Weak Intra- and Inter-molecular Interactions in a Binaphthol Imine : An Experimental Charge Density Study on (±)-8-Benzhydrylideneamino-2'-hydroxy-1,1'-binaphthyl.

Louis J. Farrugia*, Pavel Kočovský, Hans Martin Senn and Štěpán Vyskočil.

Contribution from WestCHEM, Department of Chemistry, University of Glasgow, Glasgow G12 8QQ Scotland

SUPPLEMENTARY DATA

Full reference for GAUSSIAN03 program

Supplementary Tables S1 – S8

Supplementary Figures S1-S13

Full reference for GAUSSIAN03 program

Gaussian 03, Revision E.01,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

Table S1. Monopole Populations, Radial Parameters and Net Atomic Charges.

Atom	Pval	Kappa	P00	Kappa'	Atomic charge
O(1)	6.219(10)	0.986	0.000	0.983	-0.219(10)
N(1)	5.102(11)	0.994	0.000	0.956	-0.101(11)
C(1)	4.095(15)	0.998	0.000	0.927	-0.094(15)
C(2)	3.999(18)	0.999	0.000	0.928	+0.000(18)
C(3)	4.030(19)	0.999	0.000	0.928	-0.029(19)
C(4)	4.103(19)	0.999	0.000	0.928	-0.102(19)
C(5)	4.091(20)	0.999	0.000	0.928	-0.091(20)
C(6)	4.059(20)	0.999	0.000	0.928	-0.059(20)
C(7)	4.019(19)	0.999	0.000	0.928	-0.019(19)
C(8)	4.123(16)	0.995	0.000	0.883	-0.123(16)
C(9)	4.069(16)	0.998	0.000	0.927	-0.069(16)
C(10)	4.058(16)	0.998	0.000	0.927	-0.058(16)
C(11)	4.038(18)	0.998	0.000	0.927	-0.038(18)
C(12)	4.105(17)	0.988	0.000	0.859	-0.104(17)
C(13)	3.984(22)	0.999	0.000	0.928	+0.015(22)
C(14)	3.993(22)	0.999	0.000	0.928	+0.007(22)
C(15)	4.061(24)	0.999	0.000	0.928	-0.061(24)
C(16)	4.107(24)	0.999	0.000	0.928	-0.107(24)
C(17)	4.007(22)	0.999	0.000	0.928	-0.007(22)
C(18)	4.008(19)	0.999	0.000	0.928	-0.008(19)
C(19)	3.969(17)	0.998	0.000	0.927	+0.031(17)
C(20)	4.064(18)	0.998	0.000	0.927	-0.064(18)
C(21)	4.009(14)	1.001	0.000	0.920	-0.009(14)
C(22)	4.029(17)	0.998	0.000	0.927	-0.029(17)
C(23)	4.058(19)	0.999	0.000	0.928	-0.058(19)
C(24)	4.056(22)	0.999	0.000	0.928	-0.055(22)
C(25)	4.084(22)	0.999	0.000	0.928	-0.083(22)
C(26)	4.029(21)	0.999	0.000	0.928	-0.028(21)
C(27)	4.077(20)	0.999	0.000	0.928	-0.077(20)
C(28)	4.027(17)	0.998	0.000	0.927	-0.027(17)
C(29)	4.032(18)	0.999	0.000	0.928	-0.031(18)
C(30)	4.060(20)	0.999	0.000	0.928	-0.060(20)
C(31)	4.164(22)	0.999	0.000	0.928	-0.163(22)
C(32)	3.881(21)	0.999	0.000	0.928	+0.119(21)
C(33)	4.067(19)	0.999	0.000	0.928	-0.067(19)
H(2)	0.914(10)	1.141	0.000	1.183	+0.085(10)
H(3)	0.942(10)	1.141	0.000	1.183	+0.057(10)
H(4)	0.960(10)	1.141	0.000	1.183	+0.039(10)
H(5)	0.956(10)	1.141	0.000	1.183	+0.044(10)
H(6)	0.911(10)	1.141	0.000	1.183	+0.088(10)
H(7)	0.906(10)	1.141	0.000	1.183	+0.094(10)
H(13)	0.936(11)	1.141	0.000	1.183	+0.063(11)
H(14)	0.935(10)	1.141	0.000	1.183	+0.065(10)
H(15)	0.892(11)	1.141	0.000	1.183	+0.107(11)
H(16)	0.859(12)	1.141	0.000	1.183	+0.140(12)
H(17)	0.942(12)	1.141	0.000	1.183	+0.057(12)
H(18)	0.906(10)	1.141	0.000	1.183	+0.094(10)
H(23)	0.911(10)	1.141	0.000	1.183	+0.089(10)
H(24)	0.961(11)	1.141	0.000	1.183	+0.038(11)
H(25)	0.938(11)	1.141	0.000	1.183	+0.062(11)
H(26)	0.843(11)	1.141	0.000	1.183	+0.156(11)
H(27)	0.898(10)	1.141	0.000	1.183	+0.101(10)
H(29)	0.917(10)	1.141	0.000	1.183	+0.082(10)
H(30)	0.979(11)	1.141	0.000	1.183	+0.021(11)
H(31)	0.951(11)	1.141	0.000	1.183	+0.048(11)
H(32)	0.919(11)	1.141	0.000	1.183	+0.081(11)
H(33)	0.902(10)	1.141	0.000	1.183	+0.097(10)
H(1)	0.842(9)	1.094	0.000	1.233	+0.158(9)

Total charge in the ASU : +0.0002
Sum of monopoles in ASU : 165.9998

Table S2. Dipole Population Parameters.

Atom	D11+	D11-	D10	Kappa'
O(1)	-0.092(7)	-0.005(6)	-0.006(5)	0.983
N(1)	0.005(6)	-0.095(5)	0.009(4)	0.956
C(1)	-0.003(8)	0.060(8)	0.000	0.927
C(2)	0.025(9)	-0.023(9)	0.000	0.928
C(3)	0.027(9)	0.013(10)	0.000	0.928
C(4)	0.043(10)	0.021(9)	0.000	0.928
C(5)	-0.003(10)	0.051(10)	0.000	0.928
C(6)	-0.012(11)	0.038(9)	0.000	0.928
C(7)	-0.019(10)	0.011(9)	0.000	0.928
C(8)	0.050(9)	0.007(8)	0.000	0.883
C(9)	-0.003(8)	0.004(8)	0.000	0.927
C(10)	-0.015(9)	-0.019(9)	0.000	0.927
C(11)	-0.007(9)	0.049(8)	0.000	0.927
C(12)	0.093(11)	0.126(10)	0.000	0.859
C(13)	-0.067(11)	0.096(12)	0.000	0.928
C(14)	-0.021(13)	-0.016(11)	0.000	0.928
C(15)	-0.024(13)	-0.020(14)	0.000	0.928
C(16)	-0.002(15)	0.015(12)	0.000	0.928
C(17)	-0.002(12)	0.033(11)	0.000	0.928
C(18)	0.029(10)	0.023(10)	0.000	0.928
C(19)	-0.010(10)	0.019(9)	0.000	0.927
C(20)	0.012(12)	0.002(10)	0.000	0.927
C(21)	-0.022(7)	-0.024(8)	0.000	0.920
C(22)	-0.013(9)	0.062(8)	0.000	0.927
C(23)	0.042(10)	0.040(10)	0.000	0.928
C(24)	0.000(11)	0.110(12)	0.000	0.928
C(25)	-0.075(13)	0.076(11)	0.000	0.928
C(26)	-0.076(12)	0.002(10)	0.000	0.928
C(27)	-0.008(10)	0.008(10)	0.000	0.928
C(28)	0.015(8)	0.060(8)	0.000	0.927
C(29)	0.016(9)	0.035(9)	0.000	0.928
C(30)	-0.040(10)	0.101(11)	0.000	0.928
C(31)	-0.110(12)	0.146(11)	0.000	0.928
C(32)	-0.149(12)	0.048(10)	0.000	0.928
C(33)	0.034(10)	0.007(10)	0.000	0.928
H(2)	0.025(4)	0.022(6)	0.127(6)	1.183
H(3)	0.018(4)	0.009(7)	0.152(6)	1.183
H(4)	-0.045(4)	-0.044(7)	0.157(6)	1.183
H(5)	-0.038(4)	0.042(7)	0.139(6)	1.183
H(6)	-0.032(4)	-0.009(7)	0.146(6)	1.183
H(7)	-0.069(4)	-0.008(6)	0.147(6)	1.183
H(13)	0.042(4)	0.032(8)	0.154(7)	1.183
H(14)	0.027(4)	-0.017(8)	0.149(7)	1.183
H(15)	-0.002(4)	0.033(8)	0.118(7)	1.183
H(16)	0.006(4)	0.002(8)	0.125(7)	1.183
H(17)	0.006(4)	-0.012(8)	0.139(8)	1.183
H(18)	0.021(4)	0.006(7)	0.161(6)	1.183
H(23)	0.012(4)	0.012(7)	0.158(7)	1.183
H(24)	0.005(4)	0.013(7)	0.169(7)	1.183
H(25)	0.031(4)	-0.014(8)	0.148(7)	1.183
H(26)	0.024(4)	0.014(8)	0.121(7)	1.183
H(27)	0.005(4)	0.005(7)	0.133(7)	1.183
H(29)	0.012(4)	0.003(7)	0.165(6)	1.183
H(30)	-0.002(4)	0.026(7)	0.170(7)	1.183
H(31)	0.012(4)	0.019(7)	0.164(7)	1.183
H(32)	-0.007(4)	0.000(7)	0.153(7)	1.183
H(33)	0.015(4)	-0.012(7)	0.138(6)	1.183
H(1)	0.032(5)	0.008(5)	0.189(6)	1.233

Table S3. Quadrupole Population Parameters.

