Supporting Information for Experimental and Theoretical Charge Density Distribution in Pigment Yellow 101

Table S1 Selected bond lengths and angles in complex **1**. The values in parentheses are from the geometry optimisation, and the excited state (S1) respectively, at the B3LYP/6-31+G* level of theory.

	Lengths (Å)		Angle (°)
O(1) – C(3)	1.341 (7)	N(1) – N(1)$^{\#}$ – C(1)	113.6 (4)
N(1) – N(1)$^{\#}$	1.385 (8)	N(1) – C(1) – C(2)	121.5 (4)
N(1) – C(1)	1.298 (7)	C(1) – C(2) – C(3)	120.1 (4)
C(1) – C(2)	1.446 (7)	C(1) – C(2) – C(11)	120.6 (4)
C(2) – C(3)	1.404 (7)	C(3) – C(2) – C(11)	119.2 (4)
C(3) – C(4)	1.416 (7)	O(1) – C(3) – C(2)	122.6 (4)
C(4) – C(5)	1.369 (6)	O(1) – C(3) – C(4)	116.1 (5)
C(5) – C(6)	1.423 (7)	C(2) – C(3) – C(4)	120.8 (4)
C(6) – C(7)	1.419 (7)	C(3) – C(4) – C(5)	120.1 (4)
C(6) – C(11)	1.425 (7)	C(4) – C(5) – C(6)	121.3 (4)
C(7) – C(8)	1.377 (6)	C(5) – C(6) – C(7)	120.5 (4)
C(8) – C(9)	1.413 (7)	C(5) – C(6) – C(11)	119.3 (5)
C(9) – C(10)	1.380 (8)	C(7) – C(6) – C(11)	120.1 (5)
C(10) – C(11)	1.421 (9)	C(6) – C(7) – C(8)	120.6 (4)
		C(7) – C(8) – C(9)	119.5 (4)
		C(8) – C(9) – C(10)	120.8 (3)
		C(9) – C(10) – C(11)	121.0 (4)
		C(2) – C(11) – C(6)	119.1 (5)
		C(2) – C(11) – C(10)	123.1 (4)
		C(6) – C(11) – C(10)	117.7 (4)

Table S2 Topological analysis of intramolecular covalent bonds. Values in the first row is obtained from multipole refinement (exp), and in the second row from the SHADE refinement and the third row from B3LYP/6-31+G**. Standard uncertainties have been omitted from the table for clarity. They are closely scattered around 0.02 e Å^{-3} (ρ_{bcp}) and 0.05 e Å^{-5} ($\nabla^2\rho_{bcp}$).

Bond	ρ / eÅ^{-3}	$\nabla^2\rho$ / eÅ^{-5}	ε	R_{ij} / Å	d_1 / Å	d_2 / Å
N(1)-N(1)	2.21	-2.54	0.06	1.385	0.694	0.691
Shade	2.24	-2.46	0.05	1.387	0.695	0.691
DFT	2.34	-16.03	0.04		0.689	0.689
O(1)-C(3)	2.14	-19.16	0.11	1.341	0.811	0.530
	2.16	-18.90	0.09	1.343	0.811	0.531
	2.06	-8.68	0.00		0.896	0.446
O(1)-H(1A)	2.59	-26.23	0.02	0.967	0.716	0.251
	2.15	-27.64	0.02	0.967	0.757	0.210
	2.20	-44.23	0.02		0.812	0.186
N(1)-C(1)	2.53	-26.68	0.24	1.299	0.773	0.526
	2.55	-26.95	0.24	1.30	0.776	0.524
	2.48	-19.51	0.18		0.861	0.443
C(1)-C(2)	1.92	-14.27	0.21	1.446	0.734	0.712
	1.91	-14.47	0.20	1.446	0.734	0.712
	1.94	-17.94	0.16		0.742	0.702
C(2)-C(3)	2.15	-18.23	0.27	1.404	0.681	0.723
	2.15	-18.22	0.28	1.404	0.684	0.719
	2.07	-19.68	0.25		0.683	0.729

