

CSD Organic Space Group Statistics – Space Group Frequency Ordering

Space group frequency ranking for the 653,326 organic CSD structures for which the space group is fully defined. Statistics for enantiomorphous space groups are as reported in the CSD. 460,797 (71 %) structures adopt centrosymmetric space groups, 192,529 (29 %) adopt non-centrosymmetric space groups, and 157,933 (24 %) structures adopt Sohncke space groups.

Rank	SG No.	Space Group	No. organics in CSD	% of organics in CSD
1	14	P21/c	223,278	34.2
2	2	P-1	143,374	21.9
3	19	P212121	71,945	11.0
4	4	P21	54,347	8.3
5	15	C2/c	41,165	6.3
6	61	Pbca	22,827	3.5
7	33	Pna21	10,107	1.5
8	1	P1	9,160	1.4
9	5	C2	7,821	1.2
10	9	Cc	6,630	1.0
11	29	Pca21	6,202	0.9
12	62	Pnma	4,762	0.7
13	60	Pbcn	4,440	0.7
14	7	Pc	3,427	0.5
15	18	P21212	3,252	0.5
16	148	R-3	2,959	0.5
17	13	P2/c	2,820	0.4
18	11	P21/m	2,248	0.3
19	43	Fdd2	2,030	0.3
20	56	Pccn	1,944	<0.3
21	12	C2/m	1,653	<0.3
22	88	I41/a	1,643	<0.3
23	92	P41212	1,260	<0.3
24	20	C2221	1,045	<0.3
25	96	P43212	1,015	<0.3
26	146	R3	908	<0.3
27	36	Cmc21	722	<0.3
28	145	P32	714	<0.3
29	76	P41	708	<0.3
30	144	P31	690	<0.3
31	78	P43	676	<0.3
32	169	P61	640	<0.3
33	41	Aba2	606	<0.3
34	86	P42/n	602	<0.3
35	64	Cmca	600	<0.3
36	82	I-4	571	<0.3
37	170	P65	551	<0.3
38	114	P-421c	526	<0.3
39	167	R-3c	499	<0.3
40	152	P3121	494	<0.3
41	57	Pbcm	458	<0.3
42	161	R3c	443	<0.3

43	154	P3221	409	<0.3
44	176	P63/m	390	<0.3
45	45	Iba2	373	<0.3
46	147	P-3	355	<0.3
=47	31	Pmn21	327	<0.3
=47	85	P4/n	327	<0.3
49	63	Cmcm	313	<0.3
50	173	P63	301	<0.3
51	70	Fddd	298	<0.3
52	52	Pnna	294	<0.3
53	205	Pa-3	268	<0.3
54	113	P-421m	192	<0.3
=55	8	Cm	184	<0.3
=55	122	I-42d	184	<0.3
57	58	Pnnm	183	<0.3
58	54	Pcca	170	<0.3
59	79	I4	167	<0.3
60	110	I41cd	164	<0.3
61	160	R3m	160	<0.3
62	217	I-43m	148	<0.3
63	68	Ccca	146	<0.3
=64	80	I41	143	<0.3
=64	142	I41/acd	143	<0.3
66	166	R-3m	141	<0.3
67	129	P4/nmm	135	<0.3
68	3	P2	133	<0.3
69	72	Ibam	129	<0.3
70	87	I4/m	127	<0.3
71	155	R32	125	<0.3
72	198	P213	118	<0.3
73	34	Pnn2	117	<0.3
74	59	Pmmn	114	<0.3
75	159	P31c	111	<0.3
=76	165	P-3c1	110	<0.3
=76	81	P-4	110	<0.3
78	178	P6122	103	<0.3
79	55	Pbam	101	<0.3
80	40	Ama2	96	<0.3
81	73	Ibca	95	<0.3
82	194	P63/mmc	92	<0.3
83	143	P3	90	<0.3
=84	26	Pmc21	89	<0.3
=84	225	Fm-3m	89	<0.3
=84	23	I222	89	<0.3
=87	32	Pba2	80	<0.3
=87	130	P4/ncc	80	<0.3
89	163	P-31c	74	<0.3
90	179	P6522	73	<0.3
91	94	P42212	72	<0.3
=92	77	P42	69	<0.3
=92	150	P321	69	<0.3
94	126	P4/nnc	64	<0.3
=95	137	P42/nmc	63	<0.3
=95	37	Ccc2	63	<0.3
97	186	P63mc	61	<0.3
98	106	P42bc	57	<0.3

