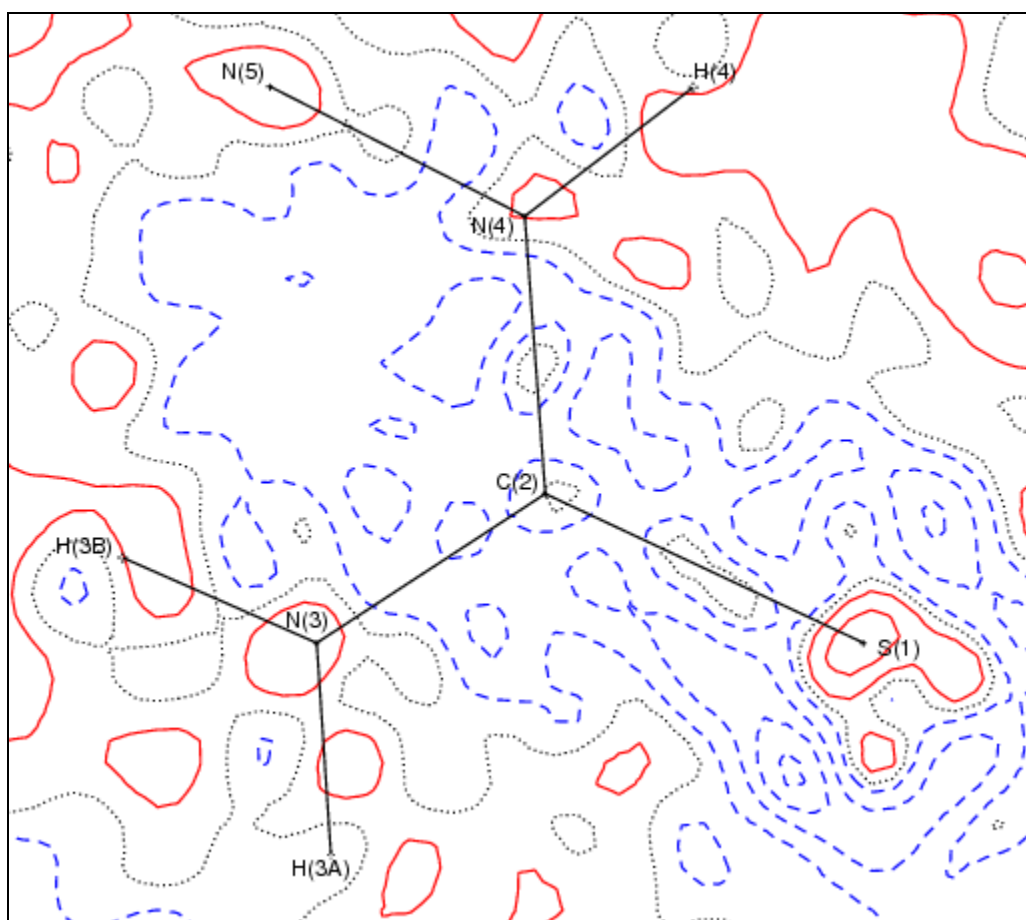
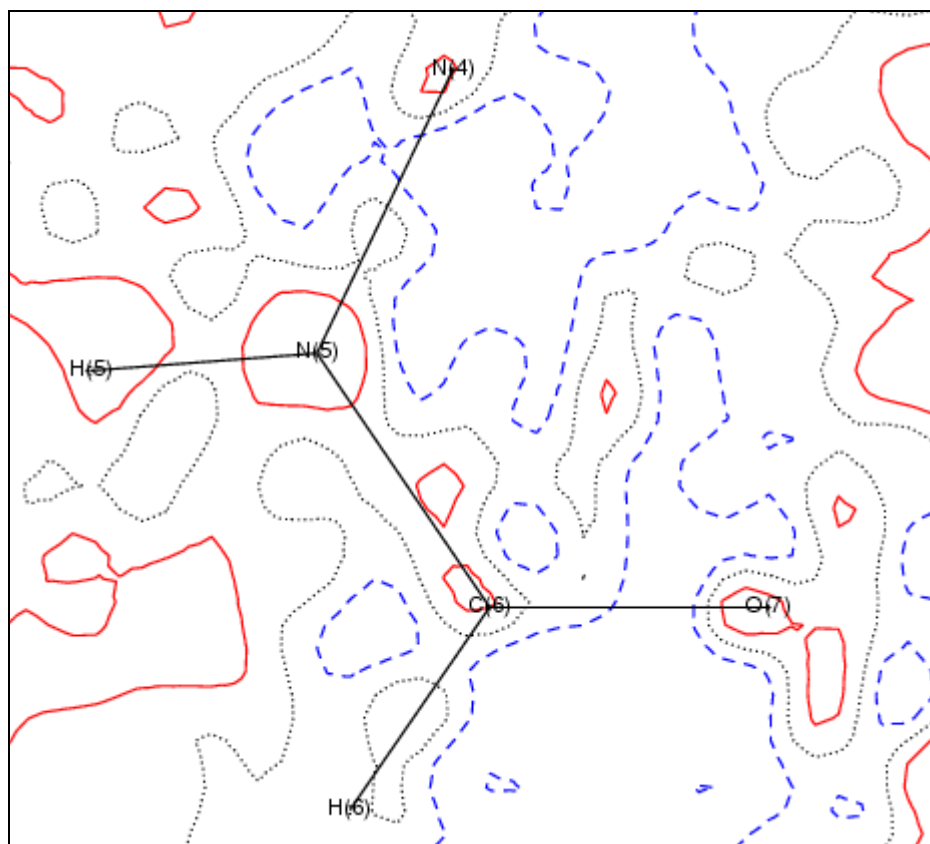


