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Supporting Information

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Enhanced Two-photon Absorption Cross-sections of Zinc(II) tetraphenylporphyrins Peripherally substituted with d^6-Metal Alkynyl Complexes

Including:

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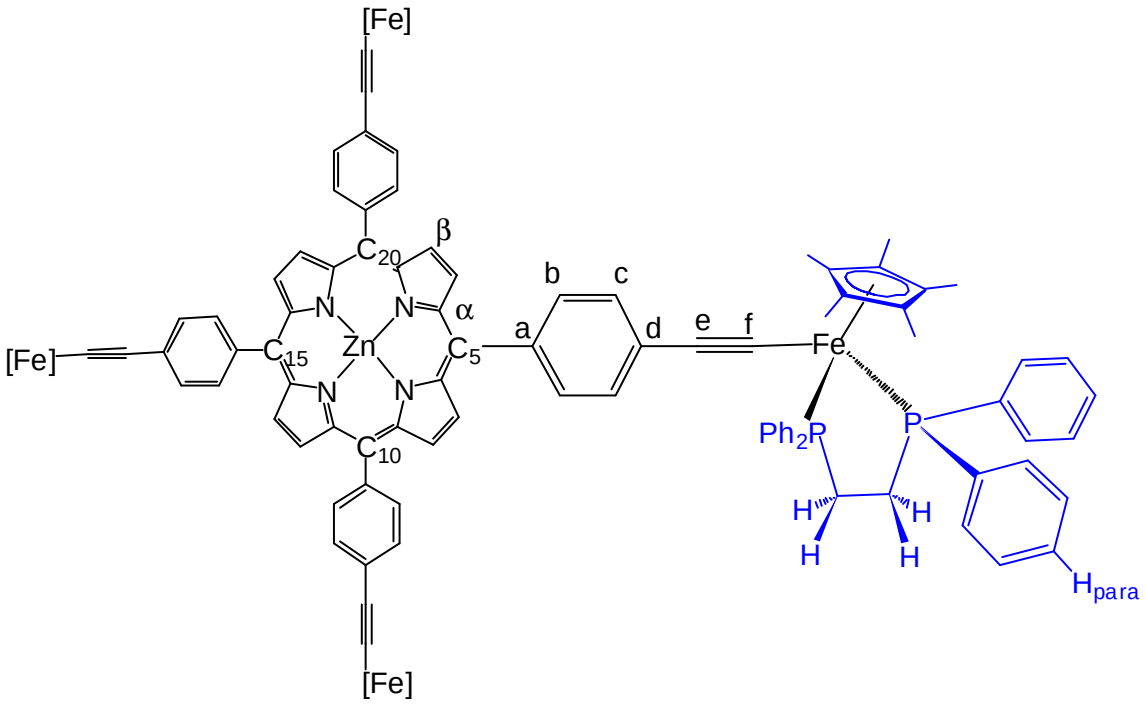
1. Labelling Scheme used for 4 in ^{13}C NMR



4

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2. Cyclic Voltammograms of 4 and 7

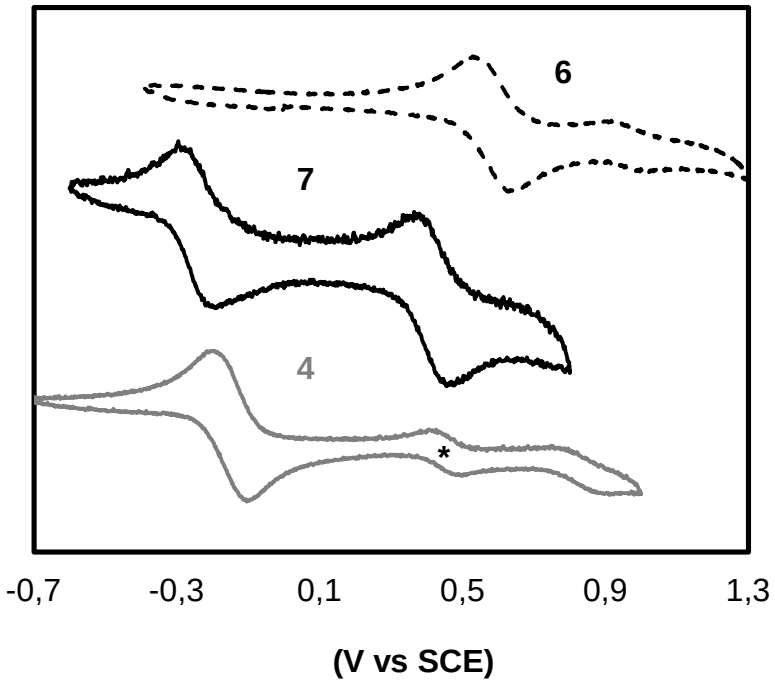

Figure S1. Cyclic voltammograms of compounds **4**, **6** and **7** showing the Fe- and/or Ru-centered redox processes as the most intense redox event(s) and, for **4** and **6**, the first oxidation of the ZnTPP core as a redox event of one quarter the intensity in the 0.9-1.0 V range. In the CV of **4**, the asterisk corresponds to ferrocene (FcH, *ca.* 1 equivalent) added as internal calibrant. Conditions: CH_2Cl_2, 20 °C, [^{n}Bu$_4$N][PF_6] 0.1 M, scan rate: 0.1 V/s. Potential given *vs.* saturated calomel electrode (SCE).

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3. Nonlinear Absorption Measurements (Z-scan)

Third-order nonlinear optical properties were investigated with an amplified femtosecond laser system using a Clark-MXR CPA-2001 Ti-sapphire regenerative amplifier pumping a Light Conversion TOPAS optical parametric amplifier. Experiments were performed over a wide range of wavelengths using different modes of the OPA output and employing polarizing optics, spatial filtering and colour glass filters to reject unwanted wavelengths. The pulse duration was approximately 150 fs and the repetition rate was 250 Hz. The pulse energy was adjusted to maintain the nonlinear phase shifts obtained from the samples in the range ca. 0.3 -1.5 rad, which typically corresponded to light intensities of the order of 100 GW/cm^2. Solutions of the compounds in dichloromethane of *ca.* 0.5 w/w% concentration were placed in 1 mm stoppered Starna glass cells. An identical cell was used for measurements of Z-scans on pure solvent. All measurements were calibrated by referencing to signals obtained from a 3 mm thick fused silica plate, and the NLO properties of the solute were determined as described previously.[1,2]

[1] B. Babgi, L. Rigamonti, M. P. Cifuentes, T. C. Corkery, M. D. Randles, T. Schwich, S. Petrie, R. Stranger, A. Teshome, I. Asselberghs, K. Clays, M. Samoc and M. G. Humphrey *J. Am. Chem. Soc.* **2009**, *131*, 10293-10307.
[2] M. Samoc, A. Samoc, G. T. Dalton, M. P. Cifuentes, M. G. Humphrey and P. A. Fleitz, *Multiphoton Processes in Organics and Their Application*; I. Rau and F. Kajzar, Eds.; Old City Publishing: Philadelphia, 2011, p 341-355.

