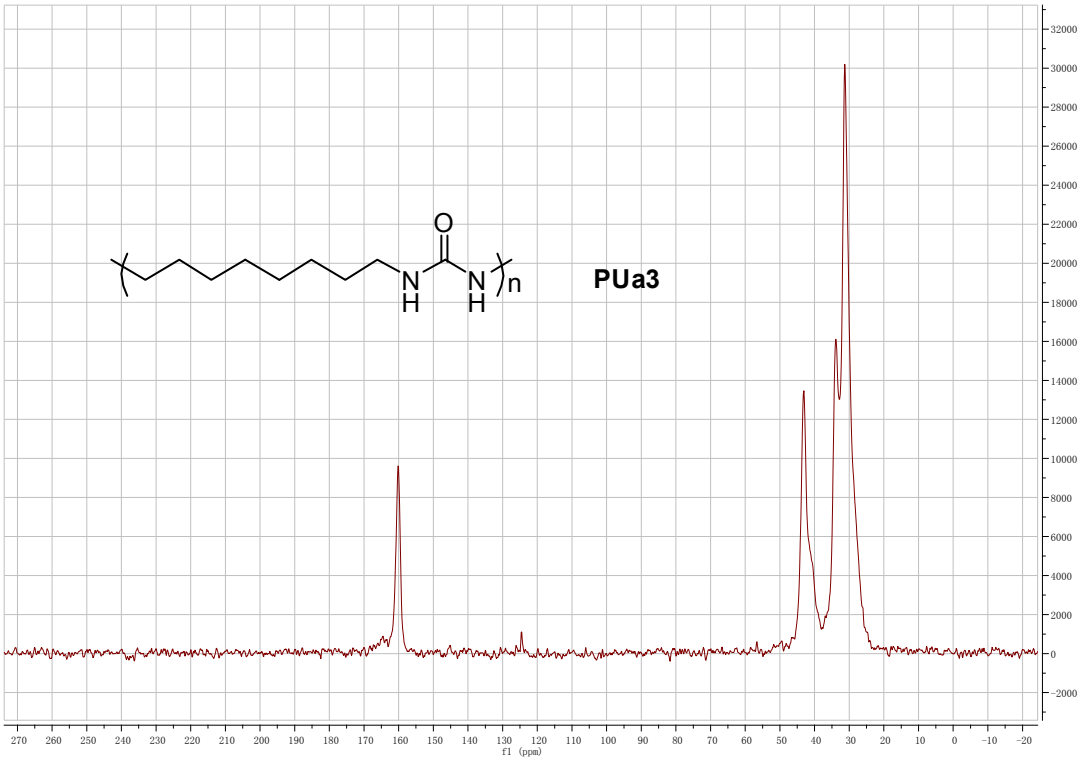
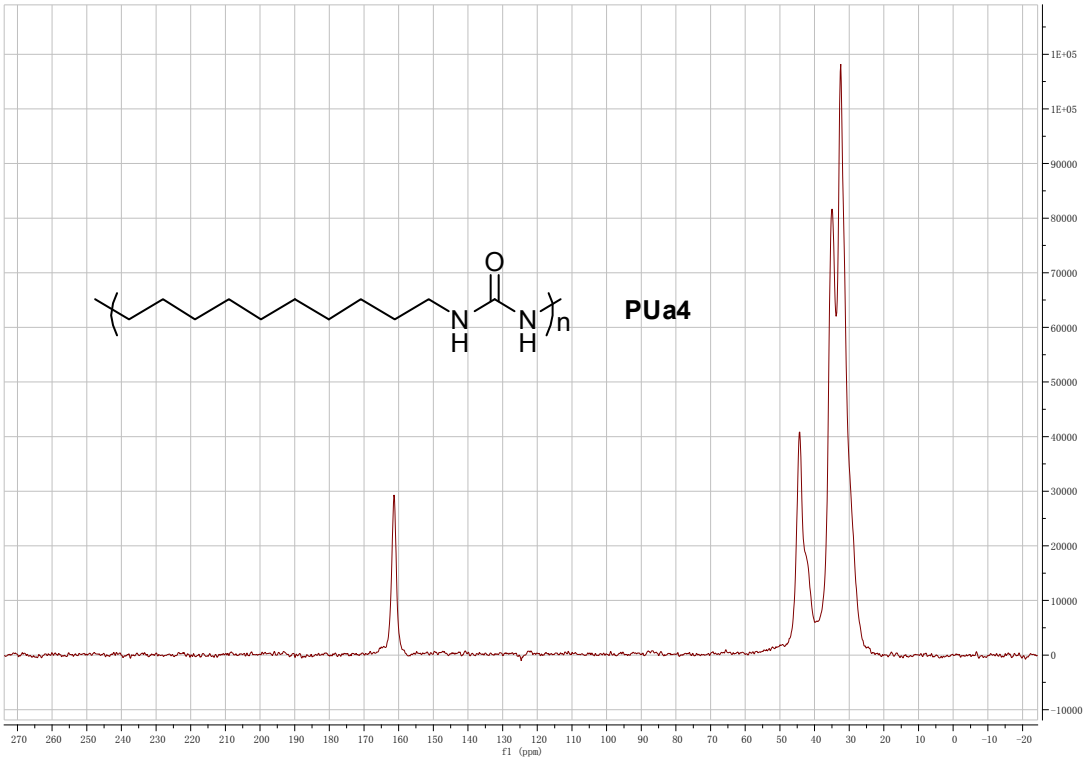