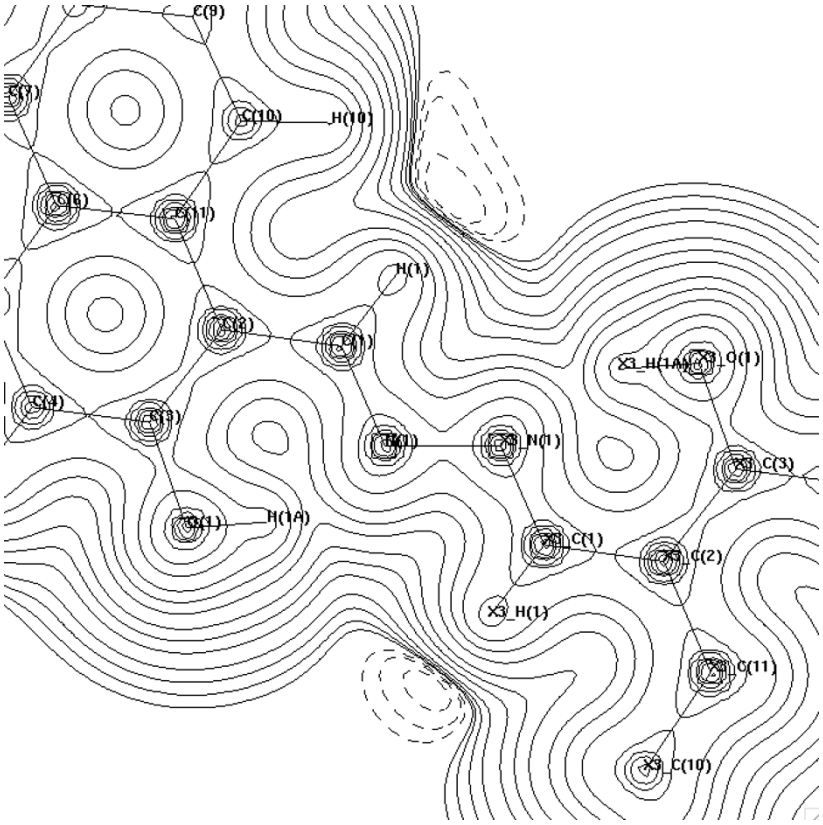
C(2)-C(11)	1.87	-13.51	0.22	1.442	0.718	0.723
	1.88	-13.59	0.21	1.442	0.715	0.726
	1.90	-16.88	0.16		0.726	0.724
C(3)-C(4)	2.05	-16.01	0.22	1.417	0.736	0.681
	2.06	-16.47	0.21	1.416	0.730	0.686
	2.06	-20.34	0.19		0.735	0.684
C(4)-C(5)	2.18	-18.96	0.25	1.370	0.682	0.688
	2.19	-19.45	0.25	1.369	0.677	0.692
	2.21	-22.25	0.25		0.688	0.682
C(5)-C(6)	2.00	-15.53	0.19	1.423	0.719	0.704
	2.02	-16.090	0.20	1.423	0.7131	0.710
	2.01	-18.99	0.14		0.718	0.708
C(6)-C(7)	2.00	-15.57	0.18	1.420	0.711	0.709
	2.01	-15.83	0.20	1.419	0.709	0.710
	2.03	-19.20	0.17		0.712	0.707
C(6)-C(11)	2.00	-15.35	0.19	1.426	0.714	0.712
	2.00	-15.809	0.18	1.425	0.717	0.708
	1.98	-18.26	0.16		0.712	0.721
C(7)-C(8)	2.23	-19.81	0.19	1.378	0.680	0.698
	2.23	-20.04	0.22	1.377	0.673	0.705
	2.17	-21.66	0.24		0.685	0.694
C(8)-C(9)	2.03	-15.98	0.19	1.414	0.698	0.716
	2.03	-16.40	0.19	1.413	0.699	0.705
	2.05	-19.70	0.17		0.708	0.703

C(9)-C(10)	2.14	-18.32	0.25	1.380	0.681	0.699
	2.14	-18.34	0.25	1.379	0.684	0.696
	2.16	-21.31	0.24		0.691	0.692
C(10)-C(11)	2.03	-16.30	0.19	1.422	0.706	0.715
	2.05	-16.48	0.19	1.421	0.707	0.714
	2.01	-18.82	0.17		0.704	0.718

Table S3 Geometrical details of hydrogen bonds and non-covalent interactions. Values in the first row are obtained from multipole refinement, and in the second row (for intramolecular contacts only) from B3LYP/6-31+G**.