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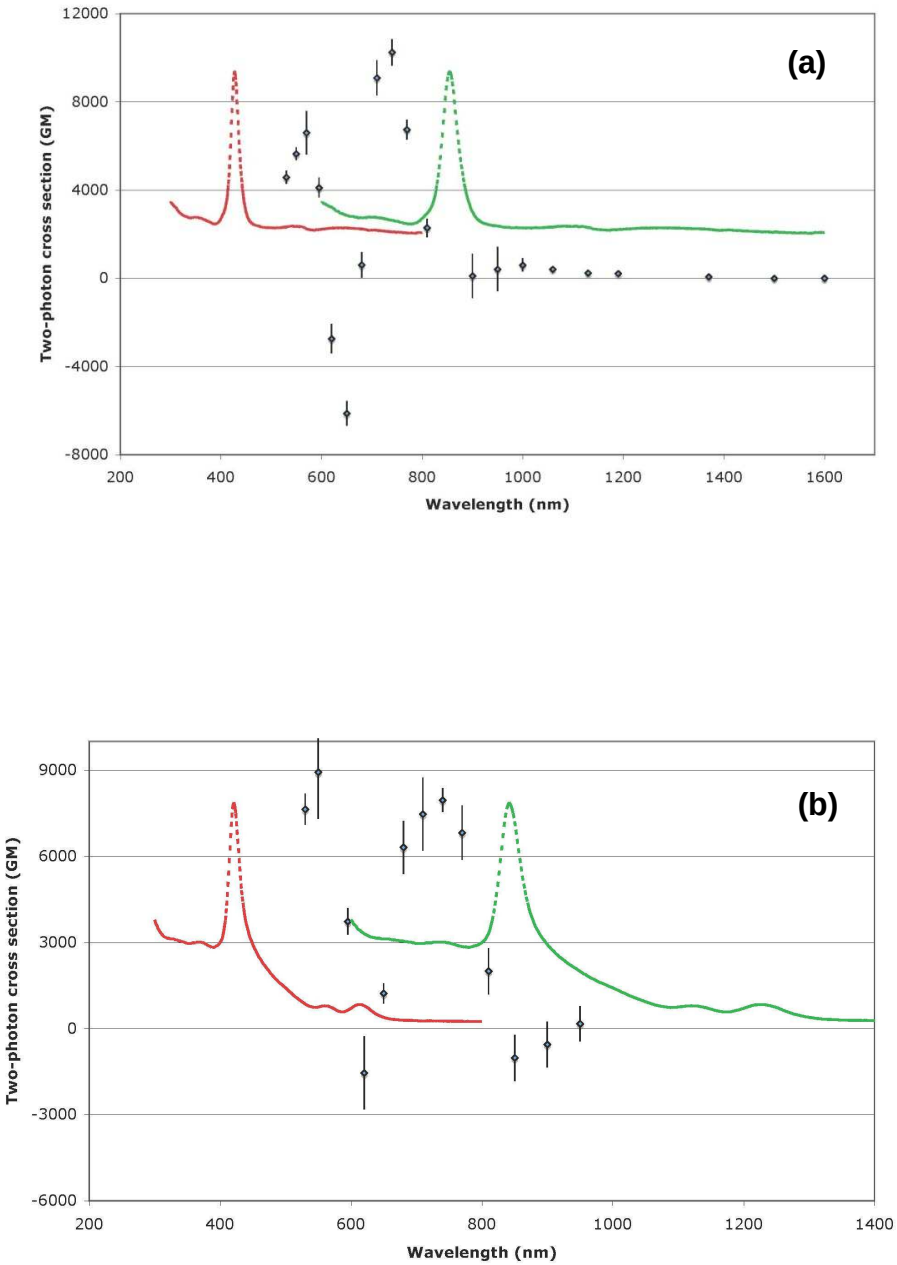

Figure S2. Nonlinear absorption measurements represented as effective two-photon absorption cross-sections overlayed with the one-photon absorption (OPA) spectrum (red curve) and the same OPA spectrum plotted against twice the wavelength (green curve) for compounds **4** (a) and **7** (b). Due to sample evolution, no data could be obtained for **7** above 1000 nm.

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4. ESR of $4[PF_6]_4$

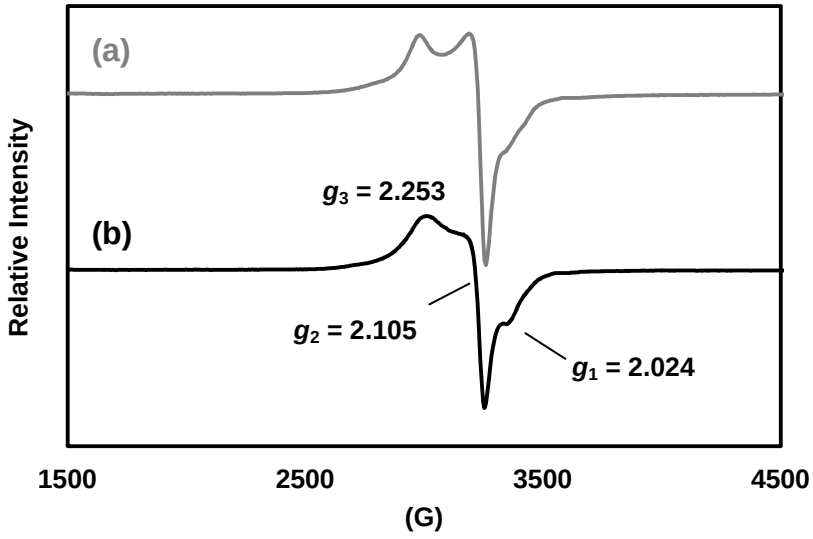

Figure S3. a) ESR spectra of **4**$[PF_6]_4$ generated in situ from **4** and [FcH][PF_6] (> 4 eq.) in THF glass at 70 K. b) ESR spectra of **4**$[PF_6]_4$ in CH_2Cl_2/1,2-$C_2H_4Cl_2$ (1:1) glass at 70 K.

