Deposition

Table 10
Summary of topological data at the bond critical points (BCP, located at $\mathbf{r}_b$ where $\nabla\rho(\mathbf{r}_b) = 0$). The quantities given are ($\rho(\mathbf{r}_b)$ and $\nabla^2\rho(\mathbf{r}_b)$) and the ellipticity ϵ (defined by $\epsilon = \frac{\lambda_1}{\lambda_2} - 1$, with λ_1, λ_2 being the two principal curvatures of $\rho(\mathbf{r})$ at a BCP), a measure for the charge asphericity. First row experimental results after multipole refinement, second an third subsequent rows: single point *ab initio* calculations at the experimental geometry, fourth and fifth row: single point ab initio calculations after geometry optimization at the HF/6-311+G(d,p) level. Bond length are experimental (first row) and optimized theoretically (second row).

bond/bond length [Å]	$\rho\,[e\text{Å}^{-3}]$	$\nabla^2\rho\,[e\text{Å}^{-5}]$	ellipticity	method
C(1)–C(2)	1.60(2)	-10.66(8)	0.10	multipole
1.5612(7)	1.59	-13.2	0.02	HF/6-311+G(d,p)(exp. geo.)
1.5386	1.52	-10.4	0.02	B3LYP/6-311+G(d,p)(exp. geo.)
	1.67	-14.8	0.02	HF/6-311+G(d,p)(opt. geo.)
	1.54	-11.8	0.02	B3LYP/6-311+G(d,p)(opt. geo.)
C(1)–C(4)	1.53(3)	-9.69(9)	0.15	multipole
1.5548(7)	1.62	-13.9	0.02	HF/6-311+G(d,p)(exp. geo.)
1.5472	1.55	-10.9	0.02	B3LYP/6-311+G(d,p)(exp. geo.)
	1.63	-14.0	0.02	HF/6-311+G(d,p)(opt. geo.)
	1.56	-11.0	0.02	B3LYP/6-311+G(d,p)(opt. geo.)
C(1)–C(5)	1.59(3)	-11.39(8)	0.09	multipole
1.5553(6)	1.60	-13.5	0.03	HF/6-311+G(d,p)(exp. geo.)
1.5510	1.53	-10.6	0.02	B3LYP/6-311+G(d,p)(exp. geo.)
	1.61	-13.6	0.03	HF/6-311+G(d,p)(opt. geo.)
	1.54	-10.7	0.03	B3LYP/6-311+G(d,p)(opt. geo.)
C(3)–C(2)	1.65(2)	-13.07(7)	0.15	multipole
1.5613(6)	1.63	-14.0	0.02	HF/6-311+G(d,p)(exp. geo.)
1.5476	1.54	-10.9	0.02	B3LYP/6-311+G(d,p)(exp. geo.)
	1.67	-14.7	0.02	HF/6-311+G(d,p)(opt. geo.)
	1.59	-11.5	0.01	B3LYP/6-311+G(d,p)(opt. geo.)
C(3)–C(4)	1.63(3)	-12.63(9)	0.08	multipole
1.5493(7)	1.66	-14.6	0.00	HF/6-311+G(d,p)(exp. geo.)
1.5409	1.58	-11.5	0.00	B3LYP/6-311+G(d,p)(exp. geo.)
	1.69	-15.1	0.01	HF/6-311+G(d,p)(opt. geo.)
	1.60	-11.9	0.00	B3LYP/6-311+G(d,p)(opt. geo.)
C(3)–C(5)	1.67(3)	-13.07(7)	0.10	multipole
1.5554(7)	1.65	-14.3	0.02	HF/6-311+G(d,p)(exp. geo.)
1.5475	1.56	-11.2	0.02	B3LYP/6-311+G(d,p)(exp. geo.)
	1.67	-14.7	0.02	HF/6-311+G(d,p)(opt. geo.)
	1.59	-11.5	0.01	B3LYP/6-311+G(d,p)(opt. geo.)
C(1)–C(11)	1.94(3)	-21.4(10)	0.03	multipole
1.4949(6)	1.88	-20.6	0.07	HF/6-311+G(d,p)(exp. geo.)
1.4913	1.79	-16.2	0.07	B3LYP/6-311+G(d,p)(exp. geo.)
	1.90	-20.8	0.07	HF/6-311+G(d,p)(opt. geo.)
	1.80	-16.5	0.07	B3LYP/6-311+G(d,p)(opt. geo.)
C(11)–O(1)	2.49(4)	-32.5(3)	0.23	multipole
1.3257(8)	2.10	-2.2	0.14	HF/6-311+G(d,p)(exp. geo.)
1.3295	2.10	-9.0	0.03	B3LYP/6-311+G(d,p)(exp. geo.)
	2.08	-2.2	0.14	HF/6-311+G(d,p)(opt. geo.)
	2.09	-9.3	0.03	B3LYP/6-311+G(d,p)(opt. geo.)
C(11)–O(2)	3.09(5)	-36.1(4)	0.10	multipole
1.2274(7)	2.75	-5.8	0.07	HF/6-311+G(d,p)(exp. geo.)

