Electronic Supplementary Material for PCCP

Supporting Information

for the paper

"The Progression of Strong and Weak Hydrogen Bonds in a Series of Ethylenediammonium Dithiocyanate Derivatives"

David J. Wolstenholme*[†], Jan J. Weigand[‡], Elinor Cameron[†], T. Stanley Cameron[†]

Department of Chemistry, Dalhousie University, Halifax, Nova Scotia, Canada, B3H 4J3, and Westfälische Wilhelms-Universität Münster, Institut für Anorganische und Analytische Chemie, Corrensstrasse 30/36, D-48149 Münster, Germany

* To whom the correspondence should be addressed. D. W.: phone, +1-(902)-494-3759, e-mail, dwolsten@dal.ca.
† Dalhousie University
‡ Westfälische Wilhelms-Universität Münster

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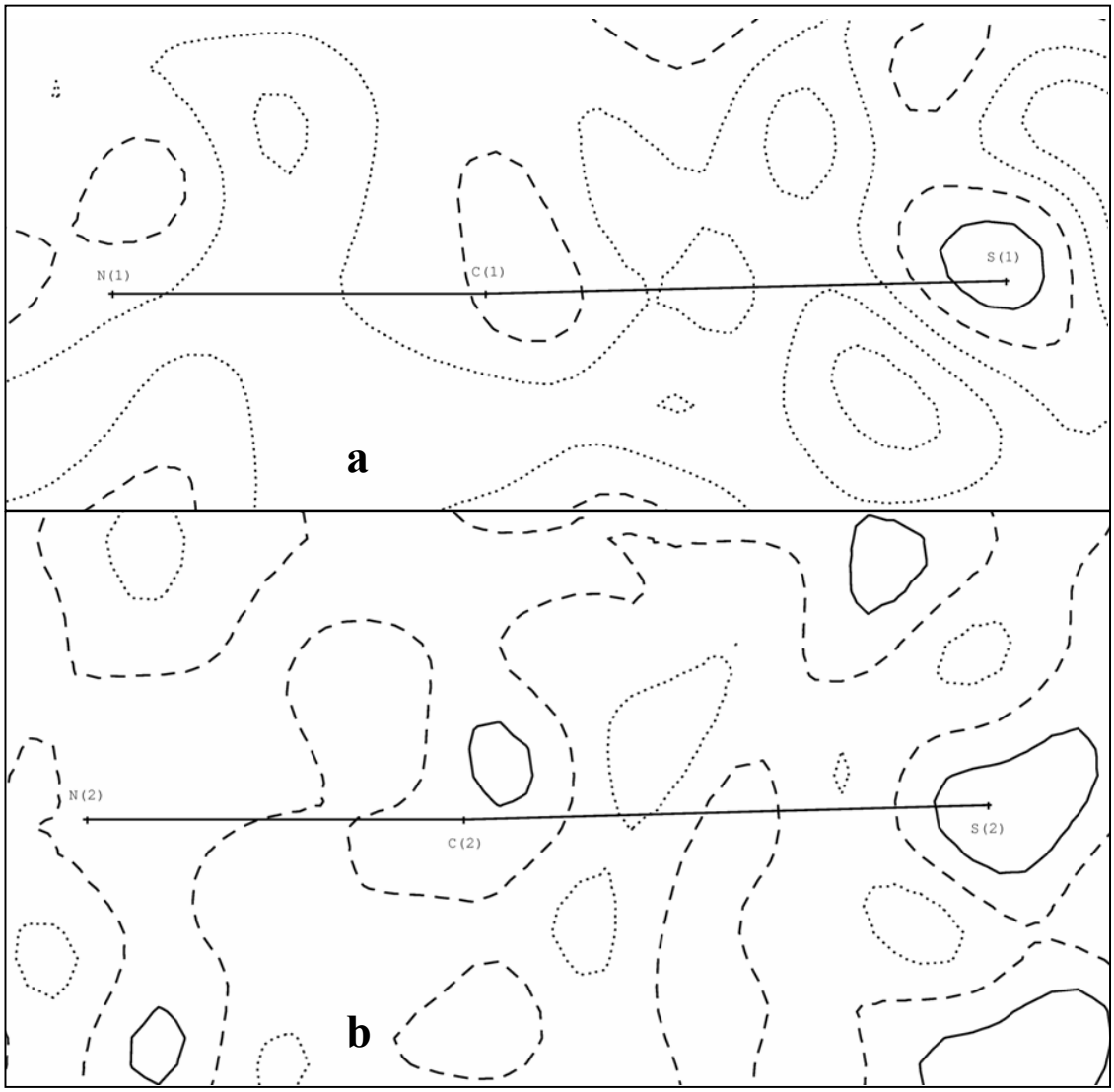
Residual Maps:



