

Synthesis and Characterization of a Novel Fluorinated Bismaleimide via Nucleophilic Addition-Elimination Reaction and its Polymeric Networks

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X-Ray Structure Elucidation of OFCP-BMI

Crystallographic data for monomer OFCP-BMI has been submitted to the Cambridge Crystallographic Data Center with publication number CCDC 1054069. Copies can be obtained free of charge from CCDC, 12 Union Road, Cambridge, CB2 1EZ, UK (e-mail: deposit@ccdc.cam.ac.uk).

A colorless crystalline fragment ($\sim 0.04 \times 0.3 \times 0.4 \text{ mm}^3$) of OFCP-BMI was chosen to study the crystal structure. Crystal data for OFCP-BMI: $\text{C}_{25}\text{H}_{12}\text{F}_6\text{N}_2\text{O}_6$, $M_r = 550.37$, Monoclinic, space group $P2_1/n$, $a = 15.802(3) \text{ \AA}$, $b = 7.0481(16) \text{ \AA}$, $c = 19.530(4) \text{ \AA}$, $\beta = 96.341(10)^\circ$, $V = 2161.7(8) \text{ \AA}^3$, $T = 105 \text{ K}$, $Z = 4$, $F(000) = 1112$, $D_x = 1.691 \text{ g cm}^{-3}$, $\mu(\text{Mo K}\alpha) = 0.16 \text{ mm}^{-1}$, 10886 measured reflections, 10886 independent reflections, 8064 reflections with $I > 2\sigma(I)$, $R_{\text{int}} = 0.076$, $\theta_{\text{max}} = 30.6^\circ$, $\theta_{\text{min}} = 2.6^\circ$, full-matrix least-squares refinement on F^2 , $R_1[F^2 > 2\sigma(F^2)] = 0.060$, $wR_2(F^2) = 0.133$, $S = 1.02$, 353 parameters, 0 restraints, $w = 1 / [\sigma^2(F_o^2) + (0.0517P)^2 + 1.408P]$, $\Delta\rho_{\text{max}} = 0.48 \text{ e \AA}^{-3}$, $\Delta\rho_{\text{min}} = -0.34 \text{ e \AA}^{-3}$, Non-merohedral twin, Twin Law = (0.235 0 - 0.765, 0 -1 0, -1.236 0 -0.235), BASF = 0.429 (1), crystallization solvent = THF, CCDC number is CCDC 1054069. Note: when examining the dihedral angles of rings within this compound, the maleimide substituents are nearly orthogonal to each other ($\sim 86^\circ$) while the phenyl rings are closer to packing parallel ($\sim 9^\circ$). Relative to the central fluorinated cyclopentene ring, one of the two maleimide substituents (contain atomic sites “C1”, “C2”, “C3”, “C4”, “N1”, “O1”, and “O2”) has the smallest dihedral angle of $\sim 12^\circ$ of all the rings. The phenyl ring to adjacent maleimide substituent dihedral angles are $\sim 54^\circ$ and $\sim 43^\circ$. There are also close contacts between neighboring halogen (F) atoms. The intermolecular distance between atomic sites “F1” and “F6” is $2.770(2) \text{ \AA}$.

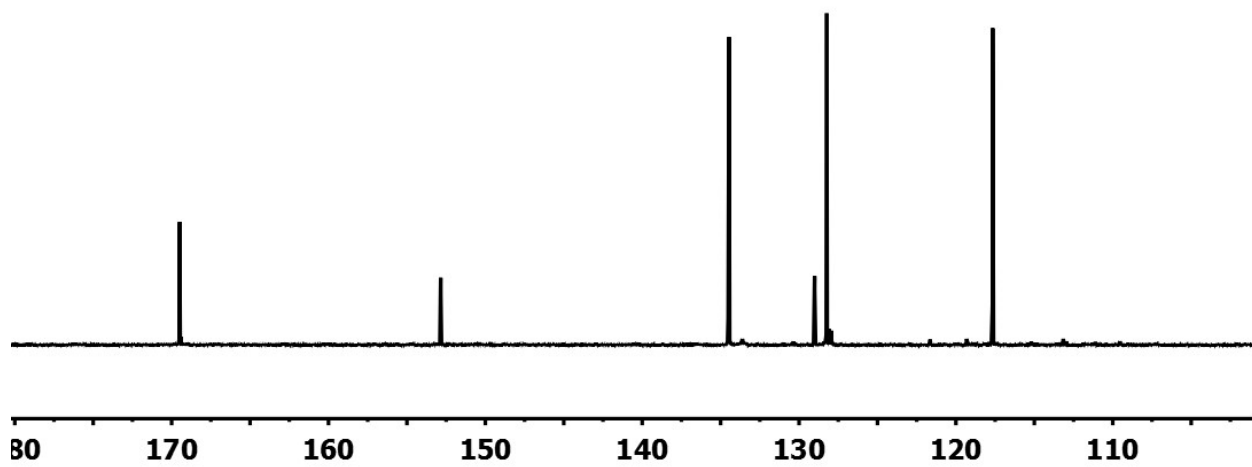


Figure S1. ^{13}C -NMR spectrum of monomer **OFCP-BMI**.

