

Supplementary Material

Distribution of members of particular crystallographic point groups over Wyckoff positions in One-R. Point groups with less than 75 members.

C₄ Total 38

C ₄	22
C ₁	12
C ₂	4

C_{4h} Total 17

C _i	10
C _{4h}	7

C_{4v} Total 36

C ₁	18
C _s	7
C ₄	6
C ₂	3
C _{2v}	2

D₄ Total 37

C ₂	23
C ₁	4
D ₂	4
D ₄	4
C ₄	2

C_{3h} Total 55

C _{3h}	27
C ₃	15
C ₁	11
C _s	2

C₆ Total 2

C ₁	1
C ₆	1

C_{6h} Total 1

C _i	1
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C_{6v} Total 0

D₆ Total 1

C ₂	1
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D_{6h} Total 20

C _i	12
C ₁	3
S ₆	2

C ₂	1
C _{2h}	1
D _{2h}	1

O_h Total 22

C _s	6
C _i	5
S ₆	4
C ₃	4
D _{3d}	1
C _{2v}	1
C ₂	1

T Total 9

T	5
C ₂	2
C ₃	2

T_h Total 1

T	1
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Favourite sites for molecules of particular crystallographic point group symmetries in One-R. Only point groups that have less than 75 members.

C₄, Total 38

C ₄ in P4/n	9	
C ₁ in Pna2 ₁	9	
C ₄ in P4nc	5	
C ₄ in I4		4
C ₄ in P4/ncc	2	
C ₂ in C2/c	2	
Rest	7	

C_{4h}, Total 17

C _{4h} in I4/m	7
C _i in P2 ₁ /c	4
C _i in P-1	3
C _i in Pccn	2
C _i in Pbca	1
Rest	0

C_{4v}, Total 36

C ₁ in P2 ₁ /c	6
C ₁ in P-1	5
C _s in Pnma	5
C ₄ in I4mm	3
C ₁ in Pbca	2
C _s in P2 ₁ /m	2
Rest	13

D₄, Total 37

C ₂ in C2/c	10
C ₂ in I4 ₁ /acd	5
D ₄ in P4/nnc	3
D ₂ in I4 ₁ /acd	3
C ₂ in Pnn2	3
C ₂ in Pbcn	3
Rest	0

C_{3h}, Total 55

C _{3h} in P63/m	27
C ₃ in R-3	7
C ₁ in P2 ₁ /c	5
C ₃ in P213	3
C ₁ in P-1	3
C ₃ in P-3c1	2
Rest	8

C₆ Total 2

C ₁ in P-1	1
C ₆ in P6cc	1

C_{6h} Total 1

C _i in C2/c	1
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C_{6v} Total 0**D₆ Total 1**

C ₂ in I2/c	1
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D_{6h}, Total 20

C _i in P2 ₁ /c	9
C _i in Pbca	2
S ₆ in Pa3	2
C ₁ in P2 ₁ /c	2
D _{2h} in Fmmm	1
C _i in C2/c	1
Rest	3

O_h, Total 22

C _s in Pnma	4
C _i in P2 ₁ /c	3
S ₆ in R-3	3
C _i in P-1	2
C ₃ in Fd-3c	2
D _{3d} in R-3m	1