Atom	Q20	Q21+	Q21-	Q22+	Q22-	Kappa'
O(1)	0.031(5)	0.006(5)	0.006(4)	0.008(6)	0.022(6)	0.983
N(1)	-0.136(4)	0.012(4)	-0.005(4)	0.029(5)	0.034(5)	0.956
C(1)	-0.173(5)	0.000	0.000	-0.009(6)	-0.025(6)	0.927
C(2)	-0.205(6)	0.000	0.000	0.002(7)	0.011(7)	0.928
C(3)	-0.215(6)	0.000	0.000	0.020(7)	-0.010(7)	0.928
C(4)	-0.211(6)	0.000	0.000	0.044(7)	-0.029(7)	0.928
C(5)	-0.200(6)	0.000	0.000	-0.006(7)	-0.048(8)	0.928
C(6)	-0.214(7)	0.000	0.000	0.010(8)	-0.025(8)	0.928
C(7)	-0.179(6)	0.000	0.000	-0.005(7)	0.005(7)	0.928
C(8)	-0.204(6)	0.000	0.000	0.037(7)	-0.018(7)	0.883
C(9)	-0.185(5)	0.000	0.000	0.007(6)	-0.003(6)	0.927
C(10)	-0.197(6)	0.000	0.000	0.004(7)	-0.008(7)	0.927
C(11)	-0.162(6)	0.000	0.000	0.034(7)	-0.032(7)	0.927
C(12)	-0.234(6)	0.000	0.000	0.048(9)	-0.066(8)	0.859
C(13)	-0.203(6)	0.000	0.000	-0.037(9)	-0.031(9)	0.928
C(14)	-0.196(7)	0.000	0.000	0.018(9)	-0.025(9)	0.928
C(15)	-0.205(7)	0.000	0.000	0.004(10)	-0.026(10)	0.928
C(16)	-0.212(8)	0.000	0.000	0.031(10)	-0.018(10)	0.928
C(17)	-0.198(7)	0.000	0.000	-0.036(9)	-0.037(9)	0.928
C(18)	-0.215(6)	0.000	0.000	0.008(8)	-0.031(8)	0.928
C(19)	-0.199(6)	0.000	0.000	0.026(7)	0.015(7)	0.927
C(20)	-0.219(6)	0.000	0.000	0.016(9)	-0.011(8)	0.927
C(21)	-0.238(5)	0.000	0.000	-0.026(6)	0.032(7)	0.920
C(22)	-0.197(5)	0.000	0.000	0.002(7)	-0.026(7)	0.927
C(23)	-0.234(6)	0.000	0.000	0.021(8)	-0.014(8)	0.928
C(24)	-0.236(7)	0.000	0.000	0.020(8)	-0.035(9)	0.928
C(25)	-0.207(7)	0.000	0.000	-0.018(9)	-0.053(9)	0.928
C(26)	-0.204(7)	0.000	0.000	0.001(9)	0.018(9)	0.928
C(27)	-0.213(6)	0.000	0.000	-0.019(8)	-0.010(8)	0.928
C(28)	-0.199(6)	0.000	0.000	0.015(7)	-0.027(7)	0.927
C(29)	-0.212(6)	0.000	0.000	0.000(7)	-0.020(8)	0.928
C(30)	-0.232(7)	0.000	0.000	0.033(8)	-0.063(8)	0.928
C(31)	-0.240(7)	0.000	0.000	-0.037(9)	-0.096(9)	0.928
C(32)	-0.198(7)	0.000	0.000	-0.036(9)	-0.034(9)	0.928
C(33)	-0.198(6)	0.000	0.000	-0.017(8)	0.005(8)	0.928
H(2)	0.044(7)	-0.004(5)	0.005(7)	0.016(7)	0.006(5)	1.183
H(3)	0.075(8)	-0.010(5)	0.011(8)	0.001(7)	0.016(5)	1.183
H(4)	0.089(8)	-0.010(5)	-0.029(7)	-0.013(7)	0.008(6)	1.183
H(5)	0.083(8)	-0.014(5)	-0.002(8)	-0.029(7)	0.004(6)	1.183
H(6)	0.045(8)	0.000(5)	0.000(8)	0.011(8)	-0.002(6)	1.183
H(7)	0.050(8)	-0.014(5)	0.027(7)	-0.003(7)	-0.001(5)	1.183
H(13)	0.083(9)	0.044(6)	-0.022(8)	-0.023(7)	0.009(6)	1.183
H(14)	0.069(8)	0.021(5)	-0.006(8)	-0.024(8)	0.005(6)	1.183
H(15)	0.037(8)	0.017(6)	0.006(9)	-0.006(8)	0.037(6)	1.183
H(16)	0.027(9)	-0.007(6)	0.015(9)	-0.007(8)	0.005(6)	1.183
H(17)	0.051(9)	0.012(6)	0.005(8)	-0.002(8)	-0.013(6)	1.183
H(18)	0.063(8)	0.004(5)	-0.005(7)	0.012(7)	0.005(5)	1.183
H(23)	0.077(8)	0.014(5)	-0.001(8)	-0.011(7)	-0.016(5)	1.183
H(24)	0.086(9)	0.011(6)	-0.002(8)	-0.020(8)	-0.048(6)	1.183
H(25)	0.072(8)	-0.009(6)	-0.004(8)	-0.018(8)	-0.039(6)	1.183
H(26)	0.035(8)	0.008(5)	0.034(8)	0.020(8)	-0.010(6)	1.183
H(27)	0.070(8)	-0.001(5)	0.023(8)	0.015(7)	-0.006(5)	1.183
H(29)	0.059(7)	0.000(5)	0.011(7)	0.019(7)	0.000(5)	1.183
H(30)	0.105(8)	-0.013(6)	0.024(8)	0.027(8)	-0.023(6)	1.183
H(31)	0.080(8)	-0.014(6)	0.018(8)	0.001(8)	-0.009(6)	1.183
H(32)	0.057(8)	-0.001(5)	-0.001(8)	0.014(8)	-0.026(6)	1.183
H(33)	0.027(8)	-0.004(5)	0.017(8)	0.015(7)	0.002(5)	1.183
H(1)	0.067(7)	0.013(6)	0.009(7)	0.018(6)	-0.001(5)	1.233

Table S4. Octupole Population Parameters.

Atom	O30	O31+	O31-	O32+	O32-	O33+	O33-	Kappa'
O(1)	-0.011(3)	-0.004(3)	-0.025(3)	0.022(3)	-0.002(3)	0.091(4)	-0.026(4)	0.983
N(1)	-0.009(4)	0.004(4)	-0.033(3)	0.000(3)	0.007(3)	0.107(4)	0.009(4)	0.956
C(1)	0.000	0.011(5)	0.030(5)	0.000	0.000	0.286(7)	-0.024(6)	0.927
C(2)	0.000	0.031(6)	0.029(5)	0.000	0.000	0.268(7)	0.008(8)	0.928
C(3)	0.000	-0.016(6)	0.037(6)	0.000	0.000	0.287(7)	-0.004(8)	0.928
C(4)	0.000	0.017(6)	0.019(6)	0.000	0.000	0.292(7)	0.011(8)	0.928
C(5)	0.000	0.010(6)	0.001(6)	0.000	0.000	0.300(8)	-0.004(8)	0.928
C(6)	0.000	0.058(7)	0.011(6)	0.000	0.000	0.280(8)	-0.014(8)	0.928
C(7)	0.000	0.027(6)	0.028(6)	0.000	0.000	0.266(7)	-0.011(8)	0.928
C(8)	0.000	0.039(6)	0.064(6)	0.000	0.000	0.337(8)	0.001(8)	0.883
C(9)	0.000	0.011(5)	-0.005(5)	0.000	0.000	0.283(7)	0.031(7)	0.927
C(10)	0.000	0.004(6)	-0.005(5)	0.000	0.000	0.278(7)	-0.006(8)	0.927
C(11)	0.000	0.027(6)	0.000(5)	0.000	0.000	0.291(7)	0.006(7)	0.927
C(12)	0.000	0.034(7)	0.015(6)	0.000	0.000	0.355(9)	0.021(9)	0.859
C(13)	0.000	0.023(6)	0.013(7)	0.000	0.000	0.305(9)	-0.010(10)	0.928
C(14)	0.000	0.027(8)	0.018(6)	0.000	0.000	0.263(10)	0.028(10)	0.928
C(15)	0.000	0.001(7)	0.029(7)	0.000	0.000	0.276(10)	0.021(11)	0.928
C(16)	0.000	0.012(9)	0.018(6)	0.000	0.000	0.323(11)	0.007(11)	0.928
C(17)	0.000	0.004(7)	0.018(6)	0.000	0.000	0.263(9)	0.035(10)	0.928
C(18)	0.000	0.021(6)	0.014(6)	0.000	0.000	0.281(8)	-0.008(9)	0.928
C(19)	0.000	0.000(6)	-0.008(6)	0.000	0.000	0.254(8)	-0.003(8)	0.927
C(20)	0.000	-0.019(7)	0.004(6)	0.000	0.000	0.297(9)	0.017(9)	0.927
C(21)	0.000	-0.028(5)	-0.067(6)	0.000	0.000	0.320(7)	-0.018(6)	0.920
C(22)	0.000	0.025(6)	0.007(5)	0.000	0.000	0.272(7)	0.017(7)	0.927
C(23)	0.000	-0.012(6)	0.009(6)	0.000	0.000	0.289(7)	0.005(8)	0.928
C(24)	0.000	0.038(7)	-0.025(7)	0.000	0.000	0.299(9)	-0.018(9)	0.928
C(25)	0.000	0.057(7)	0.007(7)	0.000	0.000	0.301(9)	0.038(10)	0.928
C(26)	0.000	0.032(7)	0.031(6)	0.000	0.000	0.256(9)	-0.004(9)	0.928
C(27)	0.000	0.041(6)	0.013(6)	0.000	0.000	0.304(7)	0.001(8)	0.928
C(28)	0.000	0.016(6)	0.021(5)	0.000	0.000	0.257(7)	0.018(7)	0.927
C(29)	0.000	0.021(6)	0.014(5)	0.000	0.000	0.293(7)	0.011(8)	0.928
C(30)	0.000	0.030(6)	-0.020(6)	0.000	0.000	0.280(8)	-0.042(9)	0.928
C(31)	0.000	0.067(7)	-0.039(6)	0.000	0.000	0.362(9)	0.024(9)	0.928
C(32)	0.000	0.083(7)	0.012(6)	0.000	0.000	0.192(8)	0.029(9)	0.928
C(33)	0.000	0.015(6)	0.040(6)	0.000	0.000	0.289(7)	-0.014(8)	0.928
H(1)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.233

Table S5. Hexadecapole Population Parameters.

