Supplementary Information for:

Möhlau's anthradipyrazole revisited: a new look at an old molecular system

Angelo Maspero,[a] Giovanni B. Giovenzana,[b] Norberto Masciocchi,[a] Giovanni Palmisano,[a] Angiolina Comotti,[c] Piero Sozzani,[c] Irene Bassanetti, [c] Luca Nardo[d]

a) Dipartimento di Scienza e Alta Tecnologia, Università dell'Insubria, Via Valleggio 11, 22100 Como (Italy); b) Dipartimento di Scienze del Farmaco, Università degli Studi del Piemonte Orientale "A. Avogadro", Largo Donegani 2/3, 28100 Novara (Italy); c) Dipartimento di Scienza dei Materiali, Università di Milano Bicocca, Via R. Cozzi 53, 20125 Milano (Italy); d) Dipartimento di Scienze della Salute, Università di Milano Bicocca, Via Cadore 48, 20900 Monza (Italy)

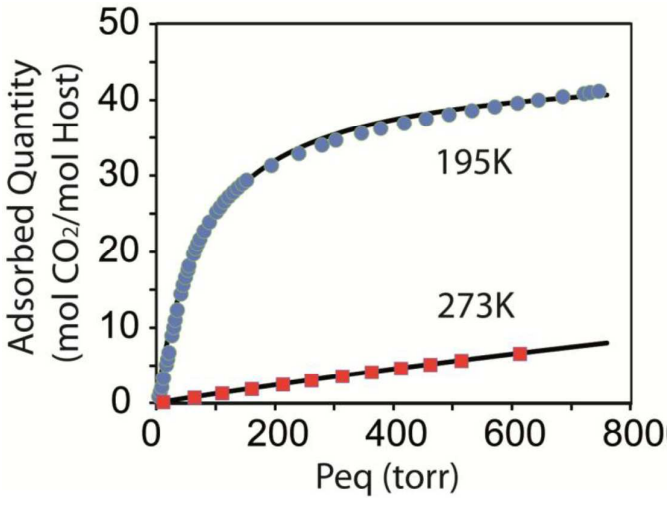

Figure S1. CO_2 adsorption isotherms of polymorph β at 195 K and 273 K. The black lines represent the best fitting Langmuir curves.

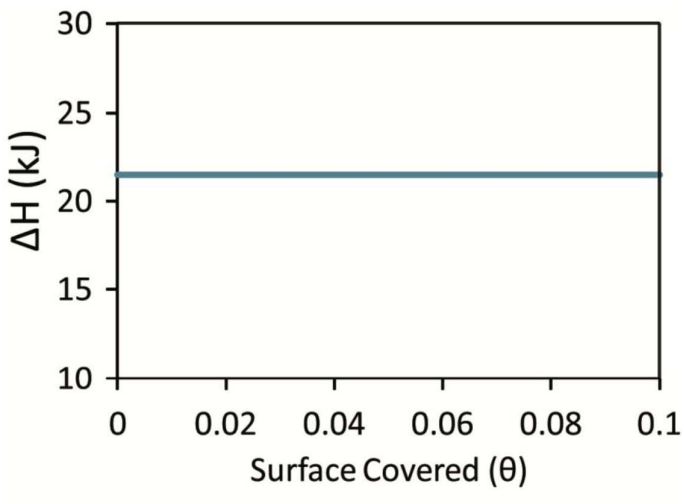

Figure S2. Heat of adsorption of CO_2 in the polymorph **β** as a function of surface covered.

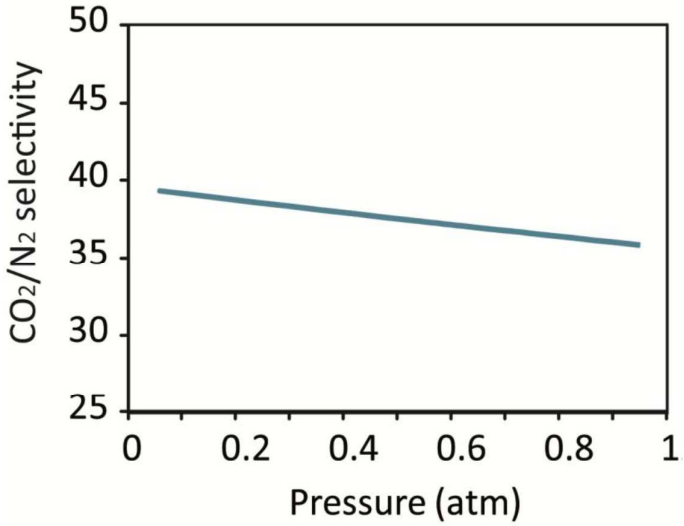

Figure S3. CO_2/N_2 selectivity as calculated by IAST theory on single-component isotherms at 273 K.

