

## 6 Kristallographischer Anhang



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## 6.1 [ReOCl<sub>3</sub>(H<sub>2</sub>L<sup>1</sup>)]

Tabelle 6.1: Kristallographische Daten und Parameter der Strukturrechnung von [ReOCl<sub>3</sub>(H<sub>2</sub>L<sup>1</sup>)]

Summenformel	C <sub>19</sub> H <sub>18</sub> NCl <sub>3</sub> PORe	
M (g/mol)	599.86	
Messtemperatur	200(2) K	
Wellenlänge	0.71073 Å	
Kristallsystem, Raumgruppe	triklin, P $\bar{1}$	
Elementarzelle	a = 9.448(1) Å	$\alpha = 101.64(1)^\circ$
	b = 9.913(1) Å	$\beta = 103.78(1)^\circ$
	c = 13.075(1) Å	$\gamma = 114.20(1)^\circ$
Volumen	1021.0(2) Å <sup>3</sup>	
Z	2	
Berechnete Dichte	1.951 g/cm <sup>3</sup>	
Linearer Absorptionskoeffizient	6.430 mm <sup>-1</sup>	
F(000)	576	
Kristallgröße	0.08 x 0.06 x 0.06 mm <sup>3</sup>	
Theta-Bereich	1.70 - 29.24°	
Indizes	-10 ≤ h ≤ 12, -13 ≤ k ≤ 13, -17 ≤ l ≤ 17	
Zahl der gemessenen Reflexe	11171	
Zahl der unabhängigen Reflexe	5438 [R(int) = 0.0683]	
Absorptionskorrektur	Integration	
Zahl der verfeinerten Parameter	236	
Goof	1.129	
R <sub>1</sub> / wR <sub>2</sub> [I > 2σ(I)]	R <sub>1</sub> = 0.0524, wR <sub>2</sub> = 0.1491	
R <sub>1</sub> / wR <sub>2</sub> (alle Reflexe)	R <sub>1</sub> = 0.0674, wR <sub>2</sub> = 0.1583	
Restelektronendichte	1.748 und -1.512 e · Å <sup>-3</sup>	
Programm zur Strukturlösung	SHELXS 97 [119]	

Tabelle 6.2: Atomkoordinaten ( $\cdot 10^4$ ) und isotrope Temperaturparameter ( $\text{\AA}^2 \cdot 10^3$ ) von  $[\text{ReOCl}_3(\text{H}_2\text{L}^1)]$

	x	y	z	E(eq)
Re(1)	5297(1)	5687(1)	7334(1)	33(1)
O(10)	6225(10)	7569(9)	8156(7)	46(2)
Cl(1)	3430(3)	3147(3)	5837(2)	37(1)
Cl(2)	5928(4)	4428(4)	8542(2)	50(1)
Cl(3)	7475(3)	5655(3)	6714(2)	43(1)
P(1)	2637(3)	5102(3)	7557(2)	32(1)
C(1)	1425(12)	5359(12)	6352(8)	36(2)
C(11)	2361(13)	6996(12)	6350(8)	36(2)
C(12)	1807(15)	8087(14)	6574(9)	44(2)
C(13)	2674(15)	9605(14)	6579(11)	49(3)
C(14)	4141(17)	10084(14)	6391(11)	50(3)
C(15)	4751(15)	9043(14)	6174(10)	45(2)
C(16)	3863(13)	7519(12)	6137(8)	37(2)
N(1)	4529(11)	6445(10)	5955(7)	38(2)
C(21)	1435(12)	3149(11)	7582(9)	37(2)
C(22)	141(14)	1953(13)	6633(11)	49(3)
C(23)	-727(16)	414(15)	6709(16)	73(5)
C(24)	-220(20)	186(16)	7692(15)	64(4)
C(25)	1027(19)	1357(15)	8589(14)	60(3)
C(26)	1873(15)	2829(13)	8556(10)	44(2)
C(31)	2634(13)	6373(12)	8778(8)	36(2)
C(32)	4041(16)	7603(13)	9599(9)	47(2)
C(33)	3926(19)	8539(15)	10508(10)	56(3)
C(34)	2390(20)	8211(16)	10542(11)	58(3)
C(35)	970(20)	6980(20)	9728(14)	69(4)

C(36)

1073(15)

6048(15)

8853(10)

51(3)

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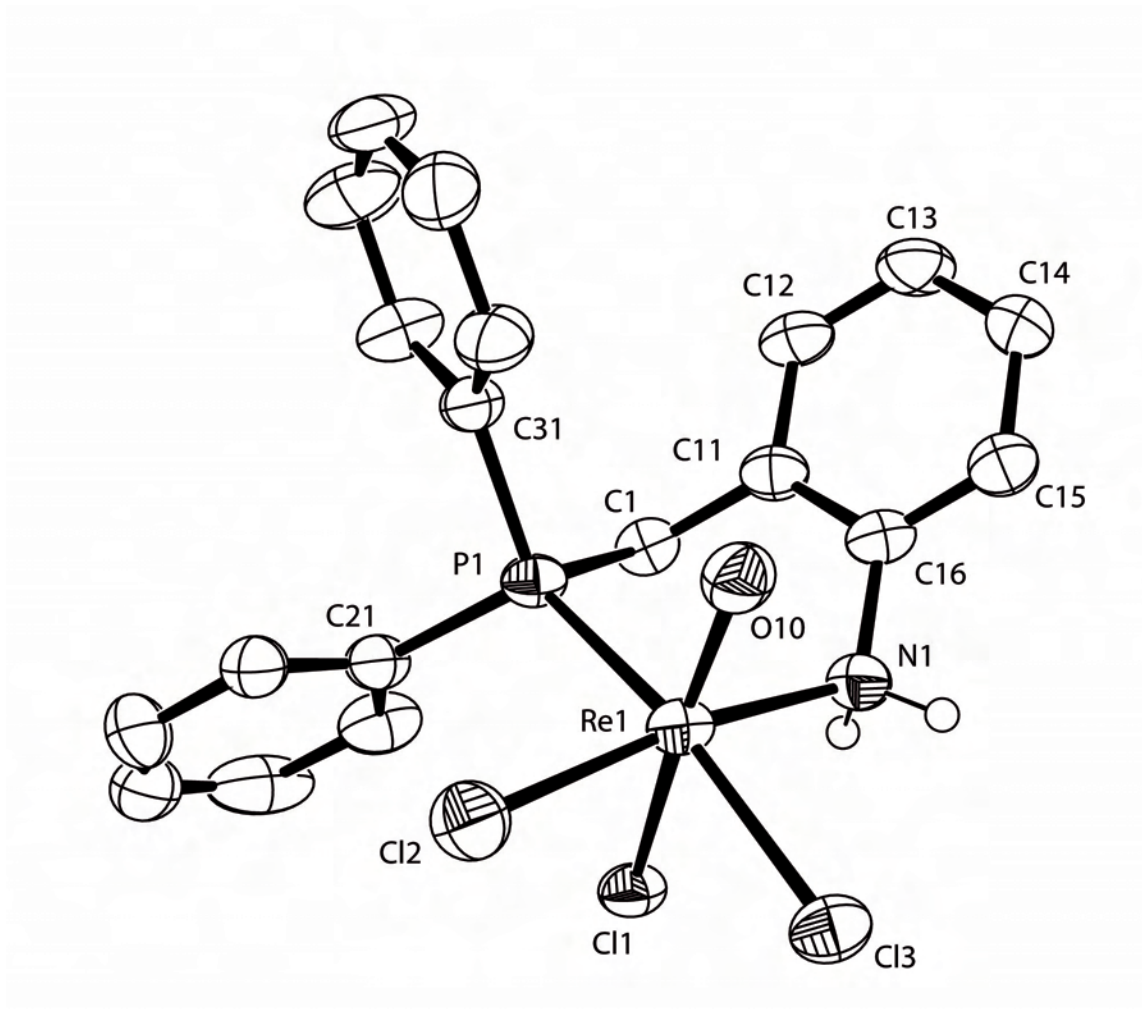