Atom	H40	H41+	H41-	H42+	H42-	H43+	H43-	H44+	H44-	Kappa'
O(1)	0.013(4)	-0.009(4)	-0.005(4)	-0.005(4)	0.016(4)	0.011(4)	-0.008(4)	0.033(4)	0.017(5)	0.983
N(1)	0.001(5)	-0.009(4)	0.005(4)	-0.005(5)	0.003(4)	0.011(4)	0.003(4)	0.000(5)	0.023(4)	0.956
C(1)	0.031(7)	0.000	0.000	0.018(6)	-0.004(7)	0.000	0.000	-0.011(8)	0.021(8)	0.927
C(2)	0.034(7)	0.000	0.000	0.018(7)	-0.023(7)	0.000	0.000	-0.021(10)	-0.016(9)	0.928
C(3)	0.036(7)	0.000	0.000	-0.014(7)	-0.011(7)	0.000	0.000	0.026(10)	-0.005(10)	0.928
C(4)	0.039(7)	0.000	0.000	-0.013(7)	-0.002(7)	0.000	0.000	0.002(10)	0.000(9)	0.928
C(5)	0.034(7)	0.000	0.000	0.006(7)	0.005(8)	0.000	0.000	0.019(10)	0.002(10)	0.928
C(6)	0.037(7)	0.000	0.000	0.011(7)	0.001(8)	0.000	0.000	-0.009(11)	0.012(10)	0.928
C(7)	0.044(7)	0.000	0.000	0.015(7)	-0.002(7)	0.000	0.000	-0.010(10)	-0.002(9)	0.928
C(8)	0.031(7)	0.000	0.000	0.016(8)	0.001(8)	0.000	0.000	0.007(11)	-0.034(10)	0.883
C(9)	0.043(6)	0.000	0.000	0.004(7)	0.005(7)	0.000	0.000	-0.009(9)	0.010(9)	0.927
C(10)	0.034(7)	0.000	0.000	-0.010(7)	0.013(7)	0.000	0.000	0.007(10)	-0.021(10)	0.927
C(11)	0.044(7)	0.000	0.000	-0.007(7)	-0.005(7)	0.000	0.000	-0.020(9)	-0.006(9)	0.927
C(12)	0.038(8)	0.000	0.000	0.023(8)	0.014(9)	0.000	0.000	-0.012(14)	-0.039(12)	0.859
C(13)	0.028(7)	0.000	0.000	-0.002(8)	-0.004(8)	0.000	0.000	0.047(12)	0.023(11)	0.928
C(14)	0.018(7)	0.000	0.000	0.006(8)	-0.035(8)	0.000	0.000	-0.027(13)	-0.014(11)	0.928
C(15)	0.020(8)	0.000	0.000	0.017(8)	-0.032(9)	0.000	0.000	-0.004(14)	-0.002(13)	0.928
C(16)	0.015(8)	0.000	0.000	0.024(9)	-0.009(9)	0.000	0.000	-0.018(14)	0.049(13)	0.928
C(17)	0.023(8)	0.000	0.000	-0.012(8)	0.005(8)	0.000	0.000	-0.030(13)	0.040(11)	0.928
C(18)	0.033(7)	0.000	0.000	0.009(7)	-0.005(8)	0.000	0.000	-0.027(11)	0.005(10)	0.928
C(19)	0.027(7)	0.000	0.000	0.010(8)	-0.005(7)	0.000	0.000	-0.007(11)	0.008(11)	0.927
C(20)	0.035(7)	0.000	0.000	-0.003(8)	0.002(8)	0.000	0.000	-0.028(12)	-0.037(13)	0.927
C(21)	0.021(7)	0.000	0.000	-0.002(7)	0.036(7)	0.000	0.000	0.008(8)	0.012(9)	0.920
C(22)	0.043(7)	0.000	0.000	0.014(7)	-0.001(7)	0.000	0.000	-0.005(10)	-0.028(9)	0.927
C(23)	0.035(7)	0.000	0.000	-0.015(7)	0.001(7)	0.000	0.000	0.034(11)	-0.021(10)	0.928
C(24)	0.036(8)	0.000	0.000	0.015(8)	0.003(8)	0.000	0.000	0.017(12)	0.018(11)	0.928
C(25)	0.023(8)	0.000	0.000	0.012(8)	0.014(8)	0.000	0.000	-0.013(13)	0.024(12)	0.928
C(26)	0.029(8)	0.000	0.000	0.004(8)	-0.029(8)	0.000	0.000	-0.029(12)	0.006(10)	0.928
C(27)	0.021(7)	0.000	0.000	0.011(7)	-0.012(7)	0.000	0.000	0.004(10)	-0.009(9)	0.928
C(28)	0.038(7)	0.000	0.000	0.010(7)	-0.021(7)	0.000	0.000	-0.006(8)	-0.009(9)	0.927
C(29)	0.036(7)	0.000	0.000	-0.007(7)	0.011(7)	0.000	0.000	0.024(10)	-0.005(9)	0.928
C(30)	0.037(7)	0.000	0.000	-0.002(7)	0.009(8)	0.000	0.000	0.024(11)	0.005(10)	0.928
C(31)	0.033(8)	0.000	0.000	0.041(8)	0.011(8)	0.000	0.000	-0.048(12)	0.068(11)	0.928
C(32)	0.016(7)	0.000	0.000	0.022(8)	0.017(8)	0.000	0.000	-0.061(12)	-0.010(10)	0.928
C(33)	0.016(7)	0.000	0.000	-0.003(7)	-0.007(8)	0.000	0.000	0.009(10)	0.031(10)	0.928

Table S6. Critical Point Properties in Experimental Molecular Graph :

		A	–	B	d1	d2	ρ	$\nabla^2\rho$	λ_1	λ_2	λ_3	ε	G_b	G_b/f	V_b	E_b
1	(3,-1)	C(12)		-O(1)	0.4999	0.8704	2.04	-19.84	-15.72	-14.78	10.66	0.06	1.71	0.84	-4.81	-3.10
2	(3,-1)	H(1)		-O(1)	0.1926	0.7781	2.29	-54.35	-41.53	-39.43	26.61	0.05	0.67	0.29	-5.14	-4.47
3	(3,-1)	C(8)		-N(1)	0.6213	0.7897	2.07	-16.30	-15.64	-15.04	14.39	0.04	1.94	0.94	-5.02	-3.08
4	(3,-1)	N(1)		-C(11)	1.3734	1.4428	0.11	1.22	-0.32	-0.18	1.72	0.83	0.08	0.70	-0.07	0.01
5	(3,-1)	C(21)		-N(1)	0.4903	0.7985	2.59	-29.42	-21.78	-17.61	9.97	0.24	2.57	0.99	-7.19	-4.63
6	(3,-1)	C(2)		-C(1)	0.6808	0.7061	2.19	-19.80	-16.55	-13.72	10.46	0.21	2.04	0.93	-5.47	-3.43
7	(3,-1)	C(1)		-C(9)	0.7153	0.7225	1.97	-15.51	-14.42	-12.24	11.15	0.18	1.77	0.90	-4.63	-2.86
8	(3,-1)	C(11)		-C(1)	0.7396	0.7521	1.78	-13.49	-12.45	-11.99	10.95	0.04	1.48	0.83	-3.91	-2.43
9	(3,-1)	H(2)		-C(2)	0.3601	0.7230	1.89	-20.64	-18.43	-17.68	15.47	0.04	1.35	0.72	-4.15	-2.80
10	(3,-1)	C(2)		-C(3)	0.6815	0.7312	2.10	-19.34	-15.85	-13.93	10.44	0.14	1.86	0.89	-5.08	-3.22
11	(3,-1)	H(3)		-C(3)	0.3739	0.7092	1.91	-21.29	-18.26	-17.72	14.69	0.03	1.37	0.72	-4.23	-2.86
12	(3,-1)	C(3)		-C(4)	0.6614	0.7111	2.26	-21.73	-17.21	-14.61	10.09	0.18	2.12	0.94	-5.76	-3.64
13	(3,-1)	C(10)		-C(4)	0.7014	0.7180	2.08	-18.38	-15.60	-13.59	10.81	0.15	1.88	0.90	-5.04	-3.16
14	(3,-1)	H(4)		-C(4)	0.3832	0.7007	1.92	-21.78	-18.14	-17.87	14.23	0.02	1.38	0.72	-4.28	-2.90
15	(3,-1)	C(6)		-C(5)	0.6608	0.7125	2.26	-21.63	-17.22	-14.51	10.11	0.19	2.12	0.94	-5.75	-3.63
16	(3,-1)	C(10)		-C(5)	0.7081	0.7121	2.07	-18.07	-15.42	-13.45	10.79	0.15	1.86	0.90	-4.99	-3.13
17	(3,-1)	H(5)		-C(5)	0.3793	0.7043	1.88	-20.42	-17.60	-17.38	14.56	0.01	1.34	0.72	-4.11	-2.77
18	(3,-1)	H(6)		-C(6)	0.3689	0.7144	1.86	-19.95	-17.63	-17.22	14.90	0.02	1.33	0.72	-4.06	-2.73
19	(3,-1)	C(7)		-C(6)	0.6801	0.7316	2.09	-18.29	-15.46	-13.50	10.67	0.14	1.89	0.91	-5.07	-3.17
20	(3,-1)	H(7)		-C(7)	0.3652	0.7185	1.89	-20.73	-18.01	-17.77	15.04	0.01	1.36	0.72	-4.16	-2.81
22	(3,-1)	C(7)		-C(8)	0.6830	0.7036	2.20	-20.69	-16.80	-13.83	9.94	0.21	2.03	0.92	-5.51	-3.48
22	(3,-1)	H(7)		-H(33)	1.0745	1.2394	0.05	0.76	-0.18	-0.07	1.02	1.39	0.04	0.78	-0.03	0.01
23	(3,-1)	C(8)		-C(9)	0.7111	0.7316	1.99	-16.46	-14.62	-12.58	10.73	0.16	1.76	0.88	-4.67	-2.91
24	(3,-1)	C(9)		-C(10)	0.7128	0.7211	2.02	-16.86	-14.95	-12.90	10.99	0.16	1.81	0.90	-4.81	-2.99
25	(3,-1)	C(11)		-C(12)	0.6836	0.6983	2.25	-21.37	-16.94	-13.96	9.53	0.21	2.11	0.94	-5.71	-3.60
26	(3,-1)	C(19)		-C(11)	0.6981	0.7318	2.03	-17.15	-14.94	-13.11	10.90	0.14	1.81	0.89	-4.83	-3.01
27	(3,-1)	C(13)		-C(12)	0.6814	0.7341	2.10	-20.34	-16.20	-13.53	9.39	0.20	1.81	0.87	-5.05	-3.24
28	(3,-1)	H(13)		-C(13)	0.3769	0.7069	1.89	-21.07	-17.86	-17.59	14.38	0.02	1.35	0.71	-4.17	-2.82
29	(3,-1)	C(14)		-C(13)	0.6472	0.7269	2.27	-21.46	-16.95	-14.50	9.99	0.17	2.15	0.95	-5.80	-3.65
30	(3,-1)	C(23)		-C(13)	1.6081	1.6237	0.05	0.49	-0.10	-0.07	0.66	0.44	0.03	0.57	-0.02	0.01
31	(3,-1)	H(14)		-C(14)	0.3730	0.7103	1.92	-21.66	-18.20	-18.05	14.59	0.01	1.36	0.71	-4.25	-2.88
32	(3,-1)	C(14)		-C(20)	0.6999	0.7222	2.07	-17.38	-15.11	-13.36	11.09	0.13	1.90	0.92	-5.01	-3.12
33	(3,-1)	C(15)		-C(16)	0.6775	0.7007	2.22	-20.68	-17.16	-13.82	10.30	0.24	2.07	0.93	-5.59	-3.52
34	(3,-1)	C(15)		-C(20)	0.7056	0.7167	2.04	-17.14	-15.06	-13.01	10.94	0.16	1.84	0.90	-4.88	-3.04
35	(3,-1)	H(15)		-C(15)	0.3563	0.7271	1.83	-19.23	-17.84	-16.98	15.59	0.05	1.31	0.72	-3.97	-2.66
36	(3,-1)	H(16)		-C(16)	0.3520	0.7310	1.79	-18.54	-17.14	-16.84	15.44	0.02	1.26	0.70	-3.82	-2.56
37	(3,-1)	H(17)		-C(17)	0.3762	0.7068	1.83	-18.25	-16.93	-16.41	15.09	0.03	1.34	0.73	-3.96	-2.62
38	(3,-1)	C(17)		-C(16)	0.6865	0.7299	2.07	-18.65	-15.74	-13.38	10.46	0.18	1.84	0.89	-4.99	-3.15
39	(3,-1)	C(18)		-C(17)	0.6834	0.6950	2.24	-21.57	-17.33	-14.47	10.23	0.20	2.08	0.93	-5.67	-3.59
40	(3,-1)	H(18)		-C(18)	0.3738	0.7093	1.88	-21.17	-18.06	-17.30	14.19	0.04	1.31	0.70	-4.09	-2.79
41	(3,-1)	H(29)		-C(18)	1.0544	1.5841	0.06	0.76	-0.14	-0.08	0.98	0.63	0.04	0.69	-0.03	0.01

