Supplemental Data for Phanstiel manuscript

Tables SI-SV. Detailed X-ray data for **5**

Fig S1. ORTEP of **5** showing disorder (i.e., the alternative position of the phenyl ring).

Fig S2. Raman spectra of different regions observed by the Raman microscope

Table SI. Crystal data and structure refinement for 5.

Identification code	Diamide Diacid(5)/op2fin
Empirical formula	C24 H26 N2 O6
Formula weight	438.47
Temperature	193(2) K
Wavelength	0.71073 A
Crystal system	Hexagonal
Space group	P6(5)
Unit cell dimensions	a = 22.3876(7) A alpha = 90 deg. b = 22.3876(7) A beta = 90 deg. c = 9.4793(4) A gamma = 120 deg.
Volume, Z	4114.5(3) A^3, 6
Density (calculated)	1.062 Mg/m^3
Absorption coefficient	0.077 mm^-1
F(000)	1392
Crystal size	0.16 x 0.18 x 0.26 mm
Theta range for data refinement	1.82 to 20.81 deg.
Limiting indices	-24<=h<=21, -18<=k<=24, -10<=l<=9
Reflections collected	14117
Independent reflections	2813 [R(int) = 0.0466] [Rsigma = 0.0350]
Observed reflections	2668
Absorption correction	SADABS (empirical)
Max & Min Transmission	0.693 0.623
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2810 / 1 / 308
Goodness-of-fit on F^2	1.140
Final R indices [I>2sigma(I)]	R1 = 0.0723, wR2 = 0.2038
R indices (all data)	R1 = 0.0777, wR2 = 0.2279
Largest diff. peak and hole	0.670 and -0.419 e.A^-3
Max Shift/esd	0.000

Table SII. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 5. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	2814(2)	-3872(2)	3290(5)	40(1)
O(2)	2622(2)	-4743(2)	1816(5)	42(1)
O(3)	2420(2)	-3473(2)	-1392(4)	40(1)
O(4)	371(2)	-4677(2)	-2287(4)	35(1)
O(5)	-535(2)	-4324(2)	-4434(5)	39(1)
O(6)	347(2)	-4345(2)	-5523(5)	37(1)
N(1)	1834(2)	-4374(3)	41(5)	30(1)
N(2)	1158(2)	-3699(3)	-3311(6)	34(1)
C(1)	2548(3)	-4266(4)	2152(7)	33(2)
C(2)	2147(3)	-3990(3)	1316(6)	28(2)
C(3)	1593(3)	-3960(3)	2257(6)	32(2)
C(4)	1336(3)	-3528(3)	1589(7)	35(2)
C(5)	716(3)	-3804(3)	884(7)	39(2)
C(6)	493(4)	-3401(4)	243(8)	53(2)
C(7)	900(4)	-2687(5)	304(11)	69(2)
C(8)	1507(4)	-2403(4)	1036(11)	68(3)
C(9)	1731(3)	-2809(3)	1675(10)	53(2)
C(10)	1970(3)	-4076(3)	-1207(6)	25(2)
C(11)	1534(3)	-4492(3)	-2452(6)	26(1)
C(12)	1947(3)	-4427(3)	-3828(7)	34(2)
C(13)	1481(4)	-5186(4)	-4094(9)	55(2)
C(14)	1229(3)	-5285(3)	-2530(7)	37(2)
C(15)	973(4)	-4296(3)	-2660(6)	32(2)
C(16)	67(3)	-4113(3)	-4550(7)	30(2)
C(17)	617(3)	-3541(3)	-3688(7)	32(2)
C(18)	938(4)	-2849(3)	-4505(9)	52(2)
C(19)	456(6)	-2645(5)	-4882(13)	40(3)
C(20)	187(7)	-2787(7)	-6243(16)	57(4)
C(21)	-305(9)	-2616(10)	-6724(22)	89(6)
C(22)	-562(13)	-2346(13)	-5795(42)	143(12)
C(23)	-322(19)	-2206(16)	-4408(35)	181(15)
C(24)	267(11)	-2305(10)	-3963(21)	96(6)
C(19A)	1265(6)	-2183(5)	-3922(15)	60(5)
C(20A)	971(5)	-1994(5)	-2846(17)	96(4)
C(21A)	1361(7)	-1369(6)	-2151(16)	96(4)
C(22A)	2044(6)	-933(5)	-2532(17)	96(4)
C(23A)	2338(5)	-1122(6)	-3609(18)	96(4)
C(24A)	1948(6)	-1747(6)	-4304(16)	96(4)

