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Thermodynamics Properties of 1,1-Carbonyldiimidazole (CDI) and 4-Imidazole Acrylic Acid, Obtained by DSC and Combustion Calorimetry

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Supplementary Information

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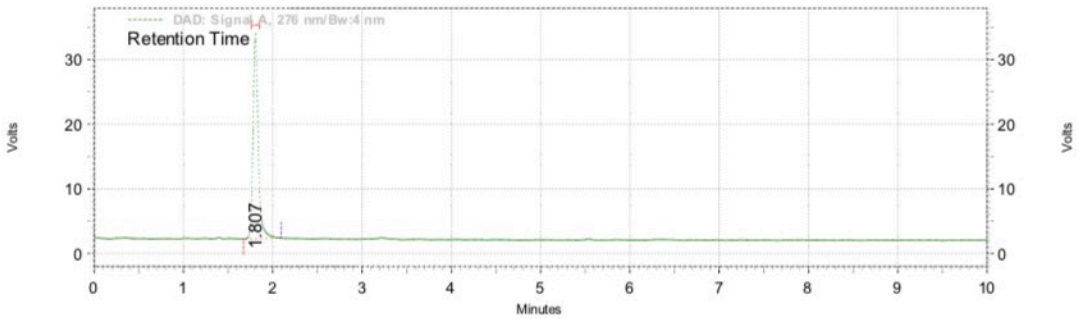
UCA purity chromatograms

Area % Report

Data File: C:\Users\admin\Desktop\RESULTADOS\chema puri y conc.rslt\027-Rep1.dat
Method: C:\Users\Public\Documents\Method\ACIDO IMIDAZOL ACRILICO BUFFER FOSFATOS.met

Acquired: 6/12/2019 8:50:55 AM (GMT -05:00)
Printed: 7/24/2019 4:27:34 PM (GMT -05:00)



DAD: Signal A, 276 nm/Bw:4 nm Results

Retention Time	Area	Area %	Height	Height %
1.807	266411	100.00	66404	100.00
Totals	266411	100.00	66404	100.00

J. Mex. Chem. Soc. **2020**, *64*(4)
Regular Issue

ISSN-e 2594-0317

Normalization Report **Page 1 of 1**

Method Name: C:\Users\Public\Documents\Method\ACIDO IMIDAZOL ACRILICO BUFFER FOSFATOS.met

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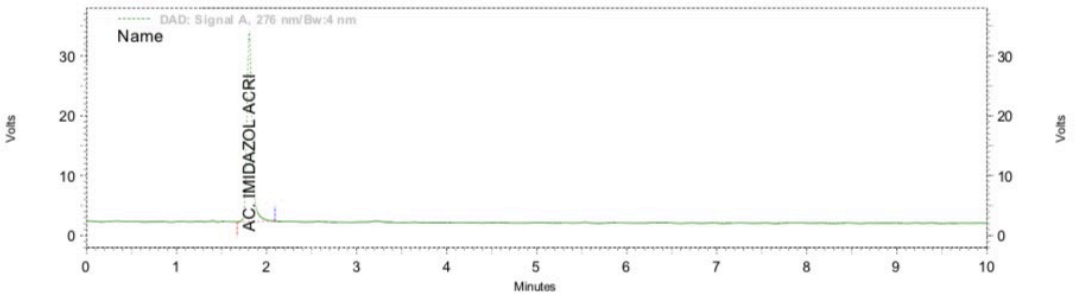

DAD: Signal A, 276 nm/Bw:4 nm Results

Pk #	*Name*	*Retention Time*	*Area*	*Concentration*
1	AC. IMIDAZOL ACRI	1.807	266411	**0.000**
Totals			266411	**0.000**

DSC results of CDI

Number	**Compound**	**purification method**	**Purity**	$\Delta_{fus}H$	T_{fus}
			x	**KJ·mol^{-1}**	**K**
1	CDI purificado	Sublimation	99.96	24.87	363.23
2	CDI purificado	Sublimation	99.97	25.06	361.53
3	CDI purificado	Sublimation	99.98	24.69	362.37
4	CDI purificado	Sublimation	99.98	24.59	361.66
		mean	99.97	24.80 ± 0.46	361.95 ± 0.93

