

Anhang

Daten der Röntgeneinkristallstrukturanalysen

Anhang A Daten zur Strukturbestimmung des Acetonitriladdukts des (Diphenylcyanomethanido-*N*)-(phenanthrolin)(triphenylphosphan)-kupfer(I) $[\text{Cu}(\text{NCCPh}_2)(\text{phen})(\text{PPh}_3)] \cdot 1/2\text{L}$ (L = CH₃CN)

24a

Kristalldaten: Summenformel: C₄₅H_{34,50}CuN_{3,50}P; Molmasse: 718,82 g/mol; Meßtemperatur 220(2) K; Kristallgröße: 0,418×0,260×0,095 mm³; Kristallsystem: triklin; Raumgruppe $P\bar{1}$; Z = 2; a = 8,8228(10) Å; b = 13,2181(15) Å; c = 17,0153(16) Å; α = 72,95(1)°; β = 85,44(1)°; γ = 72,78(1)°; V = 1812,06(30) Å³; ρ_{ber} = 1,317 g/cm³; μ(Mo-Kα) = 0,684 mm⁻¹; Bestimmung der Gitterparameter: Meßbereich (Θ) 1,25-25,98°; Reflexe: 7090 gemessen, 7090 unabhängig, 4749 beobachtet; Verfeinerung: wR₂ = 0,1551; wR₁ = 0,1240; S (alle Daten) 1,168; Zahl der verfeinerten Parameter: 452; Restelektronendichte: max. 0,772/min. -0,533 e Å⁻³.

Tabelle A Atomkoordinaten und äquivalente isotrope Auslenkungsparameter für $[\text{Cu}(\text{NCCPh}_2)(\text{phen})(\text{PPh}_3)] \cdot 1/2\text{L}$ (L = CH₃CN)

Atom	x	y	z	U(eq)
Cu1	0.81847(7)	0.38711(5)	0.22744(3)	0,03274(17)
P1	0.69289(13)	0.42570(9)	0.33644(7)	0,0273(3)
C1	0.6561(7)	0.2613(4)	0.1492(3)	0,0514(14)
C2	0.6038(7)	0.2369(5)	0.0836(4)	0,0591(16)
C3	0.6100(7)	0.3020(5)	0.0057(4)	0,0550(15)
C4	0.6678(6)	0.3941(5)	-0.0080(3)	0,0439(13)
C5	0.6759(6)	0.4702(5)	-0.0876(3)	0,0540(15)
C6	0.7322(6)	0.5569(5)	-0.0959(3)	0,0522(15)
C7	0.7864(6)	0.5767(4)	-0.0270(3)	0,0424(15)
C8	0.8446(7)	0.6671(5)	-0.0327(3)	0,0524(12)
C9	0.8985(6)	0.6785(5)	0.0361(3)	0,0500(14)
C10	0.8938(6)	0.6004(4)	0.1119(3)	0,0383(11)
C11	0.7814(5)	0.5040(4)	0.0526(3)	0,0332(10)
C12	0.7195(5)	0.4123(4)	0.0618(3)	0,0351(11)
C13	0.4762(5)	0.4653(4)	0.3307(3)	0,0322(10)
C14	0.4068(6)	0.3916(5)	0.3152(3)	0,0410(12)
C15	0.2438(7)	0.4166(6)	0.3092(3)	0,0528(15)
C16	0.1481(6)	0.5175(6)	0.3170(3)	0,0605(18)
C17	0.2156(6)	0.5922(5)	0.3310(4)	0,0585(16)
C18	0.3789(5)	0.5655(4)	0.3392(3)	0,0424(12)
C19	0.7312(5)	0.5406(4)	0.3627(3)	0,0280(9)
C20	0.7140(5)	0.6396(4)	0.2998(3)	0,0362(14)
C21	0.7458(6)	0.7284(4)	0.3151(3)	0,0474(12)
C22	0.7952(6)	0.7205(5)	0.3917(4)	0,0533(14)

