Electronic Supplementary Information

Dynamics and local ordering of pentachloronitrobenzene: a molecular dynamics investigation

Jonathan F. Gebbia[a,b], Andrés Henao Aristizabal[c], Philippe Negrier[d], David Aguilà[e,f], Josep Lluís Tamarit[a,b], Luis Carlos Pardo[a,b]

[a] Grup de Caracterització de Materials, Departament de Física, EEBE, Universitat Politècnica de Catalunya , Eduard Maristany, 10-14, 08019 Barcelona, Catalonia, Spain

[b] Barcelona Research Center in Multiscale Science and Engineering, Universitat Politècnica de Catalunya , Eduard Maristany, 10-14, 08019 Barcelona, Catalonia, Spain

[c] Data Research Sociedad Limitada, Carrer Llacuna, 162, 08018, Barcelona, Spain

[d] Laboratoire Ondes et Matière d'Aquitaine, Université de Bordeaux, UMR 5798, F-33400 Talence, France

[e] Institute of Nanoscience and Nanotechnology (IN2UB), Universitat de Barcelona, Barcelona, Spain

[f] Departament de Química Inorgànica i Orgànica, Facultat de Química, Secció de Química Inorgànica, Universitat de Barcelona, Martí i Franquès, 1-11, 08028, Barcelona, Spain

Table S1. Single crystal data and structure refinement for OD phase of PCNB at 100 and 200 K. Estimated standard deviations in parenthesis.

Temperature (σ) /K	100(2)	200(2)
Crystal system	Rhombohedral	Rhombohedral
Space group	$R\bar{3}$	$R\bar{3}$
***a* (σ) /Å**	8.7160(12)	8.7440(12)
***b* (σ) /Å**	8.7160 (12)	8.7440(12)
***c* (σ) /Å**	10.946 (4)	11.068(4)
***α* (σ) /°**	90	90
***β* (σ) /°**	90	90
***γ* (σ) /°**	120	120
Cell Volume (σ) /Å^3	720.1(2)	733.9(1)
***Z* / *Z*'**	3 / 1	3 / 1
***M* /g·mol^{-1}**	295.32	295.32
D_{calc} /g·cm^{-3}	2.034	2.007
μ /mm^{-1}	1.576	1.549
***F*(000)**	432	432
Crystal shape / mm^3	0.05 × 0.02 × 0.02	
Radiation	0.72931	0.72931
Θ range for data collection	3.364-31.245	3.345–31.391
Index ranges	-11 ≤ *h* ≤ 11 -12 ≤ *k* ≤ 12 -15 ≤ *l* ≤ 15	-11 ≤ *h* ≤ 11 -12 ≤ *k* ≤ 12 -15 ≤ *l* ≤ 15
Reflections collected	7351	4573
Independent reflections	805 R_{int} = 0.1108	495 R_{int} = 0.1362
Reflections with I > 2s(I)	759	382
No. parameters	47	47
Goodness-of-fit on F^2	1.007	0.882
R_1/wR_2 indexes [I>=2σ (I)]	0.0429/0.1355	0.0543/0.1341
R_1/wR_2 indexes [all data]	0.0435/0.1371	0.0580/0.1395
Largest diff. peak/hole / e Å^{-3}	0.456/–0.330	0.258/-0.380
CCDC	2266449	2266450