The application of statistical methodology to the analysis of time-resolved X-ray diffraction data: supporting information

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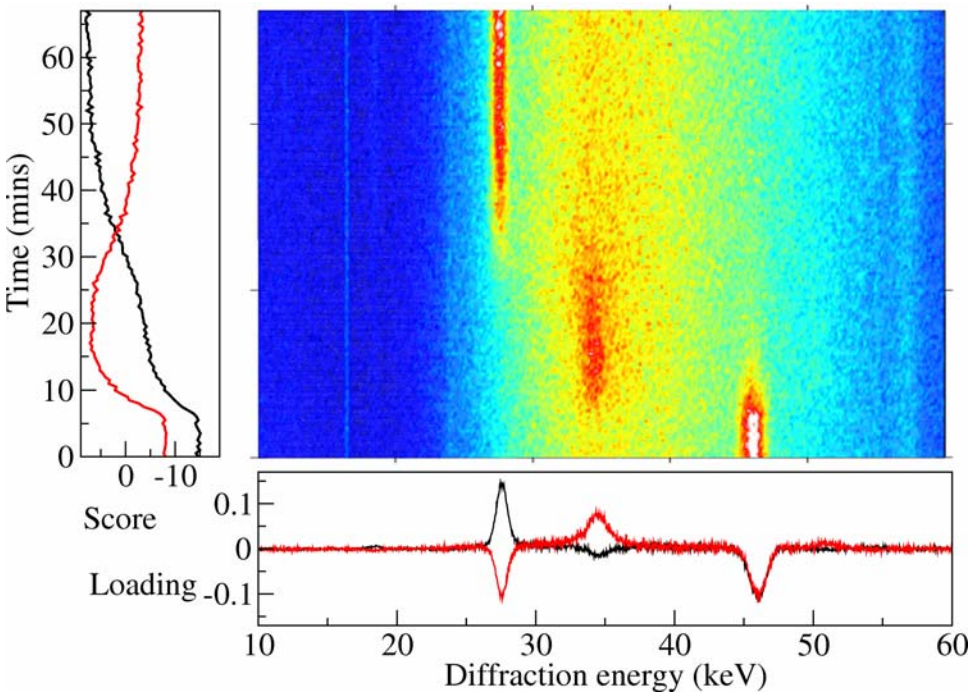

Figure S1

Variation of diffraction patterns (top right), PC1 and PC2 (top left) with time, and loadings (bottom) for the intercalation of MPA into h-$LiAl_2$-Cl at pH 4. PC1 is in black, and PC2 in red. Raw data have been mean-centred and scaled by dividing the values of each (centred) pattern by the root mean square of the entire pattern.

