Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for perylenemonoimide 1. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	21(1)	21(1)	21(1)	1(1)	2(1)	-3(1)
C(2)	16(1)	16(1)	18(1)	1(1)	0(1)	-3(1)
C(3)	16(1)	18(1)	15(1)	0(1)	0(1)	-5(1)
C(4)	16(1)	19(1)	17(1)	0(1)	1(1)	-2(1)
C(5)	22(1)	19(1)	19(1)	0(1)	-1(1)	-2(1)
C(6)	23(1)	23(1)	16(1)	1(1)	4(1)	1(1)
C(7)	23(1)	25(1)	14(1)	5(1)	0(1)	-2(1)
C(8)	17(1)	18(1)	20(1)	1(1)	1(1)	-3(1)
C(9)	17(1)	20(1)	20(1)	3(1)	-1(1)	-3(1)
C(10)	25(1)	26(1)	23(1)	4(1)	-1(1)	-2(1)
C(11)	29(1)	25(1)	25(1)	9(1)	-6(1)	-3(1)
C(12)	25(1)	23(1)	33(1)	6(1)	-4(1)	1(1)
C(13)	18(1)	20(1)	30(1)	3(1)	-1(1)	-2(1)
C(14)	23(1)	22(1)	37(2)	4(1)	1(1)	4(1)
C(15)	23(1)	25(1)	30(1)	-2(1)	6(1)	3(1)
C(16)	22(1)	23(1)	24(1)	2(1)	4(1)	0(1)
C(17)	18(1)	17(1)	23(1)	2(1)	2(1)	-2(1)
C(18)	16(1)	18(1)	18(1)	3(1)	0(1)	-3(1)
C(19)	21(1)	24(1)	18(1)	0(1)	4(1)	0(1)
C(20)	21(1)	23(1)	16(1)	4(1)	-2(1)	0(1)
C(21)	17(1)	18(1)	18(1)	3(1)	0(1)	-3(1)
C(22)	16(1)	19(1)	24(1)	3(1)	-2(1)	-4(1)
C(23)	21(1)	21(1)	21(1)	3(1)	1(1)	4(1)
C(24)	22(1)	22(1)	31(1)	3(1)	3(1)	2(1)
C(25)	38(2)	25(1)	35(2)	-1(1)	-1(1)	9(1)
C(26)	47(2)	54(2)	25(2)	0(1)	-2(1)	11(1)
C(27)	51(2)	31(1)	34(2)	10(1)	10(1)	13(1)
C(28)	62(2)	46(2)	23(1)	7(1)	9(1)	16(1)
N(1)	20(1)	18(1)	19(1)	1(1)	-1(1)	2(1)
N(2)	32(1)	22(1)	24(1)	5(1)	2(1)	8(1)
O(1)	30(1)	30(1)	21(1)	2(1)	5(1)	8(1)
O(2)	34(1)	26(1)	18(1)	6(1)	-1(1)	5(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for perylenemonoimide 1.

	x	y	z	U(eq)
H(6)	624	5419	4483	25
H(7)	3520	4197	4709	25
H(10)	6013	3107	4885	30
H(11)	9164	1944	5088	32
H(12)	11417	1291	3934	32
H(14)	12205	1181	2355	33
H(15)	11286	1667	981	31
H(16)	8270	2862	760	27
H(19)	5352	3837	559	25
H(20)	2413	5050	373	24
H(23A)	-5088	7113	2521	25
H(23B)	-4524	7073	1508	25
H(24A)	-837	8170	2779	30
H(24B)	-593	8183	1751	30
H(25A)	-4286	10127	2840	39
H(25B)	-1246	9718	3026	39
H(26A)	-6473	9037	3720	63
H(26B)	-3823	9592	4268	63
H(26C)	-3537	8549	3860	63
H(27A)	-1767	9601	1303	45
H(27B)	-4941	9909	1419	45
H(28A)	-3543	8220	509	64
H(28B)	-4901	9087	77	64
H(28C)	-6761	8443	684	64

Table 6. Torsion angles [°] for perylenemonoimide 1.