	$d_{1\text{-}2}$ / Å	$d_{1\text{-}3}$ / Å	Angle (°)
Intermolecular			
C(9)···H(1)–C(1)	2.83(1)	3.88(1)	162.3(1)
O(1) ··· H(9) – C(9)	2.46(1)	3.35(1)	138.2(1)
Intramolecular			
N(1)···H(1A) – O(1)	1.68(1)	2.57(1)	150.9(1)
	1.699	2.589	146.3
H(10)···H(1)	1.97(1)		
	1.974		

Figure S1 Total electron density plots in central region of **1** from a) experiment and b) theory.



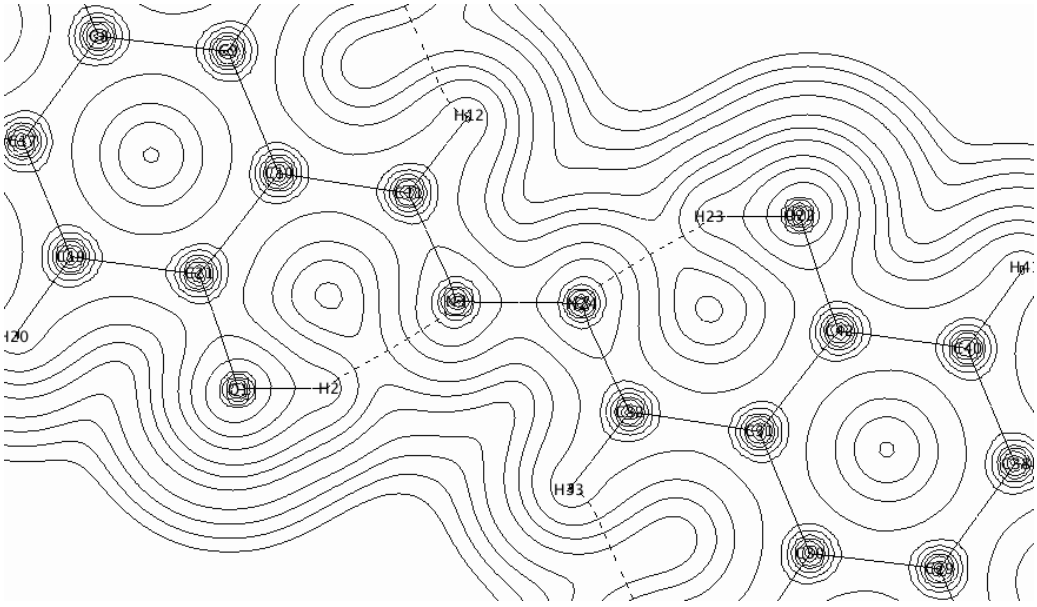


Figure S2 Total density along N—N bond close to bond critical point, and quadratic fit to this.