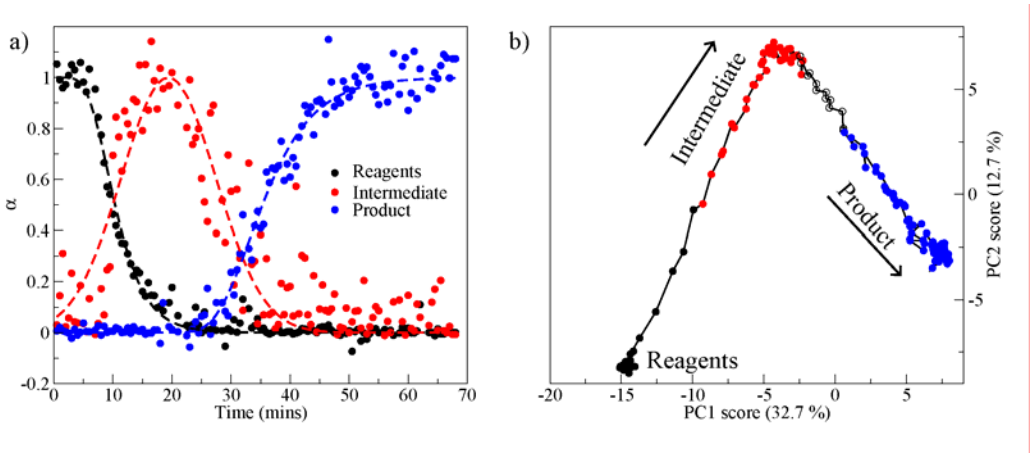

Figure S2

(a) Extent of reaction *vs.* time plot showing the change intensity of the host *002* reflection (●), intermediate *004* reflection (●) and the product *002* reflection (●) for the intercalation of MPA into h-$LiAl_2$-Cl at pH 4. **(b)** The variation in the score of PC1 as a function of PC2. Data points are colour coded as in part (a), with full circles representing situations where $\alpha > 0.5$ and empty circles situations where $\alpha < 0.5$.

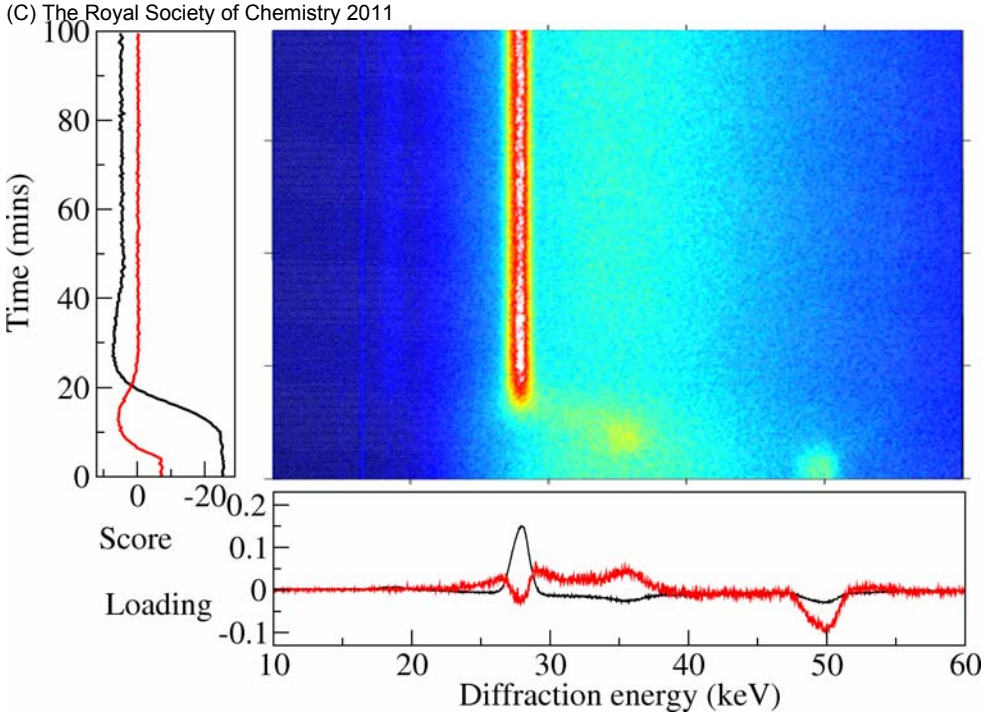

Figure S3

Variation of diffraction patterns (top right), PC1 and PC2 (top left) with time, and loadings (bottom) for the intercalation of EPA into h-$LiAl_2$-Cl at pH 8. PC1 is in black, and PC2 in red. Raw data have been mean-centred and scaled by dividing the values of each (centred) pattern by the root mean square of the entire pattern.

