

Fractional coordinates and Uiso

atom	coordinates			Uiso
	x	y	z	
O(1)	0.1172(1)	0.8311(1)	0.1242(1)	0.029
C(1)	0.1484(1)	0.9387(1)	0.2960(1)	0.028
C(2)	-0.1343(1)	0.8647(1)	0.2182(1)	0.032
H(1)	0.2850	0.8921	0.4375	0.043
H(2)	0.1788	1.0647	0.2602	0.043
H(3)	-0.3112	0.9321	0.1217	0.047
H(4)	-0.2027	0.7636	0.3044	0.047

Uij values

atom	U11	U22	U33	U12	U13	U23
O(1)	0.0342(2)	0.02514(17)	0.0292(2)	0.0030(2)	0.00966(19)	-0.00383(17)
C(1)	0.0318(2)	0.02463(14)	0.02690(16)	-0.00004(14)	0.00516(14)	-0.00206(14)
C(2)	0.0300(2)	0.03357(17)	0.03388(19)	-0.00343(15)	0.01159(16)	0.00051(16)
H(1)	0.0453	0.046178	0.035411	0.002546	0.00423	0.005772
H(2)	0.051247	0.030759	0.047823	0.001095	0.013786	-0.000034
H(3)	0.044875	0.049165	0.046149	0.001802	0.008638	0.004251
H(4)	0.052954	0.042944	0.048024	0.003232	0.019566	-0.00758

Bond distances in Å

O(1) - C(1)	1.4334(7)
O(1) - C(2)	1.4417(6)
C(1) - C(2)	1.4568(8)
C(1) - H(1)	1.0990
C(1) - H(2)	1.0989
C(2) - H(3)	1.0988
C(2) - H(4)	1.0990

Bond angles in °

C(1) - O(1) - C(2)	60.89(4)
O(1) - C(1) - C(2)	59.84(3)
O(1) - C(1) - H(1)	113.82(4)
O(1) - C(1) - H(2)	115.94(4)
C(2) - C(1) - H(1)	119.32(3)
C(2) - C(1) - H(2)	118.54(4)
H(1) - C(1) - H(2)	116.59(4)
O(1) - C(2) - C(1)	59.27(3)
O(1) - C(2) - H(3)	115.45(4)
O(1) - C(2) - H(4)	113.60(4)
C(1) - C(2) - H(3)	120.84(4)
C(1) - C(2) - H(4)	118.23(4)
H(3) - C(2) - H(4)	116.22(4)

Torsion angles in degrees

C(2) - O(1) - C(1) - H(1)	111.3(1)
C(2) - O(1) - C(1) - H(2)	-109.4(1)
C(1) - O(1) - C(2) - H(3)	112.2(1)
C(1) - O(1) - C(2) - H(4)	-109.9(1)
O(1) - C(1) - C(2) - H(3)	-103.1(1)
O(1) - C(1) - C(2) - H(4)	102.1(1)
H(1) - C(1) - C(2) - O(1)	-102.1(1)
H(1) - C(1) - C(2) - H(3)	154.8(1)
H(1) - C(1) - C(2) - H(4)	0.0(1)
H(2) - C(1) - C(2) - O(1)	105.1(1)
H(2) - C(1) - C(2) - H(3)	1.9(1)
H(2) - C(1) - C(2) - H(4)	-152.8(1)

local atomic coordinate systems

center of coordinate system	showing to	with axis	showing to	with axis
O(1)	DUM0	Z	C(1)	Y
C(1)	C(2)	X	O(1)	Y
C(2)	C(1)	X	O(1)	Y
H(1)	C(1)	Z	H(2)	Y
H(2)	C(1)	Z	H(1)	Y
H(3)	C(2)	Z	H(4)	Y
H(4)	C(2)	Z	H(3)	Y

Kappa parameters

atom group	kappa	kappa prime
O	0.994915	0.959128
C	1.014054	1.024548
H	1.130000	1.290000