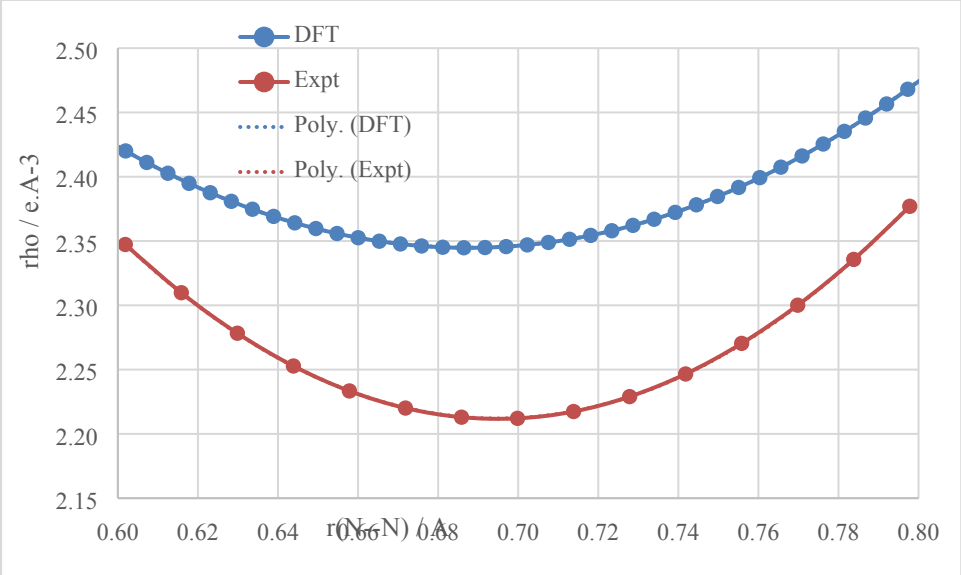


Table S4 Effect of functional, basis set and geometry on selected bond critical point properties.

Bond	Method/Basis/Geom [a]	ρ	$\nabla^2\rho$	%δr [b]	$\%\delta\nabla^2\rho$ [b]
N-N	1	2.345	-16.029		
	2	2.308	-15.538	-1.6	-3.1
	3	2.324	-14.978	-0.9	-6.6
	4	2.340	-16.190	-0.2	1.0
	5	2.349	-16.462	0.2	2.7
N…H	1	0.356	2.920		
	2	0.366	3.163	2.9	8.3
	3	0.363	2.793	1.9	-4.4
	4	0.352	2.947	-1.2	0.9
	5	0.351	3.004	-1.3	2.9

[a] 1: B3LYP/6-31+G(d,p) at optimised geometry; 2: B3LYP/6-31+G(d,p) at Xray geometry; 3: B3LYP/6-311++G(d,p) at optimised geometry; 4: M06-2X/6-31+G(d,p) at optimised geometry; 5: ωB97x-D/6-31+G(d,p) at optimised geometry. b Percentage difference from B3LYP/6-31+G(d,p) at optimised geometry

Table S5a *Experimental* Monopole Populations, Radial Parameters and Net Atomic Charges.

Atom	Pval	Kappa	P00	Kappa'	Net charge
O(1)	6.249(28)	0.991(2)	0.000	1.000	-0.248(28)
N(1)	5.214(28)	0.993(2)	0.000	1.000	-0.214(28)
C(1)	3.989(25)	1.014(2)	0.000	1.000	+0.011(25)
C(2)	4.014(20)	1.014(2)	0.000	1.000	-0.013(20)
C(3)	4.022(22)	1.014(2)	0.000	1.000	-0.022(22)
C(4)	3.991(23)	1.014(2)	0.000	1.000	+0.008(23)
C(5)	3.991(24)	1.014(2)	0.000	1.000	+0.009(24)
C(6)	4.004(21)	1.014(2)	0.000	1.000	-0.003(21)
C(7)	3.948(23)	1.014(2)	0.000	1.000	+0.051(23)
C(8)	4.055(26)	1.014(2)	0.000	1.000	-0.054(26)
C(9)	3.971(25)	1.014(2)	0.000	1.000	+0.029(25)
C(10)	4.009(24)	1.014(2)	0.000	1.000	-0.009(24)
C(11)	3.996(22)	1.014(2)	0.000	1.000	+0.003(22)
H(1A)	0.981(18)	1.200	0.000	1.200	+0.018(18)
H(1)	0.904(15)	1.200	0.000	1.200	+0.096(15)
H(4)	0.984(14)	1.200	0.000	1.200	+0.015(14)
H(5)	0.890(15)	1.200	0.000	1.200	+0.109(15)
H(7)	0.951(15)	1.200	0.000	1.200	+0.048(15)
H(8)	0.982(15)	1.200	0.000	1.200	+0.018(15)
H(9)	0.965(15)	1.200	0.000	1.200	+0.035(15)
H(10)	0.890(14)	1.200	0.000	1.200	+0.109(14)

Table S5b *Experimental* Dipole Population Parameters.

