Supplementary materials.

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Charge-density analysis and electrostatic properties of 2-Carboxy-4-methylanilinium chloride monohydrate obtained using a multipolar model and a spherical charges model.

Table S1. 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)

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

Figure S1. Analysis of experimental vs. expected $\Delta\rho$.

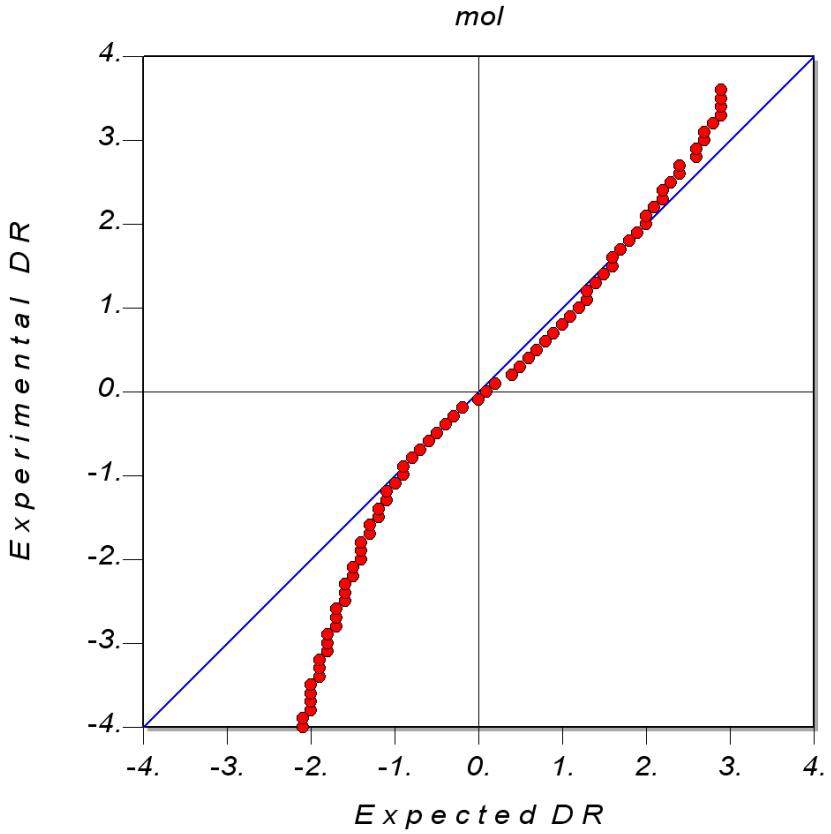


Figure S2. Analysis of <*F*o>/<*F*c> as a function of reciprocal resolution.

