
Population analysis using the SCF density.

Orbital symmetries:

Occupied (SG) (SG) (SG) (PI) (PI) (SG) (SG) (PI) (PI)
(SG) (PI) (PI)
Virtual (SG)

The electronic state is 1-SG.

Alpha occ. eigenvalues -- -103.41466 -19.43576 -10.14396 -7.60338 -7.56711
Alpha occ. eigenvalues -- -7.56711 -1.20593 -0.44578 -0.31050 -0.31050
Alpha occ. eigenvalues -- 0.04341 0.31315 0.31315
Alpha virt. eigenvalues -- 1.24297

Molecular Orbital Coefficients

		1	2	3	4	5
		(SG)--0	(SG)--0	(SG)--0	(SG)--0	(PI)--0
EIGENVALUES	--	-103.41466	-19.43576	-10.14396	-7.60338	-7.56711
1 1	C1 1S	0.99448	0.00015	-0.37667	-0.01304	0.00000
2	2S	0.01582	-0.00243	1.05138	0.03785	0.00000
3	2PX	0.00000	0.00000	0.00000	0.00000	0.98992
4	2PY	0.00000	0.00000	0.00000	0.00000	0.00000
5	2PZ	-0.00018	-0.00037	-0.03108	0.98691	0.00000
6	3S	-0.00171	-0.01769	0.03713	0.00072	0.00000
7	3PX	0.00000	0.00000	0.00000	0.00000	0.04059
8	3PY	0.00000	0.00000	0.00000	0.00000	0.00000
9	3PZ	0.00017	0.01489	-0.00020	0.04302	0.00000
10 2	0 1S	0.00005	0.99265	-0.00431	0.00646	0.00000
11	2S	0.00035	0.04212	0.00150	0.00210	0.00000
12	2PX	0.00000	0.00000	0.00000	0.00000	-0.00302
13	2PY	0.00000	0.00000	0.00000	0.00000	0.00000
14	2PZ	-0.00032	0.01441	0.01435	-0.01603	0.00000
		6	7	8	9	10
		(PI)--0	(SG)--0	(SG)--0	(PI)--0	(PI)--0
EIGENVALUES	--	-7.56711	-1.20593	-0.44578	-0.31050	-0.31050
1 1	C1 1S	0.00000	0.06910	0.05935	0.00000	0.00000
2	2S	0.00000	-0.26002	-0.17914	0.00000	0.00000
3	2PX	0.00000	0.00000	0.00000	0.00000	-0.22243
4	2PY	0.98992	0.00000	0.00000	-0.22243	0.00000
5	2PZ	0.00000	0.13172	-0.16911	0.00000	0.00000
6	3S	0.00000	0.33218	0.91555	0.00000	0.00000
7	3PX	0.00000	0.00000	0.00000	0.00000	0.74430
8	3PY	0.04059	0.00000	0.00000	0.74430	0.00000
9	3PZ	0.00000	-0.11384	0.44970	0.00000	0.00000
10 2	0 1S	0.00000	-0.20806	0.11572	0.00000	0.00000

11	2S	0.00000	0.64371	-0.48911	0.00000	0.00000
12	2PX	0.00000	0.00000	0.00000	0.00000	0.48081
13	2PY	-0.00302	0.00000	0.00000	0.48081	0.00000
14	2PZ	0.00000	0.37193	-0.07243	0.00000	0.00000
		11	12	13	14	
		(SG)--0	(PI)--0	(PI)--0	(SG)--V	
	EIGENVALUES --	0.04341	0.31315	0.31315	1.24297	
1	1 C1 1S	0.01581	0.00000	0.00000	-0.01033	
2	2S	-0.06950	0.00000	0.00000	-0.05780	
3	2PX	0.00000	0.17498	0.00000	0.00000	
4	2PY	0.00000	0.00000	0.17498	0.00000	
5	2PZ	0.13904	0.00000	0.00000	-0.18363	
6	3S	-0.02776	0.00000	0.00000	-1.35693	
7	3PX	0.00000	-0.80611	0.00000	0.00000	
8	3PY	0.00000	0.00000	-0.80611	0.00000	
9	3PZ	-0.35271	0.00000	0.00000	1.62487	
10	2 0 1S	0.12405	0.00000	0.00000	-0.13074	
11	2S	-0.65911	0.00000	0.00000	1.70055	
12	2PX	0.00000	0.95412	0.00000	0.00000	
13	2PY	0.00000	0.00000	0.95412	0.00000	
14	2PZ	0.77614	0.00000	0.00000	1.04546	