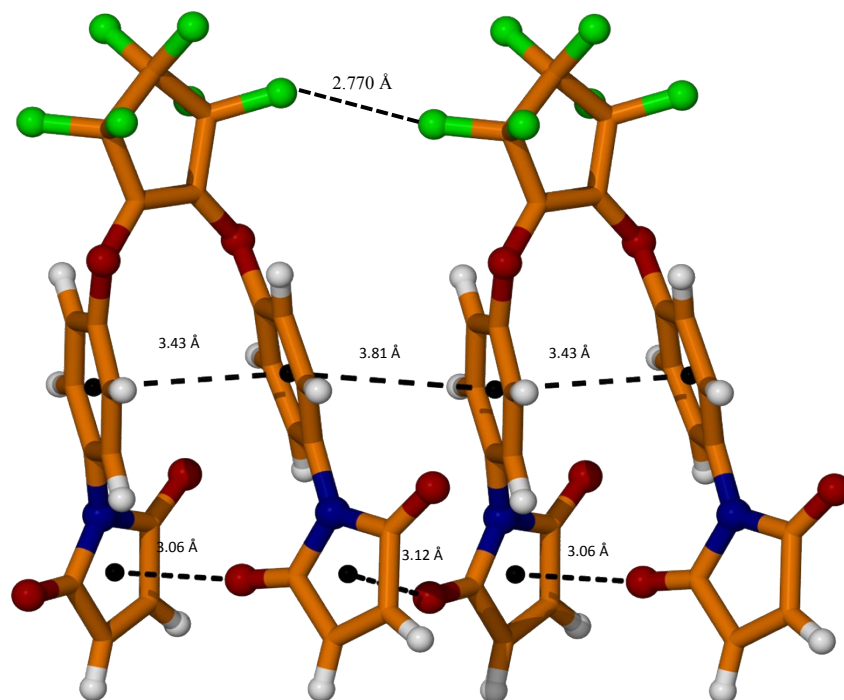


Figure S2. The two important interactions in crystal structure of monomer **OFCP-BMI**

