

Coefficient matrix **C**

O-1s	-0.99	0.00	0.22	0.13	-0.00	-0.00	0.01	0.00	0.00	-0.12
O-2s	-0.03	-0.01	-0.78	-0.63	0.00	0.00	-0.08	-0.00	-0.00	0.93
O-2p _x	-0.00	-0.00	0.00	-0.00	-0.75	0.29	0.00	-0.23	0.59	0.00
O-2p _y	-0.00	-0.00	0.00	-0.00	-0.29	-0.75	0.00	0.59	0.23	0.00
O-2p _z	0.01	0.00	0.19	-0.58	-0.00	-0.00	-0.47	-0.00	-0.00	-0.93
C-1s	-0.00	0.99	0.12	-0.18	0.00	0.00	0.16	0.00	0.00	0.12
C-2s	0.01	0.03	-0.25	0.62	-0.00	-0.00	-0.71	-0.00	-0.00	-0.84
C-2p _x	-0.00	0.00	-0.00	0.00	-0.42	0.16	0.00	0.33	-0.86	0.00
C-2p _y	-0.00	0.00	-0.00	0.00	-0.16	-0.42	0.00	-0.86	-0.33	0.00
C-2p _z	0.01	0.01	-0.16	0.05	0.00	0.00	0.58	0.00	0.00	-1.15
	ψ_1 (-20.3914 Ht)	ψ_2 (-11.0902 Ht)	ψ_3 (-1.4047 Ht)	ψ_4 (-0.6899 Ht)	ψ_5 (-0.5094 Ht)	ψ_6 (-0.5094 Ht)	ψ_7 (-0.4409 Ht)	ψ_8 (0.2865 Ht)	ψ_9 (0.2865 Ht)	ψ_{10} (0.9253 Ht)

Molecular orbital