

NHO DIRECTIONALITY AND BOND BENDING (deviations from line of nuclear centers)

[Thresholds for printing: angular deviation > 1.0 degree]
 p- or d-character > 25.0%
 orbital occupancy > 0.10e

NBO	Line of Centers		Hybrid 1			Hybrid 2		
	Theta	Phi	Theta	Phi	Dev	Theta	Phi	Dev
1. BD (1) C 1- C 2	90.0	180.0	90.0	203.5	23.5	90.0	-23.5	23.5
2. BD (1) C 1- C 3	90.0	120.0	90.0	96.5	23.5	90.0	323.5	23.5
3. BD (1) C 1- H 4	32.6	330.0	34.8	330.0	2.2	--	--	--
4. BD (1) C 1- H 7	147.4	330.0	145.2	330.0	2.2	--	--	--
5. BD (1) C 2- C 3	90.0	60.0	90.0	83.5	23.5	90.0	216.5	23.5
6. BD (1) C 2- H 6	32.6	210.0	34.8	210.0	2.2	--	--	--
7. BD (1) C 2- H 9	147.4	210.0	145.2	210.0	2.2	--	--	--
8. BD (1) C 3- H 5	32.6	90.0	34.8	90.0	2.1	--	--	--
9. BD (1) C 3- H 8	147.4	90.0	145.2	90.0	2.1	--	--	--