Table SIII. Bond lengths [A] and angles [deg] for 5.

O(1)-C(1)	1.332(8)
O(2)-C(1)	1.201(8)
O(3)-C(10)	1.228(7)
O(4)-C(15)	1.233(7)
O(5)-C(16)	1.190(7)
O(6)-C(16)	1.356(8)
N(1)-C(10)	1.318(8)
N(1)-C(2)	1.445(8)
N(2)-C(15)	1.337(8)
N(2)-C(17)	1.465(8)
C(1)-C(2)	1.540(9)
C(2)-C(3)	1.556(8)
C(3)-C(4)	1.494(9)
C(4)-C(5)	1.376(9)
C(4)-C(9)	1.398(9)
C(5)-C(6)	1.373(9)
C(6)-C(7)	1.389(11)
C(7)-C(8)	1.366(12)
C(8)-C(9)	1.380(11)
C(10)-C(11)	1.519(8)
C(11)-C(15)	1.535(9)
C(11)-C(14)	1.553(9)
C(11)-C(12)	1.563(9)
C(12)-C(13)	1.505(10)
C(13)-C(14)	1.562(11)
C(16)-C(17)	1.499(9)
C(17)-C(18)	1.551(9)
C(18)-C(19A)	1.405(11)
C(18)-C(19)	1.412(13)
C(19)-C(24)	1.36(2)
C(19)-C(20)	1.39(2)
C(20)-C(21)	1.41(2)
C(21)-C(22)	1.35(4)
C(22)-C(23)	1.40(4)
C(23)-C(24)	1.50(3)
C(19A)-C(20A)	1.39
C(19A)-C(24A)	1.39
C(20A)-C(21A)	1.39
C(21A)-C(22A)	1.39
C(22A)-C(23A)	1.39
C(23A)-C(24A)	1.39
C(10)-N(1)-C(2)	121.9(5)
C(15)-N(2)-C(17)	118.2(5)
O(2)-C(1)-O(1)	126.1(6)
O(2)-C(1)-C(2)	126.0(6)
O(1)-C(1)-C(2)	107.9(6)
N(1)-C(2)-C(1)	113.4(5)
N(1)-C(2)-C(3)	110.2(5)
C(1)-C(2)-C(3)	111.1(5)
C(4)-C(3)-C(2)	111.0(5)
C(5)-C(4)-C(9)	117.5(6)
C(5)-C(4)-C(3)	123.0(6)
C(9)-C(4)-C(3)	119.5(6)
C(6)-C(5)-C(4)	122.4(6)
C(5)-C(6)-C(7)	119.5(7)
C(8)-C(7)-C(6)	119.0(7)
C(7)-C(8)-C(9)	121.4(7)
C(8)-C(9)-C(4)	120.2(7)

