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A critical analysis of dipole moment calculations as obtained from experimental and theoretical structure factors.

Constrains/restraints imposed on the symmetry and simmilarity of the equivalent atoms:

a) symmetry:

atom	constrained symemtry
C1	*mymz*
C2	*mymz*
C3	*mymz*
C4	*mymz*
C5	*mymz*
C6	*mymz*
C7	*mz*
C8	*mz*
C9	*mz*
C71	*3m*
C91	*cy*
N1	*mymz*
N2	*mymz*
N8	*mymz*
N91	*cy*
O81	*mz*
O82	*mz*

where m – mirror plane, 3m – threefold axe, cy – cyllindrical symmetry.

b) equivalent atoms for similarity constraints/restraints on Plm, Pval, κ, κ':

C2 and C6
C3 and C5
O81 and O82
H2 and H6
H3 and H5
H71, H72 and H73

Table S1. MM of theoretical data with scale factor refined to reduce the effect of different wave functions.

Model	Multipolar expansion level of non-hydrogen / hydrogen atoms	Treatment of κ and κ' of hydrogen atoms	Parameter refined in order to remove the negative electron density	No reflections/ No parameters	Restraints/ Constraints	RF factor *w*R2F factor	Goof	Dipole moment value (module charge dipole/atomic dipole) [D]	Residual density [e/A^3] **up to 1.2Å^{-1}**
1m	HEX / QUA	refined	SCA	15074 / 532	-	0.548 0.526	0.064	14.85 (13.82/2.29)	0.287(15)/ -0.260(15)
1n	HEX / QUA	1.16	SCA	15074 / 532	-	0.554 0.531	0.064	15.32 (14.49/2.12)	0.291(15)/ -0.258(15)
1o	OCT / DIP	refined	SCA	15074 / 339	-	0.629 0.636	0.076	12.92 (12.94/1.45)	0.287(18)/ -0.248(18)
1p	OCT / DIP	1.16	SCA	15074 / 339	-	0.630 0.646	0.078	13.04 (12.62/1.40)	0.283(18)/ -0.252(18)
1q	HEX / QUA	refined	SCA	15074 / 532	R_{free} restraints	0.560 0.542	0.053	15.17 (13.63/2.39)	0.288(16)/ -0.261(16)
1r	HEX / QUA	1.16	SCA	15074 / 532	R_{free} restraints	0.565 0.546	0.060	15.64 (14.29/2.22)	0.292(16)/ -0.258(16)
1s	OCT / DIP	refined	SCA	15074 / 339	R_{free} restraints	0.638 0.649	0.068	13.50 (12.96/1.32)	0.287(18)/ -0.248(18)
1t	OCT / DIP	1.16	SCA	15074 / 339	R_{free} restraints	0.637 0.660	0.076	13.28 (12.26/1.49)	0.282(19)/ -0.252(19)

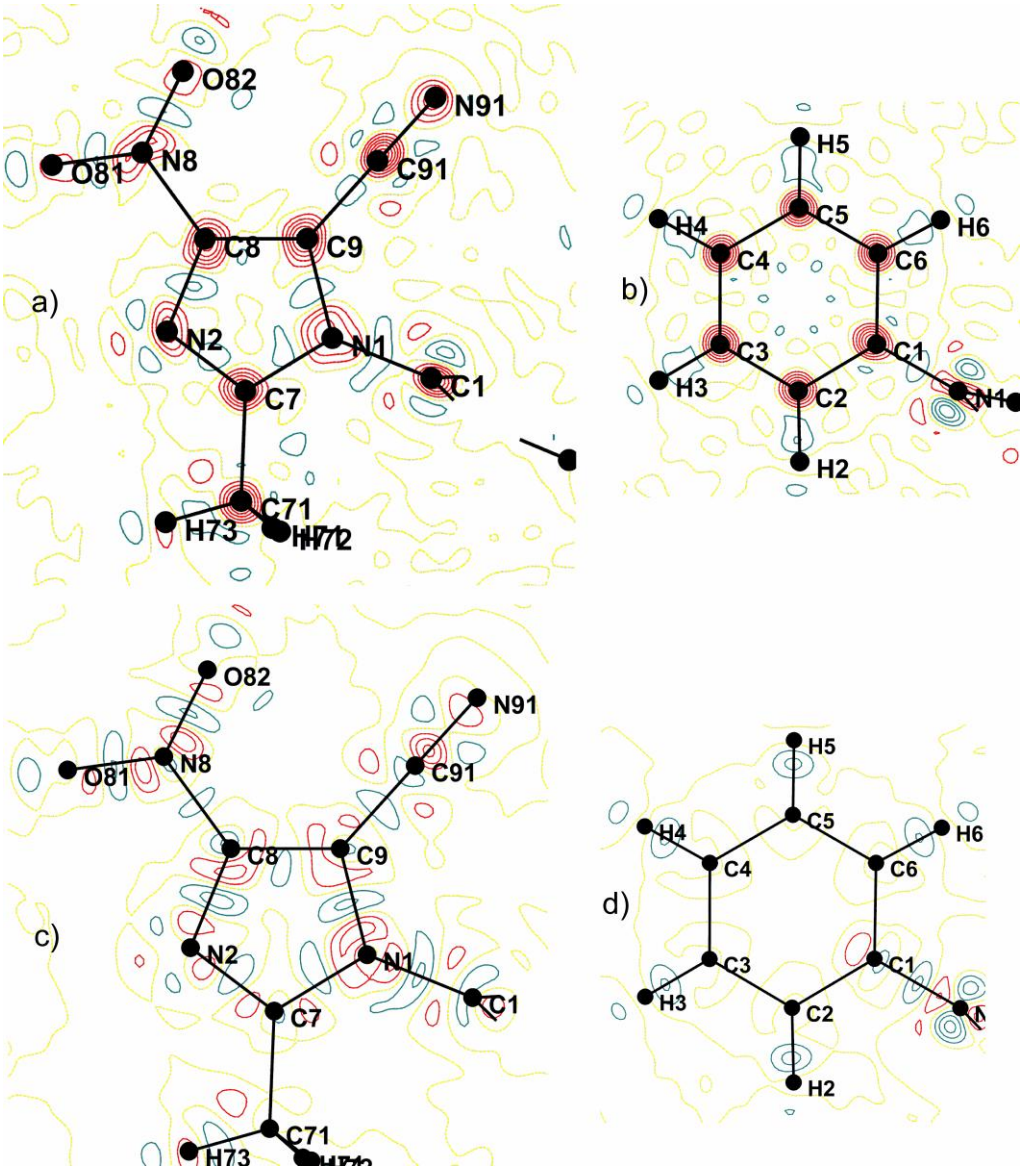
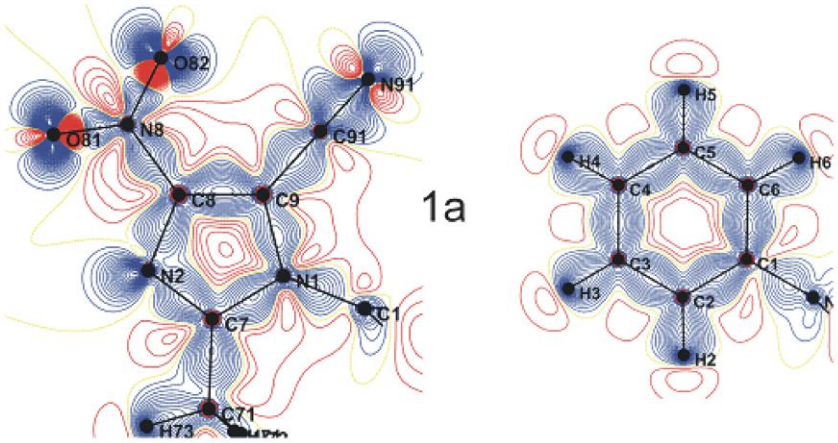
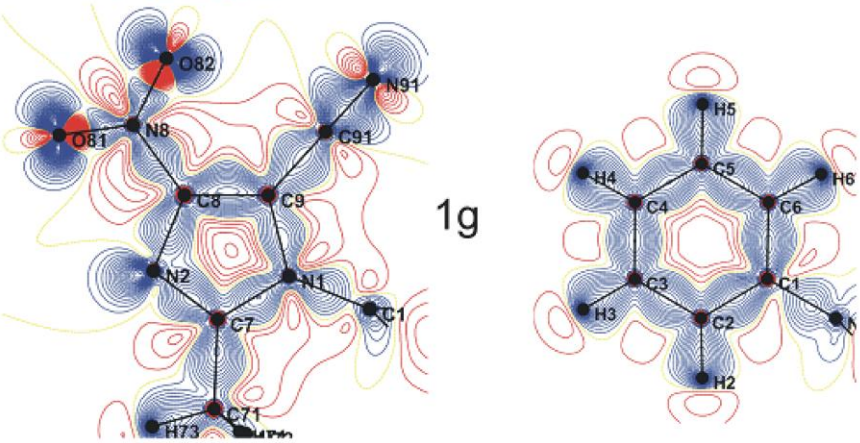


Figure S1. Example of residual Fourier density map for model 1c (*cf.* Table 1). a), b) without proper core scaling and c), d) after κ_{core} refinement; contours 0.05 e/Å^3, s_{max} = 1 Å^{-1}, red negative, blue positive.


O82
N91
O81
N8
C91
C8
C9
N2
N1
C1
C7
C71
H73
1a
H5
C5
H4
H6
C4
C6
C3
C1
H3
C2
H2


O82
N91
O81
N8
C91
C8
C9
N2
N1
C1
C7
C71
H73
1g
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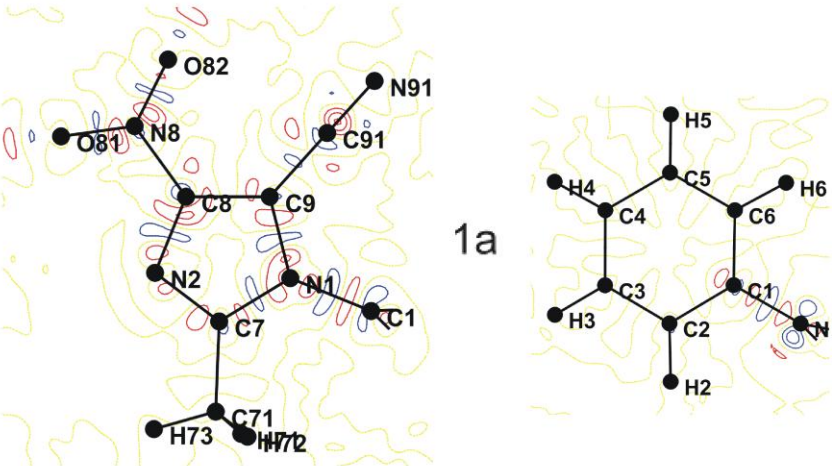
C5
H4
H6
C4
C6
C3
C1
H3
C2
H2


O82
N91
O81
N8
C91
C8
C9
N2
N1
C1
C7
C71
H73
1a
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C5
H4
H6
C4
C6
C3
C1
H3
C2
H2

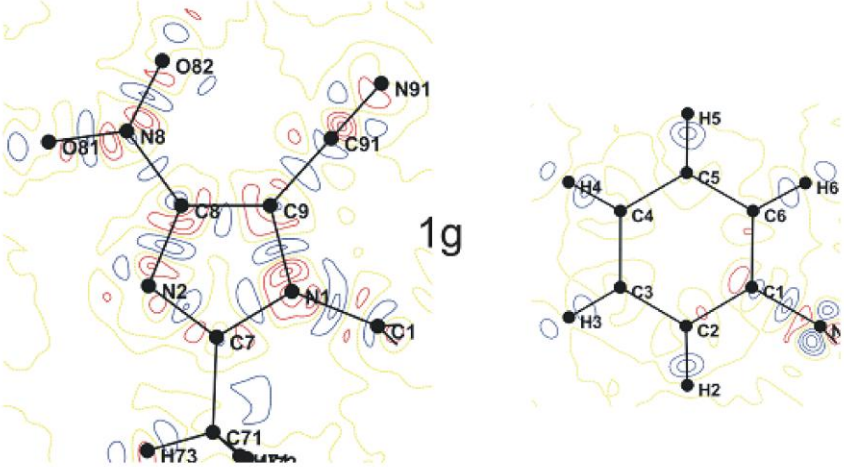

O82
N91
O81
N8
C91
C8
C9
N2
N1
C1
C7
C71
H73
1g
H5
C5
H4
H6
C4
C6
C3
C1
H3
C2
H2

Figure S2. Static deformation and Fourier residual maps for models 1c and 1g; contours ±0.05e/A^3, reciprocal resolution up to s = 1Å^{-1}.

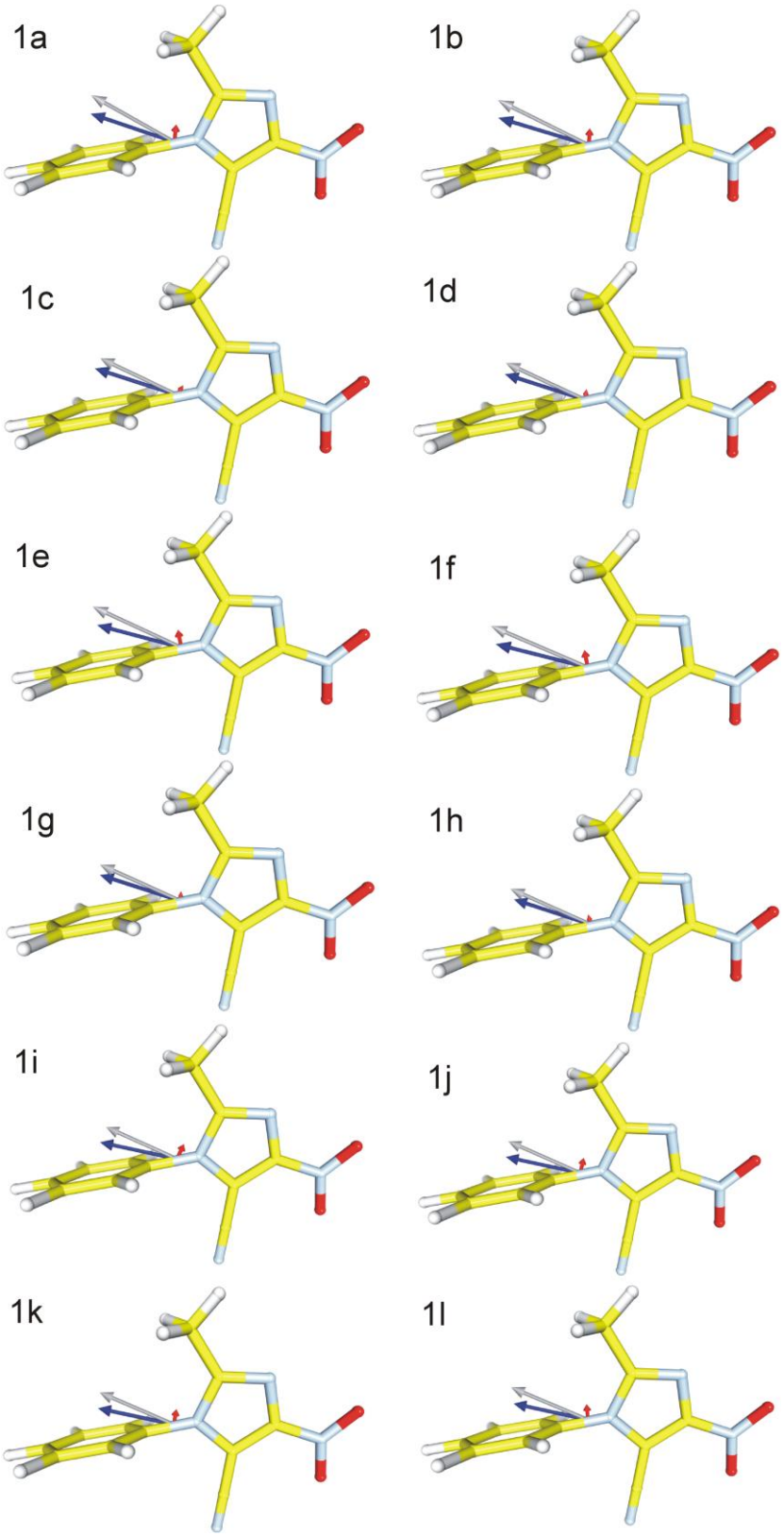


Figure S3. Dipole moment directions (grey – total, red – contribution from atomic dipoles, blue – contribution from atomic charges) for models 1a-1l.

