

## Figure Captions

Fig. S1 Difference Fourier map of **1** at 350K on O1-C1-N1-C2-O2-N2 plane. Contour level is 0.1 e Å<sup>-3</sup>.

Fig. S2 Difference Fourier map of **1** at 350K on C11-C12-C13 plane. Contour level is 0.1 e Å<sup>-3</sup>.

Fig. S3 Difference Fourier map of **1** at 350K on C13-C14-C15 plane. Contour level is 0.1 e Å<sup>-3</sup>.

Fig. S4 Difference Fourier map of **1** at 350K on N2-C21-C22 plane. Contour level is 0.1 e Å<sup>-3</sup>.

Fig. S5 Difference Fourier map of **1** at 374K on O1-C1-N1-C2-O2-N2 plane. Contour level is 0.1 e Å<sup>-3</sup>.

Fig. S6 Difference Fourier map of **1** at 374K on C11A-C12A-C13A plane. Contour level is 0.1 e Å<sup>-3</sup>.

Fig. S7 Difference Fourier map of **1** at 374K on C13A-C14A-C15A plane. Contour level is 0.1 e Å<sup>-3</sup>.

Fig. S8 Difference Fourier map of **1** at 374K on C11B-C12B-C13B plane. Contour level is 0.1 e Å<sup>-3</sup>.

Fig. S9 Difference Fourier map of **1** at 374K on C13B-C14B-C15B plane. Contour level is 0.1 e Å<sup>-3</sup>.

Fig. S10 Difference Fourier map of **1** at 374K on N2-C21-C22 plane. Contour level is 0.1 e Å<sup>-3</sup>.

Fig. S11 Difference Fourier map of **2** at 348K on O1-C1-N1-C2-O2-N2 plane. Contour level is 0.1 e Å<sup>-3</sup>.

Fig. S12 Difference Fourier map of **2** at 348K on C11-C12-C13 plane. Contour level is 0.1 e Å<sup>-3</sup>.

Fig. S13 Difference Fourier map of **2** at 348K on C13-C14-C15 plane. Contour level is 0.1 e Å<sup>-3</sup>.

Fig. S14 Difference Fourier map of **2** at 348K on C21-C22-C23 plane. Contour level is 0.1 e Å<sup>-3</sup>.

