R free Factor and Experimental charge density analysis

1-(2'-aminophenyl)-2-methyl-4-nitroimidazole: a crystal structure with Z'=2

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Figures

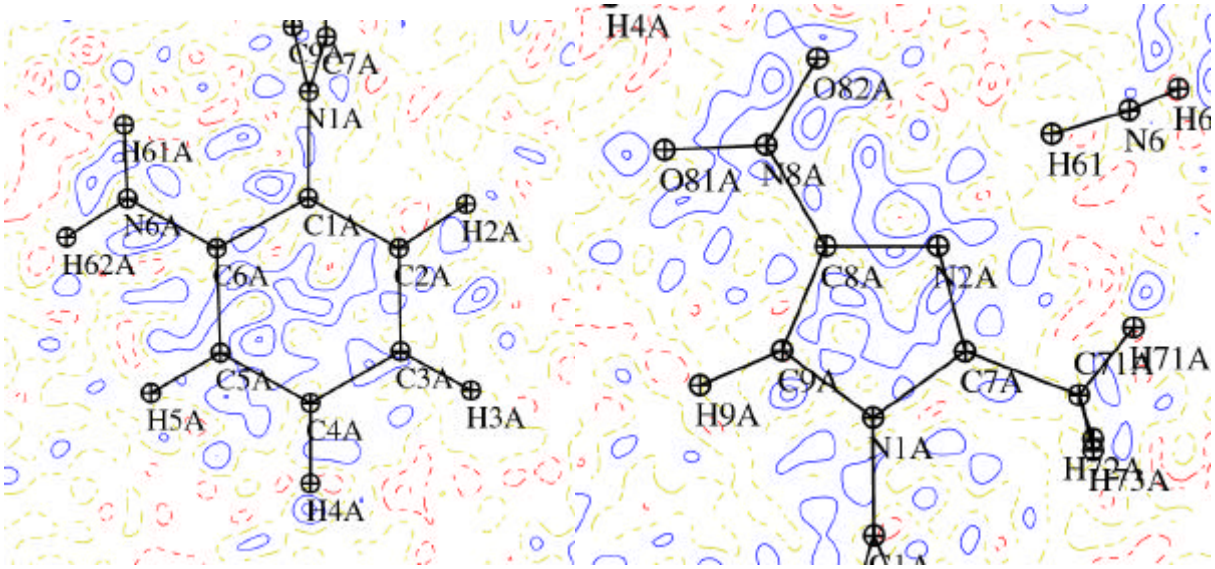


Figure 1a-b). Residual electron density maps for the second molecule. sigma cutoff 2I/sigma, resolution 0-09Å^{-1}, contour 0.05e/Å^3, blue-negative, red-positive.

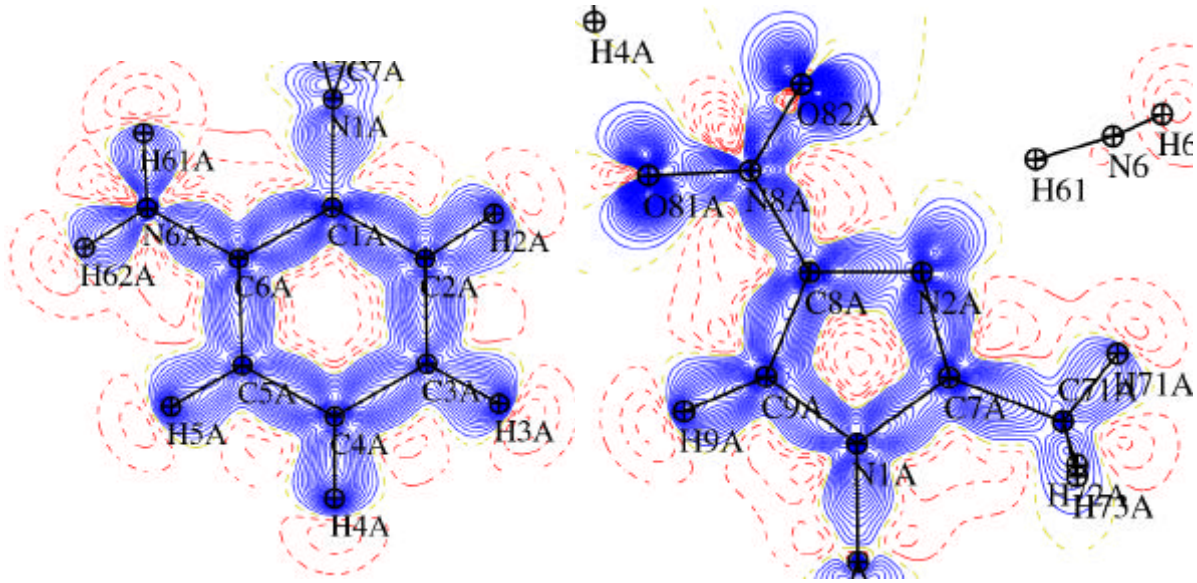
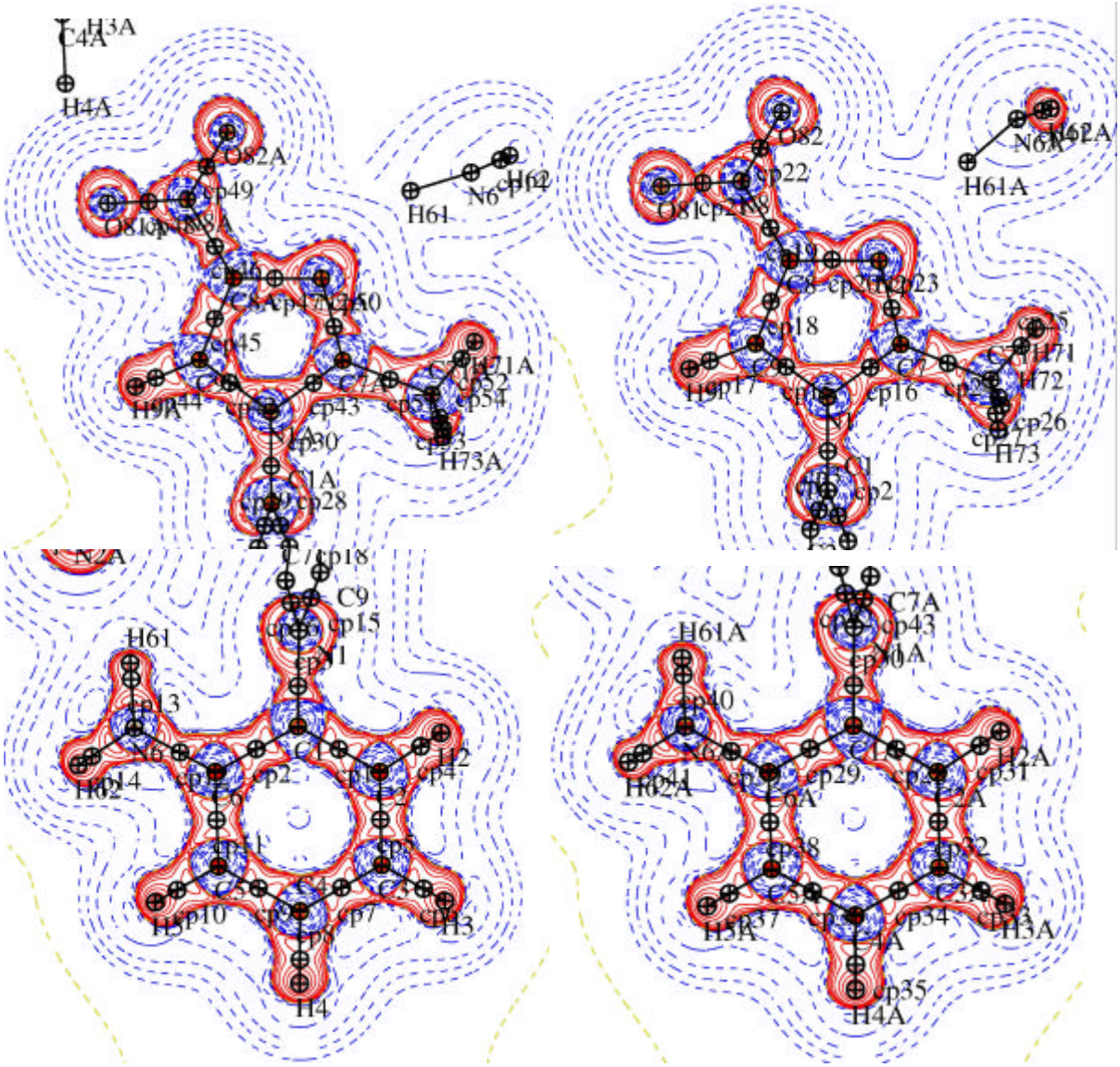