		A – B	d1	d2	ρ	$\nabla^2\rho$	λ_1	λ_2	λ_3	ε	G_b	G_b/f	V_b	E_b
43	(3,-1)	C(19) –C(20)	0.7071	0.7203	2.03	-18.09	-15.43	-13.20	10.54	0.17	1.77	0.87	-4.80	-3.03
44	(3,-1)	C(22) –C(21)	0.7353	0.7524	1.85	-15.16	-13.79	-12.32	10.95	0.12	1.54	0.83	-4.14	-2.60
45	(3,-1)	C(28) –C(21)	0.7293	0.7680	1.84	-15.00	-13.10	-12.88	10.98	0.02	1.52	0.83	-4.09	-2.57
46	(3,-1)	C(22) –C(23)	0.6770	0.7268	2.17	-20.45	-16.55	-14.32	10.42	0.16	1.97	0.91	-5.38	-3.40
47	(3,-1)	C(27) –C(22)	0.6837	0.7184	2.14	-18.89	-15.95	-13.63	10.69	0.17	1.97	0.92	-5.26	-3.29
48	(3,-1)	H(23) –C(23)	0.3721	0.7111	1.88	-21.28	-18.14	-17.47	14.33	0.04	1.31	0.70	-4.11	-2.80
49	(3,-1)	H(27) –C(27)	0.3537	0.7293	1.91	-21.97	-19.16	-18.10	15.30	0.06	1.34	0.70	-4.22	-2.88
50	(3,-1)	C(23) –C(24)	0.6933	0.6954	2.19	-20.09	-16.51	-14.15	10.56	0.17	2.04	0.93	-5.49	-3.45
51	(3,-1)	H(24) –C(24)	0.3914	0.6916	1.88	-20.93	-17.83	-16.89	13.78	0.06	1.33	0.71	-4.13	-2.80
52	(3,-1)	C(25) –C(24)	0.6502	0.7480	2.18	-20.50	-16.52	-14.01	10.03	0.18	1.99	0.91	-5.41	-3.42
53	(3,-1)	H(25) –C(25)	0.3733	0.7098	1.89	-20.77	-18.16	-17.34	14.72	0.05	1.36	0.72	-4.17	-2.81
54	(3,-1)	C(26) –C(25)	0.6399	0.7544	2.20	-20.60	-16.31	-14.30	10.01	0.14	2.02	0.92	-5.48	-3.46
55	(3,-1)	H(26) –C(26)	0.3413	0.7419	1.83	-19.88	-18.19	-17.48	15.80	0.04	1.28	0.70	-3.94	-2.67
56	(3,-1)	C(26) –C(27)	0.6871	0.7099	2.16	-19.57	-16.28	-13.88	10.59	0.17	1.99	0.92	-5.36	-3.36
57	(3,-1)	C(28) –C(29)	0.6979	0.7007	2.14	-19.49	-16.21	-13.80	10.52	0.17	1.95	0.91	-5.27	-3.32
58	(3,-1)	C(33) –C(28)	0.6942	0.7050	2.14	-18.88	-15.98	-13.59	10.69	0.18	1.98	0.92	-5.28	-3.30
59	(3,-1)	H(29) –C(29)	0.3739	0.7093	1.89	-20.93	-18.24	-17.17	14.47	0.06	1.35	0.71	-4.17	-2.82
60	(3,-1)	H(33) –C(33)	0.3600	0.7230	1.85	-18.78	-17.52	-16.93	15.67	0.04	1.36	0.74	-4.04	-2.68
61	(3,-1)	C(30) –C(29)	0.6901	0.7015	2.20	-21.10	-16.87	-14.61	10.38	0.16	2.01	0.91	-5.50	-3.49
62	(3,-1)	H(30) –C(30)	0.3971	0.6859	1.89	-20.83	-17.73	-16.70	13.60	0.06	1.35	0.71	-4.16	-2.81
63	(3,-1)	C(31) –C(30)	0.6463	0.7466	2.19	-20.31	-16.47	-13.86	10.01	0.19	2.02	0.92	-5.46	-3.44
64	(3,-1)	H(31) –C(31)	0.3807	0.7023	1.93	-22.02	-18.47	-17.73	14.18	0.04	1.38	0.71	-4.29	-2.92
65	(3,-1)	C(32) –C(31)	0.5549	0.8409	2.12	-19.12	-14.34	-12.53	7.75	0.14	1.93	0.91	-5.20	-3.27
66	(3,-1)	H(32) –C(32)	0.3727	0.7103	1.86	-19.92	-17.72	-16.94	14.75	0.05	1.34	0.72	-4.07	-2.73
67	(3,-1)	C(33) –C(32)	0.6790	0.7209	2.18	-20.09	-16.53	-14.22	10.66	0.16	2.01	0.92	-5.42	-3.41
1	(3,+1)	–	0.0000	4.0997	0.09	1.40	-0.27	0.37	1.31	0.00	0.08	0.86	-0.06	0.02
2	(3,+1)	–	0.0000	3.3062	0.02	0.30	-0.04	0.14	0.20	0.00	0.02	0.66	-0.01	0.01
3	(3,+1)	–	0.0000	4.2836	0.05	0.66	-0.07	0.05	0.68	0.00	0.04	0.78	-0.02	0.01
4	(3,+1)	–	0.0000	4.1683	0.15	3.24	-0.46	1.73	1.97	0.00	0.19	1.22	-0.15	0.04
5	(3,+1)	–	0.0000	4.4402	0.15	3.27	-0.42	1.70	2.00	0.00	0.19	1.27	-0.14	0.04
6	(3,+1)	–	0.0000	4.8265	0.15	3.37	-0.44	1.79	2.02	0.00	0.19	1.28	-0.15	0.05
7	(3,+1)	–	0.0000	3.3407	0.14	3.35	-0.40	1.74	2.01	0.00	0.19	1.33	-0.14	0.05
8	(3,+1)	–	0.0000	7.0155	0.16	3.50	-0.49	1.94	2.04	0.00	0.20	1.24	-0.16	0.04
9	(3,+1)	–	0.0000	3.6893	0.15	3.59	-0.40	1.95	2.04	0.00	0.20	1.33	-0.15	0.05
10	(3,+1)	–	0.0000	5.7025	0.03	0.40	-0.04	0.12	0.32	0.00	0.02	0.67	-0.01	0.01

Table S7 QTAIM integrated atomic properties

Atom	$q(\Omega)_{exp}$	$q(\Omega)_{theo}$	$V_{001}(\Omega)_{exp}$	$V_{001}(\Omega_{theo})$	$L(\Omega)_{exp}$	$L(\Omega)_{theo}$
O(1)	-1.194	-1.089	17.47	17.77	0.000093	0.000091
N(1)	-0.996	-1.104	13.70	14.44	-0.000398	0.000123
C(1)	-0.071	-0.031	9.04	9.07	0.000238	0.000023
C(2)	-0.001	-0.022	11.67	12.05	0.001315	-0.000010
C(3)	-0.065	-0.021	12.19	12.56	-0.001645	-0.000134
C(4)	-0.170	-0.016	12.12	12.28	0.000652	0.000065
C(5)	-0.134	-0.019	12.11	12.45	-0.000239	-0.000014
C(6)	-0.088	-0.012	12.25	12.44	0.000425	-0.000003
C(7)	-0.074	-0.005	11.93	11.92	0.001920	0.000040
C(8)	0.236	0.346	9.24	9.11	0.003162	0.000067
C(9)	-0.087	-0.012	10.72	10.58	-0.001191	-0.000005
C(10)	-0.060	0.001	10.44	10.38	0.000216	0.000056
C(11)	-0.079	0.009	9.10	9.03	0.000653	-0.000006
C(12)	0.440	0.506	8.07	8.15	0.001997	0.000057
C(13)	-0.092	0.001	11.34	11.46	0.002897	-0.000186
C(14)	-0.001	-0.005	11.64	12.17	0.001054	-0.000109
C(15)	-0.077	-0.023	12.06	12.28	0.001546	-0.000100
C(16)	-0.136	-0.028	12.35	12.53	0.001856	0.000055
C(17)	-0.041	-0.021	12.07	12.19	0.000258	-0.000144
C(18)	-0.049	-0.024	11.50	11.71	0.001730	-0.000185
C(19)	0.040	-0.006	9.66	9.71	0.000596	-0.000140
C(20)	-0.058	-0.007	10.47	10.35	0.000873	0.000129
C(21)	0.580	0.653	7.89	7.84	0.002553	-0.000396
C(22)	-0.041	-0.011	10.46	10.38	-0.001244	-0.000270
C(23)	-0.125	-0.004	11.33	11.25	0.001285	0.000130
C(24)	-0.125	-0.014	12.14	12.63	-0.000926	0.000041
C(25)	-0.136	-0.020	12.31	12.60	0.001363	-0.000028
C(26)	-0.038	-0.016	12.39	12.64	0.001116	-0.000109
C(27)	-0.101	-0.021	12.18	12.33	-0.001526	-0.000024
C(28)	-0.033	-0.026	9.18	9.28	0.001683	-0.000418
C(29)	-0.083	-0.014	11.81	11.65	-0.002218	0.000094
C(30)	-0.169	-0.013	12.54	12.46	0.000702	0.000049
C(31)	-0.222	-0.016	12.37	12.54	0.000360	0.000042
C(32)	0.103	-0.015	11.80	12.56	0.000492	0.000316
C(33)	-0.058	-0.008	11.96	11.93	0.000268	0.000182
H(2)	0.097	0.029	6.68	7.27	0.000001	0.000036
H(3)	0.104	0.022	6.40	7.37	0.000013	0.000015
H(4)	0.081	0.019	6.46	7.34	-0.000002	0.000040
H(5)	0.082	0.015	6.51	7.39	0.000010	0.000037
H(6)	0.120	0.019	6.33	7.40	0.000011	0.000017
H(7)	0.128	0.019	5.90	6.83	-0.000012	0.000004
H(13)	0.113	0.040	6.37	7.28	-0.000005	0.000053
H(14)	0.098	0.022	6.41	7.40	-0.000001	0.000058
H(15)	0.124	0.017	6.50	7.42	-0.000002	0.000037
H(16)	0.169	0.013	6.24	7.47	0.000007	0.000020
H(17)	0.097	0.016	6.53	7.46	0.000002	0.000034
H(18)	0.131	0.032	6.12	6.88	-0.000111	0.000068
H(23)	0.147	0.067	5.80	6.46	-0.000028	0.000019
H(24)	0.087	0.018	6.43	7.40	-0.000027	0.000026
H(25)	0.104	0.017	6.45	7.41	0.000044	0.000016
H(26)	0.192	0.018	6.11	7.40	0.000006	0.000017
H(27)	0.136	0.039	5.99	6.63	-0.000132	0.000080
H(29)	0.123	0.049	5.38	5.91	0.000270	0.000132
H(30)	0.078	0.020	6.63	7.60	0.000005	0.000036
H(31)	0.091	0.017	6.40	7.41	0.000004	0.000017
H(32)	0.134	0.019	6.15	7.39	0.000005	0.000018
H(33)	0.129	0.016	6.19	7.11	0.000047	0.000031
H(1)	0.661	0.569	2.75	3.24	0.000124	0.000133
sum	0.020	0.000	540.24	566.17	0.022144	0.000224

Table S8. Stockholder integrated atomic charges

Atom	q_{exp}
O(1)	-0.228
N(1)	-0.146
C(1)	-0.030
C(2)	-0.029
C(3)	-0.036
C(4)	-0.075
C(5)	-0.061
C(6)	-0.056
C(7)	-0.094
C(8)	-0.024
C(9)	-0.074
C(10)	-0.076
C(11)	-0.065
C(12)	0.022
C(13)	-0.041
C(14)	-0.075
C(15)	-0.042
C(16)	-0.012
C(17)	-0.027
C(18)	-0.011
C(19)	-0.009
C(20)	-0.032
C(21)	0.074
C(22)	-0.050
C(23)	-0.044
C(24)	-0.027
C(25)	-0.075
C(26)	-0.070
C(27)	-0.062
C(28)	-0.028
C(29)	-0.042
C(30)	-0.060
C(31)	-0.061
C(32)	-0.061
C(33)	-0.069
H(2)	0.055
H(3)	0.072
H(4)	0.063
H(5)	0.060
H(6)	0.083
H(7)	0.070
H(13)	0.074
H(14)	0.064
H(15)	0.066
H(16)	0.095
H(17)	0.069
H(18)	0.083
H(23)	0.081
H(24)	0.090
H(25)	0.069
H(26)	0.089
H(27)	0.051
H(29)	0.062
H(30)	0.074
H(31)	0.074
H(32)	0.090
H(33)	0.072
H(1)	0.186