C23	0.8127(6)	0.6234(4)	0.4546(3)	0,0473(13)
C24	0.7801(5)	0.5342(4)	0.4402(3)	0,0382(11)
C25	0.7410(5)	0.3109(4)	0.4305(3)	0,0297(10)
C26	0.6313(6)	0.2906(4)	0.4921(3)	0,0400(12)
C27	0.6744(7)	0.2004(5)	0.5607(3)	0,0511(14)
C28	0.8269(7)	0.1321(4)	0.5697(3)	0,0521(14)
C29	0.9370(7)	0.1518(5)	0.5097(3)	0,0557(15)
C30	0.8931(6)	0.2411(4)	0.4398(3)	0,0426(12)
C31	1.1206(6)	0.1859(4)	0.2426(3)	0,0360(11)
C32	1.2421(6)	0.0910(4)	0.2418(3)	0,0392(12)
C33	1.3873(7)	0.0716(4)	0.2874(3)	0,0471(13)
C34	1.3781(9)	0.1066(5)	0.3587(4)	0,0691(19)
C35	1.5158(13)	0.0967(6)	0.3988(6)	0,112(4)
C36	1.6609(12)	0.0512(6)	0.3719(7)	0,118(4)
C37	1.6756(9)	0.0139(5)	0.3032(6)	0,097(3)
C38	1.5391(7)	0.0239(4)	0.2610(4)	0,0610(17)
C39	1.2102(6)	0.0185(4)	0.1992(3)	0,0393(12)
C40	1.3071(7)	-0.0905(4)	0.2079(3)	0,0444(13)
C41	1.2706(8)	-0.1585(5)	0.1700(4)	0,0643(17)
C42	1.1374(10)	-0.1239(6)	0.1215(5)	0,087(2)
C43	1.0394(9)	-0.0172(6)	0.1122(4)	0,081(2)
C44	1.0743(7)	0.0519(5)	0.1499(4)	0,0557(15)
C45	0.5940(14)	-0.0599(11)	0.0449(7)	0.104(5)
C46	0.703(2)	-0.1282(16)	0.1075(10)	0.168(10)
N1	0.7119(4)	0.3465(3)	0.1395(2)	0,0360(9)
N2	0.8363(4)	0.5157(3)	0.1211(2)	0,0338(9)
N3	1.0197(5)	0.2673(3)	0.2397(2)	0,0403(10)
N4	0	0	0.222(8)	0,222(8)

Anhang B Daten zur Strukturbestimmung des Tetrahydrofuranaddukts des (Diphenylcyano-methanido-*N*)-(phenanthrolin)(triphenylphosphan)-kupfer(I) $[\text{Cu}(\text{NCCPh}_2)(\text{phen})(\text{PPh}_3)] \cdot 1/2\text{L}$ (L = THF) **24b**

Kristalldaten: Summenformel: $\text{C}_{46}\text{H}_{37}\text{CuN}_3\text{O}_{0,50}\text{P}$; Molmasse: 734,34 g/mol; Meßtemperatur 220(2) K; Kristallsystem: triklin; Raumgruppe $\text{P}\bar{1}$; $Z = 2$; $a = 8,934(2)$ Å; $b = 13,353(3)$ Å; $c = 17,151(5)$ Å; $\alpha = 71,74(3)^\circ$; $\beta = 86,23(3)^\circ$; $\gamma = 71,84(3)^\circ$; $V = 1845,0(8)$ Å³; $\rho_{\text{ber}} = 1,329$ g/cm³; $\mu(\text{Mo-K}\alpha) = 0,675$ mm⁻¹; Bestimmung der Gitterparameter: Meßbereich (Θ) 2,40-25,00°; Reflexe: 10776 gemessen, 6131 unabhängig ($R_{\text{int}} 0,1182$); Verfeinerung: $wR_2 = 0,1068$; $R_1 = 0,1550$; GooF 0,804; Zahl der verfeinerten Parameter: 597; Restelektronendichte: max. 0,462/min. -0,451 e Å⁻³.

Tabelle B Atomkoordinaten und äquivalente isotrope Auslenkungsparameter für $[\text{Cu}(\text{NCCPh}_2)(\text{phen})(\text{PPh}_3)] \cdot 1/2\text{L}$ (L = THF)

