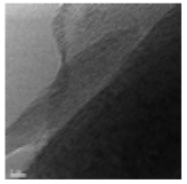
Nicanite®

Carbodeon uses its patented production technology to make Nicanite®. This high purity, graphitic carbon nitride offers new and rapidly emerging applications technology.



Micrograph showing graphitic carbon nitride layer structure

As thin films, Nicanite® produces hard, wear resistant coatings which can be made optically transparent. Films can be formed using Carbodeon's PVD Targets and are best produced using Picodeon Coldab® laser deposition or other PLD technologies. As a bulk material, Nicanite® is photoluminescent.

Further fundamental properties include:

- inertness, non-toxicity
- temperature stability to 650°C under inert atmosphere
- high optical band gap
- dielectric

Coatings properties can be adapted by the use of composites, such as with boron carbide and boron nitride to increase hardness. Carbodeon is actively developing these innovative coating materials – see PVD Targets.

Analysis of Carbodeon's Nicanite®

4th of March, 2013
Cooper Group, Group meeting

Dr. Michael J. Bojdys

University of Liverpool
m.j.bojdys.02@cantab.net
http://mjbojdys.blogspot.com/

Nicanite® graphitic carbon nitride powder

Grade A, as received from the synthesis (unground)

Chemical Formula	$C_3N_{4+x}H_y$
Chemical purity	≥ 99.5 wt.%
Color	yellow brownish
Density	2.336 g/cm^3
Particle size, d_{50}	> 30 microns
Specific surface area	> 35 m^2/g
Thermal conductivity*	1.25 W/mK
Temperature stability	
○ In inert atmosphere	650 °C
○ In air	N.A.
○ In vacuum	N.A.
Moisture content	≤ 4 wt.%