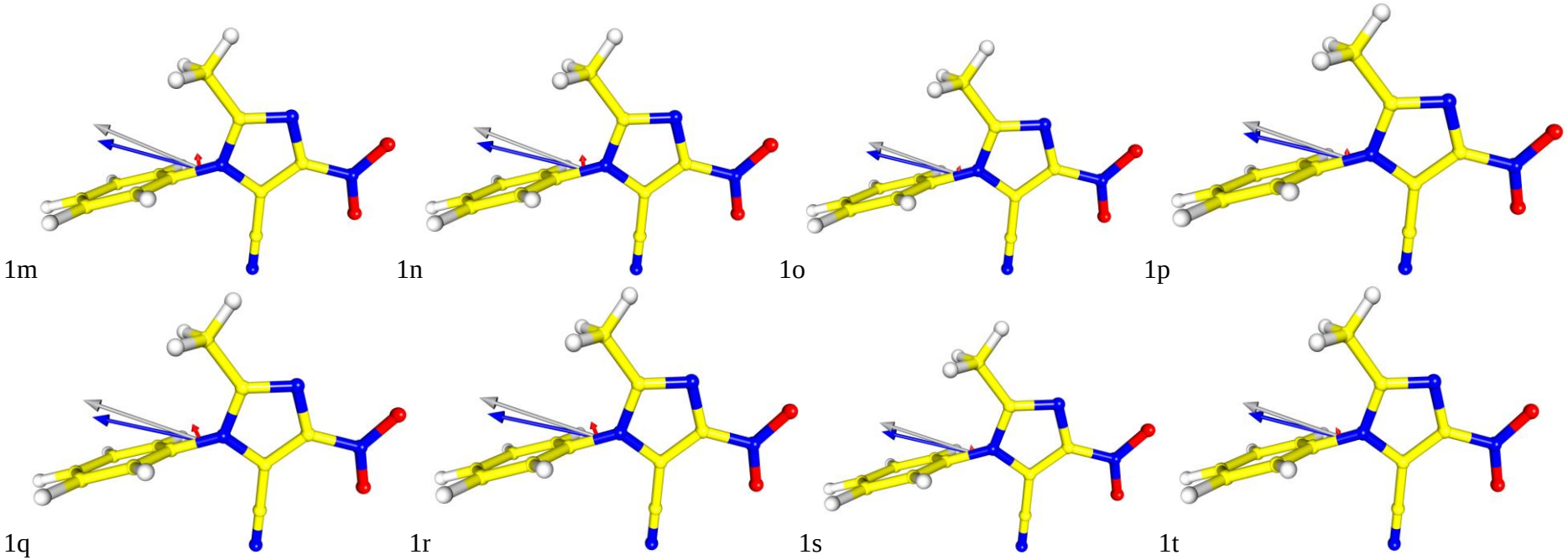


Figure S4. Dipole moments directions (grey – total, red – contribution from atomic dipoles, blue – contribution from atomic charges) for MM with scale factor refined.

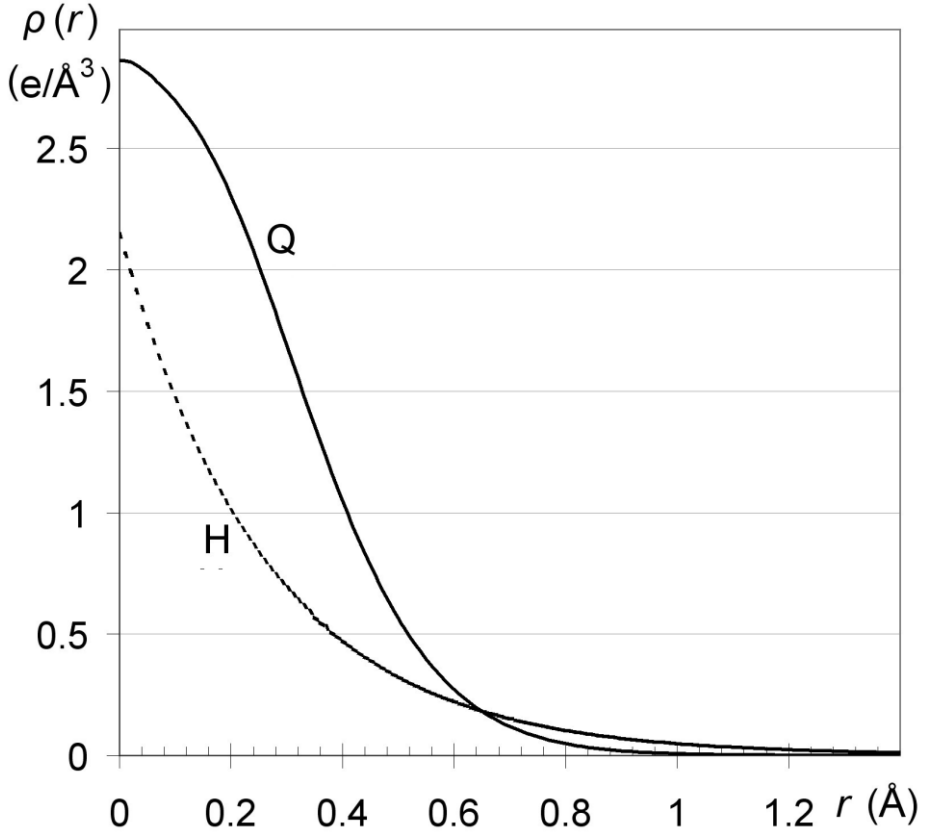


Figure S5. Electron density of a spherical virtual atom with P_{vir}=1 as a function of the distance r to the nucleus. For comparison, the same curve is shown for a hydrogen atom.

Table S2. Wave function coefficients and orbital exponents for the virtual atom described as a combination of Slater functions.
Slater(N_l, ξ,r) = coeff * r^{Nl} * exp(-ξr)

N_l	ξ	Coeff.
0	6.26445	0.07360
1	6.06204	0.13954
2	3.73854	0.87683

Table S3. κ, P_{val}, P_{10}, P_{11+} and P_{11-} parameters for models 1a-h.

	kp1							
	1a	1b	1c	1d	1e	1f	1g	1h
C1	0.990	0.990	0.989	0.989	0.997	0.997	0.996	0.997
C2	0.991	0.989	0.993	0.995	0.990	0.989	0.993	0.995
C3	0.988	0.987	0.991	0.993	0.985	0.984	0.987	0.990
C4	0.987	0.986	0.990	0.992	0.987	0.985	0.990	0.992
C5	0.988	0.987	0.991	0.993	0.986	0.985	0.988	0.991
C6	0.989	0.989	0.991	0.995	0.990	0.988	0.992	0.994
C7	0.987	0.987	0.993	0.993	0.985	0.985	0.992	0.993
C8	1.002	1.002	1.010	1.011	1.004	1.003	1.011	1.011
C9	0.993	0.993	1.003	1.003	0.997	0.997	1.007	1.007
C71	0.997	0.994	1.006	1.012	0.998	0.995	1.007	1.013
C91	0.982	0.981	0.988	0.988	0.982	0.981	0.988	0.989
N1	0.995	0.995	0.993	0.993	0.995	0.995	0.993	0.993
N2	0.987	0.987	0.991	0.991	0.988	0.988	0.991	0.991
N8	0.986	0.986	0.988	0.988	0.986	0.986	0.988	0.988
N91	0.991	0.991	0.994	0.994	0.992	0.991	0.994	0.994
O81	0.988	0.988	0.988	0.988	0.987	0.987	0.988	0.988
O82	0.988	0.988	0.988	0.988	0.987	0.987	0.988	0.988
H6	1.153	1.160	1.198	1.160	1.150	1.160	1.196	1.160
H2	1.149	1.160	1.192	1.160	1.149	1.160	1.195	1.160
H3	1.150	1.160	1.195	1.160	1.153	1.160	1.200	1.160
H4	1.148	1.160	1.192	1.160	1.150	1.160	1.192	1.160

H5	1.149	1.160	1.200	1.160	1.151	1.160	1.199	1.160
H73	1.149	1.160	1.184	1.160	1.151	1.160	1.187	1.160
H72	1.148	1.160	1.183	1.160	1.150	1.160	1.187	1.160
H71	1.160	1.160	1.196	1.160	1.151	1.160	1.187	1.160
	P_{val}							
	1a	1b	1c	1d	1e	1f	1g	1h
C1	4.05	4.04	4.08	4.09	3.98	3.97	3.97	3.98
C2	4.01	4.03	4.05	4.00	4.03	4.05	4.08	4.02
C3	4.04	4.04	4.11	4.06	4.05	4.05	4.16	4.11
C4	4.04	4.05	4.12	4.07	4.02	4.03	4.09	4.04
C5	4.02	4.03	4.12	4.07	4.05	4.05	4.16	4.11
C6	4.01	4.03	4.06	4.00	4.03	4.05	4.08	4.02
C7	4.21	4.21	4.16	4.16	4.26	4.26	4.17	4.17
C8	3.96	3.96	3.89	3.89	3.96	3.96	3.91	3.91
C9	3.96	3.97	3.98	3.97	3.93	3.93	3.92	3.92
C71	3.88	3.94	4.05	3.91	3.88	3.94	4.03	3.90
C91	4.52	4.52	4.35	4.35	4.53	4.53	4.36	4.35
N1	4.95	4.95	5.04	5.05	4.94	4.95	5.07	5.07
N2	4.96	4.97	4.97	4.97	4.94	4.95	4.97	4.97
N8	5.03	5.03	5.01	5.01	5.03	5.03	5.01	5.01
N91	4.69	4.70	4.82	4.82	4.67	4.68	4.82	4.83
O81	6.14	6.14	6.14	6.15	6.14	6.15	6.14	6.14
O82	6.13	6.14	6.14	6.14	6.14	6.15	6.14	6.14
H6	0.92	0.90	0.84	0.90	0.92	0.90	0.84	0.89
H2	0.92	0.90	0.85	0.89	0.92	0.90	0.84	0.89
H3	0.93	0.91	0.85	0.90	0.91	0.90	0.83	0.88
H4	0.94	0.92	0.86	0.90	0.94	0.92	0.86	0.90
H5	0.91	0.89	0.82	0.88	0.91	0.90	0.83	0.88
H73	0.95	0.93	0.91	0.95	0.94	0.92	0.90	0.95
H72	0.93	0.91	0.90	0.94	0.94	0.92	0.90	0.95
H71	0.91	0.91	0.88	0.94	0.94	0.92	0.90	0.95

dip x								
C1	0.121	0.117	0.171	0.173	0.104	0.102	0.146	0.148

C2	0.013	0.009	-0.030	-0.017	0.022	0.017	-0.024	-0.010
C3	0.021	0.014	-0.010	0.003	0.013	0.008	-0.013	0.003
C4	0.022	0.016	-0.010	0.003	0.020	0.013	-0.015	-0.002
C5	0.002	-0.005	-0.028	-0.012	0.013	0.007	-0.014	0.002
C6	0.026	0.023	-0.027	-0.013	0.023	0.017	-0.023	-0.009
C7	0.018	0.018	-0.010	-0.012	0.022	0.023	-0.006	-0.008
C8	-0.079	-0.077	-0.066	-0.065	-0.085	-0.084	-0.072	-0.071
C9	0.016	0.016	0.036	0.038	0.015	0.014	0.038	0.038
C71	0.018	0.013	0.017	0.013	0.001	0.001	0.002	0.002
C91	-0.003	-0.004	0.012	0.013	0.000	0.000	0.001	0.001
N1	0.003	0.003	0.014	0.016	-0.002	-0.002	0.015	0.015
N2	-0.138	-0.138	-0.126	-0.126	-0.140	-0.140	-0.125	-0.125
N8	-0.027	-0.027	-0.021	-0.021	-0.026	-0.027	-0.020	-0.021
N91	-0.001	-0.001	0.000	0.000	0.000	0.000	0.000	0.000
O81	-0.116	-0.116	-0.115	-0.115	-0.116	-0.116	-0.115	-0.115
O82	-0.116	-0.116	-0.116	-0.115	-0.116	-0.115	-0.115	-0.115
dip y								
C1	0.002	0.003	0.002	0.003	0.000	0.000	0.000	0.000
C2	0.030	0.028	0.032	0.032	0.001	0.001	0.001	0.001
C3	0.009	0.009	0.009	0.007	0.000	0.000	0.000	0.000
C4	-0.002	-0.001	-0.002	-0.001	0.000	0.000	0.000	0.000
C5	-0.015	-0.015	-0.010	-0.007	0.000	0.000	0.000	0.000
C6	0.031	0.028	0.033	0.031	0.001	0.001	0.001	0.001
C7	0.080	0.079	0.096	0.098	0.070	0.069	0.087	0.088
C8	0.164	0.161	0.162	0.162	0.156	0.154	0.159	0.159
C9	-0.077	-0.078	-0.088	-0.089	-0.078	-0.079	-0.080	-0.081
C71	-0.006	-0.006	-0.004	-0.004	0.000	0.000	0.000	0.000
C91	0.008	0.008	0.007	0.008	0.001	0.001	0.001	0.001
N1	-0.017	-0.017	-0.014	-0.013	-0.001	-0.001	-0.001	-0.001
N2	-0.004	-0.005	-0.002	-0.001	-0.001	-0.001	0.000	0.000
N8	0.005	0.005	0.000	-0.002	0.000	0.000	0.000	0.000
N91	0.002	0.002	0.003	0.002	0.001	0.001	0.001	0.001
O81	-0.002	-0.002	-0.005	-0.005	-0.002	-0.002	-0.005	-0.005
O82	-0.002	0.002	-0.005	-0.005	-0.002	-0.002	-0.005	-0.005

