Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary information for

Structural Transformation and Tuning Behavior Induced by Propylamine Concentration in Hydrogen Clathrate Hydrates

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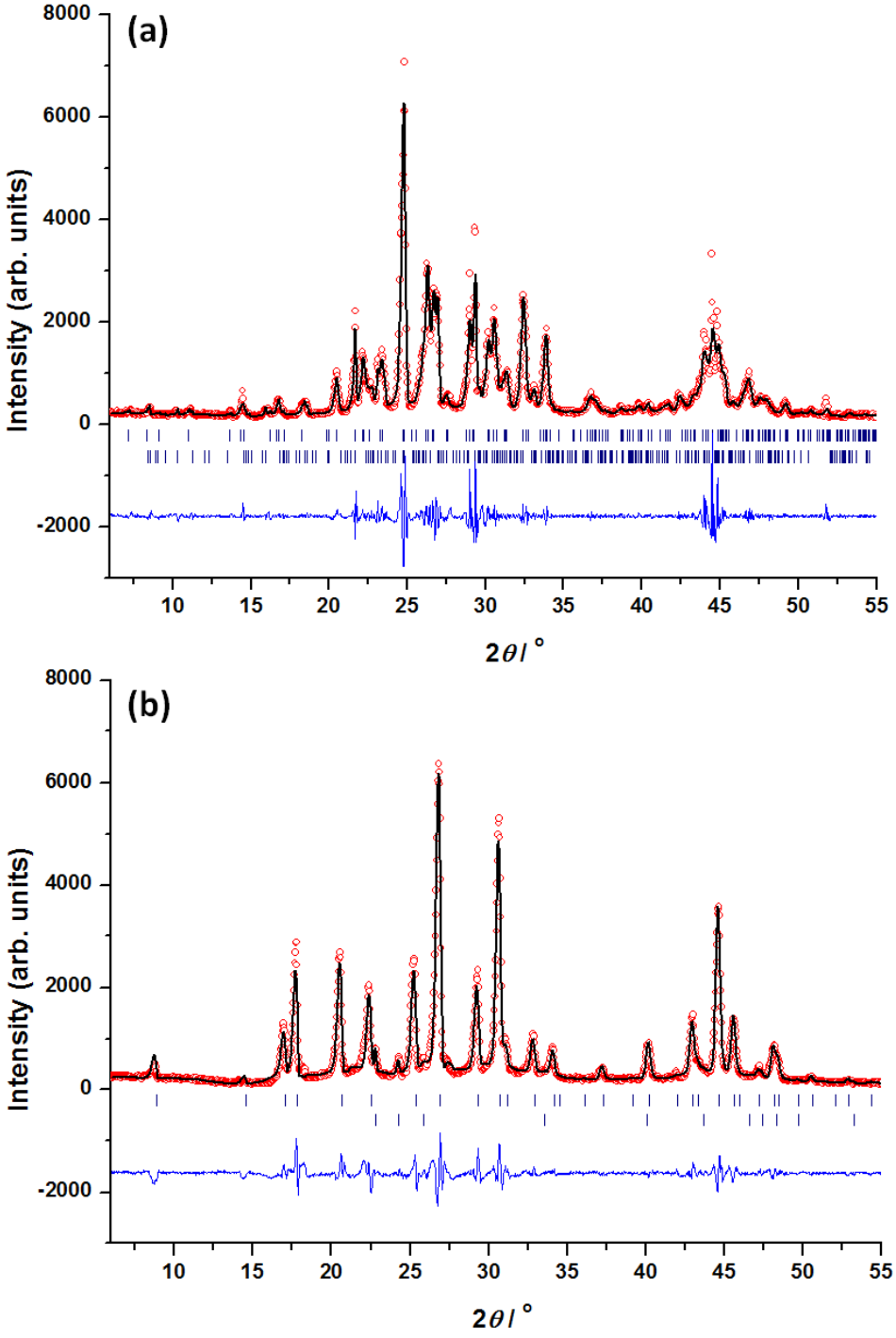

Figure S1. Refined PXRD patterns of *i*-PA + H_2 binary hydrates by structure-less Le Bail method. (a) 11.1 mol% *i*-PA and (b) 5.6 mol% *i*-PA samples.