Figure 2a-b). Deformation density maps of the second molecule drawn in the planes of imidazole (left) and phenyl (right) rings, contour 0.05e/Å^3, blue negative, red positive.



Figures 3 a-d). Bond critical points of both molecules.

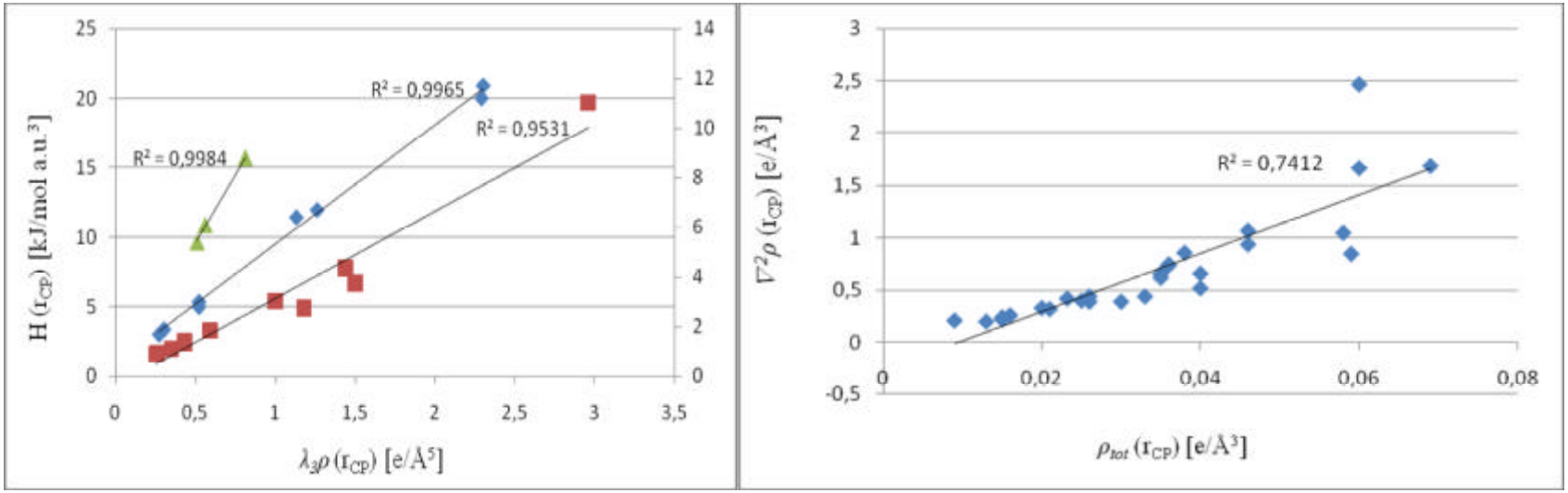
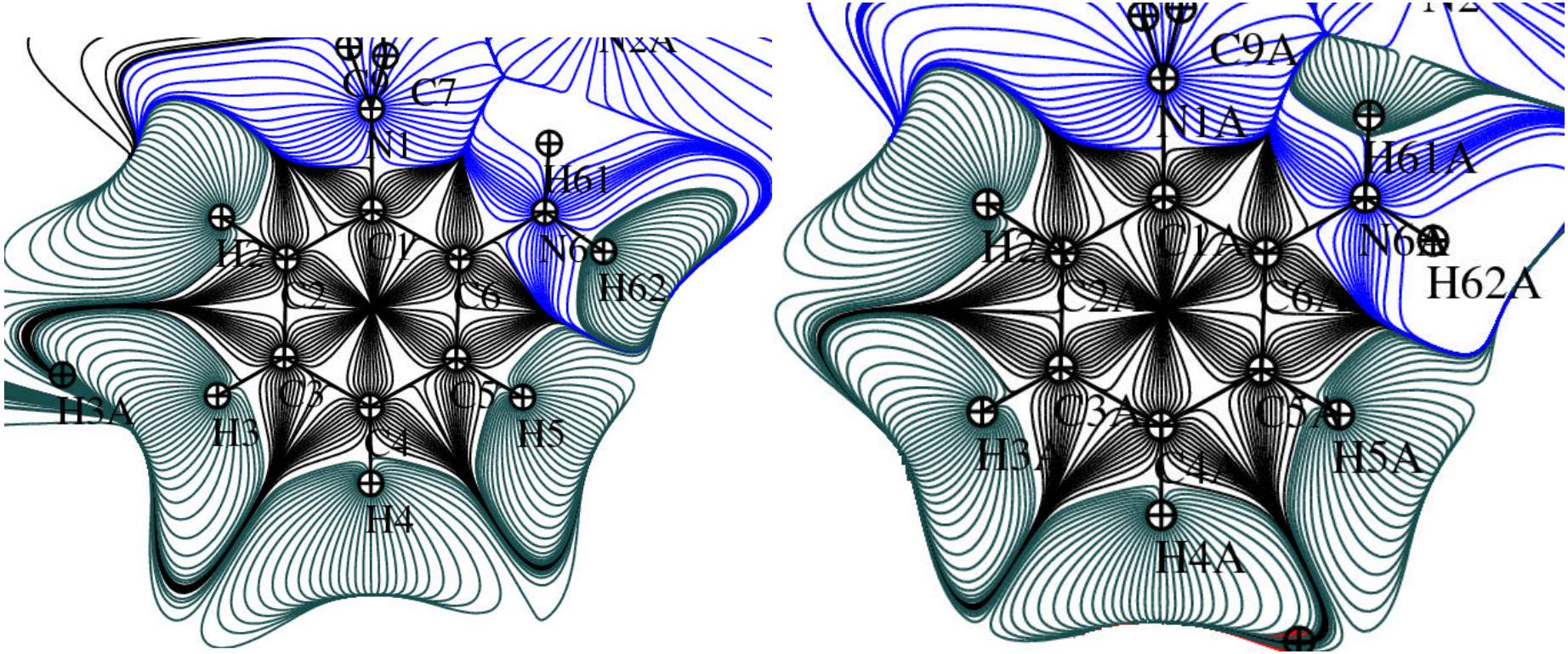


Figure 4 a-b. a) Dependence of the total energy density at the CP's on the electron density at CP's. Three lines depicts the linear dependence for different bond acceptors: blue diamonds – N, red squares – O and the green triangles – C; b) Dependance of the Laplacian at the CP's on the total electron density at CP's.