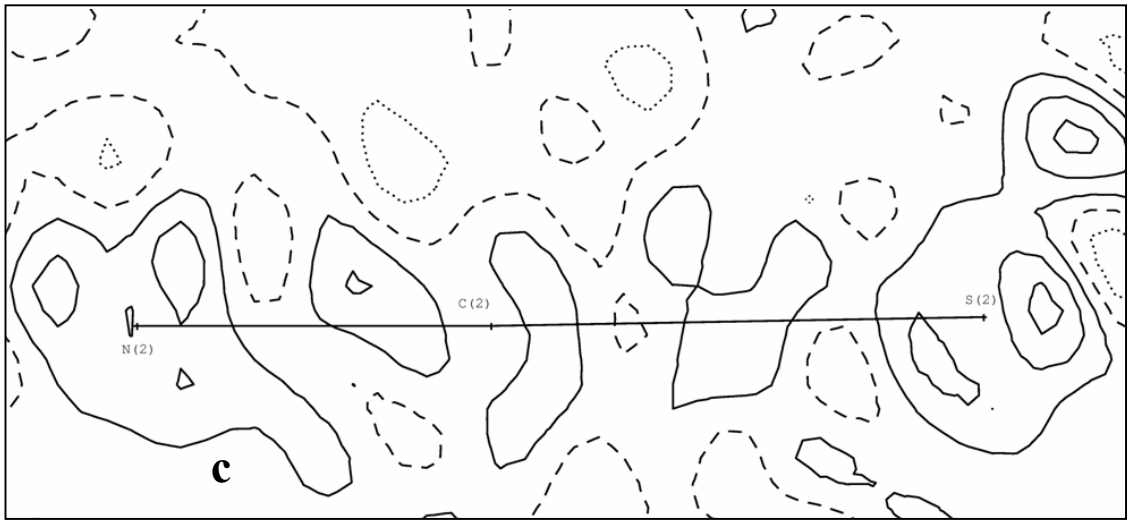
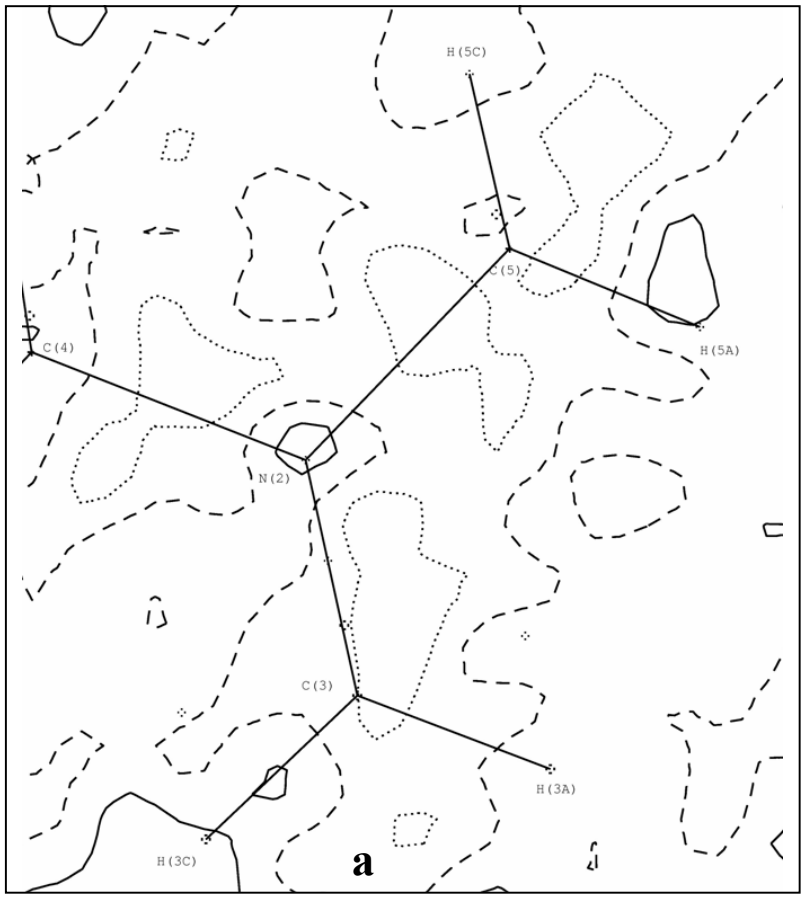


Fig. S1 Residual density maps with positive contours as solid lines, negative contour as dotted lines, and the zero contour line as dashes. a) the N1-C1-S1 plane of the thiocyanate in (I), b) the N2-C2-S2 plane of a thiocyanate in (III), and c) the N2-C2-S2 plane of a thiocyanate in (IV). All contour intervals are taken in increments of 0.1 eÅ^{-3}.



