Supporting Information for

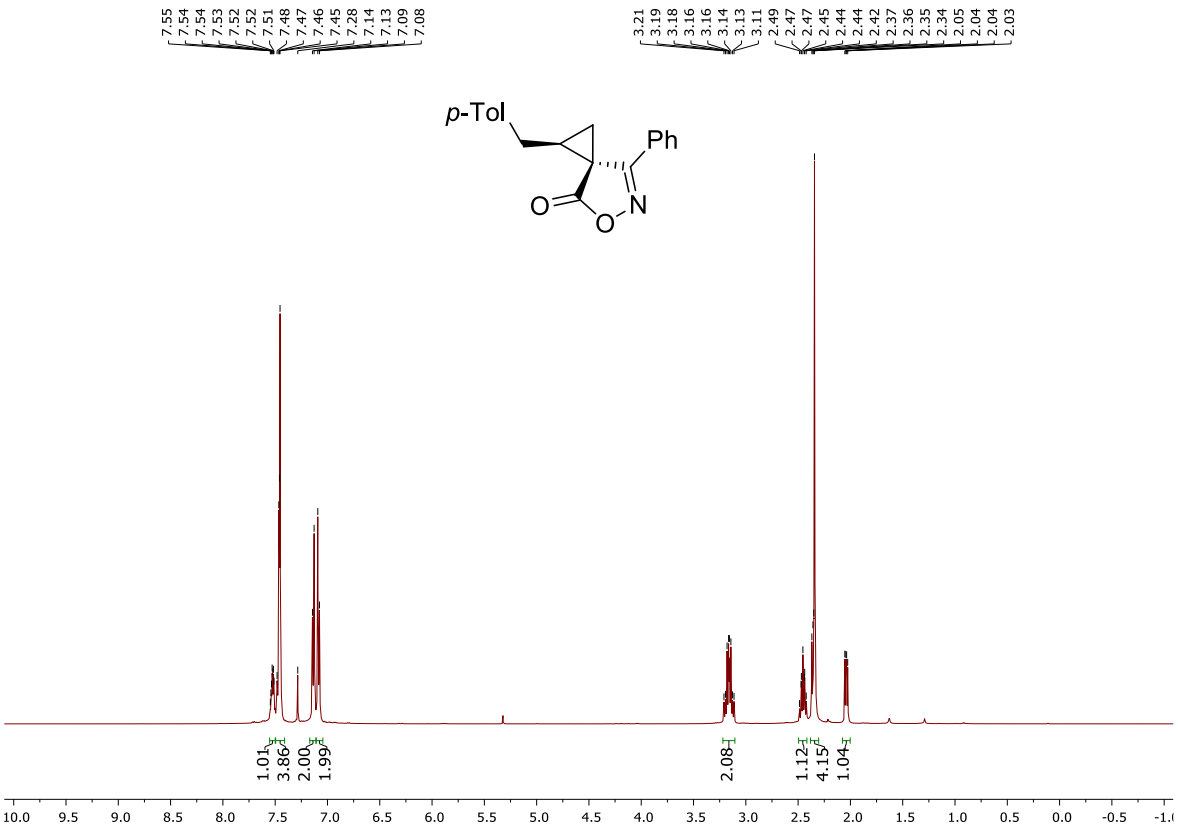
(1*RS*,3*SR*)-1-(4-Methylbenzyl)-7-phenyl-5-oxa-6-azaspiro[2.4]hept-6-en-4-one

