

igb	extdiel	AMBER/NAB consistant?				
0	default	Yes				
	1	Yes				min.in:
2	default	Yes				STOP
	1	No				&cntrl
5	default	No				imin = 1,
	1	No				ncyc = 1,
We sometimes see different energy and gradient for AMBER and NAB						maxcyc = 1,
extdiel = 1 is vacuum						igb = 0,
Looks like there are two seperate issues here:						ntb = 0,
1. AMBER and NAB treat igb2 and igb5 differently						cut = 999.99,
2. extdiel is treated differently by AMBER and NAB						rgbmax = 25.0,
						extdiel=1,
						/
Take away message: when using AMBER in vacuum, use igb=0!						