Supporting Information

Heteroleptic iron(II) complexes with naphthoquinone-type ligands

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Explanation of alerts:

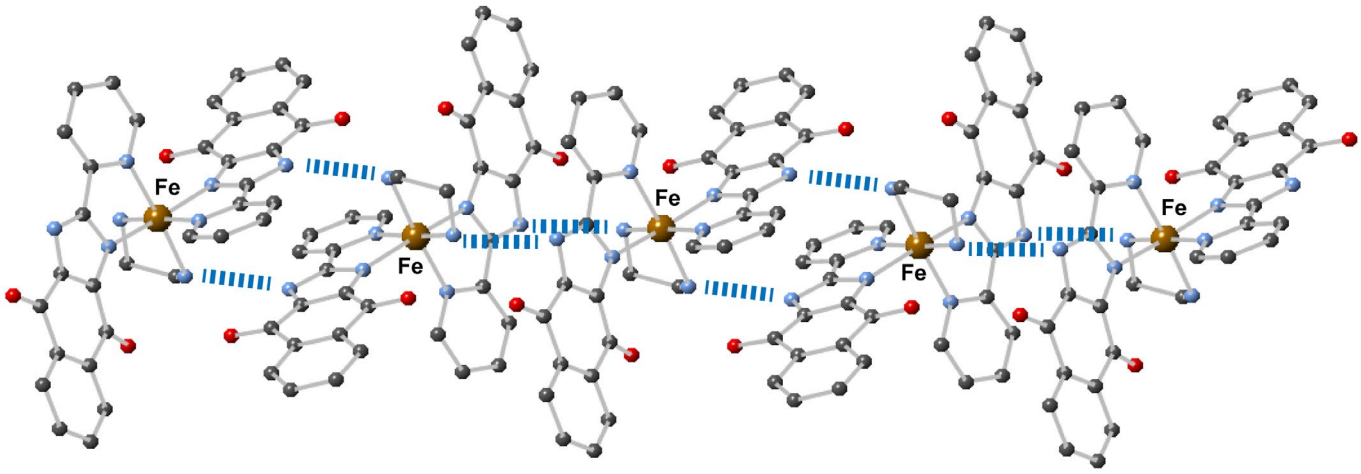

Figure S1. One dimensional network structure of **1**. Blue dotted lines represent intrachain hydrogen bond interactions.

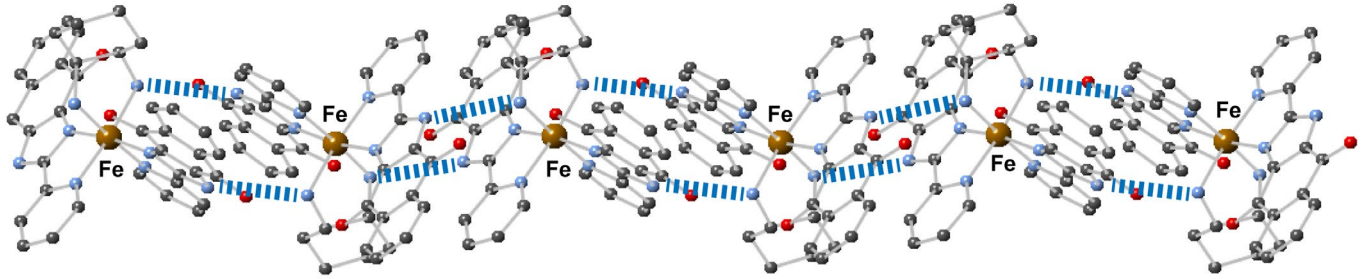

Figure S2. One dimensional network structure of **2**. Blue dotted lines represent intrachain hydrogen bond interactions.

