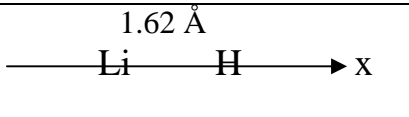


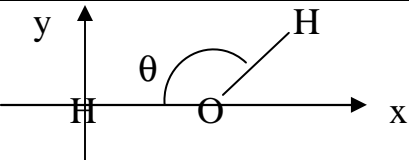
## Z-Matrix Construction

The first atom is always at the origin. The second is displaced along the x-axis. The third is in the +y direction, with the first three atoms all in the x-y plane.

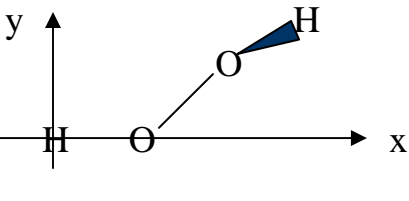
### LiH

		r						
1	Li							
2	H	1.62					1	

### H<sub>2</sub>O

		r    θ						
1	H							
2	O	0.982					1	
3	H	0.982	104.5				2	1

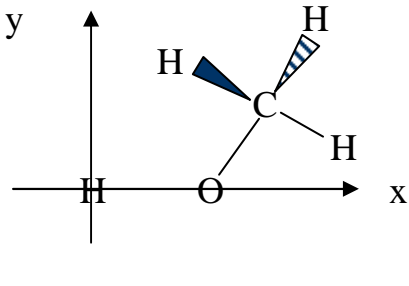
### H<sub>2</sub>O<sub>2</sub>

		r    θ    ϕ						
1	H							
2	O	0.960					1	
3	O	1.480	104.5				2	1
4	H	0.960	104.5	93.0			3	2

Here is the Z-matrix from the Distance Geometry program. This Z-matrix uses a different order than above but is otherwise equivalent. The “1” after each parameter means that the value will be optimized. The first oxygen atom is at the origin.

O	0.0000000	0	0.000000	0	0.000000	0	0	0	0
O	1.4799479	1	0.000000	0	0.000000	0	1	0	0
H	0.9600627	1	104.50000	1	0.000000	0	1	2	0
H	0.9600042	1	104.50000	1	93.000000	1	2	1	3

### CH<sub>3</sub>OH

		r    θ    ϕ						
1	H							
2	O	0.991					1	
3	C	1.583	104.5				2	1
4	H	0.983	109.5	60.0			3	2
5	H	0.983	109.5	-60.0			3	2
6	H	0.983	109.5	180.0			3	2