=99	221	Pm-3m	56	<0.3
=99	227	Fd-3m	56	<0.3
101	30	Pnc2	55	<0.3
102	53	Pmna	53	<0.3
=103	141	I41/amd	51	<0.3
=103	171	P62	51	<0.3
=103	118	P-4n2	51	<0.3
106	46	Ima2	50	<0.3
107	136	P42/mnm	49	<0.3
=108	17	P2221	47	<0.3
=108	172	P64	47	<0.3
=110	220	I-43d	46	<0.3
=110	210	F4132	46	<0.3
=112	197	I23	45	<0.3
=112	190	P-62c	45	<0.3
=114	158	P3c1	44	<0.3
=114	90	P4212	44	<0.3
=116	121	I-42m	42	<0.3
=116	84	P42/m	42	<0.3
118	128	P4/mnc	41	<0.3
=119	182	P6322	39	<0.3
=119	206	Ia-3	39	<0.3
121	10	P2/m	37	<0.3
=122	42	Fmm2	36	<0.3
=122	139	I4/mmm	36	<0.3
124	67	Cmma	34	<0.3
=125	187	P-6m2	33	<0.3
=125	191	P6/mmm	33	<0.3
=125	211	I432	33	<0.3
=128	138	P42/ncm	31	<0.3
=128	164	P-3m1	31	<0.3
130	229	Im-3m	30	<0.3
=131	120	I-4c2	29	<0.3
=131	124	P4/mcc	29	<0.3
=131	180	P6222	29	<0.3
=131	218	P-43n	29	<0.3
=131	135	P42/mbc	29	<0.3
=136	50	Pban	28	<0.3
=136	39	Abm2	28	<0.3
=136	207	P432	28	<0.3
=139	203	Fd-3	27	<0.3
=139	21	C222	27	<0.3
=139	175	P6/m	27	<0.3
=139	230	Ia-3d	27	<0.3
143	117	P-4b2	26	<0.3
144	75	P4	25	<0.3
=145	228	Fd-3c	24	<0.3
=145	71	Immm	24	<0.3
=145	91	P4122	24	<0.3
=145	226	Fm-3c	24	<0.3
=145	204	Im-3	24	<0.3
=145	133	P42/nbc	24	<0.3
=151	74	Imma	23	<0.3
=151	223	Pm-3n	23	<0.3
=153	215	P-43m	22	<0.3
=153	219	F-43c	22	<0.3

=153	123	P4/mmm	22	<0.3
=153	193	P63/mcm	22	<0.3
=157	199	I213	21	<0.3
=157	66	Cccm	21	<0.3
=157	222	Pn-3n	21	<0.3
=160	65	Cmmm	20	<0.3
=160	44	Imm2	20	<0.3
=160	51	Pmma	20	<0.3
=163	104	P4nc	19	<0.3
=163	16	P222	19	<0.3
=163	202	Fm-3	19	<0.3
=163	69	Fmmm	19	<0.3
=167	48	Pnnn	18	<0.3
=167	168	P6	18	<0.3
=169	95	P4322	17	<0.3
=169	140	I4/mcm	17	<0.3
=169	98	I4122	17	<0.3
=172	214	I4132	16	<0.3
=172	27	Pcc2	16	<0.3
=174	24	I212121	15	<0.3
=174	109	I41md	15	<0.3
=174	38	Amm2	15	<0.3
=174	112	P-42c	15	<0.3
=178	22	F222	14	<0.3
=178	153	P3212	14	<0.3
=178	201	Pn-3	14	<0.3
=178	213	P4132	14	<0.3
=182	97	I422	13	<0.3
=182	103	P4cc	13	<0.3
=184	185	P63cm	12	<0.3
=184	6	Pm	12	<0.3
=184	196	F23	12	<0.3
=184	116	P-4c2	12	<0.3
=184	174	P-6	12	<0.3
=184	162	P-31m	12	<0.3
=190	189	P-62m	11	<0.3
=190	212	P4332	11	<0.3
=190	195	P23	11	<0.3
=190	181	P6422	11	<0.3
194	151	P3112	10	<0.3
=195	192	P6/mcc	8	<0.3
=195	216	F-43m	8	<0.3
=195	108	I4cm	8	<0.3
=195	47	Pmmm	8	<0.3
=195	208	P4232	8	<0.3
=195	107	I4mm	8	<0.3
=201	177	P622	7	<0.3
=201	102	P42nm	7	<0.3
=201	83	P4/m	7	<0.3
=201	184	P6cc	7	<0.3
=201	28	Pma2	7	<0.3
=206	188	P-6c2	6	<0.3
=206	35	Cmm2	6	<0.3
=206	157	P31m	6	<0.3
=209	127	P4/mbm	5	<0.3
=209	100	P4bm	5	<0.3

=209	134	P42/nnm	5	<0.3
=212	131	P42/mmc	4	<0.3
=212	25	Pmm2	4	<0.3
=212	89	P422	4	<0.3
=212	149	P312	4	<0.3
=216	101	P42cm	3	<0.3
=216	224	Pn-3m	3	<0.3
=216	99	P4mm	3	<0.3
=216	209	F432	3	<0.3
=220	49	Pccm	2	<0.3
=220	105	P42mc	2	<0.3
=220	125	P4/nbm	2	<0.3
=220	115	P-4m2	2	<0.3
=220	93	P4222	2	<0.3
=220	183	P6mm	2	<0.3
=220	200	Pm-3	2	<0.3
227	119	I-4m2	1	<0.3