Abbildung 6.1: Ellipsoiddarstellung von  $[\text{ReOCl}_3(\text{H}_2\text{L}^1)]$ . Die Schwingungsellipsoide repräsentieren 50% der Aufenthaltswahrscheinlichkeit. [121]



## 6.2 [ReOCl<sub>3</sub>(H<sub>2</sub>L<sup>1</sup>)(OMe)]

Tabelle 6.3: Kristallographische Daten und Parameter der Strukturrechnung von [ReOCl<sub>3</sub>(H<sub>2</sub>L<sup>1</sup>)(OMe)]

Summenformel	C <sub>20</sub> H <sub>21</sub> NCl <sub>2</sub> PO <sub>2</sub> Re	
M (g/mol)	595.45	
Messtemperatur	200(2) K	
Wellenlänge	0.71073 Å	
Kristallsystem, Raumgruppe	monoklin, P <sub>2</sub> <sub>1</sub> /c	
Elementarzelle	a = 12.769(2) Å	α = 90°
	b = 9.936(1) Å	β = 92.77(1)°
	c = 16.646(2) Å	γ = 90°
Volumen	2024.5(5) Å <sup>3</sup>	
Z	4	
Berechnete Dichte	1.954 g/cm <sup>3</sup>	
Linearer Absorptionskoeffizient	6.361 mm <sup>-1</sup>	
F(000)	1152	
Kristallgröße	0.10 x 0.10 x 0.02 mm <sup>3</sup>	
Theta-Bereich	2.45 - 26.67°	
Indizes	-16 ≤ h ≤ 13, -11 ≤ k ≤ 12, -21 ≤ l ≤ 21	
Zahl der gemessenen Reflexe	10775	
Zahl der unabhängigen Reflexe	4389 [R(int) = 0.1075]	
Absorptionskorrektur	Integration	
Zahl der verfeinerten Parameter	245	
Goof	0.857	
R <sub>1</sub> / wR <sub>2</sub> [I > 2σ(I)]	R <sub>1</sub> = 0.0517, wR <sub>2</sub> = 0.1141	
R <sub>1</sub> / wR <sub>2</sub> (alle Reflexe)	R <sub>1</sub> = 0.1311, wR <sub>2</sub> = 0.1764	
Restelektronendichte	1.539 und -2.597 e · Å <sup>-3</sup>	
Programm zur Strukturlösung	SHELXS 97 [119]	

Tabelle 6.4: Atomkoordinaten ( $\cdot 10^4$ ) und isotrope Temperaturparameter ( $\text{\AA}^2 \cdot 10^3$ ) von  $[\text{ReOCl}_3(\text{H}_2\text{L}^1)(\text{OMe})]$

	x	y	z	E(eq)
Re(1)	1883(1)	903(1)	904(1)	36(1)
O(10)	1056(10)	-273(11)	447(6)	43(3)
Cl(1)	1218(4)	403(5)	2243(2)	54(1)
Cl(2)	3317(4)	-634(4)	1137(2)	53(1)
P(1)	2392(4)	1609(4)	-412(2)	36(1)
C(1)	1322(18)	2756(16)	-819(8)	57(6)
C(11)	1328(15)	3992(19)	-246(9)	49(4)
C(12)	1662(16)	5296(17)	-482(10)	48(5)
C(13)	1791(18)	6442(19)	78(11)	62(6)
C(14)	1458(17)	6262(19)	856(10)	56(5)
C(15)	1015(17)	4970(18)	1055(9)	55(5)
C(16)	966(12)	3857(14)	528(8)	34(3)
N(1)	637(12)	2506(14)	790(7)	46(4)
C(21)	2467(13)	175(17)	-1131(9)	39(4)
C(22)	1629(14)	-433(17)	-1452(8)	43(4)
C(23)	1722(17)	-1612(19)	-1975(9)	51(5)
C(24)	2630(20)	-2090(20)	-2162(10)	66(6)
C(25)	3550(20)	-1480(20)	-1824(11)	68(6)
C(26)	3530(17)	-340(19)	-1294(10)	56(5)
C(31)	3564(12)	2572(16)	-507(9)	35(3)
C(32)	4399(13)	2384(17)	39(9)	40(4)
C(33)	5377(16)	3060(20)	-59(11)	58(5)
C(34)	5511(17)	3870(20)	-725(11)	58(5)
C(35)	4690(14)	4090(20)	-1262(10)	56(4)
C(36)	3733(15)	3462(18)	-1156(9)	47(4)

O(2)	2636(9)	2354(11)	1376(5)	42(3)
C(2)	3195(19)	3310(20)	1895(11)	67(6)

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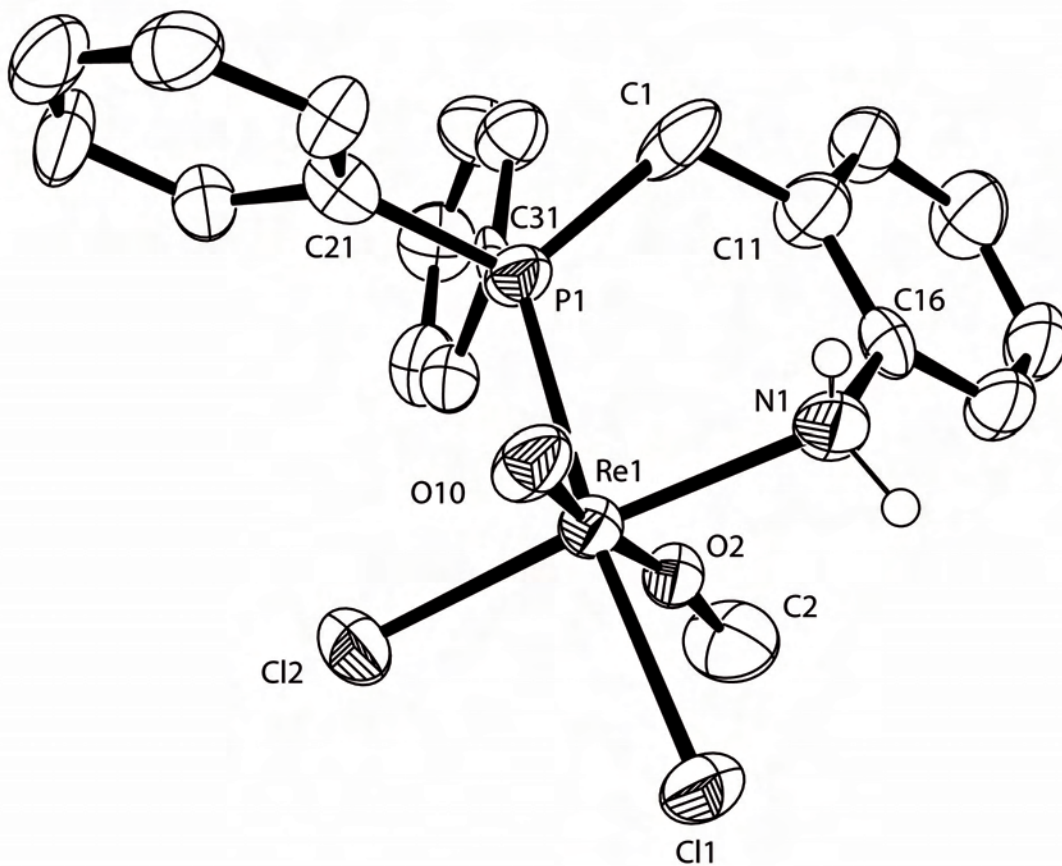


