Supplementary information

A combined experimental and theoretical study on the formation of crystalline vanadium nitride (VN) in low temperature through a fully solid-state synthesis route

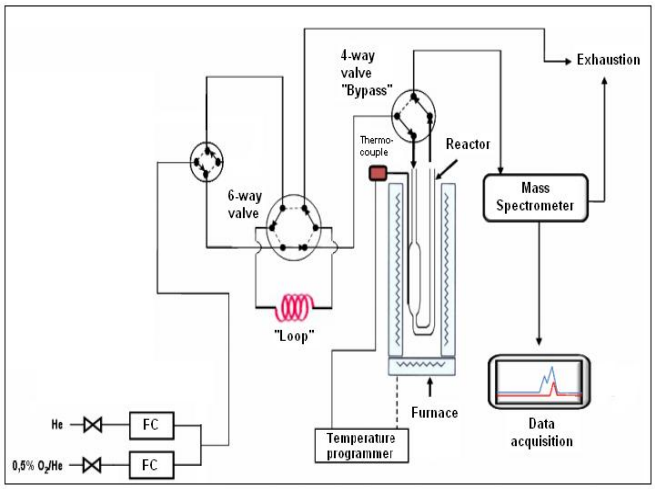
*Eugenio F. de Souza** [1], *Carlos A. Chagas*[2], *Teodorico C. Ramalho*[3], *Victor Teixeira da Silva*[3], *Daniel L.M. Aguiar*[1], *Rosane San Gil*[1], *Ricardo B. de Alencastro*[1].

[1] Universidade Federal do Rio de Janeiro. Rio de Janeiro, Instituto de Química. Programa PG Química.

[2] Universidade Federal do Rio de Janeiro, Núcleo de Catálise, Programa de Engenharia Química, COPPE.

[3] Universidade Federal de Lavras, Departamento de Química

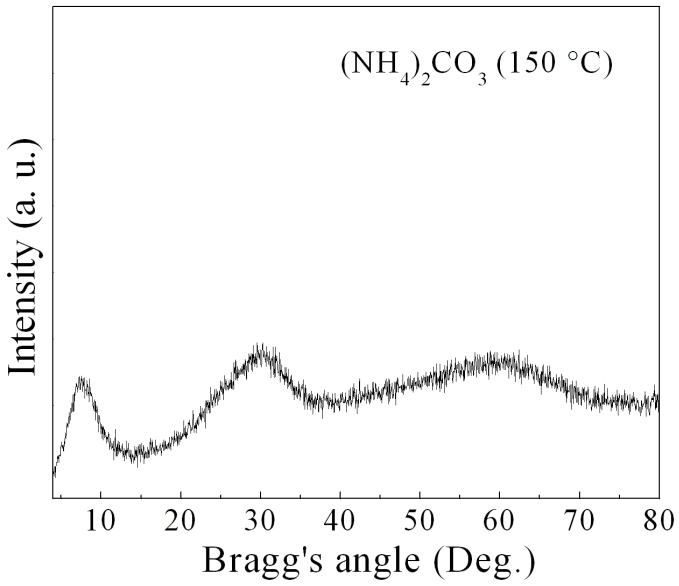
S.1. Multipurpose unit used in the synthesis (FC rely on “flow controller”).



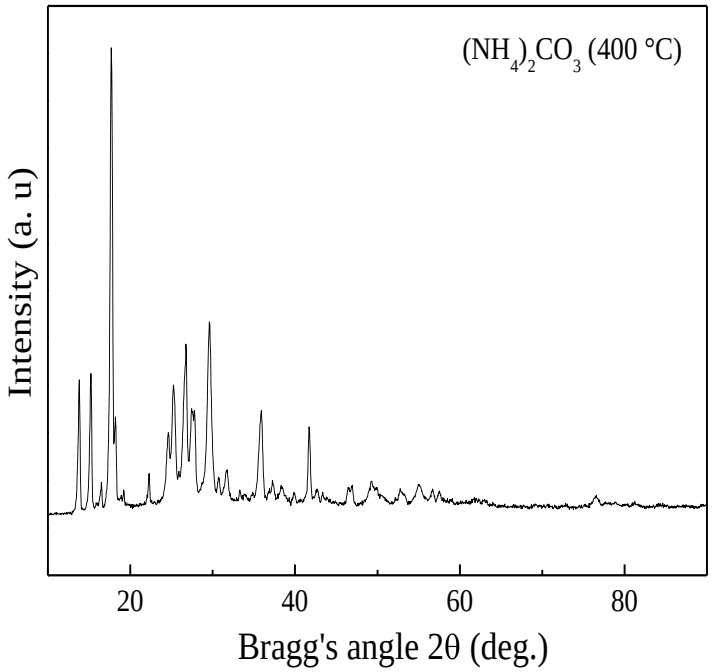
S.2. Diffraction pattern of Ammonium Carbonate (150°C).