J. Mex. Chem. Soc. **2020**, *64*(4)
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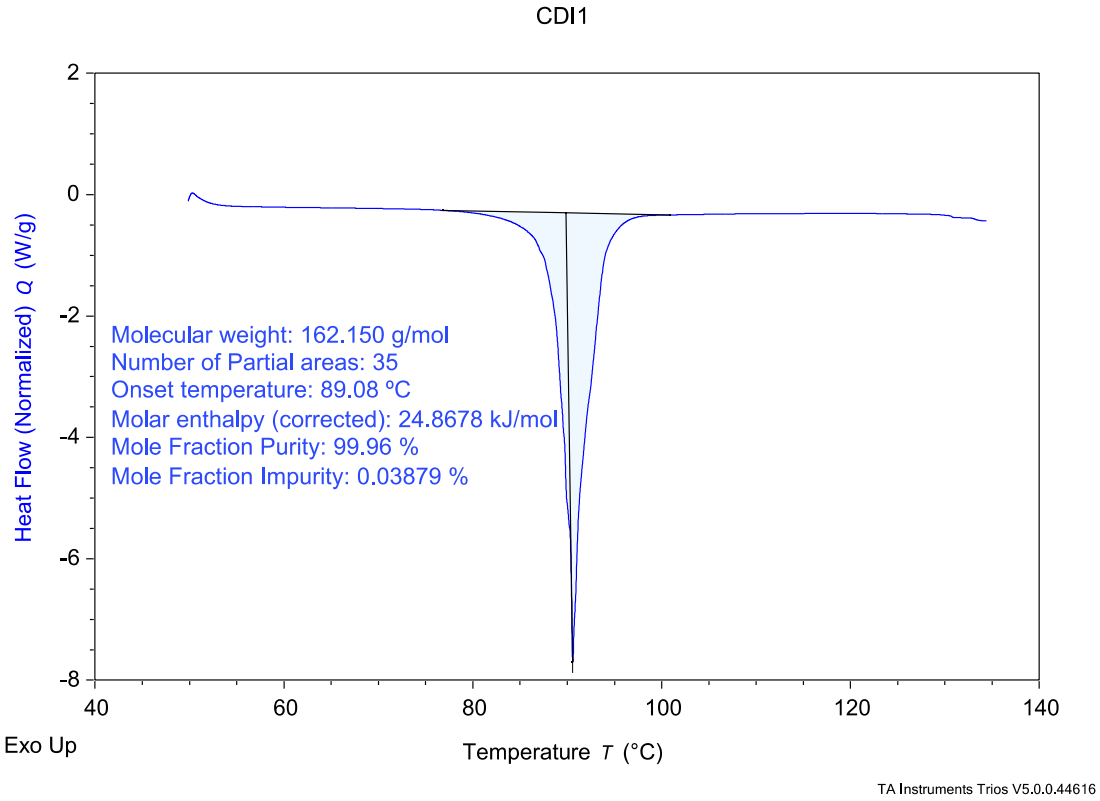