Atom	x	y	z	U(eq)
C(1)	8433(7)	7241(6)	8494(5)	39(2)
C(2)	8881(8)	7530(7)	9158(5)	47(2)
C(3)	8786(6)	6866(6)	9937(4)	40(2)
C(4)	8254(6)	5961(5)	10072(3)	31(2)
C(5)	8138(7)	5201(7)	10879(4)	42(2)
C(6)	7583(7)	4362(7)	10971(4)	43(2)
C(7)	7055(6)	4146(5)	10277(3)	29(2)
C(8)	6412(7)	3301(6)	10334(4)	39(2)
C(9)	5913(7)	3195(6)	9652(4)	37(2)
C(10)	6018(6)	3928(5)	8882(4)	33(2)
C(11)	7160(5)	4869(5)	9474(3)	23(1)
C(12)	7788(5)	5761(5)	9372(3)	24(1)
C(13)	10255(6)	5279(5)	6701(3)	24(1)
C(14)	10932(7)	6006(6)	6861(3)	37(2)
C(15)	12560(8)	5770(8)	6902(4)	49(2)
C(16)	13494(8)	4804(8)	6810(4)	57(3)
C(17)	12885(7)	4055(7)	6677(4)	50(2)
C(18)	11242(7)	4310(6)	6621(4)	40(2)
C(19)	7583(6)	6835(5)	5693(3)	26(1)
C(20)	8642(7)	7079(6)	5080(4)	38(2)
C(21)	8160(9)	7988(6)	4408(4)	49(2)
C(22)	6663(9)	8681(7)	4304(4)	55(2)
C(23)	5600(8)	8453(6)	4897(4)	50(2)
C(24)	6051(7)	7543(5)	5583(4)	40(2)
C(25)	7746(5)	4522(5)	6394(3)	25(1)
C(26)	7920(6)	3533(6)	7036(4)	33(2)
C(27)	7628(7)	2665(7)	6886(5)	42(2)
C(28)	7135(8)	2747(7)	6114(5)	47(2)
C(29)	6928(7)	3709(6)	5493(4)	44(2)
C(30)	7246(6)	4604(6)	5617(4)	32(2)
C(31)	3912(7)	8055(5)	7529(3)	28(1)
C(32)	2716(6)	9005(5)	7540(3)	34(2)
C(33)	1206(7)	9204(5)	7113(3)	35(2)
C(34)	1222(10)	8898(6)	6403(4)	61(2)
C(35)	-137(12)	8999(7)	6029(5)	87(3)
C(36)	-1604(14)	9420(8)	6310(7)	91(4)

C(37)	-1653(9)	9764(7)	6987(7)	78(3)
C(38)	-279(8)	9682(6)	7403(5)	51(2)
C(39)	3062(6)	9719(5)	7951(3)	35(2)
C(40)	2089(8)	10809(6)	7860(4)	45(2)
C(41)	2515(10)	11479(7)	8231(4)	63(2)
C(42)	3888(10)	11115(8)	8704(5)	72(2)
C(43)	4837(10)	10042(9)	8801(5)	73(3)
C(44)	4476(8)	9374(7)	8425(4)	50(2)
O(46)	10617(13)	9082(9)	10001(7)	214(5)
C(46)	9124(14)	9718(13)	9508(10)	147(5)
N(1)	7898(5)	6405(4)	8595(3)	30(1)
N(2)	6642(4)	4745(4)	8787(2)	24(1)
N(3)	4865(5)	7252(4)	7563(3)	32(1)
P(2)	8104(2)	5667(1)	6640(1)	24(1)
Cu	6871(1)	6024(1)	7714(1)	28(1)
C(47)	8500(20)	10500(20)	9610(14)	235(11)

Anhang C Daten zur Strukturbestimmung von (Isocyanato-*N*)-(phenanthrolin)-(triphenylphosphan)-kupfer(I) [Cu(NCO)(phen)(PPh₃)] **25**

Kristalldaten: Summenformel: C₃₁H₂₃CuN₃OP; Molmasse: 548,03 g/mol; Meßtemperatur 293(2) K; Kristallgröße: 0,456 × 0,367 × 0,266 mm³; Kristallsystem: monoklin; Raumgruppe A2/n; Z = 8; $a = 19,459(2)$ Å; $b = 10,8001(15)$ Å; $c = 24,649(3)$ Å; $\alpha = 90,0^\circ$; $\beta = 104,509(16)^\circ$; $\gamma = 90^\circ$; $V = 5015,1(11)$ Å³; $\rho_{\text{ber}} = 1,452$ mg/m³; $\mu(\text{Mo-K}\alpha) = 0,965$ mm⁻¹; Bestimmung der Gitterparameter: Meßbereich (Θ) 1,71-25,95°; Reflexe: 9816 gemessen, 4908 unabhängig ($R_{\text{int}} 0,0212$), 3976 beobachtet; Verfeinerung: $wR_2 = 0,0863$; $R_1 = 0,0451$; GooF 1,082; Zahl der verfeinerten Parameter: 426; Restelektronendichte: max. 0,304/min. -0,243 e Å⁻³.

