Table 1. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for Molecule 5.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
F1	0.25288(5)	0.24470(11)	0.16615(6)	0.0385(3)
F2	0.35512(5)	0.26785(9)	0.29537(5)	0.0299(2)
F3	0.42060(5)	0.66986(10)	0.20302(5)	0.0319(2)
F5	0.25097(5)	0.21621(11)	0.36996(7)	0.0439(3)
F6	0.15299(5)	0.25127(10)	0.42183(6)	0.0357(2)
F7	0.08365(5)	0.64067(10)	0.26695(5)	0.0331(2)
N1	0.28130(7)	0.44133(15)	0.12443(7)	0.0285(3)
N2	0.44971(6)	0.47822(13)	0.32083(7)	0.0224(3)
N3	0.48494(7)	0.35534(14)	0.33301(7)	0.0240(3)
N4	0.22258(7)	0.41106(15)	0.30301(8)	0.0324(3)
F4	0.30762(5)	0.63876(11)	0.08192(5)	0.0384(3)
N5	0.05685(6)	0.45798(14)	0.36610(7)	0.0242(3)
N6	0.02123(7)	0.33526(14)	0.35121(7)	0.0258(3)
C1	0.29461(8)	0.35136(17)	0.17756(9)	0.0271(4)
C2	0.34760(8)	0.36125(16)	0.24332(9)	0.0233(3)
C3	0.39240(7)	0.47026(16)	0.25472(8)	0.0218(3)
C4	0.37918(8)	0.56393(16)	0.19785(9)	0.0239(3)
C5	0.32263(8)	0.54564(17)	0.13561(9)	0.0265(3)
C6	0.54000(8)	0.34680(16)	0.39226(8)	0.0230(3)
C7	0.56347(8)	0.45719(17)	0.44216(8)	0.0240(3)
C8	0.52264(8)	0.58148(17)	0.42846(9)	0.0242(3)
F8	0.19524(5)	0.60518(11)	0.23612(5)	0.0376(2)
C9	0.46550(8)	0.59068(16)	0.36670(8)	0.0227(3)
C10	0.55412(8)	0.67327(17)	0.48767(9)	0.0274(4)
C11	0.61161(8)	0.60953(18)	0.53360(9)	0.0301(4)
C12	0.61842(8)	0.47770(18)	0.50649(9)	0.0285(4)
C13	0.42113(8)	0.71293(16)	0.34940(8)	0.0232(3)
C14	0.44994(9)	0.84302(17)	0.35257(9)	0.0275(4)
C15	0.41050(9)	0.96069(18)	0.34024(9)	0.0319(4)
C16	0.34217(9)	0.94923(18)	0.32455(10)	0.0335(4)

	x/a	y/b	z/c	U(eq)
C17	0.31353(9)	0.82036(18)	0.32161(9)	0.0309(4)
C18	0.35247(8)	0.70255(17)	0.33382(8)	0.0256(3)
C19	0.57489(7)	0.21186(16)	0.40250(9)	0.0237(3)
C20	0.58078(8)	0.14304(17)	0.34299(9)	0.0276(4)
C21	0.61393(9)	0.01773(19)	0.35316(10)	0.0347(4)
C22	0.64072(9)	0.95910(19)	0.42222(10)	0.0375(4)
C23	0.63400(9)	0.02557(19)	0.48110(10)	0.0346(4)
C24	0.60166(8)	0.15121(18)	0.47172(9)	0.0289(4)
C25	0.18105(8)	0.51488(18)	0.27947(9)	0.0286(4)
C26	0.12533(8)	0.53582(17)	0.29681(9)	0.0256(3)
C27	0.11353(8)	0.44663(16)	0.34569(9)	0.0240(3)
C28	0.15846(8)	0.33907(17)	0.37193(9)	0.0275(4)
C29	0.20994(8)	0.32445(17)	0.34727(10)	0.0315(4)
C30	0.96542(8)	0.33151(16)	0.36437(8)	0.0238(3)
C31	0.94164(8)	0.44596(16)	0.39208(8)	0.0231(3)
C32	0.98280(8)	0.57063(16)	0.40949(8)	0.0230(3)
C33	0.04090(8)	0.57454(16)	0.39612(8)	0.0230(3)
C34	0.94992(8)	0.66737(17)	0.43911(9)	0.0261(4)
C35	0.89170(8)	0.60657(18)	0.43767(9)	0.0282(4)
C36	0.88603(8)	0.47077(17)	0.40936(8)	0.0262(3)
C37	0.92982(7)	0.19700(17)	0.34792(9)	0.0241(3)
C38	0.92334(8)	0.12488(18)	0.28451(9)	0.0289(4)
C39	0.89095(9)	0.99860(18)	0.27014(10)	0.0346(4)
C40	0.86500(9)	0.94267(18)	0.31870(10)	0.0348(4)
C41	0.87131(9)	0.01392(18)	0.38171(10)	0.0330(4)
C42	0.90323(8)	0.14000(18)	0.39647(9)	0.0289(4)
C43	0.08720(8)	0.69399(17)	0.41426(8)	0.0239(3)
C44	0.06085(9)	0.82510(17)	0.39222(9)	0.0274(4)
C45	0.10241(9)	0.93943(18)	0.41109(9)	0.0317(4)
C46	0.17031(9)	0.92406(18)	0.45118(10)	0.0338(4)
C47	0.19697(9)	0.79402(18)	0.47370(9)	0.0309(4)
C48	0.15559(8)	0.67947(17)	0.45567(8)	0.0256(3)