*measured from a sintered compact with approximately 80% theoretical density

Carbodeon
SUPERHARD NANOMATERIALS

Carbodeon Ltd Oy
Pakkalankuja 5
FI-01510 Vantaa, Finland

Tel. +358 50 5678 828

www.carbodeon.com

Nicanite® – Powder X-Ray Diffraction

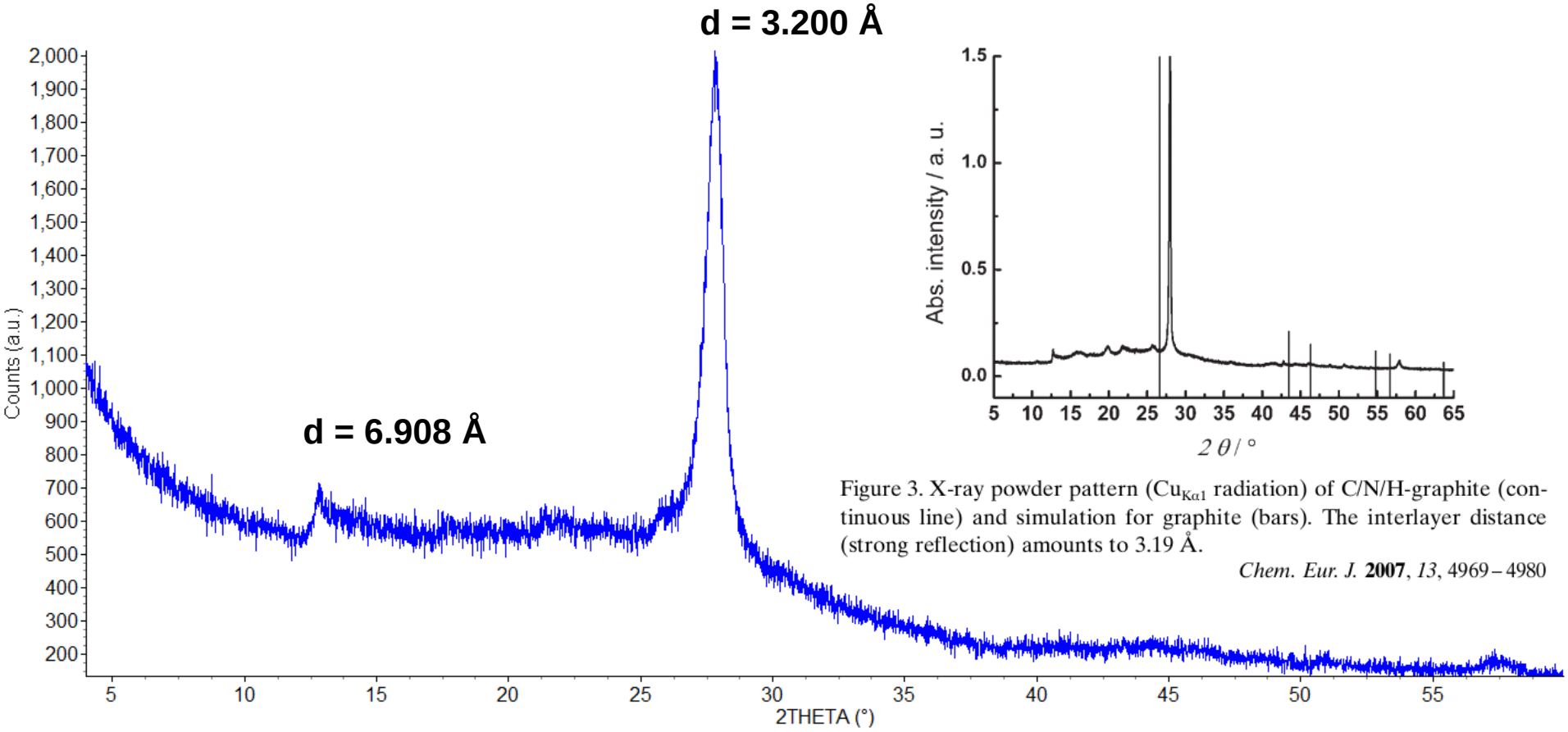


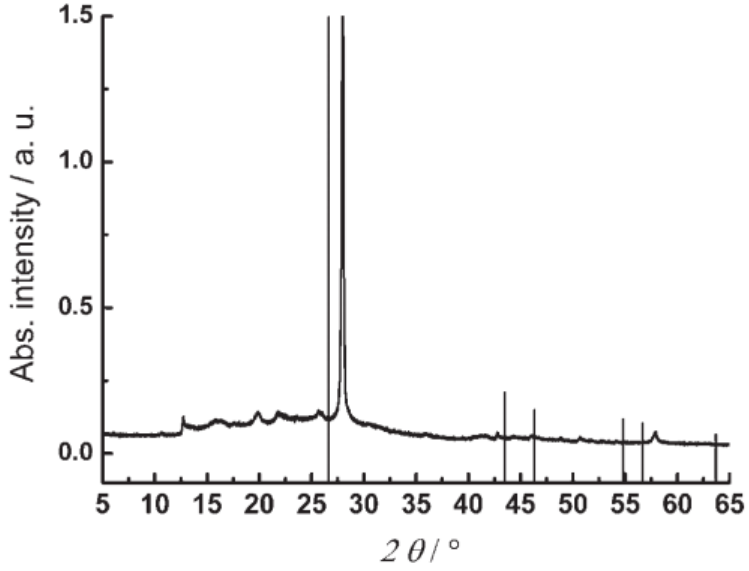
Figure 3. X-ray powder pattern ($Cu_{K\alpha1}$ radiation) of C/N/H-graphite (continuous line) and simulation for graphite (bars). The interlayer distance (strong reflection) amounts to 3.19 Å.

Chem. Eur. J. **2007**, *13*, 4969 – 4980

Instrument:
Bruker D8 Advance
capillary stage
Cu Kα1 radiation

PXRD profile matches Melon as published in e.g. *Chem. Eur. J.* **2007**, *13*, 4969-4980.