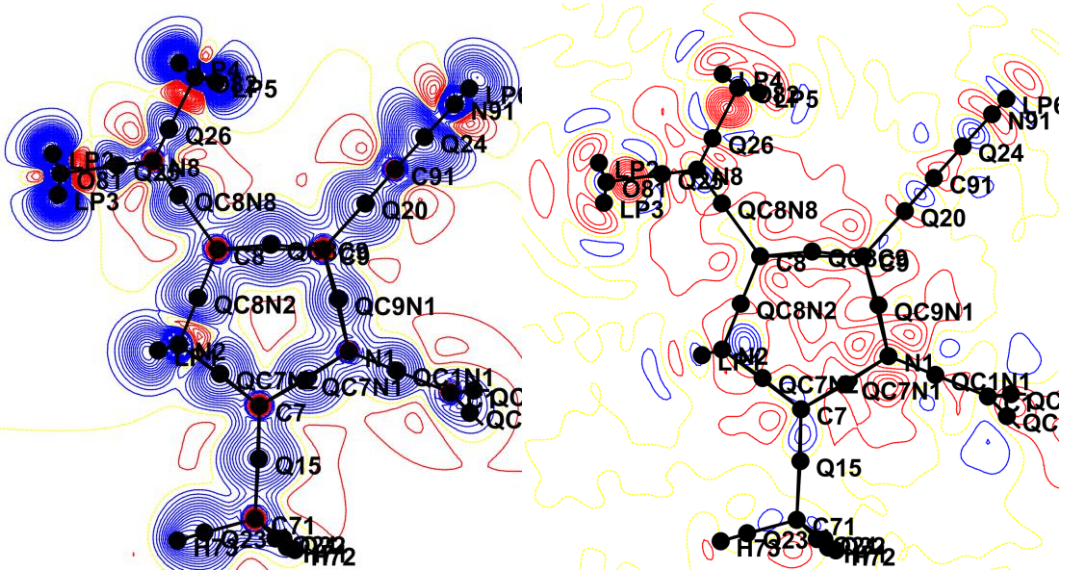
dip z								
C1	0.000	0.000	0.003	0.003				
C2	0.005	0.005	0.002	0.002				
C3	-0.005	-0.005	-0.002	-0.003				
C4	-0.001	-0.001	0.002	0.002				
C5	0.000	0.000	0.000	0.000				
C6	-0.001	-0.001	0.001	0.000				
C7	0.006	0.006	0.006	0.006				
C8	-0.002	-0.002	-0.001	-0.001				
C9	0.003	0.003	0.000	-0.001				
C71	-0.065	-0.068	-0.091	-0.082	-0.067	-0.071	-0.086	-0.078
C91	0.385	0.382	0.316	0.312	0.387	0.384	0.306	0.302
N1	-0.004	-0.004	-0.003	-0.002	-0.001	-0.001	0.000	0.000
N2	0.001	0.001	0.001	0.001	0.000	0.000	0.000	0.000
N8	-0.002	-0.002	-0.003	-0.003	0.000	0.000	0.000	0.000
N91	-0.133	-0.133	-0.120	-0.119	-0.133	-0.133	-0.119	-0.118
O81	0.000	0.000	0.001	0.001	0.000	0.000	0.000	0.000
O82	-0.001	-0.001	-0.001	-0.001	0.000	0.000	0.000	0.000
H6	0.168	0.167	0.130	0.154	0.167	0.169	0.131	0.158
H2	0.173	0.175	0.134	0.162	0.168	0.170	0.132	0.159
H3	0.163	0.165	0.125	0.151	0.167	0.170	0.125	0.154
H4	0.161	0.166	0.121	0.151	0.164	0.169	0.122	0.151
H5	0.166	0.171	0.127	0.157	0.168	0.171	0.126	0.155
H73	0.157	0.150	0.112	0.133	0.151	0.146	0.112	0.135
H72	0.149	0.140	0.106	0.128	0.150	0.146	0.111	0.134
H71	0.156	0.155	0.117	0.142	0.151	0.147	0.112	0.136

Table S4 Results of the VIRAT$_{theo}$ refinement (no additional atoms on N=O bonds)

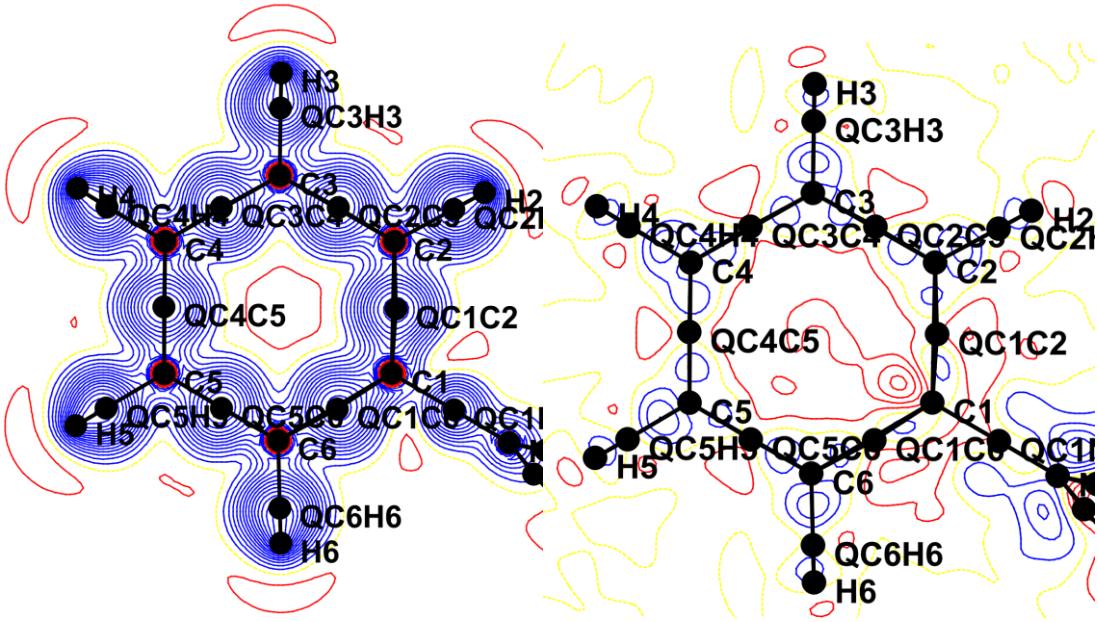
Model	Restraints/Constraints	No reflections/ No parameters	RF factor *w*R2F factor	Goof	Dipole moment value [D]	Residual density [e/A^3] up to 1.2Å^{-1}
2j	Default restraints*	15074 / 213	0.986 1.123	0.134	17.30	0.605(33)/ -0.688(33)
2k	Modified rest**	15074 / 213	0.840 0.987	0.118	17.33	0.329(29)/ -0.644(29)
2l	No restraints	15074 / 213	0.819 0.977	0.117	18.70	0.297(29)/ -0.578(29)
2m	Modified rest κ_{HYD} = **1.1**	15074 / 205	0.863 1.018	0.122	11.30	0.322(30)/ -0.646(30)
2n	Modified rest κ_{HYD} = **1.13**	15074 / 205	0.853 1.004	0.120	12.84	0.324(30)/ -0.644(30)
2o	Modified rest κ_{HYD} = **1.16**	15074 / 205	0.847 0.995	0.119	14.31	0.326(29)/ -0.644(29)

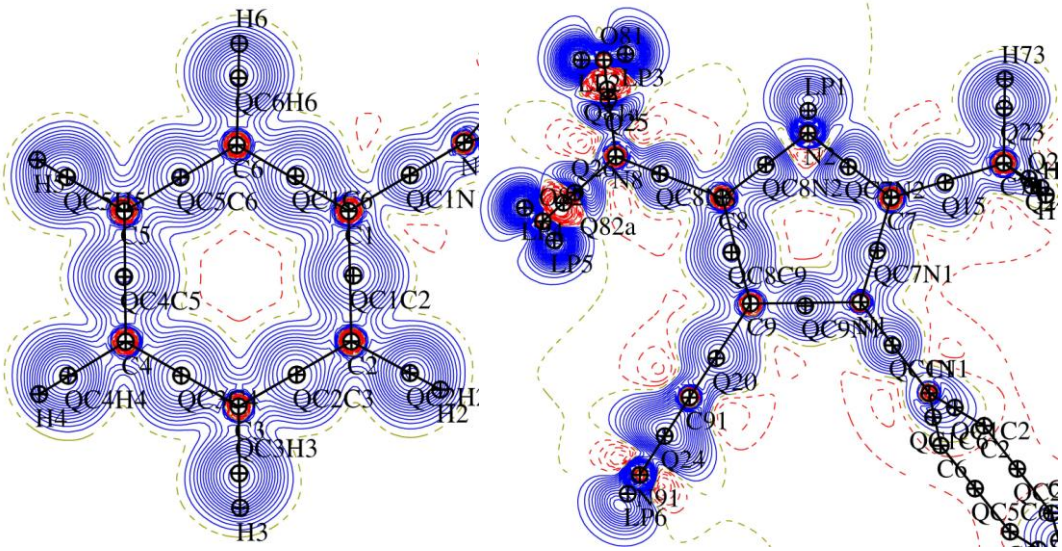
***Default restraints:** Linearity 0.001; Distances: H-Q 0.37 0.01, LP 0.28 0.01; Distance similarities: LP 0.01; Angles LP 0.1; Planarity (LP) 0.001.

****Modified restraints:** Linearity 0.1; Distances: H-Q 0.37 0.01, LP 0.28 0.01; Distance similarities: LP 0.01; Planarity (LP) 0.001


Q26
Q24
C91
Q20
QC8N8
C8
QC9
QC8N2
QC9N1
N1
QC1N1
QC7N1
C7
Q15
C71
H73
H72
LP3
O81
N91

2k


H3
QC3H3
C3
H4
QC4H4
QC3C4
QC2C9
H2
C4
C2
QC4C5
QC1C2
C5
C1
H5
QC5H5
QC5C6
QC1C6
C6
QC6H6
H6


H6
QC6H6
C6
QC5C6
QC1C6
QC1N1
C5
C1
QC4C5
QC1C2
C4
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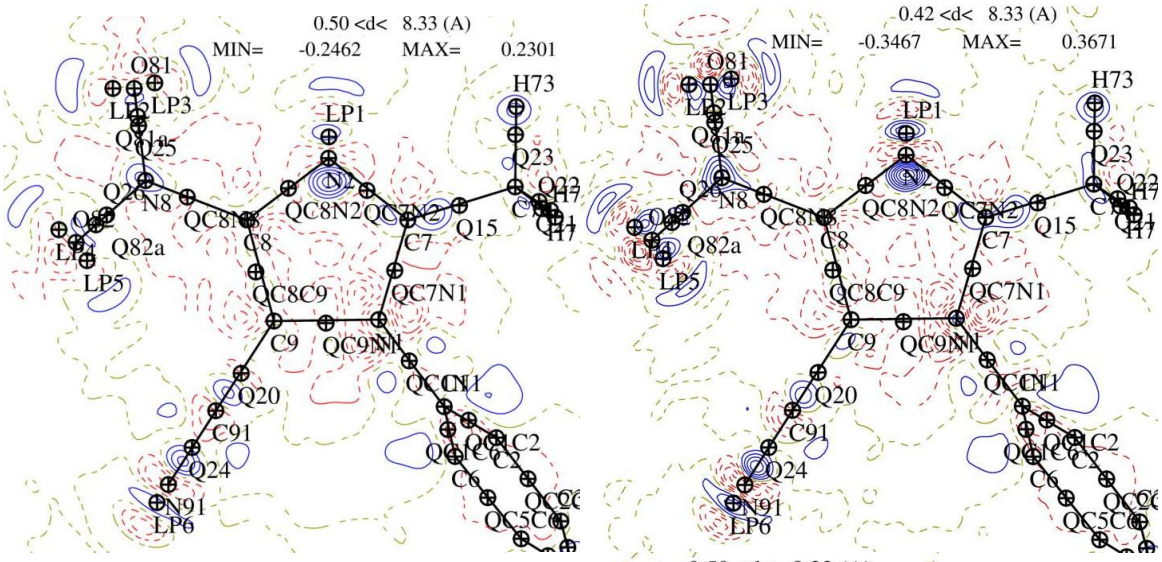
QC4H4
QC2C3
QC2H2
H4
H2
C3
QC3H3
H3
O81
LP3
Q25
H73
Q23
LP1
N2
Q20
N8
QC8N2
QC7N2
Q15
C7
C8
Q82a
LP5
QC8C9
QC7N1
C9
QC9N1
Q20
C91
Q24
N91
LP6