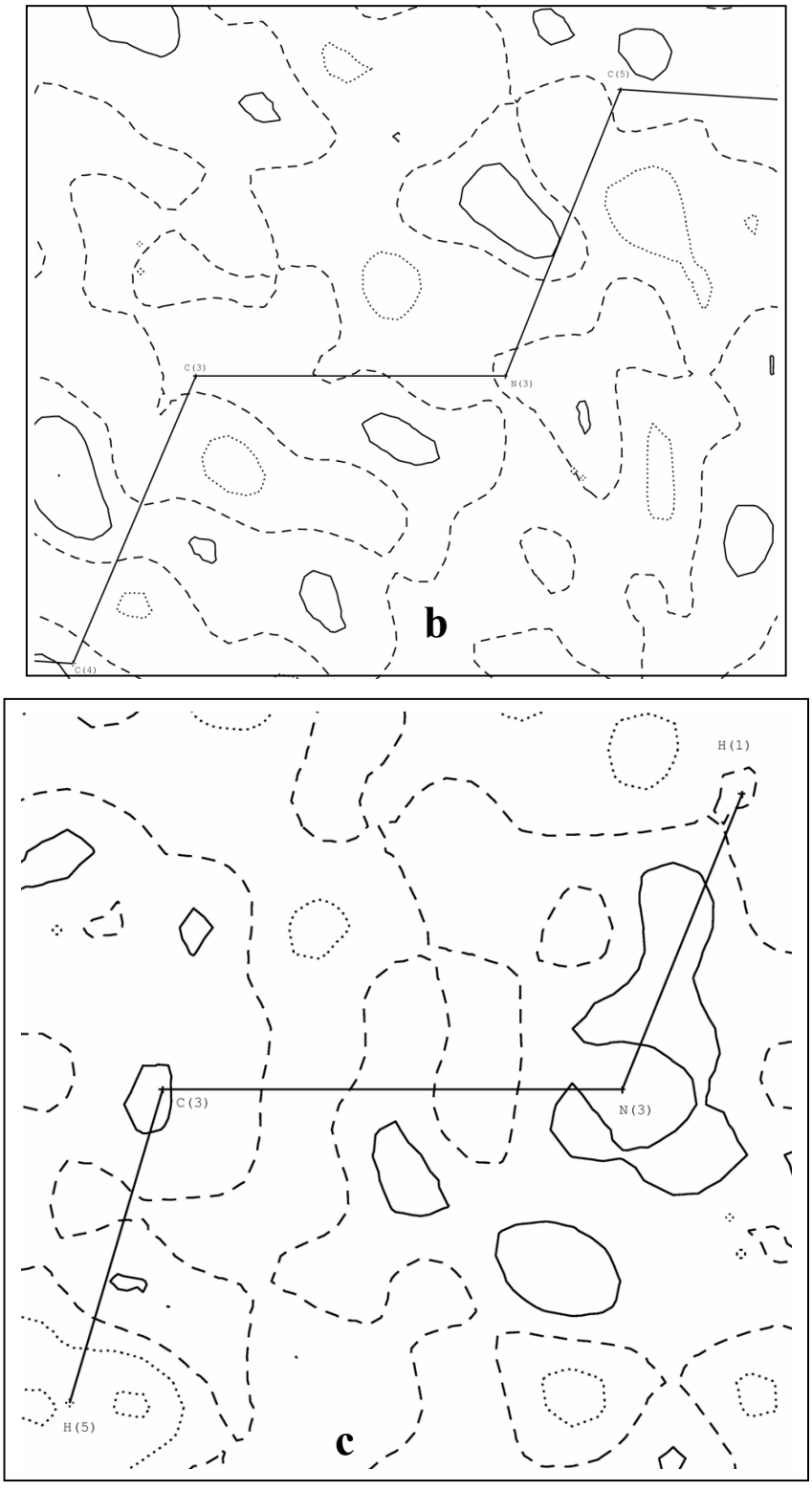


Fig. S2 Residual density maps with positive contours as solid lines, negative contour as dotted lines, and the zero contour line as dashes. a) the C4-N4-C5 plane of the dication in (I), b) the C3-N3-C5 plane of a dication in (III), and c) the C3-N3-H1 plane of a dication in (IV). All contour intervals are taken in increments of 0.1 eÅ^{-3}.