Abbildung 6.2: Ellipsoiddarstellung von  $[\text{ReOCl}_3(\text{H}_2\text{L}^1)(\text{OMe})]$ . Die Schwingungsellipsoide repräsentieren 50% der Aufenthaltswahrscheinlichkeit. [121]

### 6.3 [(ReOCl<sub>2</sub>{H<sub>2</sub>L<sup>1</sup>})<sub>2</sub>O] · 1.5 CH<sub>3</sub>CN

Tabelle 6.5: Kristallographische Daten und Parameter der Strukturrechnung von [(ReOCl<sub>2</sub>{H<sub>2</sub>L<sup>1</sup>})<sub>2</sub>O] · 1.5 CH<sub>3</sub>CN

Summenformel	C <sub>41</sub> H <sub>40.5</sub> N <sub>3.5</sub> Cl <sub>4</sub> P <sub>2</sub> O <sub>3</sub> Re <sub>2</sub>	
M (g/mol)	1206.41	
Messtemperatur	200(2) K	
Wellenlänge	0.71073 Å	
Kristallsystem, Raumgruppe	triklin, P $\bar{1}$	
Elementarzelle	a = 11.685(1) Å	$\alpha = 98.07(1)^\circ$
	b = 13.807(1) Å	$\beta = 108.25(1)^\circ$
	c = 14.876(1) Å	$\gamma = 91.41(1)^\circ$
Volumen	2250.7(3) Å <sup>3</sup>	
Z	2	
Berechnete Dichte	1.780 g/cm <sup>3</sup>	
Linearer Absorptionskoeffizient	5.722 mm <sup>-1</sup>	
F(000)	1166	
Kristallgröße	0.500 x 0.367 x 0.300 mm <sup>3</sup>	
Theta-Bereich	1.84 - 29.23°	
Indizes	-16 ≤ h ≤ 15, -18 ≤ k ≤ 18, -20 ≤ l ≤ 20	
Zahl der gemessenen Reflexe	25302	
Zahl der unabhängigen Reflexe	12017 [R(int) = 0.0640]	
Absorptionskorrektur	Empirisch, DELABS	
Zahl der verfeinerten Parameter	516	
Goof	1.050	
R <sub>1</sub> / wR <sub>2</sub> [I > 2σ(I)]	R <sub>1</sub> = 0.0320, wR <sub>2</sub> = 0.0811	
R <sub>1</sub> / wR <sub>2</sub> (alle Reflexe)	R <sub>1</sub> = 0.0424, wR <sub>2</sub> = 0.0929	
Restelektronendichte	1.479 und -2.235 e · Å <sup>-3</sup>	
Programm zur Strukturlösung	SHELXS 97 [119]	

Tabelle 6.6: Atomkoordinaten ( $\cdot 10^4$ ) und isotrope Temperaturparameter ( $\text{\AA}^2 \cdot 10^3$ ) von  $[(\text{ReOCl}_2\{\text{H}_2\text{L}^1\})_2\text{O}] \cdot 1.5 \text{CH}_3\text{CN}$

	x	y	z	E(eq)
Re(1)	7389(1)	1691(1)	3086(1)	24(1)
O(10)	8840(3)	1434(2)	3540(2)	32(1)
Cl(1)	7356(1)	1232(1)	1412(1)	35(1)
Cl(2)	6462(1)	143(1)	3025(1)	36(1)
P(1)	7439(1)	2308(1)	4707(1)	25(1)
C(1)	8049(4)	3585(3)	4973(3)	30(1)
C(11)	9236(4)	3661(3)	4767(3)	30(1)
C(12)	10317(4)	3906(3)	5516(4)	35(1)
C(13)	11407(5)	3957(4)	5336(4)	46(1)
C(14)	11434(5)	3760(4)	4408(5)	49(1)
C(15)	10382(4)	3524(4)	3660(4)	40(1)
C(16)	9279(4)	3469(3)	3834(3)	30(1)
N(1)	8177(3)	3153(3)	3052(3)	30(1)
C(21)	8456(4)	1674(3)	5586(3)	30(1)
C(22)	8637(5)	685(4)	5337(4)	38(1)
C(23)	9400(6)	189(5)	6002(4)	50(1)
C(24)	9991(6)	653(5)	6912(5)	55(2)
C(25)	9809(6)	1634(5)	7174(4)	53(1)
C(26)	9048(5)	2137(4)	6521(4)	44(1)
C(31)	6052(4)	2318(3)	5012(3)	29(1)
C(32)	5347(4)	1448(4)	4833(4)	37(1)
C(33)	4330(5)	1415(4)	5122(4)	48(1)
C(34)	4017(5)	2247(5)	5590(4)	48(1)
C(35)	4712(5)	3120(4)	5766(4)	46(1)
C(36)	5729(5)	3155(4)	5475(4)	39(1)

O(12)	5874(2)	2282(2)	2609(2)	25(1)
Re(2)	4592(1)	3043(1)	2002(1)	24(1)
O(20)	3607(3)	3679(2)	1242(2)	34(1)
Cl(3)	5926(1)	4511(1)	2866(1)	37(1)
Cl(4)	3719(1)	3169(1)	3228(1)	39(1)
P(2)	3431(1)	1537(1)	1117(1)	25(1)
C(2)	4018(4)	1161(3)	124(3)	29(1)
C(41)	4019(4)	1968(3)	-454(3)	30(1)
C(42)	3269(5)	1864(4)	-1393(3)	40(1)
C(43)	3261(6)	2604(5)	-1936(4)	49(1)
C(44)	4006(6)	3460(4)	-1543(4)	50(1)
C(45)	4758(5)	3557(4)	-609(4)	39(1)
C(46)	4778(4)	2820(3)	-64(3)	30(1)
N(2)	5545(3)	2948(3)	923(3)	28(1)
C(51)	1832(4)	1680(3)	591(3)	30(1)
C(52)	1133(5)	1018(4)	-184(4)	43(1)
C(53)	-110(6)	1086(5)	-552(5)	57(2)
C(54)	-646(5)	1823(6)	-129(5)	60(2)
C(55)	37(5)	2489(6)	644(5)	59(2)
C(56)	1289(5)	2422(4)	1010(4)	45(1)
C(61)	3471(4)	464(3)	1696(3)	28(1)
C(62)	3805(5)	-434(3)	1336(4)	36(1)
C(63)	3791(5)	-1248(3)	1774(4)	37(1)
C(64)	3430(5)	-1182(4)	2576(4)	41(1)
C(65)	3074(6)	-299(4)	2934(4)	47(1)
C(66)	3098(5)	519(4)	2506(4)	39(1)
C(87)	1270(12)	5357(10)	2272(9)	55(3)
C(88)	2008(8)	5556(6)	2089(7)	31(2)

N(89)	3055(8)	5895(6)	1856(7)	44(2)
C(97)	8601(7)	5916(6)	744(6)	69(2)
C(98)	8176(6)	5011(5)	961(5)	57(2)
N(99)	7836(6)	4312(5)	1134(6)	76(2)