O(3)-C(10)-N(1)	122.7(5)
O(3)-C(10)-C(11)	119.1(5)
N(1)-C(10)-C(11)	118.2(5)
C(10)-C(11)-C(15)	107.0(5)
C(10)-C(11)-C(14)	121.2(5)
C(15)-C(11)-C(14)	111.5(5)
C(10)-C(11)-C(12)	114.9(4)
C(15)-C(11)-C(12)	113.4(5)
C(14)-C(11)-C(12)	88.1(4)
C(13)-C(12)-C(11)	89.5(5)
C(12)-C(13)-C(14)	89.9(5)
C(11)-C(14)-C(13)	87.8(5)
O(4)-C(15)-N(2)	120.6(6)
O(4)-C(15)-C(11)	122.2(6)
N(2)-C(15)-C(11)	117.1(6)
O(5)-C(16)-O(6)	124.1(6)
O(5)-C(16)-C(17)	124.8(6)
O(6)-C(16)-C(17)	111.1(5)
N(2)-C(17)-C(16)	110.6(5)
N(2)-C(17)-C(18)	109.7(5)
C(16)-C(17)-C(18)	110.7(6)
C(19A)-C(18)-C(17)	126.9(9)
C(19)-C(18)-C(17)	113.8(7)
C(24)-C(19)-C(20)	120.2(13)
C(24)-C(19)-C(18)	121.4(13)
C(20)-C(19)-C(18)	118.3(11)
C(19)-C(20)-C(21)	123(2)
C(22)-C(21)-C(20)	118(2)
C(21)-C(22)-C(23)	121(2)
C(22)-C(23)-C(24)	120(2)
C(19)-C(24)-C(23)	116(2)
C(20A)-C(19A)-C(24A)	120.0
C(20A)-C(19A)-C(18)	122.5(9)
C(24A)-C(19A)-C(18)	116.7(9)
C(19A)-C(20A)-C(21A)	120.0
C(22A)-C(21A)-C(20A)	120.0
C(21A)-C(22A)-C(23A)	120.0
C(22A)-C(23A)-C(24A)	120.0
C(23A)-C(24A)-C(19A)	120.0

Symmetry transformations used to generate equivalent atoms:

Table SIV. Anisotropic displacement parameters (A^2 x 10^3) for 5. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
O(1)	43(3)	67(3)	28(3)	-6(2)	-12(2)	40(2)
O(2)	55(3)	46(3)	44(3)	-12(2)	-14(2)	38(2)
O(3)	35(2)	38(3)	22(3)	6(2)	4(2)	0(2)
O(4)	21(2)	46(3)	32(3)	9(2)	6(2)	11(2)
O(5)	27(3)	45(3)	40(3)	-9(2)	-8(2)	14(2)
O(6)	30(2)	49(3)	29(3)	-9(2)	-5(2)	17(2)
N(1)	26(3)	34(3)	28(4)	1(3)	3(3)	13(2)
N(2)	22(3)	36(3)	37(3)	-2(3)	-3(2)	11(2)
C(1)	27(3)	50(4)	15(4)	-1(3)	-5(3)	15(3)
C(2)	33(3)	35(3)	18(4)	4(3)	-3(3)	18(3)
C(3)	30(3)	52(4)	20(4)	4(3)	6(3)	24(3)
C(4)	32(4)	42(4)	30(4)	5(3)	4(3)	18(3)
C(5)	41(4)	42(4)	29(4)	1(3)	-1(3)	17(3)
C(6)	40(4)	73(6)	56(5)	5(4)	-11(4)	34(5)
C(7)	63(6)	73(6)	92(7)	21(5)	5(5)	51(5)
C(8)	45(5)	41(4)	119(8)	4(5)	-3(5)	22(4)
C(9)	39(4)	39(4)	78(6)	1(4)	-2(4)	15(4)
C(10)	20(3)	33(4)	21(4)	9(3)	9(3)	12(3)
C(11)	24(3)	38(3)	16(3)	-2(3)	-5(3)	15(3)
C(12)	33(4)	53(4)	23(4)	-2(3)	-1(3)	26(3)
C(13)	53(5)	61(5)	44(5)	-11(4)	2(4)	23(4)
C(14)	35(4)	42(4)	33(4)	-9(3)	-1(3)	18(3)
C(15)	46(5)	42(4)	12(3)	-6(3)	-8(3)	25(4)
C(16)	30(4)	31(4)	29(4)	1(3)	-5(3)	15(3)
C(17)	31(3)	31(4)	30(4)	0(3)	-3(3)	13(3)
C(18)	47(4)	33(4)	69(6)	-1(4)	0(4)	14(4)
C(19)	46(7)	34(7)	45(9)	9(6)	0(6)	25(6)
C(20)	63(9)	51(8)	55(10)	18(7)	-1(8)	27(7)
C(21)	78(11)	112(14)	91(14)	42(12)	-14(10)	58(11)
C(22)	118(17)	147(21)	213(35)	34(21)	-43(20)	104(17)
C(23)	310(39)	236(32)	162(27)	-62(24)	-72(28)	259(34)
C(24)	152(17)	121(14)	77(12)	-22(11)	-8(12)	115(15)
C(19A)	81(14)	34(10)	55(12)	-9(9)	-5(10)	21(10)
C(20A)	72(7)	36(5)	142(11)	-1(6)	-22(7)	-2(4)
C(21A)	72(7)	36(5)	142(11)	-1(6)	-22(7)	-2(4)
C(22A)	72(7)	36(5)	142(11)	-1(6)	-22(7)	-2(4)
C(23A)	72(7)	36(5)	142(11)	-1(6)	-22(7)	-2(4)
C(24A)	72(7)	36(5)	142(11)	-1(6)	-22(7)	-2(4)