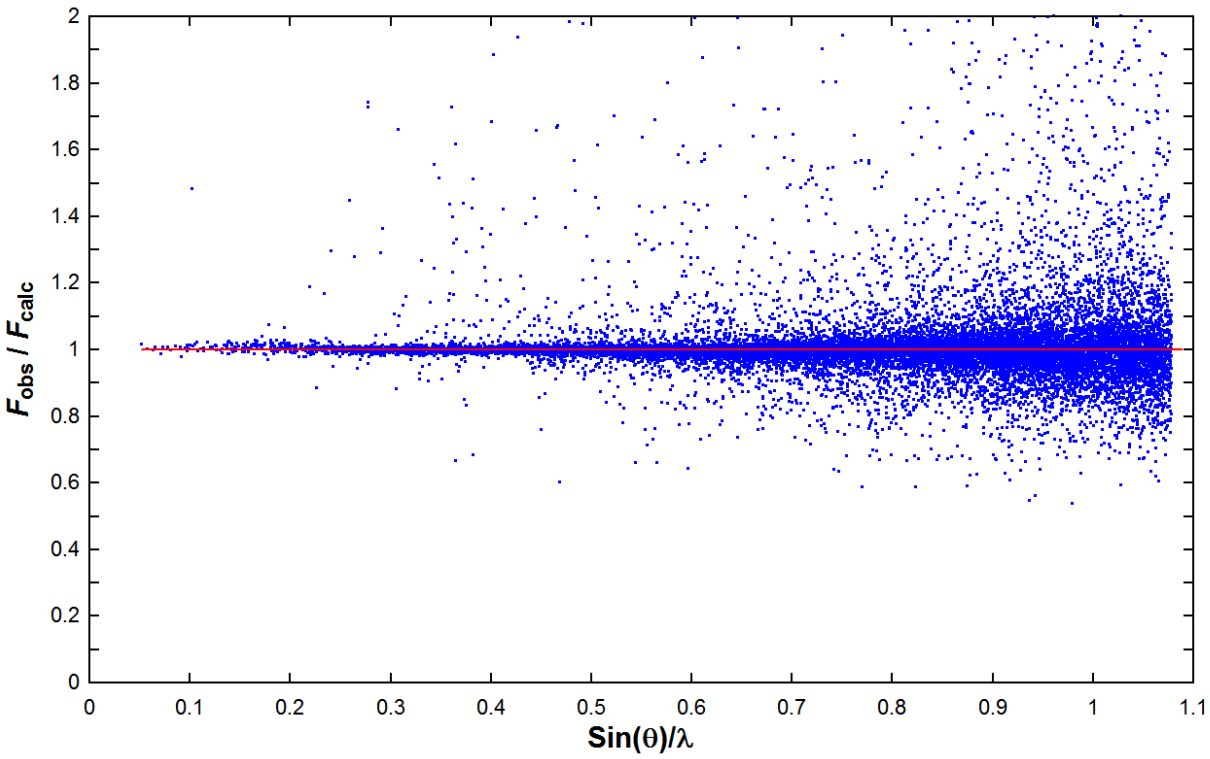


Figure S1. Scatterplot of individual scale factors against resolution, from the multipole refinement.

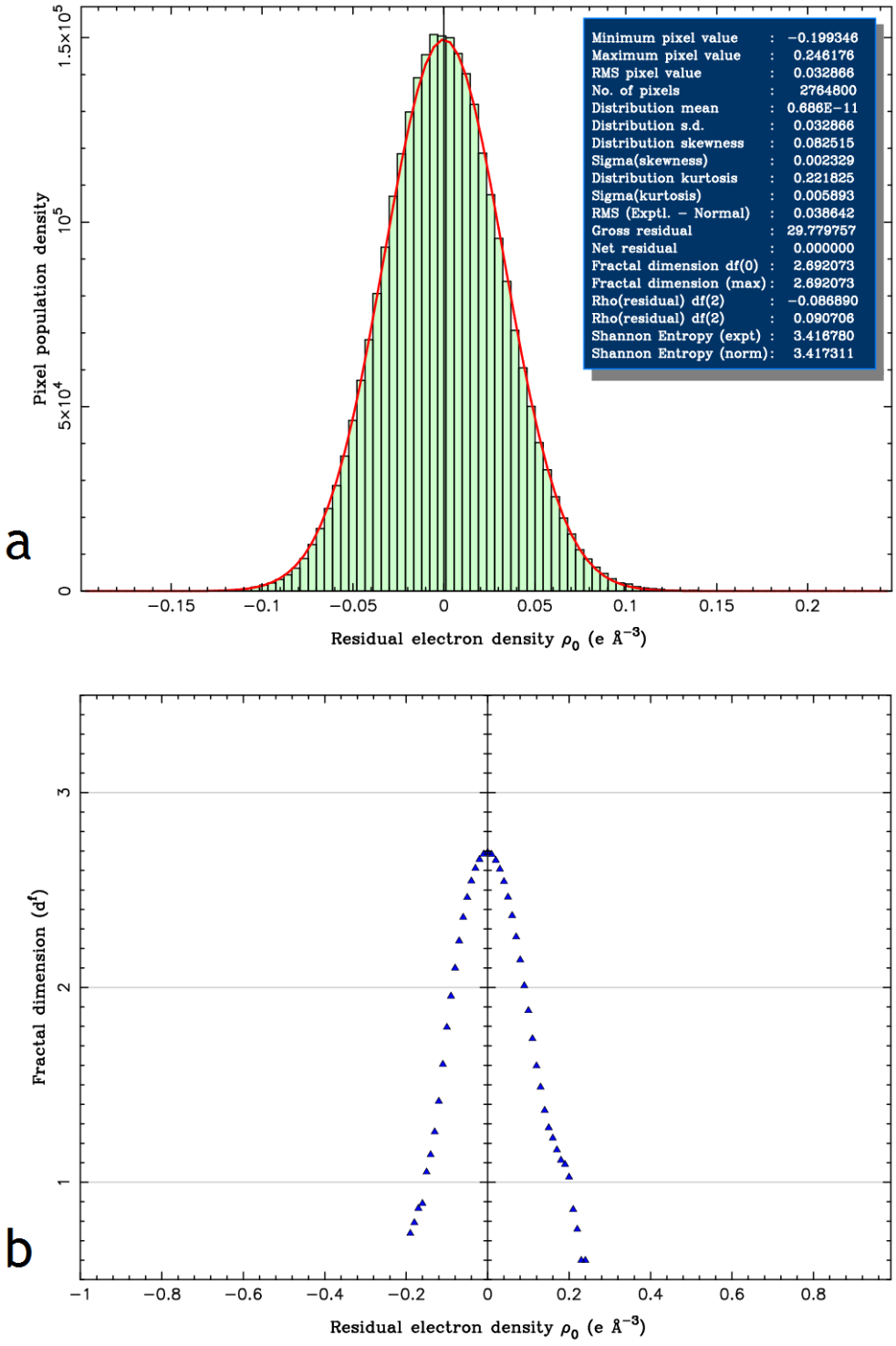


Figure S2. Residual density plots (a) histogram of residual density pixel population density (b) fractal dimension plot.

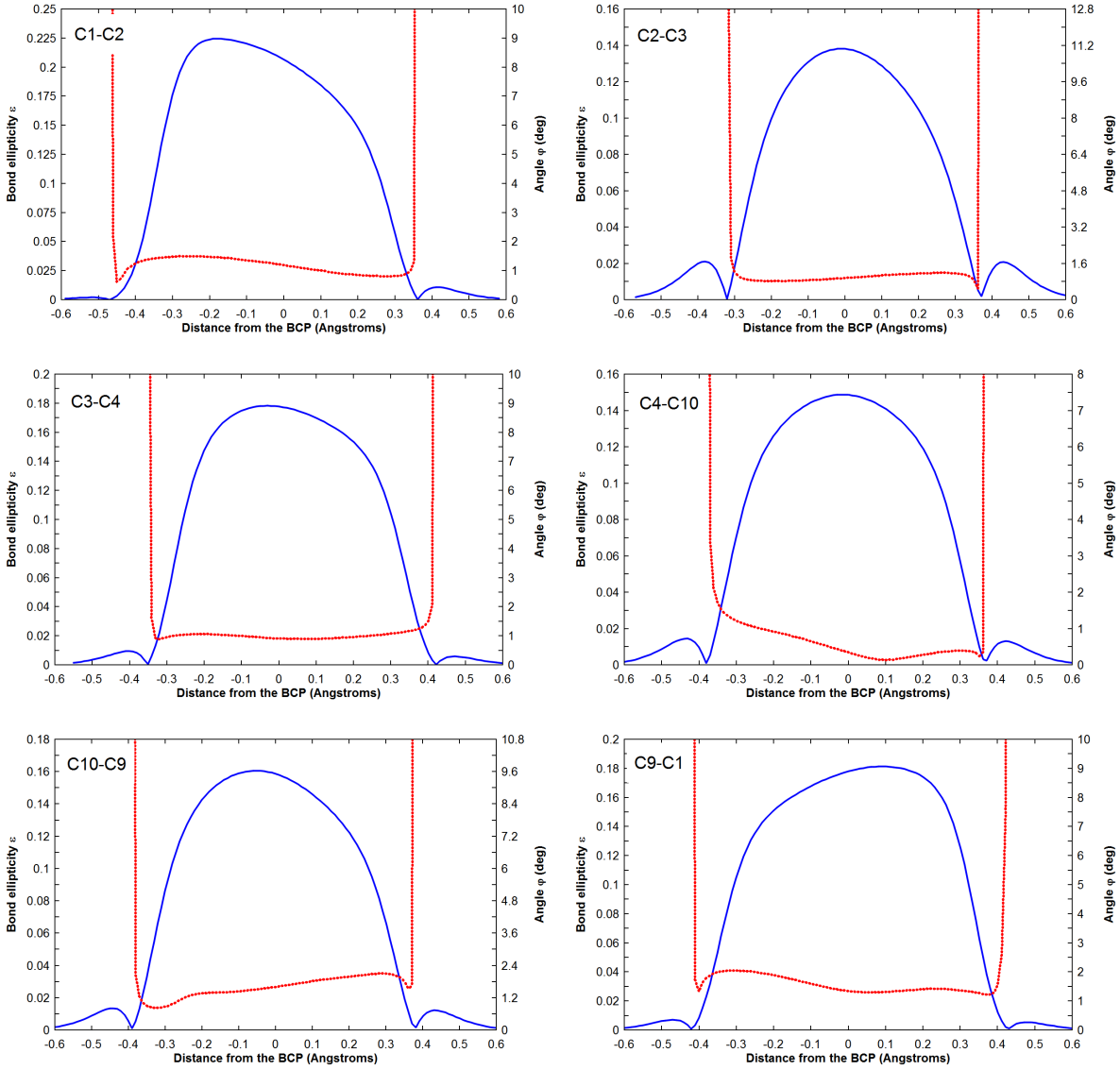


Figure S3. Plots of the experimental ellipticity ε along the bond path (solid blue line) with the φ_{ref} angle (dotted red line) for naphthalene ring C(1)-C(10). The reference vector is normal to the plane of the ring.