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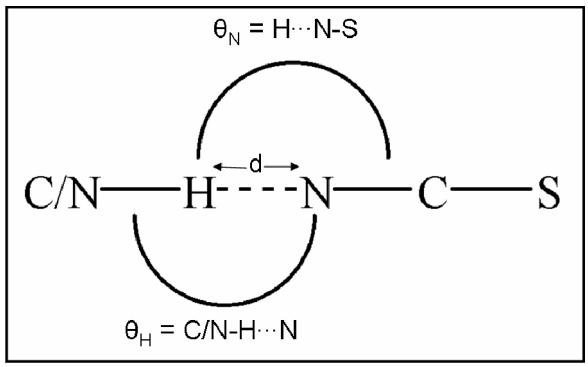
N-H···N and C-H···N Geometries:



Interaction	Internuclear Distance, d (Å)	θ_N (°)	θ_H (°)	Interaction	Internuclear Distance, d (Å)	θ_N (°)	θ_H (°)
Compound I							
N1···H2b-C2 3/2-X,1/2+Y,1/2-Z	2.9272(7)	91.18(2)	105.19(3)	N1···H3b-C3 1-X,1-Y,1-Z	2.4482(7)	141.50(3)	152.72(3)
N1···H4a-C4 1-X,1-Y,1-Z	2.4709(7)	134.57(3)	153.80(3)	N1···H4b-C4 -1/2+X,3/2-Y,-1/2+Z	2.5351(7)	133.40(3)	156.48(3)
N1···H5c-C5 -1/2+X,3/2-Y,-1/2+Z	2.5922(7)	132.73(3)	151.12(3)				
Compound II†							
N1···H2-N2 -1+X,+Y,+Z	1.7602(3)	167.45(1)	163.71(1)	N1···H2b-C2 3-X,-Y,1-Z	2.8116(3)	133.40(1)	116.17(1)
Compound III							
N1···H1-N3 -X,-Y,1-Z	1.8876(7)	131.18(4)	153.16(4)	N1···H3-N4 -X,-Y,1-Z	1.8597(7)	147.47(4)	159.58(3)
N2···H4-N4 1+X,+Y,+Z	1.7655(8)	163.18(5)	169.61(4)	N2···H6a-C6 1-X,1-Y,1-Z	2.8913(9)	85.42(3)	157.98(5)
Compound VI							
N1···H1-N3 1+X,1/2-Y,-1/2+Z	1.9382(5)	122.61(2)	163.45(3)	N1···H4-N4 +X,+Y,+Z	1.8672(5)	122.13(2)	168.86(3)
N2···H2-N3 +X,1+Y,+Z	1.8660(6)	118.60(3)	167.31(3)	N2···H6-N4 +X,3/2-Y,1/2+Z	1.8955(6)	123.69(3)	158.46(3)
N1···H3b-C3 1-X,1/2+Y,1/2-Z	2.7435(6)	133.74(2)	129.20(3)	N2···H3a-C3 -X,1-Y,1-Z	2.7165(6)	119.40(2)	132.08(3)
N2···H4a-C4 1+X,-1/2-Y,1/2+Z	2.9316(6)	99.27(2)	127.56(2)				

† Previously Published[11]

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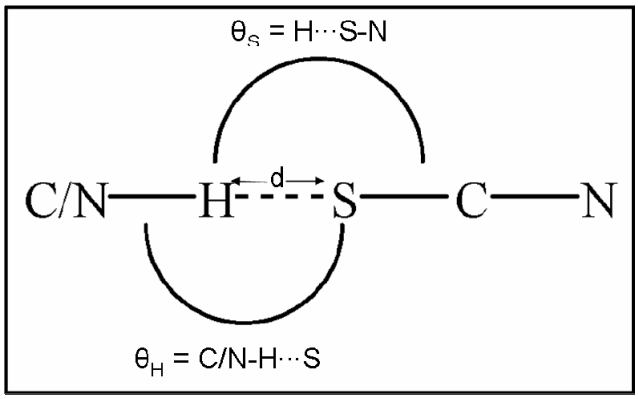
N-H···S and C-H···S Geometries:



Interaction	Internuclear Distance, d (Å)	θ_N (°)	θ_H (°)	Interaction	Internuclear Distance, d (Å)	θ_N (°)	θ_H (°)
Compound I							
S1···H2a-C2 +X,+Y,+Z	2.6920(6)	106.41(2)	168.59(3)	S1···H2b-C2 -1/2+X,1/2-Y,-1/2+Z	2.7698(5)	95.91(2)	157.22(3)
S1···H3a-C3 +X,+Y,+Z	3.0936(6)	91.22(2)	143.44(1)	S1···H4c-C4 -1/2+X,1/2-Y,-1/2+Z	2.8047(6)	80.64(2)	161.90(3)
Compound II†							
S1···H2b-C2 +X,1+Y,+Z	3.0597(1)	127.36(1)	137.75(1)	S1···H3b-C3 2-X,-Y,-Z	2.8400(1)	125.75(1)	172.62(1)
S1···H3c-C3 +X,1+Y,+Z	2.7958(1)	136.01(1)	153.05(1)	S1···H4b-C4 +X,1+Y,+Z	2.9508(1)	168.81(1))	145.57(2)
Compound III							
S1···H2-N3 1-X,-Y,1-Z	2.2107(6)	98.07(3)	170.80(3)	S2···H3a-C3 1+X,+Y,1+Z	3.0421(7)	104.51(3)	139.41(3)
S2···H3b-C3 +X,+Y,1+Z	2.8841(6)	134.83(3)	169.25(3)	S2···H5a-C5 1-X,-Y,1-Z	2.9052(7)	72.53(3)	170.67(3)
S2···H6b-C6 1+X,+Y,1+Z	3.0793(6)	145.57(3)	160.16(5)				
Compound VI							
N1···H1-N3 1+X,1/2-Y,-1/2+Z	1.9382(5)	122.61(2)	163.45(3)	N1···H4-N4 +X,+Y,+Z	1.8672(5)	122.13(2)	168.86(3)
N2···H2-N3 +X,1+Y,+Z	1.8660(6)	118.60(3)	167.31(3)	N2···H6-N4 +X,3/2-Y,1/2+Z	1.8955(6)	123.69(3)	158.46(3)
N1···H3b-C3 1-X,1/2+Y,1/2-Z	2.7435(6)	133.74(2)	129.20(3)	N2···H3a-C3 -X,1-Y,1-Z	2.7165(6)	119.40(2)	132.08(3)
N2···H4a-C4 1+X,-1/2-Y,1/2+Z	2.9316(6)	99.27(2)	127.56(2)				

† Previously Published[11]

C-H···C_π Geometries:

Interaction	Internuclear Distance, d (Å)	θ_N (°)	θ_H (°)	Interaction	Internuclear Distance, d (Å)	θ_N (°)	θ_H (°)
			Compound I				
C1···H5a-C5 +X,+Y,+Z	2.6466(5)	91.46(5)	175.22(3)				
			Compound II†				
C1···H4c-C4 2-X,-Y,1-Z	2.7957(2)	99.77(1)	140.91(2)				
			Compound III				
C1···H4b-C4 1-X,-Y,1-Z	2.5327(6)	96.44(3)	147.33(3)	C2···H4a-C4 1-X,1-Y,1-Z	2.6522(6)	90.11(4)	149.54(3)
C2···H5b-C5 1+X,+Y,1+Z	2.5648(6)	98.22(6)	167.86(4)				
			Compound VI				
C1···H4b-C4 1-X,1-Y,-Z	2.7714(4)	92.86(4)	142.23(2)				

† Previously Published[11]

Static Deformation Maps:

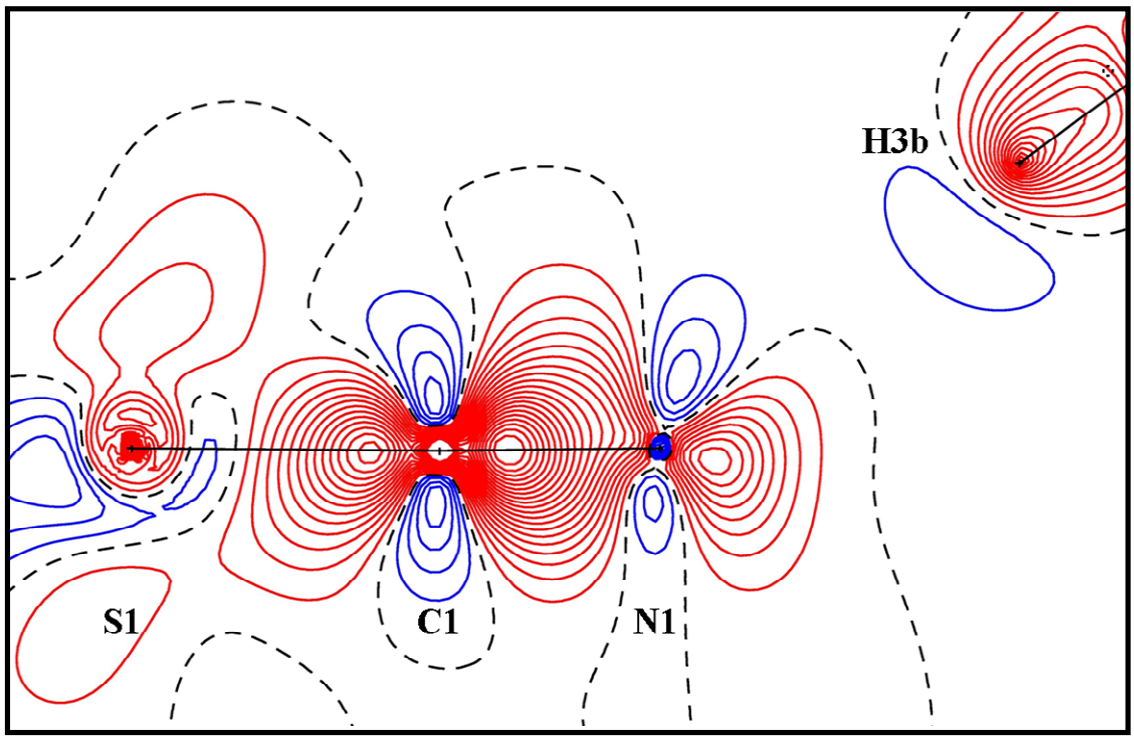


Fig. S3 The static deformation maps of a C-H···N interaction in (I). The positive (solid red lines) and negative (solid blue lines) contours are in increments of 0.05 eÅ^{-3}. The dashed line represents the zero contour line, separating the positive and negative electron density.