It is important to emphasize that the low-crystalline structure obtained for the sub-product, $(NH_4)_2CO_3$, was mainly due to the low temperatures employed over the solid-state reaction to form the intermetiate (~150°C), GmV, which consequently led to the formation of a structure predominantly amorphous (S.2). However, when the same sample was subject to higher temperatures (in this case, ~400°C) it exhibited high crystallinity and well-characterized diffraction lines of ammonium carbonate in excelent agreement with Sclar and L. C. Carrison (1963)*, as can be seen in **S.3.**

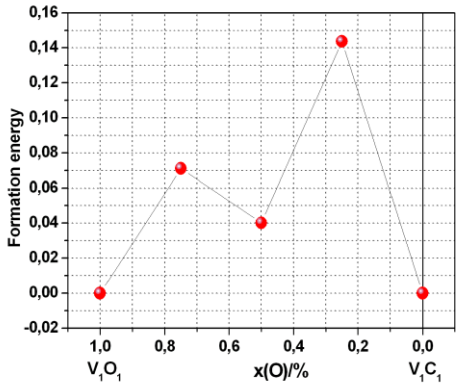
*C. B Sclar and L. C. Carrison, “Phase Composition of Commercial Ammonium Carbonate", *Science*, Vol. 140 no. 3572 pp. 1205-1207 (1963).



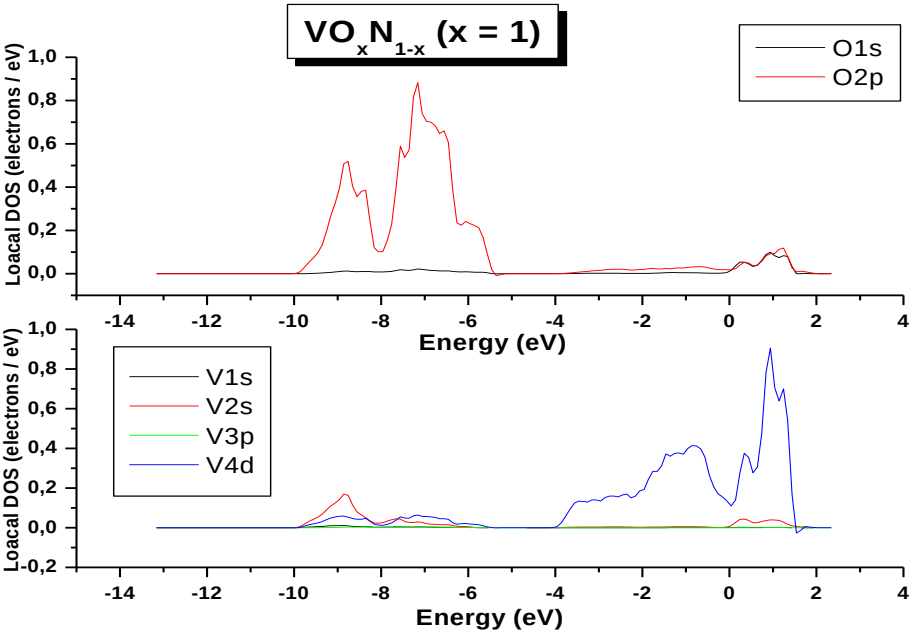
S.3. Diffraction pattern of Ammonium Carbonate (400°C).