Atom	D11+	D11-	D10	Kappa'
O(1)	-0.070(5)	-0.061(4)	-0.001(4)	1.000
N(1)	-0.039(5)	0.106(5)	0.000(5)	1.000
C(1)	-0.022(8)	0.036(8)	-0.023(7)	1.000
C(2)	0.015(8)	-0.009(7)	0.006(7)	1.000
C(3)	-0.093(8)	-0.005(8)	-0.002(7)	1.000
C(4)	-0.040(9)	-0.003(8)	0.008(7)	1.000
C(5)	-0.042(8)	-0.007(8)	0.006(7)	1.000
C(6)	-0.001(8)	-0.021(8)	-0.012(7)	1.000
C(7)	-0.033(9)	0.006(8)	-0.001(8)	1.000
C(8)	-0.026(9)	0.031(8)	-0.001(7)	1.000
C(9)	-0.052(9)	-0.008(8)	0.002(7)	1.000
C(10)	-0.030(9)	0.024(8)	0.006(8)	1.000
C(11)	0.012(8)	0.009(7)	0.021(7)	1.000
H(1A)	0.183(16)	0.009(11)	0.000	1.200
H(1)	0.191(11)	0.000	0.000	1.200
H(4)	0.190(12)	0.000	0.000	1.200
H(5)	0.181(11)	0.000	0.000	1.200
H(7)	0.172(12)	0.000	0.000	1.200
H(8)	0.183(12)	0.000	0.000	1.200
H(9)	0.184(13)	0.000	0.000	1.200
H(10)	0.161(11)	0.000	0.000	1.200

Table S5c *Experimental* Quadrupole Population Parameters.

Atom	Q20	Q21+	Q21-	Q22+	Q22-	Kappa'
O(1)	0.026(6)	-0.013(6)	0.025(6)	0.029(6)	0.049(5)	1.000
N(1)	-0.097(6)	0.035(6)	0.000(6)	0.025(6)	-0.085(5)	1.000
C(1)	-0.189(8)	-0.013(7)	0.036(7)	0.000(7)	0.015(7)	1.000
C(2)	-0.119(8)	0.002(7)	-0.034(7)	0.019(7)	0.002(8)	1.000
C(3)	-0.178(8)	-0.033(7)	-0.001(7)	-0.068(8)	-0.015(7)	1.000
C(4)	-0.147(8)	0.006(7)	-0.029(8)	-0.007(8)	-0.039(8)	1.000
C(5)	-0.178(8)	0.014(7)	-0.033(8)	-0.013(8)	-0.018(8)	1.000
C(6)	-0.168(7)	0.019(7)	0.005(7)	0.002(8)	-0.008(8)	1.000
C(7)	-0.178(8)	-0.009(7)	-0.008(8)	-0.031(9)	-0.025(8)	1.000
C(8)	-0.139(8)	0.036(7)	-0.001(8)	-0.064(9)	-0.021(8)	1.000
C(9)	-0.156(8)	-0.037(8)	0.026(8)	-0.014(9)	0.007(8)	1.000
C(10)	-0.166(8)	-0.016(7)	0.014(7)	-0.010(8)	-0.003(8)	1.000
C(11)	-0.167(7)	0.007(7)	0.032(7)	0.016(7)	-0.012(8)	1.000
H(1A)	0.000	0.000	0.000	0.000	0.000	1.200
H(1)	0.000	0.000	0.000	0.000	0.000	1.200
H(4)	0.000	0.000	0.000	0.000	0.000	1.200
H(5)	0.000	0.000	0.000	0.000	0.000	1.200
H(7)	0.000	0.000	0.000	0.000	0.000	1.200
H(8)	0.000	0.000	0.000	0.000	0.000	1.200
H(9)	0.000	0.000	0.000	0.000	0.000	1.200
H(10)	0.000	0.000	0.000	0.000	0.000	1.200

Table S5d *Experimental* Octupole Population Parameters.