Powder X-Ray Diffraction



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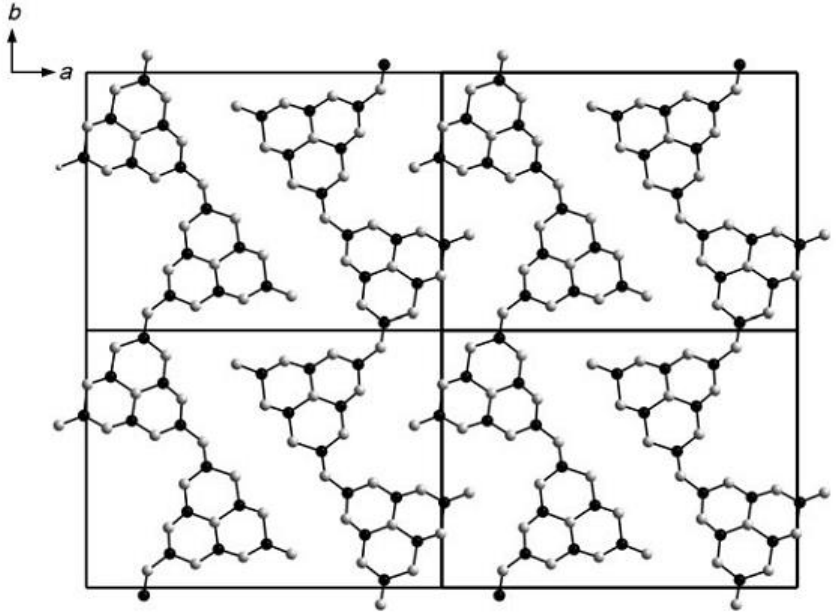
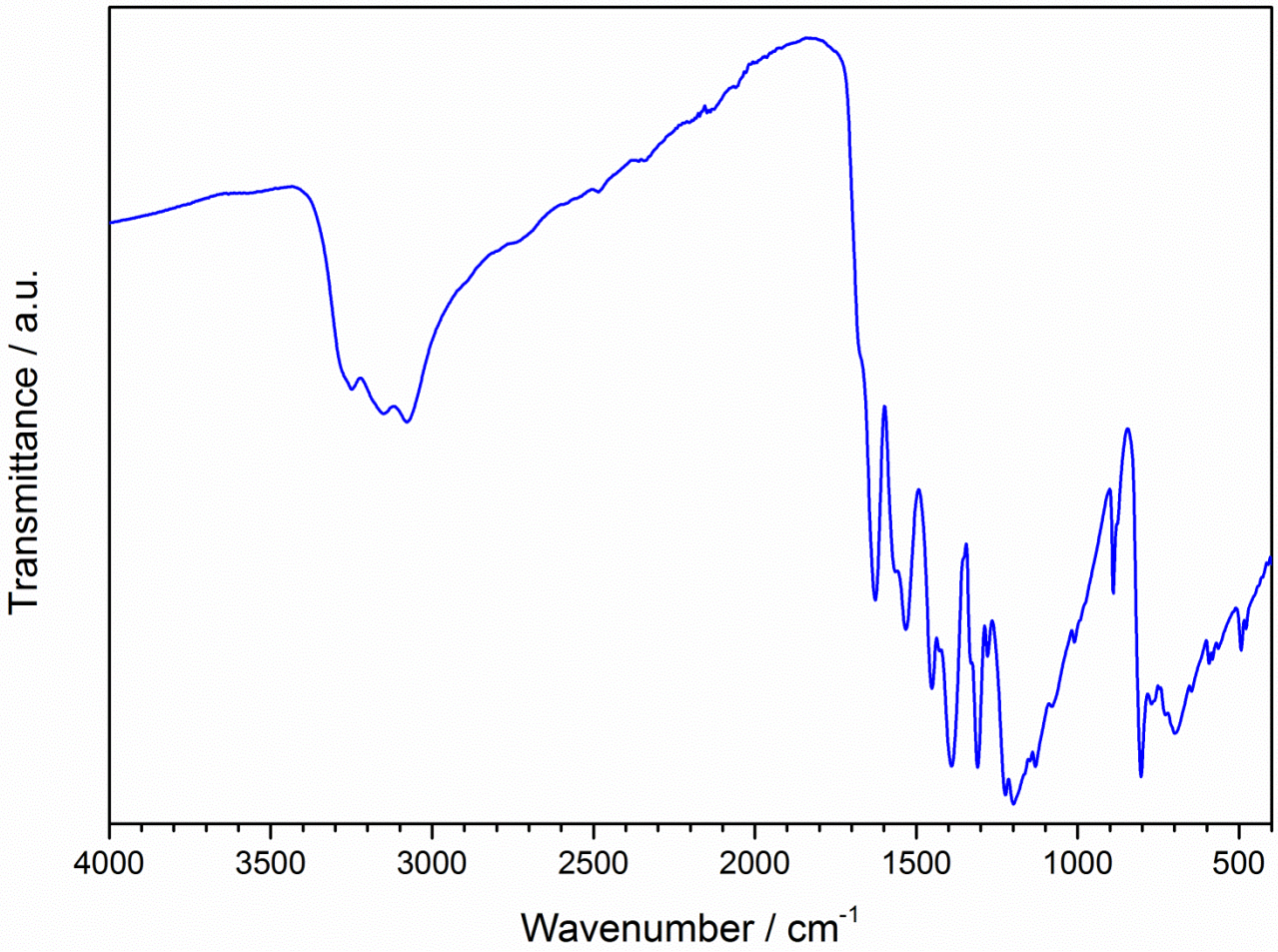


Figure 12. Projection of the structure of melon. Hydrogen atoms and molecular fragments from adjacent strands are omitted for clarity; black: C, gray: N.

Suggested structure for Melon are NH-bridged heptazine units as seen in Figure 12 above.

Nicanite® – ATR-FT Infrared Spectroscopy



ATR-FT IR spectrum shows prominent NH and NH_2 signals around 3300-3100 cm^{-1}.

