

Polymorphism in parabanic acid-urea cocrystals governed by Supramolecular Synthons: A comparative analysis

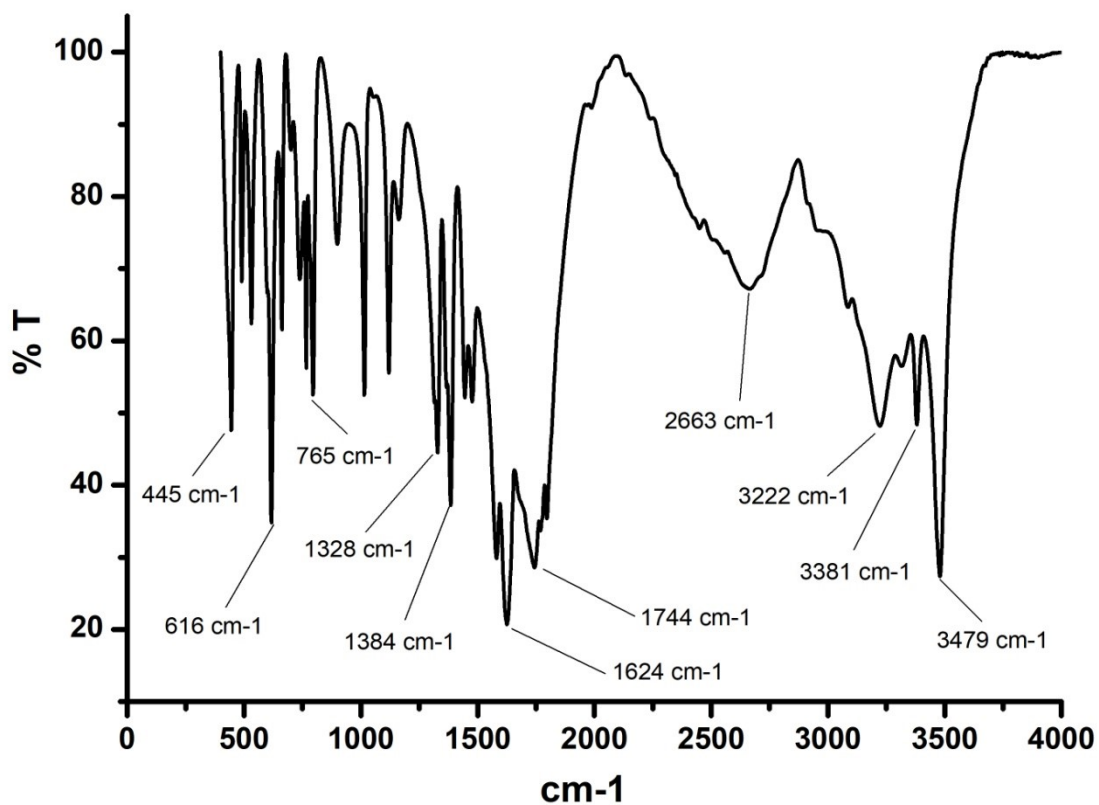
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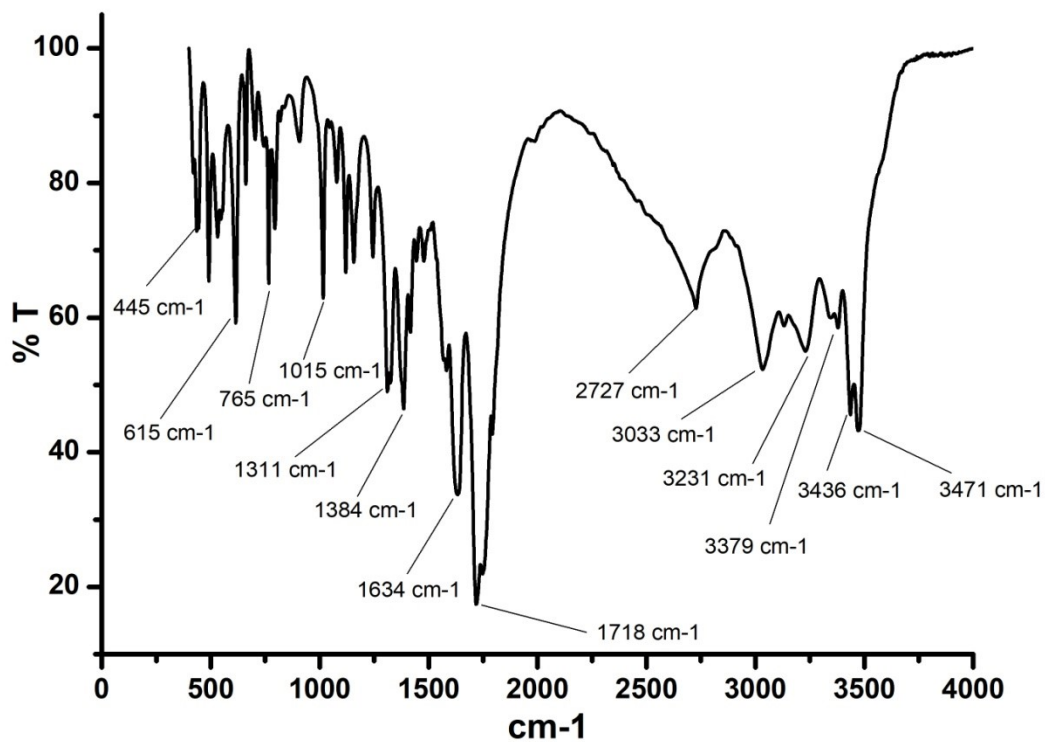
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SI 1