## Supplementary Material

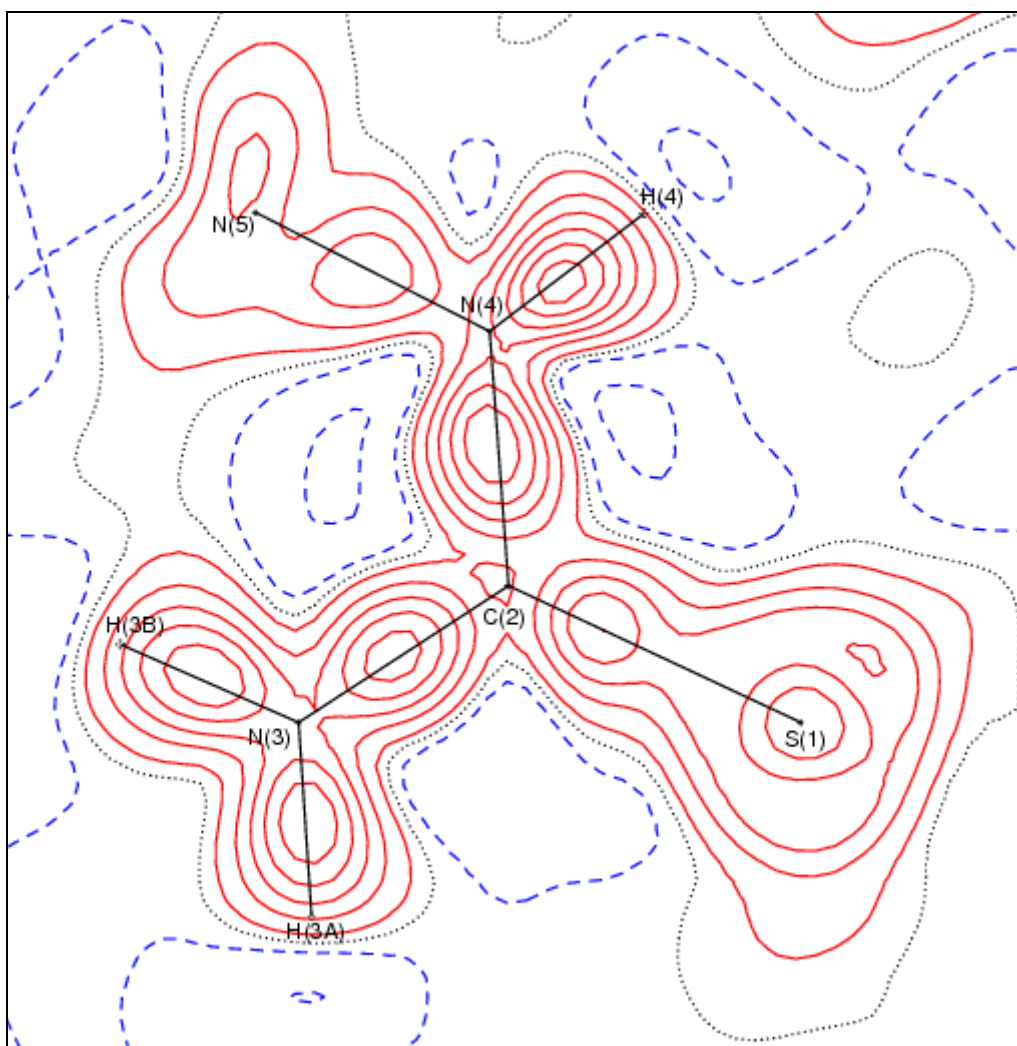
**Figure S1a.** Residual electron density map in the S(1)–N(3)–N(4) plane. For all residual density maps, the positive (solids red lines) and negative (broken blue lines) contour starts at  $\pm 0.05 \text{ e } \text{\AA}^{-3}$  and with the intervals of  $\pm 0.1 \text{ e } \text{\AA}^{-3}$ . Contours at zero are shown as black dotted lines.



