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| **PD-29-10\_Pawley** | | | | |
| Space Group: *P*3 (143)  *a* = 23.0171 Å, *b* = 23.0171 Å, *c* = 4.1494 Å  *α* = *β* = 90.00 °, *γ* = 120.00 ° | | | | |
| **Atom label** | **Atom type** | ***x*** | ***y*** | ***z*** |
| C1 | C | 0.61697 | 0.69676 | -0.01944 |
| C2 | C | 0.60046 | 0.73840 | 0.15973 |
| C3 | C | 0.64241 | 0.80801 | 0.15591 |
| C4 | C | 0.70230 | 0.83667 | -0.01850 |
| C5 | C | 0.72018 | 0.79575 | -0.19019 |
| C6 | C | 0.67775 | 0.72617 | -0.19155 |
| H7 | H | 0.55506 | 0.71708 | 0.30183 |
| H8 | H | 0.62885 | 0.83964 | 0.29168 |
| H9 | H | 0.73497 | 0.89055 | -0.01966 |
| H10 | H | 0.76660 | 0.81800 | -0.32538 |
| H11 | H | 0.69190 | 0.69530 | -0.33027 |
| C12 | C | 0.60169 | 0.58310 | 0.05868 |
| C13 | C | 0.57275 | 0.62253 | -0.01707 |
| H14 | H | 0.65470 | 0.60703 | 0.11485 |
| C16 | C | 0.26499 | 0.63449 | -0.26619 |
| N17 | N | 0.29750 | 0.59890 | -0.26498 |
| C18 | C | 0.73852 | 0.35700 | 0.20146 |
| C19 | C | 0.76335 | 0.32101 | 0.03154 |
| C20 | C | 0.83210 | 0.34584 | -0.00163 |
| C21 | C | 0.87833 | 0.40794 | 0.13250 |
| C22 | C | 0.85442 | 0.44369 | 0.30792 |
| C23 | C | 0.78553 | 0.41817 | 0.34484 |
| N24 | N | 0.98821 | 0.50475 | 0.01200 |
| C25 | C | 0.95090 | 0.43785 | 0.06981 |
| C26 | C | 0.08702 | 0.49701 | -0.08542 |
| C27 | C | 0.05433 | 0.53508 | -0.06368 |
| C28 | C | 0.08956 | 0.60408 | -0.12305 |
| C29 | C | 0.15768 | 0.63639 | -0.19888 |
| C30 | C | 0.19132 | 0.59975 | -0.22216 |
| C31 | C | 0.15510 | 0.52994 | -0.17564 |
| H32 | H | 0.72981 | 0.27393 | -0.08101 |
| H33 | H | 0.84892 | 0.31768 | -0.14447 |
| H34 | H | 0.88908 | 0.49180 | 0.41414 |
| H35 | H | 0.76926 | 0.44795 | 0.47389 |
| H36 | H | 0.06436 | 0.63305 | -0.10593 |
| H37 | H | 0.18412 | 0.69021 | -0.23459 |
| H38 | H | 0.18093 | 0.50207 | -0.20479 |
| N15 | N | 0.66667 | 0.33333 | 0.21468 |

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| **PD-29-11\_Pawley** | | | | |
| Space Group: *P*3 (143)  *a* = 23.4203 Å, *b* = 23.4203 Å, *c* = 3.9837 Å  *α* = *β* = 90.00 °, *γ* = 120.00 ° | | | | |
| **Atom label** | **Atom type** | ***x*** | ***y*** | ***z*** |
| C1 | C | 0.61327 | 0.68927 | -0.01268 |
| C2 | C | 0.59759 | 0.73012 | -0.20308 |
| C3 | C | 0.64085 | 0.79809 | -0.21033 |
| N4 | N | 0.69941 | 0.82454 | -0.04574 |
| C5 | C | 0.71721 | 0.78632 | 0.13130 |
| C6 | C | 0.67454 | 0.71831 | 0.15253 |
| H7 | H | 0.55254 | 0.70976 | -0.34676 |