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5. ^{1}H NMR of 4[PF$_6$]$_4$

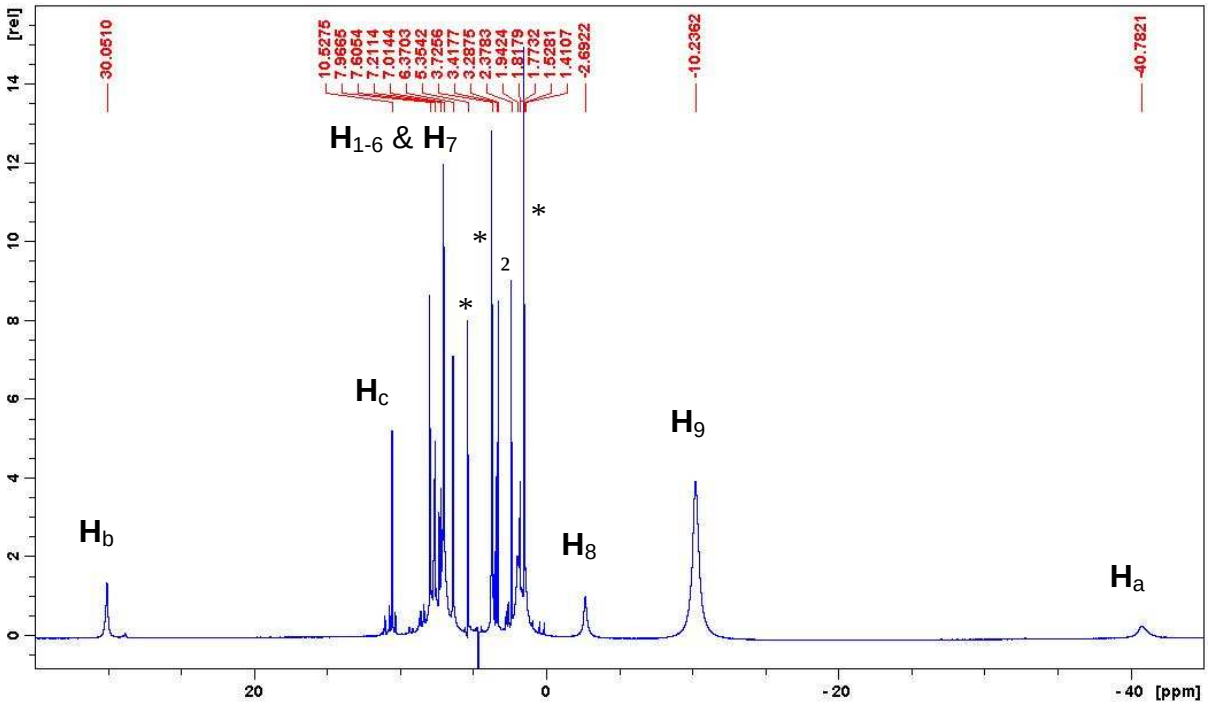

Figure S4. ^{1}H NMR spectrum of **4**[PF$_6$]$_4$ in CD_2Cl_2 at 300 K. Numbering of selected protons according to Chart S1. Signals corresponding to solvents are designated by stars.

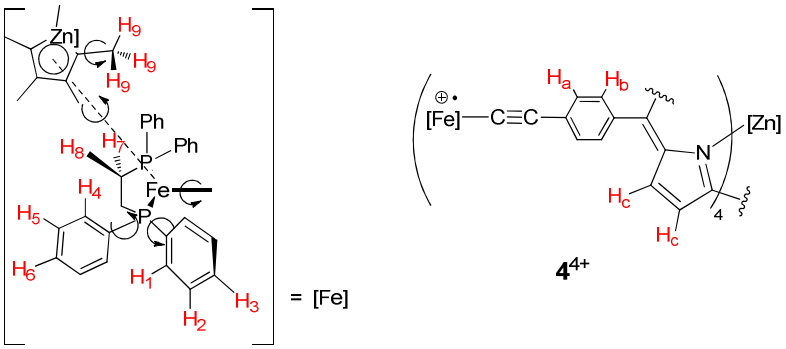

Chart S1. ^{1}H Nuclei Numbering Corresponding to the Proposed Assignment for **4**[PF$_6$]$_4$.

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6. Crystal Data and Structure Refinement Details for 4

Empirical formula	$C_{200}H_{190}Fe_4N_4OP_8Zn \bullet 4C_5H_{12}$
Formula weight	3490.67
Temperature	120(2) K
Wavelength	0.71073 Å
Crystal system, space group	Tetragonal, $I4_1/a$
Unit cell dimensions	a = 36.9262(5) Å alpha = 90 deg.
	b = 36.9262(5) Å beta = 90 deg.
	c = 14.7933(8) Å gamma = 90 deg.
Volume	20171.3(12) $Å^3$
Z, Calculated density	4, 1.140 Mg/m^3
Absorption coefficient	0.513 mm^{-1}
F(000)	7324
Crystal size	0.34 × 0.28 × 0.26 mm
Theta range for data collection	2.66 to 26.00 deg.
Limiting indices	-45<=h<=45, -45<=k<=45, -18<=l<=18
Reflections collected / unique	124179 / 9916 [R(int) = 0.0699]
Completeness to theta = 27.48	99.9 %
Absorption correction	None
Max. and min. transmission	0.989 and 0.975
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9916 / 6 / 522
Goodness-of-fit on F^2	1.133
Final R indices [I > 2σ(I)]	R1 = 0.1141, wR2 = 0.2885
R indices (all data)	R1 = 0.1684, wR2 = 0.3241
Largest diff. peak and hole	0.869 and -0.474 $e.Å^{-3}$