ATR-FT Infrared Spectroscopy

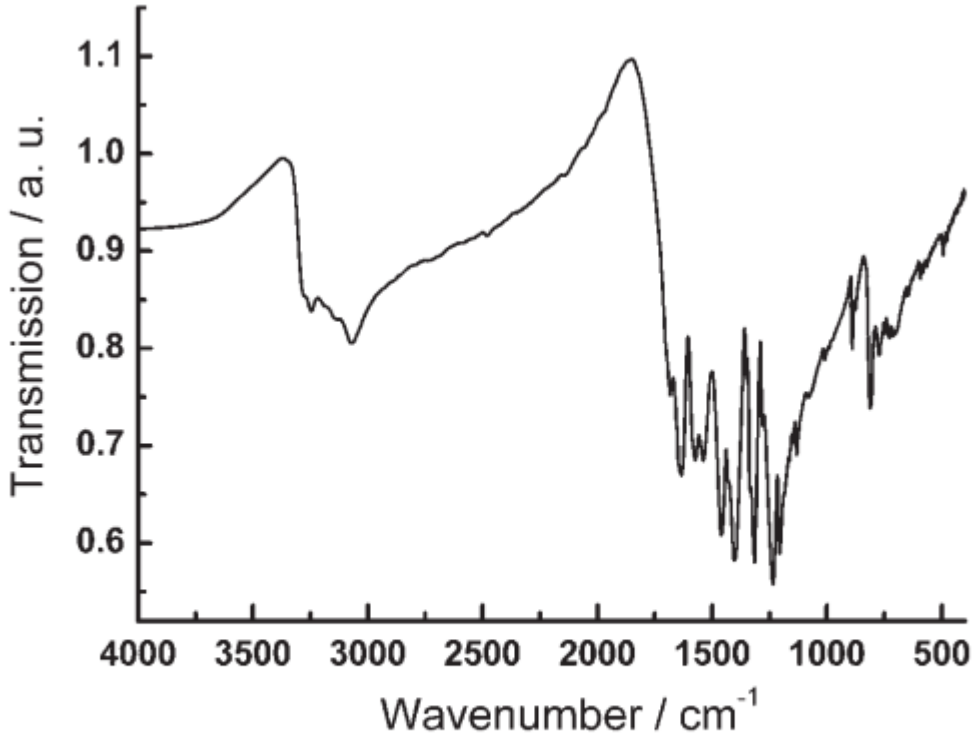
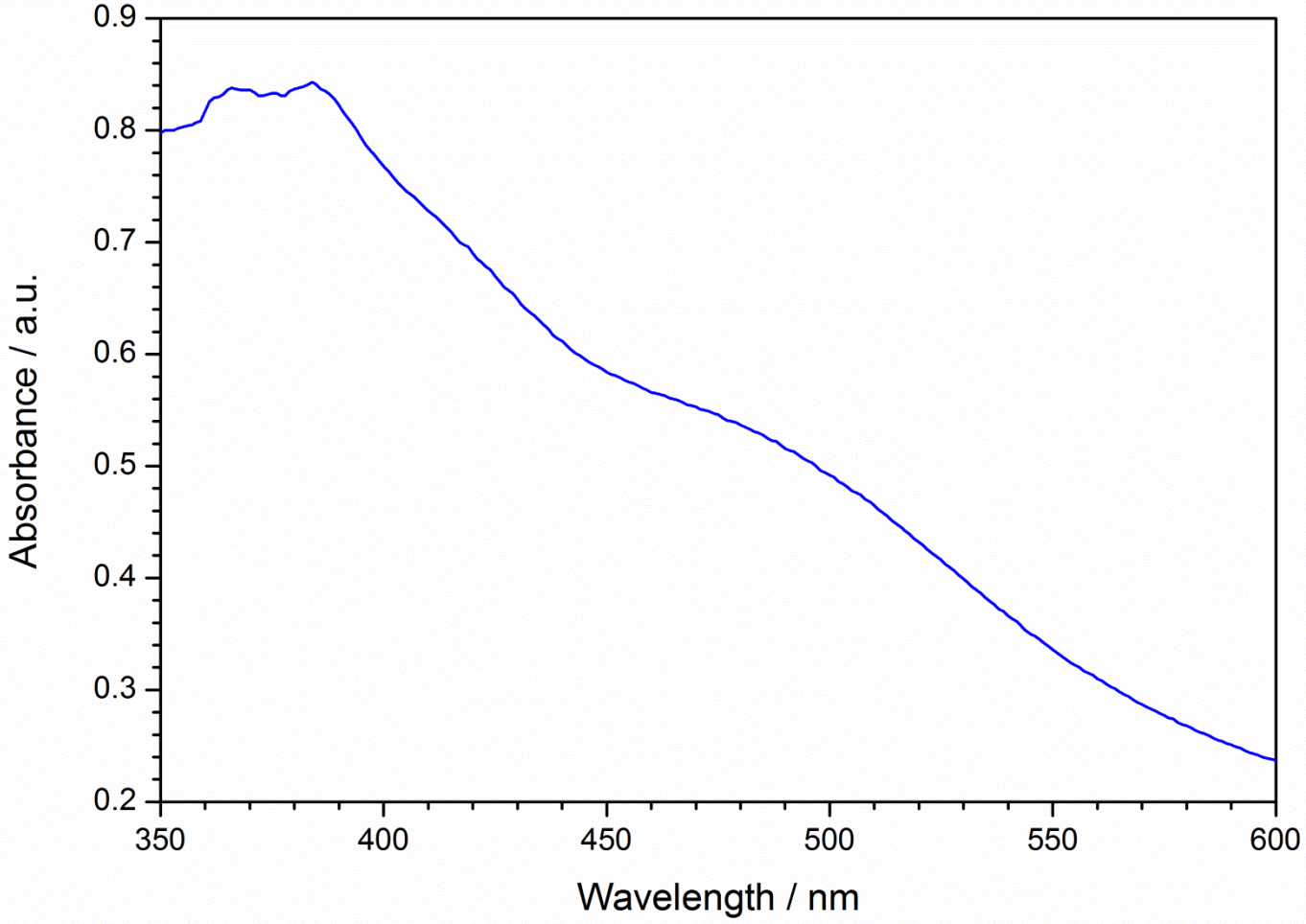