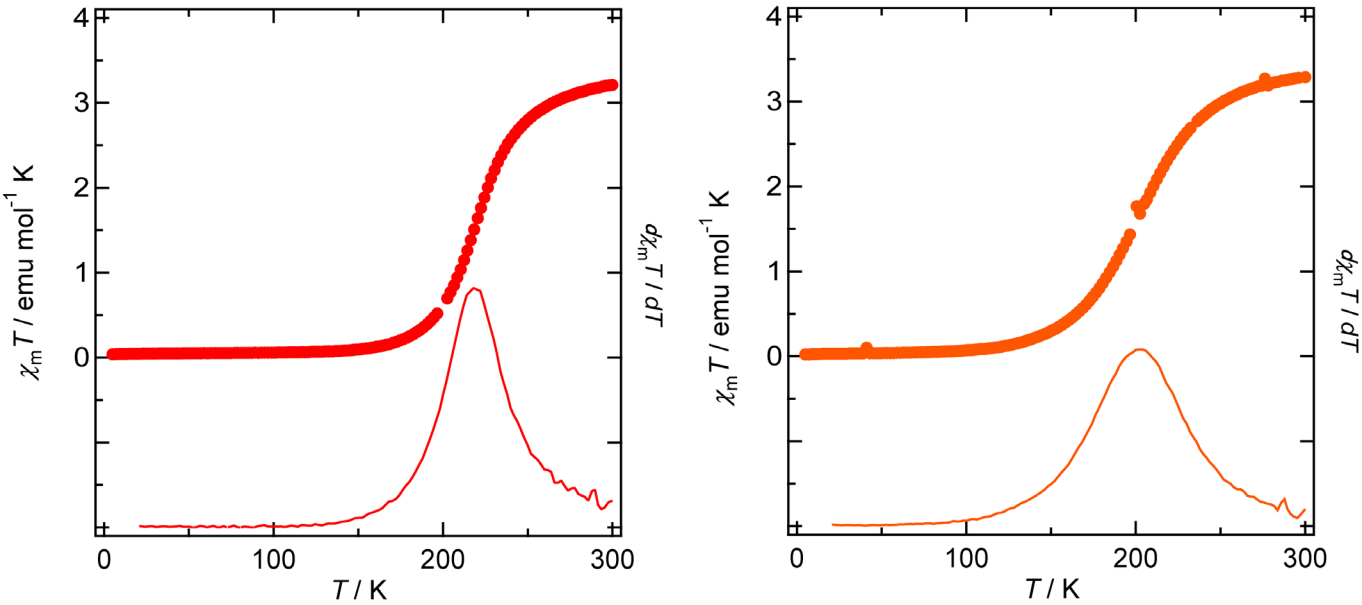

Figure S3. The derivative of the $\chi_m T$ data for complexes **1** (left) and **2** (right).