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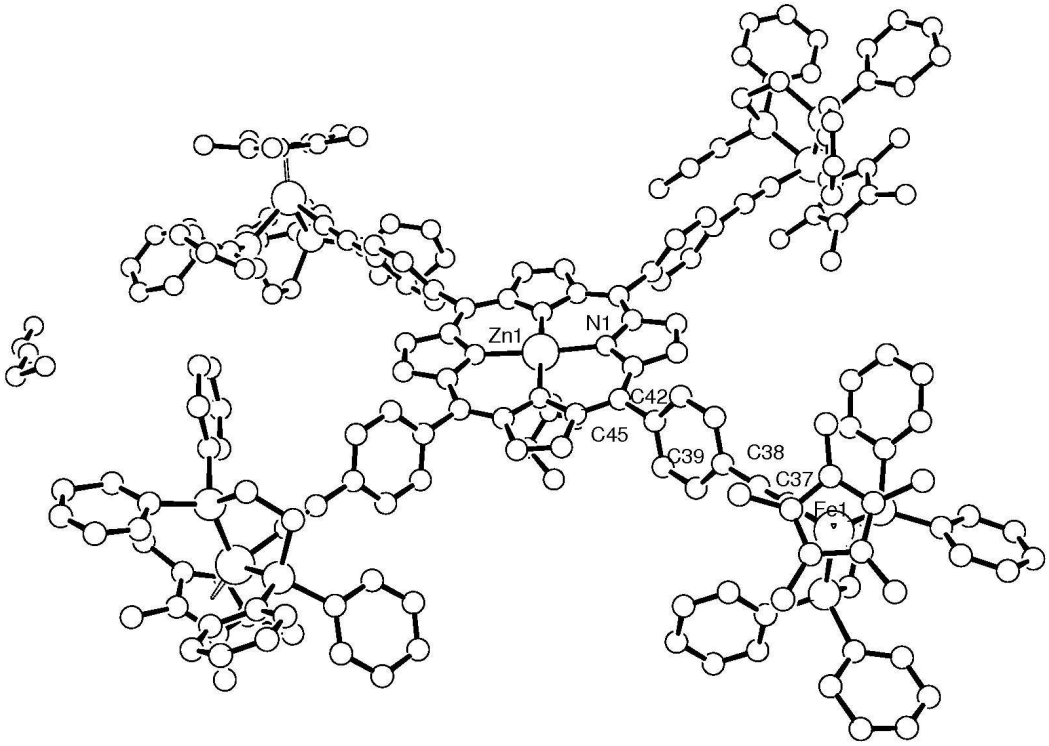

Figure S5. PLUTO plot of **4**. Hydrogen atoms have been omitted for clarity. A disordered Et_2O molecule coordinated to Zn is shown below the porphyrin plane along with one of the four pentane solvate molecules.

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Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters ($Å^2$ × 10^3) for 4. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Fe(1)	9052(1)	693(1)	8763(1)	44(1)
Zn(1)	10000	-2500	8750	67(1)
P(1)	9201(1)	746(1)	7354(2)	64(1)
P(2)	8530(1)	508(1)	8281(1)	40(1)
N(1)	10259(1)	-2012(1)	8689(4)	47(2)
C(1)	9421(2)	715(2)	9856(6)	58(2)
C(2)	9053(2)	690(2)	10185(5)	45(2)
C(3)	8868(2)	1003(2)	9873(5)	42(2)
C(4)	9112(2)	1216(2)	9352(5)	47(2)
C(5)	9452(2)	1032(2)	9352(6)	53(2)
C(6)	9722(2)	461(2)	10124(8)	76(3)
C(7)	8903(2)	398(2)	10796(6)	61(2)
C(8)	8495(2)	1117(2)	10191(5)	47(2)
C(9)	9057(2)	1597(2)	9004(6)	61(2)
C(10)	9798(2)	1200(2)	8978(7)	76(3)
C(11)	8854(2)	527(3)	6626(7)	76(3)
C(12)	8604(2)	279(2)	7190(5)	47(2)
C(13)	9219(3)	1204(3)	6778(7)	91(4)
C(14)	8902(5)	1395(3)	6580(10)	139(6)
C(15)	8880(5)	1735(5)	6185(12)	142(6)
C(16)	9177(6)	1895(6)	6123(19)	206(12)
C(17)	9506(4)	1768(4)	6272(12)	147(7)
C(18)	9540(5)	1381(4)	6647(11)	150(7)
C(19)	9622(3)	550(3)	6947(10)	100(4)
C(20)	9696(5)	549(5)	6004(12)	165(7)
C(21)	10042(7)	377(8)	5734(19)	239(13)
C(22)	10282(7)	241(9)	6414(18)	240(15)
C(23)	10202(4)	255(5)	7267(17)	181(8)
C(24)	9866(3)	399(3)	7575(11)	115(5)
C(25)	8277(2)	181(2)	8956(4)	34(1)
C(26)	8379(2)	-184(2)	8972(5)	42(2)
C(27)	8206(2)	-428(2)	9552(5)	51(2)
C(28)	7937(2)	-311(2)	10122(5)	51(2)
C(29)	7834(2)	48(2)	10132(5)	50(2)
C(30)	8004(2)	286(2)	9550(5)	41(2)
C(31)	8168(2)	824(2)	7951(5)	48(2)
C(32)	7838(2)	702(2)	7596(6)	66(2)
C(33)	7571(2)	944(3)	7310(7)	77(3)
C(34)	7629(3)	1301(3)	7357(7)	76(3)
C(35)	7947(3)	1429(2)	7730(7)	81(3)
C(36)	8223(2)	1191(2)	8016(6)	55(2)
C(37)	9176(2)	197(2)	8659(5)	48(2)
C(38)	9268(2)	-112(2)	8627(6)	53(2)

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C(39)	9381(2)	-491(2)	8655(6)	51(2)
C(40)	9562(2)	-644(2)	7932(6)	49(2)
C(41)	9673(2)	-1002(2)	7960(5)	44(2)
C(42)	9603(2)	-1220(2)	8707(6)	49(2)
C(43)	9421(2)	-1066(2)	9446(6)	49(2)
C(44)	9312(2)	-704(2)	9419(6)	53(2)
C(45)	9722(2)	-1608(2)	8737(5)	44(2)
C(46)	10096(2)	-1676(2)	8669(5)	44(2)
C(47)	10371(2)	-1400(2)	8628(6)	50(2)
C(48)	10694(2)	-1571(2)	8632(6)	49(2)
C(49)	10624(2)	-1951(2)	8684(5)	45(2)
O(41)	10000	-2500	7055(16)	80(5)
C(50)	10252(9)	-2455(10)	6480(20)	179(17)
C(51)	10204(9)	-2067(10)	6236(16)	164
C(61)	6462(6)	392(6)	7401(15)	206(9)
C(62)	6241(7)	685(7)	6876(19)	240(11)
C(63)	6468(8)	1030(8)	6660(20)	261(12)
C(64)	6503(10)	1454(10)	6070(20)	315(17)
C(65)	6707(10)	1793(9)	5870(20)	307(16)

Bond lengths [Å] and angles [deg] for 4.