Figure 1. FTIR spectrum of melon recorded as a KBr pellet between 400 and 4000 cm^{-1}.

Chem. Eur. J. **2007**, *13*, 4969 – 4980

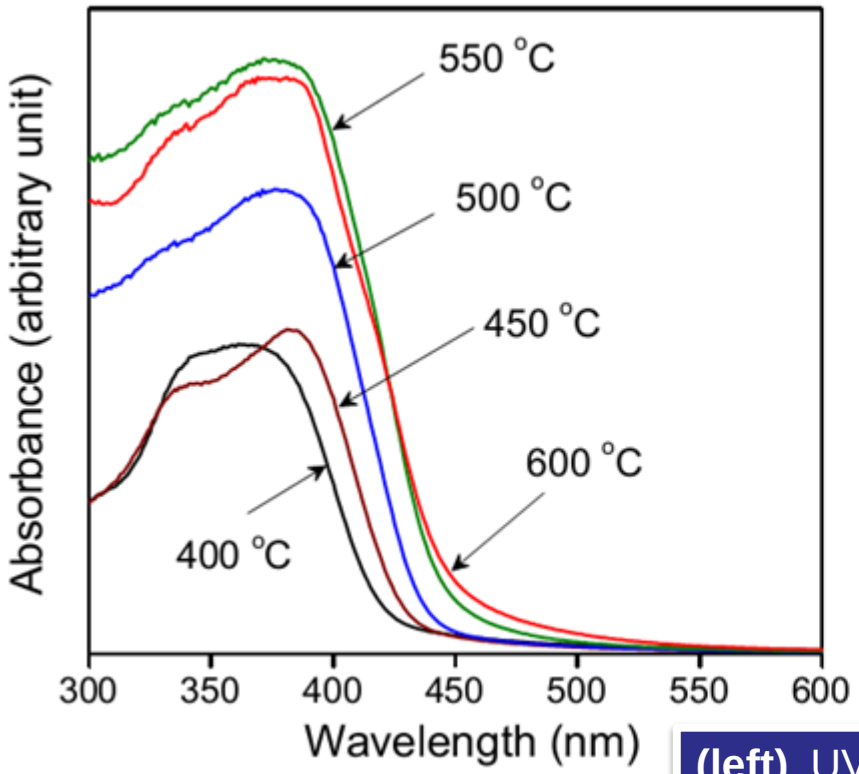
ATR-FT IR spectra of Melon and Nicanite show a similar content of NH and NH_2 groups.