Tabelle C Atomkoordinaten und äquivalente isotrope Auslenkungsparameter für [Cu(NCO)(phen)(PPh₃)]·

Atom	x	y	z	U(eq)
Cu(1)	185(1)	1470(1)	1057(1)	39(1)
P(1)	-915(1)	1286(1)	1134(1)	33(1)
C(1)	-1(1)	1927(2)	-244(1)	47(1)
C(2)	91(2)	2589(3)	-707(1)	57(1)
C(3)	453(2)	3682(3)	-624(1)	57(1)
C(4)	728(1)	4125(2)	-77(1)	47(1)
C(5)	1100(2)	5280(3)	53(1)	58(1)
C(6)	1358(1)	5655(2)	582(1)	58(1)
C(7)	1287(1)	4907(2)	1046(1)	47(1)
C(8)	1566(1)	5227(3)	1615(1)	55(1)
C(9)	1493(1)	4443(3)	2024(1)	54(1)
C(10)	1108(1)	3349(2)	1880(1)	46(1)
C(11)	916(1)	3779(2)	937(1)	38(1)
C(12)	624(1)	3384(2)	367(1)	38(1)
C(13)	-1291(1)	2505(2)	1489(1)	33(1)
C(14)	-898(1)	3574(2)	1661(1)	42(1)
C(15)	-1168(1)	4526(2)	1925(1)	48(1)
C(16)	-1836(1)	4431(2)	2017(1)	48(1)
C(17)	-2237(2)	3381(2)	1845(1)	49(1)
C(18)	-1966(1)	2417(2)	1591(1)	42(1)
C(19)	-1573(1)	1121(2)	463(1)	35(1)
C(20)	-2118(1)	1960(2)	261(1)	44(1)
C(21)	-2573(2)	1800(3)	-269(1)	58(1)
C(22)	-2488(2)	815(3)	-595(1)	62(1)
C(23)	-1947(2)	-22(3)	-404(1)	58(1)
C(24)	-1491(1)	133(3)	121(1)	50(1)
C(25)	-1057(1)	-91(2)	1528(1)	35(1)
C(26)	-1666(1)	-823(2)	1398(1)	44(1)
C(27)	-1740(2)	-1810(2)	1739(1)	52(1)
C(28)	-1214(2)	-2061(2)	2218(1)	53(1)
C(29)	-611(2)	-1342(2)	2348(1)	54(1)
C(30)	-524(1)	-375(2)	2003(1)	45(1)
C(31)	1239(1)	-670(2)	1495(1)	48(1)
N(1)	262(1)	2292(2)	283(1)	38(1)
N(2)	814(1)	3024(2)	1352(1)	39(1)

N(3)	838(1)	91(2)	1300(1)	54(1)
O(1)	1660(1)	-1460(2)	1689(1)	91(1)

Anhang D Daten zur Strukturbestimmung von [(*o*-Cyano-phenyl)cyanomethanido-C])(phenanthrolin)(triphenylphosphan)-kupfer(I) [Cu{C(H)CN(2-CN-C₆H₄)}(phen)(PPh₃)] **30**

Kristalldaten: Summenformel: C₃₉H₂₈CuN₄P; Molmasse: 647,16 g/mol; Meßtemperatur 220(2) K; Kristallsystem: monoklin; Raumgruppe C 1 c 1; Z = 4; *a* = 17,291(3) Å; *b* = 9,2401(13) Å; *c* = 22,501(3) Å; $\alpha = 90,0^\circ$; $\beta = 116,02(1)^\circ$; $\gamma = 90^\circ$; *V* = 3230,56(80) Å³; $\rho_{\text{ber}} = 1,331 \text{ mg/m}^3$.