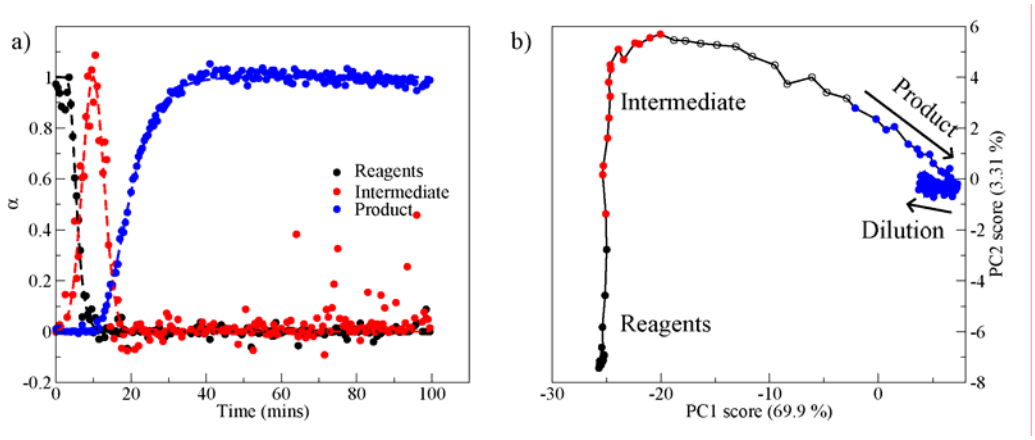

Figure S4

(a) Extent of reaction *vs.* time plot showing the change intensity of the host *002* reflection (●), intermediate *004* reflection (●) and the product *002* reflection (●) for the intercalation of EPA into h-$LiAl_2$-Cl at pH 8. **(b)** The variation in the score of PC1 as a function of PC2. Data points are colour coded as in part (a), with full circles representing situations where $\alpha > 0.5$ and empty circles situations where $\alpha < 0.5$.

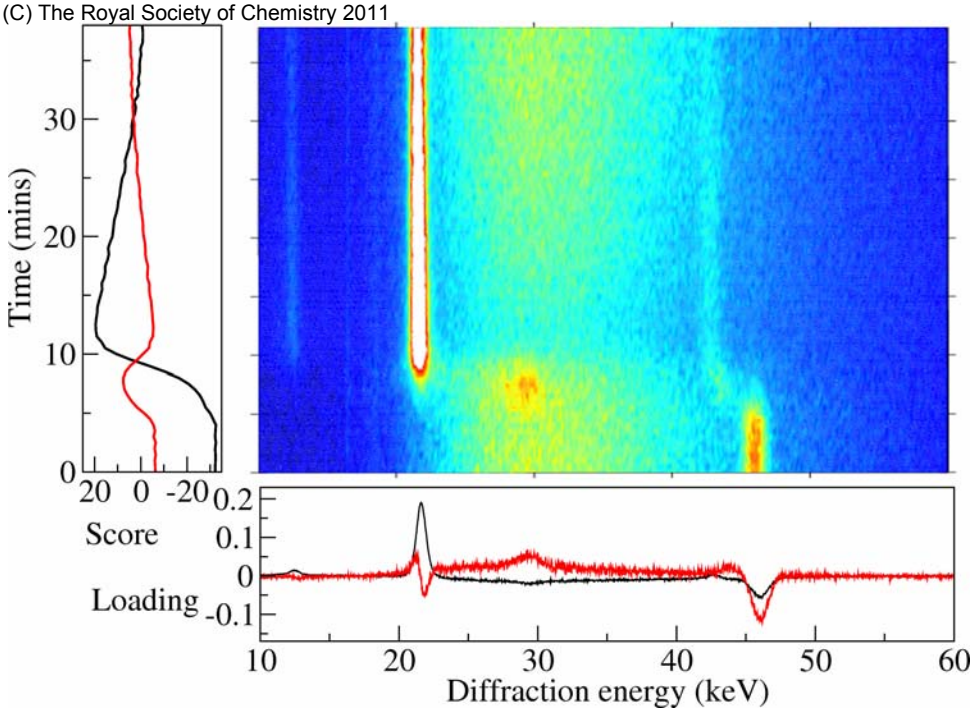

Figure S5

Variation of diffraction patterns (top right), PC1 and PC2 (top left) with time, and loadings (bottom) for the intercalation of BPA into h-$LiAl_2$-Cl at pH 8. PC1 is in black, and PC2 in red. Raw data have been mean-centred and scaled by dividing the values of each (centred) pattern by the root mean square of the entire pattern.