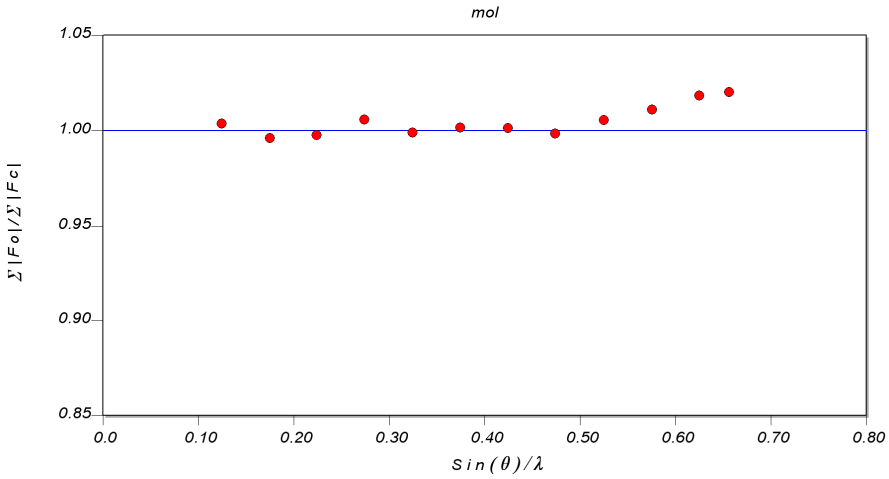
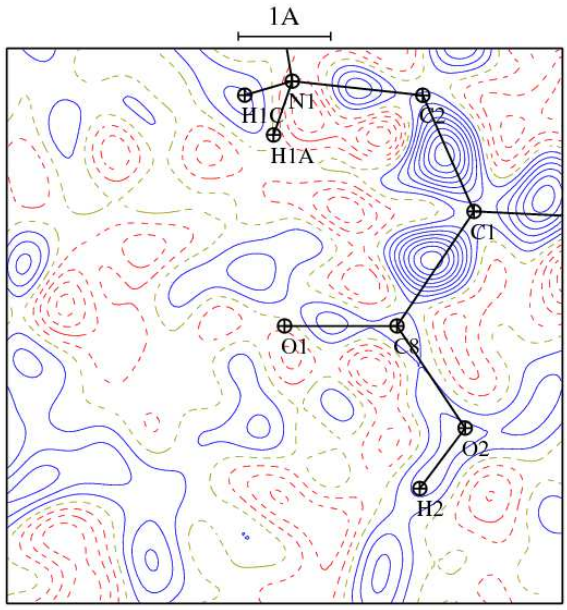
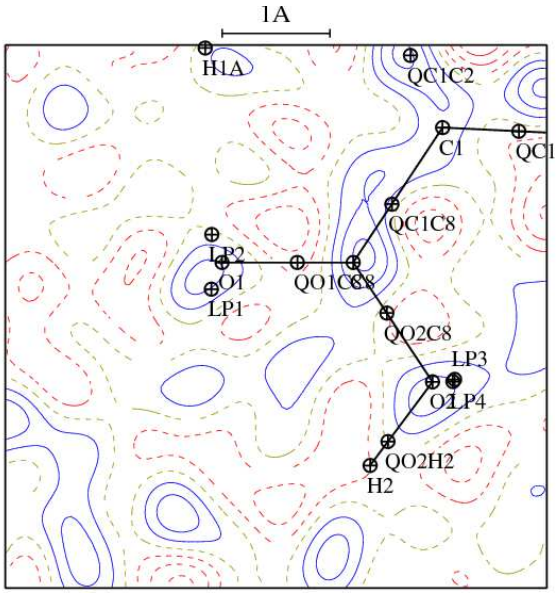


Figure S3.

Experimental residual electron density in the lone pairs planes.

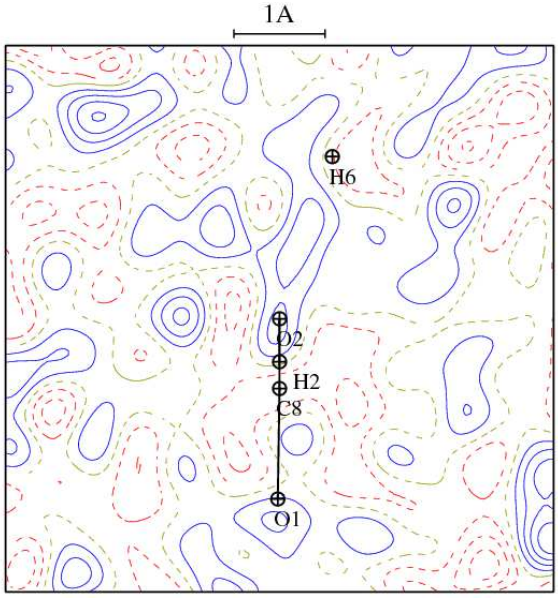
Contour level: ± 0.05 e/Å^3. Blue solid lines and red dashed lines denote positive and negative contours, respectively. The zero contours is shown as yellow line.

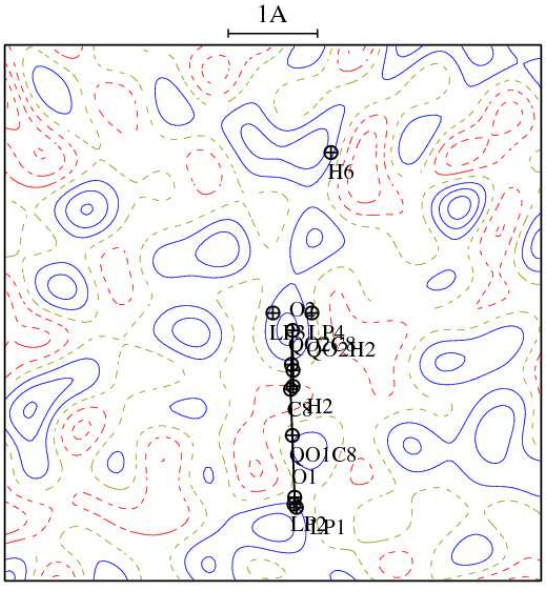




(a) EXP_IAM (b) EXP_VIR

in the C8O1O2 plane





(c) EXP_IAM (d) EXP_VIR

in the oxygen atom O2 lone pairs plane.