| H8 | H | 0.62840 | 0.82967 | -0.35301 |
| H9 | H | 0.76412 | 0.80885 | 0.26031 |
| H10 | H | 0.68884 | 0.68883 | 0.30163 |
| C11 | C | 0.56817 | 0.61633 | 0.00189 |
| C12 | C | 0.59596 | 0.57568 | -0.04251 |
| H13 | H | 0.64830 | 0.59770 | -0.09053 |
| C15 | C | 0.26608 | 0.63591 | 0.17539 |
| N16 | N | 0.29719 | 0.60003 | 0.17445 |
| C17 | C | 0.73839 | 0.36034 | -0.08823 |
| C18 | C | 0.76658 | 0.32671 | 0.07257 |
| C19 | C | 0.83481 | 0.35279 | 0.08523 |
| C20 | C | 0.87777 | 0.41416 | -0.06038 |
| C21 | C | 0.85068 | 0.44849 | -0.21988 |
| C22 | C | 0.78225 | 0.42167 | -0.23662 |
| N23 | N | 0.98926 | 0.50982 | 0.00397 |
| C24 | C | 0.95041 | 0.44356 | -0.03406 |
| C25 | C | 0.08707 | 0.50106 | 0.05501 |
| C26 | C | 0.05564 | 0.53932 | 0.04585 |
| C27 | C | 0.09252 | 0.60778 | 0.08483 |
| C28 | C | 0.16069 | 0.63924 | 0.13094 |
| C29 | C | 0.19304 | 0.60246 | 0.14755 |
| C30 | C | 0.15549 | 0.53340 | 0.12023 |
| H31 | H | 0.73617 | 0.27979 | 0.18901 |
| H32 | H | 0.85386 | 0.32556 | 0.21847 |
| H33 | H | 0.88247 | 0.49606 | -0.33415 |
| H34 | H | 0.76415 | 0.45031 | -0.35820 |
| H35 | H | 0.06840 | 0.63695 | 0.07622 |
| H36 | H | 0.18801 | 0.69246 | 0.15276 |
| H37 | H | 0.18048 | 0.50565 | 0.14941 |
| N14 | N | 0.66667 | 0.33333 | -0.09420 |

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| **PD-29-13\_Pawley** | | | | |
| Space Group: *P*3 (143)  *a* = 22.9415 Å, *b* = 22.9415 Å, *c* = 3.9302 Å  *α* = *β* = 90.00 °, *γ* = 120.00 ° | | | | |
| **Atom label** | **Atom type** | ***x*** | ***y*** | ***z*** |
| N1 | N | 0.61640 | 0.69698 | -0.03760 |
| C2 | C | 0.60607 | 0.74350 | 0.11813 |
| N3 | N | 0.65829 | 0.80616 | 0.07335 |
| C4 | C | 0.70367 | 0.79904 | -0.11180 |
| C5 | C | 0.67813 | 0.73158 | -0.17835 |
| C6 | C | 0.60365 | 0.58593 | 0.05935 |
| C7 | C | 0.57429 | 0.62484 | -0.02677 |
| H8 | H | 0.65682 | 0.61067 | 0.11882 |
| C9 | C | 0.26479 | 0.63388 | -0.30328 |
| N10 | N | 0.29789 | 0.59868 | -0.30195 |
| C11 | C | 0.73886 | 0.35625 | 0.22961 |
| C12 | C | 0.76337 | 0.31852 | 0.06166 |
| C13 | C | 0.83215 | 0.34262 | 0.02516 |
| C14 | C | 0.87909 | 0.40599 | 0.15289 |
| C15 | C | 0.85583 | 0.44342 | 0.32887 |
| C16 | C | 0.78695 | 0.41842 | 0.37090 |
| N17 | N | 0.98849 | 0.50290 | 0.01472 |
| C18 | C | 0.95153 | 0.43584 | 0.07808 |
| C19 | C | 0.08741 | 0.49554 | -0.09962 |
| C20 | C | 0.05443 | 0.53347 | -0.07229 |
| C21 | C | 0.08913 | 0.60254 | -0.13791 |
| C22 | C | 0.15709 | 0.63509 | -0.22478 |