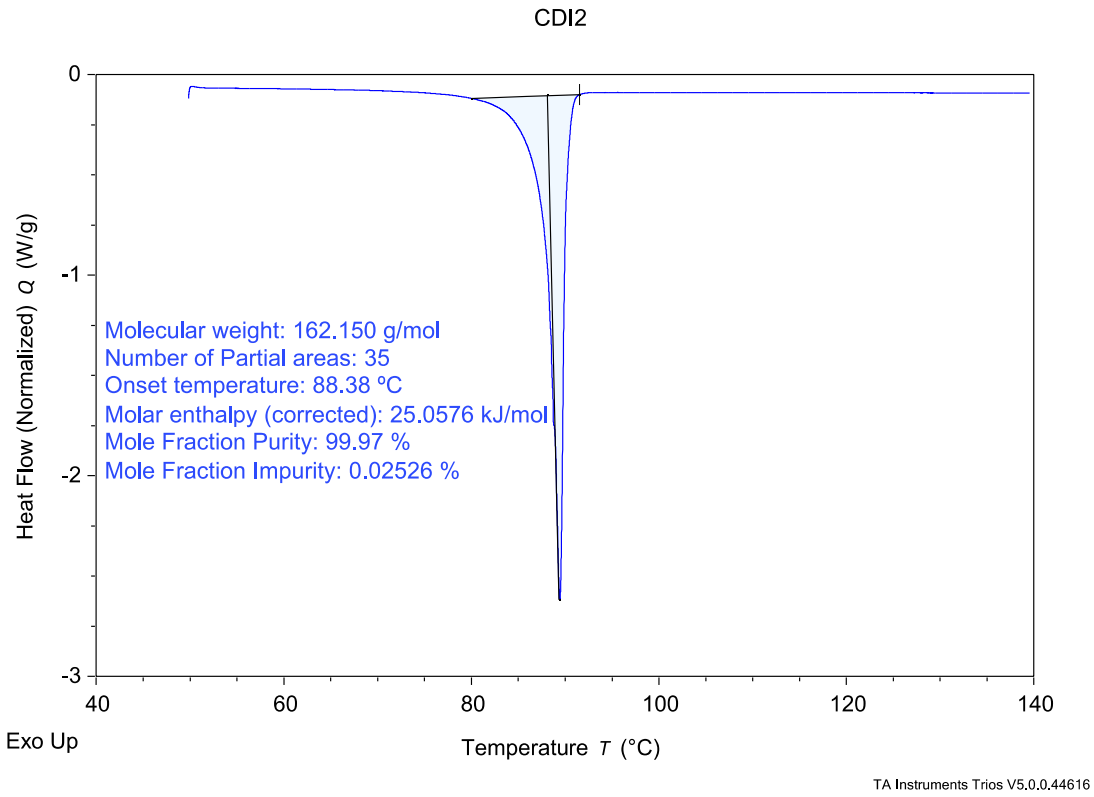
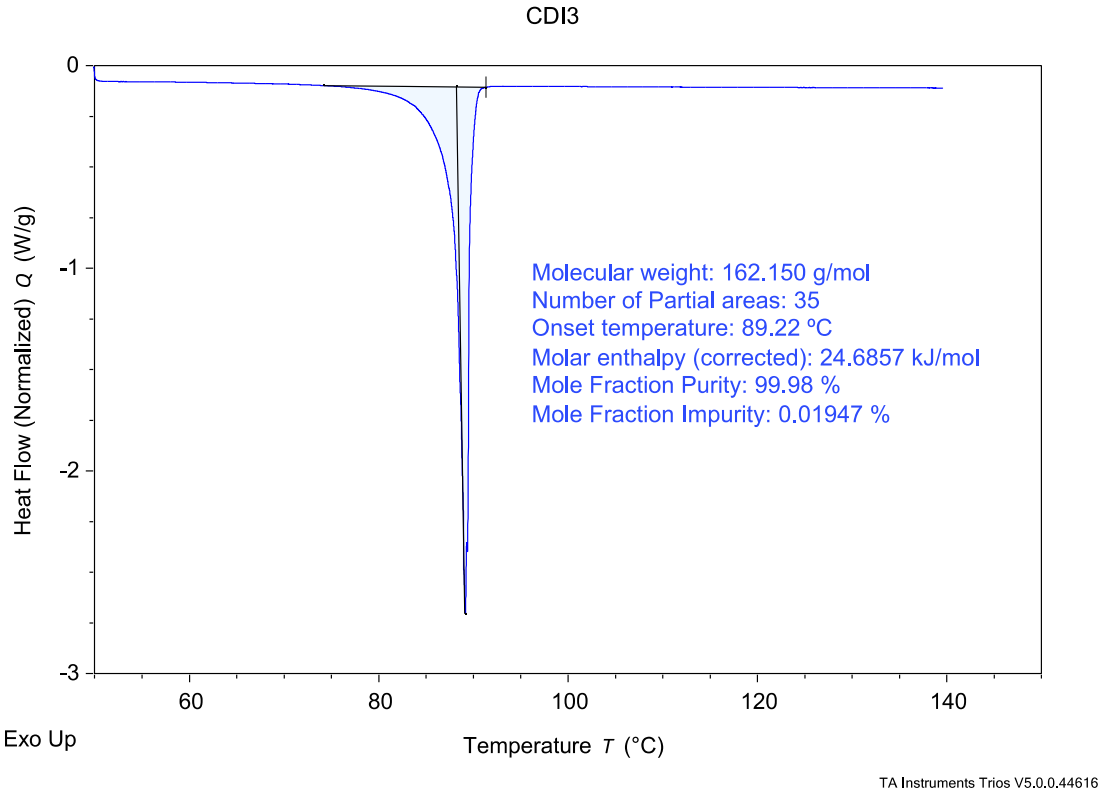
Thermograms of CDI