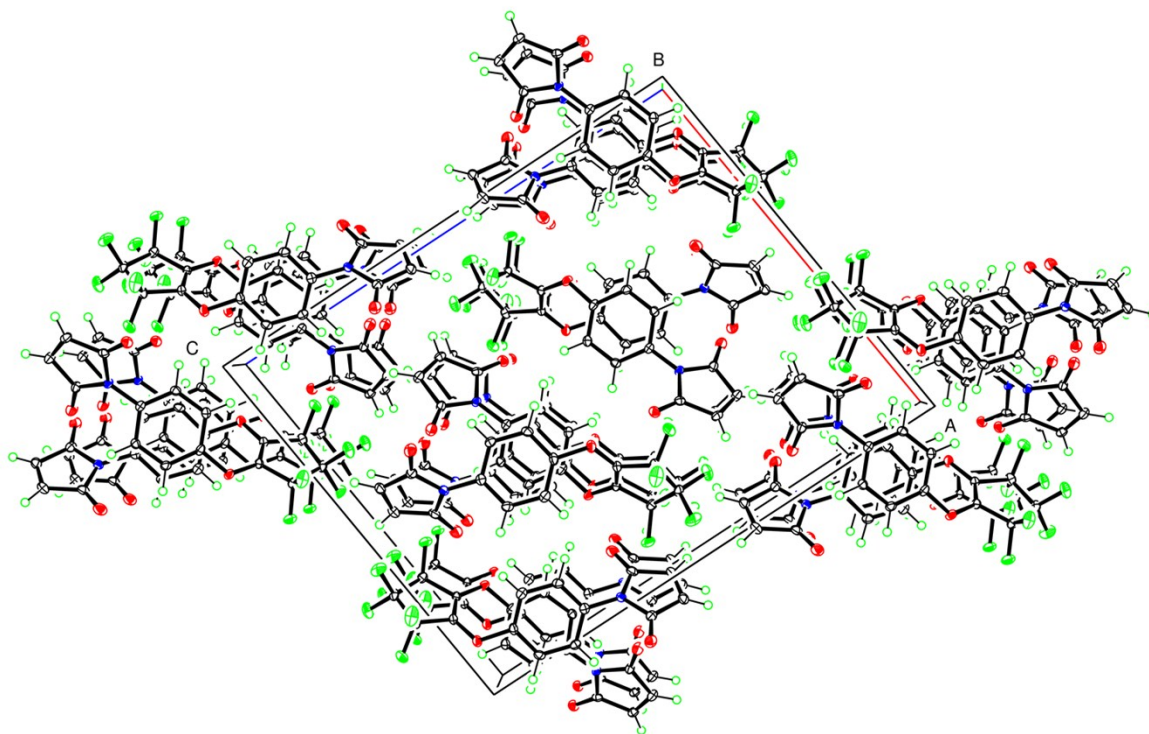


Figure S3. Packing pattern of unit cells in the crystal structure of **OFCP-BMI**

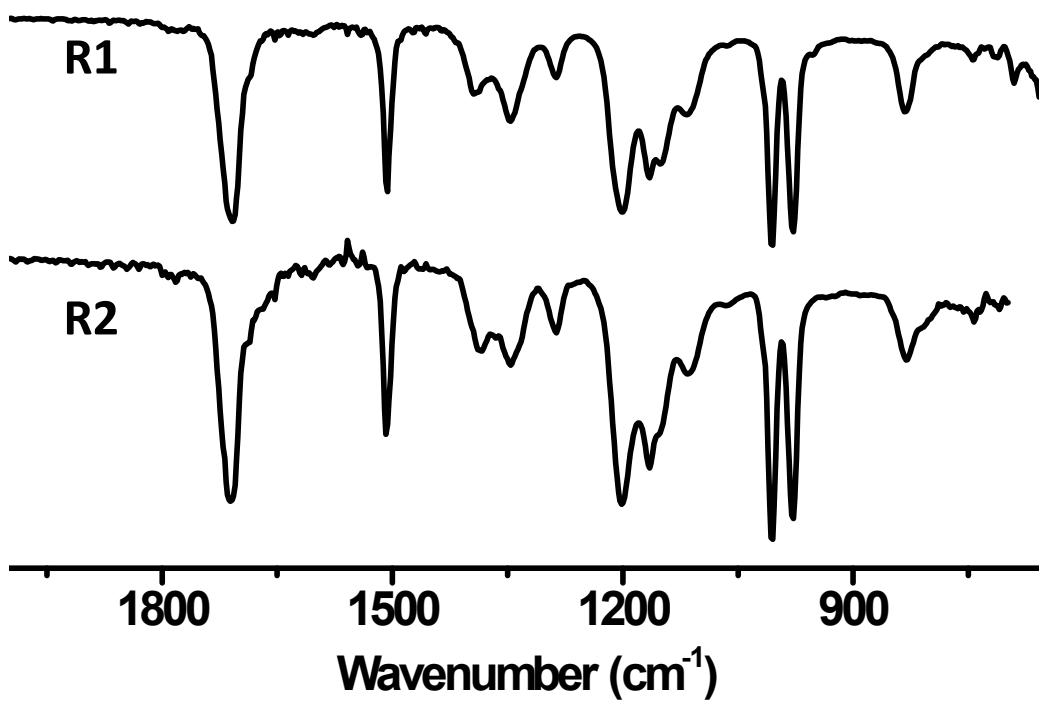


Figure S4. ATR-FTIR spectra of the resulting resins R1 and R2.

