4 atoms

Point group	\mathbf{Shape}	Example	Dihedrals
T_d	Regular Pyramidal	P_4	$\cos^{-1}\left(\frac{1}{3}\right)$
C_{3v}	Pyramidal	NH_3	$\cos^{-1}\left(\frac{\cos\theta(1-\cos\theta)}{\sin^2\theta}\right)$
C_s	Pyramidal	$\mathrm{Cl}_2\mathrm{OS}$	$\cos^{-1}\left(\frac{\cos\theta-\cos^2\varphi}{\sin^2\varphi}\right)$
C_{2v}	Pyramidal	$\mathrm{H}_{2}\mathrm{Si}_{2}$	$\cos^{-1}\left(\frac{\cos\theta - \cos^{2}\varphi}{\sin^{2}\varphi}\right)$ $\cos^{-1}\left(\frac{\cos\theta - \cos^{2}\varphi}{\sin^{2}\varphi}\right)$ $\cos^{-1}\left(\frac{\cos\theta - \cos^{2}\varphi}{\sin^{2}\varphi}\right)$
C_2	Pyramidal	$\mathrm{H_2O_2}$	$\cos^{-1}\left(\frac{\cos\theta-\cos^2\varphi}{\sin^2\varphi}\right)$
C_1	Pyramidal	$_{ m H_2OS}$	$\cos^{-1}\left(\frac{\cos\theta-\cos\varphi\cos\phi}{\sin\varphi\sin\phi}\right)$
D_{3h}	Planar	BH_3	0 or 180
C_s	Planar	HNSi_2	0 or 180
D_{2h}	Planar	$\mathrm{Br_{2}Na_{2}}$	0 or 180
C_{2h}	Planar	$(\mathrm{HI})_2$	0 or 180
C_{2v}	Planar?	O_2S_2	0 or 180
C_{2v}	Planar?	CFO_2	0 or 180
$C_{\infty v}$	Linear	CAgIO	0 or 180
$D_{\infty h}$	Linear	C_2H_2	0 or 180
C_{2v}		$(Ar_2)(HCl)$	
C_s		$(HCl)_2$	
C_2		$(HF)_2$	

5 atoms

Point group	Shape	Example	Dihedrals
T_d		O_4Os	$\cos^{-1}\left(\frac{1}{3}\right)$?
C_{3v}		${\rm ClH_3Si}$	
C_{3v}		${ m KrO_3S}$	
C_{2v}		$\mathrm{Cl_4Te}$	
C_{2v}		C_3H_2	
C_{2v}		$\mathrm{H}_{2}\mathrm{I}_{2}\mathrm{Si}$	
C_{2v}		$\mathrm{H_2O_2Si}$	
C_{2v}		$(\mathrm{CO}_2)(\mathrm{N}_2)$	
$C_s(\mathrm{syn})$		$\mathrm{BFH_2O}$	
$C_s(\text{syn-anti})$		$\mathrm{CH_{2}O_{2}}$	
C_s		CN_4	
C_s		C_2H_3	
C_s		$\mathrm{BF}_{2}\mathrm{HO}$	
C_s		$\mathrm{CH_{3}OH}$	
C_s		ClH_2NaO	
C_s		HNO_3	
C_s	NT 1	$_{\mathrm{H_2O_2Si}}$	
C_s	Non-planar	$\mathrm{CH_2N_2}$	
$C_s \ C_s$	${ m CBrF_2N} \ { m CHClF_2}$		
C_s		$(CO)(N_2O)$	
C_s (effective)		ArH_3N	
C_s (effective)		$(SO_2)(CO)$	
$C_s(\text{assumed})$		$\mathrm{H_2N_2O}$	Given!
$C_{\infty v}$	Linear	$\mathrm{CH_{3}N}$	G17 611.
$-\infty v$	Linear	(CO)(HCN)	
$D_{\infty h}$	$\begin{array}{ccc} \text{Linear} & \stackrel{\longleftarrow}{\text{C}_5} \end{array}$		
$D_{\infty h}$	$ m Linear \qquad C_3 Ge_2$		
$D_{\infty h}$	Linear	C_3H_2	
	Quasi-linear	C_3O_2	