Tabelle D Atomkoordinaten und äquivalente isotrope Auslenkungsparameter für [(*o*-Cyano)phenylcyanomethanido-C]-(phenanthrolin)(triphenylphosphan)-kupfer(I) [Cu{C(H)CN(2-CN-C₆H₄)}(phen)(PPh₃)]

Atom	x	y	z	Ueq
Cu1	0.00000	0.11697	0.00000	0.03989
P1	0.02816	0.02903	0.09796	0.03755
N1	0.07189	0.30558	0.00639	0.04676
N2	0.06373	0.05161	-0.05581	0.04522
N3	-0.14763	-0.07256	-0.14865	0.07909
N4	-0.18869	0.41319	0.00695	0.12443
C1	-0.05407	-0.06935	0.11202	0.04494
C2	-0.06880	-0.04906	0.16752	0.06606
C3	-0.13297	-0.12694	0.17487	0.08440
C4	-0.18065	-0.22611	0.12845	0.09117
C5	-0.16697	-0.24810	0.07364	0.08414
C6	-0.10387	-0.16868	0.06498	0.06515
C7	0.05553	0.17876	0.15711	0.04113
C8	-0.00830	0.28097	0.14627	0.05653
C9	0.00800	0.40054	0.18715	0.06999
C10	0.08823	0.42007	0.23854	0.07601
C11	0.15151	0.32076	0.24910	0.07388
C12	0.13634	0.19910	0.20871	0.05454
C13	0.12243	-0.08893	0.13313	0.04164
C14	0.18451	-0.07248	0.11014	0.05070
C15	0.25988	-0.15433	0.13714	0.06391
C16	0.27184	-0.25318	0.18552	0.06844
C17	0.21064	-0.27329	0.20778	0.07006
C18	0.13565	-0.19202	0.18175	0.05793
C19	0.07723	0.42901	0.03824	0.06123
C20	0.11867	0.55261	0.03036	0.07600
C21	0.15511	0.54706	-0.01174	0.07850
C22	0.15083	0.42121	-0.04703	0.06186
C23	0.18673	0.40440	-0.09349	0.07724
C24	0.18125	0.28010	-0.12501	0.07892
C25	0.13969	0.15546	-0.11475	0.06183
C26	0.13116	0.02311	-0.14700	0.07942
C27	0.09057	-0.09030	-0.13418	0.07767
C28	0.05765	-0.07112	-0.08763	0.05988
C29	0.10353	0.16574	-0.06930	0.04659
C30	0.10883	0.29949	-0.03587	0.04669
C31	-0.12525	0.15413	-0.07660	0.04541
C32	-0.13934	0.02895	-0.11673	0.05281
C33	-0.12043	0.29153	-0.10751	0.04632

C34	-0.13686	0.42468	-0.08435	0.06510
C35	-0.12697	0.55551	-0.10978	0.08567
C36	-0.10268	0.55981	-0.15914	0.10058
C37	-0.08829	0.43241	-0.18489	0.08865
C38	-0.09625	0.29797	-0.15898	0.06100
C39	-0.16624	0.41991	-0.03308	0.08341

Anhang E Daten zur Strukturbestimmung von (Dicyanomethanido-*N*)-(phenanthrolin)(triphenylphosphan)-kupfer(I) [Cu(NCC(H)CN)(phen)(PPh₃)] **32**

Kristalldaten: Summenformel: C₃₃H₂₄CuN₄P; Molmasse: 571,07 g/mol; Meßtemperatur 220(2) K; Kristallgröße: 0,30 × 0,19 × 0,11 mm³; Kristallsystem: monoklin; Raumgruppe P2₁/c; Z = 4; a = 16,635(2) Å; b = 9,139(2) Å; c = 18,417(3) Å; α = 90,0°; β = 97,923(16)°; γ = 90°; V = 2773,1(9) Å³; ρ_{ber} = 1,368 mg/m³; μ(Mo-Kα) = 0,875 mm⁻¹; Bestimmung der Gitterparameter: Meßbereich (Θ) 1,24-25,98°; Reflexe: 5635 gemessen, 5446 unabhängig (R_{int} 0,0932), 3203 beobachtet; Verfeinerung: wR₂ = 0,1220; R₁ = 0,1567; GooF 1,183; Zahl der verfeinerten Parameter: 356; Restelektronendichte: max. 0,532/min. -0,370 e Å⁻³.