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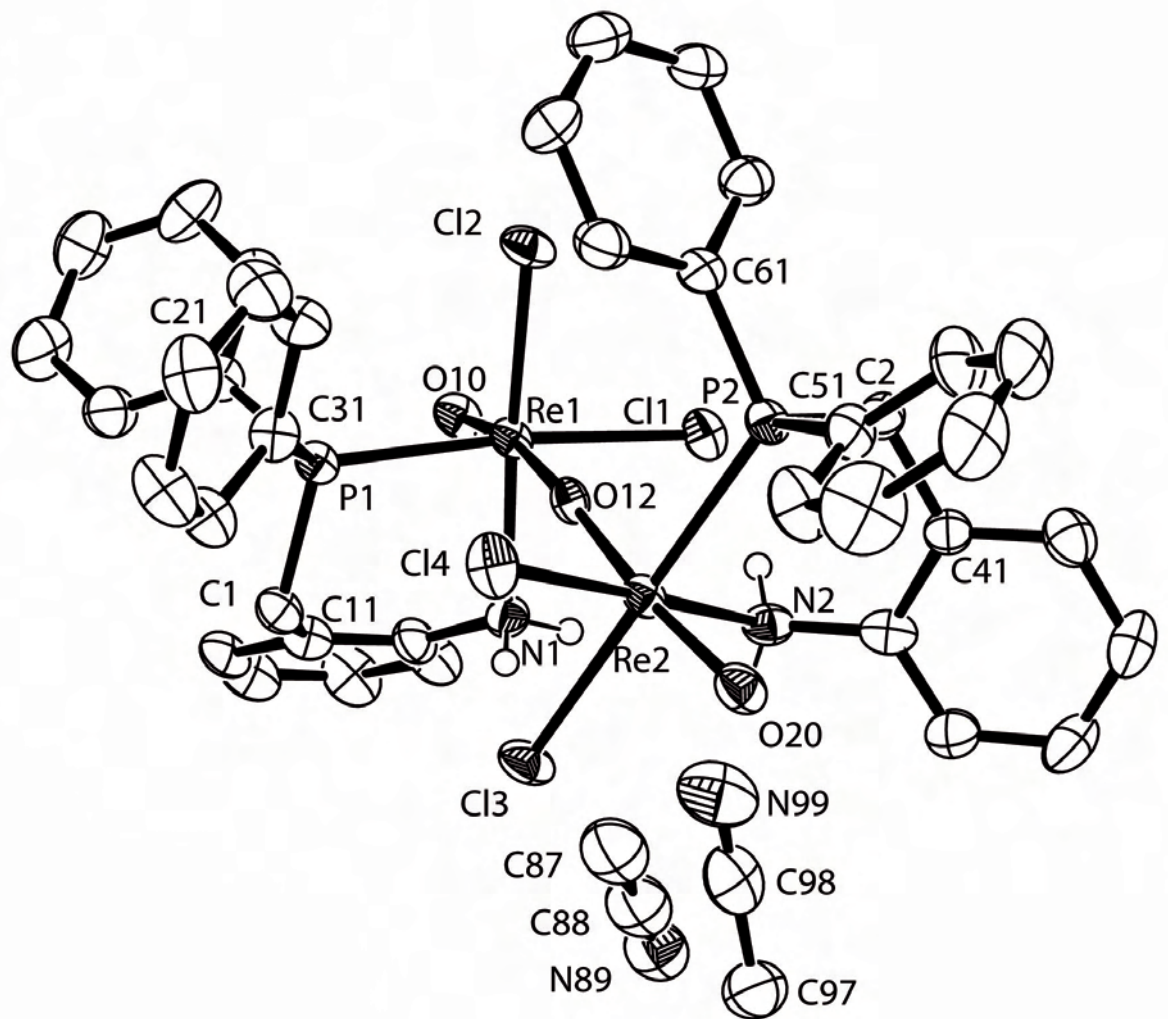


Abbildung 6.3: Ellipsoiddarstellung von  $[(\text{ReOCl}_2\{\text{H}_2\text{L}^1\})_2\text{O}] \cdot 1.5 \text{CH}_3\text{CN}$ . Die Schwingungsellipsoide repräsentieren 50% der Aufenthaltswahrscheinlichkeit. [121]



## 6.4 [(ReOCl{H<sub>2</sub>L<sup>1</sup>})<sub>3</sub>O<sub>3</sub>] · 2 CH<sub>2</sub>Cl<sub>2</sub> · 2 H<sub>2</sub>O

Tabelle 6.7: Kristallographische Daten und Parameter der Strukturrechnung von [(ReOCl{H<sub>2</sub>L<sup>1</sup>})<sub>3</sub>O<sub>3</sub>] · 2 CH<sub>2</sub>Cl<sub>2</sub> · 2 H<sub>2</sub>O

Summenformel	C <sub>59</sub> H <sub>58</sub> N <sub>3</sub> Cl <sub>7</sub> P <sub>3</sub> O <sub>8</sub> Re <sub>3</sub>	
M (g/mol)	1836.74	
Messtemperatur	200(2) K	
Wellenlänge	0.71073 Å	
Kristallsystem, Raumgruppe	triklin, P $\bar{1}$	
Elementarzelle	a = 13.532(2) Å	$\alpha = 75.36(1)^\circ$
	b = 16.606(2) Å	$\beta = 76.15(1)^\circ$
	c = 17.555(2) Å	$\gamma = 79.55(1)^\circ$
Volumen	3675.0(8) Å <sup>3</sup>	
Z	2	
Berechnete Dichte	1.638 g/cm <sup>3</sup>	
Linearer Absorptionskoeffizient	5.293 mm <sup>-1</sup>	
F(000)	1748	
Kristallgröße	0.300 x 0.167 x 0.100 mm <sup>3</sup>	
Theta-Bereich	2.68 - 29.16°	
Indizes	-17 ≤ h ≤ 17, -20 ≤ k ≤ 21, -21 ≤ l ≤ 22	
Zahl der gemessenen Reflexe	31362	
Zahl der unabhängigen Reflexe	15925 [R(int) = 0.1099]	
Absorptionskorrektur	Integration	
Zahl der verfeinerten Parameter	791	
Goof	0.850	
R <sub>1</sub> / wR <sub>2</sub> [I > 2σ(I)]	R <sub>1</sub> = 0.0666, wR <sub>2</sub> = 0.1554	
R <sub>1</sub> / wR <sub>2</sub> (alle Reflexe)	R <sub>1</sub> = 0.1352, wR <sub>2</sub> = 0.1795	
Restelektronendichte	2.184 und -4.464 e · Å <sup>-3</sup>	
Programm zur Strukturlösung	SHELXS 97 [119]	

Tabelle 6.8 : Atomkoordinaten ( $\cdot 10^4$ ) und isotrope Temperaturparameter ( $\text{\AA}^2 \cdot 10^3$ ) von  $[(\text{ReOCl}\{\text{H}_2\text{L}^1\})_3\text{O}_3] \cdot 2 \text{CH}_2\text{Cl}_2 \cdot 2 \text{H}_2\text{O}$

	x	y	z	E(eq)
Re(1)	644(1)	3470(1)	2961(1)	30(1)
P(1)	5228(2)	3126(2)	1218(2)	37(1)
C(1)	4987(10)	3800(8)	253(8)	45(3)
C(11)	4382(10)	3391(8)	-106(7)	44(3)
C(12)	3367(10)	3257(8)	273(7)	40(3)
C(13)	2814(11)	2833(9)	-42(8)	48(3)
C(14)	3272(13)	2522(10)	-707(10)	60(4)
C(15)	4248(13)	2624(11)	-1087(9)	68(5)
C(16)	4827(10)	3083(10)	-801(8)	53(4)
N(1)	2923(7)	3531(6)	1019(6)	34(2)
C(41)	6078(10)	2200(9)	964(9)	48(3)
C(42)	6831(11)	2295(10)	297(10)	57(4)
C(43)	7524(14)	1591(13)	108(13)	78(5)
C(44)	7425(18)	820(14)	587(17)	103(8)
C(45)	6628(16)	725(12)	1327(16)	92(7)
C(46)	5987(12)	1441(10)	1493(12)	69(5)
C(51)	6008(9)	3678(7)	1550(8)	38(3)
C(52)	6892(10)	3270(10)	1833(8)	49(3)
C(53)	7451(11)	3682(10)	2116(9)	57(4)
C(54)	7145(13)	4491(10)	2184(11)	65(4)
C(55)	6251(13)	4923(10)	1905(12)	69(5)
C(56)	5734(13)	4539(10)	1608(10)	62(4)
Cl(1)	899(2)	3135(2)	4382(2)	42(1)
Re(2)	3593(1)	2878(1)	2058(1)	33(1)
P(2)	1220(2)	5958(2)	3101(2)	31(1)