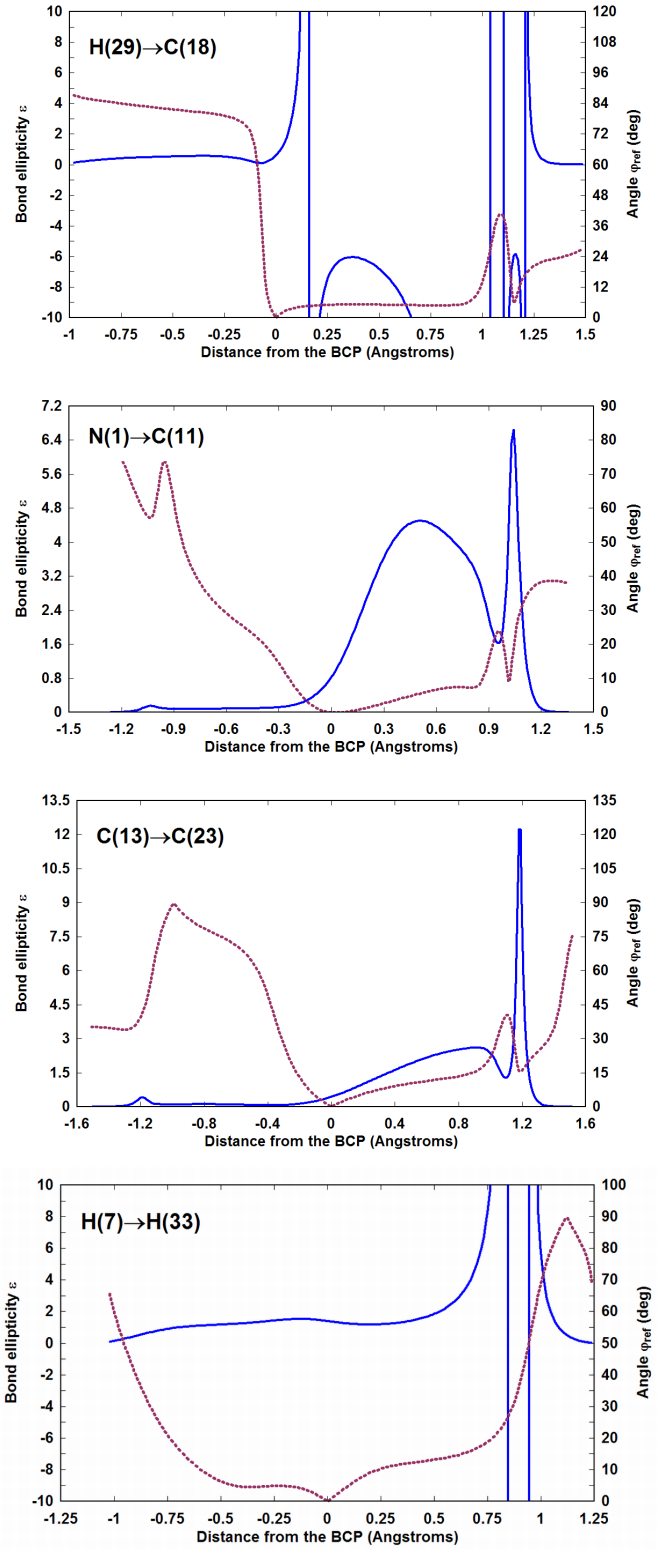


Figure S4. Plots of the experimental ellipticity ε along the bond path (solid blue line) with the φ_{ref} angle (dotted violet line) for the weak intra-molecular interactions. The reference vector is the major axis of ellipticity at the bcp.

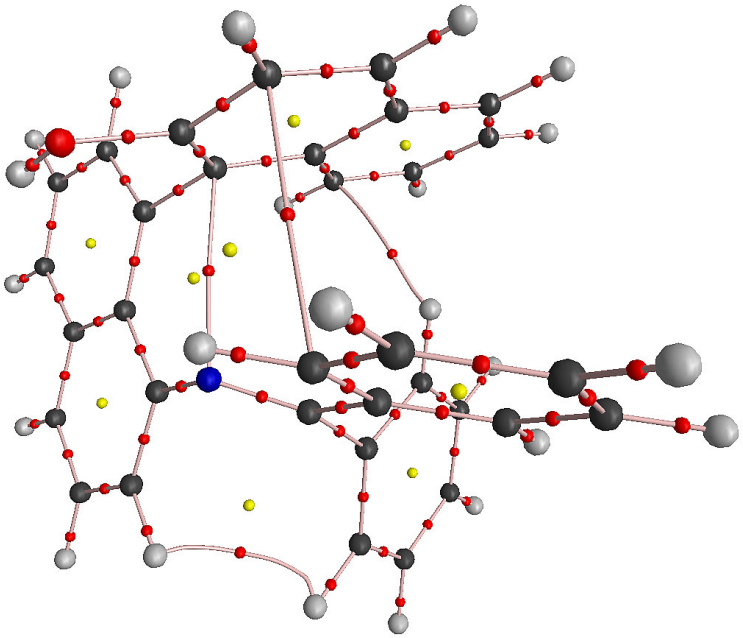


Figure S5. The virial graph of compound **1**.

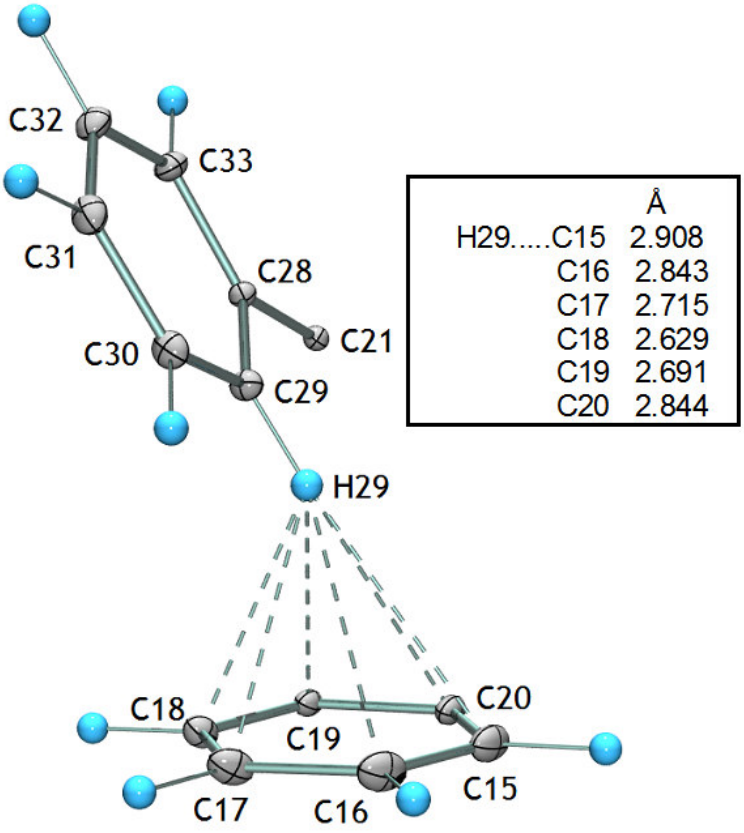
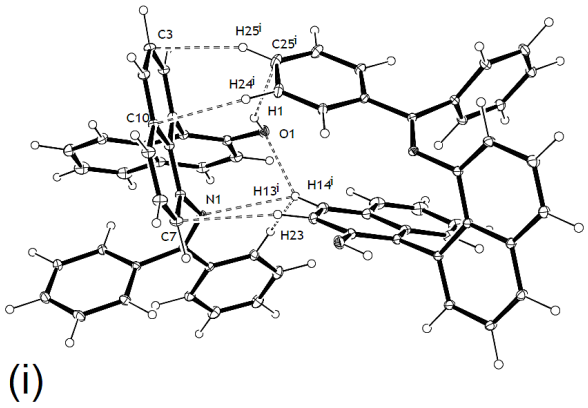
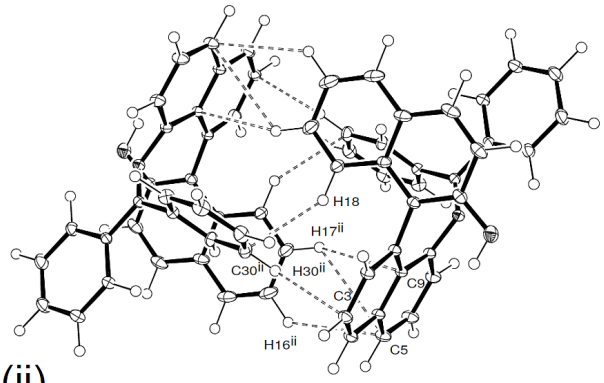


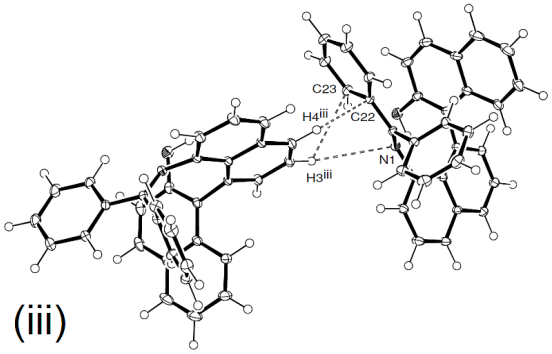
Figure S6. Geometric details of the intramolecular CH…C(π) interaction in compound **1**.



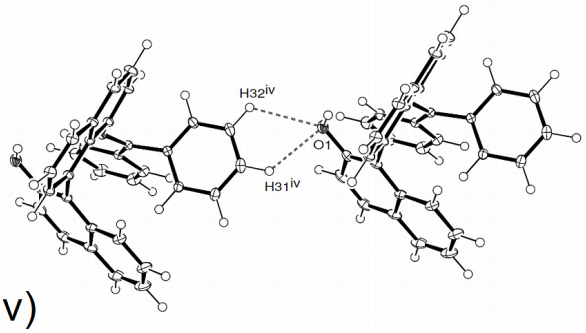
(i)



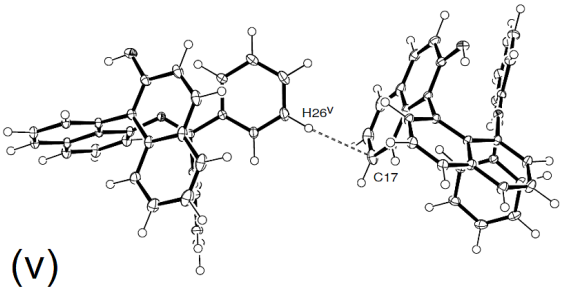
(ii)



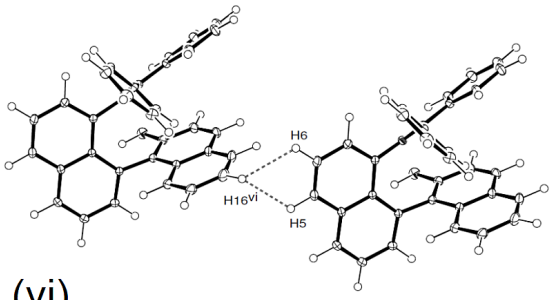
(iii)



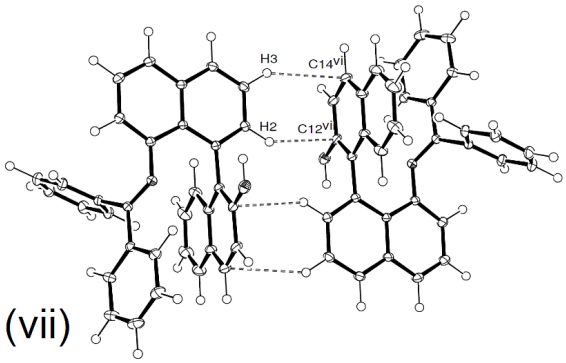
(iv)



(v)



(vi)



(vii)

Figure S7. Interactions between the seven unique dimers in the crystal structure of **1**.