Tabelle E Atomkoordinaten und äquivalente isotrope Auslenkungsparameter für (Dicyanomethanido-*N*)-(phenanthrolin)(triphenylphosphan)-kupfer(I) [Cu(NCC(H)CN)(phen)(PPh₃)]

Atom	x	y	z	U(eq)
Cu1	2118(1)	7696(1)	861(1)	41(1)
P1	3216(1)	6639(2)	566(1)	35(1)
N1	1080(3)	6554(5)	1053(2)	42(1)
N2	1272(2)	8530(5)	-4(2)	41(1)
N3	2185(3)	9110(5)	1685(3)	48(1)
N4	1877(6)	13332(8)	2772(4)	141(4)
C1	4166(3)	6893(6)	1190(3)	35(1)
C2	4256(3)	8172(6)	1599(3)	46(2)
C3	4998(4)	8434(8)	2036(3)	62(2)
C4	5614(3)	7443(8)	2088(3)	59(2)
C5	5520(3)	6153(8)	1697(3)	54(2)
C6	4790(3)	5889(7)	1246(3)	45(2)
C7	3204(3)	4646(6)	453(3)	35(1)
C8	3374(3)	3942(6)	-167(3)	47(2)
C9	3382(3)	2418(7)	-204(3)	56(2)
C10	3235(3)	1615(7)	386(4)	55(2)
C11	3065(3)	2288(7)	1016(3)	50(2)
C12	3040(3)	3806(6)	1049(3)	44(2)
C13	3478(3)	7311(6)	-307(3)	39(1)
C14	4246(3)	7788(7)	-410(3)	56(2)
C15	4390(4)	8309(8)	-1083(4)	70(2)
C16	3766(4)	8401(8)	-1661(3)	67(2)
C17	3011(4)	7928(6)	-1568(3)	54(2)
C18	2856(3)	7395(6)	-904(3)	42(1)
C19	982(4)	5645(7)	1585(3)	57(2)
C20	233(4)	5013(8)	1677(4)	70(2)
C21	-429(4)	5338(8)	1176(4)	67(2)
C22	-354(4)	6302(7)	592(4)	54(2)
C23	-1018(4)	6678(8)	44(4)	71(2)
C24	-903(3)	7617(9)	-496(4)	72(2)
C25	-140(3)	8282(7)	-543(3)	53(2)
C26	-2(4)	9285(8)	-1086(4)	70(2)
C27	747(4)	9880(7)	-1085(4)	62(2)
C28	1368(3)	9486(7)	-526(3)	49(2)

C29	525(3)	7923(6)	-5(3)	41(1)
C30	417(3)	6893(6)	561(3)	43(2)
C31	2198(3)	9824(6)	2199(3)	40(1)
C32	2221(4)	10678(8)	2817(3)	54(2)
C33	2032(4)	12139(9)	2792(4)	68(2)

Anhang F Daten zur Strukturbestimmung des Tetrahydrofuranaddukts des Tris(phenanthrolin)-zink(II)-bis(dicyanomethanat) $[\text{Zn}(\text{phen})_3]^{2+}[\text{NCCHCN}]_2 \cdot \text{L}$ (L = THF) **34**

Kristalldaten: Summenformel: $\text{C}_{46}\text{H}_{34}\text{N}_{10}\text{OZn}$; Molmasse: 808,24 g/mol; Meßtemperatur 220(2) K; Kristallgröße: $0,19 \times 0,15 \times 0,50 \text{ mm}^3$ Kristallsystem: monoklin; Raumgruppe $\text{P2}_1/\text{n}$; $Z = 4$; $a = 11,1486(19) \text{ \AA}$; $b = 14,709(2) \text{ \AA}$; $c = 23,985(5) \text{ \AA}$; $\alpha = 90,0^\circ$; $\beta = 98,51(2)^\circ$; $\gamma = 90^\circ$; $V = 3890,0(11) \text{ \AA}^3$; $\rho_{\text{ber}} = 1,366 \text{ g/cm}^3$; $\mu(\text{Mo-K}\alpha) = 0,682 \text{ mm}^{-1}$; Bestimmung der Gitterparameter: Meßbereich (Θ) $1,92\text{-}26,07^\circ$; Reflexe: 27112 gemessen, 7601 unabhängig ($R_{\text{int}} 0,0865$); Verfeinerung: $wR_2 = 0,1117$; $R_1 = 0,1011$; GooF 0,932; Zahl der verfeinerten Parameter: 653; Restelektronendichte: max. $0,504/\text{min. } -0,307 \text{ e \AA}^{-3}$.