C8
C7
N1
H61
H2
C1
N6
C2
C6
H62
H3A
C3
C5
H3
C4
H5
H4
C9A
N1A
H61A
H2A
C1A
N6A
H62A
C2A
C6A
H3A
C3A
C5A
H5A
C4A
H4A

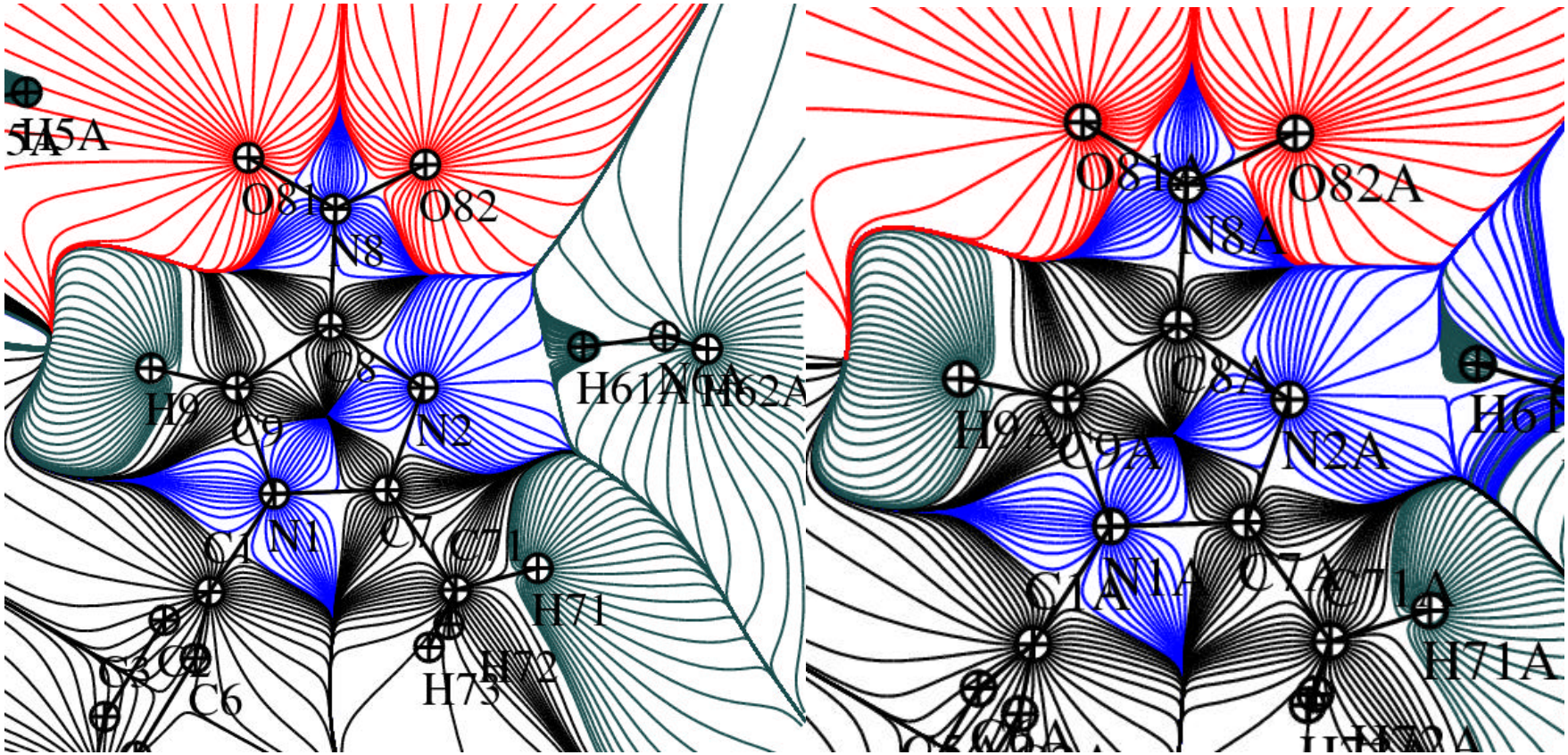


Figure 5 a-d). Representation of the gradient lines of the static electron density in the planes of aromatic rings of both molecules.

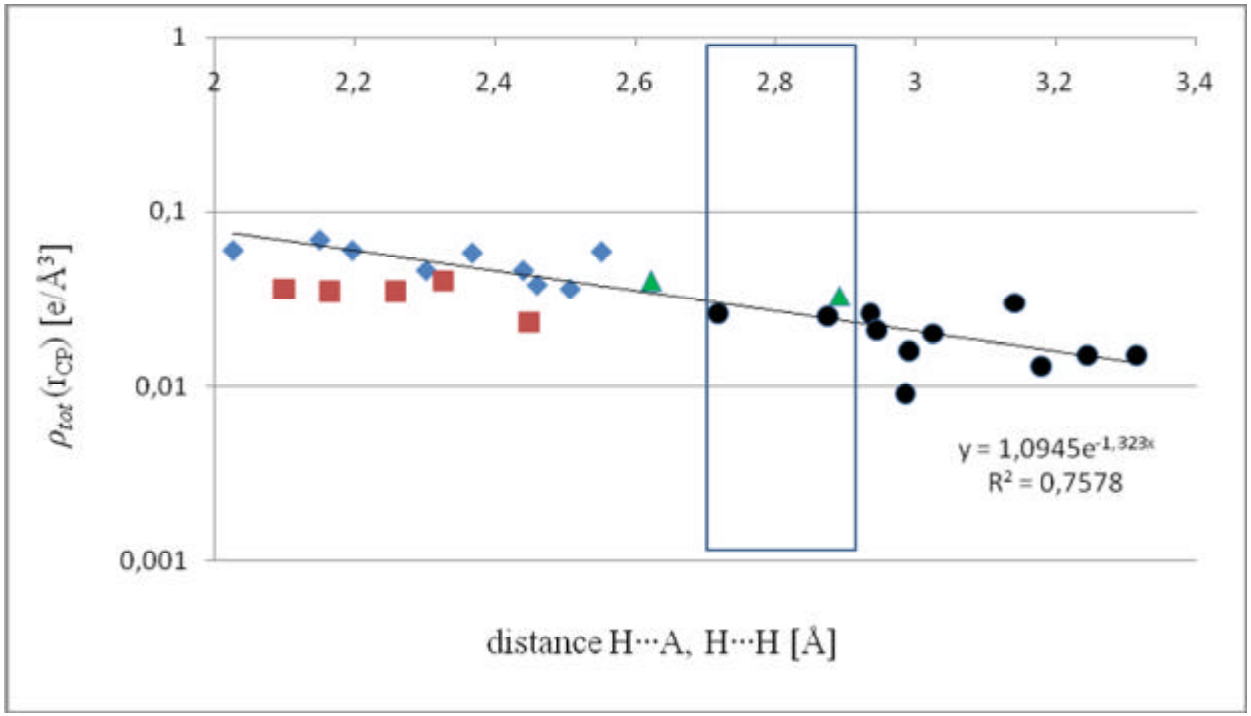


Figure 6. The exponential dependence of the total electron density at CP's on H???A distance. The blue diamond's – cp1-9, the green triangles – cp10-11, black dots – cp 12-22, red squares – cp23-27. The rectangle shows the region of overlap for hydrogen bonds – van der Waals interactions. H-H contacts not included in the exponential fitting. The rectangle shows the region of overlap for hydrogen bonds – van der Waals interactions.