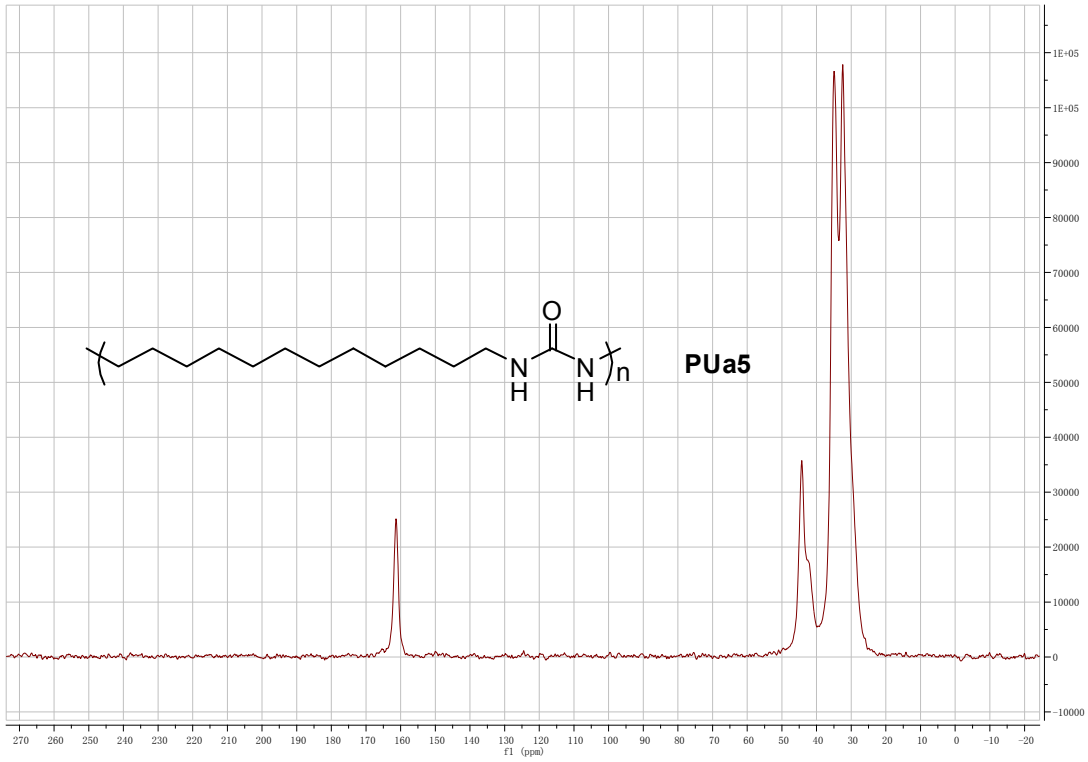
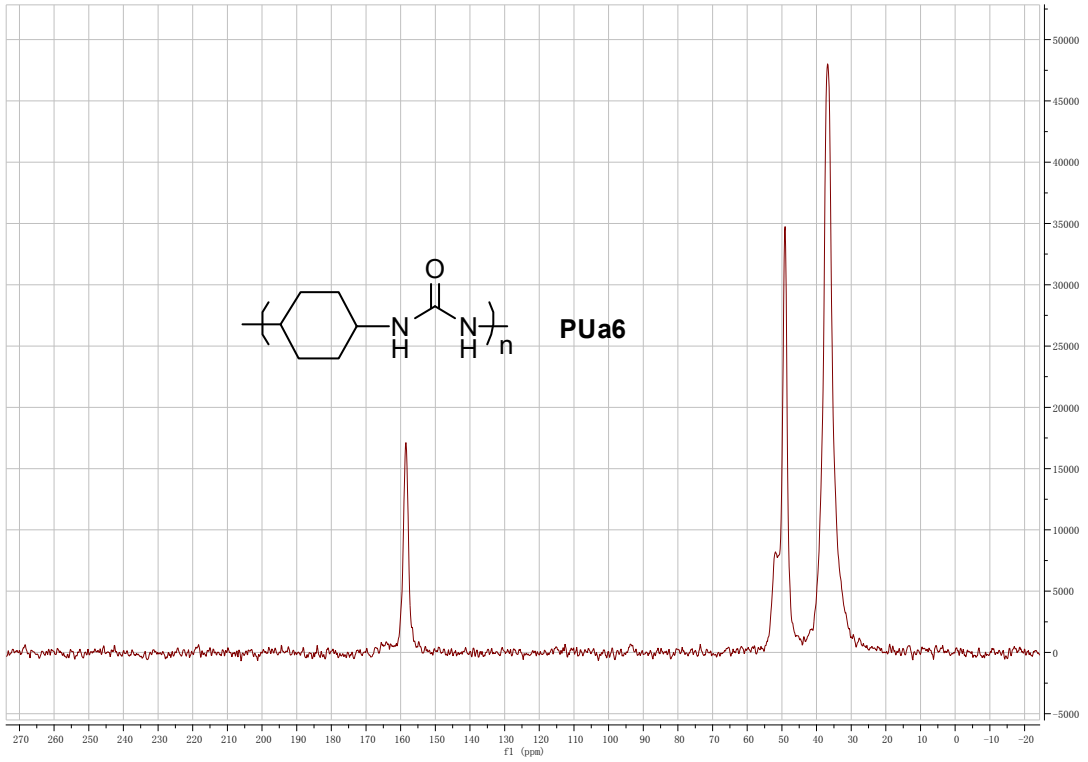


