

COMPUTATIONAL CHEMIST

4
19 June 96

BLYP/aug-cc-pVDZ sym. relaxed UHF

r (Å)

BLYP

	1.10	-149.890988839
Sp wrong with this	1.11	-149.893260068
	1.115	-149.892802792
①	1.12	-149.893174980
	1.125	-149.893433969
	1.13	UHF unable to resolve instability - claims 2
	1.14	-149.893611856
	1.15	-149.893260068

② → obviously an odd surface. Going to look @ s.c. BLYP.

③ → will have all of these check for instability and optimize.

	r (Å)	BLYP 1	BLYP 2	charge / dipole?
*	1.00	-149.842029270	-149.842029270	okay
	1.10	-149.890976811	-149.890976939	"
	1.11	-149.892302486	-149.892302612	"
	1.125	-149.892786915	-149.892787041	"
*	1.12	-149.893158488	-149.893158468	okay.
	1.13	-149.893158468	-149.89315	"
	1.14	-149.893580217	-149.893580348	BLYP 3 " BLYP 4
	1.15	-149.893600832	-149.893600832	-149.893600968
	1.15	-149.893251227	-149.893251367	"

④ → * found second instability, unable to resolve it.

Additional pts:

1.16 -149.892560527 -149.892560527 -149.892560527 -149.89256065

1.17 -149.891555562 -149.891555707

⑤ → I think there's only 1 instability, but it has trouble getting there. Note identical energies for multiple instabilities.

1.18 -149.890261689 -149.890261831