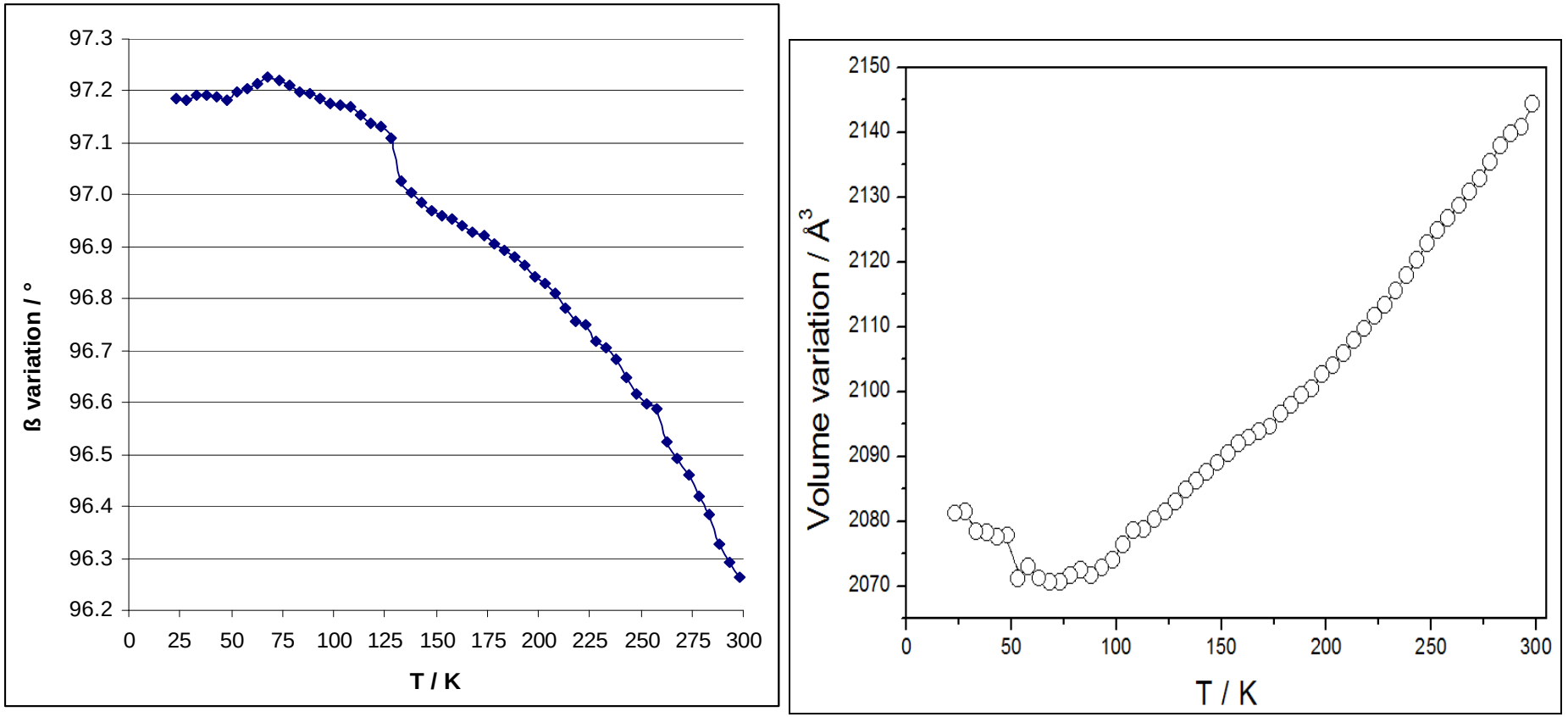


Figure 7. ß and volume value in the powder diffractions experiment.

Tables

Table 1. Rigid bond test for non-hydrogen atoms.

Atom A mol 1	Atom B mol 1	Z^2_A [Å^2]	Z^2_B [Å^2]	? $Z_{AB}{}^2$ [Å^2]	Atom A mol 2	Atom B mol 2	Z^2_A [Å^2]	Z^2_B [Å^2]	? $Z_{AB}{}^2$[Å^2]
C1	N1	0,0095	0,0091	0,0004(2)	N1A	C7A	0,0107	0,0113	-0,0006(2)
C1A	N1A	0,0103	0,0102	0,0001(1)	N1	C9	0,0122	0,0127	-0,0005(2)
C1	C6	0,0112	0,0114	-0,0001(2)	N1A	C9A	0,0125	0,0132	-0,0007(2)
C1A	C6A	0,0114	0,0116	-0,0002(2)	C9	C8	0,0117	0,0116	0,0001(2)
C1	C2	0,0130	0,0132	-0,0002(2)	C9A	C8A	0,0102	0,0102	<0,0001(2)
C1A	C2A	0,0121	0,0123	-0,0002(2)	C8	N8	0,0101	0,0104	-0,0003(2)
C2	C3	0,0144	0,0144	-0,0001(3)	C8A	N8A	0,0122	0,0128	-0,0006(2)
C2A	C3A	0,0143	0,0144	-0,0001(2)	C8	N2	0,0143	0,0147	-0,0004(2)
C3	C4	0,0230	0,0231	-0,0002(2)	C8A	N2A	0,0132	0,0139	-0,0007(2)
C3A	C4A	0,0195	0,0193	0,0002(3)	N8	O82	0,0192	0,0186	0,0007(3)
C4	C5	0,0201	0,0199	0,0002(2)	N8A	O82A	0,0127	0,0130	-0,0003(2)
C4A	C5A	0,0159	0,0161	-0,0002(3)	N8	O81	0,0211	0,0212	-0,0002(2)
C5	C6	0,0100	0,0098	0,0003(2)	N8A	O81A	0,0165	0,0171	-0,0007(2)
C5A	C6A	0,0106	0,0104	0,0002(1)	N2	C7	0,0104	0,0105	-0,0002(2)
C6	N6	0,0143	0,0145	-0,0002(2)	N2A	C7A	0,0128	0,0130	-0,0002(1)
C6A	N6A	0,0122	0,0129	-0,0007(3)	C7	C71	0,0125	0,0127	-0,0002(3)
N1	C7	0,0123	0,0125	-0,0002(2)	C7A	C71A	0,0130	0,0139	-0,0009(3)

Table 2. Geometric data after multipole refinement (distances, angles, dihedral angles)

Bonded atoms	distance	Molecule 1/Molecule 2
C1—N1	1.4378 (3)	1,0025
C1A—N1A	1.4342 (3)	
C1—C6	1.4054 (4)	1,0016

C1A—C6A	1.4031 (4)	
C1—C2	1.3934 (4)	1,0004
C1A—C2A	1.3928 (4)	
C2—C3	1.3908 (4)	1,0013
C2A—C3A	1.3890 (4)	
C3—C4	1.3967 (5)	0,9999
C3A—C4A	1.3968 (4)	
C4—C5	1.3870 (5)	1,0004
C4A—C5A	1.3865 (4)	
C5—C6	1.4103 (4)	1,0011
C5A—C6A	1.4087 (4)	
C6—N6	1.3717 (4)	0,9982
C6A—N6A	1.3742 (4)	
N1—C7	1.3785 (4)	1,0005
N1A—C7A	1.3778 (3)	
N1—C9	1.3695 (4)	0,9995
N1A—C9A	1.3702 (4)	
C9—C8	1.3709 (4)	0,9974
C9A—C8A	1.3745 (4)	
C8—N8	1.4244 (4)	0,9966
C8A—N8A	1.4292 (4)	
C8—N2	1.3666 (4)	1,0025
C8A—N2A	1.3632 (4)	
N8—O82	1.2246 (4)	1,0028
N8A—O82A	1.2238 (3)	
N8—O81	1.2324 (4)	0,9960
N8A—O81A	1.2373 (4)	
N2—C7	1.3190 (3)	0,9988
N2A—C7A	1.3206 (4)	
C7—C71	1.4794 (4)	0,9976
C7A—C71A	1.4830 (4)	