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# ELMAM2 MODEL  CHARGE DENSITY PARAMETERS     #
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0.002 -0.024 -0.008 0.001 -0.001 -0.061 -0.001
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-0.165 0.008 -0.002 -0.038 0.012
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N1 C2  Z N1 H1A X
C1 C2 bX C1 C6 Y
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C7 C5  Z C7 H7B X
C8 O2 bX C8 O1 Y
H2 O2  Z H2 C8 X
H3 C3  Z H3 C2 X
H4 C4  Z H4 C5 X
H6 C6  Z H6 C5 X
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H1C N1  Z H1C C2 X
H7A C7  Z H7A C5 X
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H7C C7  Z H7C C5 X
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H1W OW  Z H1W H2W X
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0. 0.
0. 0. 0. 0.
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0.085 0. 0. 0. 0.
0. 0.
0. 0. 0. 0.
1.160(2) 1.44(4) 1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
H7A 1.00(1) 0. 0. 0. 0.135
0.063 0. 0. 0. 0.
0. 0.
0. 0. 0. 0.
1.160(2) 1.31(4) 1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
H7B 1.000 0. 0. 0. 0.135
0.063 0. 0. 0. 0.
0. 0.
0. 0. 0. 0.
1.160(2) 1.31(4) 1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
H7C 1.000 0. 0. 0. 0.135
0.063 0. 0. 0. 0.
0. 0.
0. 0. 0. 0.
1.160(2) 1.31(4) 1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
OW 6.26(3) 0. -0.103(8) 0.0030(60) 0.0010(41)
0.108(7) -0.005(5) -0.0010(46) 0.048(5) 0.0040(58)
0.0010(67) -0.031(7) -0.0010(65) 0.0000(64) 0.0010(64) -0.066(7) -
0.0010(64)
0. 0. 0. 0.
0.983(2) 0.98(3) 2 4.466 2 4.466 2 4.466 3 4.466 4 4.466

```
H1W 0.86(1) 0. 0. 0. 0.14(1)
0.08(1) 0. 0. 0. 0.
0. 0.
0. 0. 0. 0.
1.160(2) 1.48(7)  1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
H2W 0.85(1) 0. 0. 0. 0.14(1)
0.08(1) 0. 0. 0. 0.
0. 0.
0. 0. 0. 0.
1.160(2) 1.46(6)  1 2.000 1 2.000 2 2.000 2 2.000 2 2.000

loop_
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_atom_local_axes_atom0
_atom_local_axes_ax1
_atom_local_axes_atom1
_atom_local_axes_atom2
_atom_local_axes_ax2
CL1 OW bZ CL1 N1 X
O1 C8  X O1 O2 Y
O2 C8 bX O2 H2 Y
N1 C2  Z N1 H1A X
C1 C2 bX C1 C6 Y
C2 C1 bX C2 C3 Y
C3 C2 bX C3 C4 Y
C4 C5 bX C4 C3 Y
C5 C4 bX C5 C6 Y
C6 C5 bX C6 C1 Y
C7 C5  Z C7 H7B X
C8 O2 bX C8 O1 Y
H2 O2  Z H2 C8 X
H3 C3  Z H3 C2 X
H4 C4  Z H4 C5 X
H6 C6  Z H6 C5 X
H1A N1  Z H1A C2 X
H1B N1  Z H1B C2 X
H1C N1  Z H1C C2 X
H7A C7  Z H7A C5 X
H7B C7  Z H7B C5 X
H7C C7  Z H7C C5 X
OW H1W bX OW H2W Y
H1W OW  Z H1W H2W X
H2W OW  Z H2W H1W X

#####################################################
###-THEO_VIR_MODEL  CHARGE DENSITY PARAMETERS######

loop_
_atom_site_type_symbol
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_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
_atom_site_calc_flag
_atom_site_refinement_flags_posn
_atom_site_refinement_flags_adp
_atom_site_disorder_assembly
_atom_site_disorder_group
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```
Cl CL1 0.16000 0.49786 0.67712 0.   Uiso 1 d . .    . .
O  O1 0.17413 0.46924 0.30185 0.   Uiso 1 d . .    . .
O  O2 0.37352 0.52449 0.36549 0.   Uiso 1 d . .    . .
N  N1 0.03425 0.01228 0.32497 0.   Uiso 1 d . .    . .
C  C1 0.22773 0.20083 0.40329 0.   Uiso 1 d . .    . .
C  C2 0.12204 0.01647 0.39089 0.   Uiso 1 d . .    . .
C  C3 0.09716 -0.16926 0.44079 0.   Uiso 1 d . .    . .