Table 2. Bond lengths (Å) for Molecule 5.

F1-C1	1.3322(19)	F2-C2	1.3327(18)
F3-C4	1.3383(18)	F5-C29	1.336(2)
F6-C28	1.339(2)	F7-C26	1.3377(19)
N1-C5	1.310(2)	N1-C1	1.310(2)
N2-C9	1.376(2)	N2-N3	1.3845(18)
N2-C3	1.422(2)	N3-C6	1.318(2)
N4-C29	1.310(2)	N4-C25	1.310(2)
F4-C5	1.3360(19)	N5-C33	1.378(2)
N5-N6	1.3865(18)	N5-C27	1.421(2)
N6-C30	1.318(2)	C1-C2	1.372(2)
C2-C3	1.391(2)	C3-C4	1.387(2)
C4-C5	1.378(2)	C6-C7	1.414(2)
C6-C19	1.485(2)	C7-C12	1.386(2)
C7-C8	1.456(2)	C8-C9	1.371(2)
C8-C10	1.422(2)	F8-C25	1.3359(19)
C9-C13	1.480(2)	C10-C11	1.376(2)
C11-C12	1.415(3)	C13-C18	1.393(2)
C13-C14	1.397(2)	C14-C15	1.388(2)
C15-C16	1.387(3)	C16-C17	1.385(3)
C17-C18	1.384(2)	C19-C20	1.395(2)
C19-C24	1.397(2)	C20-C21	1.386(2)
C21-C22	1.386(3)	C22-C23	1.381(3)
C23-C24	1.381(2)	C25-C26	1.376(2)
C26-C27	1.387(2)	C27-C28	1.384(2)
C28-C29	1.371(2)	C30-C31	1.414(2)
C30-C37	1.486(2)	C31-C36	1.379(2)
C31-C32	1.462(2)	C32-C33	1.368(2)
C32-C34	1.424(2)	C33-C43	1.482(2)
C34-C35	1.373(2)	C35-C36	1.419(2)
C37-C38	1.393(2)	C37-C42	1.398(2)
C38-C39	1.385(2)	C39-C40	1.385(3)
C40-C41	1.383(3)	C41-C42	1.380(2)
C43-C44	1.395(2)	C43-C48	1.396(2)
C44-C45	1.385(2)	C45-C46	1.383(3)
C46-C47	1.389(3)	C47-C48	1.384(2)

Table 3. Bond angles (°) for Molecule 5.

