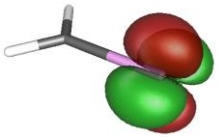
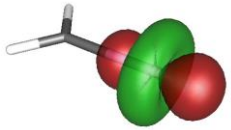
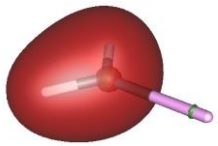
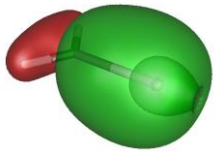
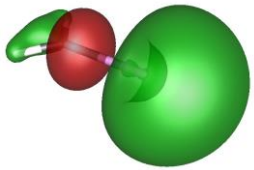
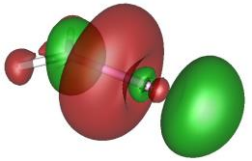
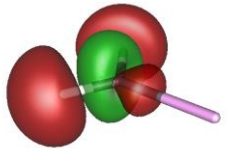
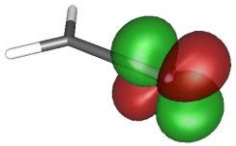
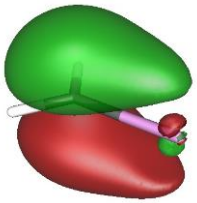
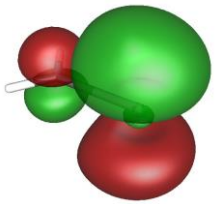
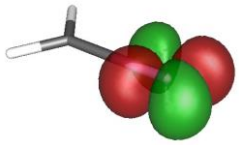
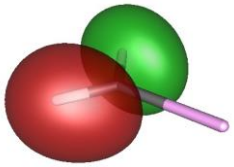
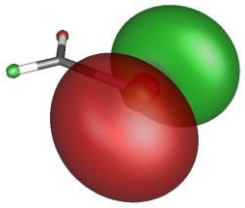
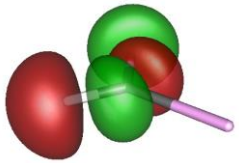
Figure SI.1 State-averaged CASSCF/aug-cc-pVTZ orbitals at the ICMRCI/aug-cc-pVTZ equilibrium geometry of the X^2B_1 state

d-orbitals		valence orbitals				
$7a_1$ -1.196532 E_h 	$8a_1$ -1.192165 E_h 	$9a_1$ -0.849439 E_h 	$10a_1$ -0.503353 E_h 	$11a_1$ -0.223780 E_h 	$12a_1$ 0.444092 E_h 	13a1 0.673044 E_h 
	$3b_1$ -1.192394 E_h 	$4b_1$ -0.168021 E_h 	$5b_1$ 0.177152 E_h 			
	$3b_2$ -1.191171 E_h 	$4b_2$ -0.544528 Eh 	$5b_2$ 0.022703 E_h 	$6b_2$ 0.686163 E_h 		
	$1a_2$ -1.196626 E_h