2d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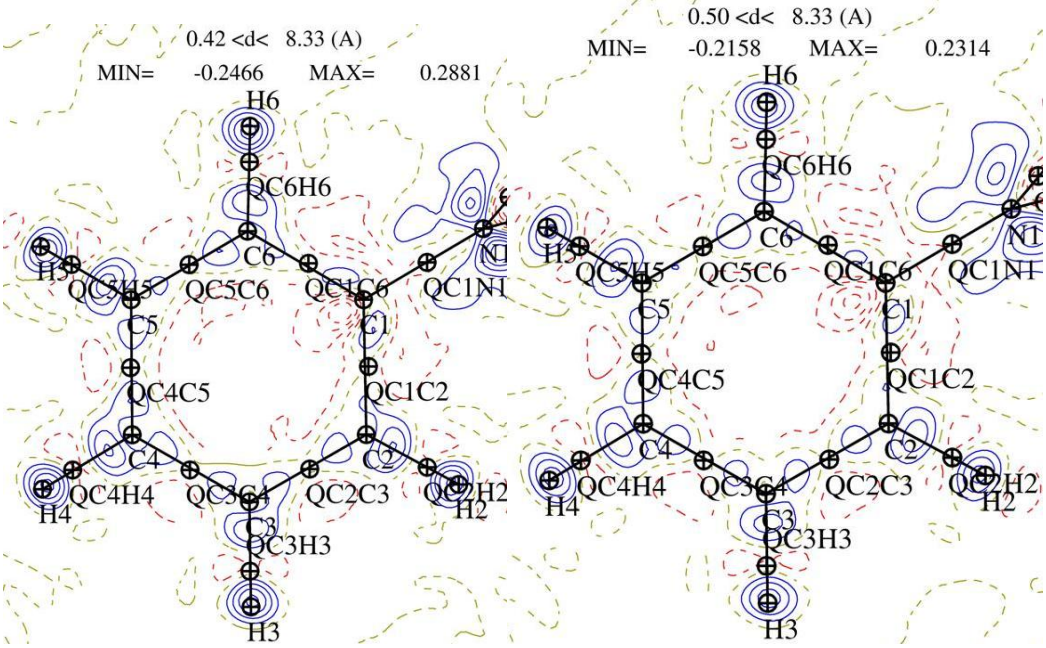
MIN= -0.3467 MAX= 0.3671
O81
LP3
H73
LP1
Q25
Q23
N2
Q20
N8
QC8N2
QC7N2
Q15
C7
C8
Q82a
LP5
QC8C9
QC7N1
C9
QC9N1
Q20
C91
Q24
N91
LP6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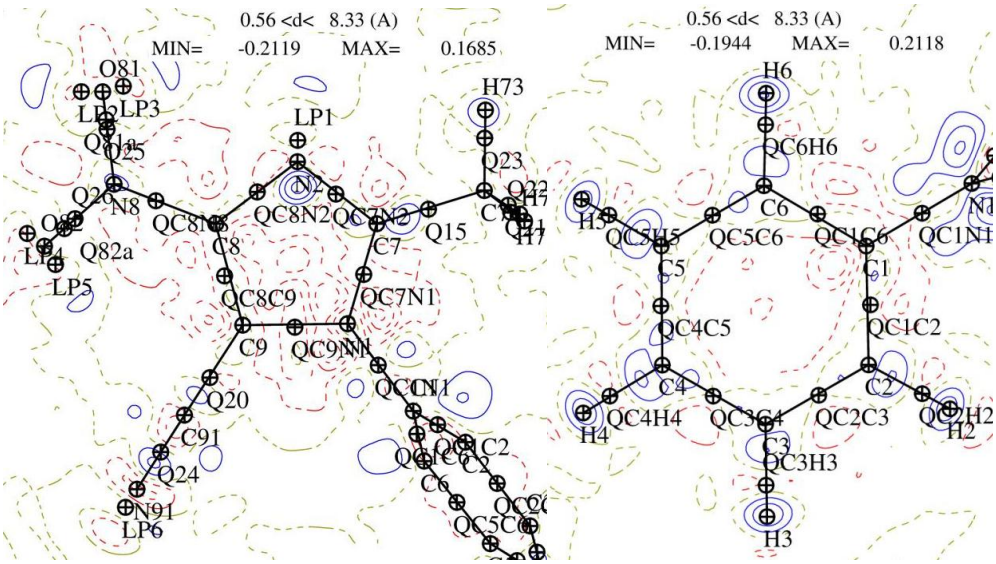
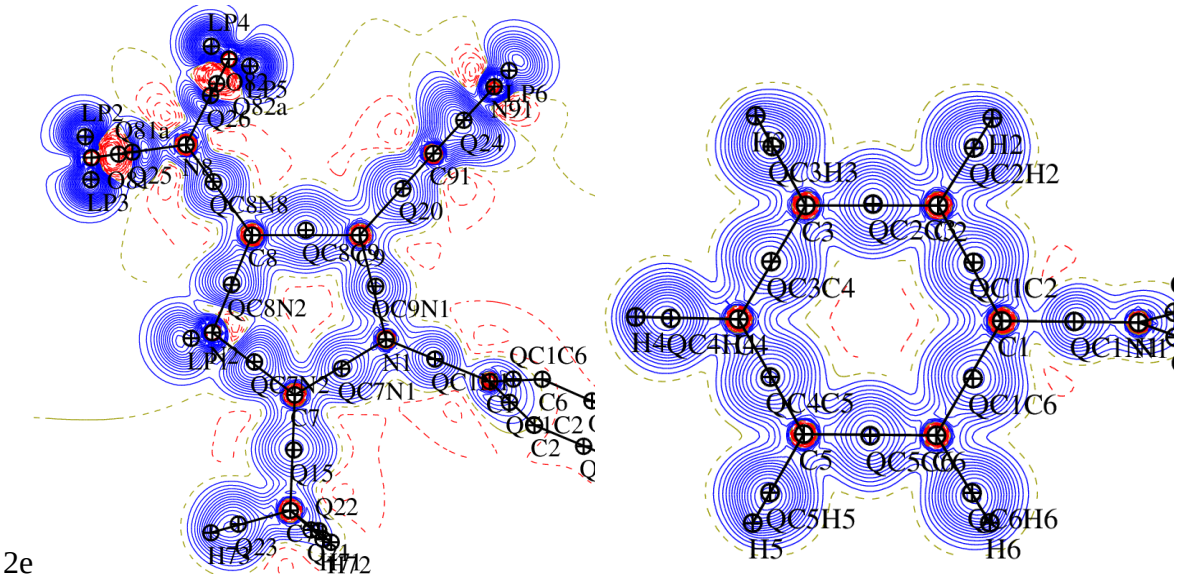
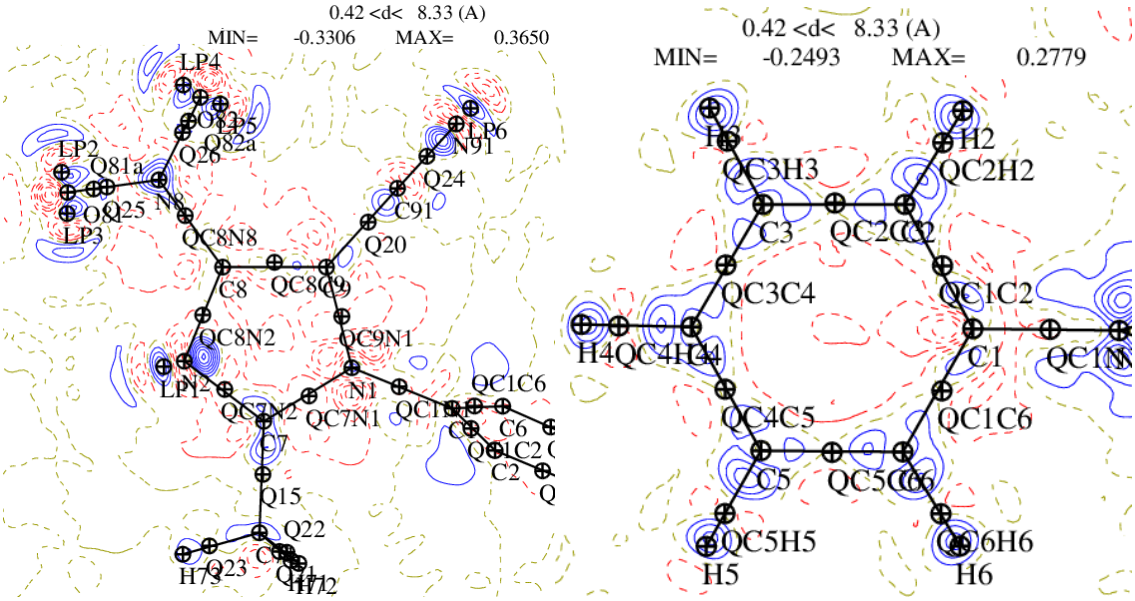
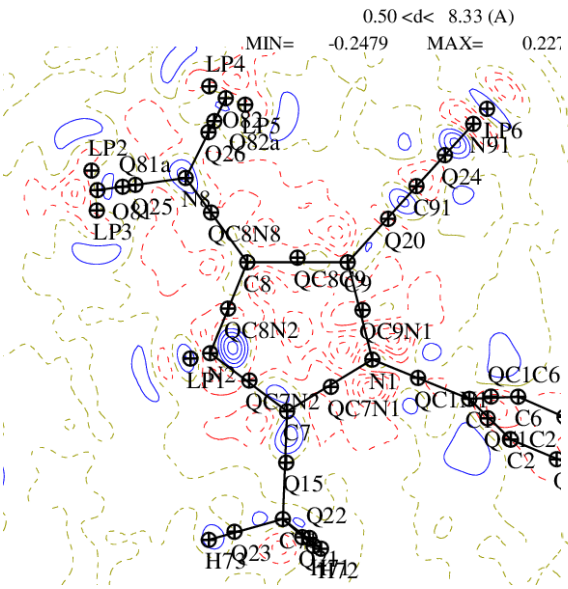
H6
QC6H6
C6
QC5C6
QC1C6
QC1N1
C5
C1
QC4C5
QC1C2
C4
C2
QC4H4
QC3C4
QC2C3
QC2H2
H4
H2
C3
QC3H3
H3

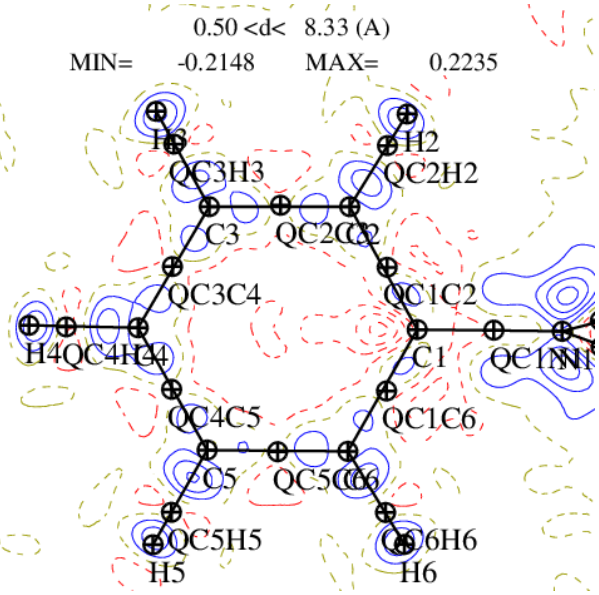

0.56 <d< 8.33 (A)
MIN= -0.2119 MAX= 0.1685
0.56 <d< 8.33 (A)
MIN= -0.1944 MAX= 0.2118

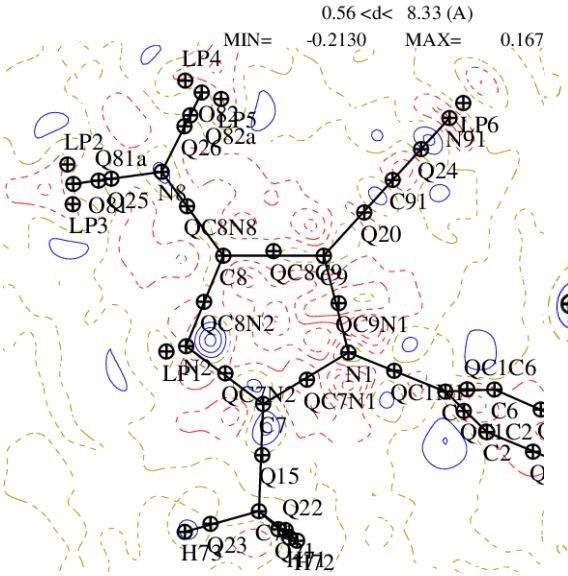
2e




0.42 <d< 8.33 (A)
MIN= -0.3306 MAX= 0.3650
0.42 <d< 8.33 (A)
MIN= -0.2493 MAX= 0.2779


0.50 <d< 8.33 (A)
MIN= -0.2479 MAX= 0.227
LP4
O82
Q25
Q82a
Q26
LP2
Q81a
O81
Q25
LP3
N8
QC8N8
C8
QC8C9
Q20
C91
Q24
LP6
N91
QC8N2
QC9N1
LP2
QC2N2
QC7N1
N1
QC1C6
C7
Q15
Q22
H73
Q23


0.50 <d< 8.33 (A)
MIN= -0.2148 MAX= 0.2235
H3
QC3H3
H2
QC2H2
C3
QC2C2
QC3C4
QC1C2
H4QC4H4
C1
QC4C5
QC1C6
C5
QC5C6
QC5H5
H5
H6


0.56 <d< 8.33 (A)
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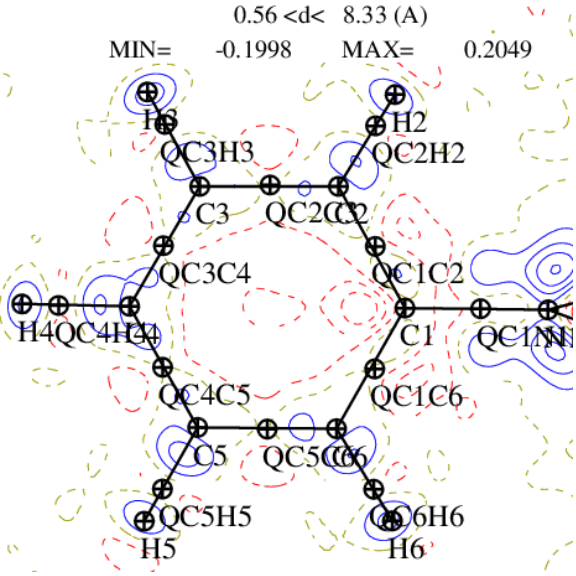
LP4
O82
Q25
Q82a
Q26
LP2
Q81a
O81
Q25
LP3
N8
QC8N8
C8
QC8C9
Q20
C91
Q24
LP6
N91
QC8N2
QC9N1
LP2
QC2N2
QC7N1
N1
QC1C6
C7
Q15
Q22
H73
Q23