J. Mex. Chem. Soc. **2020**, *64*(4)
Regular Issue

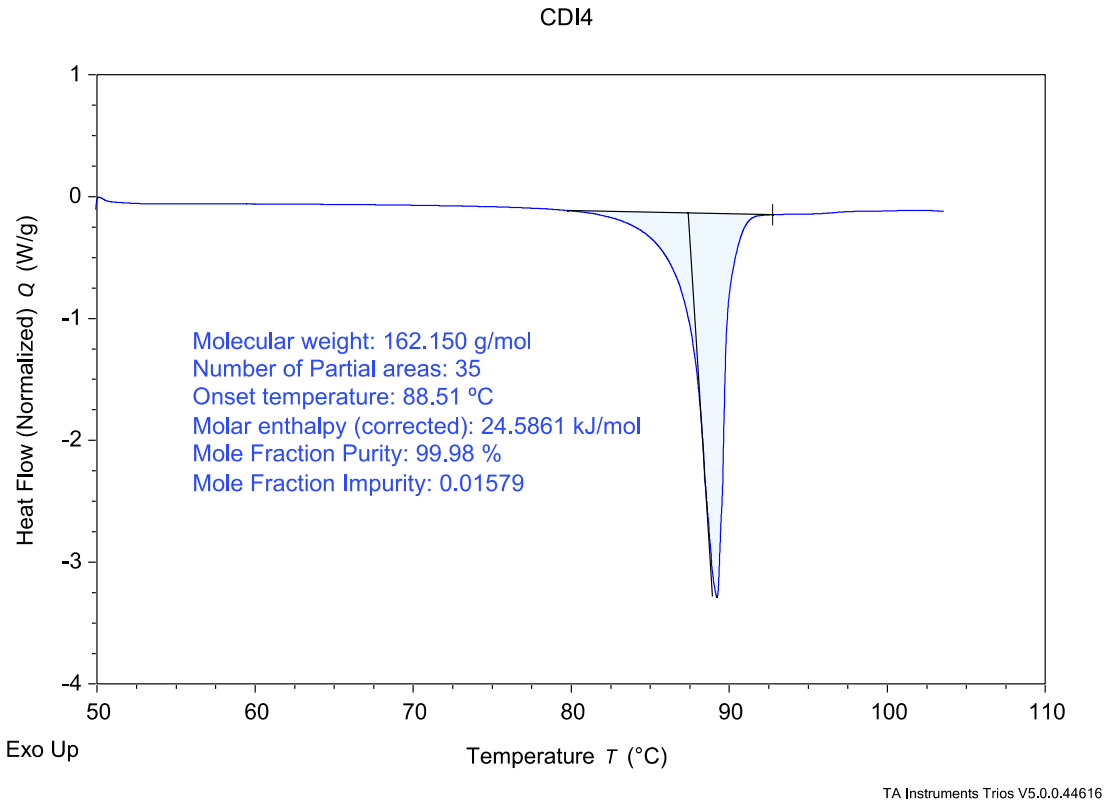
ISSN-e 2594-0317





J. Mex. Chem. Soc. **2020**, *64*(4)
Regular Issue

ISSN-e 2594-0317



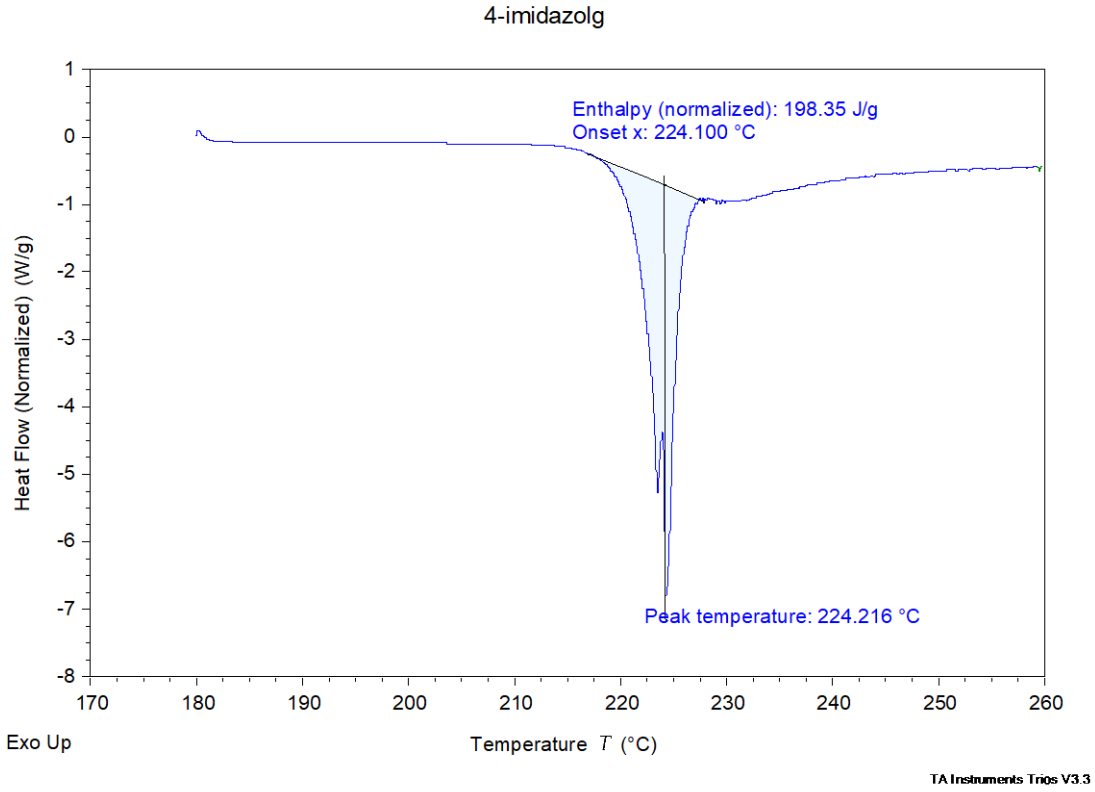