Tabelle F Atomkoordinaten und äquivalente isotrope Auslenkungsparameter für das Tetrahydrofuranaddukt des Tris(phenanthrolin)zink(II)-bis(dicyanomethanat) $[\text{Zn}(\text{phen})_3]^{2+}[\text{NCCHCN}]_2 \cdot \text{L}$ (L = THF)

Atom	x	y	z	U(eq)
C(1)	3562(3)	1145(3)	9152(2)	34(1)
C(2)	2987(3)	343(3)	9262(2)	38(1)
C(3)	3639(3)	-437(3)	9342(1)	36(1)
C(4)	4893(3)	-422(2)	9318(1)	30(1)
C(5)	5646(4)	-1208(3)	9394(1)	37(1)
C(6)	6849(4)	-1159(3)	9372(2)	39(1)
C(7)	7403(3)	-314(2)	9263(1)	34(1)
C(8)	8643(4)	-220(3)	9229(2)	49(1)
C(9)	9093(4)	605(3)	9124(2)	56(1)
C(10)	8326(3)	1353(3)	9061(2)	44(1)
C(11)	6688(3)	472(2)	9185(1)	28(1)
C(12)	5407(3)	415(2)	9209(1)	27(1)
C(13)	6934(3)	2837(3)	10175(2)	36(1)
C(14)	6930(4)	3197(3)	10713(2)	41(1)
C(15)	5946(4)	3668(3)	10826(2)	42(1)
C(16)	4963(3)	3814(2)	10398(1)	33(1)
C(17)	3887(4)	4310(3)	10475(2)	45(1)
C(18)	2987(4)	4458(3)	10043(2)	42(1)
C(19)	3073(3)	4125(2)	9487(2)	32(1)
C(20)	2185(4)	4296(3)	9018(2)	42(1)
C(21)	2328(4)	3954(3)	8500(2)	45(1)
C(22)	3346(3)	3438(3)	8450(2)	40(1)
C(23)	4082(3)	3610(2)	9399(1)	28(1)
C(24)	5043(3)	3449(2)	9864(1)	28(1)
C(25)	4667(4)	1471(3)	7746(2)	37(1)
C(26)	4577(4)	1309(3)	7169(2)	44(1)
C(27)	5317(4)	1768(3)	6868(2)	47(1)
C(28)	6149(3)	2397(3)	7136(1)	39(1)
C(29)	6970(4)	2906(3)	6853(2)	55(1)
C(30)	7765(4)	3484(3)	7131(2)	59(1)
C(31)	7820(4)	3637(3)	7727(2)	44(1)
C(32)	8633(4)	4236(3)	8040(2)	56(1)
C(33)	8627(4)	4345(3)	8606(2)	53(1)
C(34)	7810(4)	3837(2)	8871(2)	42(1)

C(35)	7018(3)	3155(2)	8021(1)	32(1)
C(36)	6180(3)	2527(2)	7719(1)	31(1)
C(37)	2516(4)	-1726(3)	8112(2)	52(1)
C(38)	1673(4)	-1481(3)	8453(2)	45(1)
C(39)	3427(4)	-1130(3)	7994(2)	47(1)
C(40)	10180(4)	2611(3)	10170(2)	50(1)
C(41)	9918(3)	3483(3)	10326(2)	43(1)
C(42)	10744(3)	2438(3)	9703(2)	51(1)
O	1036(10)	499(8)	7568(6)	233(5)
C(44)	1171(8)	1289(6)	7332(4)	116(3)
C(45)	54(12)	1736(7)	7478(8)	168(5)
C(46)	-895(10)	1074(8)	7318(9)	188(8)
C(43A)	-610(40)	1380(20)	7684(12)	70(10)
C(44A)	620(30)	1130(20)	7850(13)	83(8)
C(45A)	-220(30)	430(30)	7728(14)	86(10)
C(46A)	110(20)	125(15)	7452(8)	26(4)
OA	15(16)	572(11)	6964(7)	55(4)
C(43)	-382(15)	226(13)	7219(13)	260(12)
N(1)	4744(2)	1196(2)	9126(1)	29(1)
N(2)	7146(2)	1304(2)	9084(1)	32(1)
N(3)	6012(2)	2951(2)	9757(1)	30(1)
N(4)	4215(3)	3261(2)	8884(1)	31(1)
N(5)	5433(2)	2061(2)	8019(1)	30(1)
N(6)	7020(2)	3259(2)	8587(1)	33(1)
N(7)	977(3)	-1312(3)	8750(2)	64(1)
N(8)	4183(4)	-658(3)	7883(2)	58(1)
N(9)	9660(4)	4188(3)	10477(2)	61(1)
N(10)	11202(3)	2257(3)	9315(2)	72(1)
Zn(1)	5763(1)	2361(1)	8917(1)	29(1)