0.56 <d< 8.33 (A)
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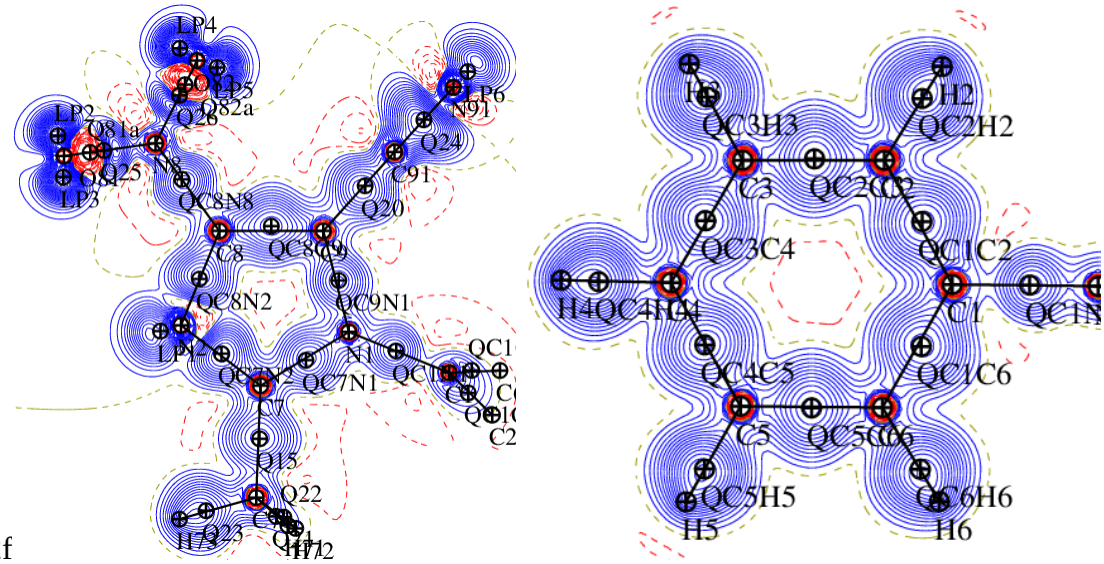
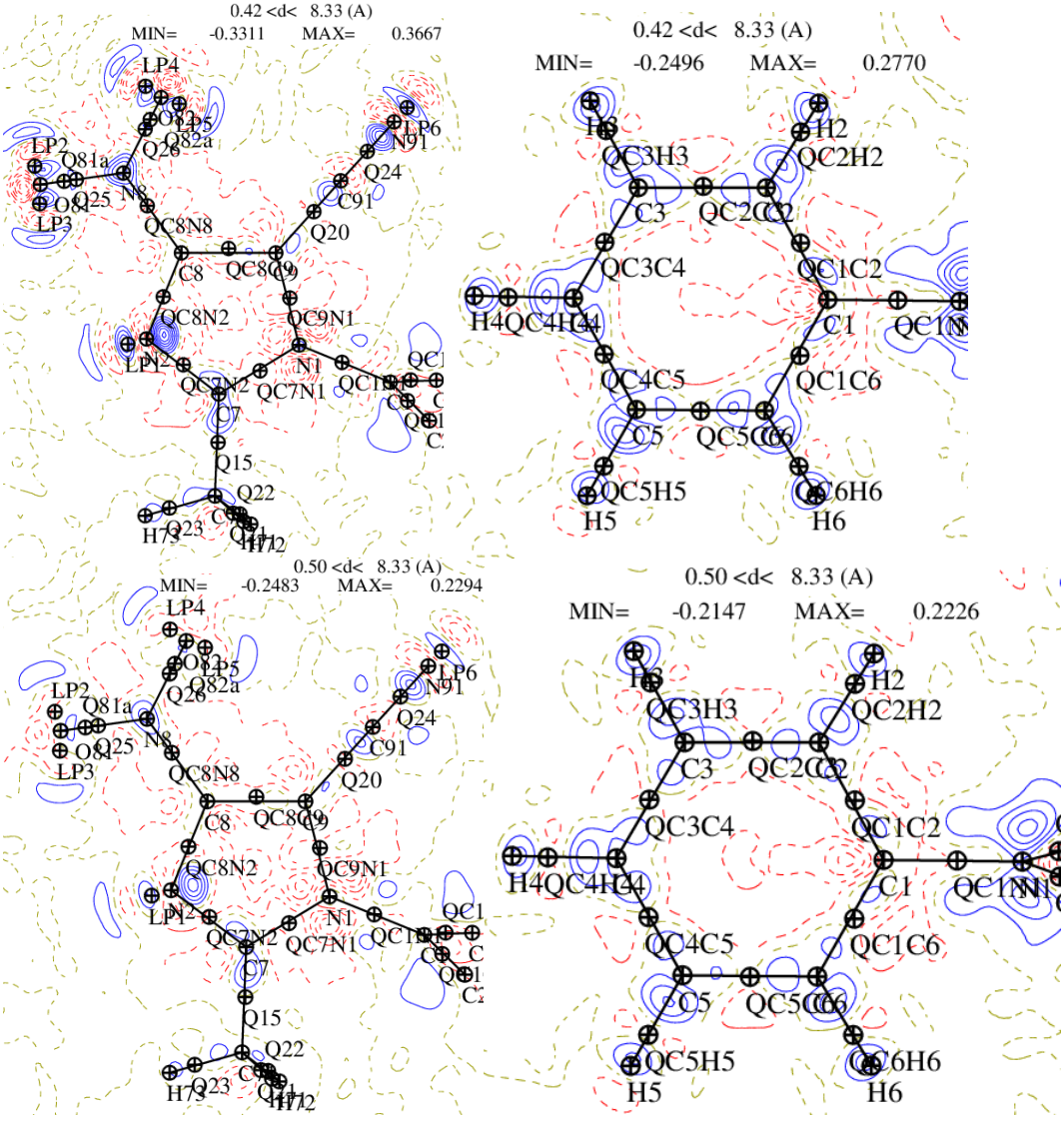
QC3H3
H2
QC2H2
C3
QC2C2
QC3C4
QC1C2
H4QC4H4
C1
QC4C5
QC1C6
C5
QC5C6
QC5H5
H5
H6


LP4
LP2
Q81a
Q25
LP3
N8
Q28
Q82a
LP6
N91
Q24
C91
Q20
QC8N8
C8
QC8C9
QC8N2
QC9N1
LP1
N1
QC7N2
QC7N1
C7
Q15
Q22
H3
H2
QC3H3
QC2H2
C3
QC2C2
QC3C4
QC1C2
H4
QC4H4
C1
QC4C5
QC1C6
C5
QC5C6
QC5H5
QC6H6
H5
H6

2f


0.42 <d< 8.33 (A)
MIN= -0.3311 MAX= 0.3667
0.42 <d< 8.33 (A)
MIN= -0.2496 MAX= 0.2770
0.50 <d< 8.33 (A)
MIN= -0.2483 MAX= 0.2294
0.50 <d< 8.33 (A)
MIN= -0.2147 MAX= 0.2226
LP4
LP2
Q81a
Q25
LP3
N8
Q28
Q82a
LP6
N91
Q24
C91
Q20
QC8N8
C8
QC8C9
QC8N2
QC9N1
LP1
N1
QC7N2
QC7N1
C7
Q15
Q22
H3
H2
QC3H3
QC2H2
C3
QC2C2
QC3C4
QC1C2
H4
QC4H4
C1
QC4C5
QC1C6
C5
QC5C6
QC5H5
QC6H6
H5
H6

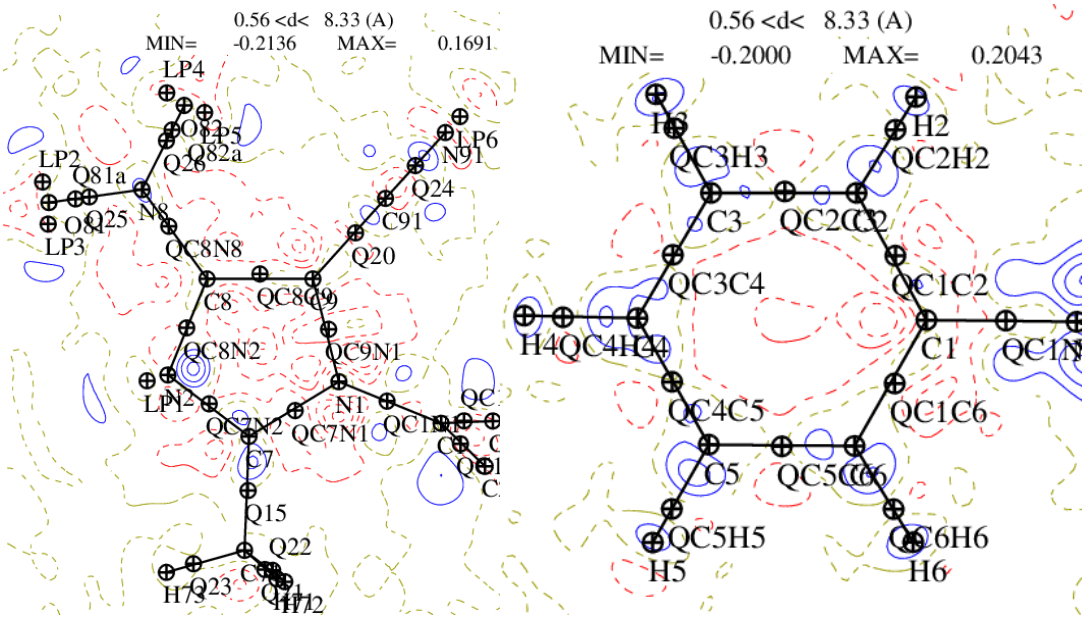


Figure S6. Static deformation and Fourier residual density maps for VIRTAT 3j, 3k, 3l, contour 0.05e/A, resolution 1.2A^{-1}.

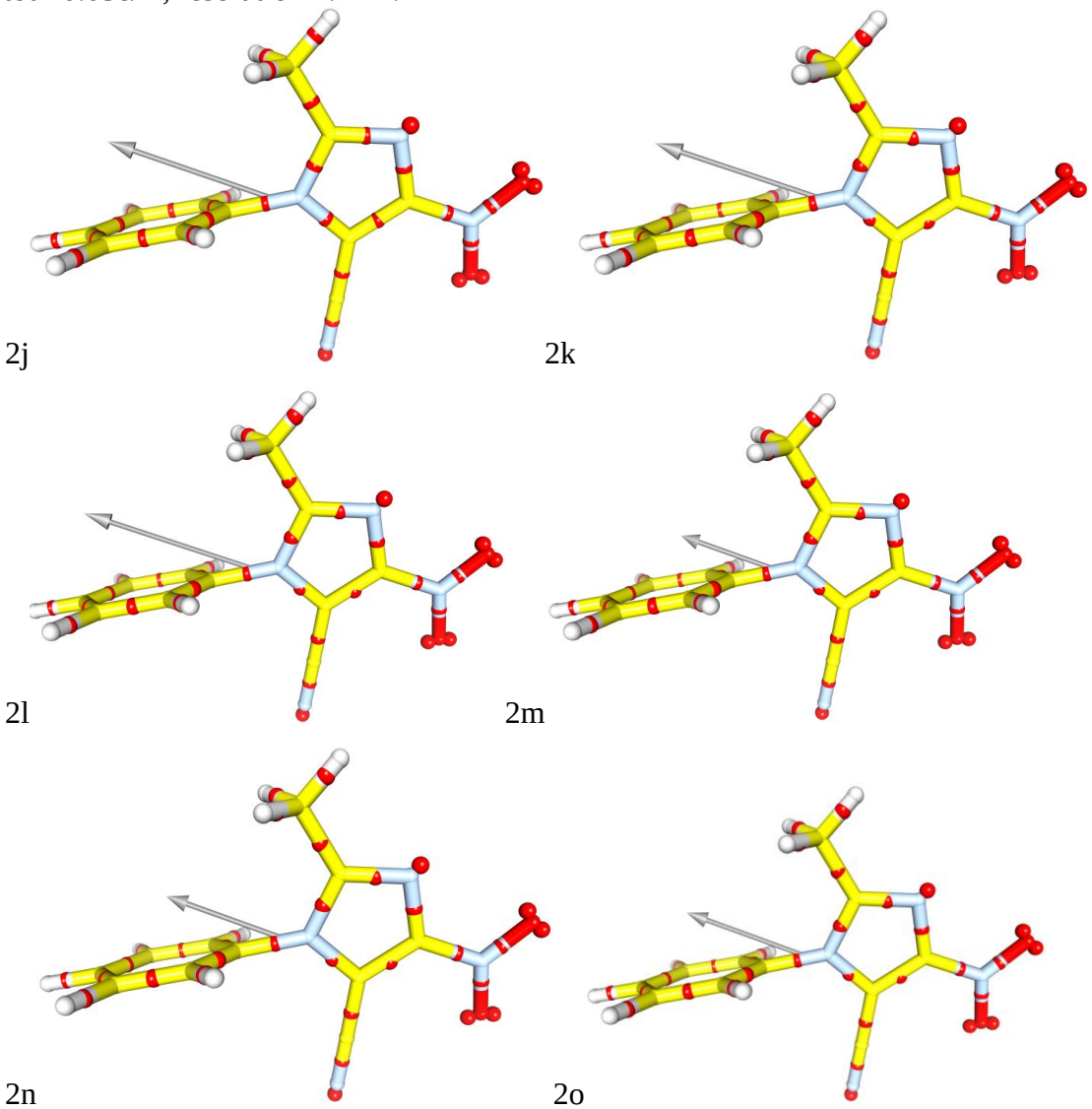


Figure S7. Dipole moment directions in sub-models 2.

Table S4. κ and P_{val} for models 2a-o.

	kp1														
	2a	2b	2c	2d	2e	2f	2g	2h	2i	2j	2k	2l	2m	2n	2o
C1	1.0387	1.0382	1.0377	1.0387	1.0349	1.0344	1.0386	1.0349	1.0346	1.0373	1.0379	1.0381	1.0396	1.0390	1.0385
C2	1.0312	1.0290	1.0268	1.0311	1.0268	1.0246	1.0302	1.0263	1.0240	1.0195	1.0236	1.0241	1.0331	1.0308	1.0287
C3	1.0294	1.0275	1.0257	1.0294	1.0252	1.0233	1.0293	1.0255	1.0237	1.0219	1.0229	1.0221	1.0300	1.0281	1.0264
C4	1.0257	1.0236	1.0215	1.0257	1.0232	1.0212	1.0256	1.0232	1.0211	1.0163	1.0171	1.0172	1.0256	1.0236	1.0215
C5	1.0293	1.0273	1.0254	1.0294	1.0259	1.0240	1.0293	1.0255	1.0237	1.0203	1.0234	1.0212	1.0309	1.0288	1.0270
C6	1.0291	1.0267	1.0246	1.0293	1.0258	1.0236	1.0302	1.0263	1.0240	1.0197	1.0214	1.0216	1.0303	1.0280	1.0258
C7	1.0528	1.0516	1.0506	1.0529	1.0509	1.0500	1.0528	1.0510	1.0503	1.0504	1.0487	1.0462	1.0526	1.0513	1.0502
C8	1.0530	1.0520	1.0512	1.0530	1.0556	1.0548	1.0532	1.0555	1.0546	1.0566	1.0519	1.0508	1.0556	1.0547	1.0538
C9	1.0434	1.0430	1.0426	1.0434	1.0430	1.0426	1.0433	1.0430	1.0428	1.0374	1.0424	1.0426	1.0437	1.0434	1.0431
C71	1.0599	1.0520	1.0450	1.0600	1.0536	1.0466	1.0602	1.0536	1.0465	1.0396	1.0380	1.0392	1.0612	1.0535	1.0472
C91	1.0072	1.0061	1.0051	1.0070	1.0055	1.0045	1.0071	1.0056	1.0045	0.9983	0.9976	0.9973	1.0013	1.0003	0.9993
N1	1.0117	1.0116	1.0116	1.0118	1.0108	1.0107	1.0118	1.0108	1.0108	1.0101	1.0110	1.0114	1.0114	1.0113	1.0112
N2	0.9549	0.9543	0.9536	0.9549	0.9554	0.9546	0.9551	0.9553	0.9547	0.9527	0.9523	0.9624	0.9549	0.9543	0.9537
N8	1.0436	1.0431	1.0424	1.0434	1.0444	1.0437	1.0424	1.0452	1.0445	1.0280	1.0293	1.0337	1.0302	1.0301	1.0296
N91	0.9382	0.9373	0.9364	0.9381	0.9364	0.9355	0.9381	0.9364	0.9354	0.9315	0.9332	0.9388	0.9368	0.9358	0.9350
O81	0.9665	0.9653	0.9652	0.9664	0.9660	0.9653	0.9670	0.9660	0.9655	0.9520	0.9408	0.9252	0.9439	0.9428	0.9423
O82	0.9660	0.9657	0.9652	0.9663	0.9669	0.9667	0.9670	0.9660	0.9655	0.9518	0.9432	0.9287	0.9458	0.9453	0.9449
H6	1.1000	1.1300	1.1600	1.1000	1.1300	1.1600	1.1000	1.1300	1.1600	1.2311	1.2335	1.2338	1.1000	1.1300	1.1600
H2	1.1000	1.1300	1.1600	1.1000	1.1300	1.1600	1.1000	1.1300	1.1600	1.2470	1.2501	1.2559	1.1000	1.1300	1.1600
H3	1.1000	1.1300	1.1600	1.1000	1.1300	1.1600	1.1000	1.1300	1.1600	1.2361	1.2266	1.2277	1.1000	1.1300	1.1600
H4	1.1000	1.1300	1.1600	1.1000	1.1300	1.1600	1.1000	1.1300	1.1600	1.2461	1.2433	1.2454	1.1000	1.1300	1.1600
H5	1.1000	1.1300	1.1600	1.1000	1.1300	1.1600	1.1000	1.1300	1.1600	1.2394	1.2271	1.2311	1.1000	1.1300	1.1600
H73	1.1000	1.1300	1.1600	1.1000	1.1300	1.1600	1.1000	1.1300	1.1600	1.2186	1.2213	1.2320	1.1000	1.1300	1.1600
H72	1.1000	1.1300	1.1600	1.1000	1.1300	1.1600	1.1000	1.1300	1.1600	1.2071	1.1930	1.2013	1.1000	1.1300	1.1600
H71	1.1000	1.1300	1.1600	1.1000	1.1300	1.1600	1.1000	1.1300	1.1600	1.2042	1.1953	1.1960	1.1000	1.1300	1.1600
QC1N1	1.1877	1.1900	1.1919	1.1877	1.2061	1.2088	1.1877	1.2061	1.2084	1.2531	1.2002	1.1971	1.1903	1.1925	1.1953
QC1C6	0.8202	0.8239	0.8269	0.8276	0.8353	0.8385	0.8280	0.8357	0.8389	0.8537	0.8304	0.8281	0.8189	0.8225	0.8259
QC1C2	0.8452	0.8487	0.8523	0.8368	0.8402	0.8435	0.8365	0.8401	0.8434	0.8629	0.8533	0.8527	0.8410	0.8450	0.8482
QC2C3	0.8347	0.8404	0.8454	0.8248	0.8389	0.8439	0.8247	0.8392	0.8441	0.8657	0.8564	0.8543	0.8371	0.8431	0.8488
QC2H2	0.9182	0.9123	0.9053	0.9153	0.9169	0.9093	0.9151	0.9169	0.9094	0.8713	0.8760	0.8750	0.9152	0.9098	0.9031

