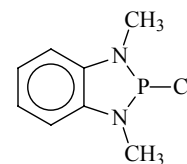
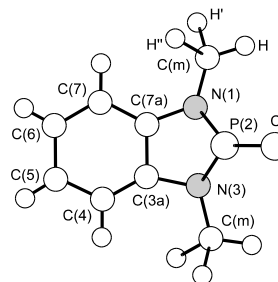


845  $C_8H_{10}ClN_2P$ ED, *ab initio*  
calculations**2-Chloro-2,3-dihydro-1,3-dimethyl-1*H*-1,3,2-benzodiazaphosphole** $C_s$ , assumed2-Chloro-1,3-dimethyl-1*H*-1,3,2-benzodiazaphospholine

2-Chloro-1,3-dimethyl-1,3,2-benzodiazaphospholine

| $r_{hl}^a)$ | $\text{\AA}^b)$ | $\theta_{hl}^a)$   | deg $^b)$ |
|-------------|-----------------|--------------------|-----------|
| P–Cl        | 2.183(5)        | N–P–Cl             | 103.0(4)  |
| P–N         | 1.698(4)        | N–P–N              | 89.1(3)   |
| N–C(m)      | 1.454(6)        | P–N–C(m)           | 124.8(4)  |
| N–C(7a)     | 1.411(4)        | C(7a)–N–C(m)       | 120.3(5)  |
| C(7a)–C(3a) | 1.405(3)        | P–N–C(7a)          | 112.3(2)  |
| C(7)–C(7a)  | 1.383(3)        | N–C(7a)–C(3a)      | 110.3(1)  |
| C(6)–C(7)   | 1.403(3)        | N–C(7a)–C(7)       | 129.2(3)  |
| C(5)–C(6)   | 1.387(3)        | C(3a)–C(7a)–C(7)   | 120.5(2)  |
| C(7)–H      | 1.068(4)        | C(7a)–C(7)–C(6)    | 119.0(4)  |
| C(6)–H      | 1.069(4)        | C(7)–C(6)–C(5)     | 120.5(2)  |
| C(m)–H      | 1.076(4)        | C(7a)–C(7)–H       | 124(2)    |
| C(m)–H'     | 1.080(4)        | C(6)–C(7)–H        | 117(2)    |
| C(m)–H''    | 1.078(4)        | C(7)–C(6)–H        | 117(2)    |
|             |                 | C(5)–C(6)–H        | 123(2)    |
|             |                 | $\varphi^c)$       | 21.3(10)  |
|             |                 | $\phi^d)$          | 71.7(5)   |
|             |                 | N–P–N–C(m)         | 177(2)    |
|             |                 | C(3a)–C(7a)–N–C(m) | 179(2)    |
|             |                 | C(7)–C(7a)–N–C(m)  | 2(2)      |
|             |                 | Cl–P–N–C(m)        | 80(2)     |
|             |                 | Cl–P–N–C(7a)       | –82(1)    |
|             |                 | P–N–C(m)–H         | 23(2)     |
|             |                 | P–N–C(m)–H'        | –97(2)    |
|             |                 | P–N–C(m)–H''       | –142(2)   |

The temperature of the measurements was *ca.* 473 K.<sup>a)</sup> Nonlinear kinematic effects were taken into account.<sup>b)</sup> Estimated standard errors including a systematic error.<sup>c)</sup> Dihedral angle between the NPN and  
NC(7a)C(3a)N planes.<sup>d)</sup> Angle between the P–Cl bond and the NPN plane.

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