Atom	O30	O31+	O31-	O32+	O32-	O33+	O33-	Kappa'
O(1)	-0.015(6)	-0.022(5)	-0.010(5)	-0.013(5)	-0.005(5)	0.088(5)	-0.054(5)	1.000
N(1)	-0.006(7)	0.000(6)	0.036(6)	-0.002(6)	0.005(6)	0.150(6)	0.009(6)	1.000
C(1)	-0.010(9)	-0.021(8)	0.040(8)	0.013(8)	-0.001(8)	0.249(9)	-0.018(8)	1.000
C(2)	0.004(9)	0.005(8)	-0.009(8)	-0.006(8)	0.020(8)	0.233(8)	-0.014(9)	1.000
C(3)	0.005(9)	-0.027(8)	0.001(8)	-0.004(8)	0.009(8)	0.271(9)	0.032(9)	1.000
C(4)	0.022(9)	-0.028(8)	0.010(8)	-0.001(8)	0.011(9)	0.211(9)	-0.008(9)	1.000
C(5)	0.004(9)	-0.019(8)	0.017(8)	0.008(8)	0.015(8)	0.241(9)	-0.016(9)	1.000
C(6)	-0.009(9)	-0.003(8)	0.007(8)	0.009(9)	-0.017(9)	0.233(9)	-0.016(9)	1.000
C(7)	0.006(9)	-0.009(9)	0.004(9)	0.011(9)	-0.003(9)	0.220(9)	0.060(9)	1.000
C(8)	-0.002(9)	0.008(8)	-0.013(9)	0.021(9)	-0.006(9)	0.220(9)	0.007(9)	1.000
C(9)	0.014(9)	0.004(9)	0.023(9)	-0.006(9)	-0.009(9)	0.228(9)	0.036(9)	1.000
C(10)	0.008(9)	-0.010(8)	0.017(9)	-0.019(9)	-0.006(8)	0.239(9)	-0.052(9)	1.000
C(11)	-0.004(9)	-0.004(8)	-0.004(8)	0.012(8)	-0.018(8)	0.237(8)	-0.019(9)	1.000

Table S6a *Shade* Monopole Populations, Radial Parameters and Net Atomic Charges.

Atom	Pval	Kappa	P00	Kappa'	Net charge
O(1)	6.380(26)	0.985(2)	0.000	1.000	-0.380(26)
N(1)	5.190(28)	0.995(2)	0.000	1.000	-0.189(28)
C(1)	4.056(25)	1.009(2)	0.000	1.000	-0.055(25)
C(2)	4.032(20)	1.009(2)	0.000	1.000	-0.032(20)
C(3)	4.054(22)	1.009(2)	0.000	1.000	-0.054(22)
C(4)	4.065(23)	1.009(2)	0.000	1.000	-0.065(23)
C(5)	4.046(24)	1.009(2)	0.000	1.000	-0.046(24)
C(6)	4.034(20)	1.009(2)	0.000	1.000	-0.034(20)
C(7)	4.021(22)	1.009(2)	0.000	1.000	-0.020(22)
C(8)	4.075(26)	1.009(2)	0.000	1.000	-0.074(26)
C(9)	4.046(25)	1.009(2)	0.000	1.000	-0.046(25)
C(10)	4.077(23)	1.009(2)	0.000	1.000	-0.077(23)
C(11)	4.028(22)	1.009(2)	0.000	1.000	-0.027(22)
H(1A)	0.720(13)	1.200	0.000	1.200	+0.280(13)
H(1)	0.839(14)	1.200	0.000	1.200	+0.161(14)
H(4)	0.906(13)	1.200	0.000	1.200	+0.093(13)
H(5)	0.866(14)	1.200	0.000	1.200	+0.134(14)
H(7)	0.861(14)	1.200	0.000	1.200	+0.139(14)
H(8)	0.942(14)	1.200	0.000	1.200	+0.058(14)
H(9)	0.881(14)	1.200	0.000	1.200	+0.119(14)
H(10)	0.881(14)	1.200	0.000	1.200	+0.118(14)

Table S6b *Shade* Dipole Population Parameters.