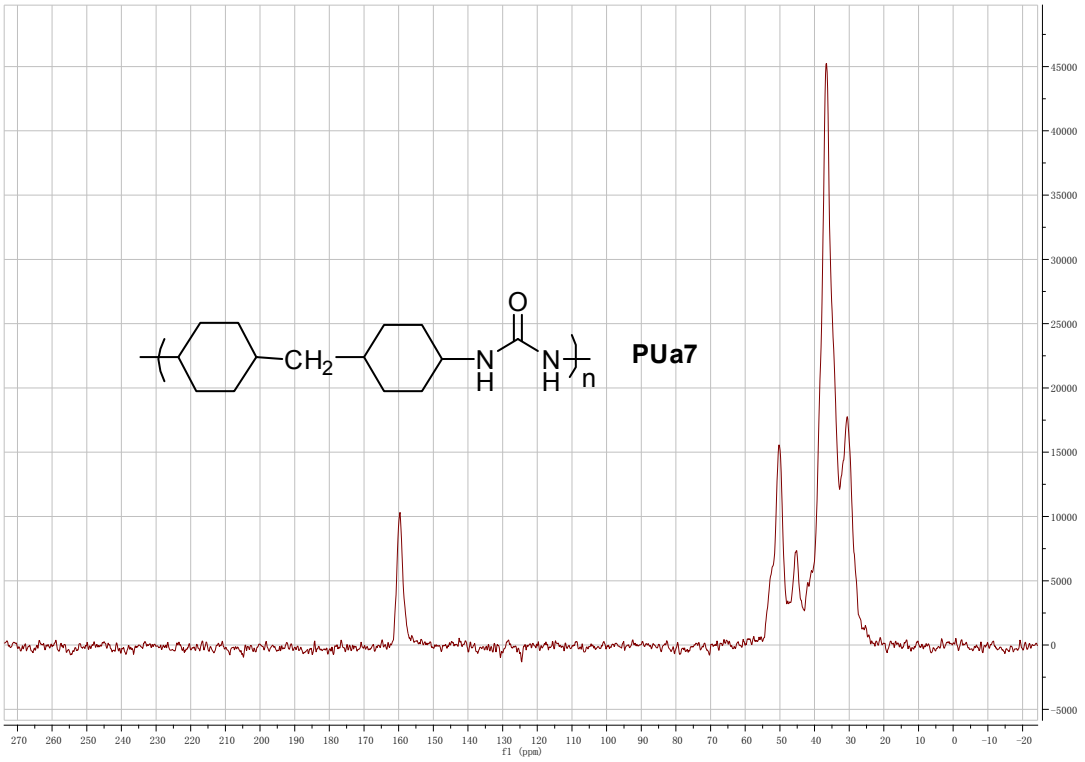


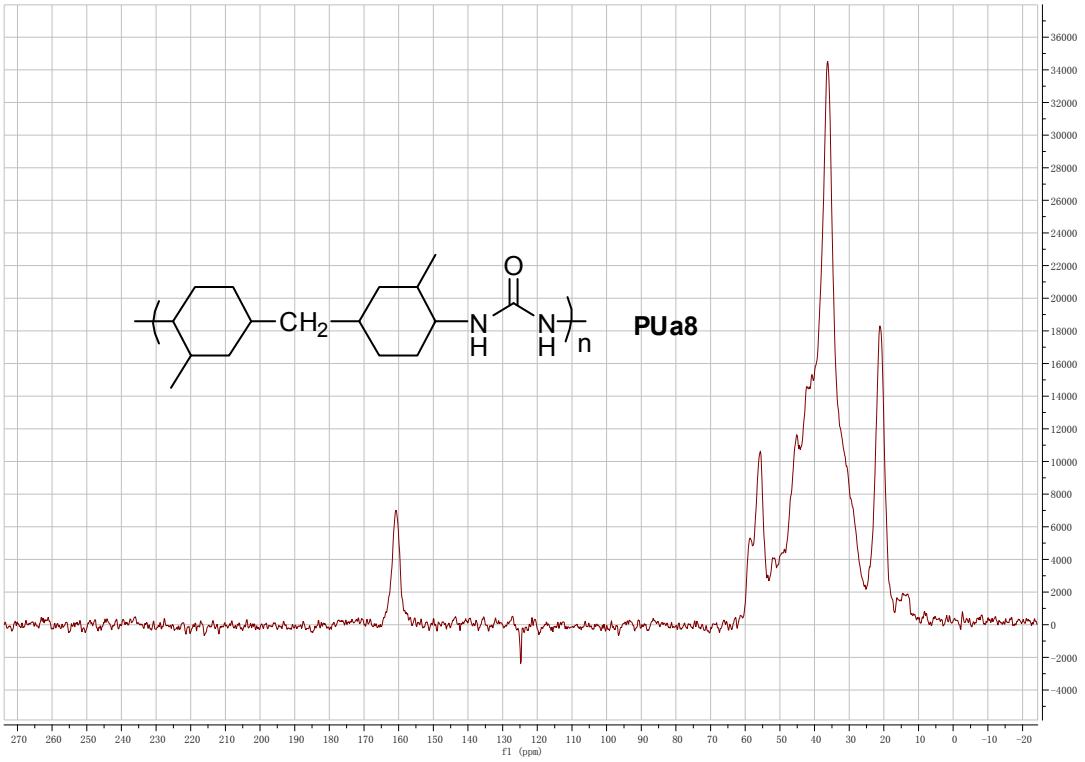

PUa3
f1 (ppm)