Fe(1)-C(37)	1.896(6)
Fe(1)-C(2)	2.104(8)
Fe(1)-C(3)	2.113(7)
Fe(1)-C(1)	2.114(8)
Fe(1)-C(5)	2.121(7)
Fe(1)-C(4)	2.129(6)
Fe(1)-P(1)	2.164(3)
Fe(1)-P(2)	2.1677(18)
Zn(1)-N(1)	2.043(5)
Zn(1)-N(1)#1	2.043(5)
Zn(1)-N(1)#2	2.043(5)
Zn(1)-N(1)#3	2.043(5)
P(1)-C(19)	1.817(10)
P(1)-C(11)	1.858(10)
P(1)-C(13)	1.895(11)
P(2)-C(25)	1.824(6)
P(2)-C(31)	1.839(6)
P(2)-C(12)	1.843(7)
N(1)-C(49)	1.369(7)
N(1)-C(46)	1.377(7)
C(1)-C(5)	1.393(11)
C(1)-C(2)	1.444(10)
C(1)-C(6)	1.509(10)
C(2)-C(3)	1.422(9)
C(2)-C(7)	1.510(11)

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C(3)-C(4)	1.423(10)
C(3)-C(8)	1.514(9)
C(4)-C(5)	1.429(9)
C(4)-C(9)	1.510(10)
C(5)-C(10)	1.523(10)
C(6)-H(6A)	0.9800
C(6)-H(6B)	0.9800
C(6)-H(6C)	0.9800
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-C(12)	1.547(10)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(18)	1.367(15)
C(13)-C(14)	1.398(18)
C(14)-C(15)	1.388(18)
C(14)-H(14)	0.9500
C(15)-C(16)	1.25(2)
C(15)-H(15)	0.9500
C(16)-C(17)	1.32(2)
C(16)-H(16)	0.9500
C(17)-C(18)	1.539(19)
C(17)-H(17)	0.9500
C(18)-H(18)	0.9500
C(19)-C(24)	1.411(19)
C(19)-C(20)	1.42(2)
C(20)-C(21)	1.48(3)
C(20)-H(20)	0.9500
C(21)-C(22)	1.43(3)
C(21)-H(21)	0.9500
C(22)-C(23)	1.30(3)
C(22)-H(22)	0.9500
C(23)-C(24)	1.424(15)
C(23)-H(23)	0.9500
C(24)-H(24)	0.9500
C(25)-C(30)	1.393(9)
C(25)-C(26)	1.400(8)
C(26)-C(27)	1.398(10)

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C(26)-H(26)	0.9500
C(27)-C(28)	1.375(10)
C(27)-H(27)	0.9500
C(28)-C(29)	1.378(10)
C(28)-H(28)	0.9500
C(29)-C(30)	1.379(10)
C(29)-H(29)	0.9500
C(30)-H(30)	0.9500
C(31)-C(36)	1.373(10)
C(31)-C(32)	1.403(11)
C(32)-C(33)	1.398(11)
C(32)-H(32)	0.9500
C(33)-C(34)	1.335(14)
C(33)-H(33)	0.9500
C(34)-C(35)	1.381(14)
C(34)-H(34)	0.9500
C(35)-C(36)	1.411(11)
C(35)-H(35)	0.9500
C(36)-H(36)	0.9500
C(37)-C(38)	1.191(9)
C(38)-C(39)	1.459(9)
C(39)-C(40)	1.382(11)
C(39)-C(44)	1.399(11)
C(40)-C(41)	1.384(8)
C(40)-H(40)	0.9500
C(41)-C(42)	1.393(10)
C(41)-H(41)	0.9500
C(42)-C(43)	1.403(10)
C(42)-C(45)	1.498(8)
C(43)-C(44)	1.398(9)
C(43)-H(43)	0.9500
C(44)-H(44)	0.9500
C(45)-C(49)#2	1.409(8)
C(45)-C(46)	1.410(8)
C(46)-C(47)	1.438(8)
C(47)-C(48)	1.349(9)
C(47)-H(47)	0.9500
C(48)-C(49)	1.430(8)
C(48)-H(48)	0.9500
C(49)-C(45)#3	1.409(8)
O(41)-C(50)#1	1.28(3)
O(41)-C(50)	1.28(3)
C(50)-C(51)	1.487(17)
C(50)-H(50A)	0.9900
C(50)-H(50B)	0.9900
C(51)-H(51A)	0.9800
C(51)-H(51B)	0.9800
C(51)-H(51C)	0.9800
C(61)-C(62)	1.56(3)
C(61)-H(61A)	0.9800

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C(61)-H(61B)	0.9800
C(61)-H(61C)	0.9800
C(62)-C(63)	1.557(16)
C(62)-H(62A)	0.9900
C(62)-H(62B)	0.9900
C(63)-C(64)	1.80(4)
C(63)-H(63A)	0.9900
C(63)-H(63B)	0.9900
C(64)-C(65)	1.487(17)
C(64)-H(64A)	0.9900
C(64)-H(64B)	0.9900
C(65)-H(65A)	0.9800
C(65)-H(65B)	0.9800
C(65)-H(65C)	0.9800

C(37)-Fe(1)-C(2)	94.3(3)
C(37)-Fe(1)-C(3)	131.6(3)
C(2)-Fe(1)-C(3)	39.4(2)
C(37)-Fe(1)-C(1)	86.7(3)
C(2)-Fe(1)-C(1)	40.1(3)
C(3)-Fe(1)-C(1)	66.0(3)
C(37)-Fe(1)-C(5)	115.8(3)
C(2)-Fe(1)-C(5)	65.9(3)
C(3)-Fe(1)-C(5)	65.6(3)
C(1)-Fe(1)-C(5)	38.4(3)
C(37)-Fe(1)-C(4)	152.2(3)
C(2)-Fe(1)-C(4)	66.2(3)
C(3)-Fe(1)-C(4)	39.2(3)
C(1)-Fe(1)-C(4)	65.6(3)
C(5)-Fe(1)-C(4)	39.3(2)
C(37)-Fe(1)-P(1)	87.0(3)
C(2)-Fe(1)-P(1)	164.47(19)
C(3)-Fe(1)-P(1)	141.3(2)
C(1)-Fe(1)-P(1)	124.8(2)
C(5)-Fe(1)-P(1)	99.6(2)
C(4)-Fe(1)-P(1)	106.6(2)
C(37)-Fe(1)-P(2)	83.28(19)
C(2)-Fe(1)-P(2)	109.15(19)
C(3)-Fe(1)-P(2)	98.02(18)
C(1)-Fe(1)-P(2)	146.7(2)
C(5)-Fe(1)-P(2)	160.14(18)
C(4)-Fe(1)-P(2)	120.86(18)
P(1)-Fe(1)-P(2)	86.38(9)
N(1)-Zn(1)-N(1)#1	175.0(4)
N(1)-Zn(1)-N(1)#2	90.114(17)
N(1)#1-Zn(1)-N(1)#2	90.110(17)
N(1)-Zn(1)-N(1)#3	90.107(17)
N(1)#1-Zn(1)-N(1)#3	90.110(17)
N(1)#2-Zn(1)-N(1)#3	175.0(4)
C(19)-P(1)-C(11)	103.0(5)