Multipole population coefficients

atom	P_v	P_{00}	P_{11}	P_{1-1}	P_{10}				
O(1)	6.28(2)	0.00(0)	0.01(1)	-0.06(1)	-0.03(1)				
C(1) and C(2)	3.99(2)	0.00(0)	-0.02(1)	-0.02(1)	0.00(0)				
H(1)	0.92(1)	0.00(0)	0.00(0)	0.00(0)	0.13(1)				
H(2)	0.97(1)	0.00(0)	0.00(0)	0.00(0)	0.15(1)				
H(3)	0.90(1)	0.00(0)	0.00(0)	0.00(0)	0.13(1)				
H(4)	0.93(1)	0.00(0)	0.00(0)	0.00(0)	0.16(1)				
atom	P_{20}	P_{21}	P_{2-1}	P_{22}	P_{2-2}				
O(1)	-0.12(1)	-0.04(1)	0.01(1)	0.08(1)	0.04(1)				
C(1) and C(2)	0.06(1)	0.00(0)	0.00(0)	0.13(1)	0.01(1)				
atom	P_{30}	P_{31}	P_{3-1}	P_{32}	P_{3-2}	P_{33}	P_{3-3}		
O(1)	-0.04(1)	-0.01(1)	0.00(1)	-0.04(1)	0.02(1)	-0.01(1)	0.00(1)		
C(1) and C(2)	0.00(0)	-0.18(1)	-0.11(1)	0.00(0)	0.00(0)	-0.02(1)	-0.09(1)		
atom	P_{40}	P_{41}	P_{4-1}	P_{42}	P_{4-2}	P_{43}	P_{4-3}	P_{44}	P_{4-4}
O(1)	-0.02(1)	-0.04(1)	-0.06(1)	-0.09(1)	-0.01(1)	-0.07(1)	0.05(1)	-0.01(1)	0.00(1)
C(1) and C(2)	0.06(1)	0.00(0)	0.00(0)	0.02(1)	0.02(1)	0.00(0)	0.00(0)	-0.03(1)	-0.05(1)

Residual density maps

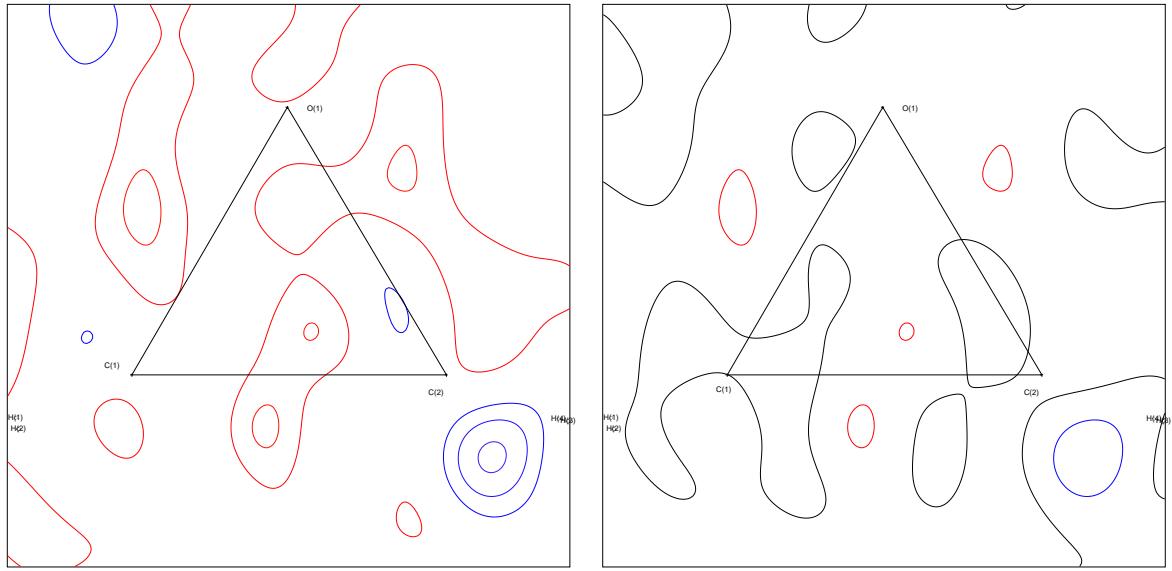


Figure S1: Residual density of full resolution in the plane of the three-membered ring; left: contour interval=0.05 $e\text{\AA}^{-3}$, red=negative, blue=positive; right: contour interval=0.1 $e\text{\AA}^{-3}$, red=negative, blue=positive, black=zero