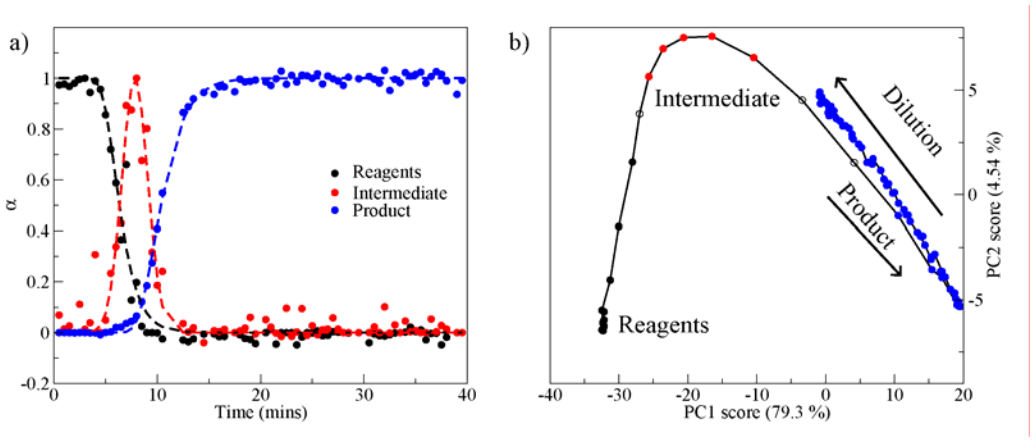

Figure S6

(a) Extent of reaction *vs.* time plot showing the change intensity of the host *002* reflection (●), intermediate *004* reflection (●) and the product *002* reflection (●) for the intercalation of BPA into h-$LiAl_2$-Cl at pH 8. **(b)** The variation in the score of PC1 as a function of PC2. Data points are colour coded as in part (a), with full circles representing situations where $\alpha > 0.5$ and empty circles situations where $\alpha < 0.5$.

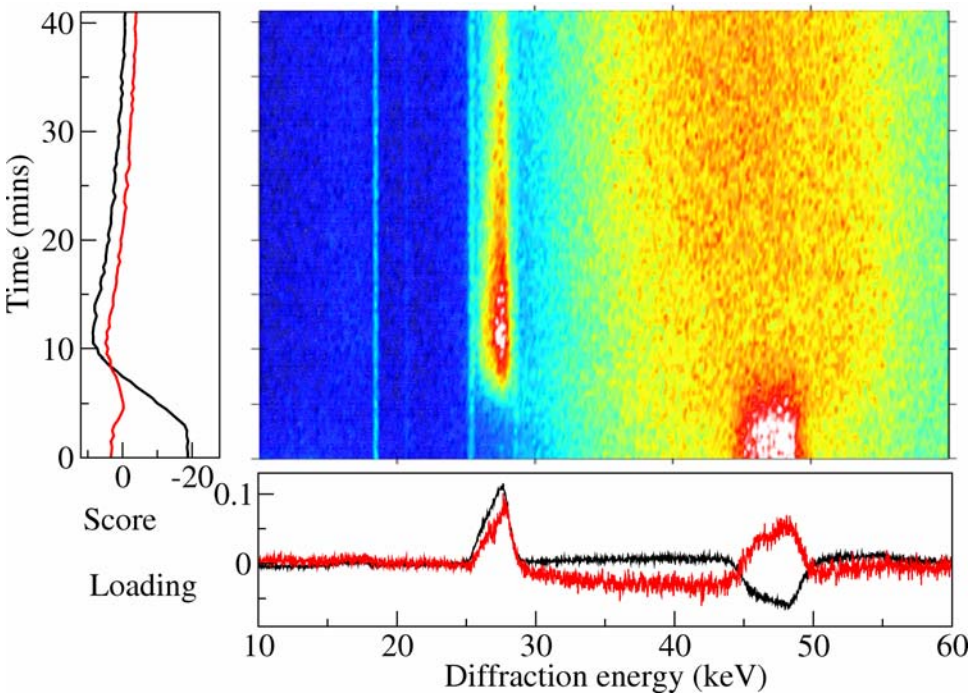

Figure S7

Variation of diffraction patterns (top right), PC1 and PC2 (top left) with time, and loadings (bottom) for the intercalation of PPA into h-$LiAl_2$-NO_3 at pH 8. PC1 is in black, and PC2 in red. Raw data have been mean-centred and scaled by dividing the values of each (centred) pattern by the root mean square of the entire pattern.