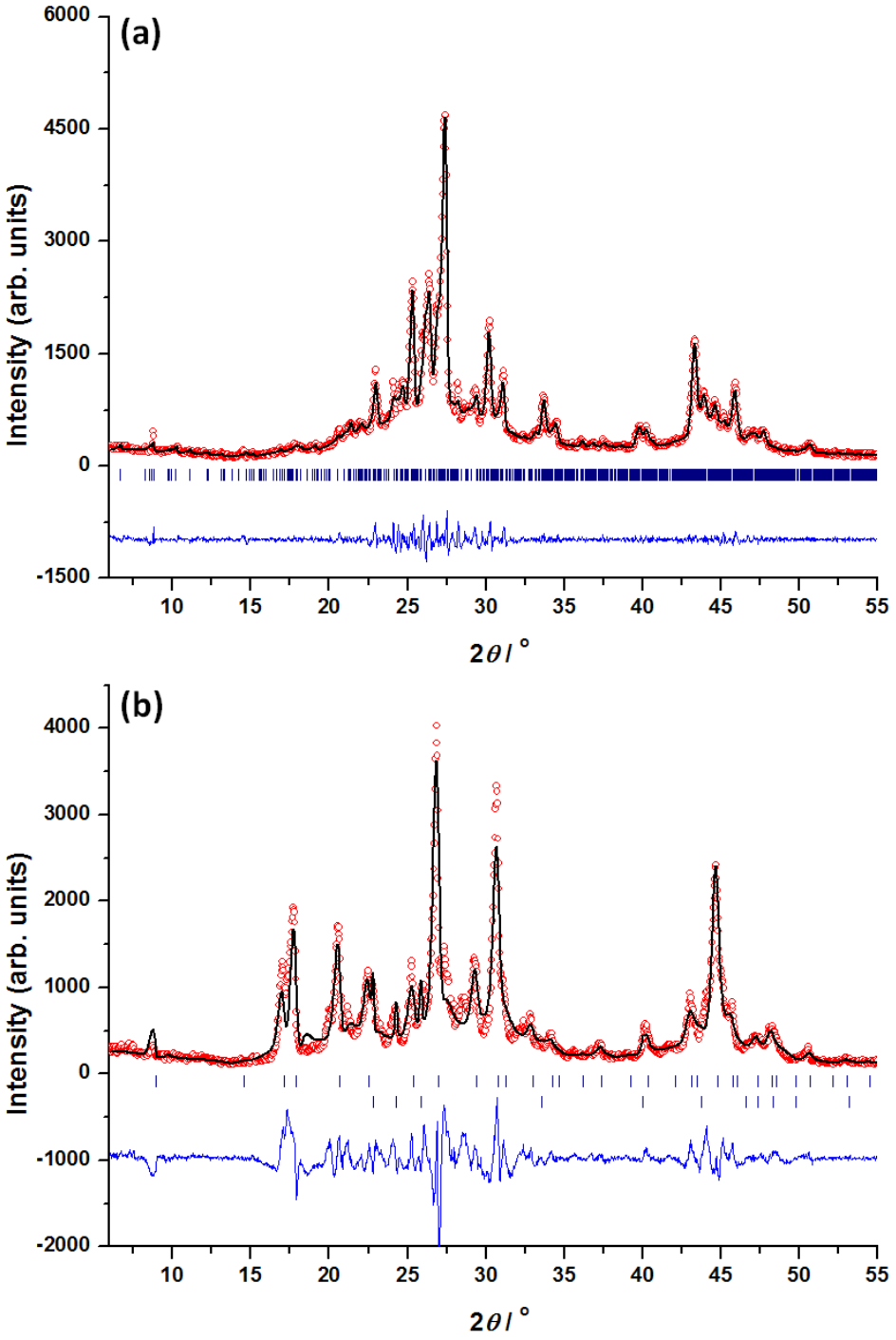

Figure S2. Refined PXRD patterns of *n*-PA + H_2 binary hydrates by structure-less Le Bail method. (a) 13.3 mol% *n*-PA and (b) 5.6 mol% *n*-PA samples. The 5.6 mol% sample contains considerable amount of monoclinic $P2_1/n$ phase, but it was not included in the Le Bail fitting because of too many reflections of the phase.