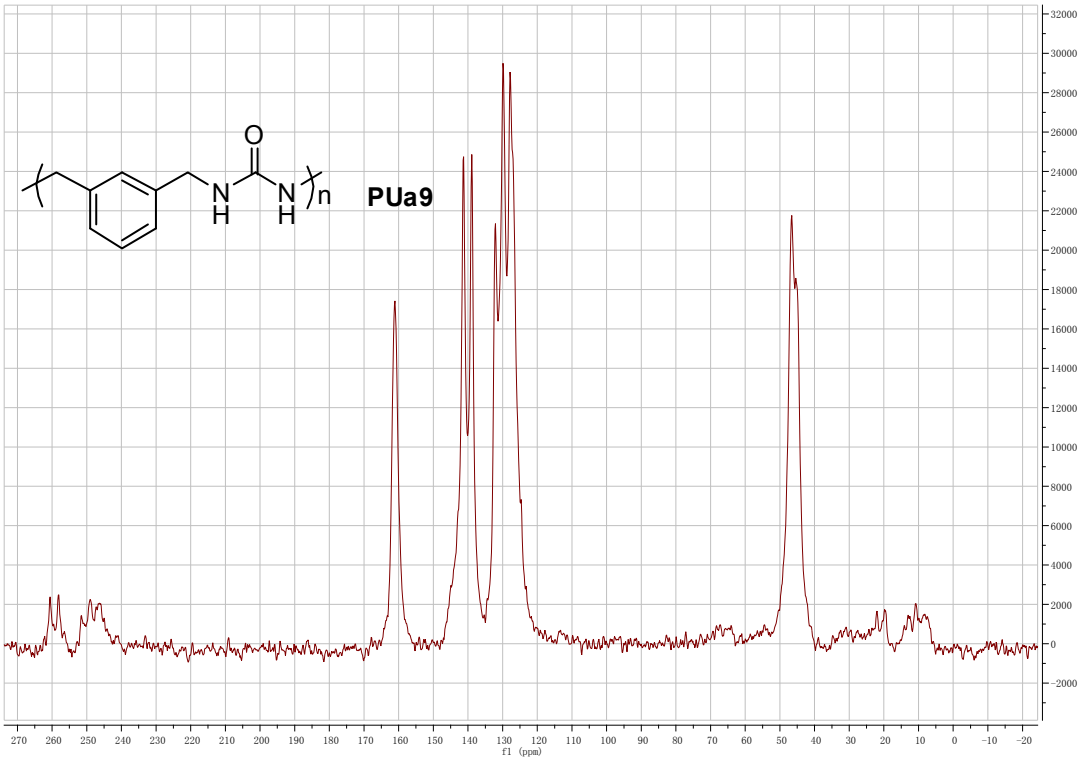

PUa4
f1 (ppm)



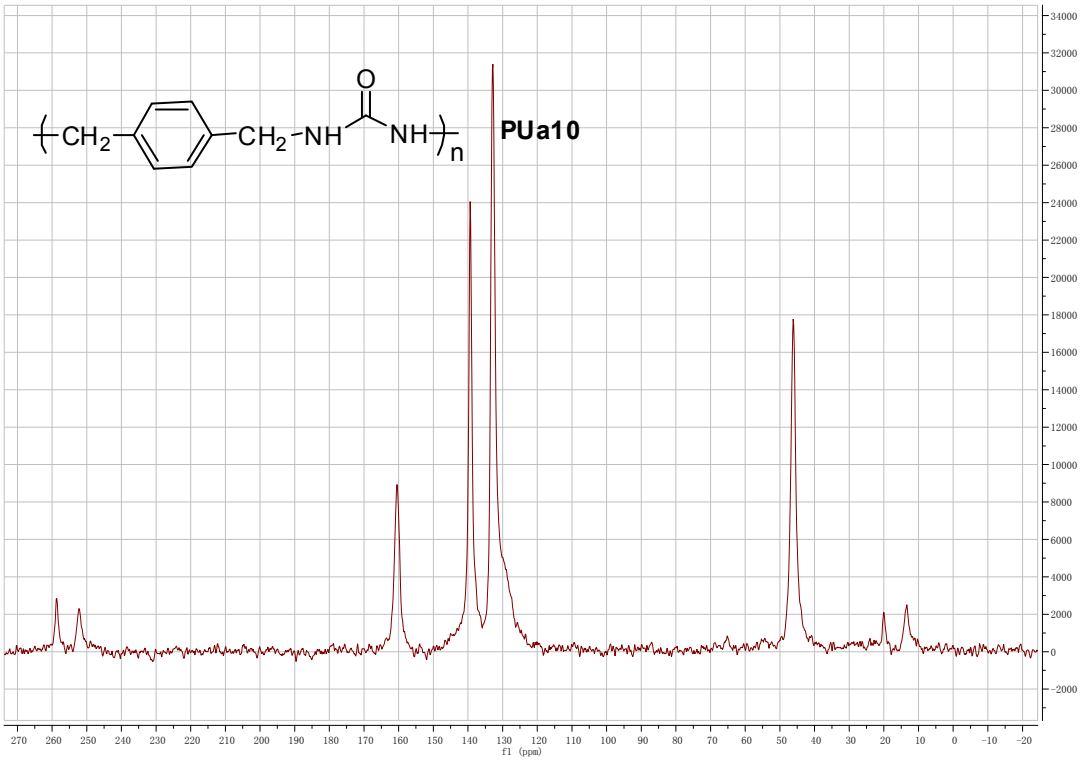








The peaks at 5-15 ppm and 240-270 ppm were caused by the side band.



The peaks at 5-25 ppm and 250-270 ppm were caused by the side band.

