

Bisphenol A		
Calculation Type	FREQ	
Calculation Method	RB3LYP	
Basis Set	6-311++G(3df,3pd)	
Charge	0	
Spin	Singlet	
E(RB3LYP)	-731.93409308	a.u.
RMS Gradient Norm	0.00000221	a.u.
Imaginary Freq	0	
Dipole Moment	0.9136	Debye
Point Group	C1	