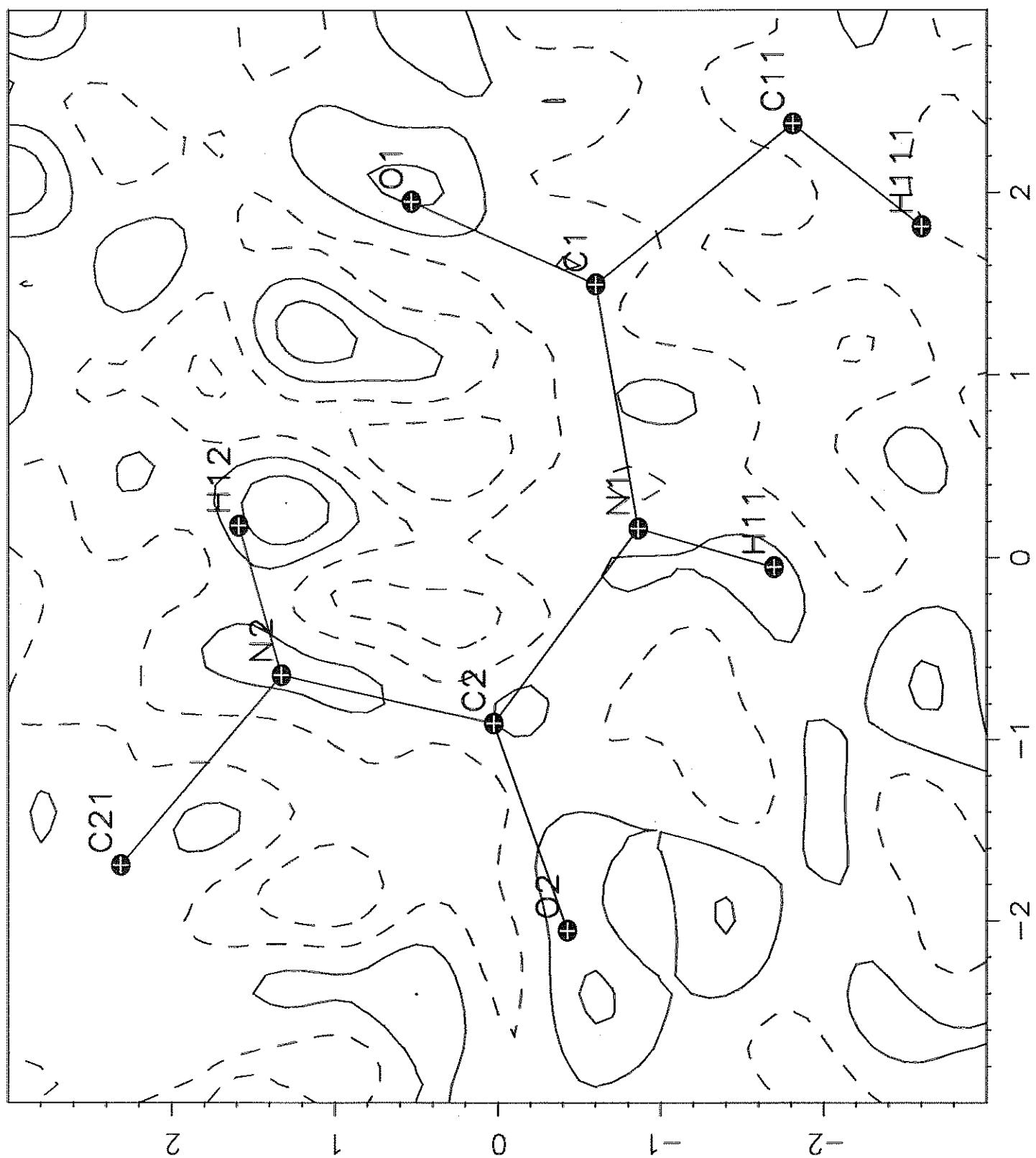


Fig. S1

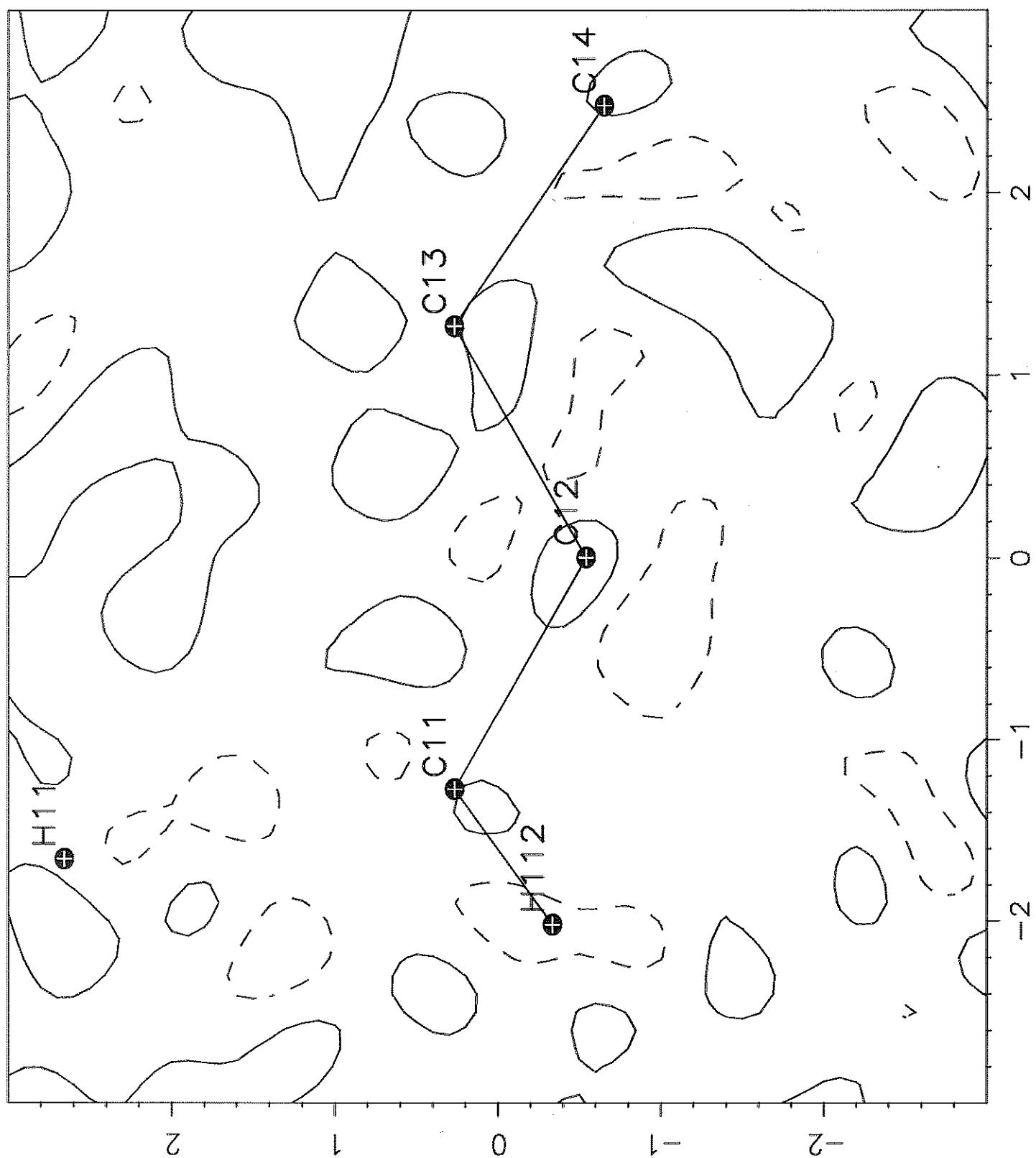


Fig. S2