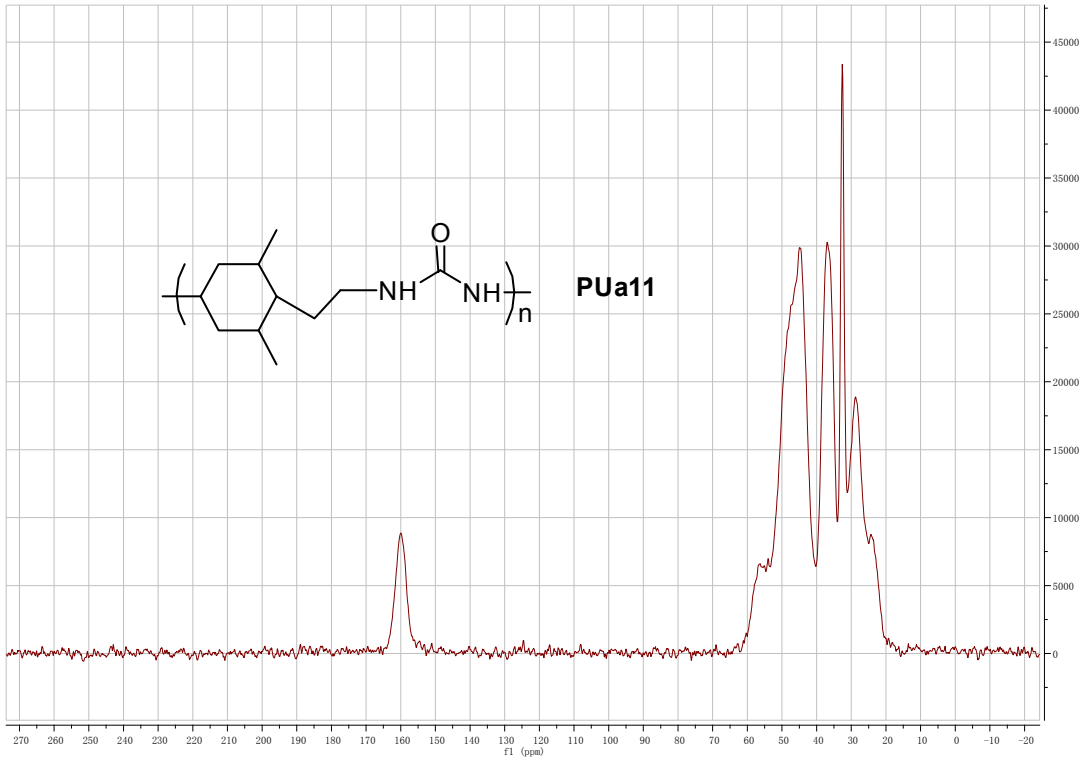
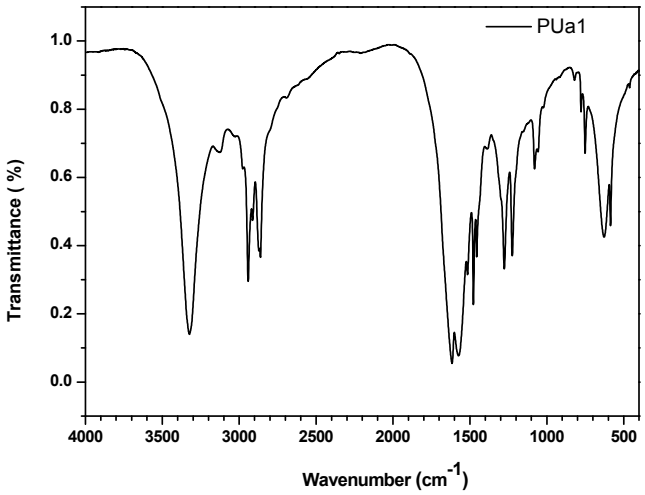
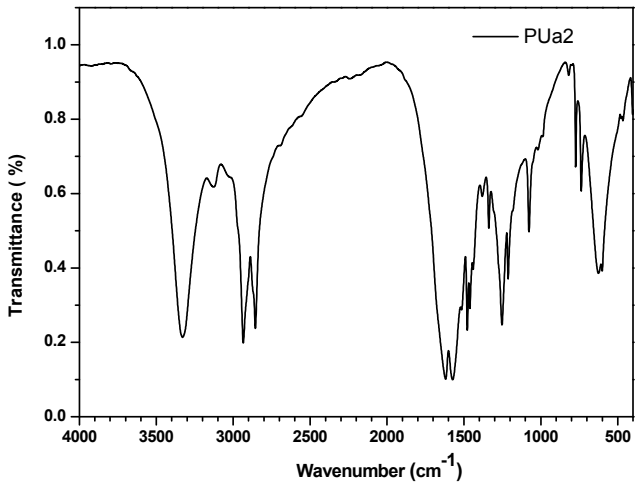
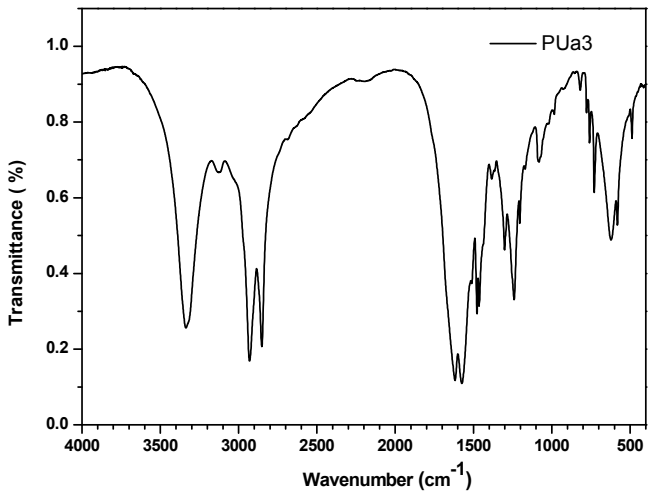
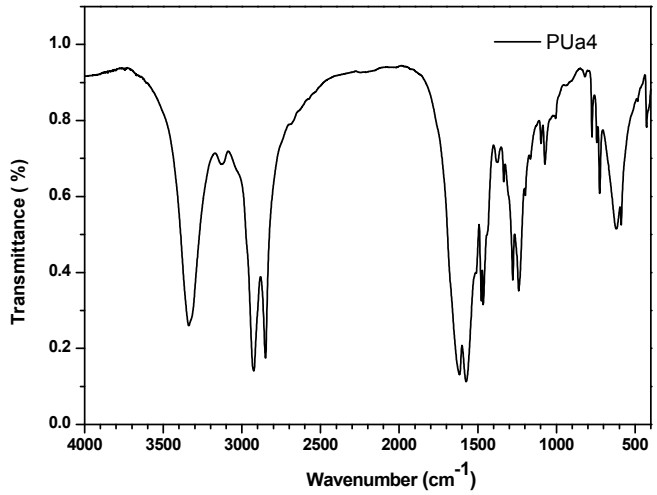