QC3C4	0.8225	0.8280	0.8324	0.8207	0.8338	0.8385	0.8207	0.8341	0.8388	0.8471	0.8380	0.8354	0.8207	0.8258	0.8313
QC3H3	0.9208	0.9147	0.9070	0.9133	0.9049	0.8975	0.9133	0.9051	0.8976	0.8764	0.8883	0.8886	0.9233	0.9175	0.9095
QC4C5	0.8141	0.8194	0.8241	0.8159	0.8323	0.8365	0.8161	0.8324	0.8365	0.8509	0.8287	0.8246	0.8118	0.8172	0.8218
QC4H4	0.9134	0.9075	0.9004	0.9134	0.9135	0.9066	0.9133	0.9135	0.9067	0.8717	0.8711	0.8715	0.9083	0.9025	0.8958
QC5C6	0.8134	0.8189	0.8236	0.8228	0.8320	0.8367	0.8232	0.8324	0.8370	0.8566	0.8347	0.8302	0.8169	0.8224	0.8277
QC5H5	0.9160	0.9107	0.9041	0.9232	0.9180	0.9111	0.9233	0.9182	0.9112	0.8817	0.8860	0.8869	0.9152	0.9101	0.9039
QC6H6	0.8987	0.8923	0.8845	0.9012	0.9056	0.8982	0.9014	0.9059	0.8985	0.8681	0.8616	0.8628	0.9002	0.8940	0.8852
QC7N1	0.9882	0.9900	0.9918	0.9880	0.9942	0.9965	0.9877	0.9942	0.9963	1.0141	0.9974	0.9957	0.9883	0.9901	0.9935
QC7N2	0.9596	0.9626	0.9655	0.9593	0.9628	0.9665	0.9586	0.9632	0.9659	0.9702	0.9652	0.9693	0.9544	0.9577	0.9599
Q15	0.8078	0.8154	0.8214	0.8077	0.8231	0.8299	0.8076	0.8231	0.8298	0.8226	0.8254	0.8267	0.8055	0.8127	0.8178
QC8N8	1.0415	1.0425	1.0436	1.0419	1.0276	1.0285	1.0431	1.0266	1.0275	1.0269	1.0254	1.0185	1.0236	1.0243	1.0249
QC8N2	1.0082	1.0115	1.0142	1.0080	1.0144	1.0163	1.0090	1.0138	1.0176	1.0307	1.0175	1.0245	1.0044	1.0075	1.0114
QC8C9	0.8671	0.8683	0.8697	0.8671	0.8697	0.8714	0.8670	0.8699	0.8715	0.8754	0.8675	0.8672	0.8625	0.8637	0.8644
QC9N1	1.1080	1.1105	1.1129	1.1080	1.1140	1.1168	1.1076	1.1142	1.1168	1.1443	1.1226	1.1191	1.1153	1.1179	1.1183
Q20	0.8771	0.8791	0.8808	0.8774	0.8927	0.8943	0.8771	0.8928	0.8943	0.8853	0.8799	0.8808	0.8736	0.8754	0.8770
Q21	0.8687	0.8654	0.8601	0.8747	0.8670	0.8616	0.8745	0.8670	0.8617	0.8331	0.8507	0.8533	0.8689	0.8656	0.8590
Q22	0.8695	0.8660	0.8596	0.8667	0.8554	0.8496	0.8666	0.8552	0.8495	0.8299	0.8509	0.8506	0.8691	0.8657	0.8583
Q23	0.8676	0.8649	0.8598	0.8642	0.8602	0.8549	0.8641	0.8601	0.8549	0.8426	0.8404	0.8353	0.8674	0.8644	0.8587
Q24	0.7969	0.7994	0.8016	0.7970	0.8000	0.8025	0.7968	0.8001	0.8026	0.8040	0.8031	0.8021	0.7937	0.7962	0.7986
Q25	1.2254	1.2266	1.2309	1.2254	1.2060	1.2091	1.2215	1.2072	1.2096	1.2431	1.2523	1.2306	1.2345	1.2429	1.2469
Q26	1.2129	1.2191	1.2230	1.2141	1.2081	1.2123	1.2154	1.2057	1.2104	1.2378	1.2303	1.2121	1.2084	1.2128	1.2193
LP1	1.0658	1.0688	1.0717	1.0655	1.0482	1.0501	1.0675	1.0475	1.0512	1.0614	1.0817	1.1330	1.0695	1.0727	1.0757
LP2	1.4787	1.4828	1.4866	1.4790	1.4873	1.4935	1.4872	1.4765	1.4808	1.5221	1.4424	1.3996	1.4370	1.4374	1.4388
LP3	1.4436	1.4472	1.4508	1.4434	1.4533	1.4607	1.4518	1.4429	1.4484	1.4990	1.4239	1.3844	1.4160	1.4182	1.4205
LP4	1.4973	1.5005	1.5043	1.4975	1.4751	1.4762	1.4874	1.4877	1.4895	1.5117	1.4583	1.4138	1.4500	1.4522	1.4552
LP5	1.4696	1.4730	1.4753	1.4702	1.4425	1.4426	1.4584	1.4552	1.4568	1.4727	1.4289	1.3942	1.4240	1.4252	1.4266
LP6	1.0295	1.0339	1.0379	1.0300	1.0309	1.0356	1.0297	1.0310	1.0356	1.0362	1.0412	1.0580	1.0256	1.0300	1.0335
Q81a	1.3201	1.3570	1.3269	1.3225	1.3709	1.3810	1.3210	1.3500	1.3531						
Q82a	1.4370	1.4179	1.4093	1.4223	1.3607	1.3424	1.3431	1.4394	1.4282						

	val														
	2a	2b	2c	2d	2e	2f	2g	2h	2i	2j	2k	2l	2m	2n	2o
C1	3.3128	3.3231	3.3328	3.3119	3.3359	3.3456	3.3121	3.3361	3.3457	3.4059	3.3300	3.3251	3.2904	3.3014	3.3118

C2	3.2614	3.2956	3.3263	3.2085	3.2778	3.3076	3.2079	3.2787	3.3088	3.3586	3.3548	3.3515	3.2425	3.2778	3.3080
C3	3.2394	3.2716	3.2971	3.2207	3.2763	3.3021	3.2211	3.2774	3.3029	3.3480	3.3453	3.3317	3.2479	3.2799	3.3076
C4	3.1908	3.2227	3.2492	3.1907	3.2656	3.2921	3.1903	3.2661	3.2931	3.3130	3.2595	3.2467	3.1621	3.1936	3.2213
C5	3.2013	3.2350	3.2635	3.2207	3.2764	3.3021	3.2211	3.2774	3.3029	3.3589	3.3020	3.2686	3.1950	3.2288	3.2588
C6	3.1563	3.1923	3.2214	3.2083	3.2777	3.3075	3.2079	3.2787	3.3088	3.3479	3.2619	3.2478	3.1580	3.1932	3.2223
C7	3.0578	3.0712	3.0833	3.0569	3.1086	3.1216	3.0568	3.1086	3.1209	3.1406	3.0897	3.0936	3.0413	3.0549	3.0671
C8	3.3705	3.3813	3.3908	3.3703	3.3628	3.3726	3.3690	3.3638	3.3739	3.4067	3.3846	3.3889	3.3425	3.3527	3.3632
C9	3.4298	3.4363	3.4429	3.4301	3.4555	3.4619	3.4299	3.4559	3.4615	3.4417	3.4388	3.4374	3.4159	3.4219	3.4266
C71	2.8256	2.9224	2.9988	2.8239	2.8905	2.9657	2.8223	2.8900	2.9667	2.9534	3.0561	3.0706	2.8067	2.9006	2.9681
C91	3.0149	3.0304	3.0442	3.0169	3.0653	3.0787	3.0153	3.0659	3.0795	3.0968	3.0616	3.0576	3.0048	3.0197	3.0343
N1	4.9256	4.9276	4.9289	4.9253	4.9245	4.9265	4.9246	4.9246	4.9259	4.9674	4.9441	4.9375	4.9363	4.9377	4.9403
N2	4.8015	4.8187	4.8346	4.8004	4.7831	4.7987	4.8031	4.7821	4.8009	4.8204	4.8646	4.9286	4.7988	4.8162	4.8319
N8	4.0976	4.1036	4.1121	4.0994	4.0763	4.0836	4.1078	4.0694	4.0768	4.0512	4.0400	3.9799	4.0173	4.0237	4.0307
N91	4.4474	4.4721	4.4946	4.4498	4.4554	4.4796	4.4487	4.4559	4.4798	4.4947	4.5173	4.5507	4.4255	4.4500	4.4734
O81	6.0630	6.0617	6.0802	6.0619	6.0675	6.0787	6.0720	6.0619	6.0717	6.1029	5.9665	5.9179	5.9297	5.9389	5.9490
O82	6.0586	6.0709	6.0812	6.0619	6.0675	6.0787	6.0720	6.0619	6.0717	6.0920	5.9725	5.9271	5.9424	5.9502	5.9586
H6	0.7667	0.7372	0.7074	0.7547	0.7327	0.7039	0.7544	0.7327	0.7038	0.6376	0.6312	0.6391	0.7636	0.7345	0.7045
H2	0.7428	0.7160	0.6888	0.7544	0.7324	0.7036	0.7544	0.7327	0.7038	0.6068	0.6023	0.5955	0.7388	0.7125	0.6859
H3	0.7813	0.7504	0.7195	0.7658	0.7303	0.7002	0.7656	0.7303	0.7002	0.6369	0.6485	0.6557	0.7770	0.7466	0.7162
H4	0.7617	0.7315	0.7012	0.7617	0.7366	0.7065	0.7613	0.7368	0.7066	0.6175	0.6179	0.6227	0.7602	0.7303	0.7002
H5	0.7501	0.7212	0.6919	0.7656	0.7300	0.6998	0.7656	0.7303	0.7002	0.6044	0.6247	0.6438	0.7452	0.7165	0.6885
H73	0.8045	0.7759	0.7453	0.7952	0.7646	0.7346	0.7950	0.7647	0.7347	0.6798	0.6792	0.6476	0.8018	0.7729	0.7427
H72	0.8026	0.7739	0.7433	0.7952	0.7649	0.7348	0.7950	0.7647	0.7347	0.6851	0.7058	0.6894	0.7946	0.7665	0.7362
H71	0.7792	0.7500	0.7195	0.7951	0.7646	0.7346	0.7950	0.7647	0.7347	0.6659	0.6856	0.6978	0.7787	0.7495	0.7187
QC1N1	0.1287	0.1277	0.1268	0.1288	0.1203	0.1194	0.1288	0.1203	0.1195	0.1049	0.1241	0.1253	0.1280	0.1270	0.1259
QC1C6	0.5687	0.5584	0.5501	0.5507	0.5248	0.5164	0.5498	0.5238	0.5156	0.4843	0.5440	0.5491	0.5752	0.5648	0.5561
QC1C2	0.5106	0.5015	0.4932	0.5289	0.5152	0.5070	0.5298	0.5154	0.5072	0.4725	0.4931	0.4946	0.5236	0.5137	0.5055
QC2C3	0.5348	0.5203	0.5082	0.5591	0.5191	0.5073	0.5598	0.5187	0.5070	0.4694	0.4853	0.4897	0.5288	0.5140	0.5012
QC2H2	0.4367	0.4388	0.4436	0.4413	0.4269	0.4328	0.4417	0.4268	0.4328	0.4853	0.4842	0.4868	0.4447	0.4461	0.4506
QC3C4	0.5649	0.5501	0.5387	0.5705	0.5349	0.5234	0.5703	0.5342	0.5228	0.5070	0.5274	0.5349	0.5702	0.5558	0.5427
QC3H3	0.4155	0.4183	0.4243	0.4306	0.4381	0.4445	0.4305	0.4378	0.4442	0.4608	0.4453	0.4428	0.4134	0.4157	0.4213
QC4C5	0.5818	0.5665	0.5540	0.5760	0.5273	0.5162	0.5758	0.5272	0.5162	0.4941	0.5461	0.5600	0.5921	0.5765	0.5634
QC4H4	0.4422	0.4452	0.4512	0.4421	0.4342	0.4397	0.4424	0.4341	0.4395	0.4872	0.4925	0.4907	0.4514	0.4545	0.4601
QC5C6	0.5817	0.5663	0.5538	0.5571	0.5292	0.5181	0.5561	0.5284	0.5173	0.4830	0.5284	0.5417	0.5725	0.5574	0.5443