Bonded atoms	Angle [°]	Angle mol1/mol2

C1—N1—C7	125.55 (3)	1,00
C1A—N1A—C7A	125.23 (3)	
C1—N1—C9	126.75 (2)	1,00
C1A—N1A—C9A	126.86 (3)	
C1—C6—N6	122.03 (3)	1,00
C1A—C6A—N6A	122.02 (3)	
C1—C6—C5	117.12 (3)	1,00
C1A—C6A—C5A	116.81 (2)	
C1—C2—C3	120.57 (4)	1,00
C1A—C2A—C3A	120.05 (2)	
C1—C2—H2	117.7	1,00
C1A—C2A—H2A	117.7	
C2—C1—N1	118.74 (3)	1,00
C2A—C1A—N1A	118.69 (3)	
C2—C1—C6	121.55 (3)	1,00
C2A—C1A—C6A	122.13 (3)	
C2—C3—C4	118.58 (4)	1,00
C2A—C3A—C4A	118.83 (3)	
C2—C3—H3	121,1	1,01
C2A—C3A—H3A	120.0	
H2—C2—C3	121.7	1,00
H2A—C2A—C3A	122.2	
C3—C4—C5	121.08 (3)	1,00
C3A—C4A—C5A	120.98 (3)	
C3—C4—H4	120.2	1,00
C3A—C4A—H4A	119,9	
H3—C3—C4	120.3	0,99
H3A—C3A—C4A	121.1	
C4—C5—C6	121.08 (3)	1,00
C4A—C5A—C6A	121.17 (3)	
C4—C5—H5	121.9	1,00
C4A—C5A—H5A	120.7	

H4—C4—C5	118.7	1,00
H4A—C4A—C5A	119.1	
C5—C6—N6	120.77 (3)	1,00
C5A—C6A—N6A	121.15 (3)	
H5—C5—C6	118,0	1,00
H5A—C5A—C6A	118.1	
C6—N6—H62	116.7	1,00
C6A—N6A—H61A	117,1	
C6—N6—H61	120.4	0,99
C6A—N6A—H62A	121.1	
C6—C1—N1	119.68 (2)	1,00
C6A—C1A—N1A	119.11 (3)	
H61—N6—H62	116.4	1,01
H61A—N6A—H62A	115.0	
N1—C7—N2	111.50 (2)	1,00
N1A—C7A—N2A	111.15 (3)	
N1—C7—C71	122.60 (2)	0,99
N1A—C7A—C71A	123.32 (3)	
N1—C9—C8	104.20 (2)	1,00
N1A—C9A—C8A	103.82 (3)	
N1—C9—H9	122.4	1,01
N1A—C9A—H9A	120,9	
C9—N1—C7	107.51 (2)	1,00
C9A—N1A—C7A	107.91 (2)	
C9—C8—N8	126.21 (3)	0,99
C9A—C8A—N8A	127.01 (4)	
C9—C8—N2	112.47 (2)	1,00
C9A—C8A—N2A	112.58 (3)	
H9—C9—C8	133.4	0,99
H9A—C9A—C8A	135.3	
C8—N8—O82	118.73 (3)	1,00
C8A—N8A—O82A	118.76 (3)	

C8—N8—O81	117.75 (3)	1,00
C8A—N8A—O81A	117.67 (3)	
C8—N2—C7	104.31 (2)	1,00
C8A—N2A—C7A	104.54 (2)	
N8—C8—N2	121. 29 (3)	1,01
N8A—C8A—N2A	120.40 (3)	
O81—N8—O82	123.51 (3)	1,00
O81A—N8A—O82A	123.57 (3)	
N2—C7—C71	125.85 (3)	1,00
N2A—C7A—C71A	125.51 (3)	
C7—C71—H73	109.7	0,99
C7A—C71A—H73A	110,6	
C7—C71—H72	109.0	0,98
C7A—C71A—H72A	111,1	
C7—C71—H71	109.1	1,01
C7A—C71A—H71A	107,8	
H71—C71—H73	109,7	1,00
H71A—C71A—H73A	109.7	
H71—C71—H72	109,5	0,99
H71A—C71A—H72A	110.2	
H72—C71—H73	109.8	1,02
H72A—C71A—H73A	107.5	

Bonded atoms	Dihedral angle [°]	Dihedral angle mol1/mol2
C1—N1—C7—N2	- 175.80 (2)	-0,98
C1A—N1A—C7A—N2A	179.87 (2)	
C1—N1—C7—C71	1.75 (2)	-0,93
C1A—N1A—C7A—C71A	- 1.89 (2)	
C1—N1—C9—C8	175.51 (2)	0,98
C1A—N1A—C9A—C8A	179.83 (2)	
C1—N1—C9—H9	- 4.2	6,00
C1A—N1A—C9A—H9A	- 0.7	

C1—C6—N6—H62	- 172.7	-1,06
C1A—C6A—N6A—H62A	162,8	
C1—C6—N6—H61	- 21,9	-1,65
C1A—C6A—N6A—H61A	13.3	
C1—C6—C5—C4	0.61 (2)	0,39
C1A—C6A—C5A—C4A	1.55 (2)	
C1—C6—C5—H5	- 179.5	1,01
C1A—C6A—C5A—H5A	- 177.0	
C1—C2—C3—C4	0.54 (3)	0,59
C1A—C2A—C3A—C4A	0.92 (3)	
C1—C2—C3—H3	179.4	1,00
C1A—C2A—C3A—H3A	179.4	
C2—C1—N1—C7	99.67 (3)	1,30
C2A—C1A—N1A—C7A	76.61 (2)	
C2—C1—N1—C9	- 74.60 (2)	0,72
C2A—C1A—N1A—C9A	- 103.08 (3)	
C2—C1—C6—N6	- 178.19 (3)	-1,00
C2A—C1A—C6A—N6A	178.88 (3)	
C2—C1—C6—C5	- 1.32 (3)	7,76
C2A—C1A—C6A—C5A	- 0.17 (2)	
C2—C3—C4—C5	- 1.24 (3)	-2,82
C2A—C3A—C4A—C5A	0.44 (3)	
C2—C3—C4—H4	177.2	-0,99
C2A—C3A—C4A—H4A	- 179.4	
H2—C2—C1—N1	3.0	
H2A—C2A—C1A—N1A	0.0	
H2—C2—C1—C6	- 178.9	-1,01
H2A—C2A—C1A—C6A	176,9	
H2—C2—C3—C4	- 179.8	1,02
H2A—C2A—C3A—C4A	- 177.0	
H2—C2—C3—H3	- 0,9	-0,56
H2A—C2A—C3A—H3A	1.6	

C3—C2—C1—N1	- 177.31 (3)	1,00
C3A—C2A—C1A—N1A	- 178.00 (3)	
C3—C2—C1—C6	0.76 (3)	-0,72
C3A—C2A—C1A—C6A	- 1.06 (3)	
C3—C4—C5—C6	0.66 (3)	-0,38
C3A—C4A—C5A—C6A	- 1.72 (3)	
C3—C4—C5—H5	- 179.2	-1,01
C3A—C4A—C5A—H5A	176.8	
H3—C3—C4—C5	179.8	-1,01
H3A—C3A—C4A—C5A	- 178.1	
H3—C3—C4—H4	- 1.7	-1,89
H3A—C3A—C4A—H4A	0.9	
C4—C5—C6—N6	177.52 (3)	-1,00
C4A—C5A—C6A—N6A	- 177.52 (3)	
H4—C4—C5—C6	- 177.8	-0,99
H4A—C4A—C5A—C6A	179.3	
H4—C4—C5—H5	2.3	-1,05
H4A—C4A—C5A—H5A	- 2.2	
C5—C6—N6—H62	10.6	-0,58
C5A—C6A—N6A—H62A	- 18.2	
C5—C6—N6—H61	161.4	-0,96
C5A—C6A—N6A—H61A	- 167.7	
C5—C6—C1—N1	176.73 (2)	1,00
C5A—C6A—C1A—N1A	176.76 (2)	
H5—C5—C6—N6	- 2.6	-0,67
H5A—C5A—C6A—N6A	3.9	
C6—C1—N1—C7	- 78.44 (2)	0,78
C6A—C1A—N1A—C7A	- 100.42 (2)	
C6—C1—N1—C9	107.29 (3)	1,34
C6A—C1A—N1A—C9A	79.88 (2)	
N6—C6—C1—N1	- 0.13 (2)	0,03
N6A—C6A—C1A—N1A	- 4.19 (2)	