Gleb D. Titov and Nikolai V. Rostovskii*

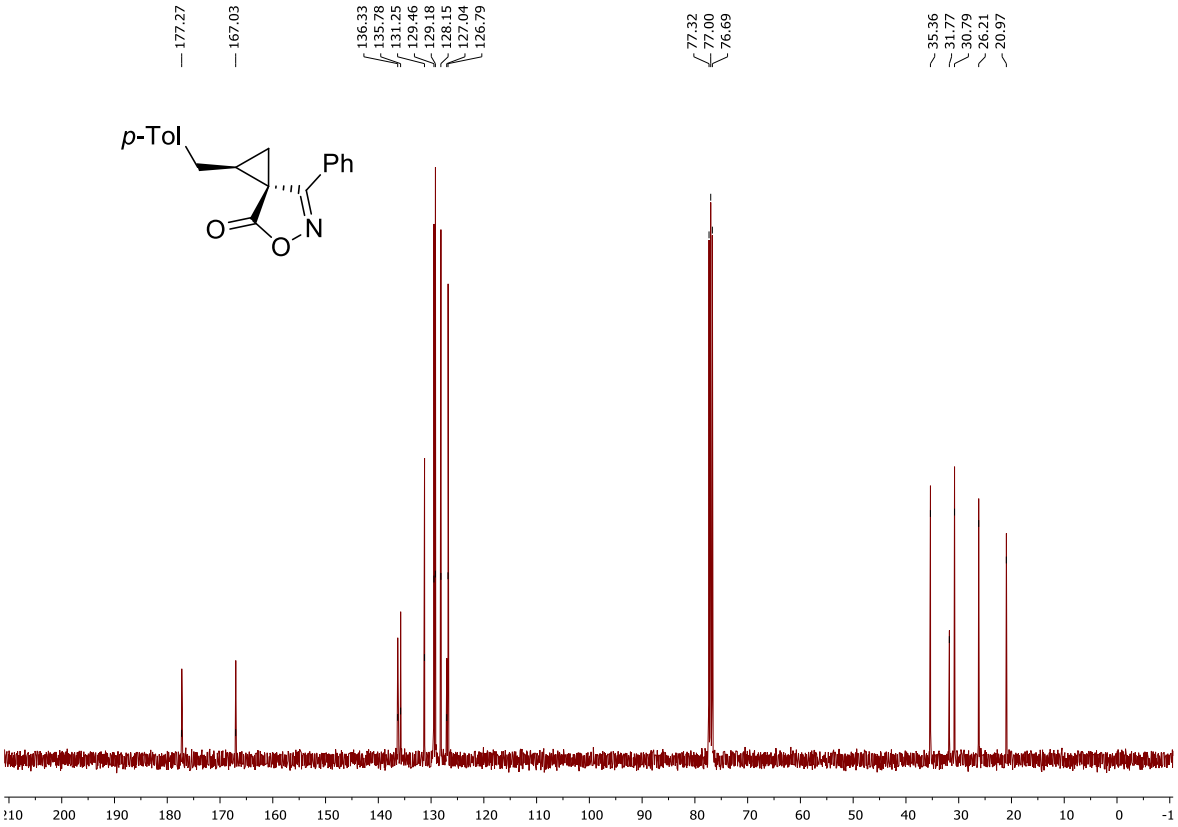
Institute of Chemistry, St. Petersburg State University, 7/9 Universitetskaya Nab., 199034 St. Petersburg, Russia
* Correspondence: n.rostovskiy@spbu.ru