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C(19)-P(1)-C(13)	100.1(5)
C(11)-P(1)-C(13)	98.7(5)
C(19)-P(1)-Fe(1)	120.0(5)
C(11)-P(1)-Fe(1)	110.2(3)
C(13)-P(1)-Fe(1)	121.5(3)
C(25)-P(2)-C(31)	101.1(3)
C(25)-P(2)-C(12)	104.5(3)
C(31)-P(2)-C(12)	99.6(3)
C(25)-P(2)-Fe(1)	119.0(2)
C(31)-P(2)-Fe(1)	122.3(2)
C(12)-P(2)-Fe(1)	107.5(2)
C(49)-N(1)-C(46)	106.4(5)
C(49)-N(1)-Zn(1)	127.2(4)
C(46)-N(1)-Zn(1)	126.3(4)
C(5)-C(1)-C(2)	108.3(6)
C(5)-C(1)-C(6)	126.9(7)
C(2)-C(1)-C(6)	124.4(8)
C(5)-C(1)-Fe(1)	71.1(5)
C(2)-C(1)-Fe(1)	69.6(4)
C(6)-C(1)-Fe(1)	130.7(5)
C(3)-C(2)-C(1)	106.8(6)
C(3)-C(2)-C(7)	126.8(6)
C(1)-C(2)-C(7)	126.3(6)
C(3)-C(2)-Fe(1)	70.7(4)
C(1)-C(2)-Fe(1)	70.3(5)
C(7)-C(2)-Fe(1)	127.0(5)
C(4)-C(3)-C(2)	108.7(6)
C(4)-C(3)-C(8)	126.2(6)
C(2)-C(3)-C(8)	124.2(6)
C(4)-C(3)-Fe(1)	71.0(4)
C(2)-C(3)-Fe(1)	69.9(4)
C(8)-C(3)-Fe(1)	133.2(5)
C(3)-C(4)-C(5)	107.1(6)
C(3)-C(4)-C(9)	127.8(6)
C(5)-C(4)-C(9)	124.2(6)
C(3)-C(4)-Fe(1)	69.8(4)
C(5)-C(4)-Fe(1)	70.1(4)
C(9)-C(4)-Fe(1)	133.7(6)
C(1)-C(5)-C(4)	109.0(6)
C(1)-C(5)-C(10)	127.4(7)
C(4)-C(5)-C(10)	122.8(7)
C(1)-C(5)-Fe(1)	70.5(4)
C(4)-C(5)-Fe(1)	70.6(4)
C(10)-C(5)-Fe(1)	132.4(6)
C(1)-C(6)-H(6A)	109.5
C(1)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
C(1)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5

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C(2)-C(7)-H(7A)	109.5
C(2)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(2)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(3)-C(8)-H(8A)	109.5
C(3)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(3)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(4)-C(9)-H(9A)	109.5
C(4)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(4)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(5)-C(10)-H(10A)	109.5
C(5)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(5)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(12)-C(11)-P(1)	110.9(7)
C(12)-C(11)-H(11A)	109.5
P(1)-C(11)-H(11A)	109.5
C(12)-C(11)-H(11B)	109.5
P(1)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	108.0
C(11)-C(12)-P(2)	106.7(5)
C(11)-C(12)-H(12A)	110.4
P(2)-C(12)-H(12A)	110.4
C(11)-C(12)-H(12B)	110.4
P(2)-C(12)-H(12B)	110.4
H(12A)-C(12)-H(12B)	108.6
C(18)-C(13)-C(14)	117.0(13)
C(18)-C(13)-P(1)	121.4(12)
C(14)-C(13)-P(1)	121.0(8)
C(15)-C(14)-C(13)	126.5(15)
C(15)-C(14)-H(14)	116.8
C(13)-C(14)-H(14)	116.8
C(16)-C(15)-C(14)	114(2)
C(16)-C(15)-H(15)	123.0
C(14)-C(15)-H(15)	123.0
C(15)-C(16)-C(17)	129(2)
C(15)-C(16)-H(16)	115.5
C(17)-C(16)-H(16)	115.5
C(16)-C(17)-C(18)	117.6(15)
C(16)-C(17)-H(17)	121.2

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C(18)-C(17)-H(17)	121.2
C(13)-C(18)-C(17)	115.1(16)
C(13)-C(18)-H(18)	122.4
C(17)-C(18)-H(18)	122.4
C(24)-C(19)-C(20)	121.5(11)
C(24)-C(19)-P(1)	119.2(9)
C(20)-C(19)-P(1)	119.3(12)
C(21)-C(20)-C(19)	115.5(19)
C(21)-C(20)-H(20)	122.2
C(19)-C(20)-H(20)	122.2
C(20)-C(21)-C(22)	120(2)
C(20)-C(21)-H(21)	120.2
C(22)-C(21)-H(21)	120.2
C(21)-C(22)-C(23)	122(2)
C(21)-C(22)-H(22)	119.0
C(23)-C(22)-H(22)	119.0
C(24)-C(23)-C(22)	122(2)
C(24)-C(23)-H(23)	119.2
C(22)-C(23)-H(23)	119.2
C(23)-C(24)-C(19)	119.6(15)
C(23)-C(24)-H(24)	120.2
C(19)-C(24)-H(24)	120.2
C(30)-C(25)-C(26)	116.9(6)
C(30)-C(25)-P(2)	122.2(5)
C(26)-C(25)-P(2)	120.6(5)
C(25)-C(26)-C(27)	120.5(6)
C(25)-C(26)-H(26)	119.7
C(27)-C(26)-H(26)	119.8
C(28)-C(27)-C(26)	120.3(6)
C(28)-C(27)-H(27)	119.9
C(26)-C(27)-H(27)	119.9
C(27)-C(28)-C(29)	120.6(7)
C(27)-C(28)-H(28)	119.7
C(29)-C(28)-H(28)	119.7
C(28)-C(29)-C(30)	118.7(7)
C(28)-C(29)-H(29)	120.7
C(30)-C(29)-H(29)	120.7
C(25)-C(30)-C(29)	123.1(6)
C(25)-C(30)-H(30)	118.4
C(29)-C(30)-H(30)	118.4
C(36)-C(31)-C(32)	118.1(7)
C(36)-C(31)-P(2)	120.0(6)
C(32)-C(31)-P(2)	121.9(6)
C(33)-C(32)-C(31)	121.4(8)
C(33)-C(32)-H(32)	119.3
C(31)-C(32)-H(32)	119.3
C(34)-C(33)-C(32)	120.1(9)
C(34)-C(33)-H(33)	119.9
C(32)-C(33)-H(33)	119.9
C(33)-C(34)-C(35)	119.7(8)