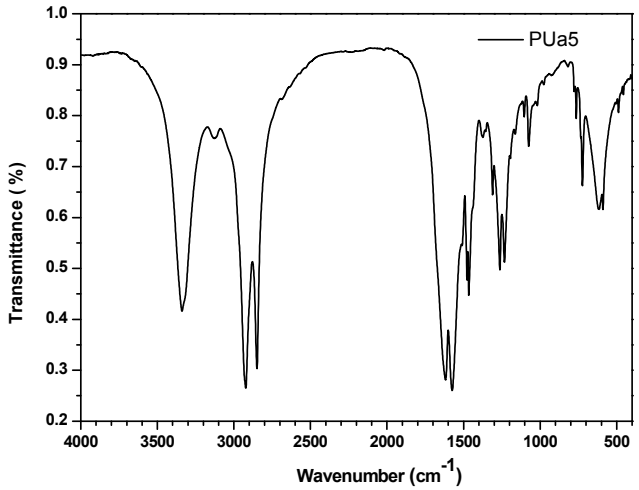
Fig. S1 CP/MAS ^{13}C NMR spectra of the products

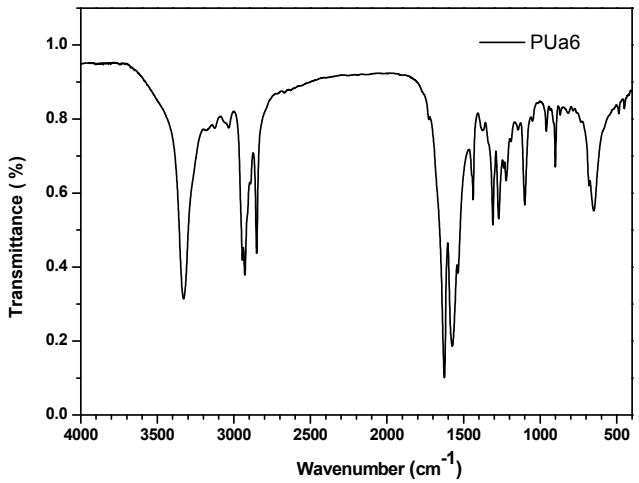


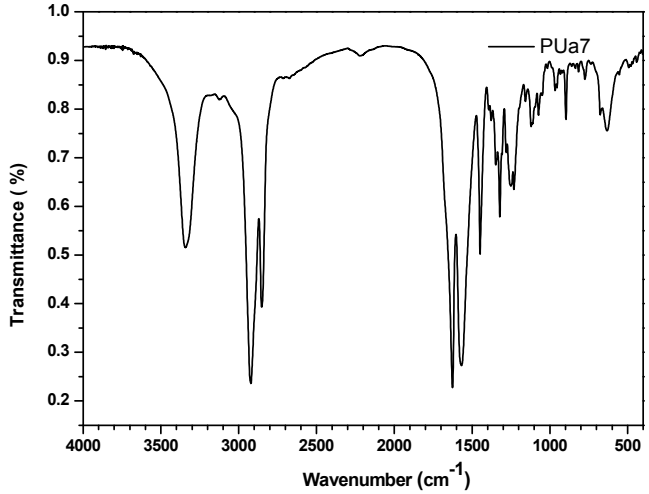


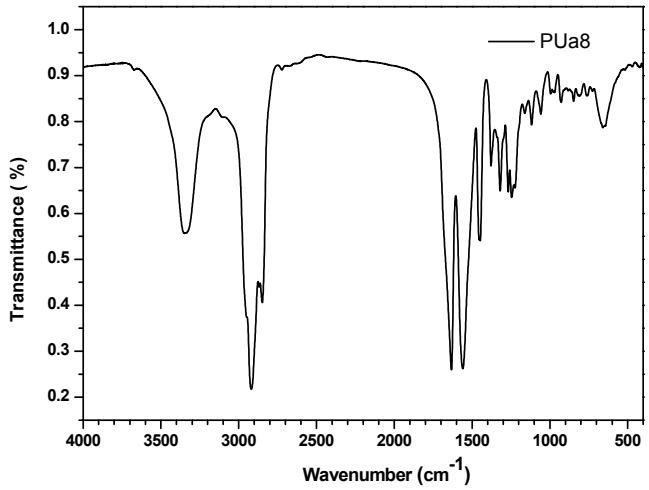


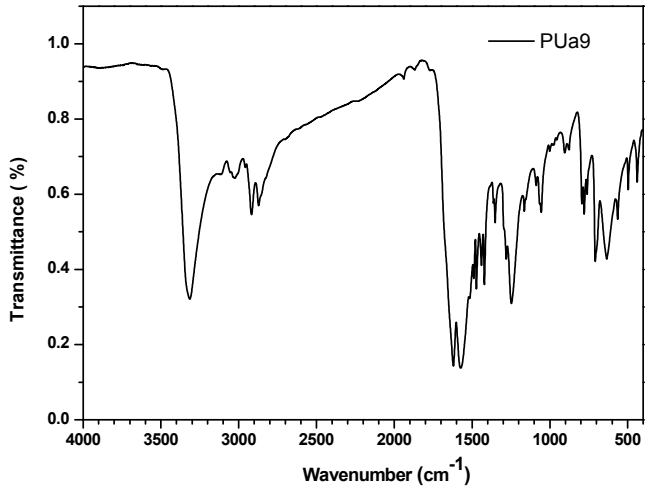







PUa7
Transmittance (%)
Wavenumber (cm-1)


PUa8
Transmittance (%)
Wavenumber (cm-1)


PUa9
Transmittance (%)
Wavenumber (cm-1)

