

1					2			3		
B1					B2			A1		
Frequencies	--	1336.0043			1383.6450			1679.5843		
Red. masses	--	1.3689			1.3442			1.1039		
Frc consts	--	1.4395			1.5162			1.8348		
IR Inten	--	0.3694			23.1585			8.6240		
Raman Activ	--	0.7657			4.5170			12.8594		
Depolar (P)	--	0.7500			0.7500			0.5908		
Depolar (U)	--	0.8571			0.8571			0.7428		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.17	0.00	0.00	0.00	0.15	0.00	0.00	0.00	0.00
2	8	-0.04	0.00	0.00	0.00	-0.08	0.00	0.00	0.00	0.08
3	1	-0.70	0.00	0.00	0.00	-0.25	-0.65	0.00	-0.35	-0.61
4	1	-0.70	0.00	0.00	0.00	-0.25	0.65	0.00	0.35	-0.61
4					5			6		
A1					A1			B2		
Frequencies	--	2028.0966			3159.3252			3231.2607		
Red. masses	--	7.2497			1.0490			1.1206		
Frc consts	--	17.5689			6.1692			6.8934		
IR Inten	--	150.1839			49.7075			135.8564		
Raman Activ	--	8.1124			137.7307			58.2883		
Depolar (P)	--	0.3281			0.1829			0.7500		
Depolar (U)	--	0.4941			0.3092			0.8571		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.00	0.58	0.00	0.00	0.06	0.00	0.10	0.00
2	8	0.00	0.00	-0.41	0.00	0.00	0.00	0.00	0.00	0.00
3	1	0.00	-0.46	-0.19	0.00	0.61	-0.35	0.00	-0.60	0.37
4	1	0.00	0.46	-0.19	0.00	-0.61	-0.35	0.00	-0.60	-0.37