C(2)	943(9)	5513(8)	4180(7)	38(3)
C(21)	1873(8)	5396(7)	4552(6)	33(2)
C(22)	1887(11)	5845(9)	5111(7)	47(3)
C(23)	2729(11)	5726(10)	5460(9)	55(4)
C(24)	3545(11)	5183(11)	5254(10)	62(4)
C(25)	3574(10)	4724(9)	4697(8)	46(3)
C(26)	2727(9)	4835(7)	4337(7)	34(2)
N(2)	2759(8)	4351(6)	3751(6)	38(2)
C(61)	1479(10)	7019(9)	2968(8)	44(3)
C(62)	1007(12)	7537(9)	3495(10)	59(4)
C(63)	1137(14)	8359(11)	3369(11)	70(5)
C(64)	1818(16)	8695(9)	2650(12)	76(5)
C(65)	2310(13)	8201(9)	2095(10)	62(4)
C(66)	2118(10)	7379(8)	2258(8)	46(3)
C(71)	2(9)	6070(7)	2803(8)	36(3)
C(72)	-30(11)	6176(11)	2015(9)	63(5)
C(73)	-959(12)	6324(11)	1748(10)	69(5)
C(74)	-1849(12)	6361(10)	2310(12)	69(5)
C(75)	-1846(13)	6227(16)	3113(11)	96(8)
C(76)	-886(11)	6082(13)	3353(9)	72(5)
Cl(2)	4183(3)	2165(3)	3262(2)	61(1)
Re(3)	2585(1)	4981(1)	2544(1)	31(1)
P(3)	341(3)	2075(2)	2976(2)	38(1)
C(3)	811(12)	1973(8)	1938(8)	49(3)
C(31)	242(10)	2634(8)	1361(8)	40(3)
C(32)	-265(12)	2391(11)	867(9)	58(4)
C(33)	-724(12)	2962(11)	329(9)	60(4)
C(34)	-728(11)	3802(11)	267(9)	56(4)

C(35)	-249(11)	4057(9)	759(8)	49(3)
C(36)	236(10)	3478(8)	1316(7)	39(3)
N(3)	715(7)	3774(6)	1789(6)	35(2)
C(81)	-954(10)	1833(8)	3251(9)	46(3)
C(82)	-1680(11)	2206(9)	3809(11)	59(4)
C(83)	-2688(13)	2055(12)	3985(14)	84(6)
C(84)	-3001(14)	1504(13)	3645(14)	78(6)
C(85)	-2296(19)	1110(15)	3113(13)	99(8)
C(86)	-1281(13)	1290(11)	2909(10)	65(4)
C(91)	1042(11)	1198(8)	3584(9)	48(3)
C(92)	1929(14)	792(10)	3273(12)	72(5)
C(93)	2485(18)	164(13)	3725(18)	104(8)
C(94)	2090(20)	-53(11)	4560(16)	97(8)
C(95)	1204(17)	382(13)	4876(13)	91(7)
C(96)	677(13)	1006(11)	4397(10)	68(5)
Cl(3)	2560(2)	5540(2)	1121(2)	42(1)
O(1)	3471(6)	3922(5)	2247(5)	38(2)
O(2)	1448(6)	4400(5)	2725(4)	30(2)
O(3)	2116(6)	2772(5)	2822(4)	31(2)
O(4)	-589(6)	3792(5)	3272(4)	35(2)
O(5)	3517(6)	5556(6)	2522(5)	44(2)
O(6)	3565(6)	1971(6)	1742(6)	45(2)
Cl(6)	5289(5)	6510(5)	3366(5)	60(2)
Cl(9)	6620(12)	7534(7)	4640(8)	109(4)
Cl(7)	3729(13)	7797(8)	3844(11)	147(7)
Cl(8)	8098(13)	8559(12)	3771(10)	148(6)
C(98)	4031(18)	6897(15)	3461(16)	40(6)
C(97)	7250(30)	8220(30)	4560(20)	86(13)

O	5085(14)	3602(13)	3594(12)	56(5)
Cl(10)	9278(11)	8582(7)	886(8)	104(4)
Cl(11)	9844(16)	9748(10)	1475(16)	198(11)
C(89)	9480(30)	8700(40)	1670(30)	150(30)
Cl(5)	2524(6)	530(5)	798(5)	61(2)
Cl(4)	4392(8)	-338(7)	1268(7)	87(3)
C(99)	3780(20)	570(20)	780(20)	66(9)
O(11)	5560(20)	9743(19)	3426(18)	99(9)
O(12)	4950(20)	9880(20)	4460(20)	111(10)
O(10)	6720(20)	8586(19)	2308(18)	99(9)

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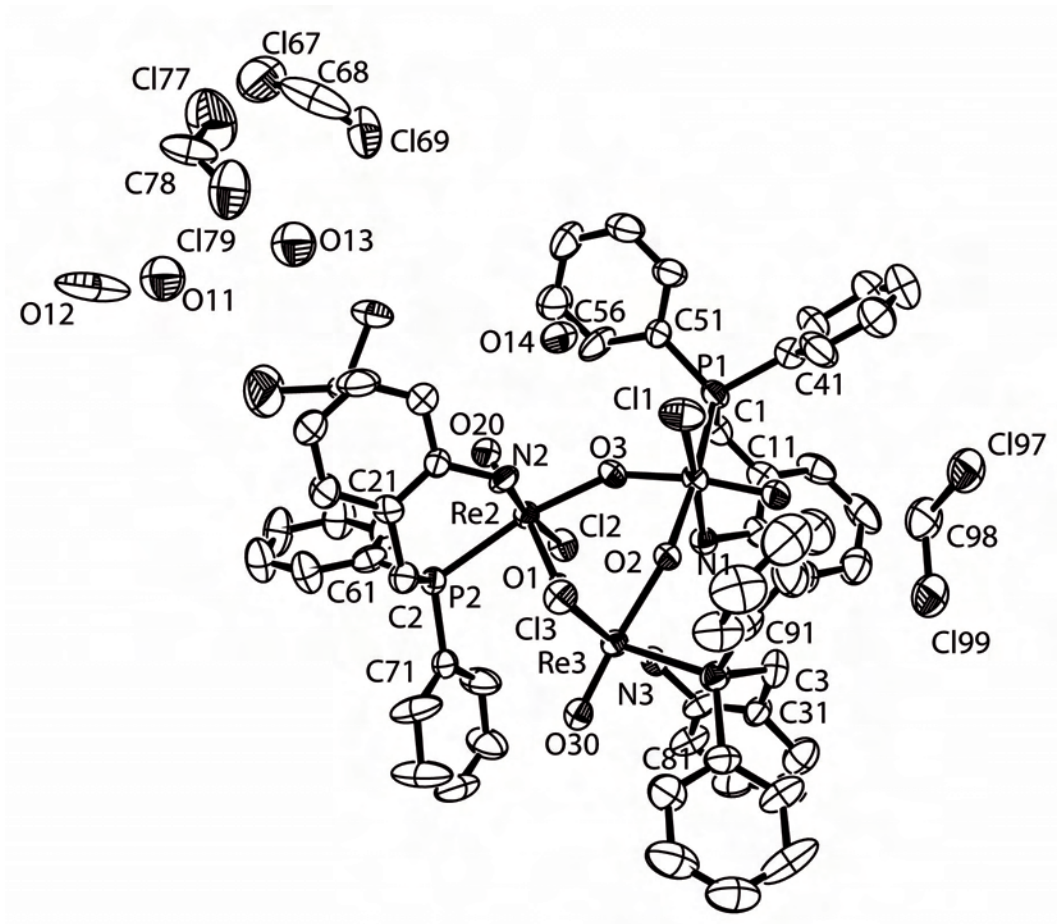