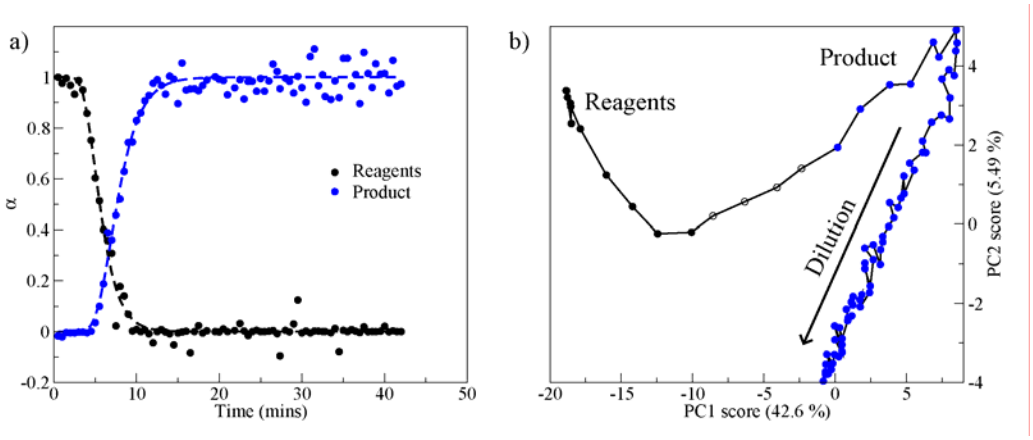

Figure S8

(a) Extent of reaction *vs.* time plot showing the change intensity of the host *002* reflection (●), and the product *002* reflection (●) for the intercalation of PPA into h-$LiAl_2$-NO_3 at pH 8. **(b)** The variation in the score of PC1 as a function of PC2. Data points are colour coded as in part (a), with full circles representing situations where $\alpha > 0.5$ and empty circles situations where $\alpha < 0.5$.