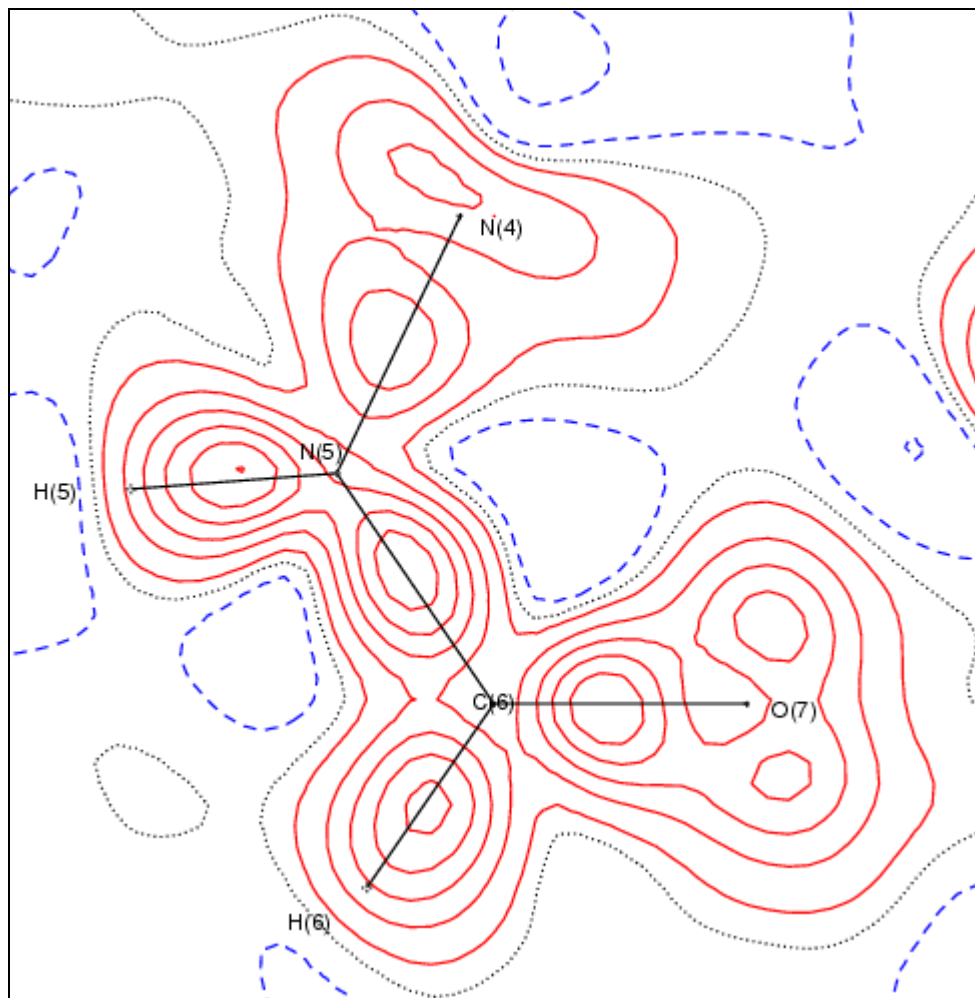
**Figure S1b.** Residual electron density map in the O(7)–C(6)–N(5)–N(4) plane.



**Figure S2a.** Dynamic deformation electron density map in the S1–N3–N4 plane. For all dynamic deformation density maps, the positive (solid red lines) and negative (broken blue lines) contour starts at  $\pm 0.05 \text{ e } \text{Å}^{-3}$  and with the intervals of  $\pm 0.1 \text{ e } \text{Å}^{-3}$ . The contours at zero are shown as black dotted lines.



**Figure S2b.** Dynamic deformation electron density map in the O7–C(6)–N5–N4 plane.



**Table S1.** Experimental and Theoretical Radial parameters.

Atoms	Experiment		Theory	
	$\kappa$	$\kappa'$	$\kappa$	$\kappa'$
S(1)	1.085(3)	0.735(7)	0.990(1)	0.907(10)
O(7)	0.987(1)	0.727(5)	0.985(1)	0.938(12)
N(3)	0.989(1)	0.832(5)	0.991(1)	0.871(5)
N(4)	0.989(1)	0.832(5)	0.991(1)	0.871(5)
N(5)	0.989(1)	0.832(5)	0.991(1)	0.871(5)
C(2)	0.991(1)	0.779(3)	0.997(2)	0.852(4)
C(6)	0.991(1)	0.779(3)	0.997(2)	0.852(4)
H(3A)	1.2	1.2	1.2	1.2
H(3B)	1.2	1.2	1.2	1.2
H(4)	1.2	1.2	1.2	1.2
H(5)	1.2	1.2	1.2	1.2
H(6)	1.2	1.2	1.2	1.2