C5-N1-C1	116.66(14)	C9-N2-N3	125.77(12)
C9-N2-C3	124.18(13)	N3-N2-C3	110.01(12)
C6-N3-N2	117.33(13)	C29-N4-C25	116.50(14)
C33-N5-N6	126.18(13)	C33-N5-C27	124.15(13)
N6-N5-C27	109.67(12)	C30-N6-N5	116.90(13)
N1-C1-F1	116.78(14)	N1-C1-C2	124.37(15)
F1-C1-C2	118.84(15)	F2-C2-C1	119.92(14)
F2-C2-C3	121.02(14)	C1-C2-C3	119.06(14)
C4-C3-C2	116.57(14)	C4-C3-N2	123.41(14)
C2-C3-N2	119.97(13)	F3-C4-C5	120.45(14)
F3-C4-C3	120.79(14)	C5-C4-C3	118.76(15)
N1-C5-F4	116.21(14)	N1-C5-C4	124.48(15)
F4-C5-C4	119.31(15)	N3-C6-C7	122.51(14)
N3-C6-C19	114.59(13)	C7-C6-C19	122.90(14)
C12-C7-C6	134.87(15)	C12-C7-C8	107.38(14)
C6-C7-C8	117.72(14)	C9-C8-C10	132.94(15)
C9-C8-C7	119.74(14)	C10-C8-C7	107.33(14)
C8-C9-N2	116.79(14)	C8-C9-C13	122.87(14)
N2-C9-C13	120.32(13)	C11-C10-C8	107.05(15)
C10-C11-C12	110.61(15)	C7-C12-C11	107.61(15)
C18-C13-C14	119.32(14)	C18-C13-C9	122.03(14)
C14-C13-C9	118.56(14)	C15-C14-C13	120.31(15)
C16-C15-C14	119.92(16)	C17-C16-C15	119.87(15)
C18-C17-C16	120.58(15)	C17-C18-C13	119.99(15)
C20-C19-C24	119.02(15)	C20-C19-C6	120.49(14)
C24-C19-C6	120.49(14)	C21-C20-C19	120.09(16)
C20-C21-C22	120.33(16)	C23-C22-C21	119.83(17)
C22-C23-C24	120.32(17)	C23-C24-C19	120.39(16)
N4-C25-F8	116.32(14)	N4-C25-C26	124.44(15)
F8-C25-C26	119.24(15)	F7-C26-C25	120.27(14)
F7-C26-C27	120.97(15)	C25-C26-C27	118.75(15)
C28-C27-C26	116.59(15)	C28-C27-N5	120.26(14)
C26-C27-N5	123.07(14)	F6-C28-C29	119.83(15)
F6-C28-C27	120.97(15)	C29-C28-C27	119.19(15)
N4-C29-F5	116.91(15)	N4-C29-C28	124.33(16)
F5-C29-C28	118.76(16)	N6-C30-C31	122.69(14)
N6-C30-C37	114.38(14)	C31-C30-C37	122.93(14)

C36-C31-C30	134.65(15)	C36-C31-C32	107.51(14)
C30-C31-C32	117.83(14)	C33-C32-C34	133.43(15)
C33-C32-C31	119.52(14)	C34-C32-C31	107.05(14)
C32-C33-N5	116.77(14)	C32-C33-C43	123.59(14)
N5-C33-C43	119.62(13)	C35-C34-C32	107.15(15)
C34-C35-C36	110.57(15)	C31-C36-C35	107.70(14)
C38-C37-C42	119.01(15)	C38-C37-C30	120.54(14)
C42-C37-C30	120.44(14)	C39-C38-C37	120.16(16)
C40-C39-C38	120.43(16)	C41-C40-C39	119.61(16)
C42-C41-C40	120.50(16)	C41-C42-C37	120.29(16)
C44-C43-C48	119.36(14)	C44-C43-C33	118.76(14)
C48-C43-C33	121.80(14)	C45-C44-C43	120.10(15)
C46-C45-C44	120.22(16)	C45-C46-C47	120.11(15)
C48-C47-C46	119.96(15)	C47-C48-C43	120.24(15)

