

All data - processed																
				Largest contribution to an MO for each atom												
				Significant secondary contribution to an MO												
C atom	MO1	MO2	MO3	MO4	MO5	MO6	MO7	MO8	MO9	MO10	MO11	MO12	MO13	MO14	MO18	
S	0.00	0.03	1.06	0.12	0.00	-0.37	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.62	0.00	
Px	0.00	0.00	0.00	0.00	0.00	0.00	0.64	0.00	0.00	0.00	0.00	1.12	0.00	0.00	0.00	
Py	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.64	0.00	0.00	0.00	0.00	1.12	0.00	0.00	
Pz	0.05	0.00	0.00	0.00	0.23	0.00	0.00	0.00	0.28	0.00	0.00	0.00	0.00	0.00	1.36	
O atom																
S	0.71	0.73	0.00	0.42	0.49	0.44	0.00	0.00	-0.30	0.00	0.00	0.00	0.00	-0.69	-0.47	
Px	0.00	0.00	0.00	0.00	0.00	0.00	0.53	0.00	0.00	0.82	0.00	-0.74	0.00	0.00	0.00	
Py	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.53	0.00	0.00	0.82	0.00	-0.74	0.00	0.00	
Pz	0.01	0.01	0.01	-0.24	-0.22	0.49	0.00	0.00	-0.60	0.00	0.00	0.00	0.00	0.82	0.82	
O atom																
S	-0.71	0.73	0.00	0.42	-0.49	0.44	0.00	0.00	0.30	0.00	0.00	0.00	0.00	-0.69	0.47	
Px	0.00	0.00	0.00	0.00	0.00	0.00	0.53	0.00	0.00	-0.82	0.00	-0.74	0.00	0.00	0.00	
Py	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.53	0.00	0.00	-0.82	0.00	-0.74	0.00	0.00	
Pz	0.01	-0.01	-0.01	0.24	-0.22	-0.49	0.00	0.00	-0.60	0.00	0.00	0.00	0.00	-0.82	0.82	
A bonding-antibonding pair of MOs							A pair of mixing MOs									
C atom	MO8	MO13					C atom	MO4	MO6							
S	0.00	0.00	MO8 is bonding - all contributions				S	0.12	-0.37	We can see that the secondary contributions						
Px	0.00	0.00	have the same sign				Px	0.00	0.00	(yellow) in MO4 line up exactly with the primary						
Py	0.64	1.12					Py	0.00	0.00	contributions (green) in MO6 and vice versa. This						
Pz	0.00	0.00					Pz	0.00	0.00	shows us that mixing is occurring.						
O atom							O atom									
S	0.00	0.00	MO13 is antibonding - the C				S	0.42	0.44							
Px	0.00	0.00	contribution has the oppostite sign to				Px	0.00	0.00							
Py	0.53	-0.74	the O contributions				Py	0.00	0.00							
Pz	0.00	0.00					Pz	-0.24	0.49							
O atom							O atom									
S	0.00	0.00					S	0.42	0.44							
Px	0.00	0.00					Px	0.00	0.00							
Py	0.53	-0.74					Py	0.00	0.00							
Pz	0.00	0.00					Pz	0.24	-0.49							
Bonding		Antibonding														