C  C4 0.17781 -0.17376 0.50395 0.   Uiso 1 d . .    . .
C  C5 0.28423 0.00540 0.51798 0.   Uiso 1 d . .    . .
C  C6 0.30797 0.19008 0.46727 0.   Uiso 1 d . .    . .
C  C7 0.37128 0.00175 0.58712 0.   Uiso 1 d . .    . .
C  C8 0.25417 0.40907 0.35124 0.   Uiso 1 d . .    . .
H  H2 0.38760 0.65111 0.32947 0.   Uiso 1 d D U    . .
H  H3 0.01517 -0.31080 0.43076 0.   Uiso 1 d D U    . .
H  H4 0.15733 -0.31896 0.54269 0.   Uiso 1 d D U    . .
H  H6 0.39072 0.32982 0.47734 0.   Uiso 1 d D U    . .
H  H1A 0.09223 0.01198 0.28473 0.   Uiso 1 d D U    . .
H  H1B -0.02454 -0.15896 0.32245 0.   Uiso 1 d D U    . .
H  H1C -0.02642 0.18091 0.32153 0.   Uiso 1 d D U    . .
H  H7A 0.31820 0.09034 0.62504 0.   Uiso 1 d D U    . .
H  H7B 0.39595 -0.19986 0.60110 0.   Uiso 1 d D U    . .
H  H7C 0.46024 0.11225 0.58333 0.   Uiso 1 d D U    . .
O  OW 0.42920 0.67298 0.76040 0.   Uiso 1 d . .    . .
H  H1W 0.48164 0.50919 0.76268 0.   Uiso 1 d D U    . .
H  H2W 0.34648 0.62584 0.73260 0.   Uiso 1 d D U    . .
Q  QO1C8 0.22014 0.43465 0.33024 0.   Uiso 1 d . .    . .
Q  QO2C8 0.30466 0.45790 0.35727 0.   Uiso 1 d . .    . .
Q  QO2H2 0.38365 0.61552 0.33959 0.   Uiso 1 d . .    . .
Q  QN1C2 0.07290 0.01413 0.35399 0.   Uiso 1 d . .    . .
Q  Q5 -0.00138 -0.09151 0.32344 0.   Uiso 1 d . .    . .
Q  Q6 -0.00197 0.11295 0.32291 0.   Uiso 1 d . .    . .
Q  Q7 0.06982 0.01210 0.30028 0.   Uiso 1 d . .    . .
Q  QC1C8 0.24276 0.31919 0.37371 0.   Uiso 1 d . .    . .
Q  QC1C2 0.17167 0.10304 0.39671 0.   Uiso 1 d . .    . .
Q  QC1C6 0.26934 0.19526 0.43647 0.   Uiso 1 d . .    . .
Q  QC2C3 0.11008 -0.07284 0.41488 0.   Uiso 1 d . .    . .
Q  QC3C4 0.13791 -0.17154 0.47270 0.   Uiso 1 d . .    . .
Q  QC3H3 0.04479 -0.25967 0.43438 0.   Uiso 1 d . .    . .
Q  QC4C5 0.23062 -0.08486 0.51091 0.   Uiso 1 d . .    . .
Q  QC4H4 0.16510 -0.26384 0.52798 0.   Uiso 1 d . .    . .
Q  QC5C6 0.29630 0.09926 0.49221 0.   Uiso 1 d . .    . .
Q  QC5C7 0.32689 0.00361 0.55186 0.   Uiso 1 d . .    . .
Q  QC6H6 0.35976 0.27753 0.47357 0.   Uiso 1 d . .    . .
Q  Q19 0.42842 0.07272 0.58469 0.   Uiso 1 d . .    . .
Q  Q20 0.38680 -0.12507 0.59591 0.   Uiso 1 d . .    . .
Q  Q21 0.33811 0.05712 0.61082 0.   Uiso 1 d . .    . .
Q  Q22 0.47033 0.54453 0.76218 0.   Uiso 1 d . .    . .
Q  Q23 0.36482 0.63629 0.73877 0.   Uiso 1 d . .    . .
Q  LP1 0.18338 0.50772 0.29455 0.   Uiso 1 d . .    . .
Q  LP2 0.15143 0.43792 0.30186 0.   Uiso 1 d . .    . .
Q  LP3 0.39373 0.48213 0.36776 0.   Uiso 1 d . .    . .
Q  LP4 0.37644 0.54653 0.37915 0.   Uiso 1 d . .    . .
Q  LP5 0.44205 0.70647 0.75197 0.   Uiso 1 d . .    . .
Q  LP6 0.42135 0.67782 0.77349 0.   Uiso 1 d . .    . .



loop_
_geom_hbond_atom_site_label_D
_geom_hbond_atom_site_label_H
_geom_hbond_atom_site_label_A
```

```
_geom_hbond_distance_DH
_geom_hbond_distance_HA
_geom_hbond_distance_DA
_geom_hbond_angle_DHA
_geom_hbond_site_symmetry_A
N1 H1A LP1 1.033 2.664 3.014 99.6  1_545
N1 H1B LP2 1.033 2.653 2.947 96.0  2_545
N1 H1A CL1 1.033 2.288 3.291 163.1  4_554
C6 H6 O2 1.083 2.379 2.732 97.0  1_555
C6 H6 LP3 1.083 2.277 2.651 97.8  1_555
C6 H6 LP4 1.083 2.191 2.618 100.7  1_555
N1 H1A O1 1.033 2.424 2.734 96.1  1_555
N1 H1A QO1C8 1.033 2.564 2.802 92.2  1_555
N1 H1A LP1 1.033 2.624 2.976 99.6  1_555
N1 H1A LP2 1.033 2.211 2.486 92.8  1_555