N1—C7—N2—C8	0.54 (2)	1,08
N1A—C7A—N2A—C8A	0.50 (2)	
N1—C7—C71—H73	49.3	0,87
N1A—C7A—C71A—H73A	56.4	
N1—C7—C71—H72	- 71.0	1,13
N1A—C7A—C71A—H72A	- 62.9	
N1—C7—C71—H71	169.5	0,96
N1A—C7A—C71A—H71A	176.3	
N1—C9—C8—N8	- 178.10 (2)	1,00
N1A—C9A—C8A—N8A	- 178.34 (2)	
N1—C9—C8—N2	- 0.08 (2)	-0,35
N1A—C9A—C8A—N2A	0.23 (2)	
C9—N1—C7—N2	- 0.61 (2)	1,56
C9A—N1A—C7A—N2A	- 0.39 (2)	
C9—N1—C7—C71	176.94 (2)	0,99
C9A—N1A—C7A—C71A	177.85 (2)	
C9—C8—N8—O82	176.26 (3)	-0,99
C9A—C8A—N8A—O82A	- 177.82 (3)	
C9—C8—N8—O81	- 3.12 (3)	-1,34
C9A—C8A—N8A—O81A	2.32 (3)	
C9—C8—N2—C7	- 0.28 (2)	0,61
C9A—C8A—N2A—C7A	- 0.46 (2)	
H9—C9—N1—C7	- 179.3	-1,00
H9A—C9A—N1A—C7A	179.6	
H9—C9—C8—N8	1.6	0,70
H9A—C9A—C8A—N8A	2.3	
H9—C9—C8—N2	- 179.6	1,00
H9A—C9A—C8A—N2A	- 179.2	
C8—N2—C7—C71	- 176.92 (2)	1,00
C8A—N2A—C7A—C71A	- 177.69 (2)	
C8—C9—N1—C7	0.40 (2)	4,44
C8A—C9A—N1A—C7A	0.09 (2)	

N8—C8—N2—C7	177.85 (2)	1,00
N8A—C8A—N2A—C7A	178.22 (2)	
O81—N8—C8—N2	179.03 (3)	-1,02
O81A—N8A—C8A—N2A	- 176.15 (3)	
O82—N8—C8—N2	- 1.59 (3)	-0,43
O82A—N8A—C8A—N2A	3.71 (3)	
N2—C7—C71—H73	- 133.5	1,06
N2A—C7A—C71A—H73A	- 125.6	
N2—C7—C71—H72	106.2	0,92
N2A—C7A—C71A—H72A	115.1	
N2—C7—C71—H71	- 13.3	2,33
N2A—C7A—C71A—H71A	- 5.7	

Table 3. Thermal motion parameters, Cijk

	U11	U22	U33	U12	U13	U23	Uiso*/Ueq	Uiso*/Ueq (mol1/mol2(
C1	0.01619 (10)	0.01349 (9)	0.00990 (8)	- 0.00213 (7)	- 0.00008 (7)	- 0.00102 (7)	0.01334 (1)	1,0917
C1A	0.01077 (8)	0.01290 (8)	0.01261 (8)	- 0.00051 (7)	0.000044 (7)	0.00081 (7)	0.01222 (1)	
C2	0.0252 (1)	0.0166 (1)	0.0155 (1)	- 0.00664 (10)	0.00156 (9)	0.00012 (8)	0.01926 (2)	1,2121
C2A	0.01453 (10)	0.01590 (10)	0.01690 (10)	- 0.00178 (8)	0.00128 (8)	0.00361 (8)	0.01589 (1)	
H2	0.0398	0.0316	0.0225	0.0026	0.0025	- 0.0058	0.03152	1,0207
H2A	0.0281	0.0339	0.0294	0.0096	- 0.0017	- 0.0001	0.03088	
C3	0.0254 (1)	0.0158 (1)	0.0216 (1)	- 0.00640 (10)	- 0.00005 (10)	- 0.00243 (9)	0.02121 (2)	1,1628
C3A	0.01409 (10)	0.0195 (1)	0.0210 (1)	- 0.00353 (9)	0.00336 (9)	0.00237 (9)	0.01824 (2)	
H3	0.0428	0.0257	0.0363	- 0.0006	0.0019	- 0.0112	0.03526	1,0368
H3A	0.0266	0.0377	0.0374	0.0086	0.0055	- 0.0067	0.03401	
C4	0.0192 (1)	0.0163 (1)	0.0183 (1)	- 0.00078 (9)	- 0.00306 (9)	- 0.00583 (8)	0.01824 (2)	1,1088

C4A	0.01108 (9)	0.0204 (1)	0.0176 (1)	- 0.00179 (8)	0.00169 (8)	- 0.00121 (8)	0.01645 (2)	
H4	0.0500	0.0333	0.0290	- 0.0111	- 0.0012	- 0.0116	0.03791	1,0810
H4A	0.0188	0.0420	0.0430	0.0059	- 0.0029	- 0.0026	0.03507	
C5	0.0219 (1)	0.0179 (1)	0.01168 (9)	- 0.00111 (9)	- 0.00196 (8)	- 0.00358 (8)	0.01741 (2)	1,1645
C5A	0.01086 (9)	0.0198 (1)	0.01378 (9)	0.00022 (8)	- 0.00018 (7)	0.00061 (8)	0.01495 (1)	
H5	0.0499	0.0393	0.0194	- 0.0016	0.0019	- 0.0101	0.03649	1,0805
H5A	0.0278	0.0366	0.0353	0.0115	- 0.0049	0.0014	0.03377	
C6	0.0190 (1)	0.01408 (9)	0.00965 (8)	- 0.00202 (8)	- 0.00065 (7)	- 0.00105 (7)	0.01443 (1)	1,0891
C6A	0.01062 (8)	0.01578 (9)	0.01301 (8)	- 0.00049 (7)	0.00030 (7)	0.00210 (7)	0.01325 (1)	
N6	0.0371 (2)	0.0186 (1)	0.01169 (8)	- 0.0094 (1)	0.00195 (9)	0.00027 (7)	0.02266 (2)	1,0193
N6A	0.01393 (9)	0.0275 (1)	0.0246 (1)	- 0.00278 (9)	- 0.00077 (8)	0.01328 (10)	0.02223 (2)	
H61	0.0370	0.0253	0.0216	- 0.0045	0.0006	- 0.0014	0.02824	1,0250
H61A	0.0212	0.0317	0.0286	0.0010	- 0.0032	- 0.0029	0.02755	
H62	0.0422	0.0337	0.0173	0.0020	- 0.0004	- 0.0036	0.03143	1,0445
H62A	0.0286	0.0297	0.0305	0.0074	- 0.0043	0.0012	0.03009	
N1	0.01335 (8)	0.01427 (8)	0.00938 (7)	- 0.00070 (6)	0.00010 (6)	- 0.00179 (6)	0.01245 (1)	1,0180
N1A	0.01083 (7)	0.01311 (7)	0.01232 (7)	0.00043 (6)	- 0.00056 (6)	- 0.00104 (6)	0.01223 (1)	
C9	0.01246 (9)	0.01620 (9)	0.01221 (8)	0.00041 (7)	0.00068 (7)	- 0.00166 (7)	0.01373 (1)	1,0409
C9A	0.01189 (9)	0.01469 (9)	0.01260 (8)	- 0.00038 (7)	- 0.00016 (7)	- 0.00228 (7)	0.01319 (1)	
H9	0.0191	0.0375	0.0333	- 0.0058	0.0017	0.0000	0.03018	0,9990
H9A	0.0289	0.0333	0.0277	- 0.0127	0.0013	- 0.0008	0.03021	
C8	0.01463 (9)	0.01308 (8)	0.01004 (8)	- 0.000065 (7)	0.00119 (7)	- 0.00135 (6)	0.01267 (1)	1,0169
C8A	0.01126 (8)	0.01237 (8)	0.01329 (8)	- 0.00011 (7)	- 0.00041 (7)	- 0.00069 (7)	0.01246 (1)	
N8	0.0229 (1)	0.01553 (9)	0.01297 (8)	0.00014 (8)	0.00399 (8)	- 0.00325 (7)	0.01717 (1)	1,1386
N8A	0.01157 (8)	0.01472 (8)	0.01855 (9)	- 0.00090 (7)	0.00058 (7)	- 0.00118 (7)	0.01508 (1)	