NMR spectra

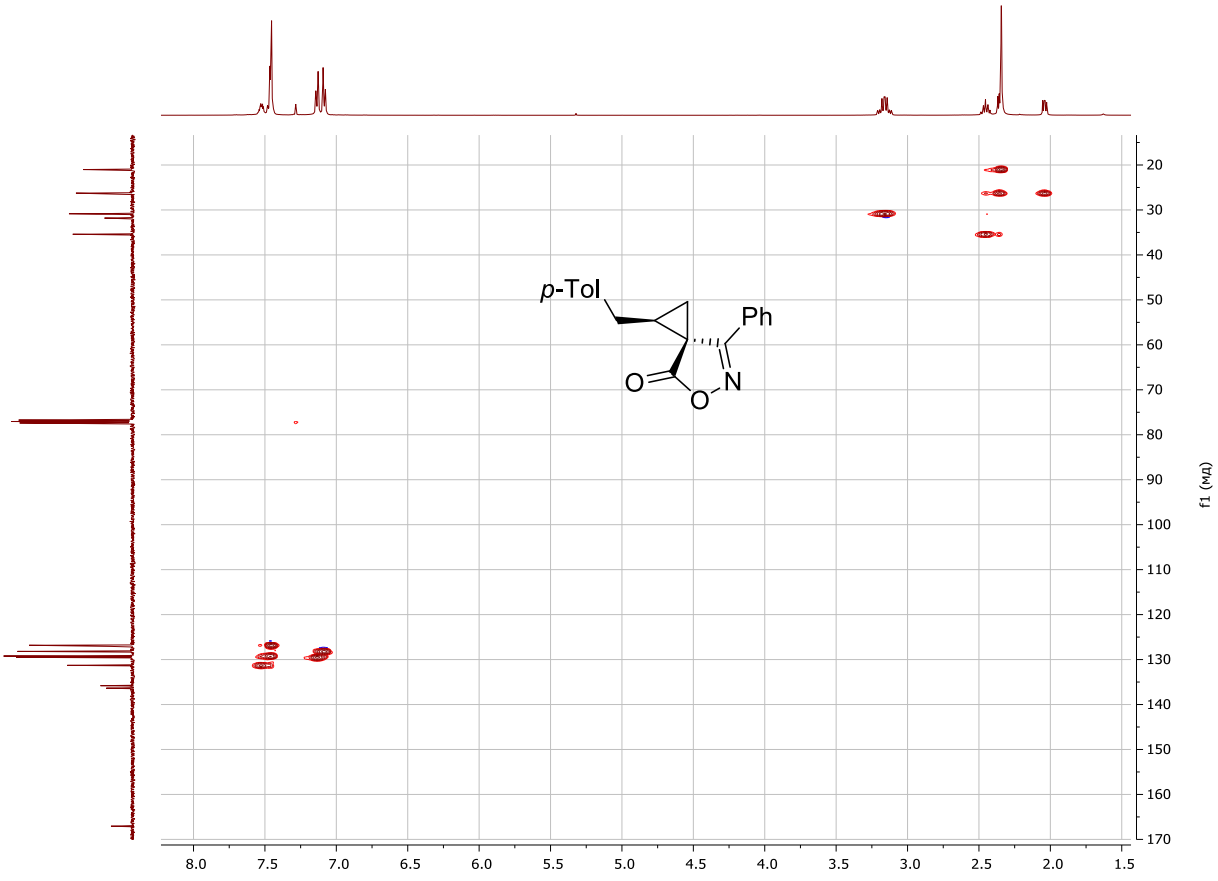
^{1}H NMR spectrum of compound **3** (400 MHz, $CDCl_3$)



