

allyl radical calculated on UHF/PM3

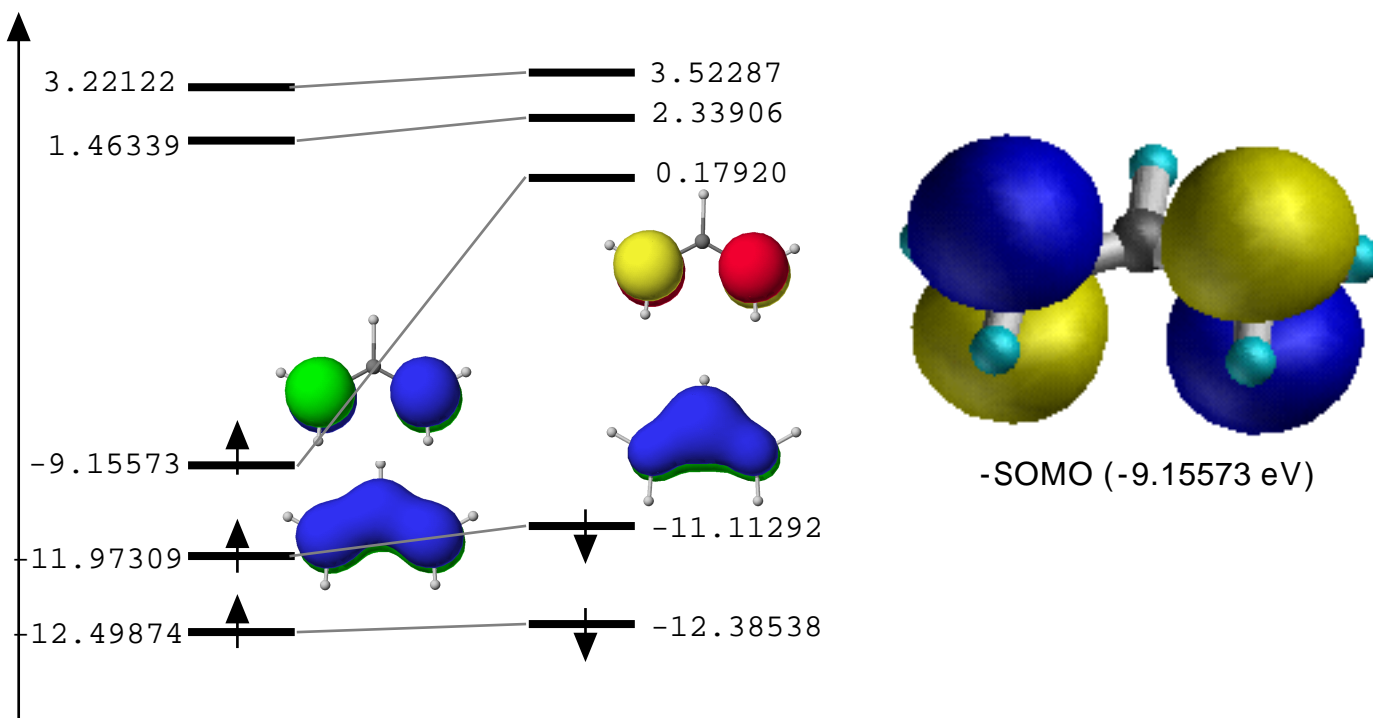
ALPHA EIGENVALUES

-34.91390 -26.20140 -19.65051 -16.68841 -15.41230 -13.22919 -12.49874 -11.97309
 -9.15573 1.46339 3.22122 3.60324 3.84215 4.49994 4.52433 5.68776
 5.78331