| C23 | C | 0.19106 | 0.59859 | -0.25257 |
| C24 | C | 0.15528 | 0.52860 | -0.20053 |
| H25 | H | 0.72985 | 0.27044 | -0.04715 |
| H26 | H | 0.84828 | 0.31292 | -0.11843 |
| H27 | H | 0.89099 | 0.49258 | 0.43080 |
| H28 | H | 0.77184 | 0.44996 | 0.49837 |
| H29 | H | 0.06365 | 0.63138 | -0.11678 |
| H30 | H | 0.18322 | 0.68902 | -0.26461 |
| H31 | H | 0.18122 | 0.50076 | -0.23396 |
| H32 | H | 0.56205 | 0.73218 | 0.26730 |
| H33 | H | 0.66307 | 0.85086 | 0.16804 |
| H34 | H | 0.75210 | 0.84001 | -0.19071 |
| H35 | H | 0.70281 | 0.70948 | -0.31943 |
| N36 | N | 0.66667 | 0.33333 | 0.24251 |

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| **PD-29-14\_Pawley** | | | | |
| Space Group: *P*3 (143)  *a* = 23.4095 Å, *b* = 23.4095 Å, *c* = 4.2474 Å  *α* = *β* = 90.00 °, *γ* = 120.00 ° | | | | |
| **Atom label** | **Atom type** | ***x*** | ***y*** | ***z*** |
| C1 | C | 0.61481 | 0.68899 | -0.03192 |
| C2 | C | 0.60443 | 0.73374 | 0.14784 |
| C3 | C | 0.64741 | 0.80171 | 0.12228 |
| C4 | C | 0.70313 | 0.82595 | -0.06941 |
| C5 | C | 0.71571 | 0.78231 | -0.23851 |
| C6 | C | 0.67173 | 0.71436 | -0.22307 |
| F7 | F | 0.55370 | 0.71185 | 0.35433 |
| F8 | F | 0.63579 | 0.84412 | 0.29054 |
| F9 | F | 0.74529 | 0.89186 | -0.08956 |
| F10 | F | 0.77012 | 0.80595 | -0.42330 |
| F11 | F | 0.68415 | 0.67360 | -0.40065 |
| C12 | C | 0.59684 | 0.57561 | 0.04026 |
| C13 | C | 0.56903 | 0.61603 | -0.01039 |
| H14 | H | 0.64965 | 0.59789 | 0.07041 |
| C16 | C | 0.26603 | 0.63612 | -0.12965 |
| N17 | N | 0.29695 | 0.59999 | -0.12872 |
| C18 | C | 0.73802 | 0.35990 | 0.12111 |
| C19 | C | 0.76547 | 0.32728 | -0.04445 |
| C20 | C | 0.83372 | 0.35351 | -0.06177 |
| C21 | C | 0.87710 | 0.41354 | 0.08641 |
| C22 | C | 0.85031 | 0.44655 | 0.25188 |
| C23 | C | 0.78185 | 0.41990 | 0.27050 |
| N24 | N | 0.98910 | 0.50961 | 0.04022 |
| C25 | C | 0.94984 | 0.44300 | 0.05730 |
| C26 | C | 0.08633 | 0.50077 | -0.03869 |
| C27 | C | 0.05544 | 0.53924 | -0.00374 |
| C28 | C | 0.09285 | 0.60808 | -0.01870 |
| C29 | C | 0.16101 | 0.63970 | -0.06463 |
| C30 | C | 0.19289 | 0.60283 | -0.10402 |
| C31 | C | 0.15474 | 0.53355 | -0.10165 |
| H32 | H | 0.73421 | 0.28144 | -0.16316 |
| H33 | H | 0.85242 | 0.32747 | -0.19947 |
| H34 | H | 0.88235 | 0.49300 | 0.36811 |
| H35 | H | 0.76335 | 0.44716 | 0.39640 |
| H36 | H | 0.06917 | 0.63742 | 0.00917 |
| H37 | H | 0.18875 | 0.69311 | -0.06676 |
| H38 | H | 0.17936 | 0.50587 | -0.14495 |
| N15 | N | 0.66667 | 0.33333 | 0.12933 |