Abbildung 6.4: Ellipsoiddarstellung von  $[(\text{ReOCl}\{\text{H}_2\text{L}^1\})_3\text{O}_3] \cdot 4\text{CH}_2\text{Cl}_2 \cdot 2\text{H}_2\text{O}$ . Die Schwingungsellipsoide repräsentieren 50% der Aufenthaltswahrscheinlichkeit. [121]



## 6.5 [ReO<sub>2</sub>(H<sub>2</sub>L<sup>1</sup>)<sub>2</sub>]Cl · 0.75 MeOH

Tabelle 6.9: Kristallographische Daten und Parameter der Strukturrechnung von [ReO<sub>2</sub>(HL<sup>1</sup>)<sub>2</sub>]Cl · 0.75 MeOH

Summenformel	C <sub>38.75</sub> H <sub>39</sub> N <sub>2</sub> ClP <sub>2</sub> O <sub>2.75</sub> Re	
M (g/mol)	860.31	
Messtemperatur	200(2) K	
Wellenlänge	0.71073 Å	
Kristallsystem, Raumgruppe	triklin, P $\bar{1}$	
Elementarzelle	a = 11.836(1) Å	$\alpha = 93.56(1)^\circ$
	b = 12.563(1) Å	$\beta = 95.41(1)^\circ$
	c = 27.119(2) Å	$\gamma = 109.07(1)^\circ$
Volumen	3775.7(5) Å <sup>3</sup>	
Z	4	
Berechnete Dichte	1.513 g/cm <sup>3</sup>	
Linearer Absorptionskoeffizient	3.411 mm <sup>-1</sup>	
F(000)	1718	
Kristallgröße	0.52 x 0.36 x 0.29 mm <sup>3</sup>	
Theta-Bereich	1.72 - 29.29°	
Indizes	-14 ≤ h ≤ 16, -17 ≤ k ≤ 17, -37 ≤ l ≤ 37	
Zahl der gemessenen Reflexe	40424	
Zahl der unabhängigen Reflexe	20155 [R(int) = 0.0723]	
Absorptionskorrektur	Integration	
Zahl der verfeinerten Parameter	854	
Goof	0.935	
R <sub>1</sub> / wR <sub>2</sub> [I > 2σ(I)]	R <sub>1</sub> = 0.0594, wR <sub>2</sub> = 0.1464	
R <sub>1</sub> / wR <sub>2</sub> (alle Reflexe)	R <sub>1</sub> = 0.0904, wR <sub>2</sub> = 0.1660	
Restelektronendichte	2.108 und -1.940 e · Å <sup>-3</sup>	
Programm zur Strukturlösung	SHELXS 97 [119]	

Tabelle 6.10: Atomkoordinaten ( $\cdot 10^4$ ) und isotrope Temperaturparameter ( $\text{\AA}^2 \cdot 10^3$ ) von  $[\text{ReO}_2(\text{H}_2\text{L}^1)_2]\text{Cl} \cdot 0.75 \text{ MeOH}$

	x	y	z	E(eq)
Re(1)	4381(1)	6719(1)	1545(1)	42(1)
O(10)	4067(5)	5569(4)	1099(2)	52(1)
O(20)	4667(5)	7809(4)	2037(2)	50(1)
P(1)	3246(2)	7599(2)	1019(1)	48(1)
C(1)	1627(8)	6934(7)	1082(3)	59(2)
C(11)	1189(7)	5663(7)	1080(3)	51(2)
C(12)	280(7)	4973(8)	718(3)	62(2)
C(13)	-100(7)	3828(7)	704(3)	64(2)
C(14)	427(8)	3321(8)	1049(3)	69(2)
C(15)	1307(8)	3965(7)	1413(3)	57(2)
C(16)	1693(7)	5149(6)	1434(2)	50(2)
N(1)	2617(5)	5816(5)	1824(2)	47(1)
C(21)	3416(7)	7412(7)	361(2)	53(2)
C(22)	4205(10)	8280(8)	148(3)	74(3)
C(23)	4448(12)	8104(9)	-334(3)	90(3)
C(24)	3933(10)	7090(9)	-598(3)	75(3)
C(25)	3180(10)	6183(9)	-390(3)	77(3)
C(26)	2888(7)	6369(7)	88(3)	59(2)
C(31)	3399(8)	9093(6)	1137(3)	55(2)
C(32)	4104(9)	9758(7)	1548(3)	67(2)
C(33)	4157(11)	10878(7)	1643(4)	79(3)
C(34)	3492(11)	11326(9)	1323(5)	89(3)
C(35)	2812(12)	10678(9)	919(5)	91(3)
C(36)	2744(10)	9554(8)	829(4)	77(3)
P(2)	6396(2)	7616(1)	1347(1)	45(1)

C(2)	7403(7)	7410(6)	1862(3)	51(2)
C(41)	7233(7)	6166(6)	1883(2)	50(2)
C(42)	8145(8)	5747(8)	1783(3)	63(2)
C(43)	7991(9)	4612(8)	1800(3)	71(2)
C(44)	6913(9)	3876(7)	1917(3)	67(2)
C(45)	5993(8)	4267(6)	2012(3)	53(2)
C(46)	6152(7)	5416(6)	1992(2)	47(1)
N(2)	5179(5)	5826(5)	2097(2)	42(1)
C(51)	6868(7)	7130(6)	782(2)	48(2)
C(52)	8086(7)	7426(7)	730(3)	60(2)
C(53)	8441(8)	7145(8)	276(3)	67(2)
C(54)	7585(9)	6563(8)	-109(3)	68(2)
C(55)	6379(9)	6258(7)	-60(3)	64(2)
C(56)	6023(7)	6538(7)	386(3)	56(2)
C(61)	6924(7)	9150(6)	1340(3)	50(2)
C(62)	7168(10)	9826(7)	1780(3)	73(2)
C(63)	7554(10)	10992(8)	1787(4)	81(3)
C(64)	7716(9)	11463(7)	1349(4)	76(3)
C(65)	7525(11)	10815(8)	920(4)	84(3)
C(66)	7111(10)	9646(7)	905(3)	70(2)
Cl'1	1482(2)	7338(2)	2489(1)	66(1)
Re(2)	4921(1)	7706(1)	3507(1)	42(1)
O'10	5523(5)	7205(4)	2999(2)	49(1)
O'20	4227(5)	8191(4)	3969(2)	52(1)
P'1	5410(2)	6390(2)	4028(1)	47(1)
C'1	4073(7)	5109(6)	4003(3)	56(2)
C'11	2899(8)	5330(7)	4040(3)	55(2)
C'12	2234(9)	4960(8)	4428(3)	69(2)