N1 H1B QC3H3 1.033 2.274 2.522 91.5  1_555
OW H2W CL1 0.967 2.148 3.113 175.4  1_555
N1 H1B CL1 1.033 2.165 3.195 174.7  3_556
O2 H2 OW 0.967 1.702 2.658 169.4  4_564
O2 H2 Q22 0.967 2.228 3.173 165.5  4_564
O2 H2 Q23 0.967 2.054 2.989 162.3  4_564
O2 H2 LP5 0.967 1.815 2.748 161.2  4_564
O2 H2 LP6 0.967 1.457 2.420 173.5  4_564
N1 H1C CL1 1.033 2.086 3.115 173.7  3_566
OW H1W OW 0.967 1.971 2.913 163.9  2_646
OW H1W Q22 0.967 2.417 3.324 156.0  2_646
OW H1W Q23 0.967 2.412 3.372 172.1  2_646
OW H1W LP5 0.967 1.726 2.677 167.0  2_646
OW H1W LP6 0.967 2.078 2.995 157.6  2_646
C7 H7B LP3 1.059 2.549 3.411 138.0  3_656
O2 H2 Q22 0.967 2.608 3.121 113.5  3_666
C7 H7C O2 1.059 2.579 3.522 148.1  3_666
C7 H7C QO2H2 1.059 2.450 3.301 136.7  3_666
C7 H7C LP3 1.059 2.606 3.525 144.9  3_666
C7 H7C LP4 1.059 2.412 3.391 153.2  3_666
OW H1W QO2H2 0.967 2.619 3.207 119.5  3_666

#-----------------------------------------------#
#   MULTIPOLE PARAMETERS                        #
#-----------------------------------------------#

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_atom_rho_multipole_coeff_Pv
_atom_rho_multipole_coeff_P00
_atom_rho_multipole_coeff_P11
_atom_rho_multipole_coeff_P1-1
_atom_rho_multipole_coeff_P10
_atom_rho_multipole_coeff_P20
_atom_rho_multipole_coeff_P21
_atom_rho_multipole_coeff_P2-1
_atom_rho_multipole_coeff_P22
_atom_rho_multipole_coeff_P2-2
_atom_rho_multipole_coeff_P30
_atom_rho_multipole_coeff_P31
_atom_rho_multipole_coeff_P3-1
_atom_rho_multipole_coeff_P32
_atom_rho_multipole_coeff_P3-2
_atom_rho_multipole_coeff_P33
_atom_rho_multipole_coeff_P3-3
_atom_rho_multipole_coeff_P40
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_atom_rho_multipole_coeff_P41
_atom_rho_multipole_coeff_P4-1
_atom_rho_multipole_coeff_P42
_atom_rho_multipole_coeff_P4-2
_atom_rho_multipole_coeff_P43
_atom_rho_multipole_coeff_P4-3
_atom_rho_multipole_coeff_P44
_atom_rho_multipole_coeff_P4-4
_atom_rho_multipole_kappa
_atom_rho_multipole_kappa_prime
_atom_rho_multipole_radial_slater_n0
_atom_rho_multipole_radial_slater_zeta0
_atom_rho_multipole_radial_slater_n1
_atom_rho_multipole_radial_slater_zeta1
_atom_rho_multipole_radial_slater_n2
_atom_rho_multipole_radial_slater_zeta2
_atom_rho_multipole_radial_slater_n3
_atom_rho_multipole_radial_slater_zeta3
_atom_rho_multipole_radial_slater_n4
_atom_rho_multipole_radial_slater_zeta4
CL1 4.60(4) 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
1.032(3) 0.     4 4.259 4 4.259 4 4.259 6 4.259 8 4.259
O1 5.7(1) 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
0.962(4) 0.     2 4.466 2 4.466 2 4.466 3 4.466 4 4.466
O2 6.3(1) 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
0.976(4) 0.     2 4.466 2 4.466 2 4.466 3 4.466 4 4.466
N1 4.1(1) 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
1.058(7) 0.     2 3.839 2 3.839 2 3.839 3 3.839 4 3.839
C1 2.98(9) 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
1.063(7) 0.     2 3.176 2 3.176 2 3.176 3 3.176 4 3.176
C2 2.92(10) 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
1.059(8) 0.     2 3.176 2 3.176 2 3.176 3 3.176 4 3.176
C3 2.7(1) 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
1.054(8) 0.     2 3.176 2 3.176 2 3.176 3 3.176 4 3.176
C4 2.69(8) 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
1.063(8) 0.     2 3.176 2 3.176 2 3.176 3 3.176 4 3.176
C5 2.9(1) 0. 0. 0. 0.
```