DSC results of UCA

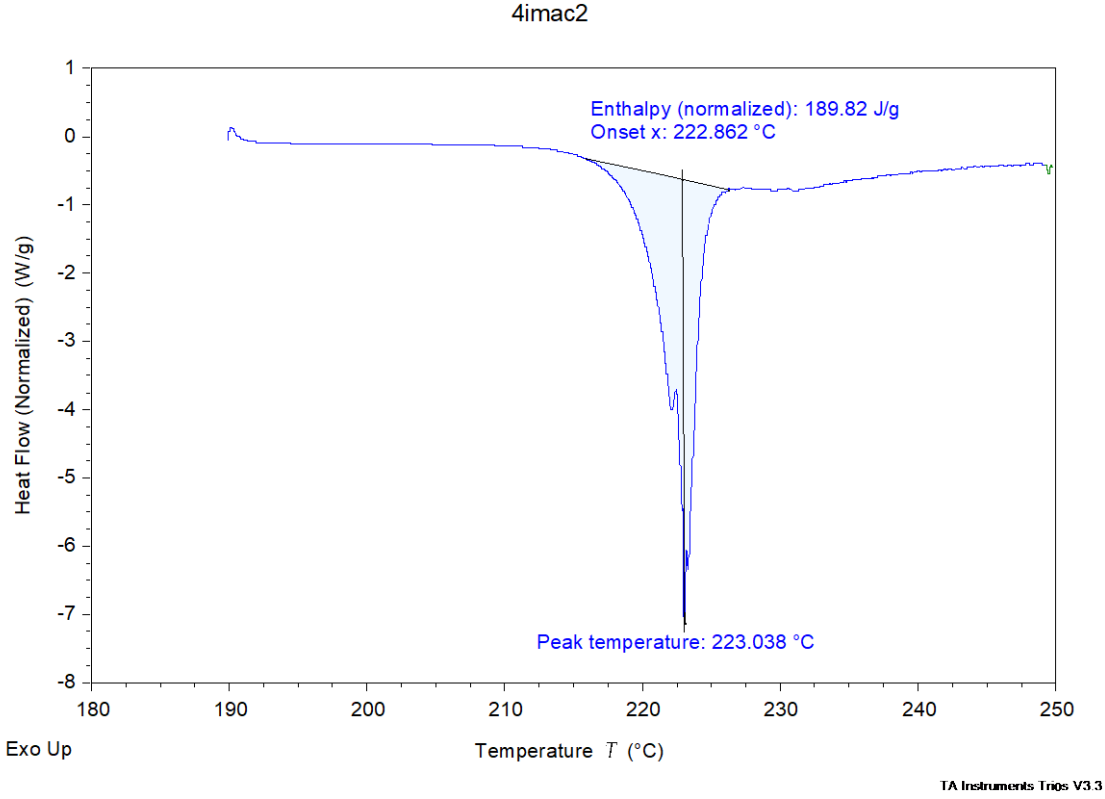
Number	Compound	$\Delta_{fus}H$	T_{fus}
		KJ·mol^{-1}	K
1	UCA	27.40	497.25
1	UCA	26.22	496.01
2	UCA	26.24	496.42
3	UCA	26.12	495.91
	mean	26.49 ± 1.35	496.40 ± 1.36