Table SV. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 5.

	x	y	z	U(eq)
H(1B)	3036(2)	-4014(2)	3762(5)	61
H(6B)	31(2)	-4665(2)	-5993(5)	56
H(1A)	1543(2)	-4821(3)	101(5)	36
H(2A)	1594(2)	-3408(3)	-3508(6)	40
H(2B)	2485(3)	-3506(3)	1029(6)	34
H(3A)	1203(3)	-4433(3)	2406(6)	39
H(3B)	1796(3)	-3765(3)	3190(6)	39
H(5A)	433(3)	-4291(3)	840(7)	47
H(6A)	63(4)	-3608(4)	-238(8)	64
H(7A)	759(4)	-2401(5)	-157(11)	83
H(8A)	1780(4)	-1915(4)	1107(11)	82
H(9A)	2156(3)	-2600(3)	2175(10)	64
H(12A)	1914(3)	-4128(3)	-4556(7)	41
H(12B)	2434(3)	-4296(3)	-3655(7)	41
H(13A)	1732(4)	-5433(4)	-4331(9)	66
H(13B)	1113(4)	-5289(4)	-4792(9)	66
H(14A)	722(3)	-5556(3)	-2423(7)	45
H(14B)	1460(3)	-5461(3)	-1900(7)	45
H(17A)	404(3)	-3493(3)	-2800(7)	38
H(18A)	1302(4)	-2484(3)	-3915(9)	63
H(18B)	1160(4)	-2892(3)	-5372(9)	63
H(20A)	342(7)	-3009(7)	-6877(16)	69
H(21A)	-452(9)	-2689(10)	-7680(22)	107
H(22A)	-911(13)	-2249(13)	-6089(42)	171
H(23A)	-531(19)	-2049(16)	-3744(35)	217
H(24B)	495(11)	-2138(10)	-3085(21)	115
H(20B)	504(6)	-2292(8)	-2585(23)	115
H(21B)	1160(9)	-1240(9)	-1415(21)	115
H(22B)	2311(9)	-506(7)	-2058(23)	115
H(23B)	2805(6)	-824(9)	-3870(25)	115
H(24A)	2149(9)	-1876(9)	-5040(20)	115