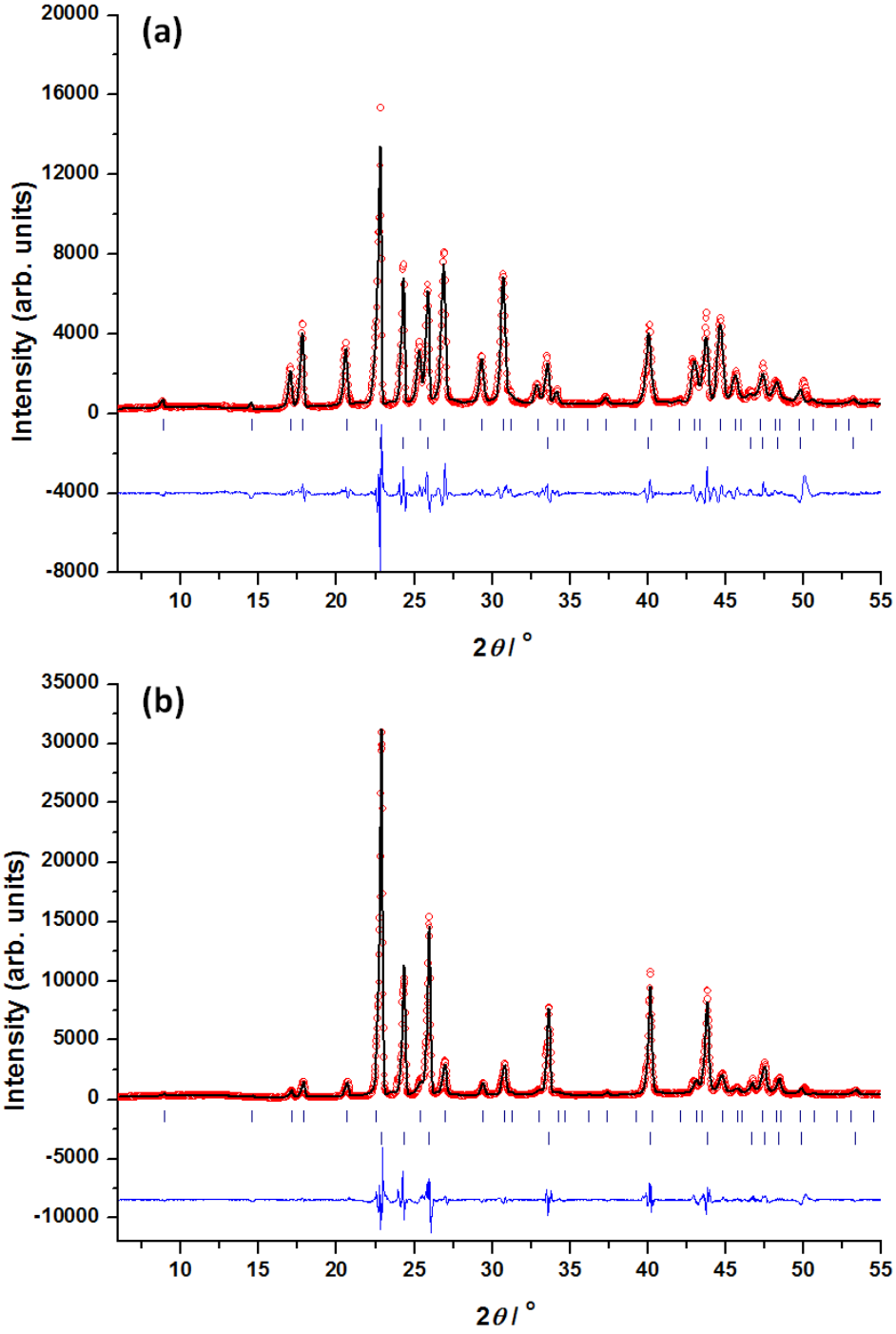

Figure S3. PXRD patterns of *i*-PA + H_2 binary hydrates. (a) 3 mol% *i*-PA (*Fd-3m* phase, a = 17.194(2) Å) and (b) 1 mol% *i*-PA (*Fd-3m* phase, a = 17.164(2) Å) samples. Tick marks of the second row indicate reflections from the hexagonal ice.