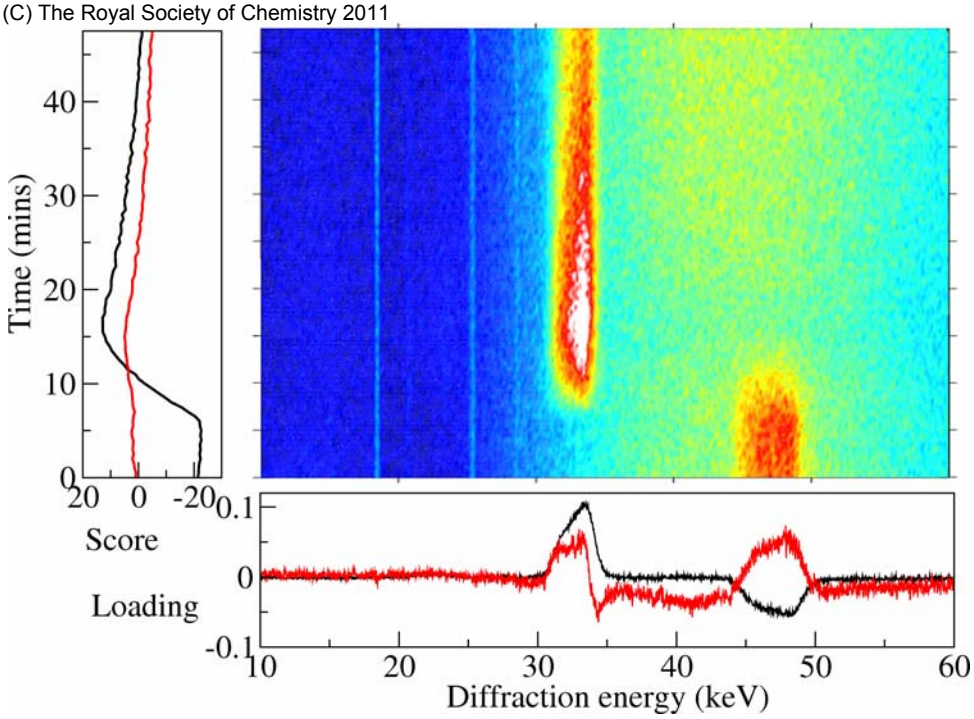

Figure S9

Variation of diffraction patterns (top right), PC1 and PC2 (top left) with time, and loadings (bottom) for the intercalation of MPA into h-$LiAl_2$-NO_3 at pH 8. PC1 is in black, and PC2 in red. Raw data have been mean-centred and scaled by dividing the values of each (centred) pattern by the root mean square of the entire pattern.

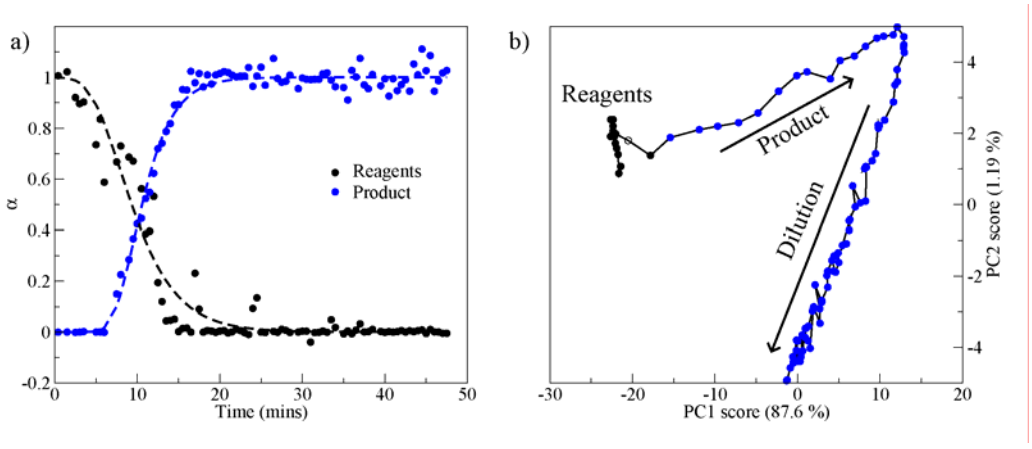

Figure S10

(a) Extent of reaction *vs.* time plot showing the change intensity of the host *002* reflection (●), and the product *002* reflection (●) for the intercalation of MPA into h-$LiAl_2$-NO_3 at pH 8. **(b)** The variation in the score of PC1 as a function of PC2. Data points are colour coded as in part (a), with full circles representing situations where $\alpha > 0.5$ and empty circles situations where $\alpha < 0.5$.