Anhang G Daten zur Strukturbestimmung von (Cyano)(phenanthrolin)(triphenylphosphan)-kupfer(I) [Cu(CN)(phen)(PPh₃)]

Kristalldaten: Summenformel: C₃₁H₂₃CuN₃P; Molmasse: 532,06 g/mol; Meßtemperatur 293(2) K; Kristallsystem: triklin; Raumgruppe P-1, Z = 2; a = 8,461(5) Å; b = 9,322(4) Å; c = 17,853(5) Å; α = 78,50(3)°; β = 77,87(4)°; γ = 69,75(4)°; V = 1279,2(10) Å³; ρ_{ber} = 1,381 g/cm³; μ(Mo-Kα) = 0,941 mm⁻¹; Bestimmung der Gitterparameter: Meßbereich (Θ) 2,35-25,00°; Reflexe: 6565 gemessen, 4490 unabhängig (R_{int} 0,0495); Verfeinerung: wR₂ = 0,1021; R₁ = 0,1057; GooF 1,093; Zahl der verfeinerten Parameter: 418; Restelektronendichte: max. 0,369/min. -0,282 e Å⁻³.

Tabelle G Atomkoordinaten und äquivalente isotrope Auslenkungsparameter für (Cyano)(phenanthrolin)(triphenylphosphan)-kupfer(I) [Cu(CN)(phen)(PPh₃)]

Atom	x	y	z	U(eq)
C(1)	-476(7)	3997(6)	4370(3)	59(2)
C(2)	-1536(8)	3947(7)	5073(3)	69(2)
C(3)	-1117(7)	2693(6)	5617(3)	56(1)
C(4)	367(5)	1455(5)	5452(2)	42(1)
C(5)	888(7)	93(6)	5983(3)	52(1)
C(6)	2301(7)	-1068(6)	5794(3)	54(1)
C(7)	3352(6)	-958(5)	5052(3)	44(1)
C(8)	4824(7)	-2140(6)	4824(3)	62(2)
C(9)	5740(7)	-1950(6)	4114(3)	61(2)
C(10)	5224(6)	-572(6)	3625(3)	52(1)
C(11)	2873(5)	372(5)	4516(2)	35(1)
C(12)	1355(5)	1604(5)	4715(2)	33(1)
C(13)	1579(6)	1018(5)	1983(2)	39(1)
C(14)	2688(7)	-440(6)	2183(3)	49(1)
C(15)	2286(8)	-1745(6)	2159(3)	58(1)
C(16)	789(9)	-1619(7)	1951(3)	70(2)
C(17)	-337(9)	-187(8)	1751(4)	76(2)
C(18)	61(8)	1135(7)	1768(3)	64(2)
C(19)	432(5)	4326(5)	1727(2)	37(1)
C(20)	509(6)	5152(5)	997(3)	45(1)
C(21)	-829(7)	6423(6)	783(3)	56(1)
C(22)	-2291(7)	6869(7)	1300(3)	60(2)
C(23)	-2423(7)	6058(7)	2025(3)	61(2)
C(24)	-1075(7)	4798(6)	2243(3)	53(1)
C(25)	3950(6)	2638(5)	1277(2)	39(1)
C(26)	4256(7)	1853(6)	659(3)	56(1)
C(27)	5611(8)	1876(7)	75(3)	69(2)
C(28)	6679(7)	2667(7)	100(3)	62(2)
C(29)	6399(7)	3458(7)	711(3)	61(2)
C(30)	5038(7)	3435(6)	1298(3)	50(1)
C(31)	4074(6)	4110(5)	3281(2)	42(1)
N(1)	928(5)	2868(4)	4175(2)	41(1)
N(2)	3817(4)	572(4)	3813(2)	39(1)
N(3)	4805(6)	4865(5)	3387(2)	64(1)
P	2178(2)	2679(1)	2069(1)	38(1)
Cu	2819(1)	2787(1)	3198(1)	45(1)