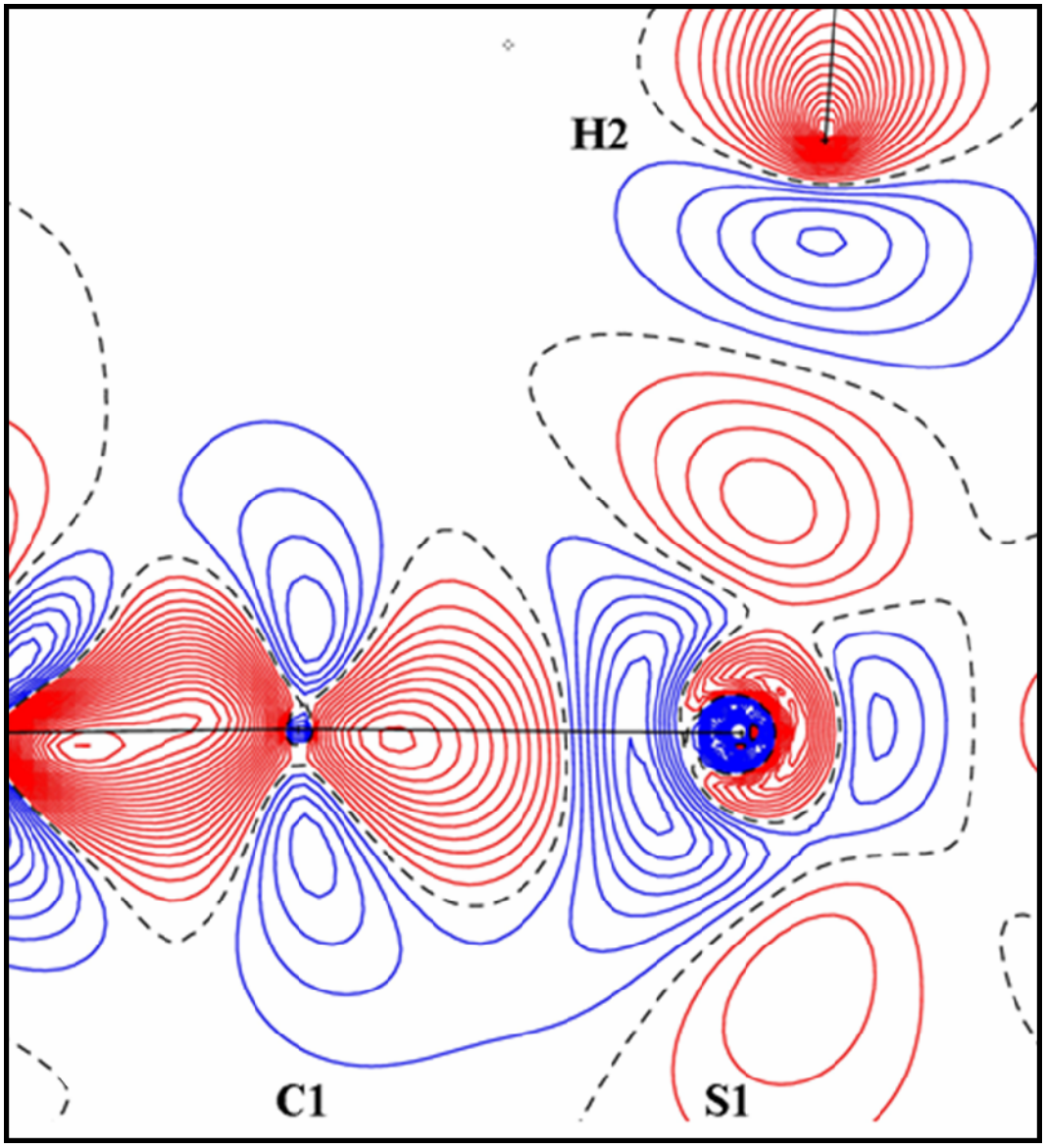


Fig. S4 The static deformation maps of the N-H···S interaction in (III). The positive (solid red lines) and negative (solid blue lines) contours are in increments of 0.05 eÅ^{-3}. The dashed line represents the zero contour line, separating the positive and negative electron

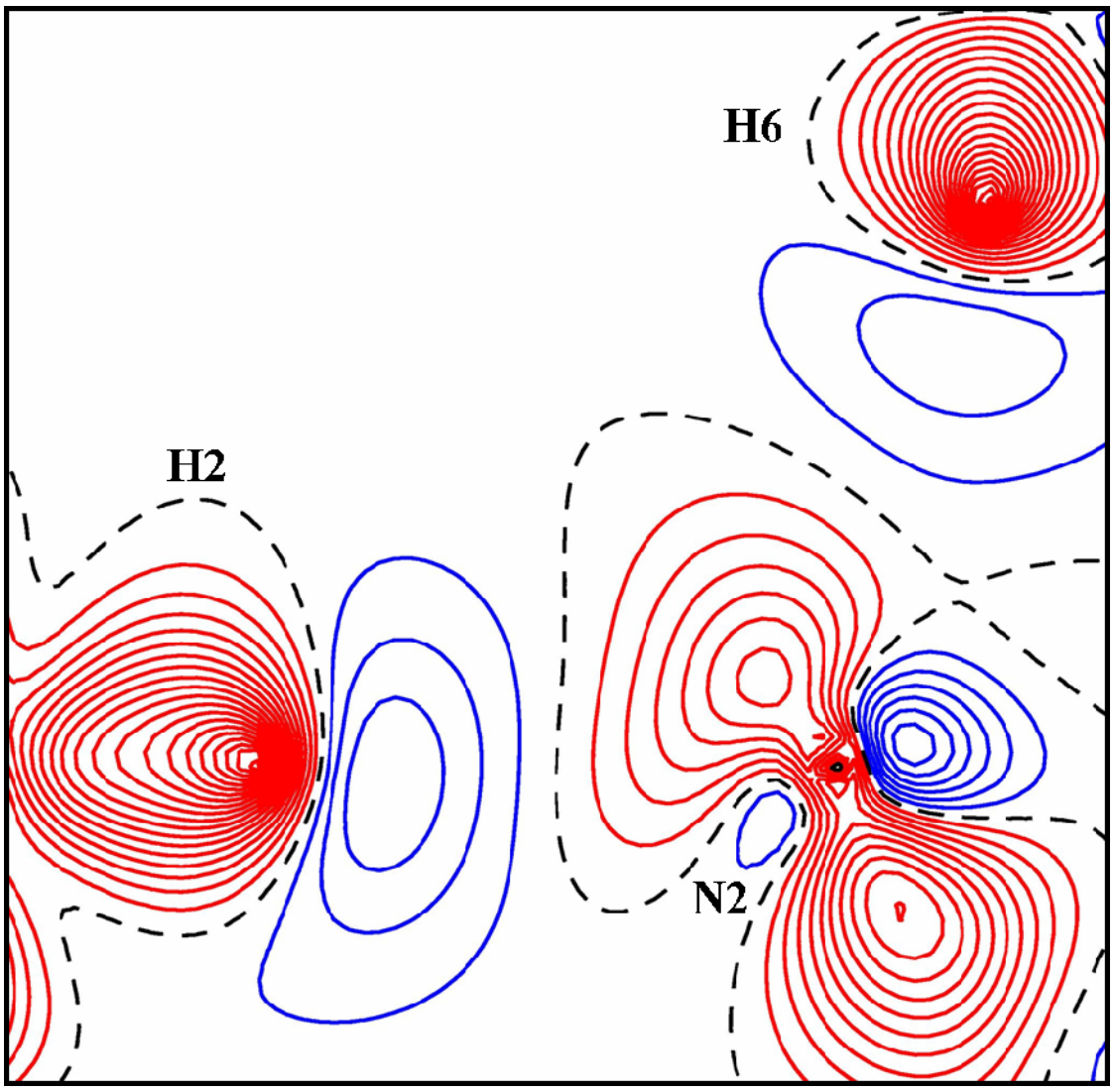


Fig. S5 The static deformation maps for a bifurcated N-H···N interaction in (IV). The positive (solid red lines) and negative (solid blue lines) contours are in increments of 0.05 eÅ^{-3}. The dashed line represents the zero contour line, separating the positive and negative electron density.