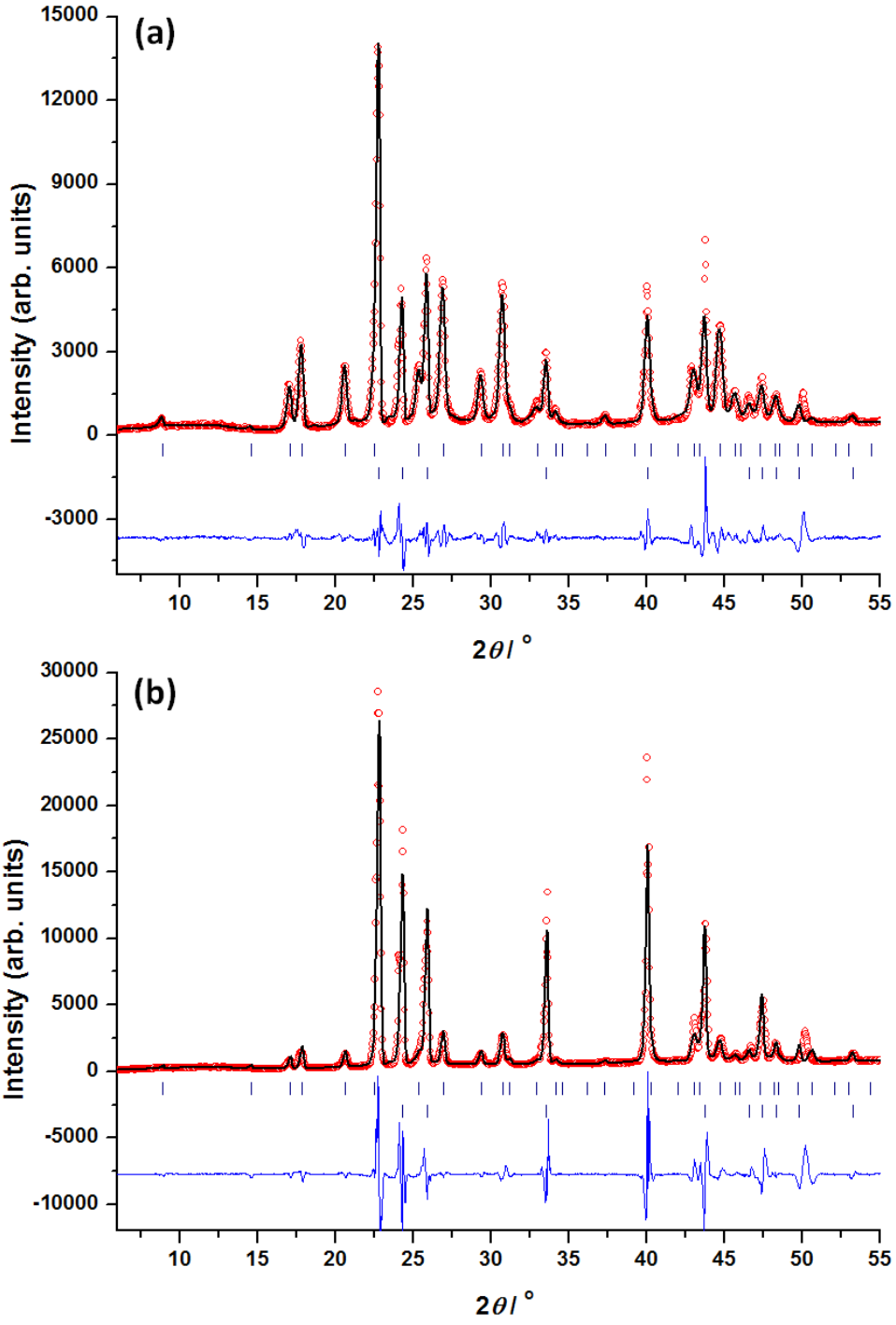

Figure S4. PXRD patterns of *n*-PA + H_2 binary hydrates. (a) 3 mol% *n*-PA (*Fd-3m* phase, *a* = 17.184(1) Å) and (b) 1 mol% *n*-PA (*Fd-3m* phase, *a* = 17.191(3) Å) samples. Tick marks of the second row indicate reflections from the hexagonal ice.