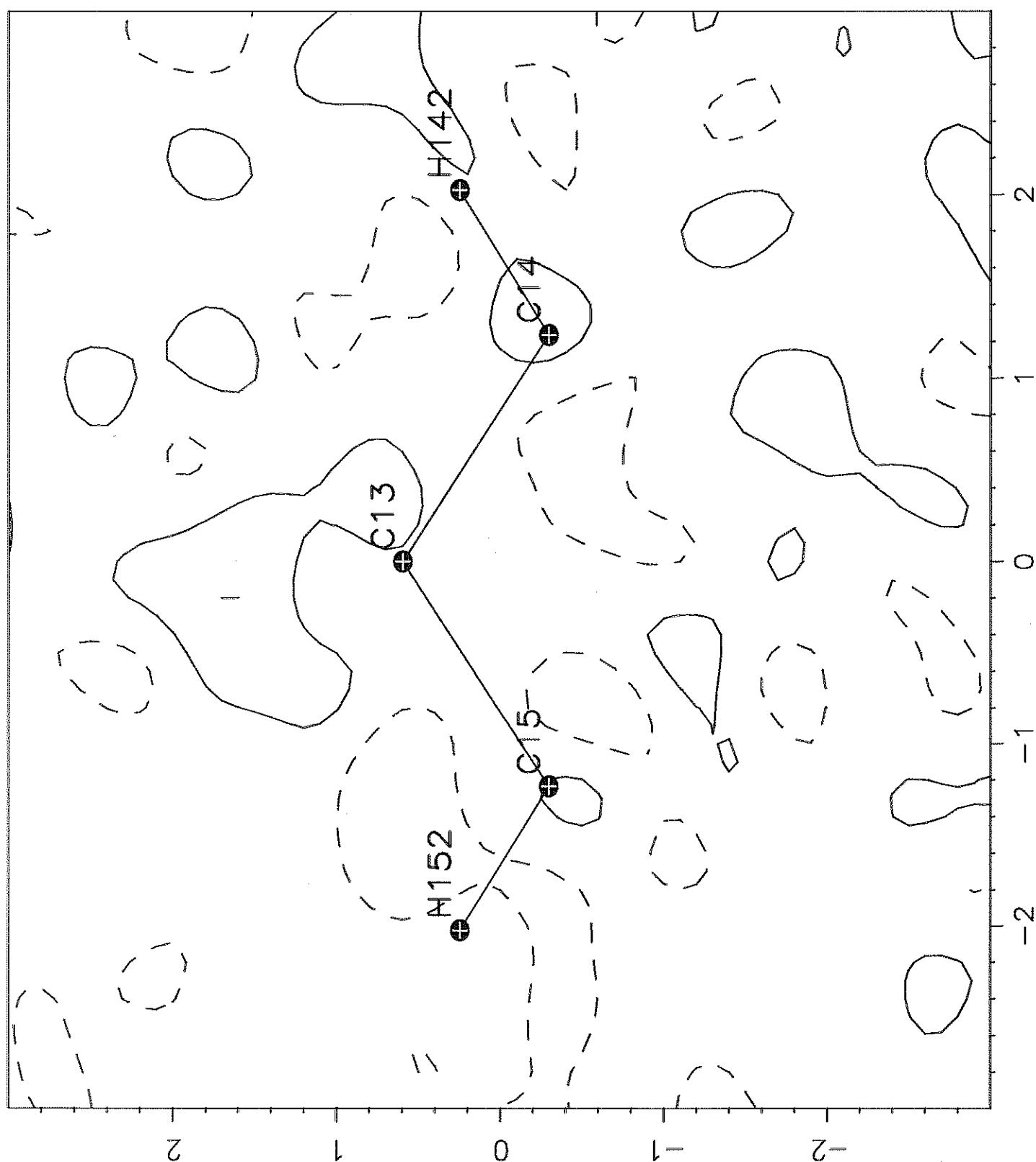


Fig. S3

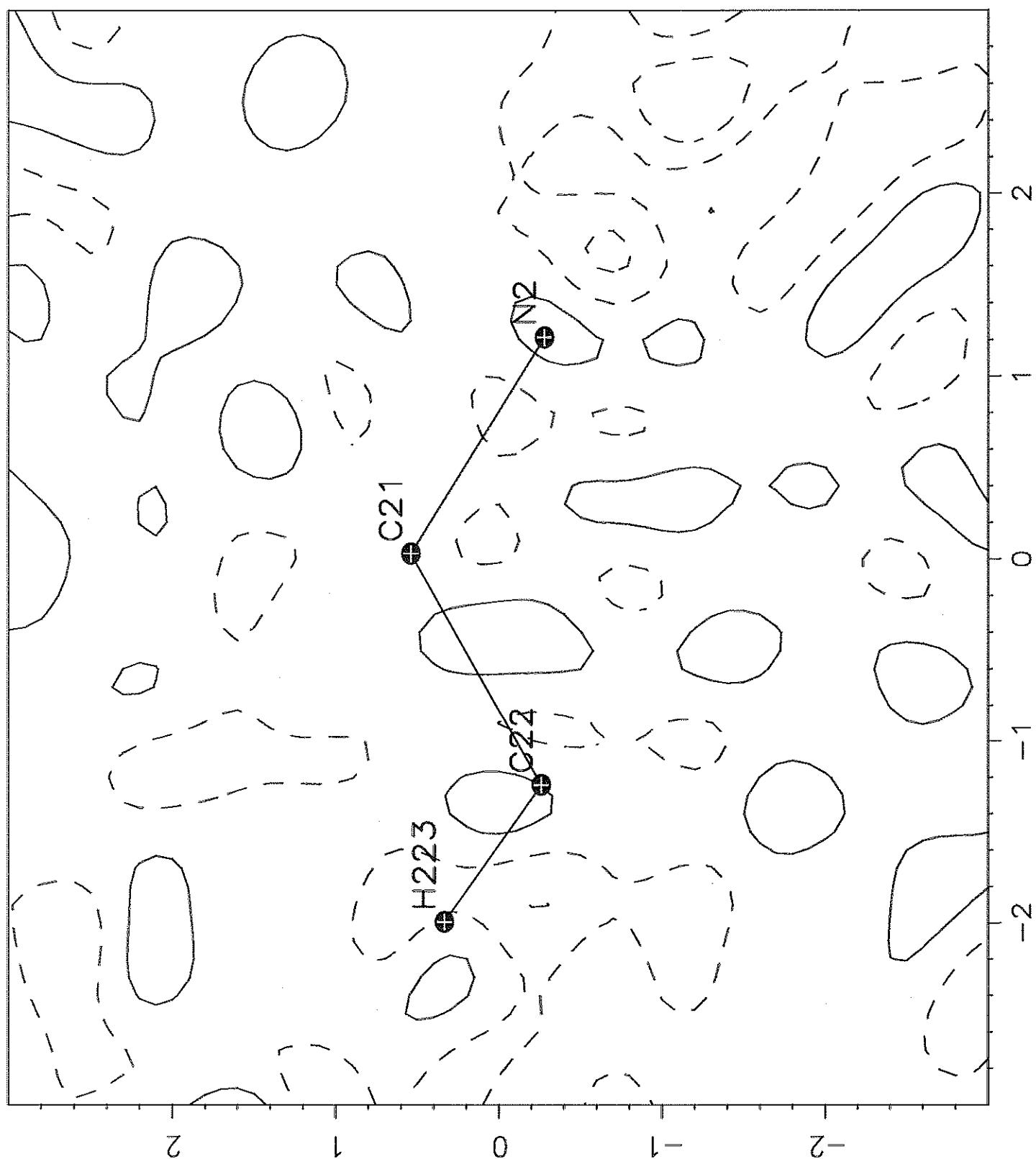


Fig. S4

