Group	
Schönflies	Abstract
K_h	O(3)
K	SO(3)
$D_{\infty h}$	$\mathrm{O}(2) \times \mathrm{Z}_2$
D_∞	O(2)
$C_{\infty v}$	O(2)
$C_{\infty h}$	$\mathrm{SO}(2) \times \mathrm{Z}_2$
C_∞	SO(2)

Continuous group		Finite group	
Schönflies	Abstract	Schönflies	Abstract
K_h	O(3)		
		I_h	$\mathrm{A}_5 \times \mathrm{Z}_2$
		O_h	$\mathrm{S}_4 \times \mathrm{Z}_2$
		T_h	$\mathrm{A}_4 \times \mathrm{Z}_2$
		T_d	S_4
K	SO(3)		
		I	A_5
		O	S_4
		T	A_4
$D_{\infty h}$	$\mathrm{O}(2) \times \mathrm{Z}_2$		
		D_{nh}	$\mathrm{Dih}_n \times \mathrm{Z}_2$
		D_{nd}	Dih_{2n}
D_∞	O(2)		
		D_n	Dih_n
$C_{\infty v}$	O(2)		
		C_{nv}	Dih_n
$C_{\infty h}$	$\mathrm{SO}(2) \times \mathrm{Z}_2$		
		C_{nh}	$\mathrm{Z}_n \times \mathrm{Z}_2$
		S_{2n}	Z_{2n}
C_∞	SO(2)		
		C_n	Z_n

Group	
Schönflies	Abstract
K_h	O(3)
I_h	$A_5 \times Z_2$
O_h	$S_4 \times Z_2$
T_h	$A_4 \times Z_2$
K	SO(3)
I	A_5
O	S_4
T_d	S_4
T	A_4
$D_{\infty h}$	$O(2) \times Z_2$
D_{nh}	$\mathrm{Dih}_n \times Z_2$
D_{nd}	Dih_{2n}
D_∞	O(2)
D_n	Dih_n
$C_{\infty v}$	O(2)
C_{nv}	Dih_n
$C_{\infty h}$	$SO(2) \times Z_2$
C_{nh}	$Z_n \times Z_2$
S_{2n}	Z_{2n}
C_∞	SO(2)
C_n	Z_n

Number of atoms	Possible groups (not including subgroups)
1	K_h
2	$D_{\infty h}, C_{\infty v}$
3	$D_{\infty h}, C_{\infty v}, D_{3h}, C_{2v}, C_s$
4	$D_{\infty h}, C_{\infty v}, D_{3h}, C_{2v}, C_s, T_d, D_{4h}, D_{2h}, D_{2d}, D_2, C_{3v}, C_{2h}, C_2, C_1$

Possible point groups for 3-atom (triatomic) molecules

Point group	Chemical formula type		
	A_3	A_2B	ABC
$D_{\infty h}$	C_3	CO_2	Not possible
$C_{\infty v}$		N_2O	HOS
D_{3h}	H_3^+	Not possible	Not possible
C_{2v}	O_3	H_2O	Not possible
C_s	Unlikely	HO_2	HNO

Impossible point groups for 3-atom (triatomic) molecules

C_1

Any three points form a plane, so any triatomic molecule will have a mirror-plane formed by the three atoms. The existence of a mirror-plane will promote the molecule to C_s.

C_i

Triple scalar product to show that 4 points are co-planar. However Sichao also says that a 5th atom must also be coplanar.

C_n,$n \geq 2$

A minimum of $2n$ atoms is needed, so for $n = 2$ we would need 4 atoms, and for $n > 2$ we would need even more.

$C_{nh}, n \geq 2$, $D_n, n \geq 2$, and $D_{nd}, n \geq 2$

These are supergroups of C_n, although D_{3h} is too and yet it's possible.

$C_{nv}, n \geq 3$

A minimum of $n + 1$ atoms is needed, so for $n = 3$ we would need 4 atoms, and for $n > 3$ we would need even more.

