Table 1 Atomic coordinates of Model I. In parentheses are those obtained by Refinement I.

Atom	*x*	*y*	*z*
Cu1	0	0	0
C1	0. 176951	0.164158	0.154347
	(0. 174(3))	(0. 148(17))	(0. 158(3))
C2	0. 203070	0. 332498	0. 264962
	(0. 198(4))	(0. 36(4))	(0. 265(5))
C3	0. 295249	0. 383876	0. 324560
	(0. 286(2))	(0. 42(3))	(0. 329(6))
C4	0. 293466	0. 558562	0. 430482
	(0. 277(3))	(0. 62(3))	(0. 432(6))
C5	0. 198911	0. 683967	0. 477902
	(0. 180(4))	(0. 74(4))	(0. 473(6))
C6	0. 107605	0. 632738	0. 418663
	(0. 096(4))	(0. 716(19))	(0. 406(8))
C7	0. 109581	0. 456489	0. 311847
	(0. 102(2))	(0. 49(4))	(0. 308(6))
C8	0. 030250	0. 358722	0. 227918
	(0. 0242(13))	(0. 330(13))	(0. 2342(19))
C9	-0. 141527	0. 347527	0. 168388
	(-0. 1413(18))	(0. 36(2))	(0. 170(3))
C10	-0. 249741	0. 433072	0. 187323
	(-0. 2442(16))	(0. 505(7))	(0. 185(2))
C11	-0. 302781	0. 605995	0. 276443
	(-0. 296(2))	(0. 686(11))	(0. 276(4))
C12	-0. 408210	0. 644404	0. 267503
	(-0. 402(2))	(0. 68(2))	(0. 278(4))
C13	-0.461728	0.509351	0.168769
	(-0.456(2))	(0.43(2))	(0.206(2))
C14	-0.408986	0.337985	0.080507
	(-0.410(3))	(0.29(2))	(0.106(4))
C15	-0.302655	0.299544	0.089703
	(-0.3024(15))	(0.328(16))	(0.095(3))
C16	-0.224559	0.137995	0.015204
	(-0.224(3))	(0.15(2))	(0.017(3))
N1	0.248111	0.016168	0.085983
	(0.248(3))	(0.017(19))	(0.085(4))
N2	0.073030	0.184294	0.134733
	(0.0686(13))	(0.140(15))	(0.1419(17))
N3	-0.068763	0.436422	0.244895

	(-0.0745(14))	(0.394(15))	(0.2519(15))
N4	-0.129030	0.171126	0.064709
	(-0.129(2))	(0.17(3))	(0.066(5))
H1	0.367266	0.288364	0.288444
H2	0.364763	0.599857	0.477527
H3	0. 198191	0. 820774	0. 561063
H4	0. 035588	0. 728252	0. 454780
H5	-0. 262020	0. 708858	0. 351643
H6	-0. 450178	0. 778526	0. 336371
H7	-0. 544456	0. 540610	0. 162437
H8	-0. 449747	0. 235124	0. 005307

Table 2 Atomic coordinates of Model II. In parentheses are those obtained by Refinement II.

Atom	*x*	*y*	*z*
Cu1	0	0	0
C1	0.225372	-0.060174	0.036695
	(0.2276(19))	(-0.08(2))	(0.036(3))
C2	0.306813	0.032743	0.118582
	(0.312(3))	(0.04(2))	(0.115(5))
C3	0.412804	-0.022718	0.119583
	(0.419(4))	(-0.02(2))	(0.117(3))
C4	0.469484	0.102456	0.212788
	(0.473(3))	(0.08(3))	(0.217(7))
C5	0.420301	0.285162	0.306273
	(0.428(7))	(0.32(3))	(0.299(6))
C6	0.315202	0.339860	0.305103
	(0.322(3))	(0.38(3))	(0.297(8))
C7	0.258186	0.213388	0.211013
	(0.265(5))	(0.25(3))	(0.204(7))
C8	0.149066	0.223292	0.181736
	(0.155(5))	(0.22(3))	(0.182(5))
C9	-0.020185	0.386371	0.224737
	(-0.016(4))	(0.38(2))	(0.232(3))
C10	-0.095852	0.554517	0.300963
	(-0.089(3))	(0.57(4))	(0.308(7))
C11	-0.089149	0.729467	0.407836
	(-0.0762(19))	(0.77(3))	(0.410(7))
C12	-0.177891	0.861543	0.458255
	(-0.163(2))	(0.89(3))	(0.467(6))

C13	-0.274603	0.819411	0.401837
	(-0.262(4))	(0.83(3))	(0.417(5))
C14	-0.281074	0.645858	0.295875
	(-0.272(4))	(0.70(3))	(0.306(5))
C15	-0.191474	0.512860	0.245181
	(-0.186(2))	(0.55(3))	(0.253(5))
C16	-0.170233	0.321006	0.137206
	(-0.168(2))	(0.34(3))	(0.143(5))
N1	0.244462	-0.235548	-0.062110
	(0.245(2))	(-0.26(2))	(-0.067(4))
N2	0.131974	0.057492	0.076988
	(0.134(2))	(0.05(2))	(0.077(5))
N3	0.079642	0.376738	0.251178
	(0.086(4))	(0.37(3))	(0.256(5))
N4	-0.067115	0.249321	0.127570
	(-0.064(2))	(0.25(2))	(0.132(3))
H1	0.450263	-0.161874	0.048381
H2	0. 551984	0. 060659	0. 214388
H3	0. 465342	0. 382521	0. 379075
H4	0. 277742	0. 479017	0. 376305
H5	-0. 015489	0. 761556	0. 450806
H6	-0. 173491	0. 998059	0. 541382
H7	-0. 343863	0. 923839	0. 441994
H8	-0. 354734	0. 613769	0. 252905