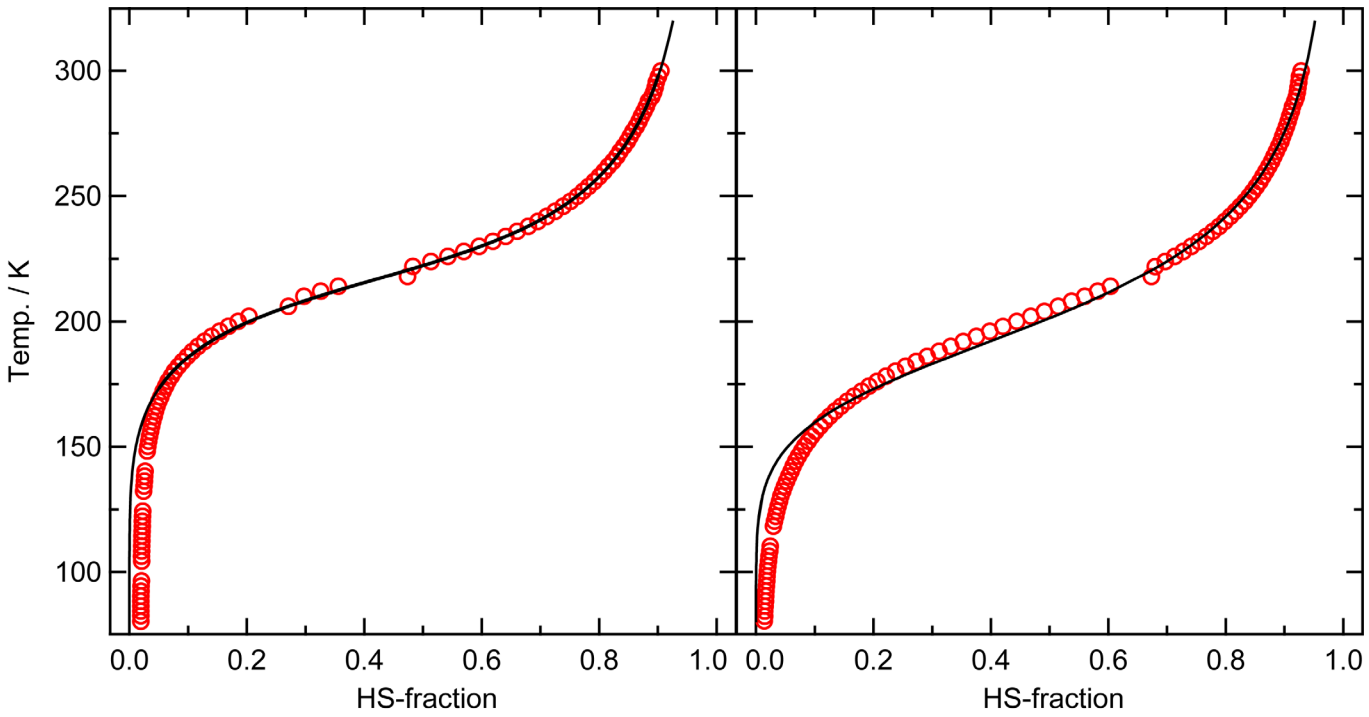

Figure S4. Simulation of magnetic data with spin crossover transition for complexes **1** (left) and **2** (right).

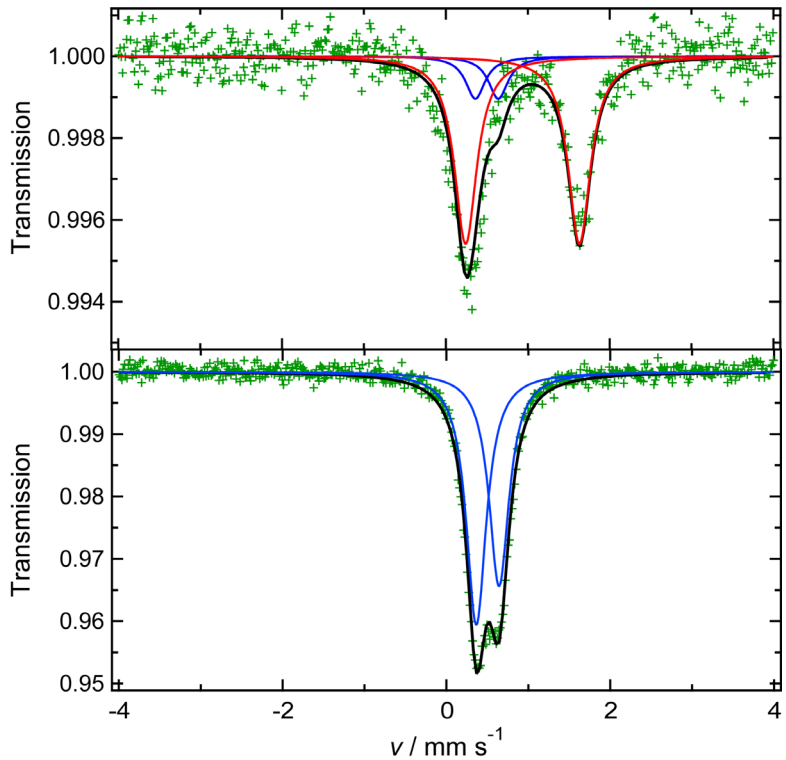

Figure S5. Mössbauer spectra of **1** at 300 K (top) and 20 K (bottom). Parameters are provided in Table S3.