Table 4. Anisotropic atomic displacement parameters (Å^2) for Molecule 5.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
F1	0.0304(5)	0.0311(6)	0.0464(6)	-0.0042(4)	0.0056(5)	-0.0105(4)
F2	0.0325(5)	0.0224(5)	0.0342(5)	0.0053(4)	0.0118(4)	-0.0010(4)
F3	0.0347(5)	0.0298(5)	0.0321(5)	0.0020(4)	0.0137(4)	-0.0081(4)
F5	0.0317(5)	0.0303(6)	0.0724(8)	0.0003(5)	0.0226(5)	0.0067(4)
F6	0.0360(5)	0.0240(5)	0.0503(6)	0.0085(4)	0.0198(5)	0.0017(4)
F7	0.0353(5)	0.0320(5)	0.0305(5)	0.0052(4)	0.0106(4)	0.0043(4)
N1	0.0249(7)	0.0304(8)	0.0276(7)	-0.0028(6)	0.0068(6)	0.0024(6)
N2	0.0213(6)	0.0208(7)	0.0236(6)	-0.0005(5)	0.0065(5)	0.0012(5)
N3	0.0248(7)	0.0219(7)	0.0260(7)	0.0000(5)	0.0103(6)	0.0031(5)
N4	0.0270(7)	0.0328(8)	0.0406(8)	-0.0089(7)	0.0161(6)	-0.0066(6)
F4	0.0448(6)	0.0361(6)	0.0288(5)	0.0092(4)	0.0074(4)	0.0039(4)
N5	0.0229(7)	0.0212(7)	0.0301(7)	-0.0031(5)	0.0116(6)	-0.0029(5)
N6	0.0253(7)	0.0216(7)	0.0308(7)	-0.0027(5)	0.0110(6)	-0.0037(5)
C1	0.0217(8)	0.0236(9)	0.0350(9)	-0.0065(7)	0.0094(7)	-0.0016(6)
C2	0.0243(8)	0.0202(8)	0.0266(8)	0.0011(6)	0.0106(7)	0.0034(6)
C3	0.0204(7)	0.0226(8)	0.0228(8)	-0.0025(6)	0.0085(6)	0.0032(6)
C4	0.0252(8)	0.0215(8)	0.0270(8)	-0.0024(6)	0.0120(7)	-0.0014(6)
C5	0.0286(8)	0.0265(9)	0.0243(8)	0.0013(7)	0.0099(7)	0.0053(7)
C6	0.0215(8)	0.0254(8)	0.0245(8)	0.0023(6)	0.0113(7)	-0.0012(6)
C7	0.0224(8)	0.0267(9)	0.0246(8)	0.0020(6)	0.0106(7)	-0.0012(6)
C8	0.0236(8)	0.0247(8)	0.0258(8)	-0.0005(6)	0.0109(7)	-0.0030(6)
F8	0.0405(6)	0.0425(6)	0.0340(5)	0.0002(4)	0.0187(5)	-0.0116(5)
C9	0.0234(8)	0.0206(8)	0.0266(8)	-0.0008(6)	0.0120(7)	-0.0029(6)
C10	0.0283(8)	0.0265(9)	0.0282(8)	-0.0049(7)	0.0114(7)	-0.0042(7)
C11	0.0270(8)	0.0350(10)	0.0247(8)	-0.0046(7)	0.0057(7)	-0.0075(7)
C12	0.0231(8)	0.0325(9)	0.0276(8)	0.0017(7)	0.0068(7)	-0.0013(7)
C13	0.0282(8)	0.0216(8)	0.0197(7)	-0.0018(6)	0.0089(6)	-0.0008(6)
C14	0.0293(8)	0.0265(9)	0.0264(8)	-0.0004(7)	0.0102(7)	-0.0016(7)
C15	0.0411(10)	0.0221(9)	0.0326(9)	0.0010(7)	0.0139(8)	-0.0012(7)
C16	0.0421(10)	0.0237(9)	0.0333(9)	0.0005(7)	0.0124(8)	0.0073(7)
C17	0.0276(9)	0.0319(9)	0.0313(9)	-0.0009(7)	0.0089(7)	0.0040(7)
C18	0.0281(8)	0.0237(8)	0.0234(8)	-0.0021(6)	0.0077(7)	-0.0010(6)
C19	0.0194(7)	0.0234(8)	0.0282(8)	0.0003(6)	0.0085(6)	-0.0005(6)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C20	0.0276(8)	0.0278(9)	0.0279(8)	-0.0005(7)	0.0109(7)	-0.0028(7)
C21	0.0402(10)	0.0302(10)	0.0364(10)	-0.0060(8)	0.0175(8)	0.0022(8)
C22	0.0384(10)	0.0274(10)	0.0444(11)	-0.0003(8)	0.0126(8)	0.0086(7)
C23	0.0372(10)	0.0300(10)	0.0320(9)	0.0041(7)	0.0075(8)	0.0058(7)
C24	0.0292(9)	0.0290(9)	0.0283(8)	-0.0007(7)	0.0104(7)	0.0018(7)
C25	0.0292(9)	0.0314(9)	0.0264(8)	-0.0057(7)	0.0117(7)	-0.0096(7)
C26	0.0261(8)	0.0237(8)	0.0249(8)	-0.0033(7)	0.0071(7)	-0.0018(6)
C27	0.0214(8)	0.0224(8)	0.0286(8)	-0.0062(6)	0.0098(6)	-0.0052(6)
C28	0.0271(8)	0.0213(9)	0.0347(9)	-0.0014(7)	0.0123(7)	-0.0048(6)
C29	0.0240(8)	0.0243(9)	0.0454(10)	-0.0072(7)	0.0120(7)	-0.0006(7)
C30	0.0225(8)	0.0256(8)	0.0214(8)	0.0017(6)	0.0060(6)	0.0005(6)
C31	0.0211(8)	0.0251(8)	0.0202(8)	0.0024(6)	0.0044(6)	0.0000(6)
C32	0.0230(8)	0.0230(8)	0.0201(7)	0.0022(6)	0.0046(6)	0.0018(6)
C33	0.0239(8)	0.0222(8)	0.0211(8)	0.0024(6)	0.0062(6)	0.0018(6)
C34	0.0294(8)	0.0241(9)	0.0238(8)	0.0003(6)	0.0087(7)	0.0028(6)
C35	0.0266(8)	0.0323(9)	0.0267(8)	0.0018(7)	0.0111(7)	0.0064(7)
C36	0.0223(8)	0.0299(9)	0.0251(8)	0.0025(7)	0.0074(6)	0.0004(6)
C37	0.0197(8)	0.0238(8)	0.0266(8)	0.0001(6)	0.0061(6)	0.0001(6)
C38	0.0297(9)	0.0294(9)	0.0278(8)	0.0003(7)	0.0110(7)	-0.0002(7)
C39	0.0404(10)	0.0300(10)	0.0308(9)	-0.0071(7)	0.0102(8)	-0.0038(8)
C40	0.0344(9)	0.0261(9)	0.0395(10)	-0.0031(7)	0.0086(8)	-0.0077(7)
C41	0.0357(9)	0.0288(9)	0.0370(9)	0.0018(7)	0.0166(8)	-0.0061(7)
C42	0.0298(9)	0.0279(9)	0.0289(9)	-0.0030(7)	0.0109(7)	-0.0020(7)
C43	0.0276(8)	0.0249(8)	0.0205(8)	-0.0012(6)	0.0104(6)	-0.0016(6)
C44	0.0297(9)	0.0267(9)	0.0261(8)	0.0013(7)	0.0108(7)	0.0006(7)
C45	0.0419(10)	0.0210(9)	0.0334(9)	0.0024(7)	0.0155(8)	-0.0016(7)
C46	0.0398(10)	0.0264(9)	0.0357(9)	-0.0022(7)	0.0148(8)	-0.0102(7)
C47	0.0282(9)	0.0337(10)	0.0291(9)	-0.0012(7)	0.0088(7)	-0.0066(7)
C48	0.0282(8)	0.0243(9)	0.0249(8)	0.0003(6)	0.0105(7)	-0.0001(6)