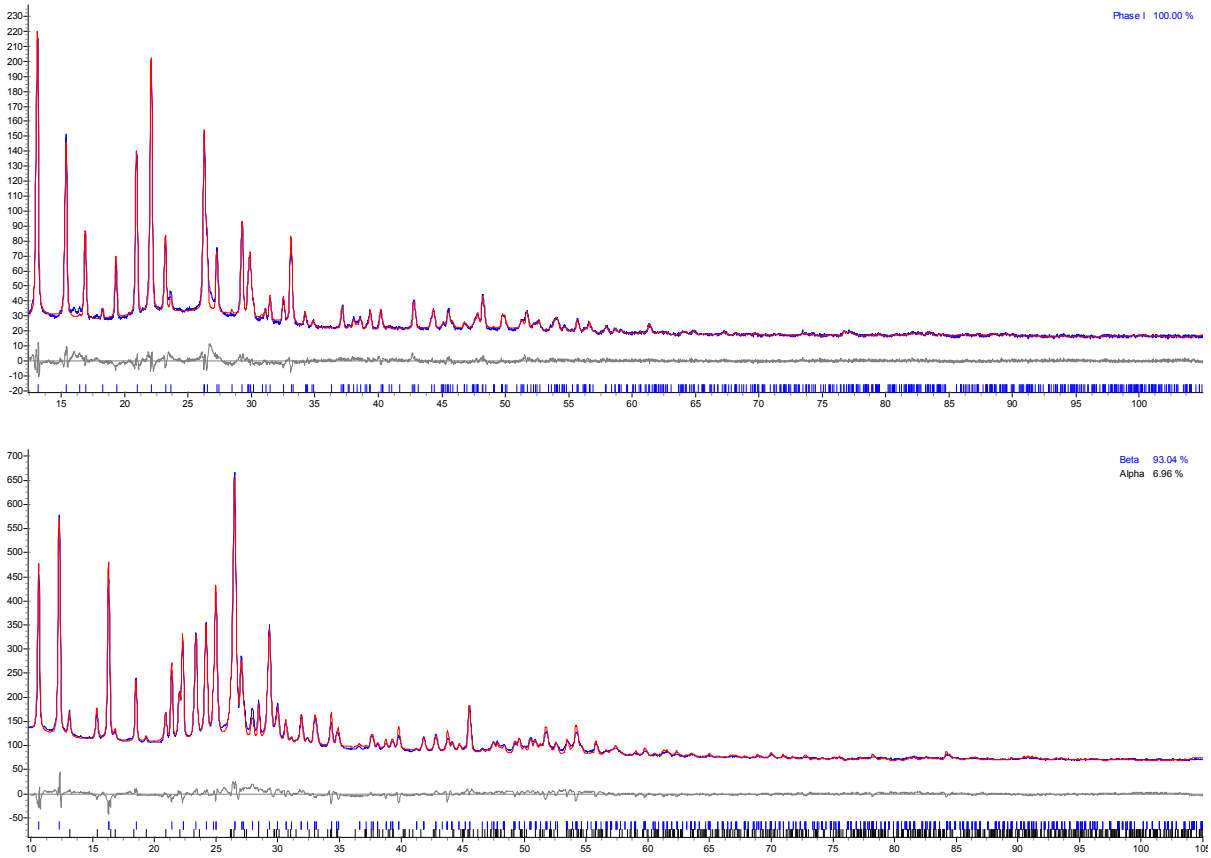

Figure S4: Rietveld refinement plots for phase **α** (top) and **β** (bottom), drawn on a "square root of counts" scale, thus magnifying the high-angle region.