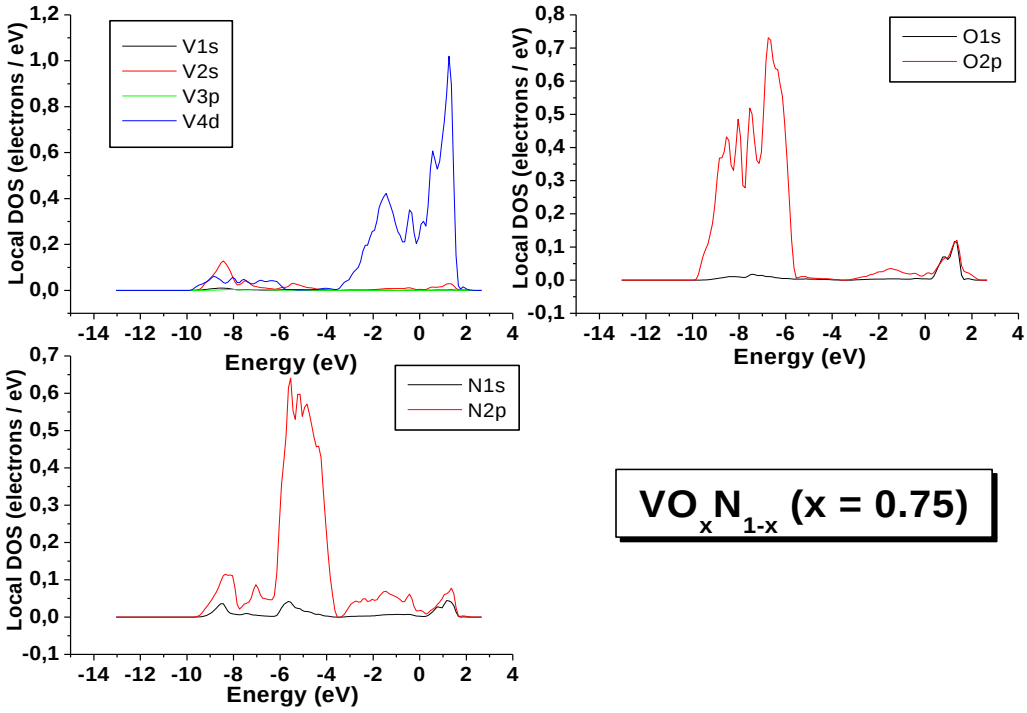


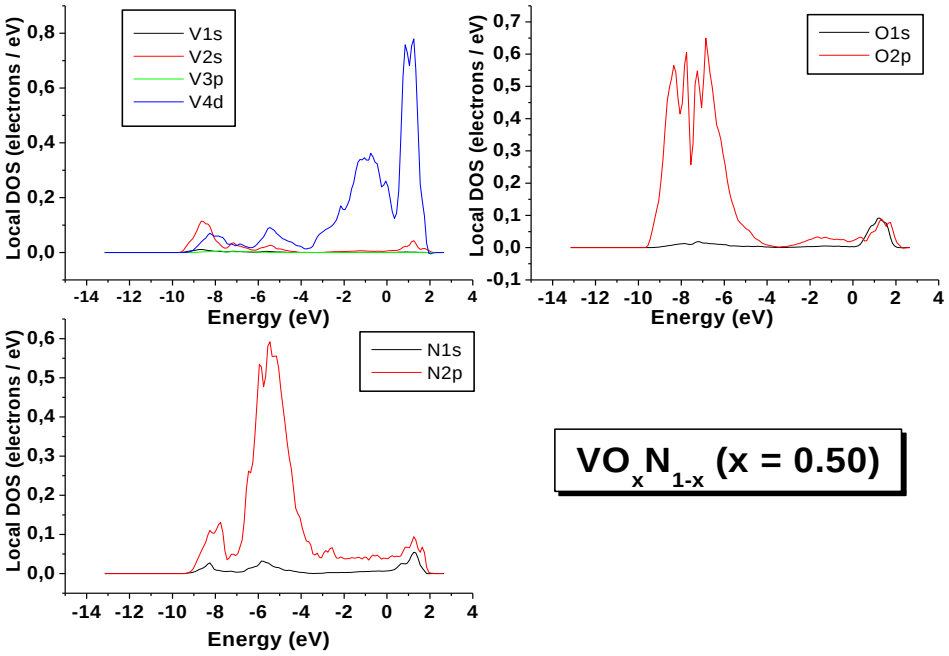
S.4 Calculated formation energy for VO_xC_{1-x}