Table 5. Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å^2) for Molecule 5.

	x/a	y/b	z/c	U(eq)
H10	0.5384	0.7619	0.4942	0.033
H11	0.6425	0.6486	0.5775	0.036
H12	0.6542	0.4147	0.5284	0.034
H14	0.4967	0.8510	0.3632	0.033
H15	0.4303	1.0490	0.3426	0.038
H16	0.3150	1.0296	0.3158	0.04
H17	0.2667	0.8128	0.3111	0.037
H18	0.3324	0.6146	0.3316	0.031
H20	0.5620	0.1822	0.2954	0.033
H21	0.6183	-0.0282	0.3126	0.042
H22	0.6636	-0.1266	0.4290	0.045
H23	0.6517	-0.0153	0.5283	0.042
H24	0.5976	0.1967	0.5126	0.035
H34	-0.0346	0.7571	0.4566	0.031
H35	-0.1403	0.6495	0.4534	0.034
H36	-0.1496	0.4082	0.4034	0.031
H38	-0.0588	0.1624	0.2510	0.035
H39	-0.1135	-0.0499	0.2267	0.041
H40	-0.1570	-0.1441	0.3088	0.042
H41	-0.1465	-0.0242	0.4151	0.04
H42	-0.0928	0.1883	0.4398	0.035
H44	0.0143	0.8360	0.3642	0.033
H45	0.0842	1.0287	0.3964	0.038
H46	0.1988	1.0026	0.4633	0.041
H47	0.2436	0.7837	0.5015	0.037
H48	0.1738	0.5907	0.4715	0.031