D_{2h}

Proof still neeeded

$D_{nh}, n \geq 4$

A minimum of n atoms is needed, so for $n = 4$ we would need 4 atoms, and for $n > 4$ we would need even more.

C_1

Any three points form a plane, so any triatomic molecule will have a mirror-plane formed by the three atoms. The existence of a mirror-plane will promote the molecule to C_s.

C_1

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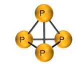
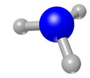
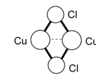
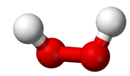
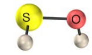
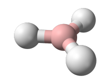
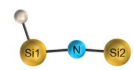
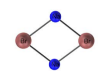
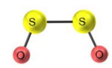
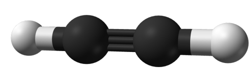
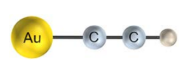
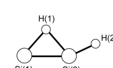
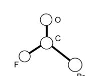
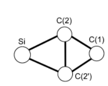
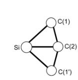
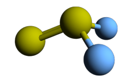
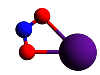
Any three points form a plane, so any triatomic molecule will have a mirror-plane formed by the three atoms. The existence of a mirror-plane will promote the molecule to C_s.

Structure	Point group	Graph	Formula	Dimensionality	Example	Dihedrals	Diagram
1	T_d	K_4	A_4	Pyramidal	P_4	$\cos^{-1}\left(\frac{1}{3}\right)$	
2	C_{3v}	S_3	A_3B	Pyramidal	H_3N	$\cos^{-1}\left(\frac{\cos\theta(1-\cos\theta)}{\sin^2\theta}\right)$	
3	C_s	S_3	A_2BC	Pyramidal	Cl_2OS	$\cos^{-1}\left(\frac{\cos\theta-\cos^2\varphi}{\sin^2\varphi}\right)$	
4	D_{2h}	K_4-e	A_2B_2	Planar	Cl_2Cu_2	0 or 180	
5	C_{2v}	K_4-e	A_2B_2	Pyramidal	H_2Si_2	$\cos^{-1}\left(\frac{\cos\theta-\cos^2\varphi}{\sin^2\varphi}\right)$	
6	C_2	P_4	A_2B_2	Pyramidal	H_2O_2	$\cos^{-1}\left(\frac{\cos\theta-\cos^2\varphi}{\sin^2\varphi}\right)$	
7	C_1	P_4	A_2BC	Pyramidal	H_2OS	$\cos^{-1}\left(\frac{\cos\theta-\cos\varphi\cos\phi}{\sin\varphi\sin\phi}\right)$	
8	D_{3h}	S_3	A_3B	Planar	BH_3	0 or 180	
9	C_s	P_4	A_2BC	Planar	$HNSi_2$	0 or 180	
10	D_{2h}	C_4	A_2B_2	Planar	Br_2Na_2	0 or 180	
11	C_{2v}	P_4	A_2B_2	Planar	O_2S_2	0 or 180	
12	C_{2v}	S_3	A_2BC	Planar	CFO_2	0 or 180	
13	$D_{\infty h}$	P_4	A_2B_2	Linear	C_2H_2	0 or 180	
14	$C_{\infty v}$	P_4	A_2BC	Linear	C_2AuH	0 or 180	
15	C_s	$T_{3,1}$	A_2B_2	Planar	H_2Si_2	0 or 180	
16	C_s	S_3	ABCD	Planar	CBrFO	0 or 180	
17	C_{2v}	K_4-e	A_3B	Planar	C_3Si	0 or 180	
18	C_{2v}	K_4-e	A_3B	Planar	C_3Si	0 or 180	

Structure	Point group	Graph	Formula	Dimensionality	Example	Dihedrals	Diagram
19	C_{3v}	K_4	A_3B	Pyramidal	AsP_3		
20	C_{2h}	P_4	A_2B_2	Planar	H_2N_2		
21	C_s	S_3	A_2B_2	Pyramidal	S_2F_2	$\cos^{-1}\left(\frac{\cos\theta-\cos^2\varphi}{\sin^2\varphi}\right)$	
22	C_{2v}	$T_{3,1}$	A_3B	Planar	C_3H	0 or 180	
23	C_{2v}	C_4	ABC_2	Planar	$CsNO_2$	0 or 180	