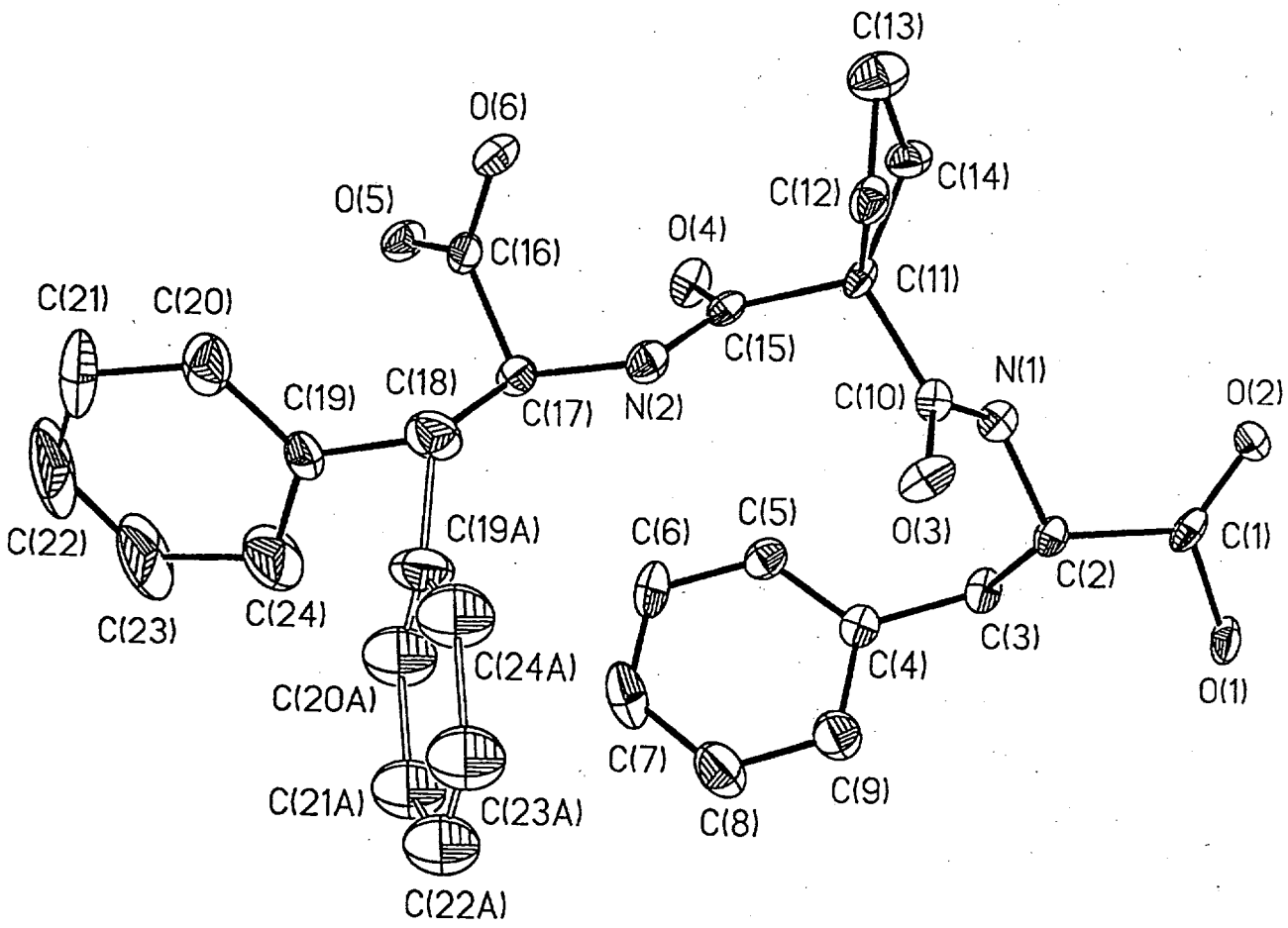
C(13)
O(6)
O(5)
C(12)
C(14)
C(16)
O(4)
C(11)
C(21)
C(20)
C(15)
C(19)
C(18)
C(17)
N(2)
C(10)
N(1)
O(2)
C(22)
C(19A)
C(6)
C(5)
O(3)
C(1)
C(23)
C(24)
C(2)
C(3)
C(24A)
C(4)
O(1)
C(20A)
C(7)
C(9)
C(21A)
C(23A)
C(8)
C(22A)

Figure SI.

Figure S2. Raman Microscope Spectra