Molecular Orbital Coefficients:

				1	2	3	4	5
				(SG)--O	**(SG)--O**	**(SG)--O**	**(PI)--O**	**(PI)--O**
EIGENVALUES --				**-25.90351**	**-1.45985**	**-0.57365**	**-0.46312**	**-0.46312**
1	1	F	1S	0.99475	-0.25068	-0.07826		
2			2S	0.02226	0.94671	0.41089		
3			2PX				1.00000	
4			2PY					1.00000
5			2PZ	-0.00267	-0.07825	0.69806		
6	2	H	1S	-0.00534	0.15042	-0.53371		

				6
				(SG)--V
EIGENVALUES --				***0.58980***
1	*1*	*F*	*1S*	*0.08057*
2			*2S*	*-0.51583*
3			*2PX*	
4			*2PY*	
5			*2PZ*	*0.81643*
6	*2*	*H*	*1S*	*1.05432*

Aus den LCAO-Koeffizienten wird die Dichte-Matrix berechnet:

DENSITY MATRIX:

				1	2	3	4	5	6
1	1	F	1S	2.11697					
2			2S	-0.49467	2.13117				
3			2PX			2.00000			
4			2PY				2.00000		
5			2PZ	-0.07535	0.42537			0.98683	
6	2	H	1S	-0.00250	-0.15401			-0.76864	0.61501

Aus der Dichte-Matrix und der Überlappmatrix wird die Populations-Matrix berechnet:

Full Mulliken population analysis:

				1	2	3	4	5	6
1	1	F	1S	2.11697					
2			2S	-0.11773	2.13117				
3			2PX			2.00000			
4			2PY				2.00000		
5			2PZ					0.98683	
6	2	H	1S	-0.00011	-0.06522			0.25807	0.61501

Gross orbital populations:

				1
1	1	F	1S	1.99913
2			2S	1.94822
3			2PX	2.00000
4			2PY	2.00000
5			2PZ	1.24490
6	2	H	1S	0.80775

z(Fluor)=9 , Z(Wasserstoff)=1)

Mulliken atomic charges:

		1
1	F	-0.192250
2	H	0.192250

Sum of Mulliken charges= 0.00000