O(1)-C(1)-C(2)-C(6)	0.2(3)	C(5)-C(4)-C(20)-C(19)	178.99(19)
N(1)-C(1)-C(2)-C(6)	-179.27(18)	C(18)-C(19)-C(20)-C(4)	-1.6(3)
O(1)-C(1)-C(2)-C(3)	179.89(19)	C(2)-C(3)-C(21)-C(8)	0.9(3)
N(1)-C(1)-C(2)-C(3)	0.4(3)	C(4)-C(3)-C(21)-C(8)	-179.42(19)
C(6)-C(2)-C(3)-C(4)	-179.02(19)	C(2)-C(3)-C(21)-C(18)	-179.54(18)
C(1)-C(2)-C(3)-C(4)	1.3(3)	C(4)-C(3)-C(21)-C(18)	0.2(3)
C(6)-C(2)-C(3)-C(21)	0.7(3)	C(7)-C(8)-C(21)-C(3)	-1.2(3)
C(1)-C(2)-C(3)-C(21)	-178.99(19)	C(9)-C(8)-C(21)-C(3)	179.23(19)
C(2)-C(3)-C(4)-C(20)	-179.34(19)	C(7)-C(8)-C(21)-C(18)	179.24(19)
C(21)-C(3)-C(4)-C(20)	0.9(3)	C(9)-C(8)-C(21)-C(18)	-0.4(3)
C(2)-C(3)-C(4)-C(5)	1.4(3)	C(19)-C(18)-C(21)-C(3)	-2.0(3)
C(21)-C(3)-C(4)-C(5)	-178.32(19)	C(17)-C(18)-C(21)-C(3)	179.29(19)
C(20)-C(4)-C(5)-O(2)	-4.5(3)	C(19)-C(18)-C(21)-C(8)	177.64(19)
C(3)-C(4)-C(5)-O(2)	174.70(19)	C(17)-C(18)-C(21)-C(8)	-1.1(3)
C(20)-C(4)-C(5)-N(1)	175.02(18)	C(14)-C(13)-C(22)-C(9)	-179.73(18)
C(3)-C(4)-C(5)-N(1)	-5.8(3)	C(12)-C(13)-C(22)-C(9)	-0.4(3)
C(3)-C(2)-C(6)-C(7)	-2.0(3)	C(14)-C(13)-C(22)-C(17)	0.0(3)
C(1)-C(2)-C(6)-C(7)	177.7(2)	C(12)-C(13)-C(22)-C(17)	179.33(19)
C(2)-C(6)-C(7)-C(8)	1.7(3)	C(10)-C(9)-C(22)-C(13)	-0.9(3)
C(6)-C(7)-C(8)-C(21)	-0.1(3)	C(8)-C(9)-C(22)-C(13)	178.13(19)
C(6)-C(7)-C(8)-C(9)	179.5(2)	C(10)-C(9)-C(22)-C(17)	179.37(19)
C(7)-C(8)-C(9)-C(10)	1.1(3)	C(8)-C(9)-C(22)-C(17)	-1.6(3)
C(21)-C(8)-C(9)-C(10)	-179.27(19)	C(16)-C(17)-C(22)-C(13)	-0.1(3)
C(7)-C(8)-C(9)-C(22)	-177.87(18)	C(18)-C(17)-C(22)-C(13)	-179.61(19)
C(21)-C(8)-C(9)-C(22)	1.7(3)	C(16)-C(17)-C(22)-C(9)	179.57(18)
C(22)-C(9)-C(10)-C(11)	1.5(3)	C(18)-C(17)-C(22)-C(9)	0.1(3)
C(8)-C(9)-C(10)-C(11)	-177.5(2)	N(1)-C(23)-C(24)-N(2)	-173.76(18)
C(9)-C(10)-C(11)-C(12)	-0.7(3)	O(2)-C(5)-N(1)-C(1)	-172.6(2)
C(10)-C(11)-C(12)-C(13)	-0.6(3)	C(4)-C(5)-N(1)-C(1)	7.9(3)
C(11)-C(12)-C(13)-C(14)	-179.5(2)	O(2)-C(5)-N(1)-C(23)	1.5(3)
C(11)-C(12)-C(13)-C(22)	1.2(3)	C(4)-C(5)-N(1)-C(23)	-178.02(19)
C(12)-C(13)-C(14)-C(15)	-179.8(2)	O(1)-C(1)-N(1)-C(5)	175.26(19)
C(22)-C(13)-C(14)-C(15)	-0.5(3)	C(2)-C(1)-N(1)-C(5)	-5.3(3)
C(13)-C(14)-C(15)-C(16)	1.1(3)	O(1)-C(1)-N(1)-C(23)	1.1(3)
C(14)-C(15)-C(16)-C(17)	-1.3(3)	C(2)-C(1)-N(1)-C(23)	-179.42(18)
C(15)-C(16)-C(17)-C(22)	0.8(3)	C(24)-C(23)-N(1)-C(5)	-88.4(2)
C(15)-C(16)-C(17)-C(18)	-179.8(2)	C(24)-C(23)-N(1)-C(1)	86.1(2)
C(16)-C(17)-C(18)-C(19)	3.1(3)	C(26)-C(25)-N(2)-C(24)	-73.3(2)
C(22)-C(17)-C(18)-C(19)	-177.45(19)	C(26)-C(25)-N(2)-C(27)	160.91(19)
C(16)-C(17)-C(18)-C(21)	-178.20(18)	C(23)-C(24)-N(2)-C(25)	128.2(2)
C(22)-C(17)-C(18)-C(21)	1.3(3)	C(23)-C(24)-N(2)-C(27)	-106.5(2)
C(21)-C(18)-C(19)-C(20)	2.7(3)	C(28)-C(27)-N(2)-C(25)	-170.0(2)
C(17)-C(18)-C(19)-C(20)	-178.59(19)	C(28)-C(27)-N(2)-C(24)	64.7(3)
C(3)-C(4)-C(20)-C(19)	-0.2(3)		