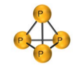
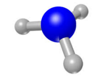
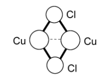
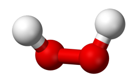
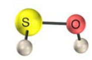
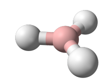
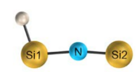
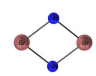
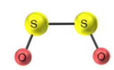
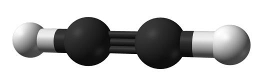
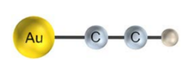
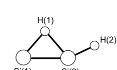
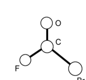
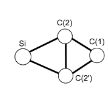
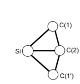
Shape	Point group	Graph	Shape	Example	Dihedrals	Diagram
1	T_d	K_4	Regular Pyramidal	P_4	$\cos^{-1}\left(\frac{1}{3}\right)$	
2	C_{3v}	S_3	Pyramidal	NH_3	$\cos^{-1}\left(\frac{\cos\theta(1-\cos\theta)}{\sin^2\theta}\right)$	
3	C_s	S_3	Pyramidal	Cl_2OS	$\cos^{-1}\left(\frac{\cos\theta-\cos^2\varphi}{\sin^2\varphi}\right)$	
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_2Si_2

Information provided	
r_1	Si-Si bond length
r_2	Si-H bond length
φ	Dihedral angle between two Si-Si-H planes

Information missing	
r_3	H-H distance
θ_1	H-Si-H bond angle
θ_2	Si-H-Si bond angle
θ_3	Si-Si-H bond angle
θ_4	H-H-Si angle
φ_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	Si, Si, H, H	θ_3	$\theta_1, \theta_3, \theta_4$
2	Si, H, Si, H	θ_3, θ_2	$\theta_1, \theta_3, \theta_4$
3	Si, H, H, Si	θ_1, θ_4	$\theta_2, \theta_3, \theta_4$
4	H, Si, Si, H	θ_2, θ_3	$\theta_1, \theta_3, \theta_4$
5	H, Si, H, Si	θ_1, θ_4	$\theta_2, \theta_3, \theta_4$
6	H, H, Si, Si	θ_4	$\theta_2, \theta_3, \theta_4$

This means that if we know θ_3 or θ_4 then we have enough to complete the planar angles column of the z-matrix, but if we only know θ_1 or θ_2, we would need to determine two of the angles rather than one. Since θ_3 is a "bond angle" in the original reference and θ_4 is not, we will present a formula for θ_3 (right now we only have θ_1 though, but soon we'll replace the equations below with θ_3 equations):

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

An alternative formula is:

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

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	θ_3		
H	1	r_3	2	θ_3	3	Dihedral