0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
1.064(9) 0. 2 3.176 2 3.176 2 3.176 3 3.176 4 3.176
C6 2.78(9) 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
1.051(8) 0. 2 3.176 2 3.176 2 3.176 3 3.176 4 3.176
C7 2.4(1) 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
1.08(1) 0. 2 3.176 2 3.176 2 3.176 3 3.176 4 3.176
C8 2.5(1) 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
1.046(9) 0. 2 3.176 2 3.176 2 3.176 3 3.176 4 3.176
H2 0.71(8) 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
1.02(8) 0. 1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
H3 0.80(8) 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
1.14(5) 0. 1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
H4 0.78(6) 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
1.17(3) 0. 1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
H6 0.779 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
1.17(3) 0. 1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
H1A 1.16(5) 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
0.77(4) 0. 1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
H1B 1.162 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
0.77(4) 0. 1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
H1C 1.162 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
0.77(4) 0. 1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
H7A 0.73(5) 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
1.19(3) 0. 1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
H7B 0.734 0. 0. 0. 0.
0. 0. 0. 0. 0.

0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
1.19(3) 0. 1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
H7C 0.734 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
1.19(3) 0. 1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
OW 6.1(1) 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
0.958(4) 0. 2 4.466 2 4.466 2 4.466 3 4.466 4 4.466
H1W 1.09(7) 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
0.57(6) 0. 1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
H2W 1.089 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
0.57(6) 0. 1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
QO1C8 0.38(9) 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
1.26(8) 0. 1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
QO2C8 -0.029(64) 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
1.8(1) 0. 1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
QO2H2 -0.085(87) 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
2.0(2) 0. 1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
QN1C2 0.22(7) 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
1.30(10) 0. 1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
Q5 0.28(7) 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
1.26(5) 0. 1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
Q6 0.284 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
1.26(5) 0. 1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
Q7 0.284 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
1.26(5) 0. 1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
QC1C8 1.05(9) 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.