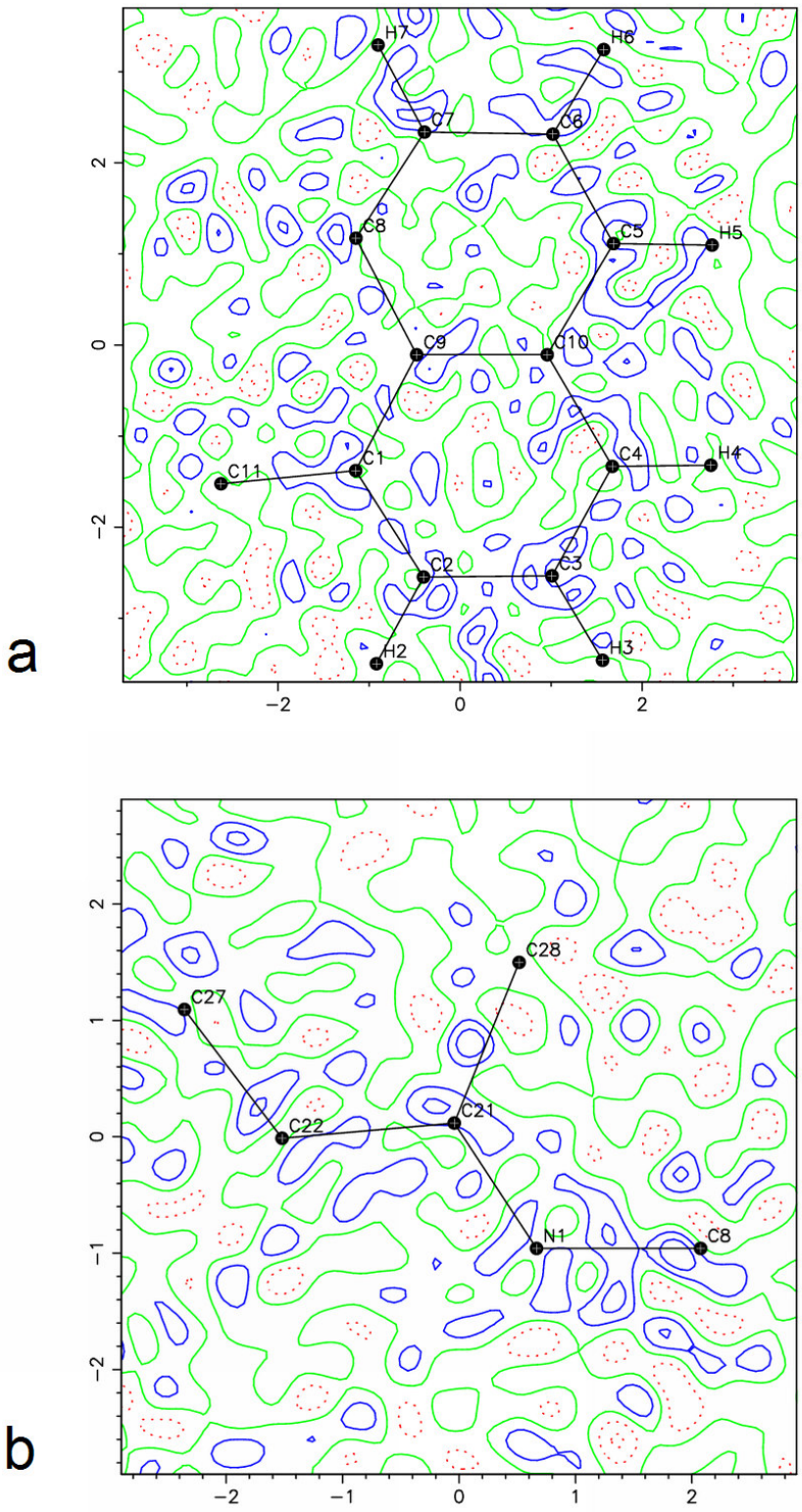


Figure S8. Difference Fourier map of **1**, (a) in the plane of naphthalene ring C1-C10 and (b) in the imine plane. Contours are drawn at 0.05 eÅ^{-3}, positive contours solid blue, negative contours in broken red, zero contour in green.

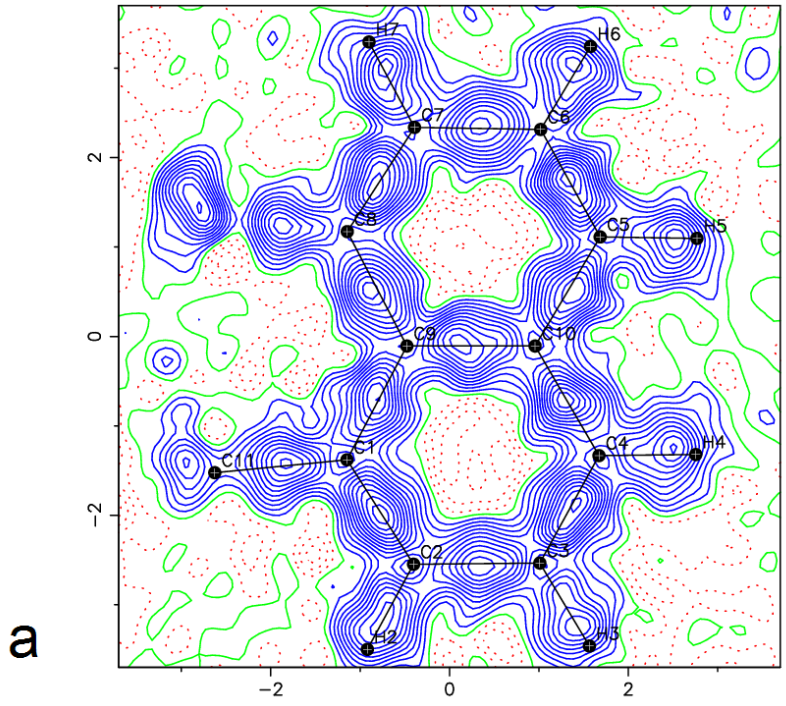


Figure S9. Experimental deformation map of **1**, (a) in the plane of naphthalene ring C1-C10 and (b) in the imine plane. Contours are drawn at 0.05 eÅ^{-3}, positive contours solid blue, negative contours in broken red, zero contour in green.

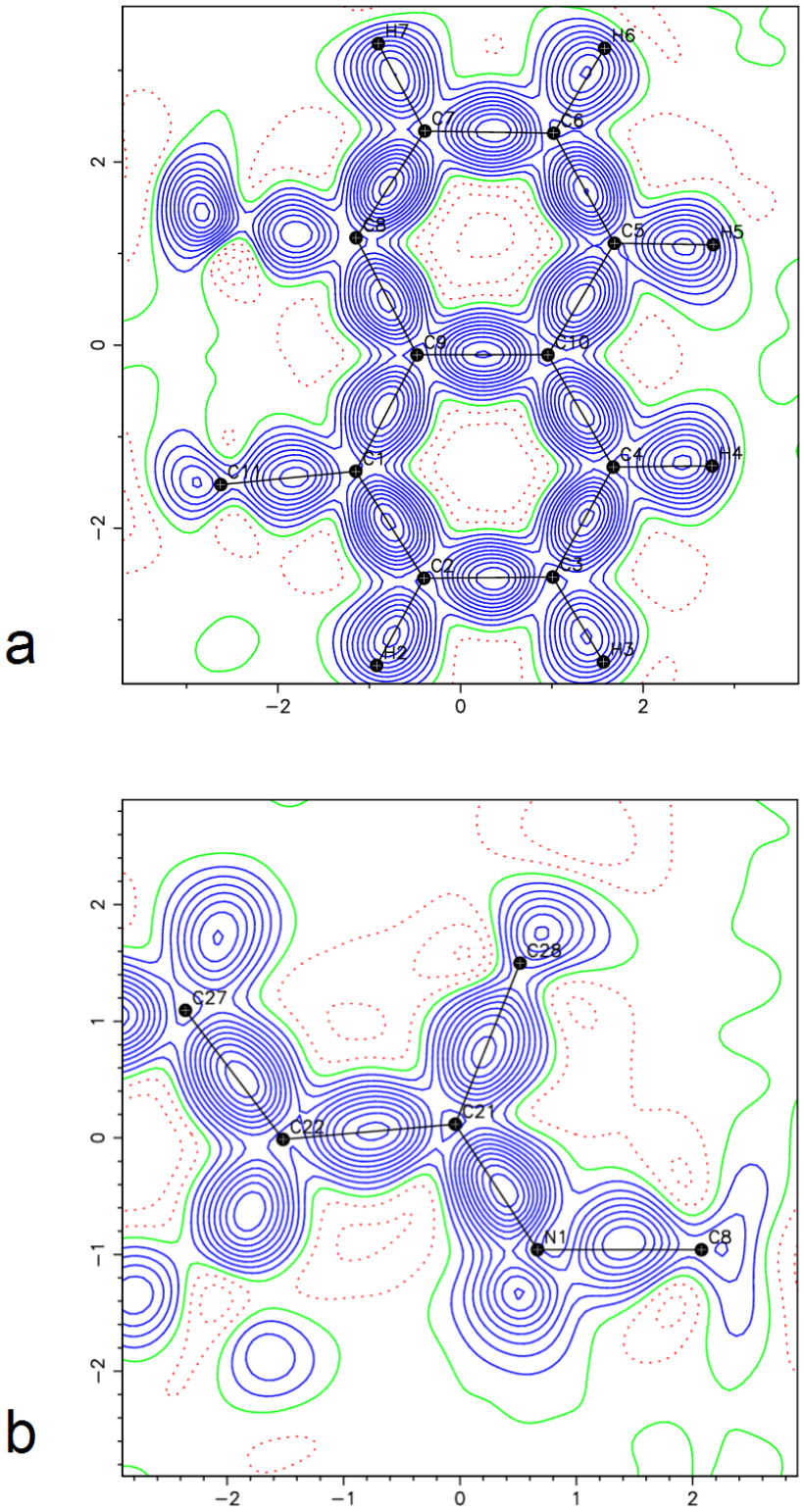


Figure S10. Dynamic model map of **1**, (a) in the plane of naphthalene ring C1-C10 and (b) in the imine plane. Contours are drawn at 0.05 eÅ^{-3}, positive contours solid blue, negative contours in broken red, zero contour in green.