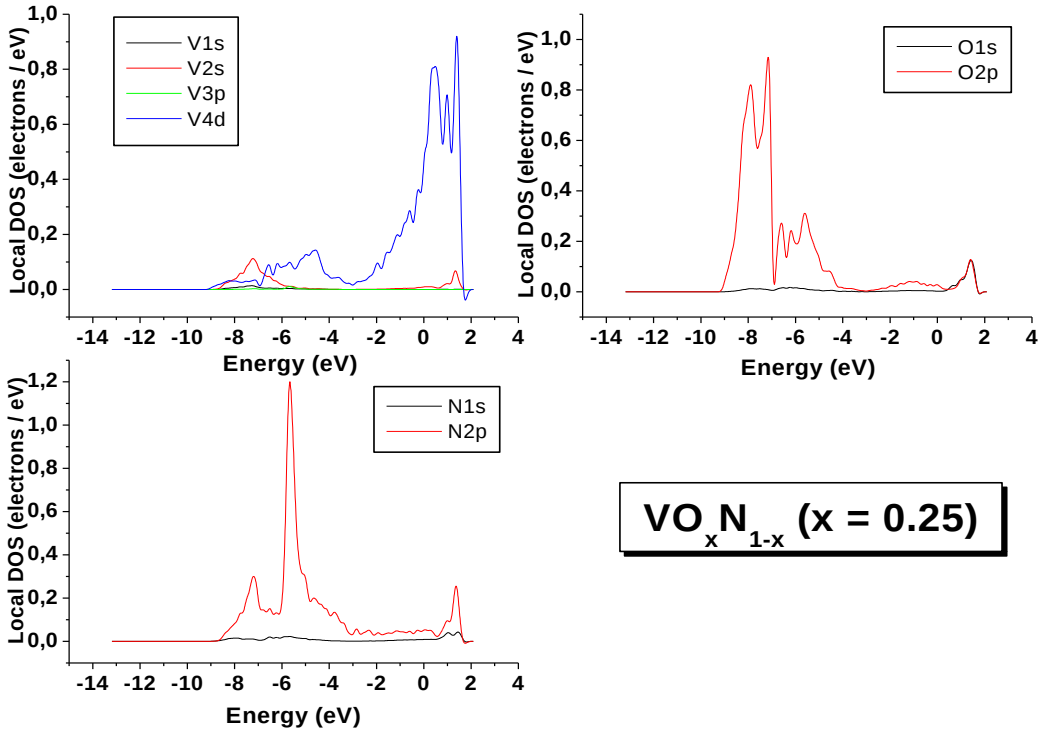
S.5 Partial DOS for the VO_xN_{1-x} models