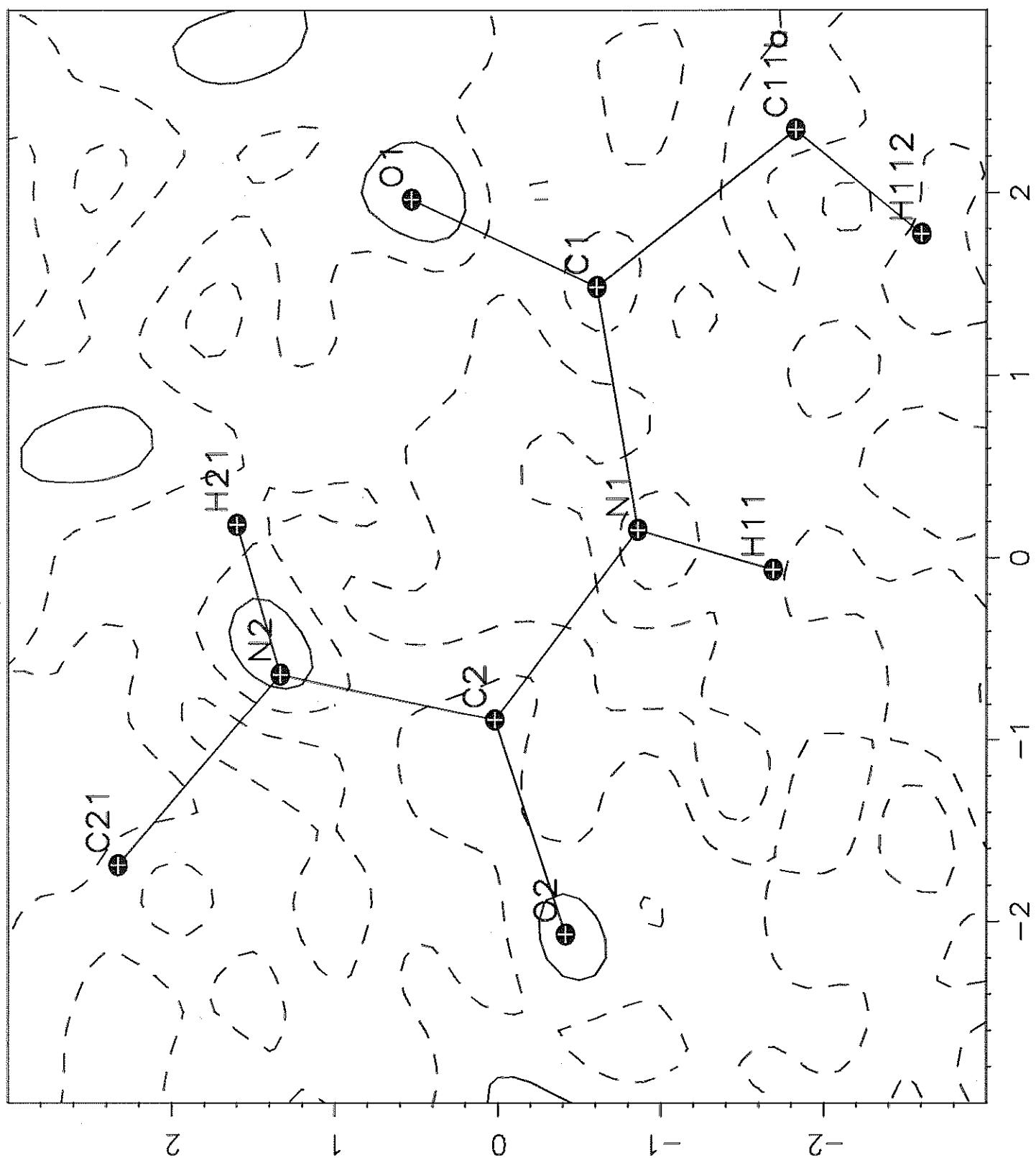


Fig. S5

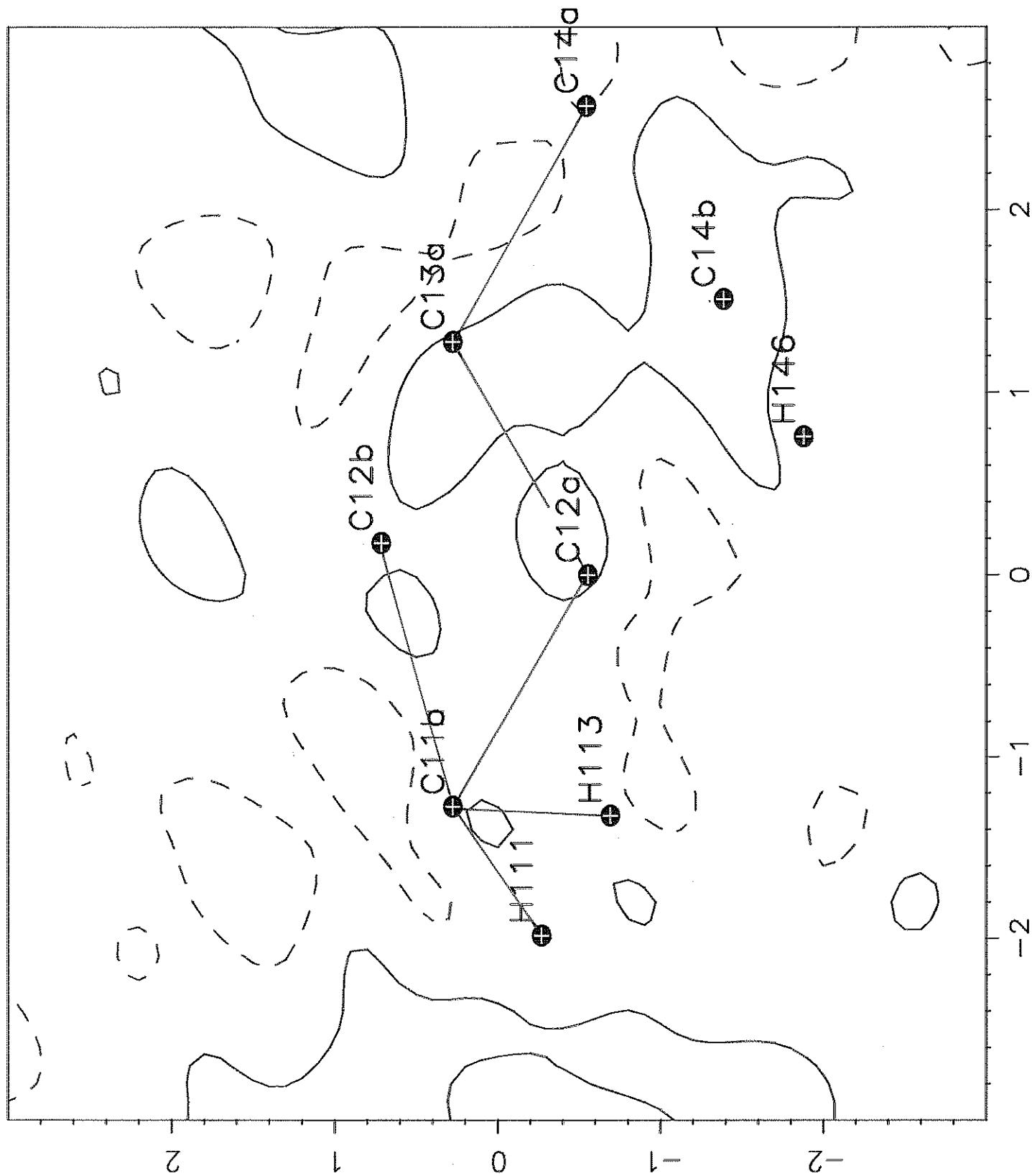


Fig. S6