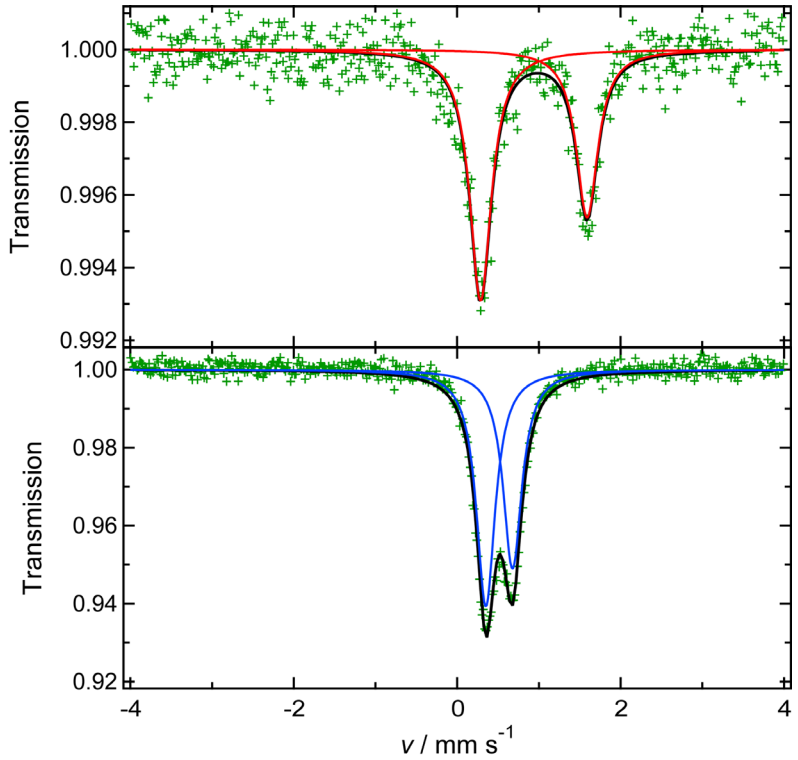

Figure S6 Mössbauer spectra of **2** at 300 K (top) and 20 K (bottom). Parameters are provided in Table S3.

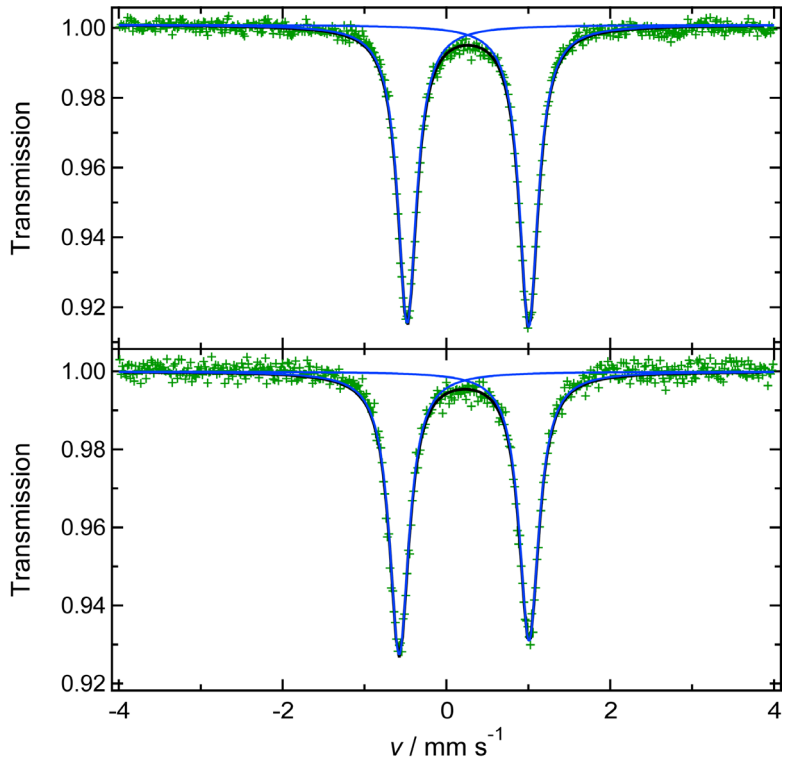

Figure S7 Mössbauer spectra of **3** (top) and **4** (bottom) at 20 K. Parameters are provided in Table S3.