Atom	D11+	D11-	D10	Kappa'
O(1)	-0.041(4)	-0.039(4)	0.002(4)	1.000
N(1)	-0.030(5)	0.074(5)	0.001(5)	1.000
C(1)	-0.008(8)	0.046(7)	-0.013(7)	1.000
C(2)	0.017(8)	0.001(7)	0.002(7)	1.000
C(3)	-0.067(8)	0.002(8)	-0.009(7)	1.000
C(4)	-0.011(8)	-0.009(8)	-0.003(7)	1.000
C(5)	-0.023(8)	-0.002(8)	0.010(7)	1.000
C(6)	-0.003(8)	-0.009(8)	-0.021(7)	1.000
C(7)	-0.008(8)	-0.009(8)	-0.009(8)	1.000
C(8)	-0.026(9)	0.043(8)	0.005(7)	1.000
C(9)	-0.037(9)	0.007(8)	-0.001(7)	1.000
C(10)	-0.018(9)	0.015(8)	-0.012(8)	1.000
C(11)	0.016(8)	-0.003(7)	0.015(7)	1.000
H(1A)	0.112(11)	0.030(8)	0.002(7)	1.200
H(1)	0.171(11)	0.000	0.000	1.200
H(4)	0.156(11)	0.000	0.000	1.200
H(5)	0.167(11)	0.000	0.000	1.200
H(7)	0.151(11)	0.000	0.000	1.200
H(8)	0.179(11)	0.000	0.000	1.200
H(9)	0.169(12)	0.000	0.000	1.200
H(10)	0.147(11)	0.000	0.000	1.200

Table S6c *Shade* Quadrupole Population Parameters.

Atom	Q20	Q21+	Q21-	Q22+	Q22-	Kappa'
O(1)	0.026(6)	-0.017(6)	0.024(6)	0.033(6)	0.052(5)	1.000
N(1)	-0.098(6)	0.035(6)	-0.005(6)	0.022(6)	-0.083(5)	1.000
C(1)	-0.186(8)	-0.014(7)	0.040(7)	0.001(7)	0.012(7)	1.000
C(2)	-0.122(8)	0.006(7)	-0.034(7)	0.026(7)	0.005(8)	1.000
C(3)	-0.178(8)	-0.036(7)	-0.002(7)	-0.074(8)	-0.013(7)	1.000
C(4)	-0.151(8)	0.003(7)	-0.030(8)	-0.007(8)	-0.031(8)	1.000
C(5)	-0.184(8)	0.008(7)	-0.030(8)	-0.008(8)	-0.021(8)	1.000
C(6)	-0.171(7)	0.019(7)	0.015(7)	-0.002(8)	-0.010(8)	1.000
C(7)	-0.178(8)	-0.015(7)	-0.013(8)	-0.020(9)	-0.026(8)	1.000
C(8)	-0.147(8)	0.046(7)	0.005(8)	-0.061(9)	-0.020(8)	1.000
C(9)	-0.154(8)	-0.037(8)	0.030(8)	-0.006(9)	0.006(8)	1.000
C(10)	-0.171(8)	-0.017(7)	0.020(7)	-0.007(8)	0.002(8)	1.000
C(11)	-0.171(7)	0.008(7)	0.028(7)	0.017(7)	-0.008(8)	1.000
H(1A)	0.000	0.000	0.000	0.000	0.000	1.200
H(1)	0.000	0.000	0.000	0.000	0.000	1.200
H(4)	0.000	0.000	0.000	0.000	0.000	1.200
H(5)	0.000	0.000	0.000	0.000	0.000	1.200
H(7)	0.000	0.000	0.000	0.000	0.000	1.200
H(8)	0.000	0.000	0.000	0.000	0.000	1.200
H(9)	0.000	0.000	0.000	0.000	0.000	1.200
H(10)	0.000	0.000	0.000	0.000	0.000	1.200

Table S6d *Shade* Octupole Population Parameters.