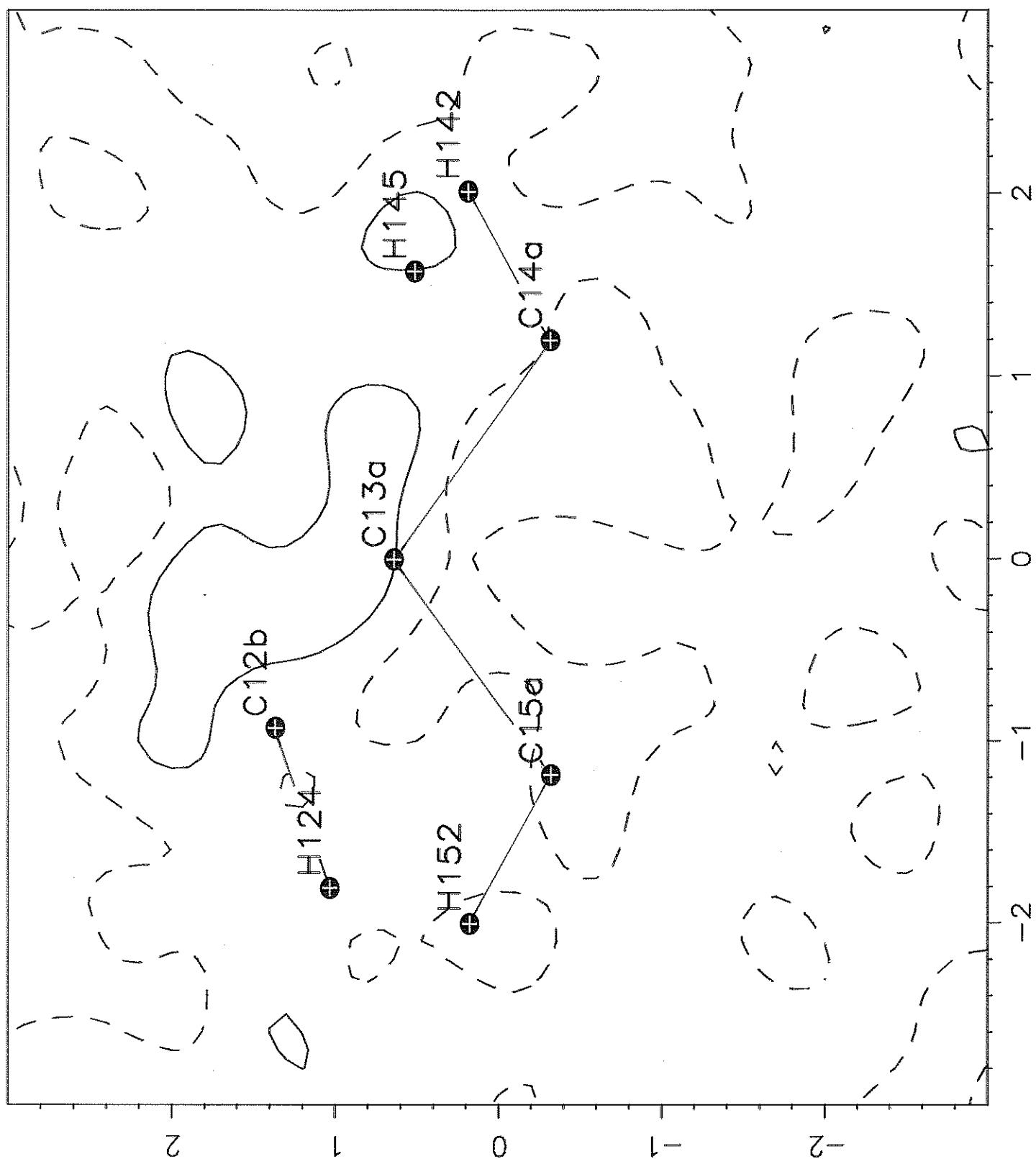


Fig. S7

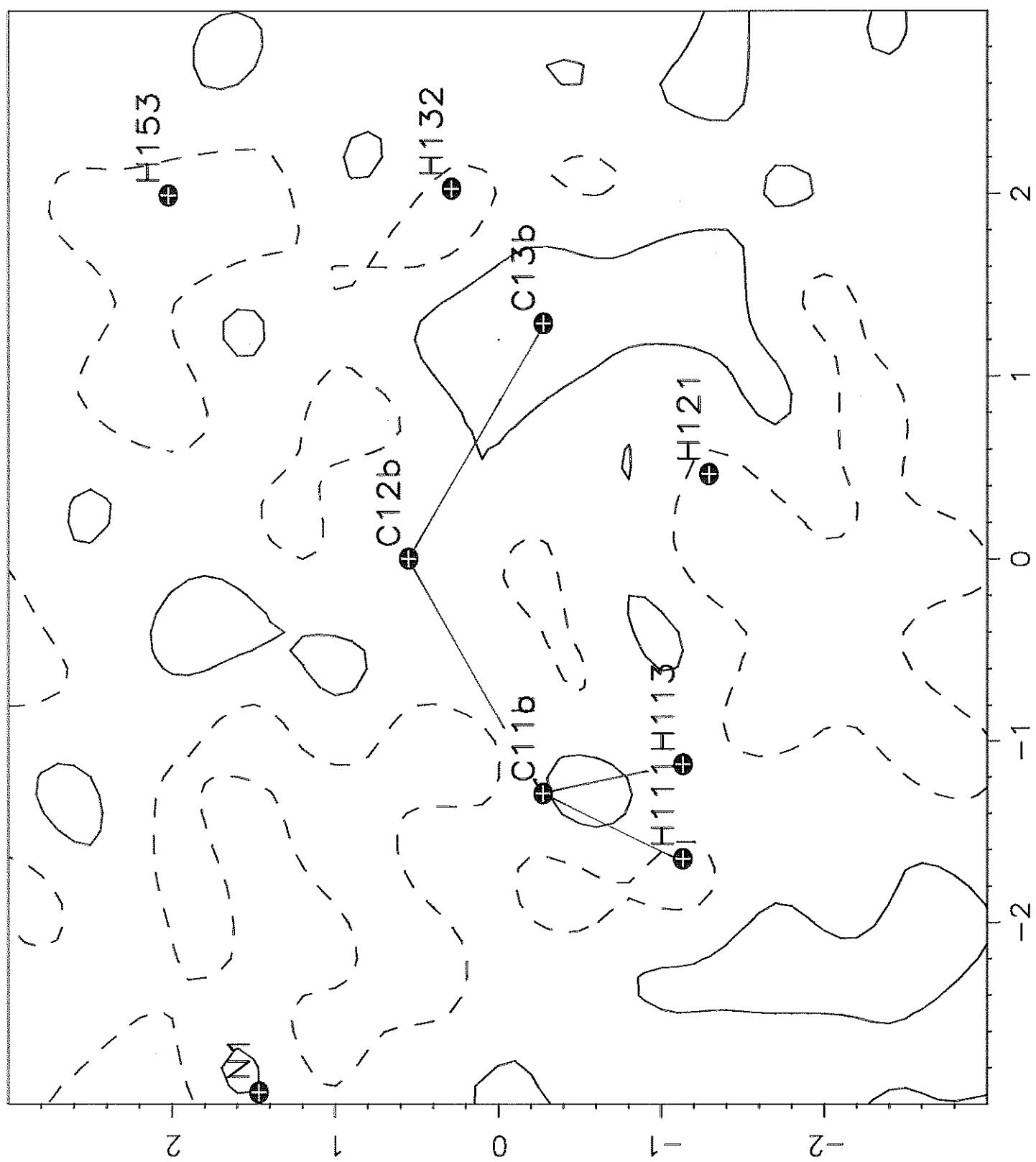


Fig. S8