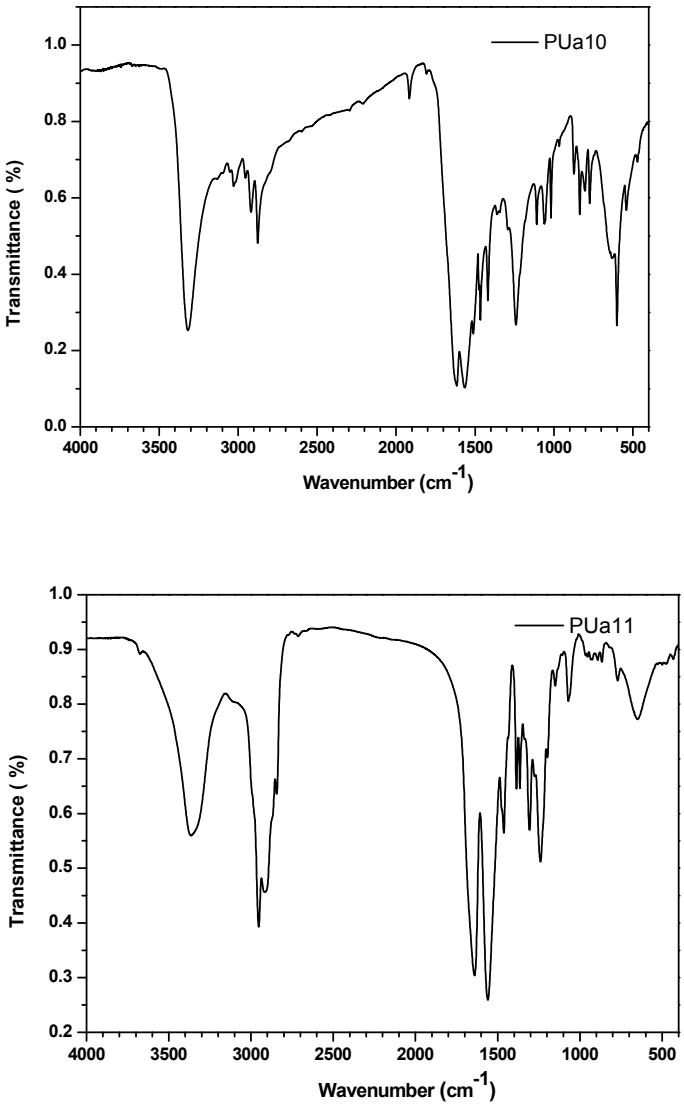


Fig. S2 FTIR spectra of the products

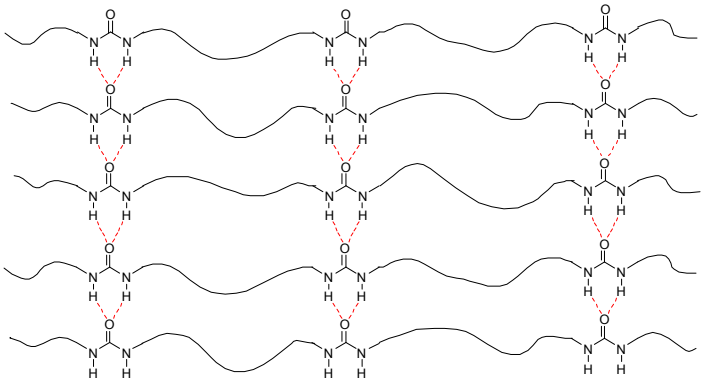


Fig. S3 The network structure of the PUas.

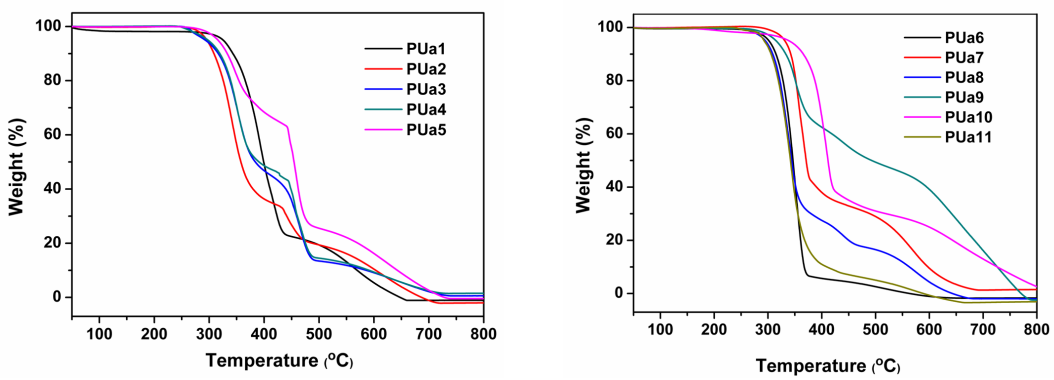


Fig. S4 TGA curves of the PUas.

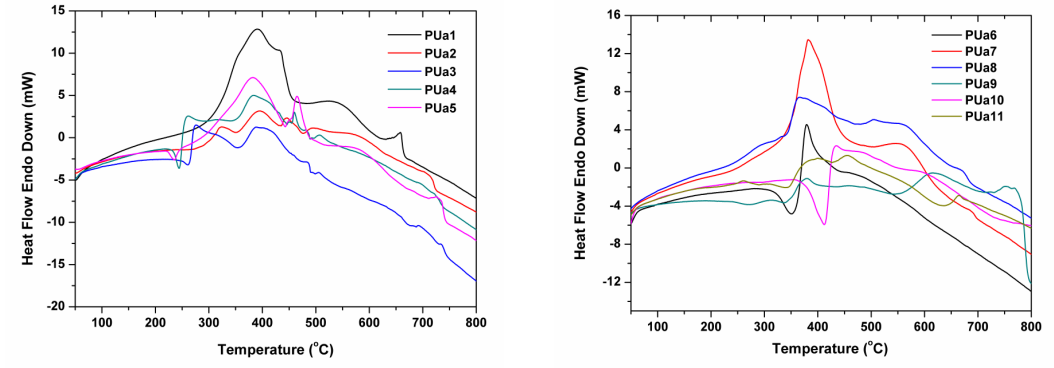


Fig. S5 DTA curves of the PUas.