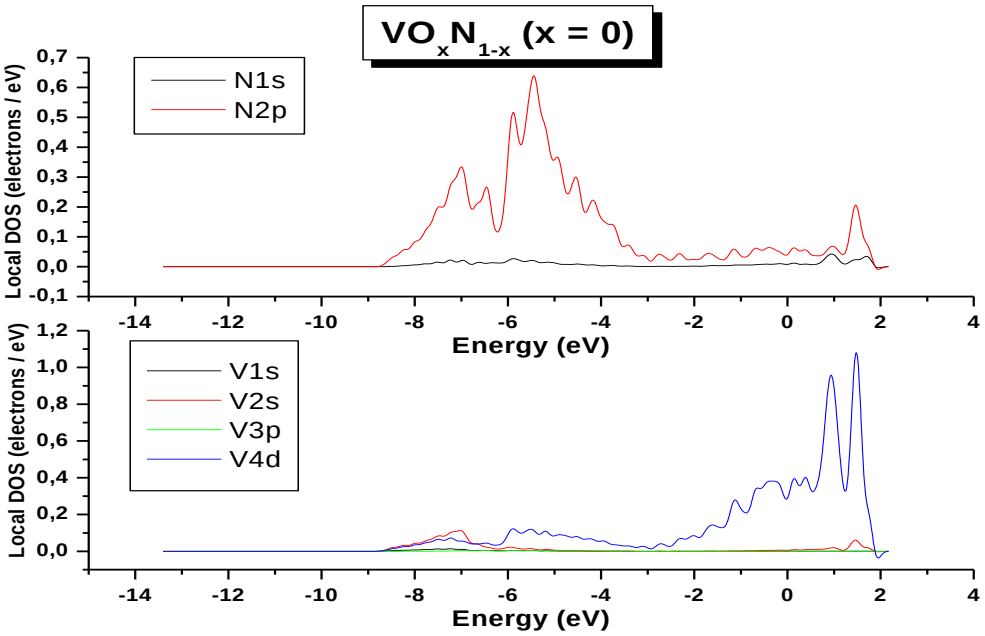




VO_xN_{1-x} (x = 0.50)

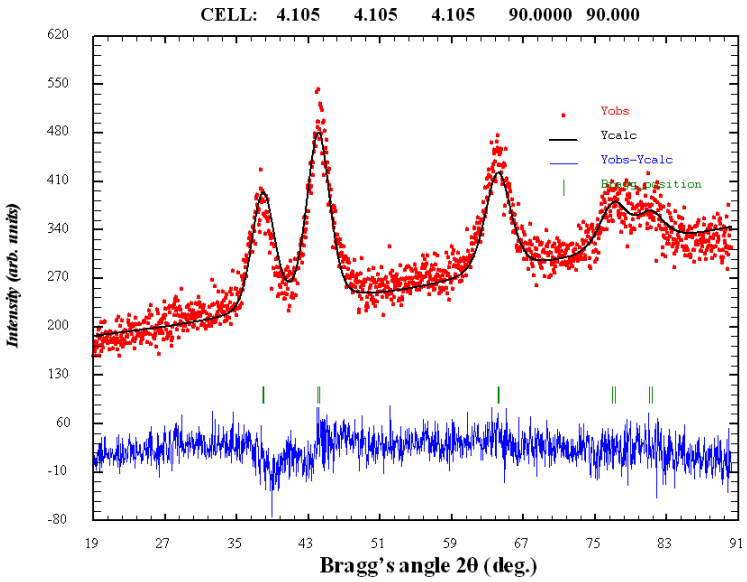


VO_xN_{1-x} (x = 0.25)

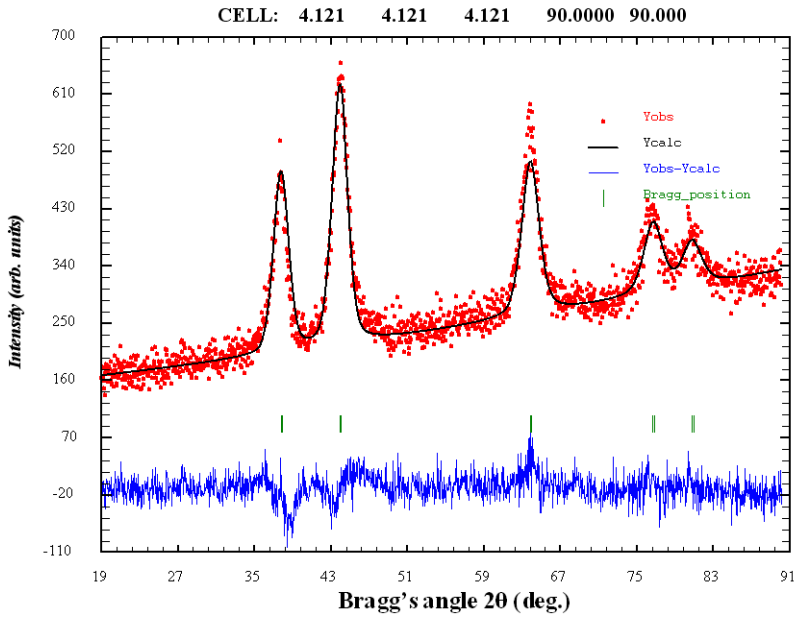


S.6 Diffraction patterns and Rietveld refinement of the thermally treated samples