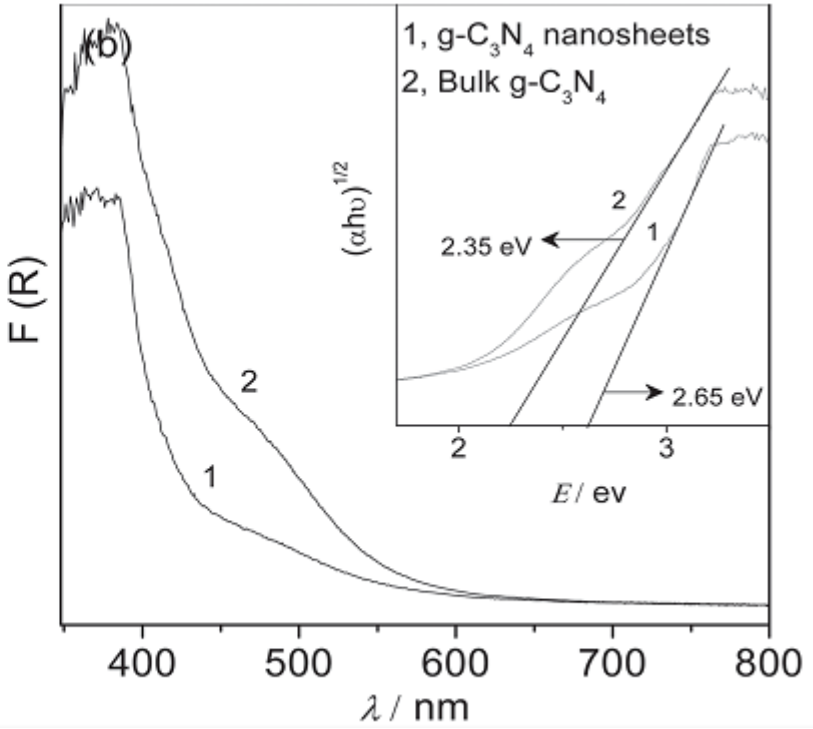
Nicanite® – UV/Vis Spectroscopy



UV/Vis spectrum shows max. absorbance at 390 nm, tailing off at ~550 nm.

UV/Vis Spectroscopy



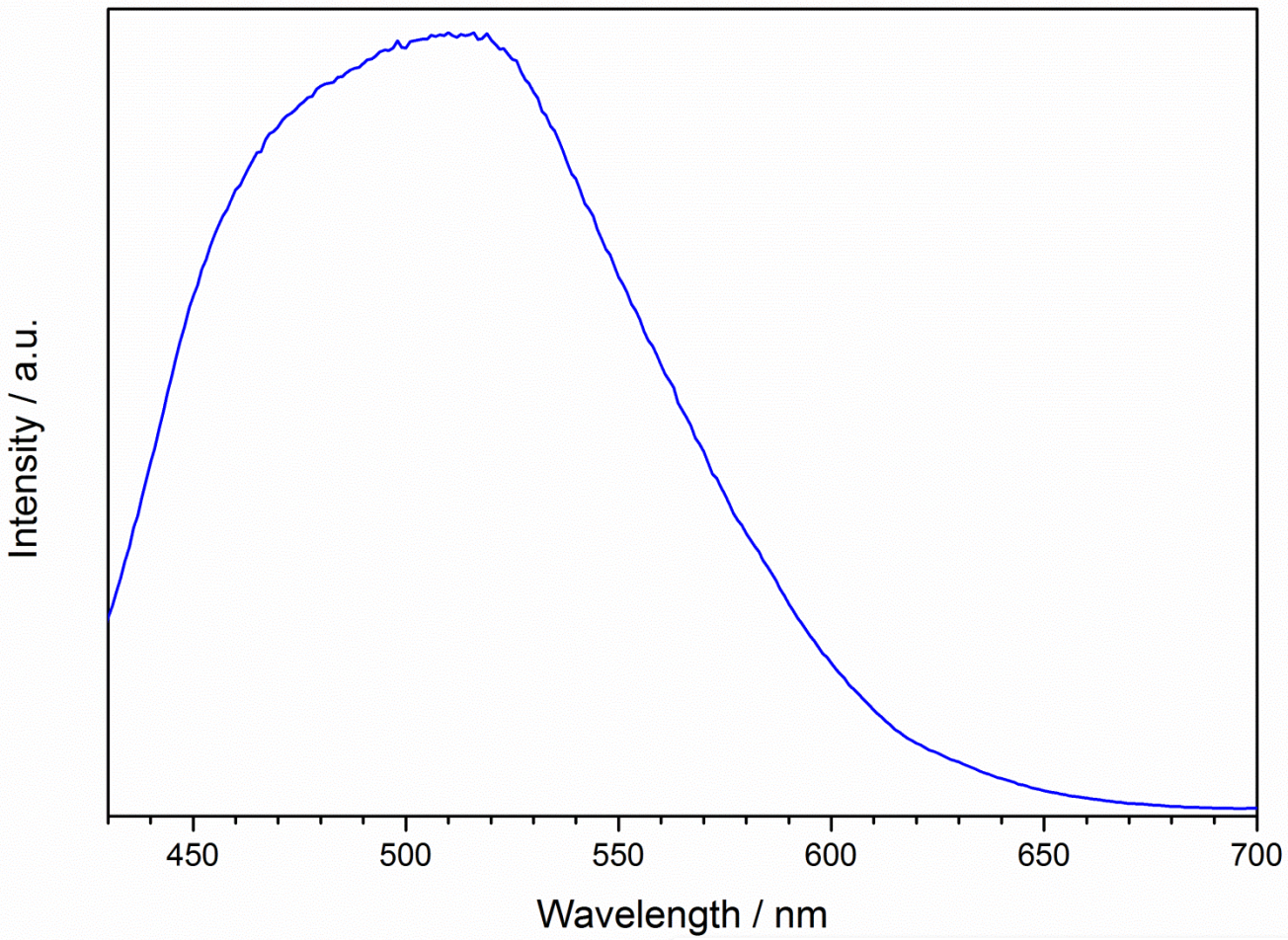


(left) UV/Vis spectra (DCDA treated at T for 16 h) show similar max. absorbance. (*Nat. Mater.* **2009**, *8*, 76-80)