QC5H5	0.4494	0.4515	0.4568	0.4344	0.4348	0.4410	0.4342	0.4346	0.4408	0.4822	0.4809	0.4745	0.4534	0.4554	0.4596
QC6H6	0.4517	0.4554	0.4625	0.4478	0.4279	0.4338	0.4475	0.4273	0.4333	0.4677	0.4944	0.4905	0.4513	0.4546	0.4627
QC7N1	0.2558	0.2538	0.2521	0.2559	0.2478	0.2456	0.2561	0.2478	0.2458	0.2308	0.2479	0.2502	0.2558	0.2539	0.2515
QC7N2	0.3389	0.3344	0.3301	0.3394	0.3365	0.3313	0.3398	0.3362	0.3315	0.3251	0.3284	0.3172	0.3457	0.3409	0.3370
Q15	0.5681	0.5463	0.5295	0.5687	0.5247	0.5081	0.5691	0.5248	0.5080	0.5163	0.5201	0.5169	0.5766	0.5553	0.5405
QC8N8	0.2734	0.2722	0.2708	0.2730	0.2891	0.2878	0.2717	0.2902	0.2890	0.3021	0.2998	0.3096	0.3034	0.3022	0.3010
QC8N2	0.2571	0.2536	0.2506	0.2574	0.2543	0.2517	0.2566	0.2547	0.2508	0.2391	0.2465	0.2358	0.2603	0.2567	0.2531
QC8C9	0.4456	0.4425	0.4395	0.4455	0.4437	0.4403	0.4459	0.4434	0.4402	0.4357	0.4455	0.4460	0.4577	0.4547	0.4522
QC9N1	0.1629	0.1616	0.1604	0.1629	0.1588	0.1574	0.1630	0.1587	0.1575	0.1449	0.1549	0.1562	0.1592	0.1580	0.1572
Q20	0.4667	0.4626	0.4591	0.4661	0.4355	0.4322	0.4666	0.4352	0.4321	0.4456	0.4618	0.4615	0.4759	0.4721	0.4686
Q21	0.4971	0.4908	0.4909	0.4834	0.4915	0.4910	0.4838	0.4917	0.4909	0.5466	0.4989	0.4868	0.4987	0.4928	0.4953
Q22	0.4611	0.4542	0.4546	0.4679	0.4795	0.4801	0.4682	0.4799	0.4803	0.5122	0.4634	0.4653	0.4663	0.4594	0.4616
Q23	0.4871	0.4792	0.4785	0.4952	0.4921	0.4912	0.4956	0.4923	0.4912	0.5095	0.5018	0.5174	0.4890	0.4819	0.4826
Q24	0.9224	0.9106	0.9004	0.9213	0.9039	0.8934	0.9223	0.9034	0.8930	0.8939	0.8997	0.8915	0.9425	0.9311	0.9197
Q25	0.4407	0.3501	0.4242	0.4338	0.3157	0.3027	0.4125	0.3488	0.3433	0.1306	0.1326	0.1418	0.1393	0.1366	0.1351
Q26	0.2634	0.2768	0.2803	0.2725	0.3277	0.3548	0.3512	0.2657	0.2696	0.1314	0.1387	0.1475	0.1467	0.1447	0.1427
LP1	0.3285	0.3251	0.3225	0.3289	0.3466	0.3447	0.3265	0.3475	0.3433	0.3379	0.3144	0.2533	0.3261	0.3226	0.3199
LP2	0.1725	0.1714	0.1704	0.1724	0.1691	0.1672	0.1693	0.1733	0.1721	0.1527	0.2240	0.2726	0.2236	0.2248	0.2240
LP3	0.1861	0.1850	0.1841	0.1862	0.1825	0.1798	0.1827	0.1869	0.1849	0.1619	0.2342	0.2834	0.2344	0.2351	0.2342
LP4	0.1623	0.1614	0.1608	0.1620	0.1705	0.1703	0.1666	0.1653	0.1651	0.1553	0.2116	0.2578	0.2122	0.2116	0.2106
LP5	0.1695	0.1690	0.1685	0.1696	0.1803	0.1808	0.1752	0.1742	0.1745	0.1649	0.2228	0.2665	0.2223	0.2220	0.2215
LP6	0.4329	0.4270	0.4221	0.4323	0.4320	0.4260	0.4327	0.4319	0.4260	0.4316	0.4228	0.3894	0.4435	0.4378	0.4327
Q81a	-0.4045	-0.3047	-0.3883	-0.3967	-0.2603	-0.2466	-0.3801	-0.2966	-0.2914						
Q82a	-0.1974	-0.2156	-0.2232	-0.2097	-0.2767	-0.3106	-0.3098	-0.1950	-0.2032						

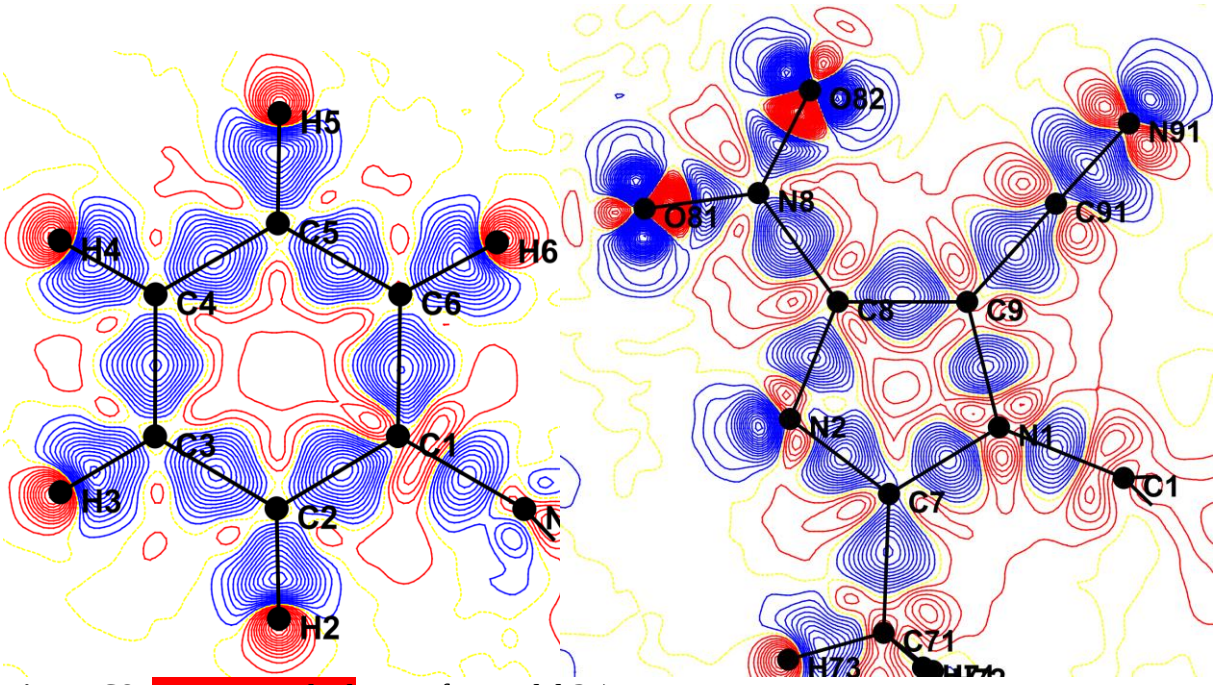


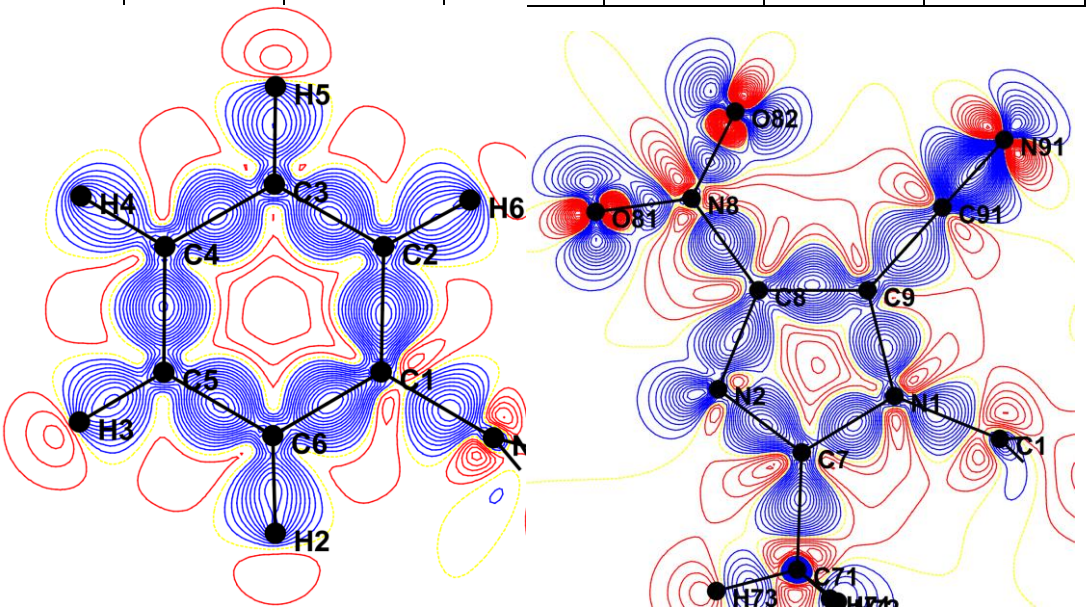
Figure S8. Fourier residual maps for model 3a).

Table S5. κ and P_{val} for models 3a-f.

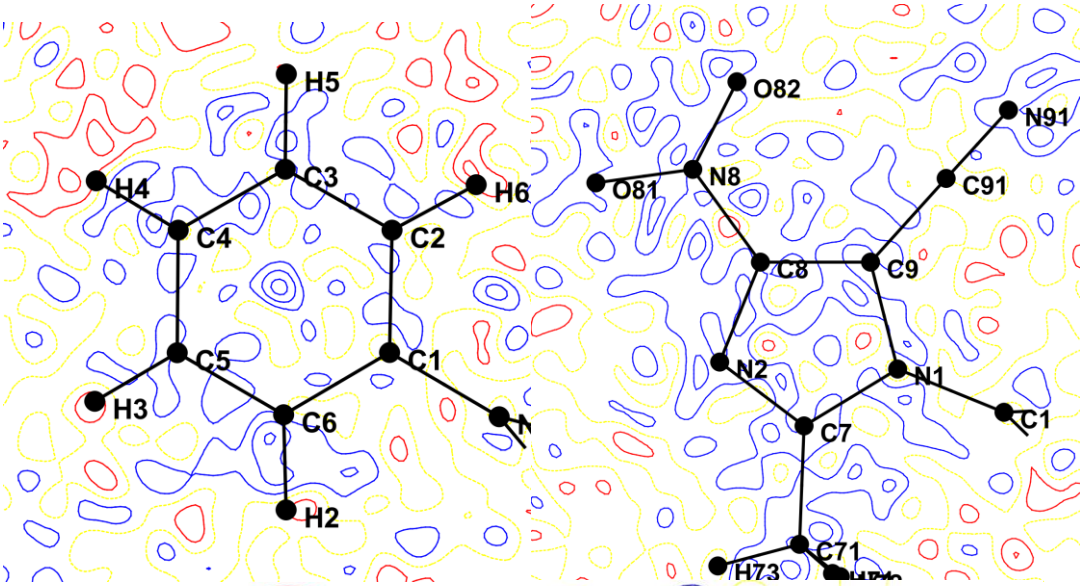
	3a	3b	3c	3d	3e	3f
	kp1					
C1	1.0376	1.0362	1.0376	1.0382	1.0369	1.0384
C2	1.0218	1.0253	1.0246	1.0227	1.0258	1.0259
C3	1.0217	1.0236	1.0243	1.0225	1.0245	1.0256
C4	1.0201	1.0183	1.0214	1.0212	1.0200	1.0228
C5	1.0217	1.0235	1.0216	1.0225	1.0241	1.0229
C6	1.0218	1.0225	1.0209	1.0227	1.0230	1.0219
C7	1.0371	1.0365	1.0356	1.0385	1.0381	1.0371
C8	1.0375	1.0372	1.0377	1.0393	1.0390	1.0401
C9	1.0384	1.0380	1.0382	1.0392	1.0388	1.0395
C71	1.0101	1.0104	1.0138	1.0113	1.0116	1.0153
C91	1.0411	1.0407	1.0413	1.0421	1.0415	1.0432
N1	1.0164	1.0160	1.0159	1.0170	1.0167	1.0163
N2	0.9988	0.9985	0.9995	0.9993	0.9992	1.0005
N8	1.0192	1.0188	1.0166	1.0199	1.0198	1.0174
N91	0.9943	0.9942	0.9951	0.9948	0.9947	0.9963
O81	0.9952	0.9963	0.9961	0.9956	0.9967	0.9965
O82	0.9952	0.9951	0.9957	0.9956	0.9956	0.9960
H6	1.4000	1.4000	1.4000	1.3353	1.3300	1.3206
H2	1.4000	1.4000	1.4000	1.3353	1.3292	1.3179
H3	1.4000	1.4000	1.4000	1.3330	1.3283	1.3221
H4	1.4000	1.4000	1.4000	1.3298	1.3302	1.3173
H5	1.4000	1.4000	1.4000	1.3330	1.3276	1.3195
H73	1.4000	1.4000	1.4000	1.3454	1.3391	1.3336
H72	1.4000	1.4000	1.4000	1.3454	1.3384	1.3246
H71	1.4000	1.4000	1.4000	1.3454	1.3386	1.3290

	3a	3b	3c	3d	3e	3f
	val					

C1	3.979	3.998	3.987	3.971	3.987	3.984
C2	4.226	4.206	4.226	4.197	4.178	4.192
C3	4.208	4.191	4.187	4.186	4.171	4.154
C4	4.218	4.236	4.211	4.195	4.211	4.176
C5	4.208	4.191	4.214	4.186	4.171	4.184
C6	4.226	4.206	4.211	4.197	4.178	4.181
C7	3.869	3.873	3.884	3.855	3.859	3.867
C8	4.043	4.045	4.038	4.022	4.021	4.005
C9	3.996	4.000	4.000	3.989	3.992	3.985
C71	4.614	4.610	4.576	4.559	4.548	4.509
C91	4.008	4.013	4.005	3.993	3.992	3.978
N1	5.009	5.011	5.009	5.003	5.003	5.004
N2	5.226	5.229	5.219	5.214	5.215	5.196
N8	4.660	4.665	4.687	4.651	4.656	4.678
N91	5.221	5.226	5.219	5.208	5.211	5.195
O81	6.181	6.174	6.183	6.173	6.166	6.175
O82	6.181	6.173	6.166	6.173	6.166	6.160
H6	0.748	0.752	0.759	0.788	0.795	0.810
H2	0.748	0.751	0.747	0.788	0.794	0.799
H3	0.747	0.751	0.760	0.787	0.794	0.809
H4	0.744	0.743	0.749	0.788	0.788	0.803
H5	0.747	0.751	0.748	0.787	0.794	0.798
H73	0.731	0.736	0.750	0.763	0.772	0.794
H72	0.731	0.734	0.732	0.763	0.771	0.782
H71	0.731	0.735	0.736	0.763	0.771	0.783