C'13	1189(9)	5192(9)	4478(3)	80(3)
C'14	783(8)	5794(8)	4139(4)	73(2)
C'15	1412(8)	6136(7)	3744(3)	62(2)
C'16	2456(7)	5921(6)	3690(3)	54(2)
N'1	3138(5)	6316(5)	3279(2)	48(1)
C'21	5864(8)	6955(6)	4684(2)	55(2)
C'22	7053(9)	7321(7)	4867(3)	67(2)
C'23	7404(11)	7874(9)	5351(3)	89(3)
C'24	6578(12)	8052(9)	5632(3)	85(3)
C'25	5401(11)	7713(10)	5445(3)	86(3)
C'26	5011(9)	7127(7)	4972(3)	66(2)
C'31	6500(7)	5729(6)	3876(3)	51(2)
C'32	6703(8)	4938(7)	4175(3)	64(2)
C'33	7443(9)	4363(7)	4053(4)	75(3)
C'34	8000(9)	4534(7)	3619(4)	72(2)
C'35	7798(8)	5300(8)	3319(4)	71(2)
C'36	7064(8)	5917(8)	3445(3)	65(2)
P'2	6769(2)	9284(2)	3664(1)	45(1)
C'2	6797(7)	10107(7)	3125(3)	54(2)
C'41	5799(7)	10597(6)	3093(2)	51(2)
C'42	6056(9)	11762(7)	3129(3)	67(2)
C'43	5136(10)	12237(7)	3109(3)	74(3)
C'44	3985(10)	11566(7)	3044(3)	67(2)
C'45	3683(8)	10395(6)	3006(3)	55(2)
C'46	4585(7)	9922(6)	3020(2)	49(2)
N'2	4258(6)	8700(4)	2957(2)	44(1)
C'51	7015(7)	10285(6)	4209(2)	46(1)
C'52	7902(8)	11347(7)	4242(3)	58(2)

C'53	8148(8)	12042(7)	4678(3)	63(2)
C'54	7538(9)	11734(7)	5080(3)	63(2)
C'55	6673(8)	10690(7)	5049(3)	58(2)
C'56	6400(7)	9969(7)	4618(3)	54(2)
C'61	8206(7)	9026(6)	3693(3)	52(2)
C'62	8952(9)	9192(8)	4137(3)	70(2)
C'63	10048(10)	9012(10)	4146(5)	89(3)
C'64	10368(11)	8631(9)	3709(5)	95(4)
C'65	9692(11)	8490(10)	3281(5)	87(3)
C'66	8596(9)	8682(8)	3266(3)	70(2)
Cl(1)	3118(2)	4053(2)	2631(1)	60(1)
C(97)	-450(20)	2044(19)	3259(8)	84(5)
O(97)	570(20)	1781(17)	3391(7)	123(6)
C(98)	241(19)	3138(18)	2498(7)	74(5)
O(98)	132(16)	4061(15)	2643(6)	103(5)
C(99)	605(19)	9820(18)	1954(7)	78(5)
O(99)	340(10)	8758(9)	1788(4)	56(2)

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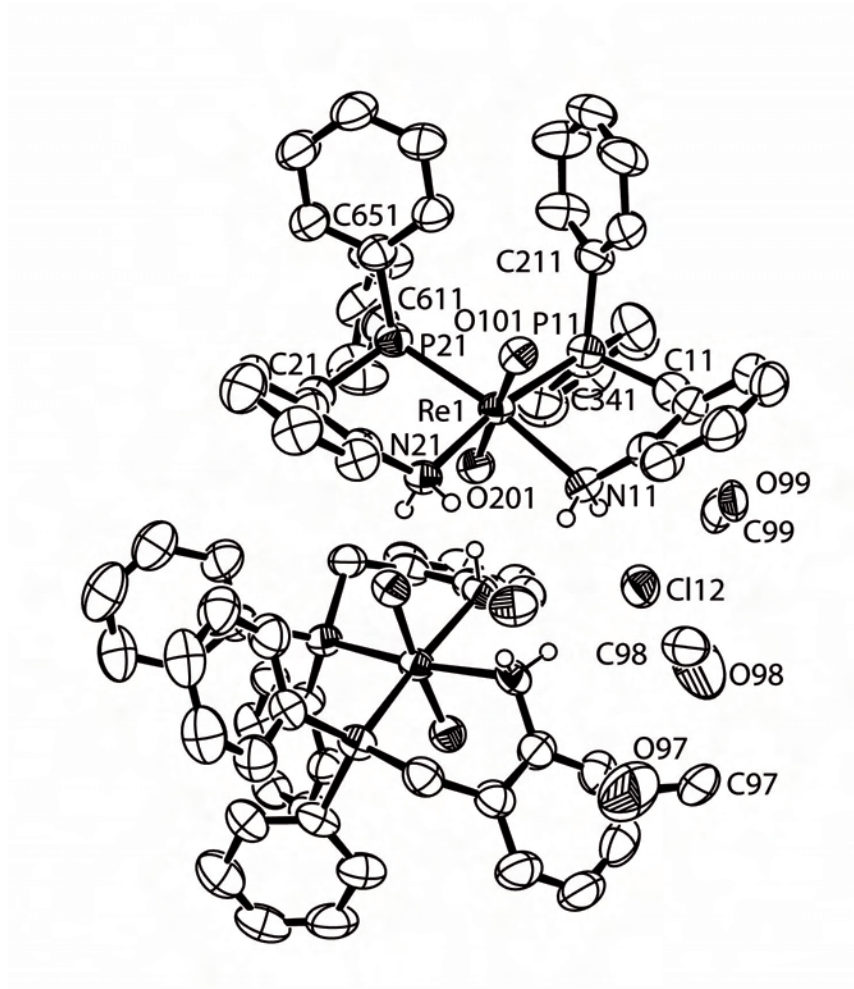


Abbildung 6.5: Ellipsoiddarstellung von  $2 [\text{ReO}_2(\text{H}_2\text{L}^1)_2]\text{Cl} \cdot 1.5 \text{ MeOH}$ . Die Schwingungsellipsoide repräsentieren 50% der Aufenthaltswahrscheinlichkeit. [121]