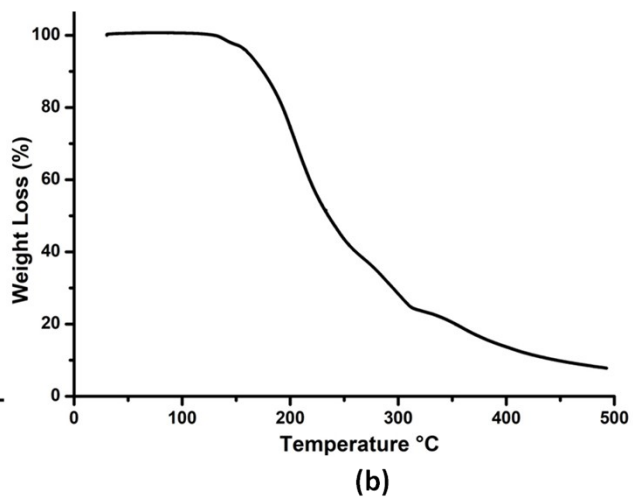
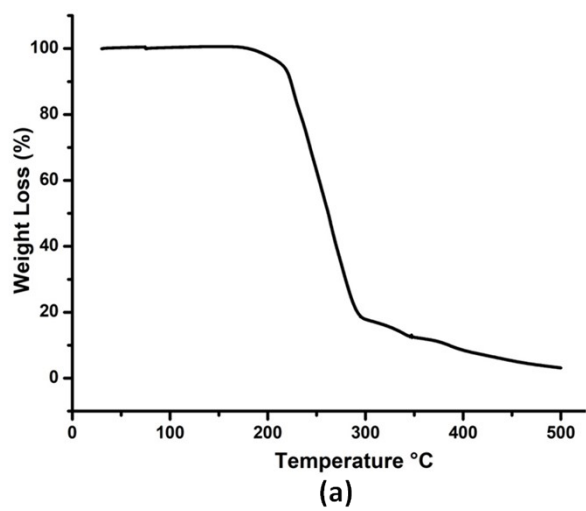


IR spectrum of *PA-UA Form I*



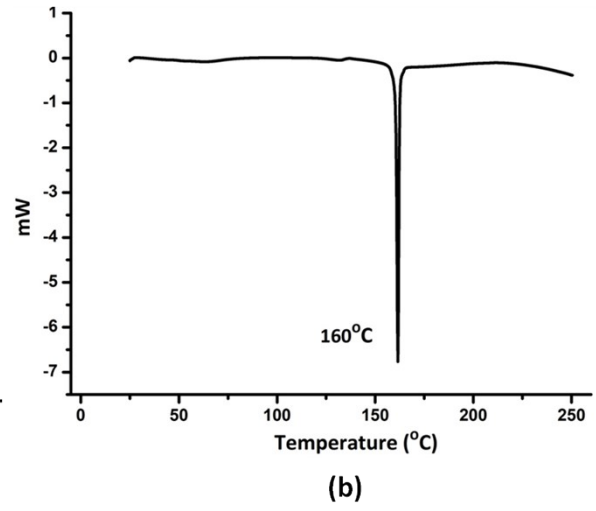
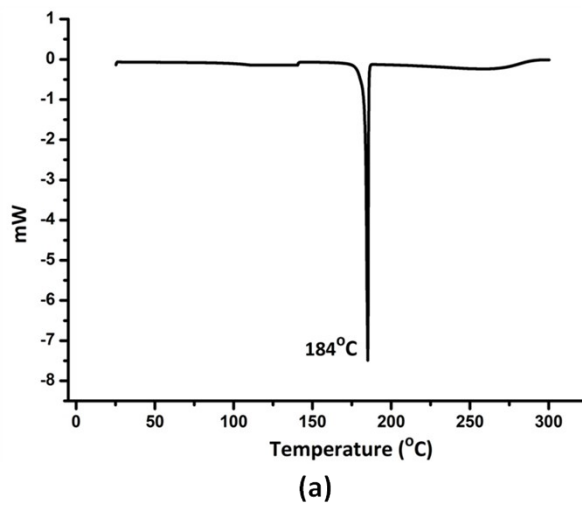
IR spectra of *PA-UA Form II*