O81	0.0287 (1)	0.0252 (1)	0.0225 (1)	0.00963 (10)	0.00728 (9)	- 0.00392 (9)	0.02539 (2)	1,0704
O81A	0.01443 (9)	0.0265 (1)	0.0303 (1)	- 0.00245 (8)	0.00610 (8)	- 0.01101 (9)	0.02372 (2)	
O82	0.0300 (1)	0.0356 (1)	0.01918 (10)	- 0.0084 (1)	0.00279 (9)	- 0.01462 (10)	0.02841 (2)	1,2325
O82A	0.01228 (8)	0.0281 (1)	0.0277 (1)	- 0.00058 (8)	- 0.00336 (8)	- 0.00603 (9)	0.02305 (2)	
N2	0.01353 (8)	0.01570 (8)	0.00992 (7)	- 0.00099 (7)	- 0.00017 (6)	- 0.00149 (6)	0.01318 (1)	0,9741
N2A	0.01280 (8)	0.01337 (8)	0.01378 (8)	0.000048 (6)	- 0.00174 (6)	- 0.00147 (6)	0.01353 (1)	
C7	0.01305 (9)	0.01540 (9)	0.00985 (8)	0.00059 (7)	0.00068 (7)	- 0.00128 (7)	0.01286 (1)	0,9772
C7A	0.01317 (9)	0.01267 (8)	0.01319 (8)	0.00108 (7)	- 0.00019 (7)	- 0.00160 (7)	0.01316 (1)	
H71	0.0236	0.0401	0.0426	- 0.0114	- 0.0001	- 0.0029	0.03578	0,9725
H71A	0.0325	0.0480	0.0287	- 0.0138	- 0.0007	- 0.0048	0.03679	
H72	0.0425	0.0210	0.0495	0.0032	0.0131	0.0017	0.03759	0,9892
H72A	0.0407	0.0341	0.0403	0.0001	0.0186	- 0.0090	0.03800	
H73	0.0417	0.0452	0.0208	0.0010	0.0045	0.0098	0.03607	0,9970
H73A	0.0384	0.0399	0.0297	0.0043	0.0040	0.0147	0.03618	
C71	0.0172 (1)	0.0266 (1)	0.0173 (1)	0.00521 (10)	0.00293 (9)	- 0.00457 (10)	0.02044 (2)	1,0493
C71A	0.0194 (1)	0.0192 (1)	0.0196 (1)	0.00248 (9)	0.00275 (9)	- 0.00578 (9)	0.01948 (2)	

C_{111}	**N6**	-0.001724(81)	**N6A**	0.000657(47)	**N8**	0.000073(36)	**O81**	0.000787(60)	**O82**	0.000494(66)
C_{222}	**N6**	0.000264(49)	**N6A**	0.000067(40)	**N8**	-0.001359(69)	**O81**	0.000246(63)	**O82**	0.000379(95)
C_{333}	**N6**	-0.000010(6)	**N6A**	0.000007(6)	**N8**	-0.000232(10)	**O81**	-0.000044(9)	**O82**	-0.000034(8)
C_{112}	**N6**	0.002705(157)	**N6A**	-0.000538(93)	**N8**	-0.000386(91)	**O81**	0.000655(138)	**O82**	-0.000725(165)
C_{122}	**N6**	-0.001220(128)	**N6A**	0.000432(92)	**N8**	0.000902(119)	**O81**	0.000411(141)	**O82**	0.000856(192)
C_{113}	**N6**	-0.000161(73)	**N6A**	0.000268(51)	**N8**	-0.000303(50)	**O81**	0.000324(71)	**O82**	0.000083(73)

C_{133}	**N6**	-0.000018(30)	**N6A**	0.000056(26)	**N8**	0.000295(34)	**O81**	0.000093(39)	**O82**	0.000009(37)
C_{223}	**N6**	-0.000009(52)	**N6A**	0.000093(46)	**N8**	-0.002084(85)	**O81**	-0.000051(71)	**O82**	-0.000378(101)
C_{233}	**N6**	-0.000015(27)	**N6A**	-0.000015(25)	**N8**	-0.001178(45)	**O81**	0.000002(39)	**O82**	0.000386(44)
C_{123}	**N6**	-0.000087(99)	**N6A**	-0.000305(75)	**N8**	0.000991(102)	**O81**	-0.000511(114)	**O82**	-0.000216(137)

Table 4. Kappa comparison of both molecules

Atom	Kp1	Kp1mol1/Kp1mol2	Atom	Kp2	Kp2mol1/Kp2mol2
C1	1,0485(23)	1,0071	C1	0,9647(145)	1,0141
C1A	1,0411(23)		C2	0,9513(161)	
C2	1,0302(23)	1,0019	C3	0,9155(167)	0,9793
C2A	1,0282(22)		C4	0,9349(138)	
H2	1,1451(112)	0,9871	C5	0,9181(163)	0,9751
H2A	1,1601(110)		C6	0,9415(143)	
C3	1,0266(24)	1,0033	N6	0,8870(166)	1,0148
C3A	1,0233(24)		N1	0,8740(161)	
H3	1,1358(116)	0,9770	C9	0,9565(141)	0,9995
H3A	1,1626(115)		C8	0,9569(123)	
C4	1,0391(24)	1,0009	N8	0,8260(99)	0,8064
C4A	1,0381(24)		O81	1,0242(351)	
H4	1,1727(118)	0,9818	O82	0,9573(276)	1,0141
H4A	1,1945(119)		N2	0,9440(182)	
C5	1,0379(25)	1,0075	C7	0,9473(138)	1,0691
C5A	1,0302(23)		C71	0,8860(166)	
H5	1,1822(119)	0,9956	C1A	0,9838(138)	1,0348
H5A	1,1874(117)		C2A	0,9507(152)	
C6	1,0396(23)	1,0093	C3A	0,8623(149)	0,9268
C6A	1,0300(23)		C4A	0,9304(135)	