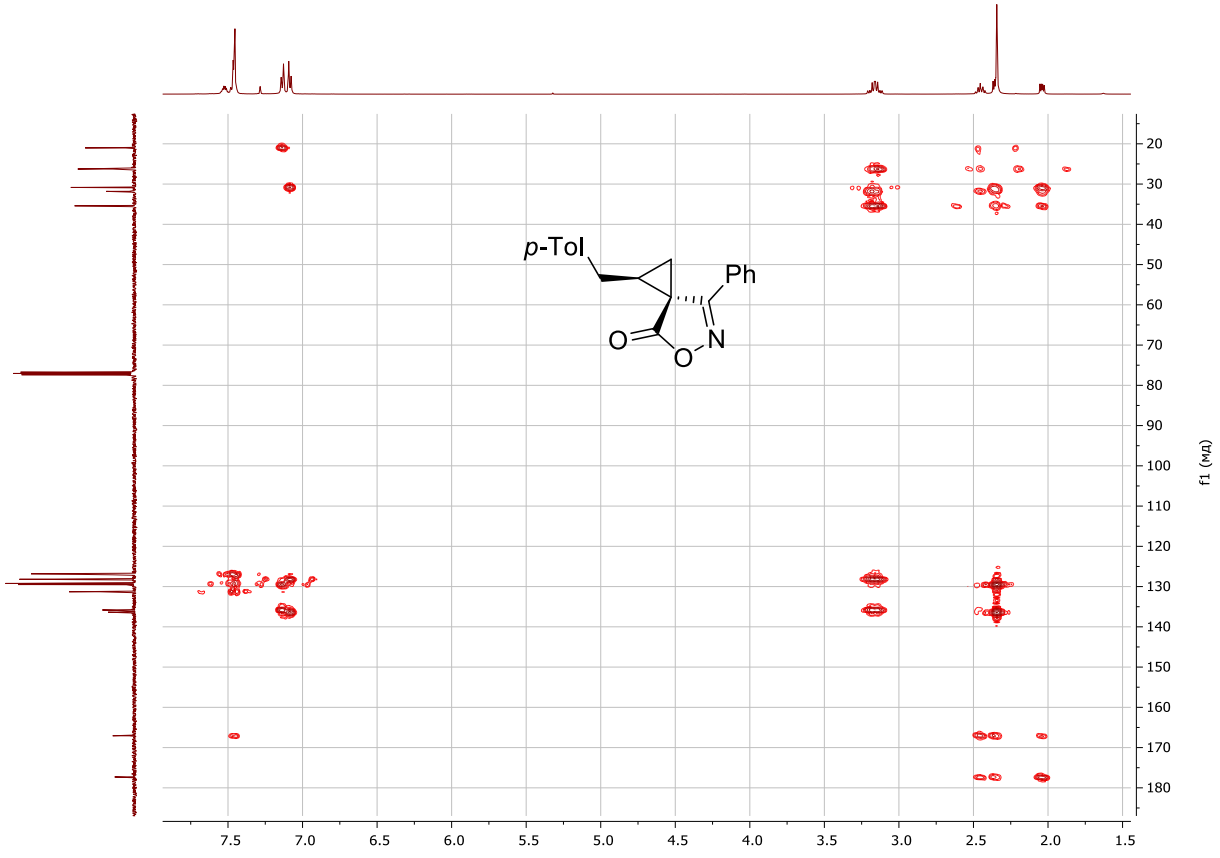
^{13}C{^{1}H} NMR spectrum of compound **3** (100 MHz, $CDCl_3$)