0. 0. 0. 0. 0. 0. 0. 0. 0.
0.83(5) 0.   1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
QC1C2 1.00(9) 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
0.83(5) 0.   1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
QC1C6 1.06(9) 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
0.84(5) 0.   1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
QC2C3 0.84(10) 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
0.97(5) 0.   1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
QC3C4 1.12(10) 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
0.89(4) 0.   1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
QC3H3 0.9(1) 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
0.89(7) 0.   1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
QC4C5 0.70(8) 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
1.03(3) 0.   1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
QC4H4 0.71(8) 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
0.98(5) 0.   1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
QC5C6 0.698 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
1.03(3) 0.   1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
QC5C7 0.15(10) 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
1.27(6) 0.   1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
QC6H6 0.708 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
0.98(5) 0.   1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
Q19 1.01(8) 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
0.81(3) 0.   1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
Q20 1.008 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.

```
0.81(3) 0.     1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
Q21 1.008 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
0.81(3) 0.     1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
Q22 0.012(70) 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
2.0(1) 0.     1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
Q23 0.012 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
2.0(1) 0.     1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
LP1 0.25(5) 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
1.7(1) 0.     1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
LP2 0.255 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
1.7(1) 0.     1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
LP3 0.06(3) 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
2.3(2) 0.     1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
LP4 0.061 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
2.3(2) 0.     1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
LP5 0.19(4) 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
1.8(2) 0.     1 2.000 1 2.000 2 2.000 2 2.000 2 2.000
LP6 0.195 0. 0. 0. 0.
0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0.
1.8(2) 0.     1 2.000 1 2.000 2 2.000 2 2.000 2 2.000

loop_
_atom_local_axes_atom_label
_atom_local_axes_atom0
_atom_local_axes_ax1
_atom_local_axes_atom1
_atom_local_axes_atom2
_atom_local_axes_ax2
CL1 OW bZ CL1 N1 X
O1 C8  X O1 O2 Y
O2 C8 bX O2 H2 Y
N1 C2  Z N1 H1A X
C1 C2 bX C1 C6 Y
C2 C1 bX C2 C3 Y
C3 C2 bX C3 C4 Y
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C4 C5 bX C4 C3 Y
C5 C4 bX C5 C6 Y
C6 C5 bX C6 C1 Y
C7 C5  Z C7 H7B X
C8 O2 bX C8 O1 Y
H2 O2  Z H2 C8 X
H3 C3  Z H3 C2 X
H4 C4  Z H4 C5 X
H6 C6  Z H6 C5 X
H1A N1  Z H1A C2 X
H1B N1  Z H1B C2 X
H1C N1  Z H1C C2 X
H7A C7  Z H7A C5 X
H7B C7  Z H7B C5 X
H7C C7  Z H7C C5 X
OW H1W bX OW H2W Y
H1W OW  Z H1W H2W X
H2W OW  Z H2W H1W X
QO1C8 O1  X QO1C8 C8 Y
QO2C8 O2  X QO2C8 C8 Y
QO2H2 O2  X QO2H2 H2 Y
QN1C2 N1  X QN1C2 C2 Y
Q5 N1  X Q5 H1B Y
Q6 N1  X Q6 H1C Y
Q7 N1  X Q7 H1A Y
QC1C8 C1  X QC1C8 C8 Y
QC1C2 C1  X QC1C2 C2 Y
QC1C6 C1  X QC1C6 C6 Y
QC2C3 C2  X QC2C3 C3 Y
QC3C4 C3  X QC3C4 C4 Y
QC3H3 C3  X QC3H3 H3 Y
QC4C5 C4  X QC4C5 C5 Y
QC4H4 C4  X QC4H4 H4 Y
QC5C6 C5  X QC5C6 C6 Y
QC5C7 C5  X QC5C7 C7 Y
QC6H6 C6  X QC6H6 H6 Y
Q19 C7  X Q19 H7C Y
Q20 C7  X Q20 H7B Y
Q21 C7  X Q21 H7A Y
Q22 OW  X Q22 H1W Y
Q23 OW  X Q23 H2W Y
LP1 O1  X LP1 C8 Y
LP2 O1  X LP2 C8 Y
LP3 O2  X LP3 C8 Y
LP4 O2  X LP4 C8 Y
LP5 OW  X LP5 H1W Y
LP6 OW  X LP6 H1W Y
```