



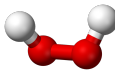




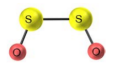

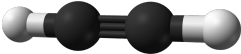
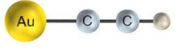






Shape	Point group	Graph	Dimensionality	Example	Dihedrals	Diagram
1	$T_d$	$K_4$	Regular Pyramidal	$P_4$	$\cos^{-1}\left(\frac{1}{3}\right)$	
2	$C_{3v}$	$S_3$	Pyramidal	$NH_3$	$\cos^{-1}\left(\frac{\cos \theta(1-\cos \theta)}{\sin^2 \theta}\right)$	
3	$C_s$	$S_3$	Pyramidal	$Cl_2OS$	$\cos^{-1}\left(\frac{\cos \theta - \cos^2 \varphi}{\sin^2 \varphi}\right)$	
4	$D_{2h}$	$K_4 - e$	Planar	$Cl_2Cu_2$	0 or 180	
5	$C_{2v}$	$K_4 - e$	Pyramidal	$H_2Si_2$	$\cos^{-1}\left(\frac{\cos \theta - \cos^2 \varphi}{\sin^2 \varphi}\right)$	
6	$C_2$	$P_4$	Pyramidal	$H_2O_2$	$\cos^{-1}\left(\frac{\cos \theta - \cos^2 \varphi}{\sin^2 \varphi}\right)$	
7	$C_1$	$P_4$	Pyramidal	$H_2OS$	$\cos^{-1}\left(\frac{\cos \theta - \cos \varphi \cos \phi}{\sin \varphi \sin \phi}\right)$	
8	$D_{3h}$	$S_3$	Planar	$BH_3$	0 or 180	
9	$C_s$	$P_4$	Planar	$HNSi_2$	0 or 180	
10	$D_{2h}$	$C_4$	Planar	$Br_2Na_2$	0 or 180	
11	$C_{2v}$	$P_4$	Planar	$O_2S_2$	0 or 180	
12	$C_{2v}$	$S_3$	Planar	$CFO_2$	0 or 180	
13	$D_{\infty h}$	$P_4$	Linear	$C_2H_2$	0 or 180	
14	$C_{\infty v}$	$P_4$	Linear	$C_2AuH$	0 or 180	
15	$C_s$	$T_{3,1}$	Planar	$H_2Si_2$	0 or 180	
16	$C_s$	$S_3$	Planar	$CBrFO$	0 or 180	
17	$C_{2v}$	$K_4 - e$	Planar	$C_3Si$	0 or 180	
18	$C_{2v}$	$K_4 - e$	Planar	$C_3Si$	0 or 180	

# H<sub>2</sub>Si<sub>2</sub>

Information provided	
$r_1$	Si-Si bond length
$r_2$	Si-H bond length
$\varphi$	Dihedral angle between two Si-Si-H planes
Information missing	
$r_3$	H-H distance
$\theta_1$	H-Si-H bond angle
$\theta_2$	Si-H-Si bond angle
$\theta_3$	Si-Si-H bond angle
$\theta_4$	H-H-Si angle
$\varphi_i$	Dihedral angles between various other pairs of planes

For a z-matrix, in addition to the information provided we would need *at least* one planar angle. For the first column of the z-matrix, we have 6 possibilities which are listed below along with the possible planar angles that could be used for each of these possibilities:

1		2		3		4		5		6	
Si	$\theta_3$ $\theta_1, \theta_3, \theta_4$	Si	$\theta_3, \theta_2$ $\theta_1, \theta_3, \theta_4$	Si	$\theta_1, \theta_4$ $\theta_2, \theta_3, \theta_4$	H	$\theta_2, \theta_3$ $\theta_1, \theta_3, \theta_4$	H	$\theta_1, \theta_4$ $\theta_2, \theta_3, \theta_4$	H	$\theta_4$ $\theta_2, \theta_3, \theta_4$
Si		H		H		Si		Si		H	
H		Si		H		Si		H		Si	
H		H		Si		H		Si		Si	

This means that if we know  $\theta_3$  or  $\theta_4$  then we have enough to complete the planar angles column of the z-matrix, but if we only know  $\theta_1$  or  $\theta_2$ , we would need to determine two of the angles rather than one. Since  $\theta_3$  is a “bond angle” in the original reference and  $\theta_4$  is not, we will present a formula for  $\theta_3$  (right now we only have  $\theta_1$  though, but soon we’ll replace the equations below with  $\theta_3$  equations):

$$\theta_1 = \cos^{-1} \left( \frac{\cos \varphi (4r_1^2 - r_2^2) + r_2^2}{4r_1^2} \right). \quad (1)$$

An alternative formula is:

$$\theta_1 = \sin^{-1} \left( \frac{\sin \left( \frac{\varphi}{2} \right) \sqrt{4r_2^2 - r_1^2}}{r_2} \right). \quad (2)$$

We can now write a z-matrix. Since the first option in the above table will lead to usage of  $r_1$  and  $r_2$  in lexicographical order (these bond angles are presented as they were in Landolt-Bornstein), we will use that option:

Si						
Si	1	$r_1$				
H	1	$r_2$	2	$\theta_3$		
H	1	$r_3$	2	$\theta_3$	3	Dihedral