Shape 1: P_4

Information provided	
r	P-P bond length
Information missing	
θ	P-P-P bond angle
φ	P-P-P-P dihedral angle

Since all faces of a regular tetrahedron are equilateral triangles, $\theta = 60°$. The dihedral angles φ in a regular tetrahedron are given by $\cos^{-1}\left(\frac{1}{3}\right)$. We therefore have the following z-matrix:

$$\boxed{\begin{array}{lllllll} \mathtt{P} & & & & & & \\ \mathtt{P} & 1 & r & & & & \\ \mathtt{P} & 1 & r & 2 & \theta_3 & & \\ \mathtt{P} & 1 & r & 2 & \theta_3 & 3 & \varphi \end{array}}.$$

Shape 2: NH_3

Information provided	
r_1	N-H bond length
θ_1	H-N-H bond angle
Information missing	
r_2	H-H distance
θ_2	H-H-H bond angle
θ_3	H-H-N bond angle
φ_i	Dihedral angles between various pairs of planes

Since the three H atoms form an equilateral triangle, $\theta_2 = 60°$. Also, (at least some of) the dihedral angles φ are given by the following simplified form for the dihedral law of cosines:

$$\varphi = \cos^{-1}\left(\frac{\cos\theta\,(1-\cos\theta)}{\sin^2\theta}\right). \tag{1}$$

We therefore have the following z-matrix:

$$\boxed{\begin{array}{lllllll} \mathtt{N} & & & & & & \\ \mathtt{H} & 1 & r_1 & & & & \\ \mathtt{H} & 1 & r_1 & 2 & \theta_1 & & \\ \mathtt{H} & 1 & r_1 & 2 & \theta_1 & 3 & \varphi \end{array}}.$$

Shape 3: Cl_2OS

Information provided	
r_1	S-O bond length
r_2	S-Cl bond length
θ_1	Cl-S-O bond angle
θ_2	Cl-S-Cl bond angle
φ	Cl-S-O-Cl dihedral angle
Information missing	
r_3	Cl-O distance
θ_3	
θ_4	
θ_5	
φ_i	Dihedral angles between various other pairs of planes

They gave the dihedral angle but didn't need to, because it's exactly what we would get from the dihedral law of cosines.

The missing geometric information is provided below:

$$r_3 = \sqrt{r_1^2 + r_2^2 - 2\cos\theta_1} \tag{2}$$

Shape 4: Cl_2Cu_2

We need to first undersatnd why one pair of atoms has a dashed line between them and the other pair does not.

Information provided	
r_1	
θ_1	
Information missing	
r_2	
θ_2	
φ_i	Dihedral angles between various pairs of planes

We therefore have the following z-matrix:

N						
H	1	r_2				
H	1	r_2	2	θ_1		
H	1	r_2	2	θ_1	3	φ

.

Shape 5: 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, despite none being provided from the experimental paper. The missing geometric information can be provided based on the information provided from the experimental paper though:

$$r_3 = \sin\frac{\varphi}{2}\sqrt{4r_2^2 - r_1^2}, \tag{3}$$

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

$$\theta_2 = \cos^{-1}\left(1 - \frac{1}{2}\left(\frac{r_1}{r_2}\right)^2\right), \tag{5}$$

$$\theta_3 = \cos^{-1}\left(\frac{r_1}{2r_2}\right), \tag{6}$$

$$\theta_4 = \frac{\pi - \theta_1}{2}. \tag{7}$$

An alternative formula for θ_1 is:

$$\theta_1 = \sin^{-1}\left(\frac{\sin\left(\frac{\varphi}{2}\right)\sqrt{4r_2^2 - r_1^2}}{r_2}\right). \tag{8}$$

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:

	Atoms	Angles (atoms 1–3)	Angles (atoms 2–4)
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:

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

Shape 6: H_2O_2

	Information provided
r_1	H-O bond length
r_2	O-O bond length
θ_1	H-O-O bond angle
φ	H-O-O-H dihedral angle
	Information missing
r_3	H...H distance
r_4	O...H distance
θ_2	H-H-B bond angle
θ_3	H-H-H angle
φ_i	Dihedral angles between various pairs of planes

We therefore have the following z-matrix:

$$\boxed{\begin{array}{lllllll} \texttt{O} & & & & & & \\ \texttt{O} & 1 & r_2 & & & & \\ \texttt{H} & 1 & r_1 & 2 & \theta_1 & & \\ \texttt{H} & 2 & r_1 & 1 & \theta_1 & 3 & \varphi \end{array}}.$$

Shape 7: H_2OS

Peilin's molecule

	Information provided
r_1	H-O bond length
r_2	O-S bond length
r_3	S-H bond length
θ_1	H-O-S bond angle
θ_2	H-S-O bond angle
φ	H-O-S-H dihedral angle
	Information missing
r_4	H...H distance
r_5	H...O distance
r_6	H...S distance
θ_3	H...H-O angle
θ_4	H...H...O angle
θ_5	H-O...H angle
θ_6	H...O-S angle
θ_7	H-S...H angle
θ_8	H...S-O angle
φ_i	Dihedral angles between various pairs of planes

We therefore have the following z-matrix:

$$\boxed{\begin{array}{lllllll} \texttt{B} & & & & & & \\ \texttt{H} & 1 & r_1 & & & & \\ \texttt{H} & 1 & r_1 & 2 & \theta_1 & & \\ \texttt{H} & 1 & r_1 & 2 & \theta_1 & 3 & \varphi \end{array}}.$$

Shape 8: BH_3

Hemanth's molecule

Information provided	
r_1	B-H bond length
Information missing	
r_2	H-H distance
θ_1	H-B-H bond angle
θ_2	H-H-B bond angle
θ_3	H-H-H angle
φ_i	Dihedral angles between various pairs of planes

Since the three H atoms form an equilateral triangle, $\theta_3 = 60°$.
We therefore have the following z-matrix:

B						
H	1	r_1				
H	1	r_1	2	θ_1		
H	1	r_1	2	θ_1	3	φ

.

Shape 9: $HNSi_2$

Mia finished this but still needs to type it in LaTeX.

Information provided	
r_1	H-Si bond length
r_2	Si-N bond length
r_3	N-Si bond length
θ_1	Si-N-Si bond angle
θ_2	H-Si-N bond angle
Information missing	
r_4	N...H distance
r_5	Si...Si distance
r_6	Si...H distance
θ_3	N=Si...Si angle
θ_4	H...Si...Si angle
θ_5	H-Si...Si angle
θ_6	H...Si-N angle
φ_i	Dihedral angles between various other pairs of planes

We have the following expressions for the missing geometric information (waiting for Mia):
But we can make the z-matrix with only information given to us originally:

Si						
N	1	r_1				
Si	2	r_2	1	θ_1		
H	3	r_3	2	θ_2	1	φ

Shape 10: Br_2Na_2

Abdul's molecule

Information provided	
r_1	Br-Na bond length
θ_1	Br-Na-Br bond angle

Information missing	
r_2	Br...Br distance
r_3	Na...Na distance
θ_1	Br...Br-Na angle
θ_2	Br-Na...Na angle
θ_3	Na-Br-Na angle
φ_i	Dihedral angles between various other pairs of planes

We have the following expressions for the missing geometric information (waiting for Abdul):
But we can make the z-matrix with only information given to us originally:

Si						
N	1	r_1				
Si	2	r_2	1	θ_1		
H	3	r_3	2	θ_2	1	φ

Shape 11: O_2S_2

Abdul's molecule

Information provided	
r_1	O-S bond length
r_2	S-S bond length
θ_1	O-S-S bond angle

Information missing	
r_3	O...O distance
r_4	O...S distance
θ_2	O...O-S angle
θ_3	O...O...S angle
θ_4	O-S...O angle
θ_5	O...S-S angle
φ_i	Dihedral angles between various other pairs of planes