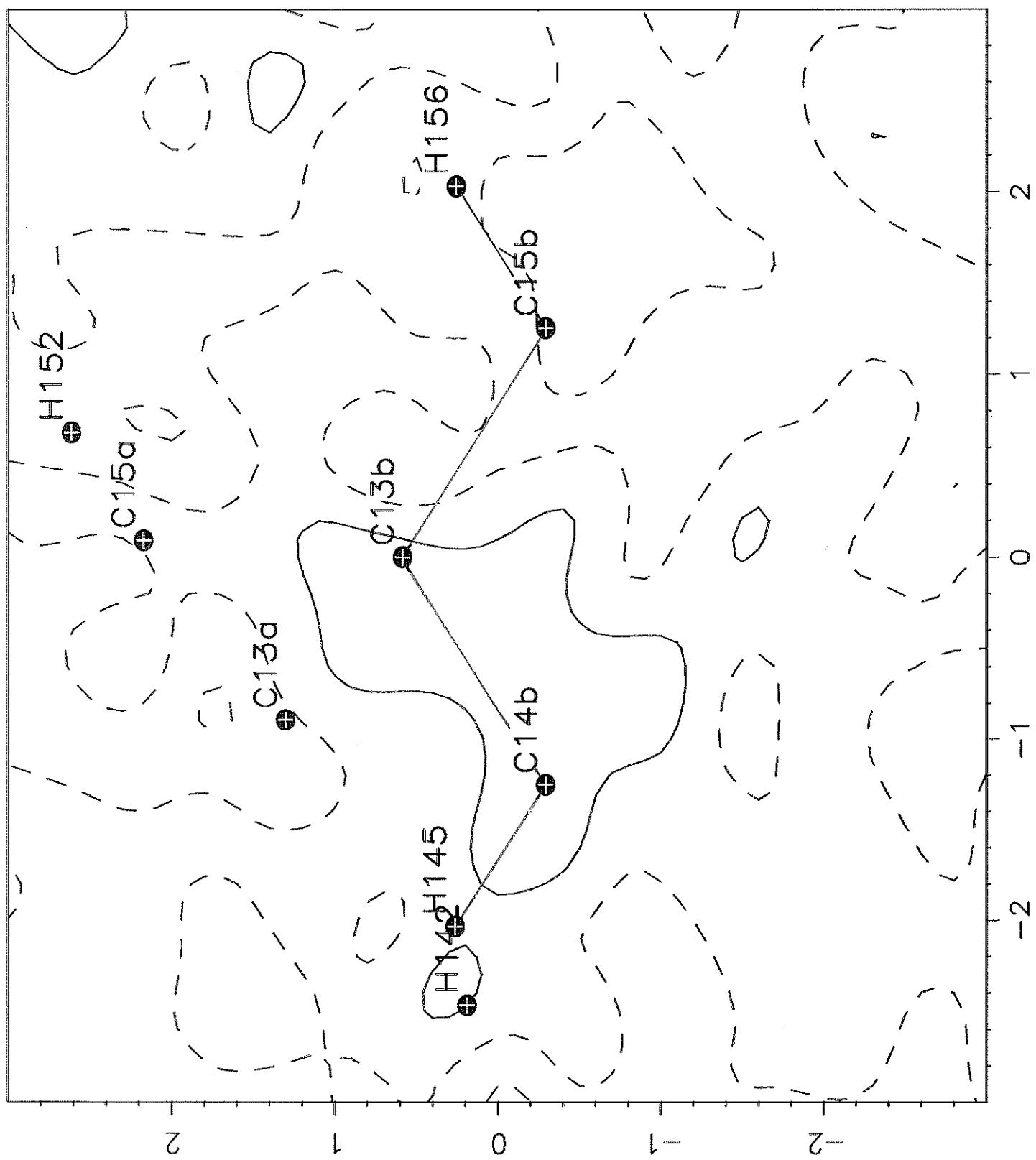


Fig. S9

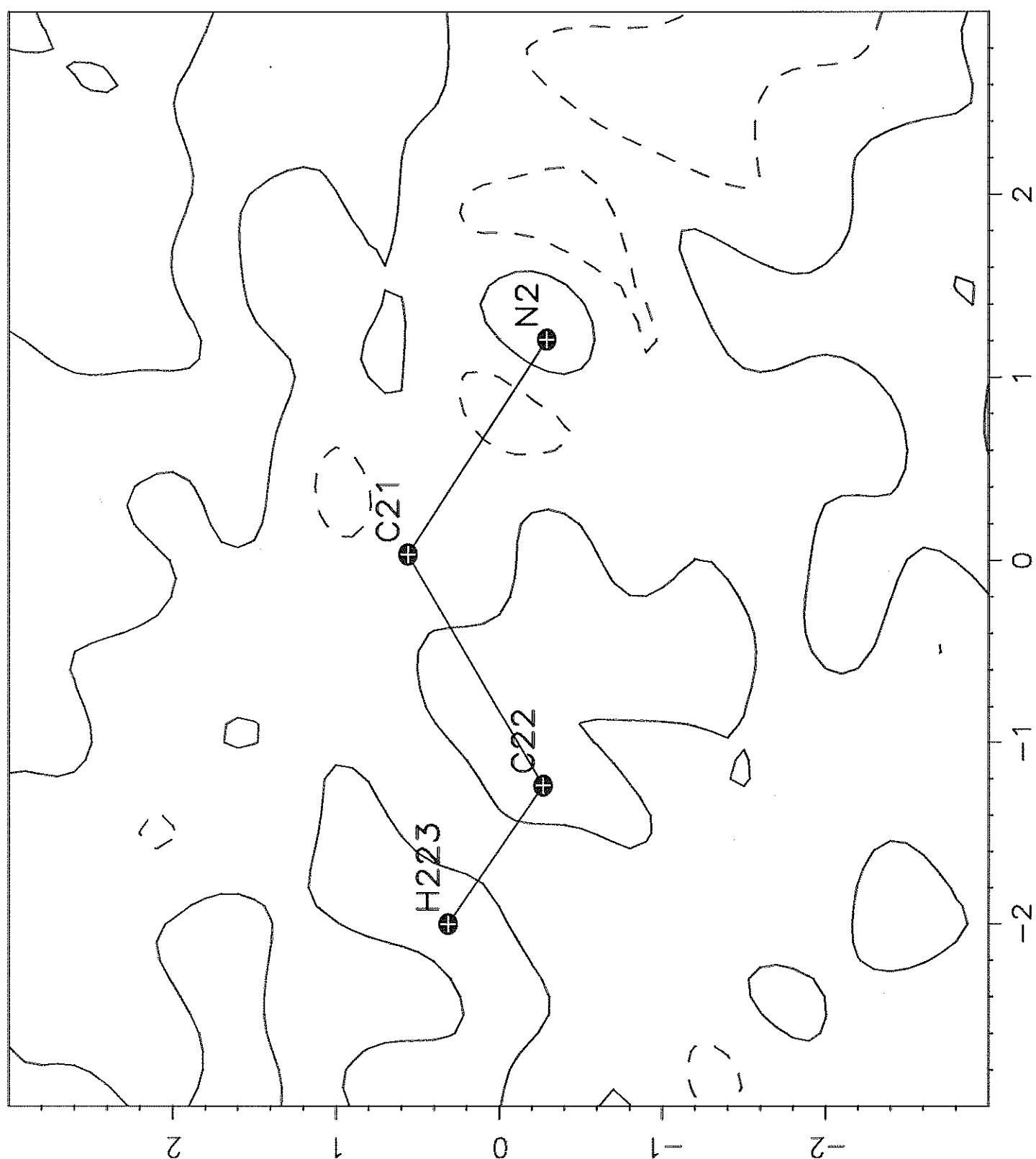


Fig. S10