^{1}H-^{13}C HSQC NMR spectrum of compound **3**



^{1}H-^{13}C HMBC NMR spectrum of compound **3**



^{1}H-^{1}H NOESY NMR spectrum of compound **3** (400 MHz, $CDCl_3$)

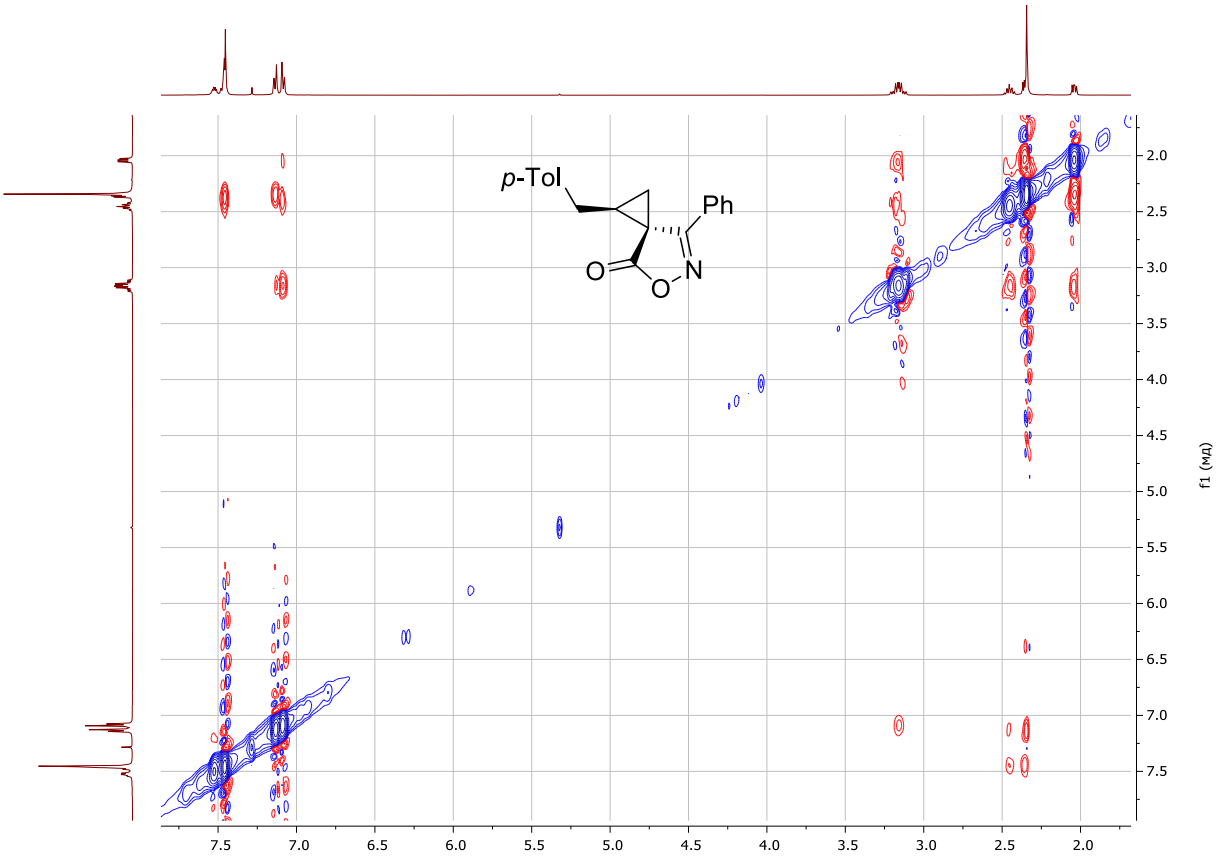


Table S1. Crystal data and structure refinement for compound 3.

Empirical formula	$C_{19}H_{17}NO_2$
Formula weight	291.33
Temperature/K	99.97(16)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	6.0246(3)
b/Å	10.1973(5)
c/Å	24.5720(14)
α/°	90
β/°	94.008(5)
γ/°	90
Volume/Å^3	1505.88(14)
Z	4
ρ_{calc}g/cm^3	1.285
μ/mm^{-1}	0.664
F(000)	616.0
Crystal size/mm^3	0.14 × 0.12 × 0.1
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	7.212 to 142.976
Index ranges	$-7 \leq h \leq 7$, $-10 \leq k \leq 12$, $-29 \leq l \leq 28$
Reflections collected	6142
Independent reflections	2770 [R_{int} = 0.0308, R_{sigma} = 0.0418]
Data/restraints/parameters	2770/0/200
Goodness-of-fit on F^2	1.086
Final R indexes [I>=2σ (I)]	R_1 = 0.0747, wR_2 = 0.1898
Final R indexes [all data]	R_1 = 0.0910, wR_2 = 0.2005
Largest diff. peak/hole / e Å^{-3}	0.32/-0.32

Table S2. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for compound 3. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O001	2797(4)	344(3)	6305.9(12)	32.8(6)
O002	982(5)	2079(3)	5923.4(13)	39.3(7)
N003	4589(5)	136(3)	6723.5(14)	31.1(7)
C004	5969(6)	5261(4)	5674.4(15)	25.7(8)
C005	7183(6)	1364(3)	7302.1(15)	25.3(8)
C006	8588(6)	6914(4)	5430.7(15)	28.5(8)
C007	4473(6)	6258(4)	5771.8(15)	26.3(8)
C11	5312(6)	1277(3)	6883.4(16)	26.1(8)
C009	2476(6)	1674(4)	6225.9(17)	30.3(9)
C00A	5025(6)	7565(4)	5702.1(16)	27.5(8)
C00B	4202(6)	2341(3)	6579.3(16)	26.8(8)
C00C	7095(6)	2225(4)	7744.4(16)	28.4(8)
C00D	8033(6)	5610(4)	5505.7(15)	27.6(8)
C00E	5577(6)	3480(3)	6350.0(16)	25.5(8)
C00F	7099(6)	7916(4)	5528.7(16)	28.3(8)
C00G	9038(6)	576(4)	7259.6(17)	31.5(9)
C00H	5326(6)	3838(4)	5754.3(16)	30.2(8)
C00I	8884(7)	2293(4)	8133.0(16)	31.9(9)
C00J	3879(6)	3770(4)	6739.1(16)	28.6(8)
C00K	10815(7)	644(4)	7652.5(17)	36.3(10)
C00L	10740(7)	1516(4)	8085.4(17)	34.7(9)
C00M	7700(7)	9333(4)	5445.8(19)	38.2(10)