(right) UV/Vis spectra of Nicanite® from Adv. Mater. 2013, DOI: 10.1002/adma.201204453

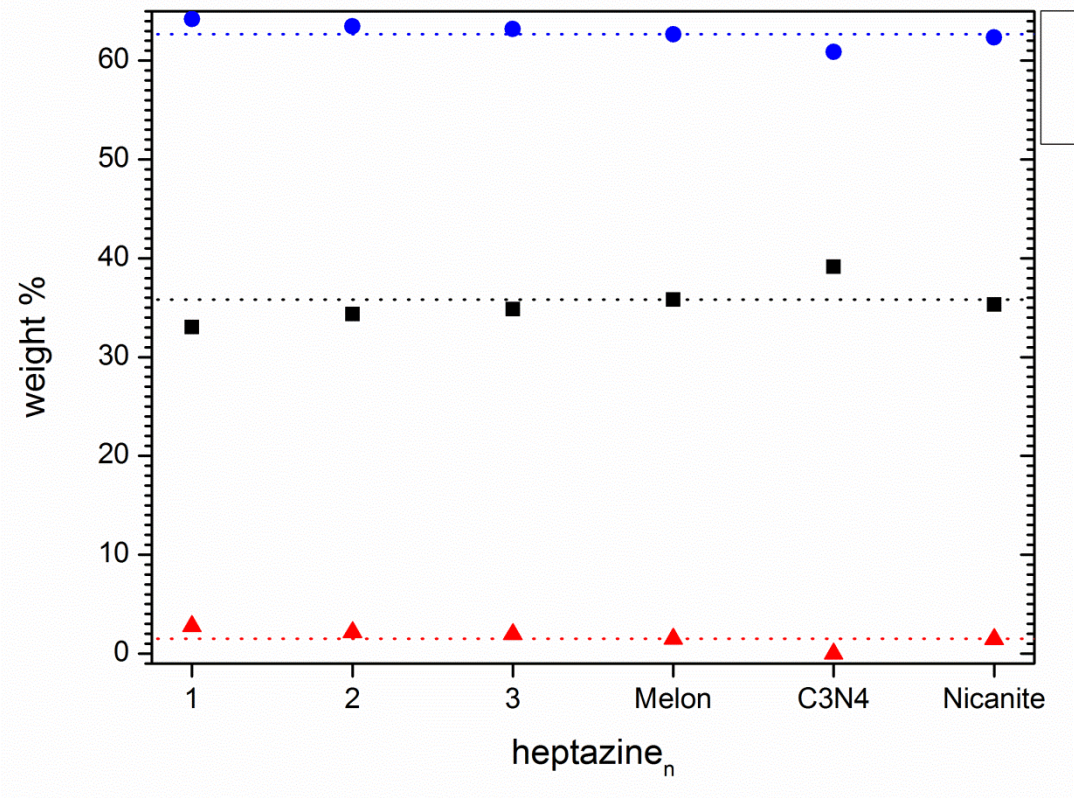
Tail at ~500-550 nm is probably an effect of bulk packing.

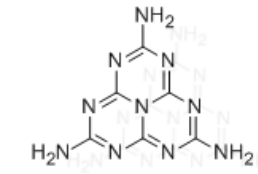
Nicanite® – Photoluminescence Spectroscopy



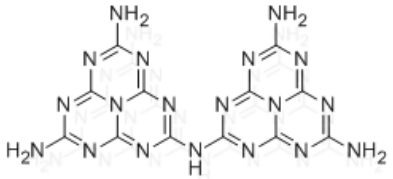
PL spectrum shows max. emission at around 520 nm (excitation at 390 nm) .

Nicanite® – C, H, N Elemental Analysis

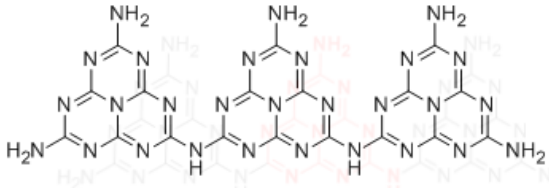




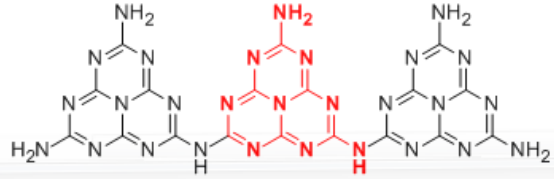
Chemical Formula: $C_6H_6N_{10}$
Elemental Analysis: C, 33.03; H, 2.77; N, 64.20