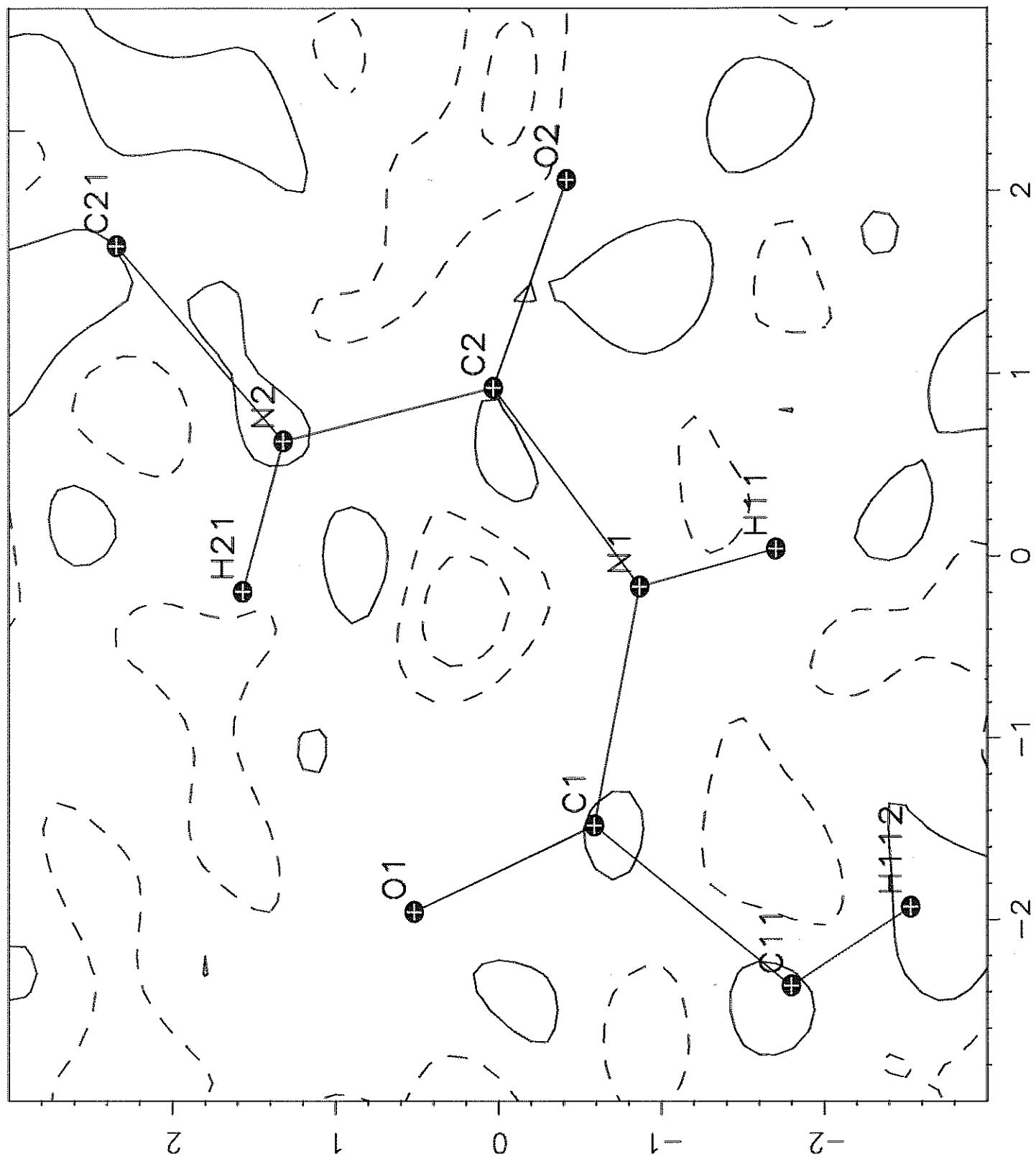


Fig. S11

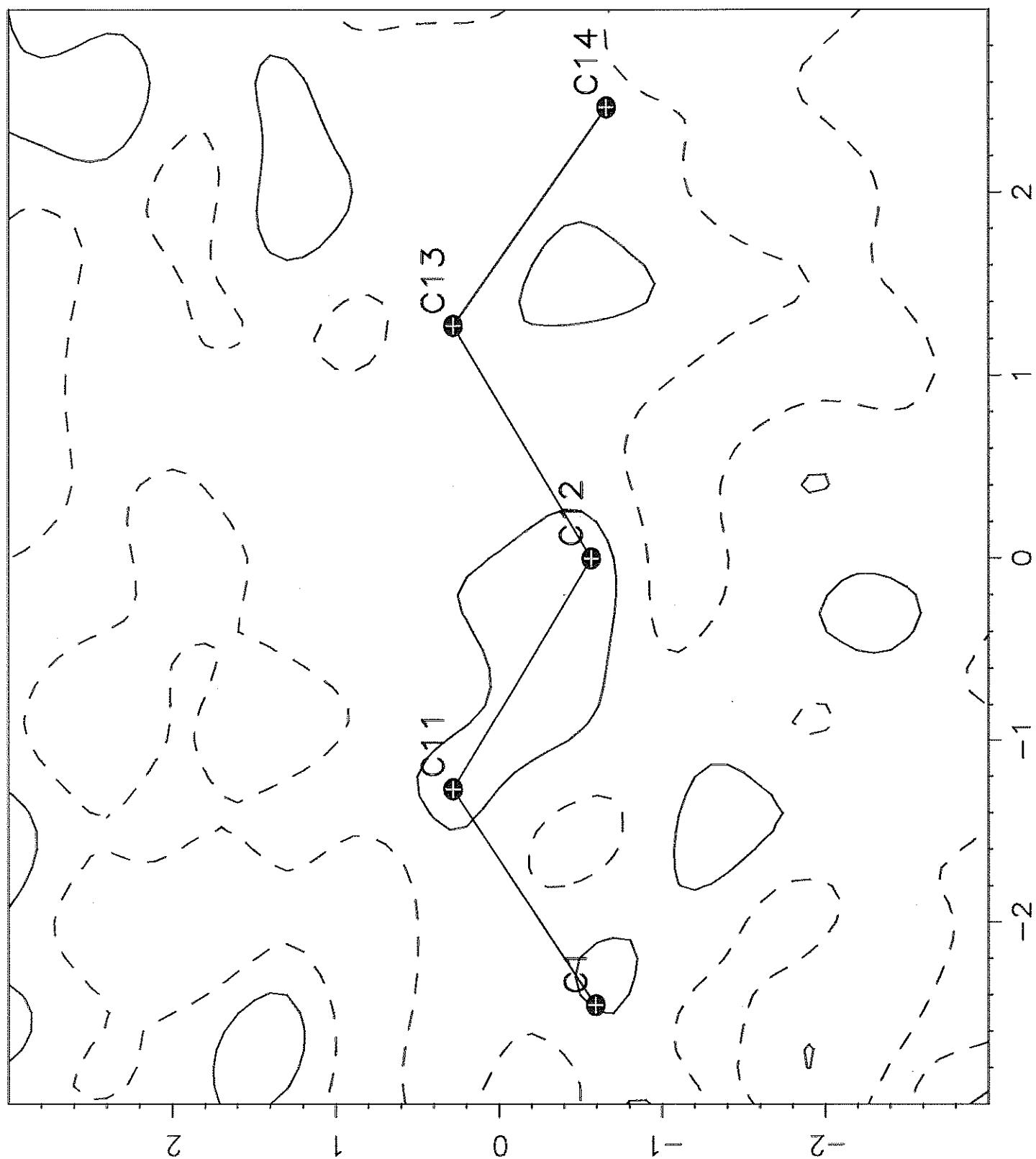


Fig. S12