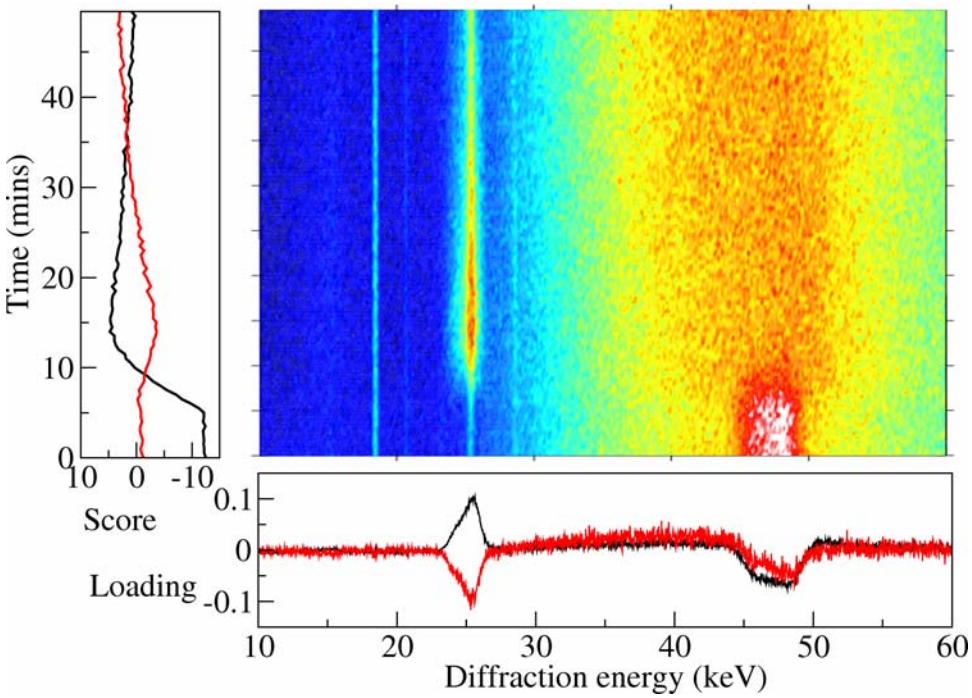

Figure S11

Variation of diffraction patterns (top right), PC1 and PC2 (top left) with time, and loadings (bottom) for the intercalation of EPA into h-$LiAl_2$-NO_3 at pH 8. PC1 is in black, and PC2 in red. Raw data have been mean-centred and scaled by dividing the values of each (centred) pattern by the root mean square of the entire pattern.

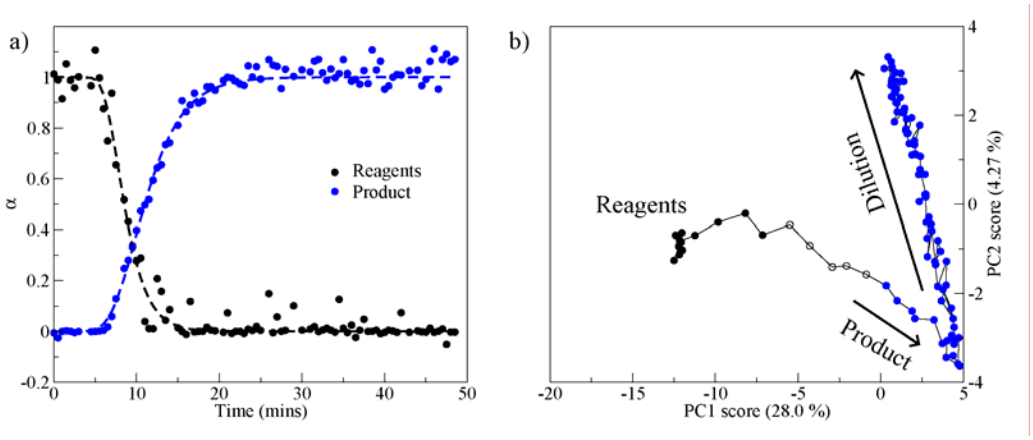

Figure S12

(a) Extent of reaction *vs.* time plot showing the change intensity of the host *002* reflection (●), and the product *002* reflection (●) for the intercalation of EPA into h-$LiAl_2$-NO_3 at pH 8. **(b)** The variation in the score of PC1 as a function of PC2. Data points are colour coded as in part (a), with full circles representing situations where $\alpha > 0.5$ and empty circles situations where $\alpha < 0.5$.