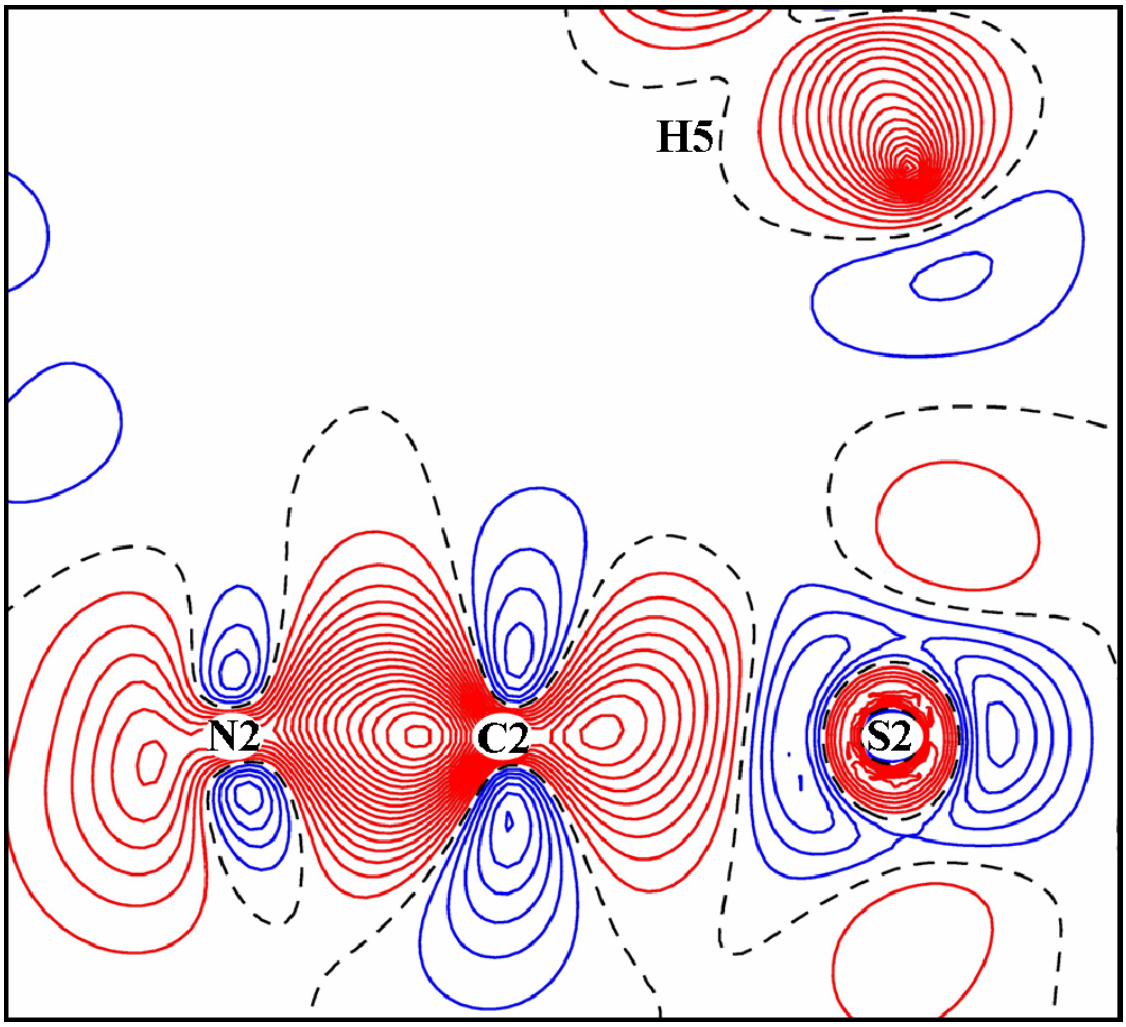


Fig. S6 The static deformation maps for an N-H···S interaction in (IV). The positive (solid red lines) and negative (solid blue lines) contours are in increments of 0.05 eÅ^{-3}. The dashed line represents the zero contour line, separating the positive and negative electron