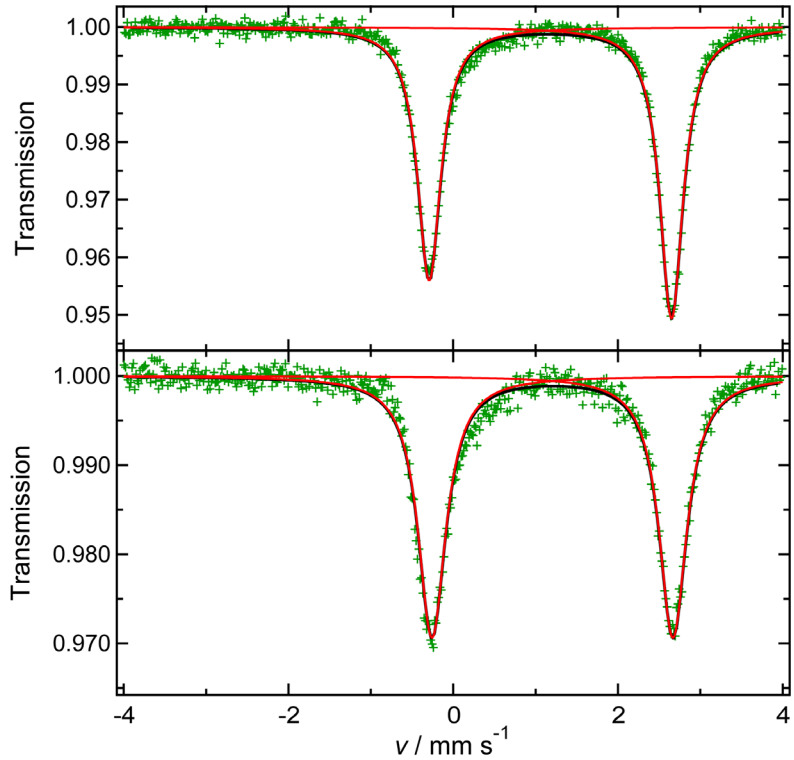

Figure S8 Mössbauer spectra of **5** (top) and **6** (bottom) at 20 K. Parameters are provided in Table S3.

Table S1. Crystal parameters of **1** and **2**.

	Comp. 1		Comp. 2	
	100 K	270 K	100 K	270 K
Formula	$C_{45}H_{47}FeN_9O_9$	$C_{45}H_{47}FeN_9O_9$	$C_{41}H_{37}FeN_9O_5$	$C_{41}H_{37}FeN_9O_5$
M / g mol^{-1}	913.76	913.76	791.64	791.64
Temp. / K	100(2)	270(2)	100(2)	270(2)
Crystal system	Triclinic	Triclinic	Monoclinic	Monoclinic
Space group	$P\bar{1}$	$P\bar{1}$	$P2_1/c$	$P2_1/c$
a / Å	11.088(3)	11.339(3)	14.218(3)	14.317(5)
b / Å	12.398(3)	12.582(3)	17.474(4)	17.962(6)
c / Å	16.239(4)	16.370(4)	15.627(4)	15.991(5)
α / °	101.544(4)	100.776(4)	-	-
β / °	100.791(4)	101.014(4)	109.818(3)	110.230(5)
γ / °	100.566(4)	101.059(4)	-	-
V / Å^3	2091.3(8)	2188.4(8)	3652.6(14)	3859(2)
Z	2	2	4	4
d / g cm^{-3}	1.451	1.387	1.440	1.363
μ / mm^{-1}	0.431	0.412	0.473	0.448
F(000)	956	956	1648	1648
Reflections				
collected / unique	10032 / 7103	12931 / 9734	20780 / 8347	18274 / 8379
R_{int}	0.0631	0.0651	0.0507	0.1810
GOF	1.067	1.028	1.039	1.219
$R1$ ($I > 2\sigma(I)$)	0.0770	0.0886	0.0603	0.1810
R_w2 ($I > 2\sigma(I)$]	0.1762	0.1564	0.1455	0.2736
$\Delta\rho_{max}$ / e Å^{-3}	1.106	0.393	1.933	0.640
$\Delta\rho_{min}$ / e Å^{-3}	-0.827	-0.480	-0.729	-0.825
CCDC No.	1956636	1956637	1956638	1956639

Table S2. Crystal parameters of **3**, **4**, **5** and **6** at 100 K.