Atom	O30	O31+	O31-	O32+	O32-	O33+	O33-	Kappa'
O(1)	-0.017(6)	-0.018(5)	-0.008(5)	-0.016(5)	-0.002(5)	0.083(5)	-0.041(5)	1.000
N(1)	-0.008(7)	0.001(6)	0.035(6)	0.003(6)	0.004(6)	0.151(6)	0.008(6)	1.000
C(1)	-0.013(9)	-0.021(8)	0.043(8)	0.009(8)	0.002(8)	0.249(9)	-0.020(8)	1.000
C(2)	0.011(8)	0.009(8)	-0.004(8)	-0.009(8)	0.013(8)	0.233(8)	-0.013(9)	1.000
C(3)	0.007(9)	-0.027(8)	0.005(8)	-0.006(8)	0.008(8)	0.265(9)	0.026(9)	1.000
C(4)	0.022(9)	-0.029(8)	0.015(8)	-0.004(8)	0.010(9)	0.217(9)	-0.006(9)	1.000
C(5)	0.003(9)	-0.016(8)	0.012(8)	0.004(8)	0.017(8)	0.246(9)	-0.032(9)	1.000
C(6)	-0.005(9)	0.004(8)	0.010(8)	0.010(9)	-0.018(9)	0.242(9)	-0.015(9)	1.000
C(7)	0.005(9)	-0.021(9)	0.008(9)	-0.005(9)	0.003(9)	0.225(9)	0.058(9)	1.000
C(8)	-0.008(9)	0.005(8)	-0.008(9)	0.027(9)	-0.005(9)	0.229(9)	-0.014(9)	1.000
C(9)	-0.001(9)	-0.002(9)	0.026(9)	0.008(9)	-0.012(9)	0.231(9)	0.019(9)	1.000
C(10)	0.010(9)	-0.012(8)	0.014(8)	-0.021(9)	-0.004(8)	0.238(9)	-0.054(8)	1.000
C(11)	-0.002(9)	-0.004(8)	-0.006(8)	0.005(8)	-0.022(8)	0.235(8)	-0.020(9)	1.000

Table S7. Topological analysis of Heavy atom – Hydrogen bonds. Standard uncertainties have been omitted from the table for clarity. They are closely scattered around 0.02 e Å^{-3} (ρ_{bcp}) and 0.05 e Å^{-5} ($\nabla^2\rho_{bcp}$).

Bond	ρ / eÅ^{-3}	$\nabla^2\rho$ / eÅ^{-5}	ε	R_{ij} / Å	d_1 / Å	d_2 / Å
O(1)-H(1A)	2.56	-26.23	0.02	0.967	0.716	0.251
Shade	2.15	-27.64	0.02	-	0.756	0.210
DFT	2.20	-44.20	0.02			
C(1)-H(1)	1.91	-18.61	0.06	1.087	0.699	0.387
	1.86	-18.01	0.06	-	0.716	0.370
	1.94	-25.56	0.02			
C(4)-H(4)	1.89	-17.01	0.05	1.087	0.677	0.410
	1.84	-16.31	0.05	-	0.702	0.385
	1.92	-24.96	0.02			
C(5)-H(5)	1.85	-17.50	0.06	1.087	0.697	0.389
	1.85	-17.44	0.06	-	0.709	0.377
	1.92	-24.82	0.01			
C(7)-H(7)	1.83	-16.13	0.06	1.087	0.683	0.404
	1.80	-16.18	0.05	-	0.709	0.377
	1.91	-24.50	0.02			
C(8)-H(8)	1.83	-15.40	0.08	1.087	0.671	0.416
	1.82	-15.77	0.08	-	0.680	0.407
	1.92	-24.67	0.02			
C(9)-H(9)	1.85	-16.50	0.09	1.087	0.678	0.409
	1.81	-16.41	0.08	-	0.699	0.387

	1.92	-24.76	0.02			
C(10)-H(10)	1.83	-16.60	0.07	1.087	0.702	0.385
	1.82	-16.37	0.07	-	0.710	0.377
	1.93	-24.71	0.02			