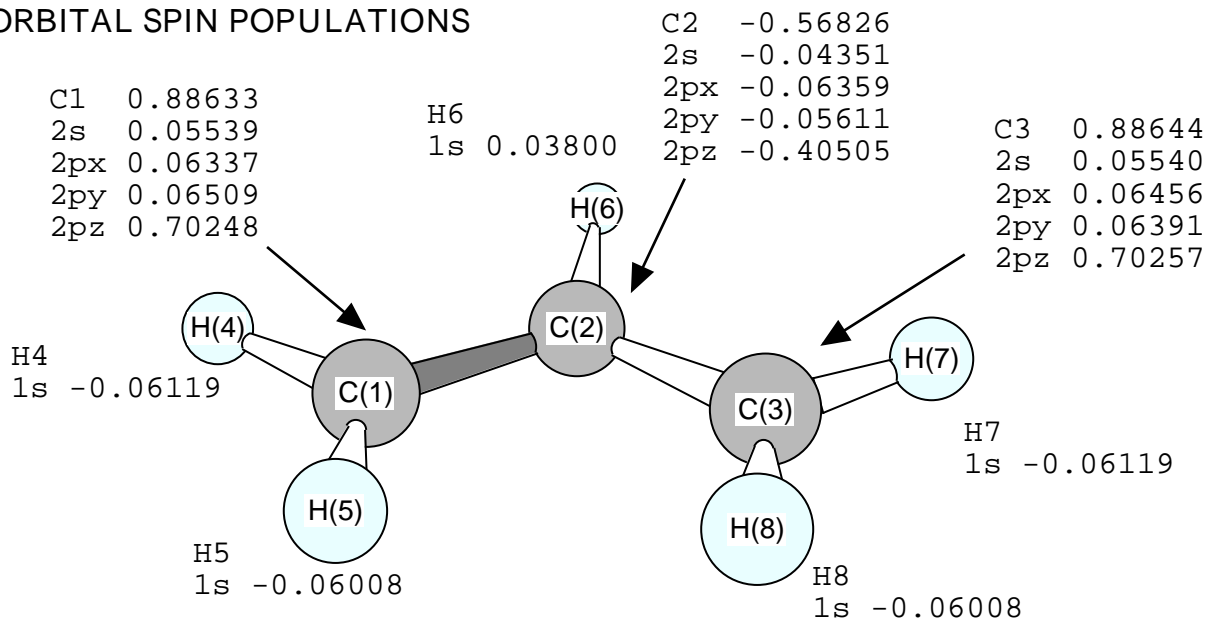
BETA EIGENVALUES

-34.54849 -25.11520 -19.56672 -16.54019 -15.21775 -12.96089 -12.38538 -11.11292
 0.17920 2.33906 3.52287 3.89818 4.11544 4.73281 4.83949 5.79533
 5.99529

E/eV



ATOMIC ORBITAL SPIN POPULATIONS



benzyl radical calculated on UHF/PM3

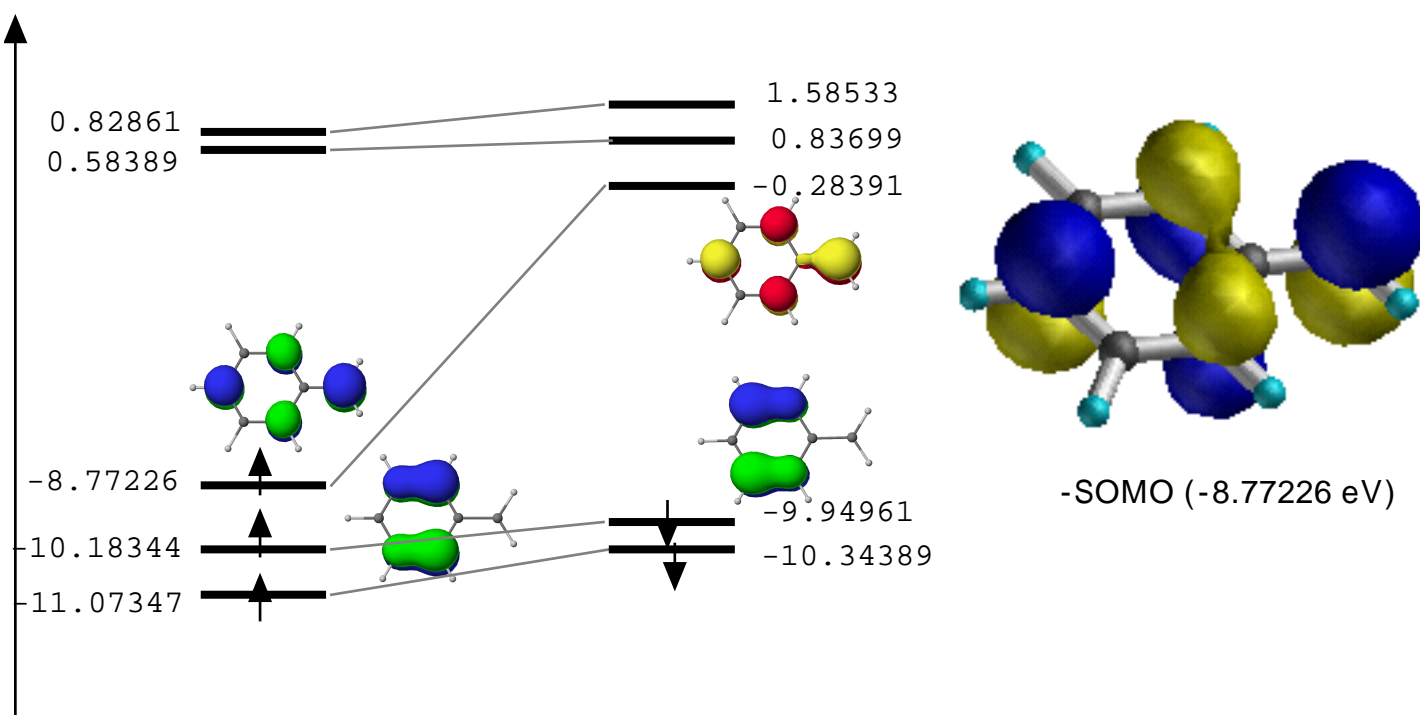
ALPHA EIGENVALUES

-39.57510	-31.94131	-29.70018	-25.29102	-21.60143	-20.43702	-17.84447	-16.69672
-15.54992	-14.68546	-14.60235	-13.63563	-13.49698	-12.78842	-12.22246	-11.07347
-10.18344	-8.77226	0.58389	0.82861	2.79698	3.01884	3.29953	3.36717
3.51125	3.79037	3.89464	4.33563	4.36131	5.00013	5.14860	5.31379
5.41966	6.15234	6.29895					

BETA EIGENVALUES

-39.44403	-31.60207	-29.62141	-24.43190	-21.56484	-20.41912	-17.70856	-16.62311
-15.44742	-14.66379	-14.52195	-13.37861	-13.20650	-12.69465	-12.19998	-10.34389
-9.94961	-0.28391	0.83699	1.58533	3.08831	3.21749	3.41795	3.45194
3.70641	3.98801	4.01110	4.43719	4.60950	5.05538	5.21839	5.43621
5.53067	6.24524	6.34109					

E/eV



ATOMIC ORBITAL SPIN POPULATIONS