Table S3. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for compound 3. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O001	30.5(14)	21.9(13)	46.4(16)	-4.0(12)	6.0(12)	-4.0(11)
O002	29.4(15)	35.0(16)	53.2(18)	0.3(14)	0.8(13)	-5.3(13)
N003	27.5(16)	22.5(16)	44.4(19)	-1.1(14)	11.0(14)	-0.9(14)
C004	23.5(18)	24.8(19)	28.9(19)	2.0(15)	4.2(14)	-0.8(15)
C005	25.1(18)	16.9(17)	35(2)	3.5(14)	11.8(15)	-1.8(14)
C006	17.9(17)	35(2)	33(2)	3.8(16)	6.2(14)	-2.3(16)
C007	16.7(16)	26.5(19)	36(2)	1.7(16)	6.8(14)	-1.8(15)
C11	24.6(18)	18.0(17)	38(2)	0.9(15)	14.9(15)	0.6(15)
C009	26.5(19)	23.0(19)	42(2)	-0.1(16)	9.2(17)	-0.5(16)
C00A	18.0(17)	25.1(19)	40(2)	1.4(16)	7.6(15)	3.5(15)
C00B	25.8(18)	16.0(17)	40(2)	-0.1(15)	9.1(16)	-1.9(15)
C00C	27.9(19)	19.0(18)	40(2)	2.6(15)	12.1(16)	3.8(15)
C00D	21.4(18)	30(2)	31.7(19)	1.9(16)	6.5(14)	6.7(16)
C00E	21.5(17)	17.1(17)	38(2)	0.0(15)	5.8(15)	-1.2(14)
C00F	24.3(18)	26.5(19)	35(2)	1.7(16)	5.5(15)	-5.9(16)
C00G	29(2)	27.2(19)	40(2)	3.4(17)	16.2(17)	4.8(17)
C00H	28.9(19)	24.4(19)	38(2)	-0.9(16)	5.9(16)	0.7(16)
C00I	35(2)	27(2)	34(2)	4.1(16)	8.8(16)	0.3(17)
C00J	26.2(19)	20.0(18)	40(2)	0.2(16)	8.4(16)	4.6(15)
C00K	30(2)	38(2)	43(2)	8.3(19)	15.6(17)	10.5(18)
C00L	29(2)	37(2)	39(2)	11.7(18)	7.0(17)	1.1(18)
C00M	35(2)	29(2)	52(3)	3.3(19)	8.1(19)	-10.5(18)

Table S4. Bond Lengths for compound 3.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O001	N003	1.452(4)	C11	C00B	1.453(5)
O001	C009	1.382(5)	C009	C00B	1.474(5)
O002	C009	1.200(5)	C00A	C00F	1.394(5)
N003	C11	1.294(5)	C00B	C00E	1.555(5)
C004	C007	1.391(5)	C00B	C00J	1.525(5)
C004	C00D	1.385(5)	C00C	C00I	1.391(6)
C004	C00H	1.518(5)	C00E	C00H	1.506(5)
C005	C11	1.474(5)	C00E	C00J	1.478(5)
C005	C00C	1.401(5)	C00F	C00M	1.507(5)
C005	C00G	1.386(5)	C00G	C00K	1.392(6)
C006	C00D	1.387(5)	C00I	C00L	1.382(6)
C006	C00F	1.392(5)	C00K	C00L	1.390(6)
C007	C00A	1.387(5)			

Table S5. Bond Angles for compound 3.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C009	O001	N003	109.5(3)	C11	C00B	C00J	130.0(4)
C11	N003	O001	107.5(3)	C009	C00B	C00E	120.2(3)
C007	C004	C00H	120.1(3)	C009	C00B	C00J	119.7(3)
C00D	C004	C007	118.0(3)	C00J	C00B	C00E	57.3(2)
C00D	C004	C00H	121.9(3)	C00I	C00C	C005	119.6(3)
C00C	C005	C11	120.7(3)	C004	C00D	C006	121.1(3)
C00G	C005	C11	119.6(3)	C00H	C00E	C00B	120.9(3)
C00G	C005	C00C	119.7(4)	C00J	C00E	C00B	60.3(2)
C00D	C006	C00F	121.1(3)	C00J	C00E	C00H	123.6(3)
C00A	C007	C004	121.1(3)	C006	C00F	C00A	117.8(3)
N003	C11	C005	119.3(3)	C006	C00F	C00M	121.1(3)
N003	C11	C00B	112.5(3)	C00A	C00F	C00M	121.1(4)
C00B	C11	C005	128.0(3)	C005	C00G	C00K	120.3(4)
O001	C009	C00B	106.4(3)	C00E	C00H	C004	110.4(3)
O002	C009	O001	121.2(4)	C00L	C00I	C00C	120.4(4)
O002	C009	C00B	132.4(4)	C00E	C00J	C00B	62.3(2)
C007	C00A	C00F	120.8(3)	C00L	C00K	C00G	119.9(4)
C11	C00B	C009	103.8(3)	C00I	C00L	C00K	120.1(4)
C11	C00B	C00E	120.4(3)				