J. Mex. Chem. Soc. **2020**, *64*(4)
Regular Issue

ISSN-e 2594-0317

Termograms of UCA





J. Mex. Chem. Soc. **2020**, *64*(4)
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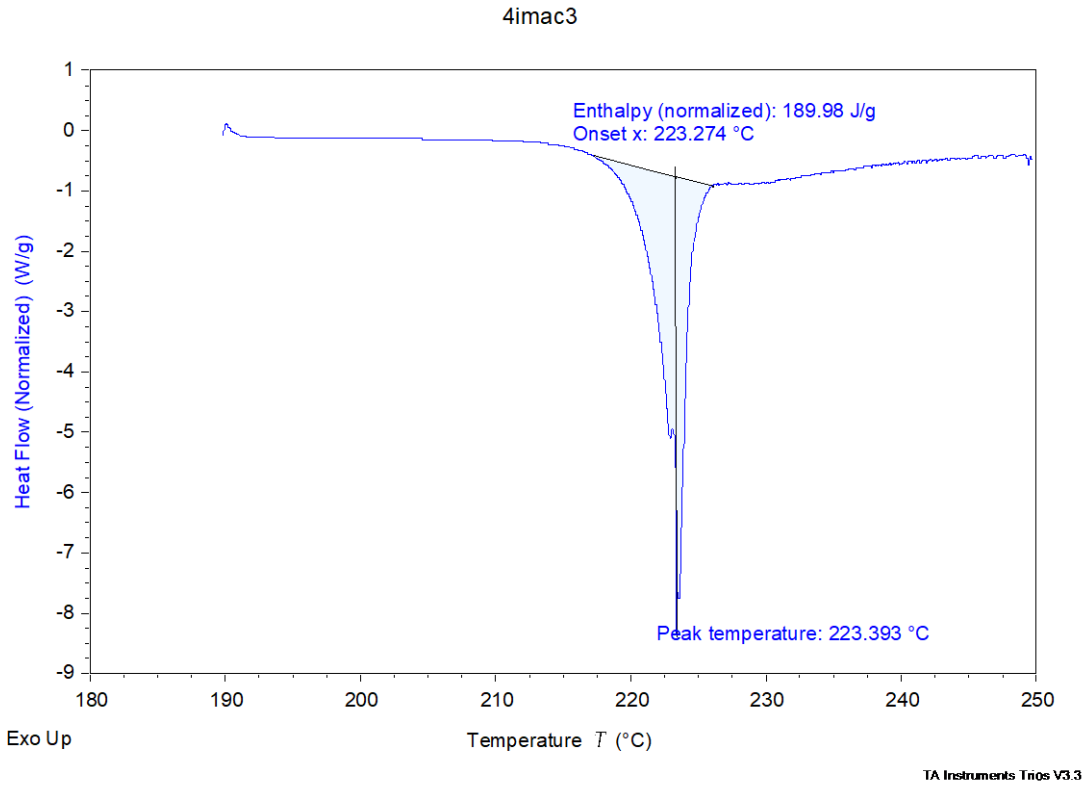