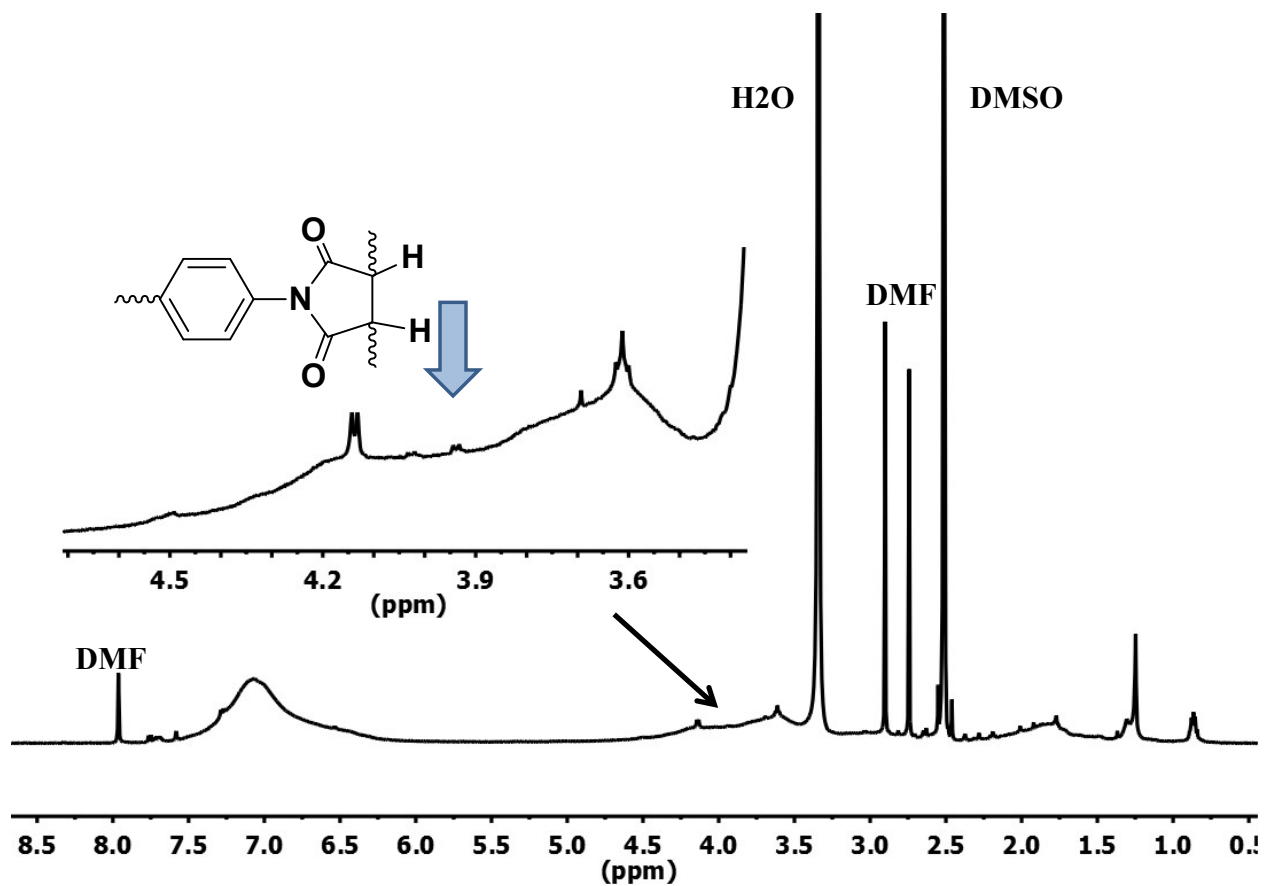


Figure S5. ^1H NMR spectrum of the resulting resin R2.

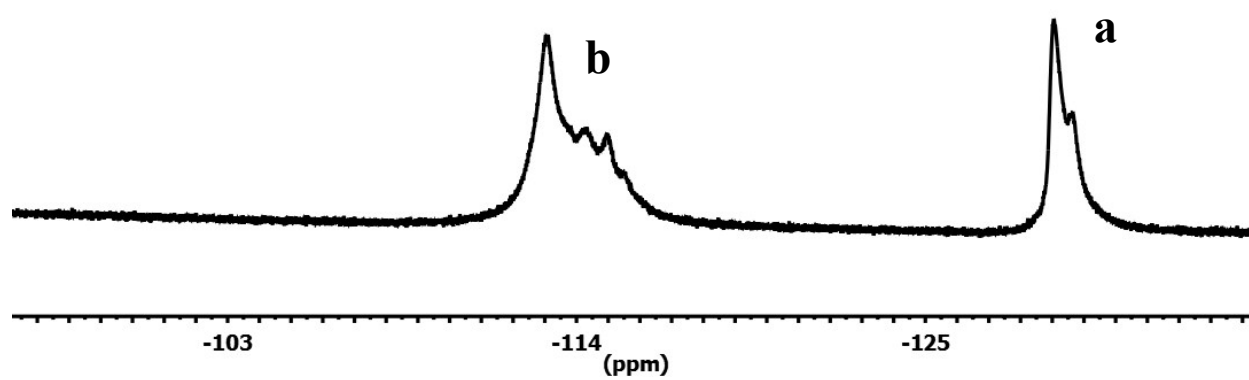
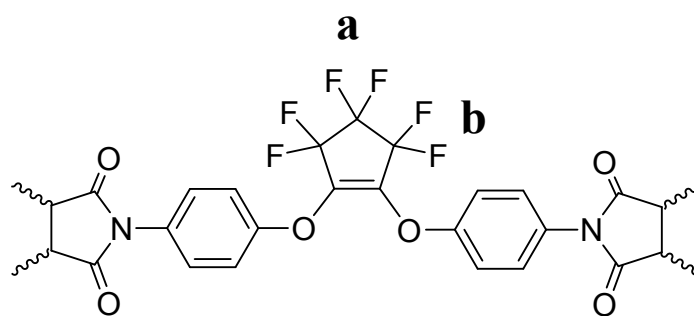


Figure S6. ^{19}F NMR spectrum of the resulting resin R2.