We have the following expressions for the missing geometric information (waiting for Abdul):
But we can make the z-matrix with only information given to us originally:

Si						
N	1	r_1				
Si	2	r_2	1	θ_1		
H	3	r_3	2	θ_2	1	φ

Shape 12: $CBrO_2$

Hemanth's molecule

Information provided	
r_1	C-Cl bond length
r_2	C=O bond length
θ_1	Cl-C-Cl bond angle

Information missing	
r_3	Cl...Cl distance
r_4	Cl...O distance
θ_2	C-Cl...Cl angle
θ_3	C-Cl...O angle
θ_4	C-O...Cl angle
θ_5	Cl-C...O angle
θ_6	Cl...Cl...O angle
θ_7	Cl...O-C angle
θ_8	Cl...O...Cl angle
φ_i	Dihedral angles between various other pairs of planes

We have the following expressions for the missing geometric information:

$$r_3 = \sqrt{2r_1^2 - 2r_1^2 \cos\theta_1}, \tag{9}$$

$$r_4 = \sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos\theta_2}, \tag{10}$$

$$\theta_2 = \tag{11}$$

But we can make the z-matrix with only information given to us originally:

Si						
N	1	r_1				
Si	2	r_2	1	θ_1		
H	3	r_3	2	θ_2	1	φ

Shape 13: C_2H_2

Aimun's molecule

Information provided	
r_1	H-Si bond length
r_2	Si-N bond length
r_3	N-Si bond length
θ_1	Si-N-Si bond angle
θ_2	H-Si-N bond angle

Information missing	
r_4	N...H distance
r_5	Si...Si distance
r_6	Si...H distance
θ_3	N=Si...Si angle
θ_4	H...Si...Si angle
θ_5	H-Si...Si angle
θ_6	H...Si-N angle
φ_i	Dihedral angles between various other pairs of planes

We have the following expressions for the missing geometric information (waiting for Mia):
But we can make the z-matrix with only information given to us originally:

`Si`						
`N`	1	r_1				
`Si`	2	r_2	1	θ_1		
`H`	3	r_3	2	θ_2	1	φ

Shape 15: H_2Si_2

Justin's molecule

Information provided	
r_1	Si-Si bond length
r_2	Si-N bond length
r_3	N-Si bond length
θ_1	Si-N-Si bond angle
θ_2	H-Si-N bond angle
Information missing	
r_4	N...H distance
r_5	Si...Si distance
r_6	Si...H distance
θ_3	N=Si...Si angle
θ_4	H...Si...Si angle
θ_5	H-Si...Si angle
θ_6	H...Si-N angle
φ_i	Dihedral angles between various other pairs of planes

We have the following expressions for the missing geometric information (waiting for Mia): But we can make the z-matrix with only information given to us originally:

`Si`						
`N`	1	r_1				
`Si`	2	r_2	1	θ_1		
`H`	3	r_3	2	θ_2	1	φ

Shape 16: CBrFO

Hemanth's molecule

Information provided	
r_1	C-F bond length
r_2	C=O bond length
θ_1	Si-N-Si bond angle
θ_2	H-Si-N bond angle
Information missing	
r_4	N...H distance
r_5	Si...Si distance
r_6	Si...H distance
θ_3	N=Si...Si angle
θ_4	H...Si...Si angle
θ_5	H-Si...Si angle
θ_6	H...Si-N angle
φ_i	Dihedral angles between various other pairs of planes

We have the following expressions for the missing geometric information (waiting for Mia): But we can make the z-matrix with only information given to us originally:

`Si`						
`N`	1	r_1				
`Si`	2	r_2	1	θ_1		
`H`	3	r_3	2	θ_2	1	φ

Shape 17: C_3Si

Sam's molecule

	Information provided
r_1	C(1)-C(2) bond length
r_2	C(2)-C(2)' bond length
r_3	C(2)-Si bond length
	Information missing
r_4	C(1)...Si distance
θ_1	C(2)-C(1)-C(2)' angle
θ_2	C(1)-C(2)-C(2)' angle
θ_3	Si-C(2)-C(2)' angle
θ_4	C(2)-Si-C(2)' angle
θ_5	Si-C(2)-C(1) angle
θ_6	Si...C(1)-C(2) angle
θ_7	C(1)...Si-C(2) angle
φ_i	Dihedral angles between various other pairs of planes