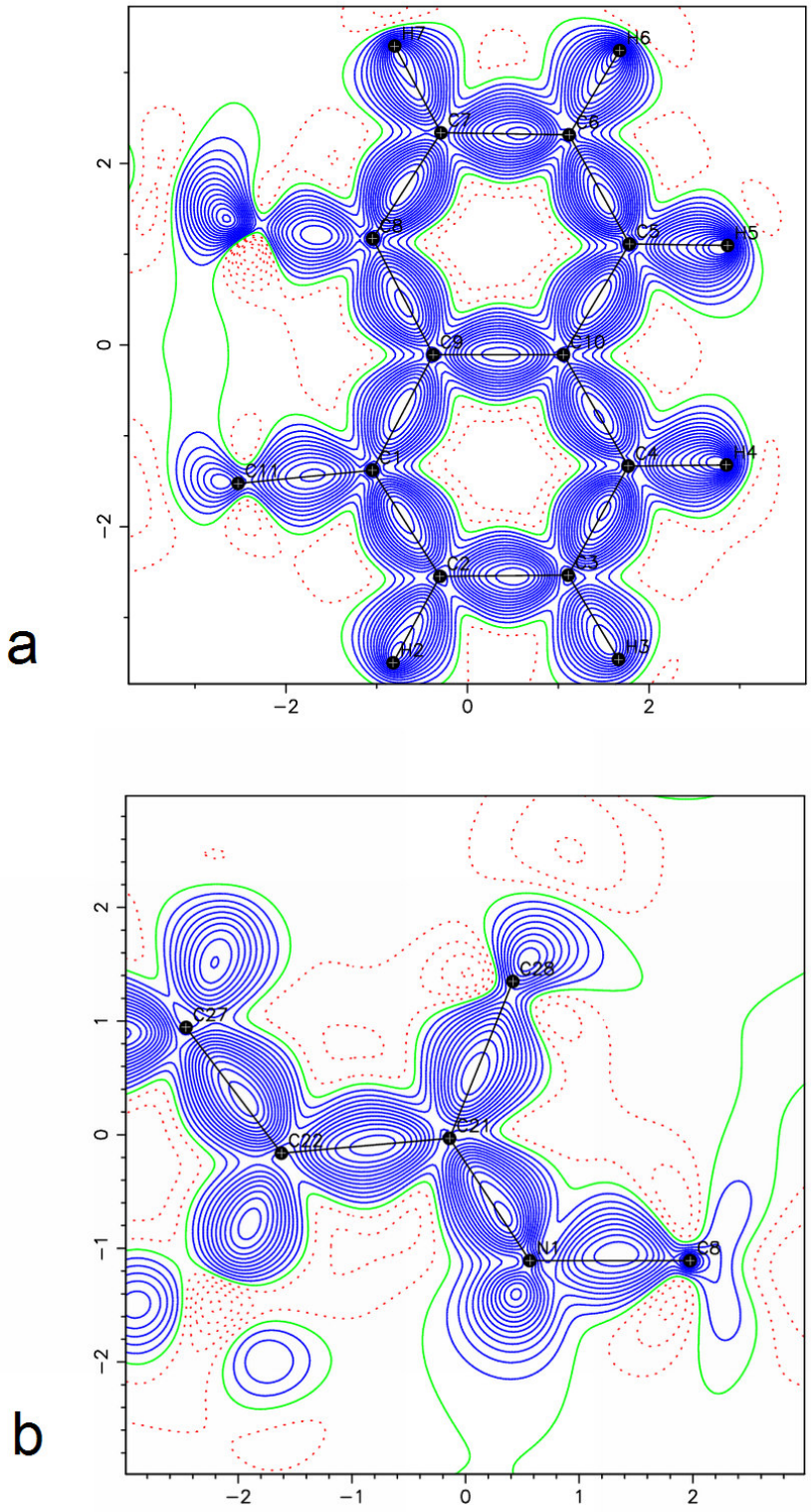


Figure S11. Deformation density map of **1**, (a) in the plane of naphthalene ring C1-C10 and (b) in the imine plane. Contours are drawn at 0.05 eÅ^{-3}, positive contours solid blue, negative contours in broken red, zero contour in green.

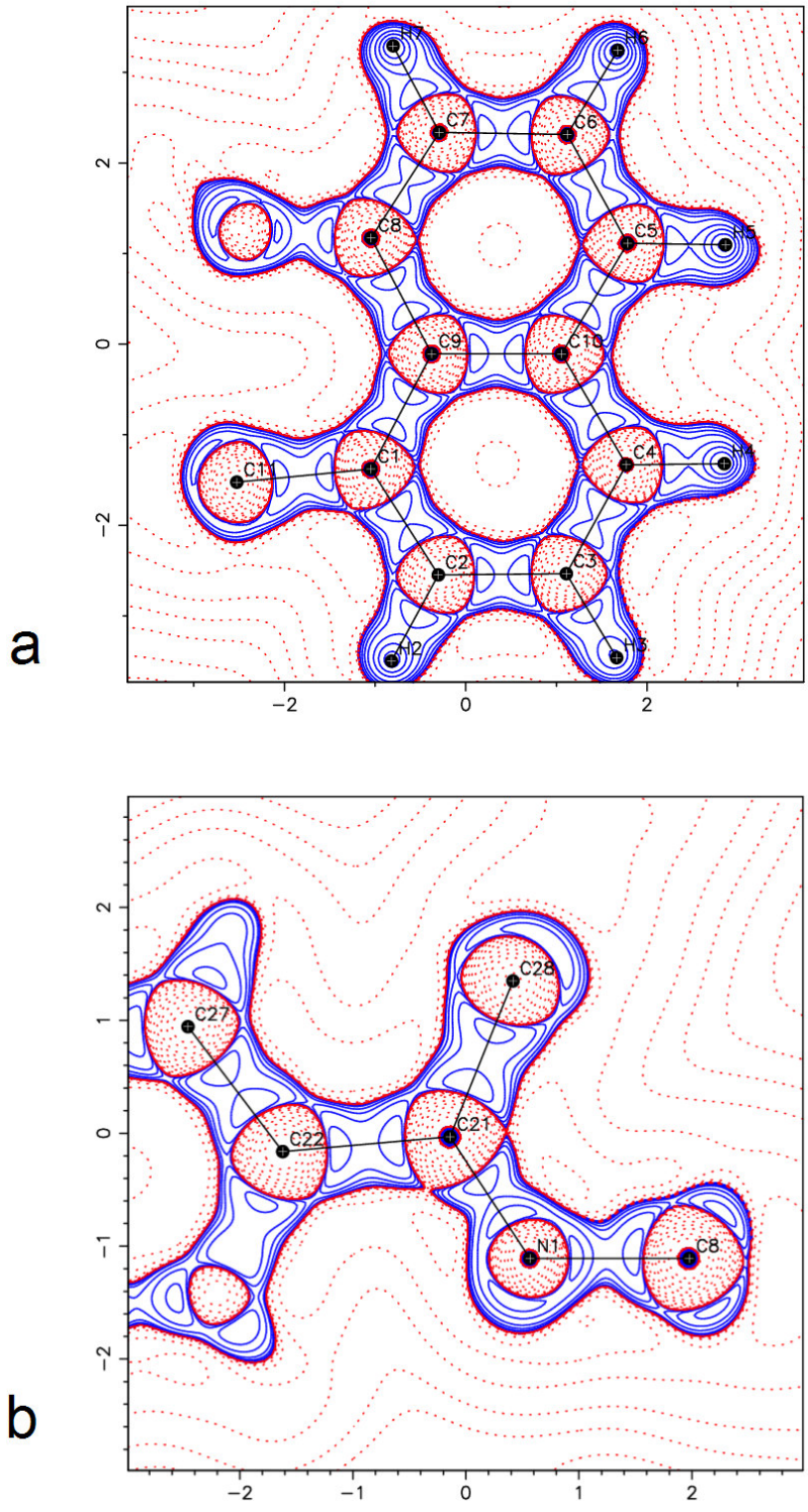


Figure S12. Negative Laplacian map of **1**, (a) in the plane of naphthalene ring C1-C10 and (b) in the imine plane. Contours are drawn at $\pm 2 \times 10^n$, $\pm 4 \times 10^n$ and $\pm 8 \times 10^n$ ($n = -3, -2, -1, 0, +1$ eÅ^{-5}): positive contours solid blue, negative contours in broken red.

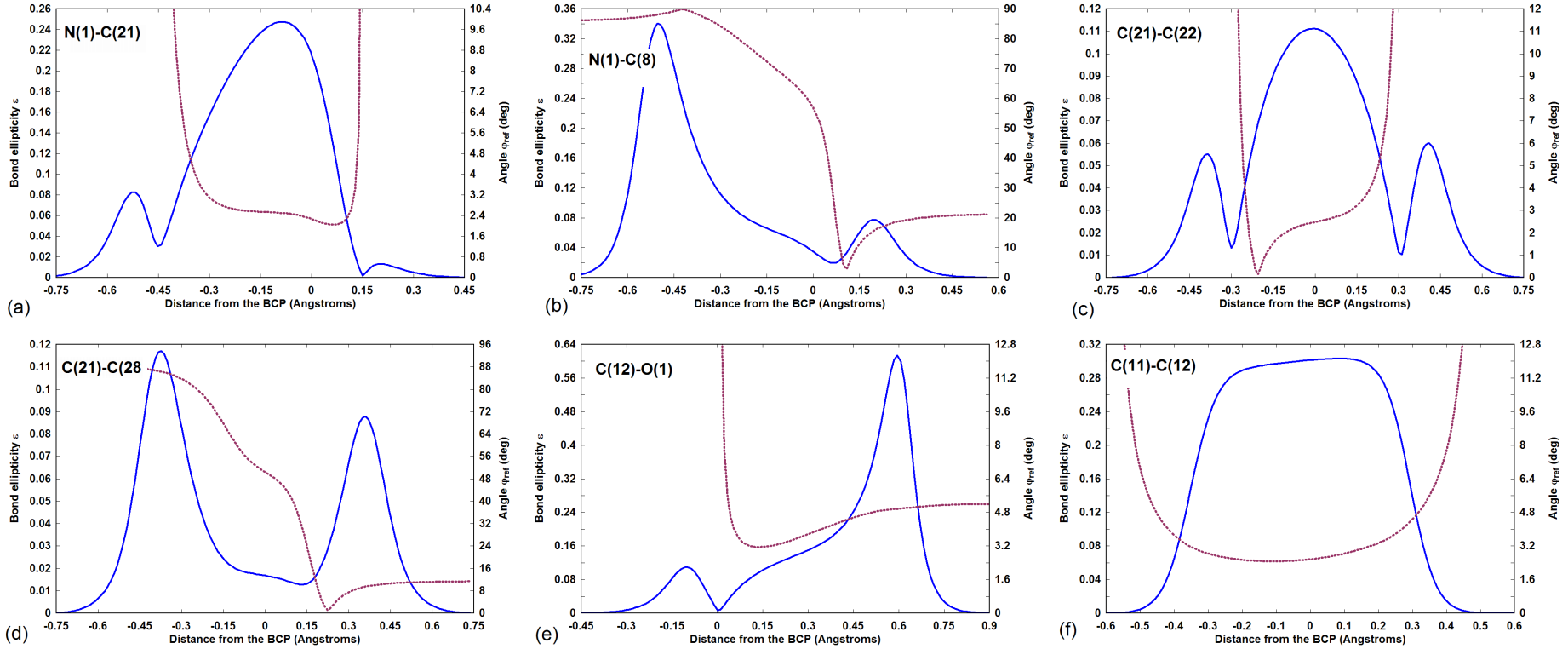


Figure S13. Plots of the theoretical (isolated molecule gas-phase DFT calculation) bond ellipticities ε along the bond path (solid blue line) with the φ_{ref} angle (dotted violet line) for the same bond paths as shown in Figure 4. For plots (a)-(d) the reference vector (see Text) is normal to the C(8)-N(1)-C(21)-C(22)-C(28) mean plane, while for (e) and (f) it is normal to the C_6 ring containing C(11) and C(12).