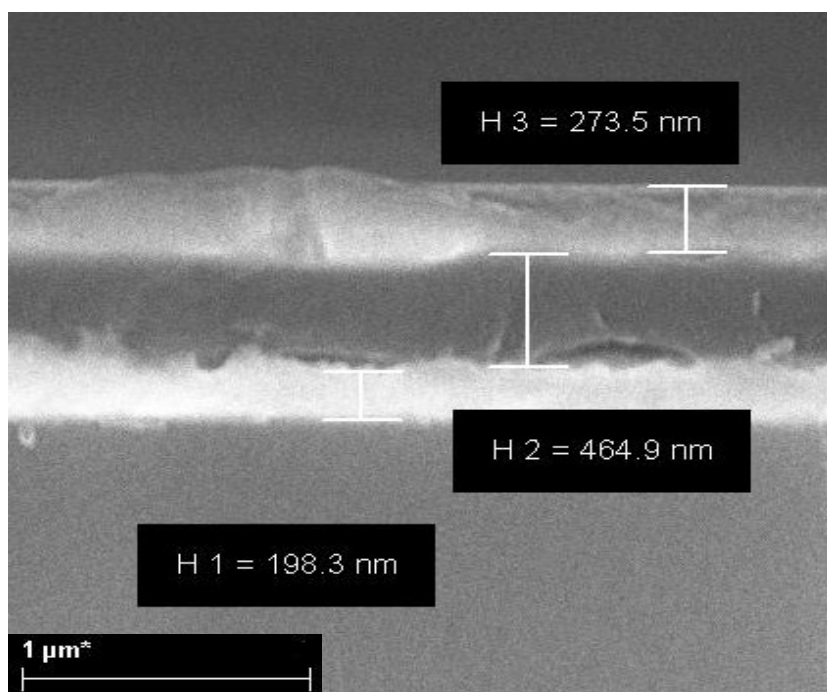


Figure S7. The measurement of the thickness of the thin film via SEM technology.

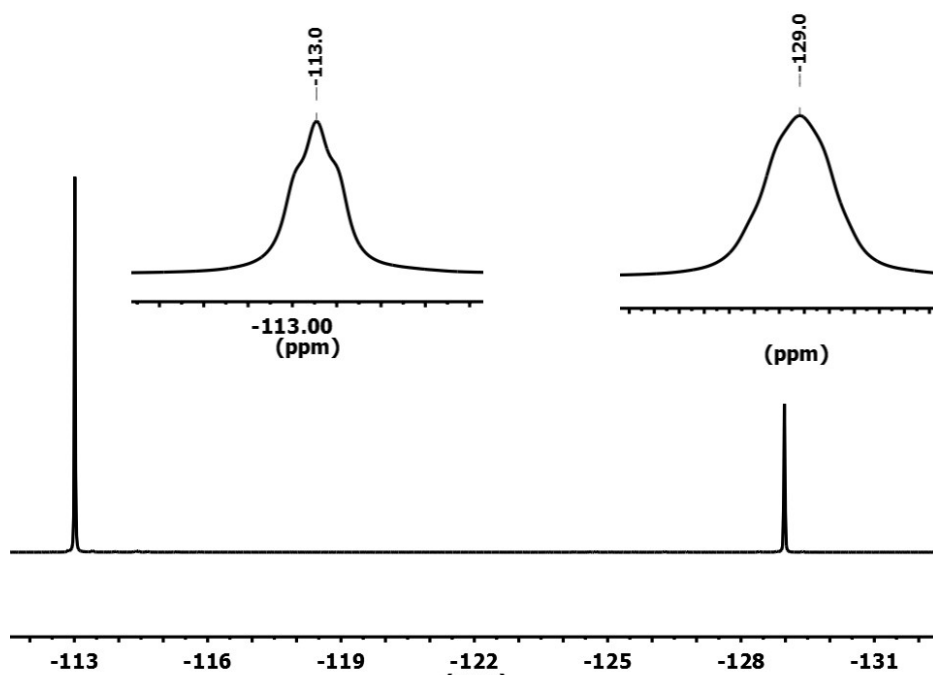


Figure S8. ^{19}F NMR spectrum of OFCP-BMI in DMSO-d_6