	Comp. 3	Comp. 4	Comp. 5	Comp. 6
Formula	$C_{44}H_{36}FeN_{10}O_6$	$C_{42}H_{32}FeN_{12}O_6$	$C_{64}H_{32}Fe_2N_{12}O_{12}$	$C_{48}H_{22}BF_4FeN_9O_6$
M / g mol^{-1}	856.68	856.64	1272.71	963.40
Temp. / K	100(2)	100(2)	100(2)	100(2)
Crystal system	Orthorhombic	Triclinic,	Triclinic	Monoclinic
Space group	*F*dd2	$P\bar{1}$	$P\bar{1}$	*C*2/c
a / Å	17.374(3)	11.6257(11)	10.55(2)	9.260(7)
b / Å	28.891(6)	13.6920(12)	13.14(3)	32.13(3)
c / Å	16.217(3)	13.7914(12)	28.26(7)	18.517(15)
α / ^{o}	-	106.5717(12)	95.12(2)	-
β / ^{o}	-	111.1607(11)	91.640(19)	103.237(9)
γ / ^{o}	-	94.9087(12)	107.52(5)	-
V / Å^3	8140(3)	1918.1(3)	3715(15)	5362(7)
Z	8	2	2	4
d / g cm^{-3}	1.398	1.483	1.138	1.193
μ / mm^{-1}	0.433	0.461	0.450	0.346
F(000)	3552	884	1296	1952
Reflections				
collected / unique	10689 / 4009	11328 / 8506	21449 / 16347	14165 / 6036
R_{int}	0.0335	0.0188	0.0410	0.1105
GOF	1.018	1.288	1.413	0.870
$R1$ ($I > 2\sigma(I)$)	0.0321	0.0541	0.1197	0.0977
R_w2 ($I > 2\sigma(I)$]	0.0662	0.1647	0.2882	0.2502
$\Delta\rho_{max}$ / e Å^{-3}	0.311	1.828	1.910	0.775
$\Delta\rho_{min}$ / e Å^{-3}	-0.311	-1.194	-1.532	-0.441
CCDC No.	1956640	1956641	1956642	1956643

Table S3. Mössbauer parameters for all complexes.

	δ_{IS} (mm / s)	ΔE_Q (mm / s)	spin state	Area fraction (%)
Comp.1 (300 K)	0.94	1.39	Fe(II) HS	83
	0.50	0.28	Fe(II) LS	17
Comp.1 (20 K)	0.50	0.28	Fe(II) LS	-
Comp.2 (300 K)	0.94	1.30	Fe(II) HS	-
Comp.2 (20 K)	0.51	0.33	Fe(II) LS	-
Comp.3 (20 K)	0.26	1.48	Fe(II) LS	-
Comp.4 (20 K)	0.22	1.59	Fe(II) LS	-
Comp.5 (20 K)	1.18	2.94	Fe(II) HS	-
Comp.6 (20 K)	1.20	2.93	Fe(II) HS	-

Explanation of alerts in CIFCHECK:

Datablock: Comp1_270K

Alert Level B

The following B-level alerts arise from the diffraction data being slightly weak.

PLAT026_ALERT_3_B Ratio Observed / Unique Reflections (too) Low .. 34% Check
PLAT260_ALERT_2_B Large Average Ueq of Residue Including O5 0.187 Check
PLAT260_ALERT_2_B Large Average Ueq of Residue Including O9 0.172 Check

The following B-level alerts arise from the movement of solvent molecules due to high-temperature measurement.

PLAT360_ALERT_2_B Short C(sp3)-C(sp3) Bond C35 - C36 . 1.24 Ang.
PLAT360_ALERT_2_B Short C(sp3)-C(sp3) Bond C37 - C38 . 1.25 Ang.
PLAT410_ALERT_2_B Short Intra H...H Contact H35A ..H48 . 1.80 Ang.
x,y,z = 1_555 Check
PLAT410_ALERT_2_B Short Intra H...H Contact H35B ..H47 . 1.81 Ang.
x,y,z = 1_555 Check
PLAT410_ALERT_2_B Short Intra H...H Contact H37A ..H38B . 1.82 Ang.
x,y,z = 1_555 Check
PLAT410_ALERT_2_B Short Intra H...H Contact H37B ..H38A . 1.81 Ang.
x,y,z = 1_555 Check

Datablock: Comp2_270K
Alert Level B

The following B-level alerts arise from the diffraction data being slightly weak.

RINTA01_ALERT_3_B The value of Rint is greater than 0.18
Rint given 0.181
PLAT020_ALERT_3_B The Value of Rint is Greater Than 0.12 ..... 0.181 Report
PLAT026_ALERT_3_B Ratio Observed / Unique Reflections (too) Low .. 36% Check
PLAT082_ALERT_2_B High R1 Value ..... 0.18 Report
PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.01608 Ang.