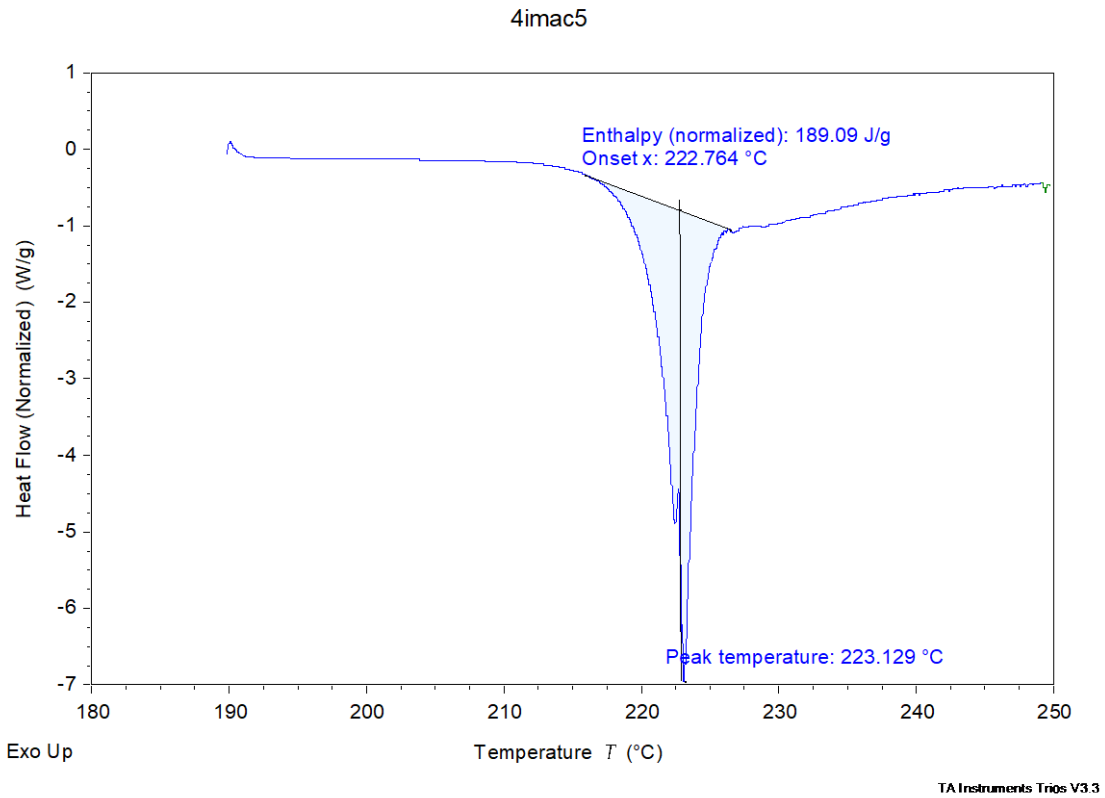

J. Mex. Chem. Soc. **2020**, *64*(4)
Regular Issue

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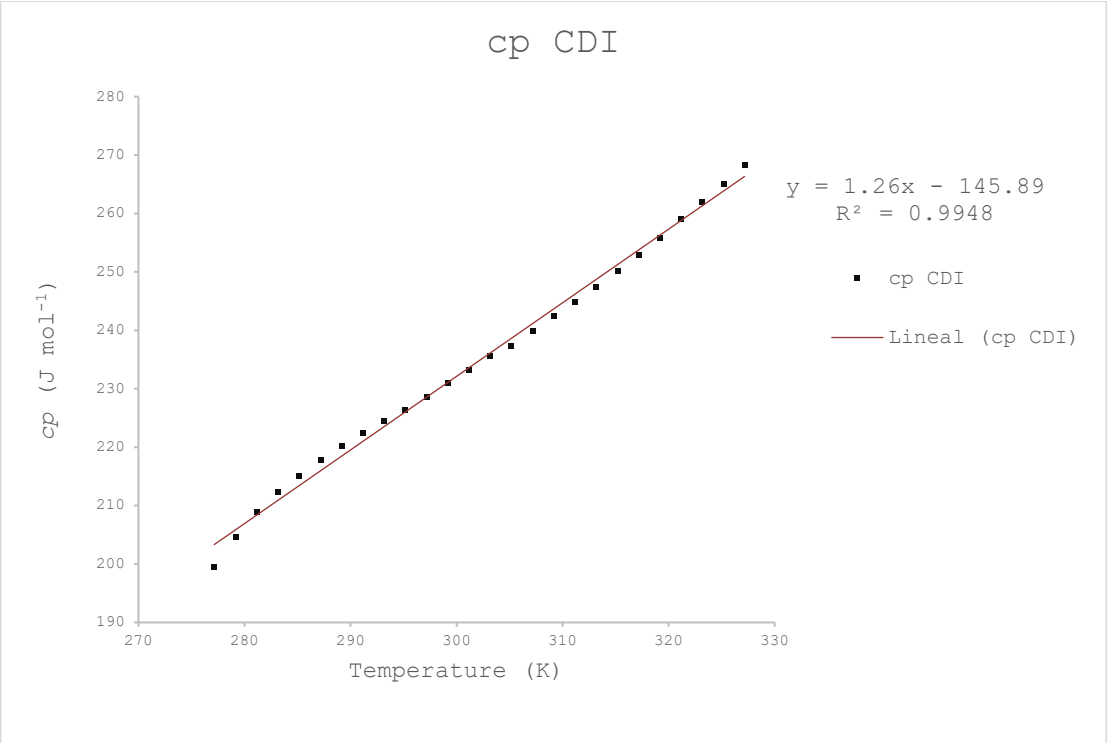
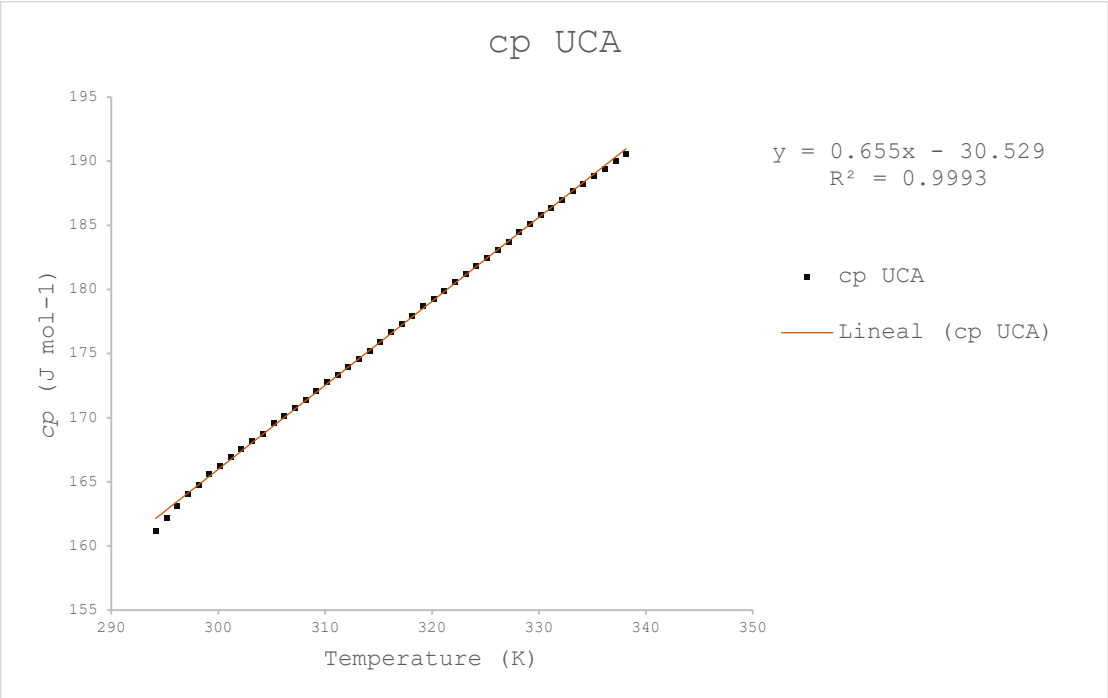
Graphs of cp of CDI and UCA