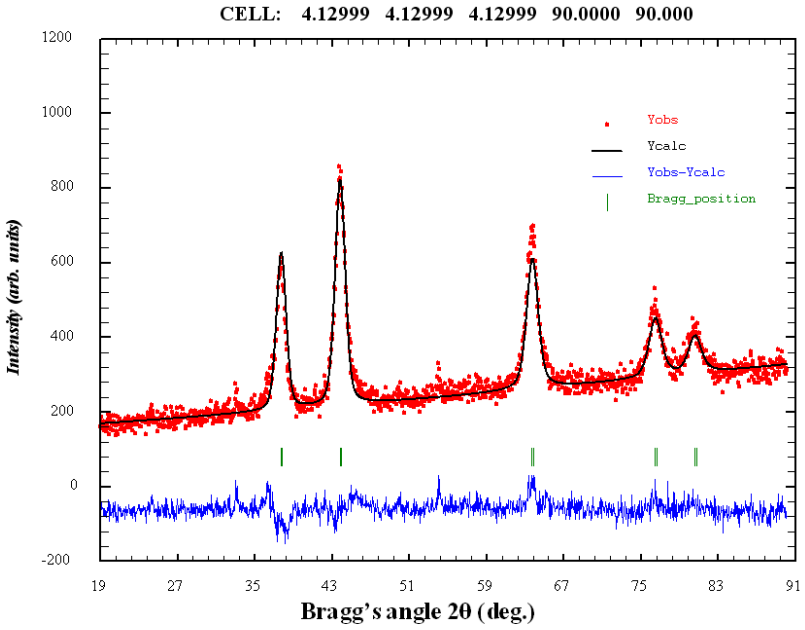
⟶ **500 °C**



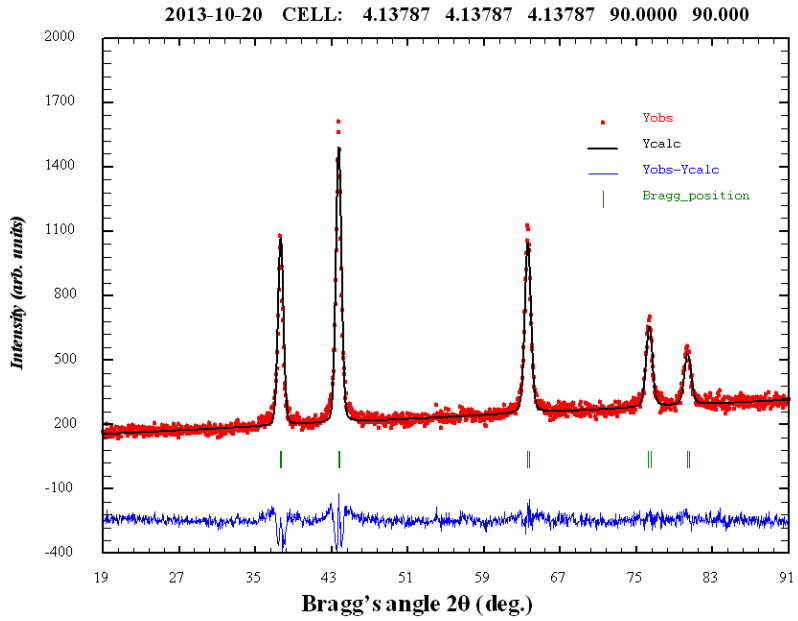
⟶ **600°C**



⟶ **700°C**



⟶ **800°C**


2013-10-20 CELL: 4.13787 4.13787 4.13787 90.0000 90.000
Yobs
Ycalc
Yobs-Ycalc
Bragg_position
Intensity (arb. units)
2000
1700
1400
1100
800
500
200
-100
-400
19
27
35
43
51
59
67
75
83
91
Bragg's angle 2θ (deg.)