SI 2



TGA of (a) *PA-UA Form I* (b) *PA-UA Form II*

SI3



DSC containing endothermic peak observed (a) *PA-UA Form I* (b) *PA-UA Form II*

SI 4

The interaction energies of the molecular pairs (kJ/mol) in *PA-UA Form I* and *Form II*.

N	Symmetry Operations	R(Å)	Electron Density	E _{ele}	E _{pol}	E _{dis}	E _{rep}	E _{tot}
PA-UA Form I								
1	-x, -y, -z	6.26	B3LYP/6-31G(d,p)	-5.4	-0.8	-5.7	3.2	-9.4
2	-x, y+1/2, -z+1/2	4.74	B3LYP/6-31G(d,p)	-24.7	-3.9	-14.3	19.6	-29.4
1	-x, -y, -z	5.77	B3LYP/6-31G(d,p)	-72.0	-15.7	-12.4	75.1	-52.1
1	-	7.71	B3LYP/6-31G(d,p)	8.5	-1.3	-5.9	0.9	3.5
2	x, y, z	5.58	B3LYP/6-31G(d,p)	8.5	-1.3	-5.9	0.9	3.5
2	x, -y+1/2, z+1/2	7.30	B3LYP/6-31G(d,p)	4.4	-0.6	-2.3	0.4	2.4
1	-	4.79	B3LYP/6-31G(d,p)	-5.4	-0.8	-5.7	3.2	-9.4
1	-	3.97	B3LYP/6-31G(d,p)	-0.2	-0.0	-0.2	0.0	-0.4
1	-	3.76	B3LYP/6-31G(d,p)	-72.0	-15.7	-12.4	75.1	-52.1
1	-	6.64	B3LYP/6-31G(d,p)	0.3	-0.0	-0.1	0.0	0.2
1	-	5.70	B3LYP/6-31G(d,p)	-24.7	-3.9	-14.3	19.6	-29.4
1	-	5.95	B3LYP/6-31G(d,p)	-24.7	-3.9	-14.3	19.6	-29.4
PA-UA Form II								
1	-	4.30	B3LYP/6-31G(d,p)	-1.8	-1.9	-10.3	4.6	-9.5
1	-x, -y, -z	7.22	B3LYP/6-31G(d,p)	-0.1	-0.6	-1.9	0.5	-1.9
2	-x, y+1/2, -z+1/2	5.89	B3LYP/6-31G(d,p)	-16.8	-4.9	-9.9	12.2	-22.5
1	-	6.23	B3LYP/6-31G(d,p)	-3.9	-2.3	-5.9	8.8	-5.4
1	-	5.52	B3LYP/6-31G(d,p)	-4.7	-0.8	-3.4	0.3	-8.4
1	-x, -y, -z	4.77	B3LYP/6-31G(d,p)	-2.3	-1.7	-14.9	8.2	-11.5
2	x, -y+1/2, z+1/2	5.49	B3LYP/6-31G(d,p)	-2.9	-1.5	-6.8	2.5	-8.6
1	-	5.59	B3LYP/6-31G(d,p)	-13.9	-5.3	-8.5	14.3	-17.1
1	-	3.55	B3LYP/6-31G(d,p)	-18.6	-6.7	-18.0	19.1	-28.5
1	-	4.86	B3LYP/6-31G(d,p)	2.9	-1.3	-8.0	3.7	-2.6
1	-	4.80	B3LYP/6-31G(d,p)	-90.4	-23.0	-12.3	89.3	-68.1
1	-	6.30	B3LYP/6-31G(d,p)	-14.2	-3.3	-4.4	18.1	-10.1

1	-x, -y, -z	6.13	B3LYP/6-31G(d,p)	-4.5	-0.5	-5.3	1.4	-8.9
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