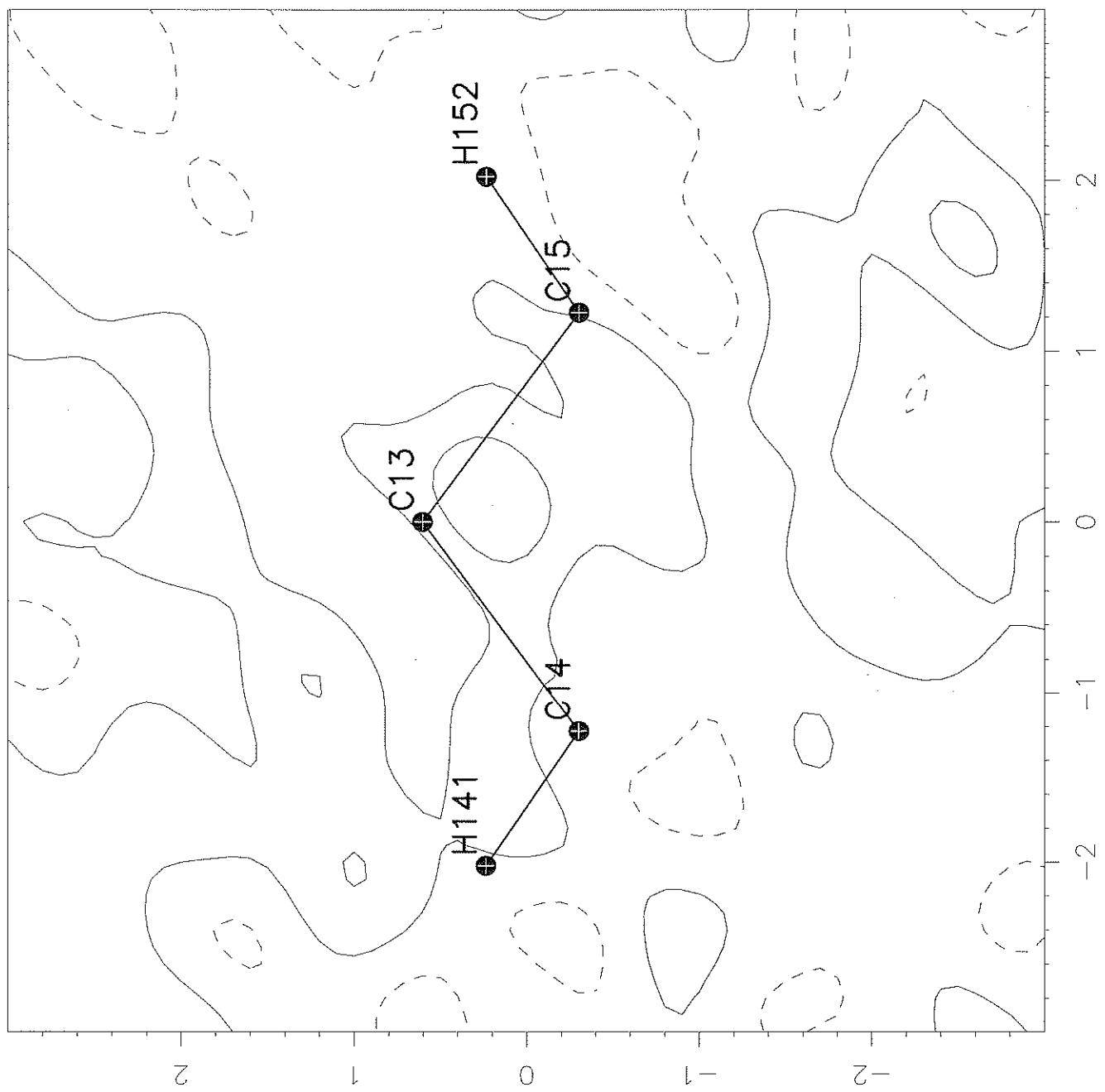


Fig. S13

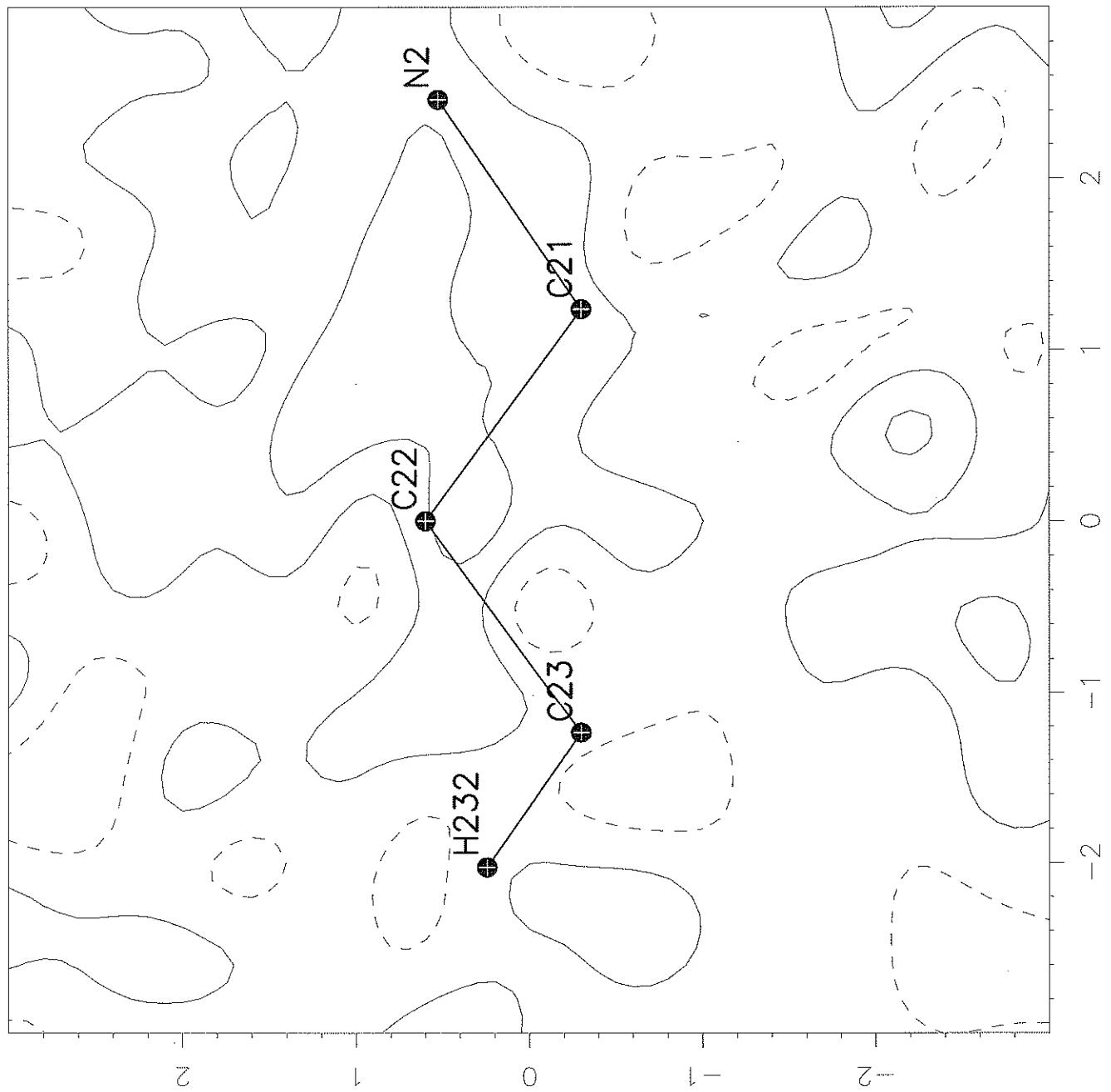


Fig. S14