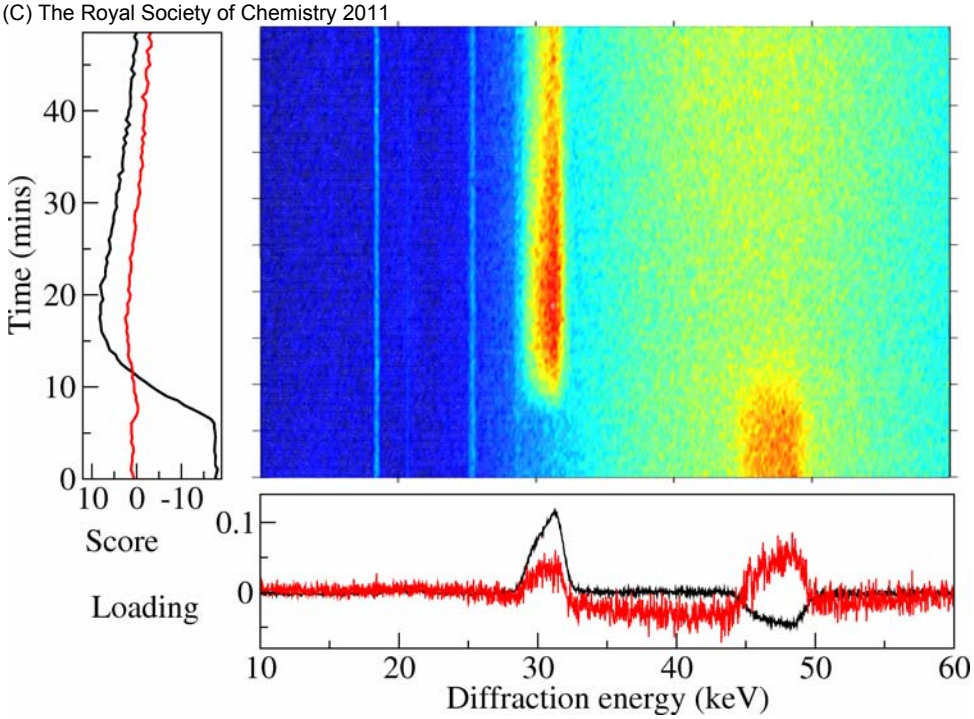

Figure S13

Variation of diffraction patterns (top right), PC1 and PC2 (top left) with time, and loadings (bottom) for the intercalation of BPA into h-$LiAl_2$-NO_3 at pH 8. PC1 is in black, and PC2 in red. Raw data have been mean-centred and scaled by dividing the values of each (centred) pattern by the root mean square of the entire pattern.

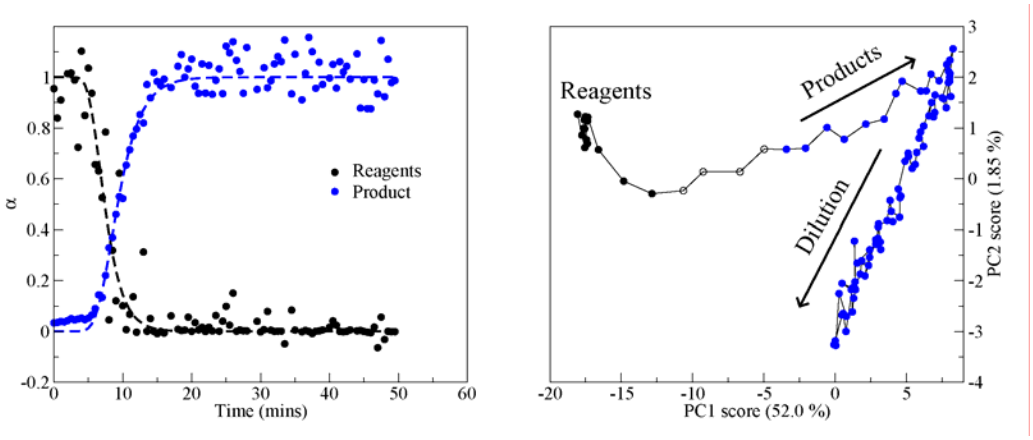

Figure S14

(a) Extent of reaction *vs.* time plot showing the change intensity of the host *002* reflection (●), and the product *002* reflection (●) for the intercalation of BPA into h-$LiAl_2$-NO_3 at pH 8. **(b)** The variation in the score of PC1 as a function of PC2. Data points are colour coded as in part (a), with full circles representing situations where $\alpha > 0.5$ and empty circles situations where $\alpha < 0.5$.