N6	0,9948(15)	1,0095	C5A	0,9030(160)	0,9379
N6A	0,9855(15)		C6A	0,9628(136)	
H61	1,2144(140)	1,0091	N6A	0,8465(152)	0,9899
H61A	1,2034(134)		N1A	0,8551(147)	
H62	1,1637(135)	0,9639	C9A	0,9295(136)	0,9931
H62A	1,2073(139)		C8A	0,9359(115)	
N1	1,0067(14)	1,0000	N8A	0,8578(99)	0,7943
N1A	1,0067(14)		O81A	1,0799(226)	
C9	1,0469(22)	1,0023	O82A	1,0888(251)	1,0419
C9A	1,0445(22)		N2A	1,0450(211)	
H9	1,1683(119)	0,9929	C7A	0,9009(126)	1,0755
H9A	1,1767(122)		C71A	0,8376(152)	
C8	1,0514(23)	0,9989			
C8A	1,0525(23)				
N8	1,0094(15)	0,9992			
N8A	1,0102(14)				
O81	0,9980(11)	0,9942			
O81A	1,0038(11)				
O82	0,9940(11)	0,9956			
O82A	0,9984(11)				
N2	1,0108(14)	1,0019			
N2A	1,0089(14)				
C7	1,0501(23)	0,9946			
C7A	1,0557(23)				
H71	1,1831(124)	1,0443			
H71A	1,1330(133)				
H72	1,1622(124)	1,0329			
H72A	1,1252(121)				
H73	1,1608(120)	0,9931			
H73A	1,1688(123)				
C71	1,0341(23)	1,0179			

C71A	1,0159(23)	

Table 5. Bond critical points and its characteristics

atom1	atom2	D12 [Å]	D1cp [Å]	D2cp [Å]	?tot [e/Å^3]	Laplac [e/Å^5]	?$_1$?$_2$?$_3$ [e/Å^5]			Elliplicity
C1	C2	1,393	0,695	0,698	2,21	-17,8	-17,7	-14,2	14,1	0,20
C1A	C2A	1,393	0,704	0,689	2,18	-17,4	-17,3	-14,1	13,9	0,18
C1	C6	1,405	0,706	0,700	2,15	-16,4	-17,0	-13,8	14,5	0,19
C1A	C6A	1,403	0,712	0,691	2,17	-17,5	-17,6	-14,0	14,1	0,20
C1	N1	1,438	0,605	0,833	1,84	-10,1	-13,7	-12,8	16,4	0,07
C1A	N1A	1,434	0,589	0,845	1,83	-11,8	-13,2	-13,2	14,7	0,00
C2	H2	1,083	0,722	0,361	1,76	-15,4	-17,0	-15,7	17,2	0,08
C2A	H2A	1,083	0,725	0,358	1,84	-16,6	-17,8	-16,8	18,0	0,05
C2	C3	1,391	0,713	0,678	2,18	-18,1	-16,8	-14,1	12,8	0,17
C2A	C3A	1,389	0,720	0,669	2,18	-18,1	-16,2	-14,1	12,3	0,13
C3	H3	1,083	0,715	0,368	1,81	-17,6	-17,2	-16,2	15,8	0,06
C3A	H3A	1,083	0,691	0,392	1,84	-17,2	-16,7	-15,7	15,3	0,06
C3	C4	1,397	0,688	0,709	2,17	-17,6	-16,7	-14,0	13,1	0,17
C3A	C4A	1,397	0,677	0,720	2,16	-18,0	-16,4	-13,9	12,4	0,15
C4	H4	1,083	0,723	0,361	1,84	-16,5	-17,6	-17,3	18,4	0,02
C4A	H4A	1,083	0,715	0,368	1,87	-17,0	-18,1	-17,2	18,3	0,05
C4	C5	1,387	0,709	0,678	2,20	-18,2	-17,4	-14,3	13,4	0,18
C4A	C5A	1,387	0,713	0,674	2,19	-18,5	-17,1	-14,2	12,8	0,17
C5	H5	1,083	0,710	0,373	1,83	-16,9	-17,4	-16,7	17,2	0,04
C5A	H5A	1,083	0,709	0,374	1,82	-15,6	-17,1	-16,1	17,6	0,06
C5	C6	1,410	0,691	0,720	2,06	-15,3	-15,9	-13,1	13,7	0,18
C5A	C6A	1,409	0,681	0,728	2,06	-16,0	-15,9	-13,2	13,0	0,17
C6	N6	1,372	0,604	0,769	2,25	-16,7	-18,5	-15,7	17,6	0,15
C6A	N6A	1,374	0,615	0,759	2,27	-17,5	-19,0	-15,7	17,2	0,17
N6	H61	1,009	0,761	0,248	2,14	-28,5	-29,4	-27,2	28,1	0,07
N6A	H61A	1,009	0,758	0,251	2,11	-27,0	-28,4	-26,0	27,4	0,08

N6	H62	1,009	0,765	0,244	2,09	-28,4	-28,5	-26,5	26,5	0,07
N6A	H62A	1,009	0,753	0,256	2,15	-27,1	-28,6	-26,2	27,6	0,08
N1	C9	1,370	0,786	0,584	2,22	-15,5	-17,7	-15,1	17,3	0,15
N1A	C9A	1,370	0,786	0,584	2,20	-15,8	-17,7	-14,9	16,7	0,15
N1	C7	1,379	0,794	0,585	2,18	-15,7	-17,9	-14,7	16,9	0,18
N1A	C7A	1,378	0,804	0,575	2,14	-14,8	-17,0	-14,3	16,5	0,16
C9	H9	1,083	0,747	0,336	1,86	-18,5	-19,4	-17,9	18,8	0,08
C9A	H9A	1,083	0,738	0,345	1,88	-18,7	-19,3	-17,6	18,2	0,09
C9	C8	1,371	0,684	0,688	2,26	-18,4	-18,7	-14,2	14,5	0,24
C9A	C8A	1,375	0,682	0,694	2,22	-17,7	-17,9	-13,8	14,0	0,23
C8	N8	1,424	0,583	0,841	1,98	-15,2	-16,9	-13,2	14,9	0,22
C8A	N8A	1,429	0,577	0,852	1,93	-14,1	-16,4	-12,8	15,1	0,22
C8	N2	1,366	0,642	0,724	2,28	-12,9	-18,1	-16,3	21,5	0,10
C8A	N2A	1,363	0,637	0,726	2,31	-13,8	-18,5	-16,4	21,1	0,11
N8	O81	1,232	0,594	0,638	3,48	-11,2	-32,3	-30,3	51,4	0,06
N8A	O81A	1,237	0,602	0,636	3,35	-7,7	-31,3	-28,3	51,8	0,09
N8	O82	1,227	0,583	0,644	3,44	-12,0	-32,6	-30,1	50,7	0,07
N8A	O82A	1,223	0,596	0,628	3,45	-8,2	-31,9	-28,5	52,2	0,11
N2	C7	1,319	0,752	0,567	2,52	-21,0	-21,5	-17,8	18,3	0,17
N2A	C7A	1,321	0,775	0,545	2,50	-21,0	-21,2	-17,5	17,8	0,18
C7	C71	1,479	0,777	0,702	1,81	-12,0	-13,3	-12,1	13,4	0,09
C7A	C71A	1,483	0,795	0,688	1,79	-11,8	-12,7	-11,5	12,3	0,09
H71	C71	1,059	0,348	0,711	1,76	-13,9	-16,7	-15,7	18,5	0,06
H71A	C71A	1,059	0,335	0,724	1,70	-15,3	-16,3	-14,8	15,8	0,09
H72	C71	1,059	0,344	0,715	1,75	-14,0	-16,5	-15,7	18,2	0,05
H72A	C71A	1,059	0,346	0,713	1,75	-14,9	-16,3	-14,7	16,2	0,10
H73	C71	1,059	0,346	0,713	1,75	-13,9	-16,5	-15,6	18,1	0,06
H73A	C71A	1,059	0,355	0,704	1,79	-14,9	-16,7	-15,0	16,8	0,10