Chemical Formula: $C_{12}H_9N_{19}$
Elemental Analysis: C, 34.37; H, 2.16; N, 63.47



Chemical Formula: $C_{18}H_{12}N_{28}$
Elemental Analysis: C, 34.84; H, 1.95; N, 63.21



Chemical Formula: $C_6H_3N_9^{2\bullet}$
Elemental Analysis: C, 35.83; H, 1.50; N, 62.67

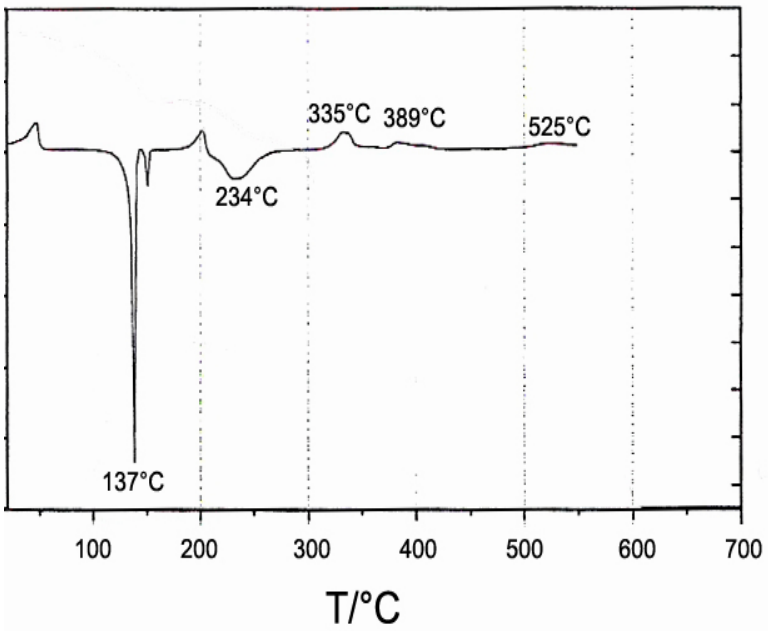
C_3N_4

Chemical Formula: C_3N_4
Elemental Analysis: C, 39.14; N, 60.86

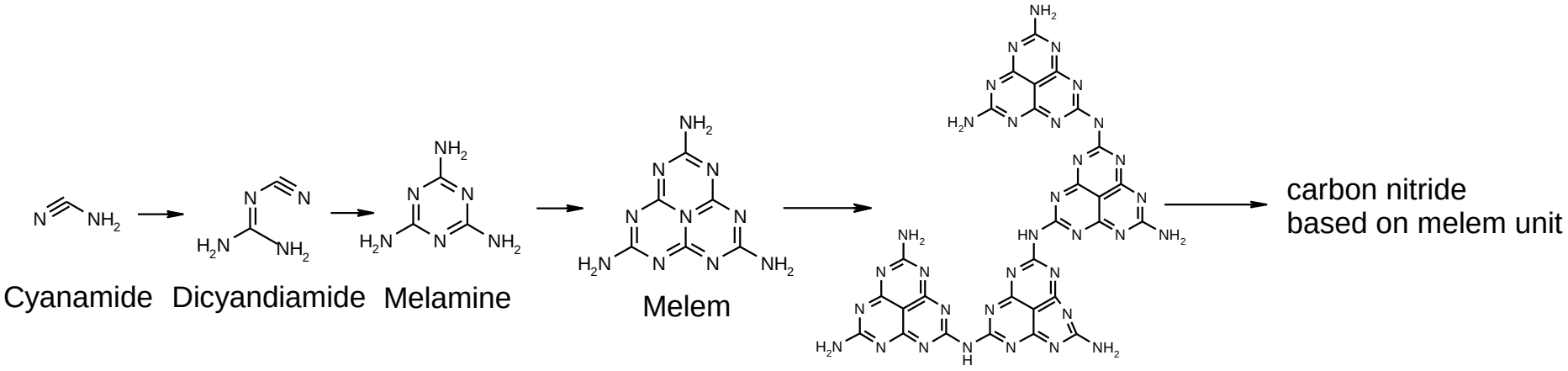
C, H, N Elemental Analysis for Nicanite® (in wt%)
C, 35.33
H, 1.46
N, 62.36

C, H, N Elemental Analysis of Nicanite® best matches poly(heptazine) (i.e. Melon, $C_6H_3N_9$)

Synthesis of Melon



T	Related process
47°C	Melting point of cyanamide
137°C	Reaction of cyanamide into dicyandiamide
203°C	Melting point of dicyandiamide
234°C	Reaction of dicyandiamide into melamine
335°C	Sublimation point of melamine
389°C	Formation of polymeric melem
525°C	Formation of carbon nitride network



Liebig, J. v. *Ann. Pharm.* **1834,** *10*, 1.