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C(33)-C(34)-H(34)	120.1
C(35)-C(34)-H(34)	120.1
C(34)-C(35)-C(36)	121.3(9)
C(34)-C(35)-H(35)	119.3
C(36)-C(35)-H(35)	119.3
C(31)-C(36)-C(35)	119.2(8)
C(31)-C(36)-H(36)	120.4
C(35)-C(36)-H(36)	120.4
C(38)-C(37)-Fe(1)	176.5(7)
C(37)-C(38)-C(39)	176.1(9)
C(40)-C(39)-C(44)	118.9(6)
C(40)-C(39)-C(38)	120.5(7)
C(44)-C(39)-C(38)	120.6(7)
C(39)-C(40)-C(41)	120.7(7)
C(39)-C(40)-H(40)	119.7
C(41)-C(40)-H(40)	119.7
C(40)-C(41)-C(42)	121.5(7)
C(40)-C(41)-H(41)	119.2
C(42)-C(41)-H(41)	119.2
C(43)-C(42)-C(41)	118.1(6)
C(43)-C(42)-C(45)	120.3(7)
C(41)-C(42)-C(45)	121.6(6)
C(42)-C(43)-C(44)	120.2(7)
C(42)-C(43)-H(43)	119.9
C(44)-C(43)-H(43)	119.9
C(39)-C(44)-C(43)	120.6(7)
C(39)-C(44)-H(44)	119.7
C(43)-C(44)-H(44)	119.7
C(49)#2-C(45)-C(46)	125.2(5)
C(49)#2-C(45)-C(42)	117.7(5)
C(46)-C(45)-C(42)	117.1(5)
N(1)-C(46)-C(45)	125.8(5)
N(1)-C(46)-C(47)	109.4(5)
C(45)-C(46)-C(47)	124.7(5)
C(48)-C(47)-C(46)	106.9(5)
C(48)-C(47)-H(47)	126.5
C(46)-C(47)-H(47)	126.5
C(47)-C(48)-C(49)	107.5(5)
C(47)-C(48)-H(48)	126.2
C(49)-C(48)-H(48)	126.2
N(1)-C(49)-C(45)#3	125.2(5)
N(1)-C(49)-C(48)	109.7(5)
C(45)#3-C(49)-C(48)	125.1(5)
C(50)#1-O(41)-C(50)	96(4)
O(41)-C(50)-C(51)	101.5(19)
O(41)-C(50)-H(50A)	111.5
C(51)-C(50)-H(50A)	111.5
O(41)-C(50)-H(50B)	111.4
C(51)-C(50)-H(50B)	111.4
H(50A)-C(50)-H(50B)	109.3

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C(50)-C(51)-H(51A)	109.5
C(50)-C(51)-H(51B)	109.5
H(51A)-C(51)-H(51B)	109.5
C(50)-C(51)-H(51C)	109.4
H(51A)-C(51)-H(51C)	109.5
H(51B)-C(51)-H(51C)	109.5
C(62)-C(61)-H(61A)	109.5
C(62)-C(61)-H(61B)	109.5
H(61A)-C(61)-H(61B)	109.5
C(62)-C(61)-H(61C)	109.5
H(61A)-C(61)-H(61C)	109.5
H(61B)-C(61)-H(61C)	109.5
C(63)-C(62)-C(61)	113(2)
C(63)-C(62)-H(62A)	109.0
C(61)-C(62)-H(62A)	109.0
C(63)-C(62)-H(62B)	109.0
C(61)-C(62)-H(62B)	109.0
H(62A)-C(62)-H(62B)	107.8
C(62)-C(63)-C(64)	148(3)
C(62)-C(63)-H(63A)	99.7
C(64)-C(63)-H(63A)	99.7
C(62)-C(63)-H(63B)	99.7
C(64)-C(63)-H(63B)	99.7
H(63A)-C(63)-H(63B)	104.1
C(65)-C(64)-C(63)	149(3)
C(65)-C(64)-H(64A)	99.4
C(63)-C(64)-H(64A)	99.3
C(65)-C(64)-H(64B)	99.3
C(63)-C(64)-H(64B)	99.3
H(64A)-C(64)-H(64B)	104.0
C(64)-C(65)-H(65A)	109.5
C(64)-C(65)-H(65B)	109.4
H(65A)-C(65)-H(65B)	109.5
C(64)-C(65)-H(65C)	109.5
H(65A)-C(65)-H(65C)	109.5
H(65B)-C(65)-H(65C)	109.5

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,-y-1/2,z #2 -y+3/4,x-5/4,-z+7/4 #3 y+5/4,-x+3/4,-z+7/4

Anisotropic displacement parameters ($Å^2 \times 10^3$) for 4.

The anisotropic displacement factor exponent takes the form: $-2\ pi^2\ [\ h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U_{12}\ ]$