bond/bond length [Å]	$\rho\,[e\text{Å}^{-3}]$	$\nabla^2\rho\,[e\text{Å}^{-5}]$	ellipticity	method
1.1826	2.72	-9.9	0.09	B3LYP/6-311+G(d,p)(exp. geo.)
	2.99	+3.5	0.08	HF/6-311+G(d,p)(opt. geo.)
	2.98	-1.9	0.08	B3LYP/6-311+G(d,p)(opt. geo.)
N(1)–C(3)	1.99(4)	-27.3(2)	0.09	multipole
1.4331(6)	1.83	-15.1	0.03	HF/6-311+G(d,p)(exp. geo.)
1.4219	1.83	-17.8	0.06	B3LYP/6-311+G(d,p)(exp. geo.)
	1.87	-15.2	0.04	HF/6-311+G(d,p)(opt. geo.)
	1.87	-18.5	0.06	B3LYP/6-311+G(d,p)(opt. geo.)
N(1)–C(6)	2.52(4)	-26.7(2)	0.26	multipole
1.3579(6)	2.26	-26.0	0.11	HF/6-311+G(d,p)(exp. geo.)
1.3577	2.21	-24.4	0.19	B3LYP/6-311+G(d,p)(exp. geo.)
	2.25	-25.1	0.10	HF/6-311+G(d,p)(opt. geo.)
	2.21	-24.1	0.19	B3LYP/6-311+G(d,p)(opt. geo.)
C(6)–O(3)	2.60(4)	-33.4(2)	0.02	multipole
1.3294(6)	2.13	-7.4	0.05	HF/6-311+G(d,p)(exp. geo.)
1.3180	2.12	-12.4	0.05	B3LYP/6-311+G(d,p)(exp. geo.)
	2.16	-5.1	0.05	HF/6-311+G(d,p)(opt. geo.)
	2.16	-10.8	0.04	B3LYP/6-311+G(d,p)(opt. geo.)
C(6)–O(4)	3.11(5)	-42.0(3)	0.05	multipole
1.2406(7)	2.72	-12.5	0.07	HF/6-311+G(d,p)(exp. geo.)
1.1922	2.68	-14.7	0.11	B3LYP/6-311+G(d,p)(exp. geo.)
	2.97	-3.1	0.08	HF/6-311+G(d,p)(opt. geo.)
	2.94	-6.8	0.10	B3LYP/6-311+G(d,p)(opt. geo.)
O(3)–C(7)	1.81(4)	-19.4(2)	0.01	multipole
1.4845(7)	1.36	+1.5	0.05	HF/6-311+G(d,p)(exp. geo.)
1.4528	1.43	-7.2	0.01	B3LYP/6-311+G(d,p)(exp. geo.)
	1.45	+3.4	0.02	HF/6-311+G(d,p)(opt. geo.)
	1.52	-6.8	0.00	B3LYP/6-311+G(d,p)(opt. geo.)
C(7)–C(8)	1.89(2)	-20.02(6)	0.08	multipole
1.5215(7)	1.79	-18.0	0.04	HF/6-311+G(d,p)(exp. geo.)
1.5252	1.70	-14.5	0.03	B3LYP/6-311+G(d,p)(exp. geo.)
	1.78	-17.8	0.04	HF/6-311+G(d,p)(opt. geo.)
	1.69	-14.3	0.04	B3LYP/6-311+G(d,p)(opt. geo.)
C(7)–C(9)	1.86(2)	-18.87(7)	0.07	multipole
1.5220(7)	1.78	-17.7	0.03	HF/6-311+G(d,p)(exp. geo.)
1.5269	1.69	-14.2	0.03	B3LYP/6-311+G(d,p)(exp. geo.)
	1.76	-17.4	0.03	HF/6-311+G(d,p)(opt. geo.)
	1.67	-13.9	0.03	B3LYP/6-311+G(d,p)(opt. geo.)
C(7)–C(10)	1.86(2)	-18.85(7)	0.07	multipole
1.5242(8)	1.77	-17.6	0.03	HF/6-311+G(d,p)(exp. geo.)
1.5269	1.68	-14.0	0.03	B3LYP/6-311+G(d,p)(exp. geo.)
	1.76	-17.4	0.03	HF/6-311+G(d,p)(opt. geo.)
	1.67	-13.9	0.03	B3LYP/6-311+G(d,p)(opt. geo.)
C(1)–C(3)	0.68(2)	11.09(6)	–	multipole
1.8680(6)	0.66	11.85	–	HF/6-311+G(d,p)(exp. geo.)
1.8538	0.67	11.09	–	B3LYP/6-311+G(d,p)(exp. geo.)
	0.68	12.21	–	HF/6-311+G(d,p)(opt. geo.)
	0.69	11.42	–	B3LYP/6-311+G(d,p)(opt. geo.)