Static deformation and Laplacian density maps

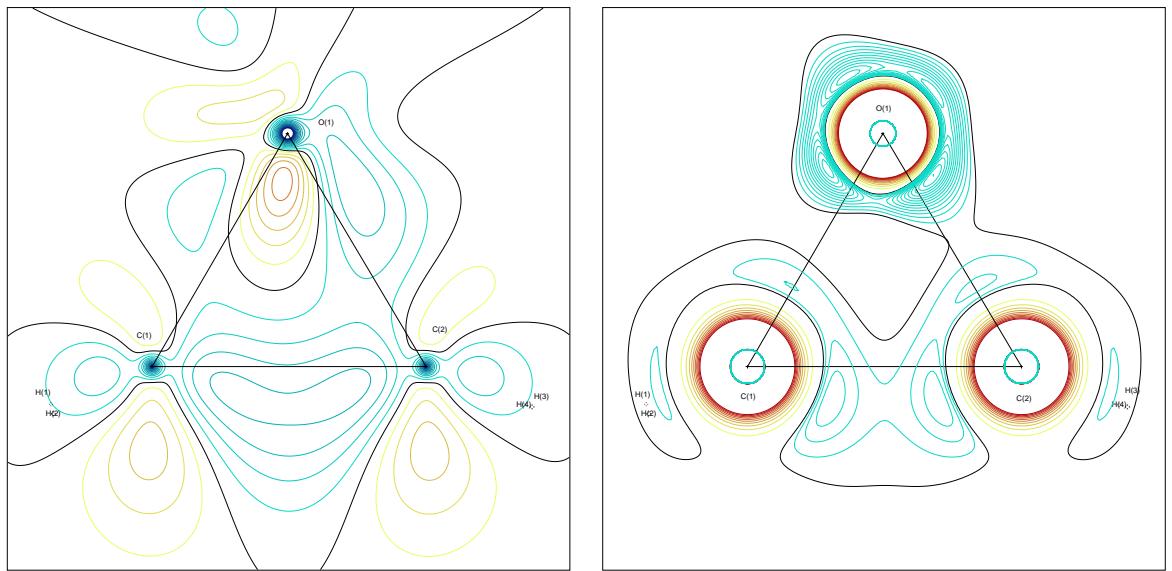


Figure S2: left: Static deformation density map in the plane of the three-membered ring with contour interval=0.1 $e\text{\AA}^{-3}$ (blue=positive, red=negative); right: Laplacian density map in the plane of the three-membered ring with contour interval=8 $e\text{\AA}^{-5}$ (blue=negative, red=positive)

Density ($e\text{\AA}^{-3}$) and Laplacian ($e\text{\AA}^{-5}$) values for all bond critical points

bond	density	Laplacian
O(1) -C(1)	1.68(2)	-2.8(1)
O(1) -C(2)	1.80(1)	-9.0(1)
C(1) -C(2)	1.72(1)	-7.6(1)
C(1) -H(1)	1.76(4)	-16.3(1)
C(1) -H(2)	1.84(4)	-17.4(1)
C(2) -H(3)	1.75(4)	-16.3(1)
C(2) -H(4)	1.82(4)	-17.7(1)

Atomic charges in e and volumes in \AA^3 for all atoms

atom	q ₀₀₁	V ₀₀₁
O(1)	-0.79	14.79
C(1)	0.18	10.33
C(2)	0.16	10.62
H(1)	0.13	6.43
H(2)	0.07	6.70
H(3)	0.15	6.70
H(4)	0.12	6.90
sum	0.01	62.47