U11	U22	U33	U23	U13	U12

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Fe(1)	27(1)	22(1)	85(1)	-10(1)	3(1)	1(1)
Zn(1)	17(1)	17(1)	168(2)	0	0	0
P(1)	53(1)	43(1)	96(2)	-20(1)	30(1)	-12(1)
P(2)	30(1)	25(1)	64(1)	2(1)	-1(1)	1(1)
N(1)	23(2)	18(2)	100(5)	-2(3)	-3(3)	3(2)
C(1)	34(3)	33(4)	108(7)	-23(4)	-21(4)	4(3)
C(2)	37(3)	30(3)	69(5)	-15(3)	-9(3)	-1(3)
C(3)	33(3)	27(3)	64(5)	-10(3)	-2(3)	0(2)
C(4)	37(3)	28(3)	77(5)	-14(3)	2(3)	0(3)
C(5)	31(3)	31(3)	99(6)	-19(4)	8(4)	-4(3)
C(6)	42(4)	54(5)	132(9)	-26(5)	-24(5)	9(4)
C(7)	69(5)	38(4)	76(6)	6(4)	-23(4)	-2(3)
C(8)	33(3)	39(4)	70(5)	-9(3)	3(3)	0(3)
C(9)	60(5)	25(3)	96(7)	-10(4)	16(4)	-6(3)
C(10)	34(4)	56(5)	138(9)	-32(5)	10(5)	-15(3)
C(11)	74(6)	68(6)	86(7)	1(5)	17(5)	-20(5)
C(12)	42(4)	41(4)	57(5)	-4(3)	6(3)	-7(3)
C(13)	118(9)	68(6)	88(7)	-11(5)	56(7)	-43(6)
C(14)	206(16)	82(8)	129(11)	36(8)	93(11)	51(10)
C(15)	127(13)	136(13)	164(15)	55(11)	34(11)	35(11)
C(16)	105(13)	153(17)	360(40)	-82(19)	-5(18)	3(13)
C(17)	110(11)	99(9)	233(19)	89(11)	34(11)	-22(8)
C(18)	179(15)	115(11)	155(13)	-25(10)	63(11)	-85(11)
C(19)	59(6)	92(8)	149(11)	-37(7)	46(7)	-3(5)
C(20)	156(14)	179(16)	161(15)	-44(12)	103(12)	19(12)
C(21)	200(20)	330(30)	190(20)	-20(20)	140(20)	40(20)
C(22)	160(20)	380(40)	180(20)	-50(20)	72(17)	110(20)
C(23)	60(8)	208(18)	280(20)	-31(17)	67(11)	21(9)
C(24)	52(6)	102(8)	191(14)	-57(9)	40(7)	7(6)
C(25)	29(3)	27(3)	45(4)	-4(3)	-9(3)	-3(2)
C(26)	39(3)	31(3)	57(4)	1(3)	-4(3)	-1(3)
C(27)	52(4)	33(3)	68(5)	8(3)	-8(4)	0(3)
C(28)	45(4)	42(4)	67(5)	5(3)	-1(4)	-7(3)
C(29)	45(4)	44(4)	61(5)	5(3)	1(3)	-3(3)
C(30)	31(3)	35(3)	58(4)	-4(3)	-6(3)	1(3)
C(31)	43(4)	46(4)	56(5)	14(3)	6(3)	13(3)
C(32)	39(4)	66(5)	93(7)	33(5)	-4(4)	12(3)
C(33)	48(5)	93(7)	89(7)	44(6)	2(4)	8(4)
C(34)	58(5)	94(7)	76(6)	32(5)	11(5)	30(5)
C(35)	103(8)	52(5)	87(7)	22(5)	21(6)	30(5)
C(36)	56(4)	38(4)	72(5)	16(4)	8(4)	10(3)
C(37)	28(3)	27(3)	89(6)	-11(3)	-7(3)	3(2)
C(38)	30(3)	32(3)	97(6)	-11(4)	-14(4)	6(3)
C(39)	27(3)	24(3)	102(6)	-5(4)	-17(4)	0(2)
C(40)	31(3)	24(3)	91(6)	-4(3)	-9(3)	-1(2)
C(41)	30(3)	25(3)	77(5)	-7(3)	-9(3)	0(2)
C(42)	18(3)	24(3)	104(6)	-16(4)	-12(3)	6(2)
C(43)	26(3)	32(3)	88(6)	1(3)	-9(3)	0(3)
C(44)	26(3)	38(4)	94(6)	-17(4)	-5(3)	9(3)

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C(45)	23(3)	20(3)	89(5)	-1(3)	-6(3)	5(2)
C(46)	30(3)	19(3)	82(5)	-4(3)	-3(3)	-1(2)
C(47)	33(3)	19(3)	98(6)	-8(3)	-4(4)	-2(2)
C(48)	27(3)	27(3)	92(6)	-4(3)	1(3)	-3(2)
C(49)	23(3)	25(3)	87(5)	-11(3)	-4(3)	-4(2)
O(41)	40(8)	60(10)	140(18)	0	0	-8(7)
C(50)	150(30)	280(50)	110(20)	-20(30)	50(20)	120(30)
C(51)	149	299	44	-43	47	36

Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for 4.

	x	y	z	U(eq)
H(6A)	9639	210	10071	114
H(6B)	9793	509	10751	114
H(6C)	9931	499	9725	114
H(7A)	8996	162	10603	92
H(7B)	8638	399	10760	92
H(7C)	8979	445	11420	92
H(8A)	8333	908	10183	71
H(8B)	8400	1305	9789	71
H(8C)	8512	1213	10808	71
H(9A)	9135	1610	8372	91
H(9B)	9200	1766	9369	91
H(9C)	8800	1660	9046	91
H(10A)	9740	1345	8442	114
H(10B)	9968	1007	8813	114
H(10C)	9908	1355	9439	114
H(11A)	8707	716	6325	91
H(11B)	8976	383	6151	91
H(12A)	8720	40	7286	56
H(12B)	8371	241	6875	56
H(14)	8680	1281	6731	167
H(15)	8659	1837	5979	171
H(16)	9164	2142	5944	247
H(17)	9714	1911	6152	177
H(18)	9767	1273	6778	179
H(20)	9534	652	5576	198
H(21)	10104	356	5113	287
H(22)	10507	139	6236	288
H(23)	10371	166	7696	217
H(24)	9807	392	8200	138
H(26)	8567	-267	8586	51
H(27)	8276	-676	9553	61
H(28)	7820	-478	10513	62
H(29)	7650	131	10531	60

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H(30)	7931	532	9554	50
H(32)	7794	449	7550	79
H(33)	7347	855	7082	92
H(34)	7453	1465	7134	91
H(35)	7980	1683	7796	97
H(36)	8444	1283	8251	66
H(40)	9611	-502	7411	59
H(41)	9799	-1101	7458	53
H(43)	9372	-1209	9967	59
H(44)	9191	-601	9923	63
H(47)	10332	-1146	8604	60
H(48)	10925	-1459	8605	59
H(50A)	10218	-2614	5943	214
H(50B)	10493	-2501	6743	214
H(51A)	10394	-1994	5810	246
H(51B)	10221	-1919	6784	246
H(51C)	9966	-2032	5956	246
H(61A)	6313	174	7478	310
H(61B)	6530	486	7996	310
H(61C)	6681	330	7059	310
H(62A)	6153	580	6302	287
H(62B)	6028	755	7240	287
H(63A)	6697	915	6466	313
H(63B)	6519	1114	7284	313
H(64A)	6468	1366	5440	378
H(64B)	6266	1560	6229	378
H(65A)	6543	1972	5603	461
H(65B)	6905	1740	5451	461
H(65C)	6807	1889	6437	461