4b


H5
H4
C3
H6
C4
C2
C5
C1
H3
C6
H2
O82
N91
O81
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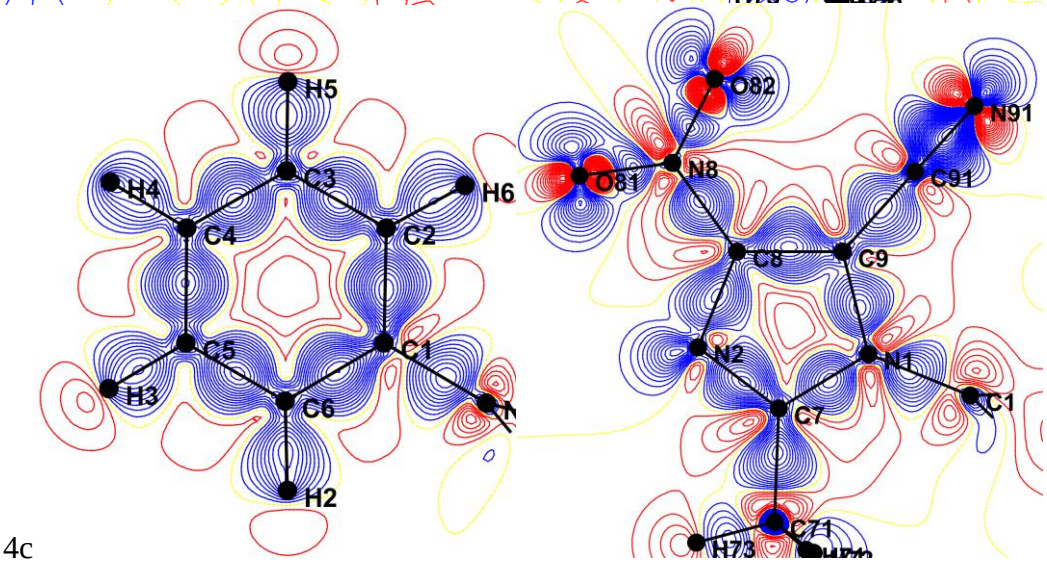
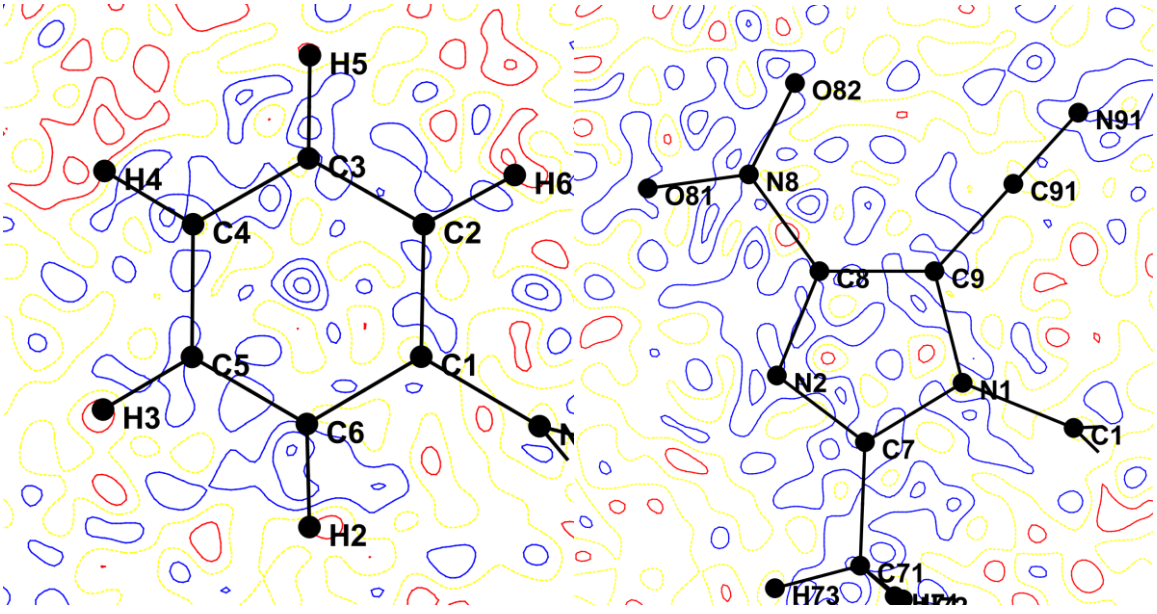
C91
C8
C9
N2
N1
C1
C7
C71
H73


H5
O82
N91
H4
C3
H6
O81
N8
C91
C4
C2
C8
C9
C5
C1
N2
N1
H3
C6
C1
C7
H2
C71
H73

4c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O82
N91
H4
C3
H6
O81
N8
C91
C4
C2
C8
C9
C5
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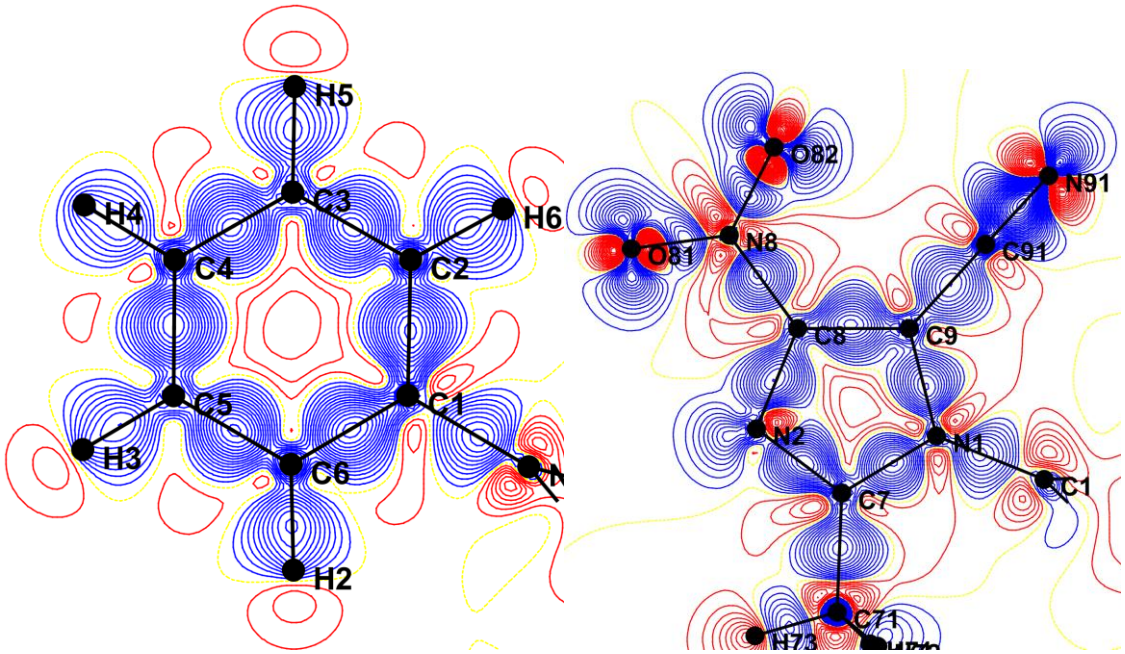
H3
C6
C1
C7
H2
C71
H73


H5
C3
H4
H6
C4
C2
C5
C1
H3
C6
H2
O82
N91
O81
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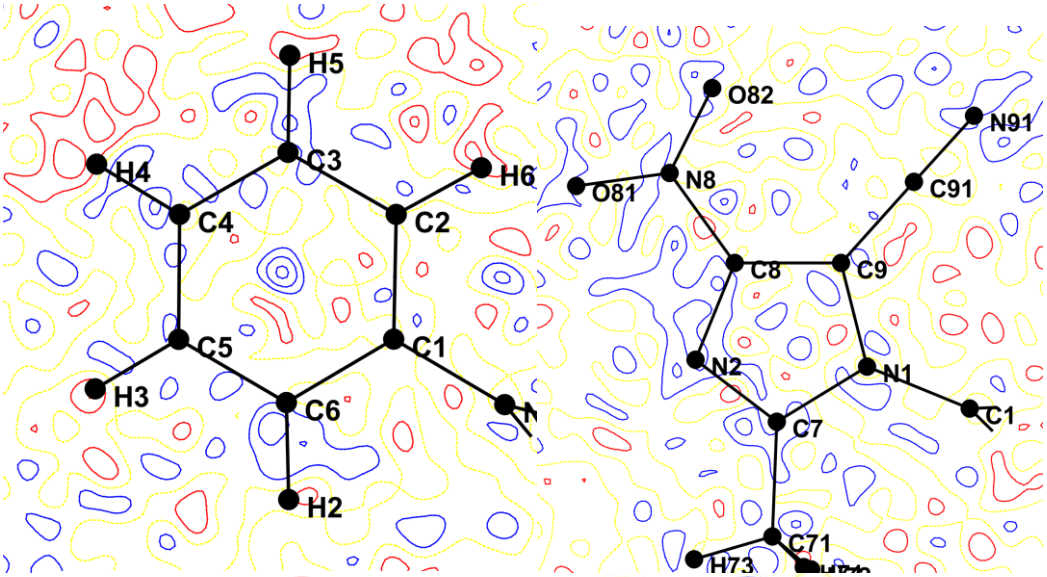
C9
N2
N1
C1
C7
C71

4d


H5
C3
H4
H6
C4
C2
C5
C1
H3
C6
H2
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O81
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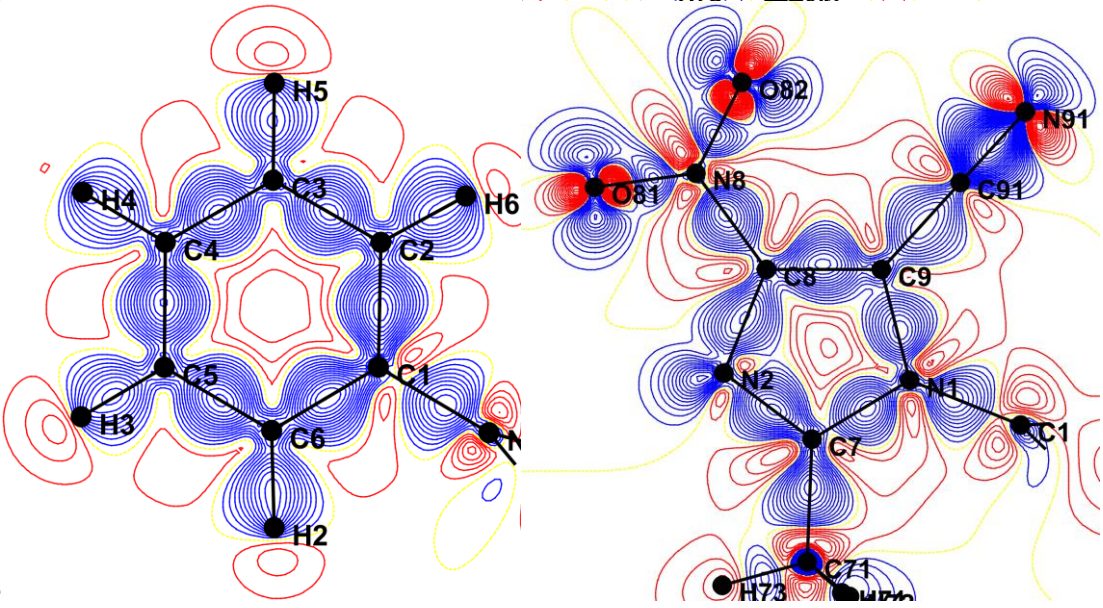
C9
N2
N1
C1
C7
C71
H73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H4
H6
C4
C2
C5
C1
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C6
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C1
C7
C71
H73

4e

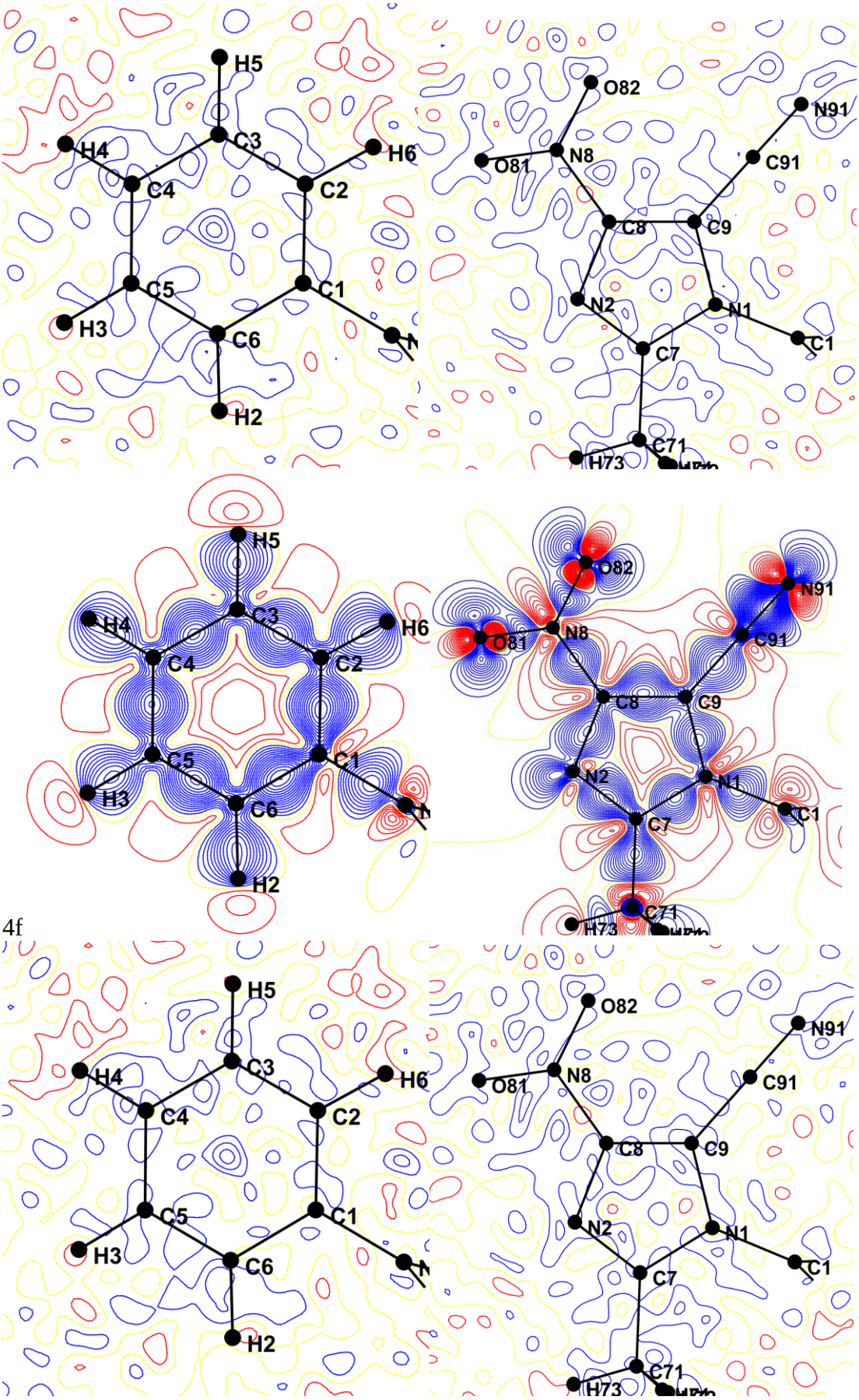

Figure S9. Fourier residual density maps for sub-models 4 not included in the main article, contour 0.05, resolution 1A^{-1}