Table S6. Torsion Angles for compound 3.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O001	N003	C11	C005	-178.7(3)	C11	C00B	C00E	C00J	-120.6(4)
O001	N003	C11	C00B	-3.1(4)	C11	C00B	C00J	C00E	104.3(4)
O001	C009	C00B	C11	-4.9(4)	C009	O001	N003	C11	-0.3(4)
O001	C009	C00B	C00E	133.4(3)	C009	C00B	C00E	C00H	-5.7(5)
O001	C009	C00B	C00J	-159.4(3)	C009	C00B	C00E	C00J	107.9(4)
O002	C009	C00B	C11	173.5(4)	C009	C00B	C00J	C00E	-108.8(4)
O002	C009	C00B	C00E	-48.2(6)	C00B	C00E	C00H	C004	155.0(3)
O002	C009	C00B	C00J	19.0(6)	C00C	C005	C11	N003	-133.8(4)
N003	O001	C009	O002	-175.2(3)	C00C	C005	C11	C00B	51.3(5)
N003	O001	C009	C00B	3.4(4)	C00C	C005	C00G	C00K	-0.3(5)
N003	C11	C00B	C009	5.0(4)	C00C	C00I	C00L	C00K	-1.0(6)
N003	C11	C00B	C00E	-133.1(4)	C00D	C004	C007	C00A	0.0(6)
N003	C11	C00B	C00J	155.8(4)	C00D	C004	C00H	C00E	100.0(4)
C004	C007	C00A	C00F	0.4(6)	C00D	C006	C00F	C00A	-0.3(6)
C005	C11	C00B	C009	-179.7(3)	C00D	C006	C00F	C00M	-179.8(4)
C005	C11	C00B	C00E	42.1(5)	C00F	C006	C00D	C004	0.8(6)
C005	C11	C00B	C00J	-29.0(6)	C00G	C005	C11	N003	45.6(5)
C005	C00C	C00I	C00L	-0.2(6)	C00G	C005	C11	C00B	-129.3(4)
C005	C00G	C00K	C00L	-0.8(6)	C00G	C005	C00C	C00I	0.8(5)
C007	C004	C00D	C006	-0.6(6)	C00G	C00K	C00L	C00I	1.5(6)
C007	C004	C00H	C00E	-79.9(4)	C00H	C004	C007	C00A	179.9(4)
C007	C00A	C00F	C006	-0.2(6)	C00H	C004	C00D	C006	179.5(4)
C007	C00A	C00F	C00M	179.3(4)	C00H	C00E	C00J	C00B	109.3(4)
C11	C005	C00C	C00I	-179.7(3)	C00J	C00B	C00E	C00H	-113.6(4)
C11	C005	C00G	C00K	-179.8(3)	C00J	C00E	C00H	C004	82.2(4)
C11	C00B	C00E	C00H	125.8(4)					

Table S7. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for compound 3.

Atom	*x*	*y*	*z*	U(eq)
H006	10009	7127	5310	34
H007	3048	6040	5888	32
H00A	3978	8229	5773	33
H00C	5820	2759	7779	34
H00D	9087	4946	5440	33
H00E	7142	3532	6513	31
H00G	9098	-12	6961	38
H00B	3764	3701	5613	36
H00F	6286	3264	5546	36
H00I	8831	2878	8433	38
H00H	2497	4212	6595	34
H00J	4410	4036	7113	34
H00K	12076	94	7625	44
H00L	11967	1578	8349	42
H00M	9100	9533	5657	57
H00N	6516	9897	5569	57
H00O	7876	9492	5058	57