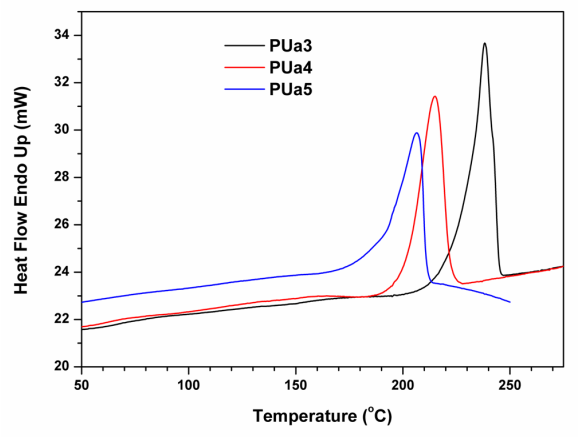


Fig. S6 The second heating runs of DSC curves of PUa3-PUa5.

Table S1. DFT calculations

Cartesian Coordinates of N, N'-dipropylurea calculated at the B3LYP/6-31G(d,p) levels of theory.

C	-0.00000500	-0.00012800	0.00096500
O	0.00001700	-0.00006300	1.22776200
N	1.15941400	-0.00084400	-0.75732800
N	-1.15950200	0.00085400	-0.75726000
H	1.07711700	-0.30200300	-1.71859200
H	-1.07721500	0.30269500	-1.71832400
C	2.45845300	-0.19892600	-0.12788500
C	3.53950000	0.69561400	-0.74088700
H	2.76823600	-1.25392800	-0.19166300
H	2.32113400	0.02767400	0.93173100
C	4.90913000	0.47963800	-0.09076800
H	3.61089300	0.49885800	-1.81997000
H	3.23008000	1.74230200	-0.63789000
H	4.87688500	0.70183000	0.98144900
H	5.24514100	-0.55737300	-0.20342500
C	-2.45834100	0.19952500	-0.12755300
C	-3.54046800	-0.69223500	-0.74265500
H	-2.76668800	1.25509000	-0.18911200
H	-2.32153000	-0.02948500	0.93160700
C	-4.90990600	-0.47588700	-0.09225800
H	-3.61147000	-0.49301300	-1.82131600
H	-3.23244900	-1.73955600	-0.64192200
H	-4.87811300	-0.70051000	0.97946600
H	-5.24453200	0.56181200	-0.20265300
H	-5.67025000	-1.11954500	-0.54490500
H	5.66869300	1.12530200	-0.54186700

Cartesian Coordinates of the dimmer of N, N'-dipropylurea calculated at the B3LYP/6-31G(d,p) levels of theory.

C	0.34836300	0.20443900	-0.19922700
O	0.75091600	0.55875600	0.90989600
N	0.72122100	-0.97650800	-0.79531000
N	-0.50911800	0.97870600	-0.96852700
H	0.41435200	-1.15397900	-1.74508500
H	-0.95122000	0.51575300	-1.75516300
C	1.71652000	-1.83679700	-0.18450300
C	3.16395300	-1.49542200	-0.57033700
H	1.49116600	-2.87489300	-0.46063100
H	1.60172900	-1.75003400	0.89979300
C	4.18231300	-2.43192200	0.08549400
H	3.26607600	-1.53817400	-1.66352400
H	3.35842000	-0.45857000	-0.27357900
H	4.11935200	-2.37962300	1.17816000
H	4.01110800	-3.47540200	-0.20501800
C	-1.20670300	2.09771300	-0.35394100
C	-2.44414500	1.70089500	0.46458500
H	-1.49134500	2.79959600	-1.14812000
H	-0.48900000	2.60563700	0.29587100
C	-3.14575900	2.91095800	1.08755600

H	-3.14482200	1.15330200	-0.18030500
H	-2.12388500	1.00586500	1.24857800
H	-2.47342900	3.45238200	1.76249800
H	-3.48188300	3.61784500	0.31942000
H	-4.02431700	2.60965500	1.66678600
H	5.20701600	-2.17306200	-0.19971600
H	-3.72590600	-4.39078700	-4.87255100
C	-3.65973500	-4.10605800	-5.92823800
C	-2.42720600	-3.23604300	-6.19042400
H	-4.58412300	-3.57759400	-6.18719300
H	-3.62717200	-5.02597200	-6.51935400
C	-2.44696700	-1.94051600	-5.37309600
H	-2.36993100	-2.99273900	-7.26061200
H	-1.51232300	-3.79013200	-5.94964600
N	-1.28696200	-1.09959200	-5.63770400
H	-3.37372500	-1.38404400	-5.57676100
H	-2.42988700	-2.15698600	-4.30297300
C	-0.52263700	-0.56223500	-4.63065500
H	-1.19929200	-0.70832300	-6.56427300
O	-0.73081200	-0.82189100	-3.43653700
N	0.47251000	0.28553500	-5.04933600
H	0.74401600	0.23922900	-6.02191700
C	1.47301300	0.81851200	-4.12714900
C	2.08731400	2.10993000	-4.67023600
H	2.26557400	0.07859000	-3.93687800
H	0.97728200	1.00741100	-3.17251700
C	3.14959900	2.68276000	-3.72802600
H	2.53669100	1.91859900	-5.65581000
H	1.28762800	2.84311500	-4.82990200
H	2.72279500	2.91222500	-2.74631900
H	3.97024500	1.97344000	-3.57495200
H	3.57774400	3.60495100	-4.13189000