J. Mex. Chem. Soc. **2020**, *64*(4)
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Combustion calorimetry

Calibration results of the combustion calorimeter performed by combustion of benzoic acid

Benzoic acid							
Experimento	**1**	**2**	**3**	**4**	**5**	**6**	**7**
***m*(benzoic acid)/g**	0.9428	0.9818	0.9638	1.0216	0.9771	1.0216	1.0114
***m*(cotton)/g**	0.0066	0.0065	0.0065	0.0066	0.0071	0.0064	0.0048
***m*(platinum)/g**	9.8301	9.8302	9.8298	9.8303	9.8304	9.8297	9.8343
ΔT_c/K	2.5525	2.6583	2.6064	2.7627	2.6446	2.7601	2.7305
ε(cont)(-ΔT_c)/kJ	0.0418	0.0440	0.0429	0.0458	0.0437	0.0459	0.0446
ΔU_{ign}/kJ	0.0042	0.0042	0.0042	0.0042	0.0042	0.0042	0.0042
-ΔU_{IBP}/kJ	25.0333	26.0638	25.5874	27.1158	25.9489	27.1137	26.8185
-$m\Delta_c U°$(cotton)/kJ	0.1124	0.1100	0.1109	0.1112	0.1207	0.1083	0.0822
-$\Delta_c U°$(benzoic acid)/kJ g^{-1}	24.9209	25.9538	25.4766	27.0046	25.8282	27.0054	26.7363
ε(calor)(-ΔT_c)/kJ	24.9957	26.0240	25.5487	27.0742	25.9094	27.0721	26.7780
ε (calor) / kJ K^{-1}	9.7926	9.7896	9.8022	9.7998	9.7971	9.8084	9.8069
ε (calor) / *cal* K^{-1}	2340.48	2339.78	2342.78	2342.21	2341.56	2344.26	2343.92
ε (calor) / kJ K^{-1} = 9.7995 ± 0.0031							

Note. The uncertainty associated with the energy equivalent represents the standard error.

Combustion results of cotton

cotton					
Experiment	**1**	**2**	**3**	**4**	**5**
***m*(cotton)/g**	0.9735	1.1261	0.9853	0.9977	0.9923
***m*(platinum)/g**	9.8300	9.8304	9.8297	9.8304	9.8308
T_i /K	296.7020	296.6490	296.646	296.663	296.6672
T_f/K	298.4924	298.6957	298.4627	298.4877	298.5039
ΔT_{corr}/K	0.1091	0.1020	0.1158	0.1012	0.1283
ΔT_c/K	1.6813	1.9446	1.7012	1.7231	1.7084
ε^i(cont)/kJ K^{-1}	0.0545	0.0548	0.0546	0.0546	0.0546
ε^f(cont)/kJ K^{-1}	0.0530	0.0533	0.0530	0.0530	0.0530
-ΔU_{IBP}/kJ	16.5626	19.1583	16.7589	16.9748	16.8303
ΔU_{ign}/kJ	0.0042	0.0042	0.0042	0.0042	0.0042
$\Delta U_{\sum}$/kJ	0.0244	0.0286	0.0247	0.0251	0.0249
-$m\Delta_c U°$(cotton)/kJ g^{-1}	16.99	16.99	16.98	16.99	16.94
-$m\Delta_c U°$(cotton)/kJ mol^{-1}	461.47	461.47	461.20	461.47	460.11
-$m\Delta_c U°$(cotton)/kJ mol^{-1} = 461.14 ± 0.60					

Note. The uncertainties associated with each average value of specific combustion energy is the standard uncertainty.