We have the following expressions for the missing geometric information:

$$r_4 = r_3\sqrt{1-\frac{r_2^2}{4r_3^2}} + r_1\sqrt{1-\frac{r_2^2}{4r_1^2}} \tag{12}$$

$$\theta_1 = \arccos\left(1-\frac{r_2^2}{2r_1^2}\right) \tag{13}$$

$$\theta_2 = \arccos\left(\frac{r_2}{2r_1}\right) \tag{14}$$

$$\theta_3 = \arccos\left(\frac{r_2}{2r_3}\right) \tag{15}$$

$$\theta_4 = \arccos\left(1-\frac{r_2^2}{2r_3^2}\right) \tag{16}$$

$$\theta_5 = \arccos\left(\frac{r_2}{2r_1}\right) + \arccos\left(\frac{r_2}{2r_3}\right) \tag{17}$$

$$\theta_6 = \frac{1}{2}\arccos\left(1-\frac{r_2^2}{2r_1^2}\right) \tag{18}$$

$$\theta_7 = \frac{1}{2}\arccos\left(1-\frac{r_2^2}{2r_3^2}\right) \tag{19}$$

The z-matrix can be constructed as shown using both calculated and originally provided information:

$C(1)$						
`C(2)`	1	r_1				
`C(2)'`	2	r_2	1	θ_2		
`Si`	3	r_3	2	θ_3	1	φ

Shape 18: C_3Si

Sam's molecule

Information provided	
r_1	C(1)-C(2) bond length
r_2	Si-C(2) bond length
r_3	Si-C(1) bond length
Information missing	
r_4	C(1)...C(1)' distance
θ_1	C(1)...C(1)'-C(2) angle
θ_2	C(1)-C(2)-C(1)' angle
θ_3	C(1)-C(2)-Si angle
θ_4	Si-C(1)-C(2) angle
θ_5	C(1)-Si-C(2) angle
θ_6	C(1)-Si-C(1)' angle
θ_7	C(1)...C(1)'-Si angle
φ_i	Dihedral angles between various other pairs of planes

We have the following expressions for the missing geometric information:

$$r_4 = 2r_1 \cos\left(90 - \arccos\left(\frac{r_1^2 + r_2^2 - r_3^2}{2r_1 r_2}\right)\right) \tag{20}$$

$$\theta_1 = 90 - \arccos\left(\frac{r_1^2 + r_2^2 - r_3^2}{2r_1 r_2}\right) \tag{21}$$

$$\theta_2 = 2\arccos\left(\frac{r_1^2 + r_2^2 - r_3^2}{2r_1 r_2}\right) \tag{22}$$

$$\theta_3 = \arccos\left(\frac{r_1^2 + r_2^2 - r_3^2}{2r_1 r_2}\right) \tag{23}$$

$$\theta_4 = \arccos\left(\frac{r_1^2 + r_3^2 - r_2^2}{2r_1 r_3}\right) \tag{24}$$

$$\theta_5 = \arccos\left(\frac{r_2^2 + r_3^2 - r_1^2}{2r_2 r_3}\right) \tag{25}$$

$$\theta_6 = 2\arccos\left(\frac{r_2^2 + r_3^2 - r_1^2}{2r_2 r_3}\right) \tag{26}$$

$$\theta_7 = 90 - \arccos\left(\frac{r_2^2 + r_3^2 - r_1^2}{2r_2 r_3}\right) \tag{27}$$

The z-matrix can be constructed as shown using both calculated and originally provided information:

C(1)						
C(2)	1	r_1				
C(1)′	2	r_1	1	θ_2		
Si	3	r_3	2	θ_4	1	φ

Shape 19: AsP_3

Sichao's molecule

Information provided	
r_1	As-P bond length
r_2	P-P bond length
Information missing	
θ_1	P-As-P angles
θ_2	As-P-P angle
θ_3	P-P-P angle
φ_1	Dihedral angle between AsP_2 plane and AsP_2 plane
φ_2	Dihedral angle between AsP_2 plane and P_3 plane

We have the following expressions for the missing geometric information:

$$\theta_1 = \cos^{-1}\left(\frac{2r_1^2 - r_2^2}{2r_1^2}\right)$$

$$\theta_2 = \frac{180 - \theta_1}{2}$$

$$\theta_3 = 60$$

$$\varphi_1 = \cos^{-1}\left(\frac{\cos\theta_1(1-\cos\theta_1)}{\sin^2\theta_1}\right)$$

$$\varphi_2 = \cos^{-1}\left(\frac{\cot\theta_2}{\sqrt{3}}\right)$$

We are able to construct the z-matrix using just the information on r_1, θ_1 and φ_1:

As						
P	1	r_1				
P	1	r_1	2	θ_1		
P	1	r_1	2	θ_1	3	φ_1

Shape 20: H_2N_2

Justin's molecule

Information provided	
r_1	H-Si bond length
r_2	Si-N bond length
r_3	N-Si bond length
θ_1	Si-N-Si bond angle
θ_2	H-Si-N bond angle
Information missing	
r_4	N...H distance
r_5	Si...Si distance
r_6	Si...H distance
θ_3	N=Si...Si angle
θ_4	H...Si...Si angle
θ_5	H-Si...Si angle
θ_6	H...Si-N angle
φ_i	Dihedral angles between various other pairs of planes

We have the following expressions for the missing geometric information (waiting for Mia):
But we can make the z-matrix with only information given to us originally:

Si						
N	1	r_1				
Si	2	r_2	1	θ_1		
H	3	r_3	2	θ_2	1	φ

Shape 21: S_2F_2

Sam's molecule

Information provided	
r_1	F-S bond length
r_2	S=S bond length
θ_1	F-S-F bond angle
θ_2	F-S=S bond angle
Information missing	
r_3	F...F distance
r_4	F...S distance
θ_3	S-F...F angle
θ_4	S...F...F angle
θ_5	S...F-S angle
θ_6	F...S=S angle
φ_1	Dihedral angle between S_2Fplane and S_2F plane
φ_2	Dihedral angle between SF_2 plane and S_2F plane

We have the following expressions for the missing geometric information:

$$r_3 = r_1\sqrt{2\left(1-\cos\theta_1\right)} \tag{28}$$

$$r_4 = \sqrt{r_1^2+r_2^2-2r_1r_2\cos\theta_2} \tag{29}$$

$$\theta_3 = \frac{180-\theta_1}{2} \tag{30}$$

$$\theta_4 = \arccos\left(r_1\sqrt{\frac{1-\cos\theta_1}{2\left(r_1^2+r_2^2-2r_1r_2\cos\theta_2\right)}}\right) \tag{31}$$

$$\theta_5 = \arccos\left(\frac{r_1-r_2\cos\theta_2}{\sqrt{r_1^2+r_2^2-2r_1r_2\cos\theta_2}}\right) \tag{32}$$

$$\theta_6 = \arccos\left(\frac{r_2-r_1\cos\theta_2}{\sqrt{r_1^2+r_2^2-2r_1r_2\cos\theta_2}}\right) \tag{33}$$

$$\varphi_1 = \arccos\left(\frac{\cos\theta_1-\cos^2\theta_2}{\sin^2\theta_2}\right) \tag{34}$$

$$\varphi_2 = \arccos\left(\frac{\cos\theta_2\left(1-\cos\theta_1\right)}{\sin\theta_1\sin\theta_2}\right) \tag{35}$$

The z-matrix can be constructed as shown using both calculated and originally provided information:

F						
S	1	r_1				
S	2	r_2	1	θ_2		
F	2	r_1	3	θ_2	1	φ_1

Shape 22: C_3H

Sam's molecule

Information provided	
r_1	C≡C bond length
r_2	C-C bond length
r_3	C-H bond length
Information missing	
r_4	C...H distance
θ_1	C≡C-C bond angle
θ_2	C-C-C bond angle
θ_3	C-C-H bond angle
θ_4	C≡C...H angle
θ_5	C-C...H angle
θ_6	C-H...C angle
φ_i	Dihedral angles between various other pairs of planes

We have the following expressions for the missing geometric information:

$$r_4 = \sqrt{r_2^2 + r_3^2 - 2r_2r_3\cos\left(90 + \arccos\left(\frac{r_1}{2r_2}\right)\right)} \tag{36}$$

$$\theta_1 = \arccos\left(\frac{r_1}{2r_2}\right) \tag{37}$$

$$\theta_2 = 180 - 2\arccos\left(\frac{r_1}{2r_2}\right) \tag{38}$$

$$\theta_3 = 90 + \arccos\left(\frac{r_1}{2r_2}\right) \tag{39}$$

$$\theta_4 = \arccos\left(\frac{r_1}{2\sqrt{r_2^2 + r_3^2 - 2r_2r_3\cos\left(90 + \arccos\left(\frac{r_1}{2r_2}\right)\right)}}\right) \tag{40}$$

$$\theta_5 = \arccos\left(\frac{r_1}{2\sqrt{r_2^2 + r_3^2 - 2r_2r_3\cos\left(90 + \arccos\left(\frac{r_1}{2r_2}\right)\right)}}\right) - \arccos\left(\frac{r_1}{2r_2}\right) \tag{41}$$

$$\theta_6 = \arcsin\left(\frac{r_1}{2\sqrt{r_2^2 + r_3^2 - 2r_2r_3\cos\left(90 + \arccos\left(\frac{r_1}{2r_2}\right)\right)}}\right) \tag{42}$$

The z-matrix can be constructed as shown using both calculated and originally provided information:

C						
C	1	r_1				
C	2	r_2	1	θ_1		
H	3	r_3	2	θ_3	1	φ

Shape 23: $CsNO_2$

Sam's molecule

	Information provided
r_1	Cs-O bond length
r_2	O-N bond length
θ_1	O-N-O bond angle
	Information missing
r_3	Cs...N distance
r_4	O...NO distance
θ_2	Cs-O-N bond angle
θ_3	O-Cs-O bond angle
θ_4	Cs...N-O angle
θ_5	Cs-O...O angle
θ_6	N...Cs-O angle
θ_7	O...O-N angle
φ_i	Dihedral angles between various other pairs of planes

We have the following expressions for the missing geometric information:

$$r_3 = \sqrt{r_1^2 + r_2^2 - 2r_1r_2\cos\left(\frac{180-\theta_1}{2} + \arccos\left(\frac{r_2}{2r_1}\sqrt{2\left(1-\cos\theta_1\right)}\right)\right)} \tag{43}$$

$$r_4 = r_2\sqrt{2\left(1-\cos\theta_1\right)} \tag{44}$$

$$\theta_2 = \frac{180-\theta_1}{2} + \arccos\left(\frac{r_2}{2r_1}\sqrt{2\left(1-\cos\theta_1\right)}\right) \tag{45}$$

$$\theta_3 = 2\arcsin\left(\frac{r_2}{2r_1}\sqrt{2\left(1-\cos\theta_1\right)}\right) \tag{46}$$

$$\theta_4 = \frac{\theta_1}{2} \tag{47}$$

$$\theta_5 = \arccos\left(\frac{r_2}{2r_1}\sqrt{2\left(1-\cos\theta_1\right)}\right) \tag{48}$$

$$\theta_6 = \arcsin\left(\frac{r_2}{2r_1}\sqrt{2\left(1-\cos\theta_1\right)}\right) \tag{49}$$

$$\theta_7 = \frac{180-\theta_1}{2} \tag{50}$$

The z-matrix can be constructed as shown using both calculated and originally provided information:

Cs						
O	1	r_1				
N	2	r_2	1	θ_2		
O	3	r_2	2	θ_1	1	φ