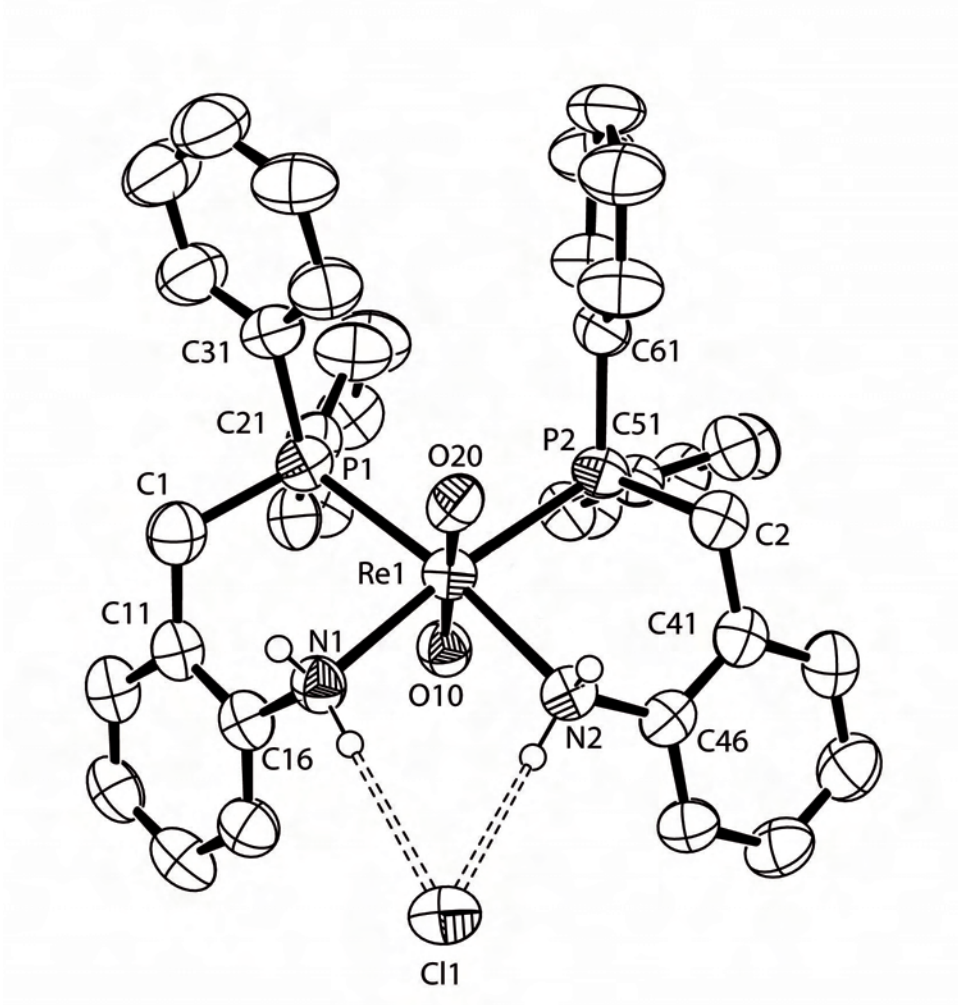


Abbildung 6.6: Ellipsoiddarstellung von  $[\text{ReO}_2(\text{H}_2\text{L}^1)_2]\text{Cl}$ . Die Schwingungsellipsoide repräsentieren 50% der Aufenthaltswahrscheinlichkeit. [121]





## 6.6 [ReO<sub>2</sub>(H<sub>2</sub>L<sup>1</sup>)<sub>2</sub>]Cl,

### [ReO<sub>2</sub>(H<sub>2</sub>L<sup>1</sup>)(H<sub>2</sub>L<sup>1b</sup>)]Cl · 2.5 CH<sub>2</sub>Cl<sub>2</sub>

Tabelle 6.11: Kristallographische Daten und Parameter der Strukturrechnung von [ReO<sub>2</sub>(H<sub>2</sub>L<sup>1</sup>)<sub>2</sub>]Cl, [ReO<sub>2</sub>(H<sub>2</sub>L<sup>1</sup>)(H<sub>2</sub>L<sup>1b</sup>)]Cl · 2.5 CH<sub>2</sub>Cl<sub>2</sub>

Summenformel	C <sub>77.5</sub> H <sub>75</sub> N <sub>4</sub> Cl <sub>7</sub> P <sub>4</sub> O <sub>4</sub> Re <sub>2</sub>	
M (g/mol)	1870.85	
Messtemperatur	200(2) K	
Wellenlänge	0.71073 Å	
Kristallsystem, Raumgruppe	triklin, P $\bar{1}$	
Elementarzelle	a = 15.047(2) Å	$\alpha = 84.05(1)^\circ$
	b = 15.087(2) Å	$\beta = 77.87(1)^\circ$
	c = 20.609(2) Å	$\gamma = 61.74(1)^\circ$
Volumen	4028.8(9) Å <sup>3</sup>	
Z	2	
Berechnete Dichte	1.543 g/cm <sup>3</sup>	
Linearer Absorptionskoeffizient	3.362 mm <sup>-1</sup>	
F(000)	1858	
Kristallgröße	0.40 x 0.30 x 0.29 mm <sup>3</sup>	
Theta-Bereich	2.05 - 29.59°	
Indizes	-19 ≤ h ≤ 18, -18 ≤ k ≤ 19, -26 ≤ l ≤ 26	
Zahl der gemessenen Reflexe	34966	
Zahl der unabhängigen Reflexe	17415 [R(int) = 0.0724]	
Absorptionskorrektur	Integration	
Zahl der verfeinerten Parameter	899	
Goof	0.961	
R <sub>1</sub> / wR <sub>2</sub> [I > 2σ(I)]	R <sub>1</sub> = 0.0594, wR <sub>2</sub> = 0.1672	
R <sub>1</sub> / wR <sub>2</sub> (alle Reflexe)	R <sub>1</sub> = 0.0835, wR <sub>2</sub> = 0.1841	

Restelektronendichte	5.195 und -2.047 e · Å <sup>-3</sup>
Programm zur Strukturlösung	SHELXS 97 [119]

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Tabelle 6.12: Atomkoordinaten ( $\cdot 10^4$ ) und isotrope Temperaturparameter ( $\text{\AA}^2 \cdot 10^3$ ) von  $[\text{ReO}_2(\text{H}_2\text{L}^1)_2]\text{Cl}$ ,  $[\text{ReO}_2(\text{H}_2\text{L}^1)(\text{H}_2\text{L}^{1b})]\text{Cl} \cdot 2.5 \text{CH}_2\text{Cl}_2$

	x	y	z	E(eq)
Re(1)	8642(1)	8265(1)	3108(1)	32(1)
O(101)	7689(5)	9380(4)	2838(3)	39(1)
O(201)	9613(4)	7082(4)	3318(3)	36(1)
P(11)	9782(2)	8939(2)	3194(1)	37(1)
C(11)	10766(8)	8563(8)	2434(4)	47(2)
C(111)	10265(7)	9051(7)	1841(4)	41(2)
C(121)	10347(9)	9863(9)	1502(5)	56(3)
C(131)	9812(11)	10327(9)	1006(6)	65(3)
C(141)	9148(10)	10046(8)	852(5)	60(3)
C(151)	9042(8)	9242(8)	1187(5)	47(2)
C(161)	9578(7)	8759(6)	1680(4)	35(2)
N(11)	9441(5)	7951(5)	2048(3)	34(1)
C(311)	9305(7)	10279(7)	3225(4)	41(2)
C(321)	9994(9)	10657(8)	3269(5)	50(2)
C(331)	9650(10)	11683(9)	3270(5)	57(3)
C(341)	8656(10)	12336(8)	3235(5)	61(3)
C(351)	7993(10)	11998(8)	3167(6)	65(3)
C(361)	8292(8)	10962(8)	3190(5)	50(2)
C(411)	10494(7)	8434(7)	3868(4)	41(2)
C(421)	10182(9)	8916(8)	4442(4)	53(2)
C(431)	10733(11)	8483(10)	4973(5)	66(3)
C(441)	11553(11)	7560(10)	4916(6)	66(3)
C(451)	11865(9)	7054(9)	4335(6)	62(3)
C(461)	11326(9)	7479(8)	3814(5)	55(2)
P(21)	7613(2)	8581(2)	4214(1)	36(1)

C(21)	6699(7)	8066(8)	4270(4)	45(2)
C(211)	6132(7)	8347(7)	3697(4)	41(2)
C(221)	5080(7)	8932(8)	3803(5)	50(2)
C(231)	4573(8)	9224(9)	3279(6)	61(3)
C(241)	5094(9)	8935(10)	2642(6)	61(3)
C(251)	6145(7)	8362(8)	2527(5)	47(2)
C(261)	6666(6)	8058(7)	3044(4)	38(2)
N(21)	7767(5)	7486(5)	2919(3)	35(1)
C(511)	8132(7)	8042(7)	4968(4)	40(2)
C(521)	9153(7)	7349(8)	4941(5)	45(2)
C(531)	9510(9)	6946(9)	5524(5)	55(3)
C(541)	8877(9)	7208(9)	6115(5)	56(3)
C(551)	7830(10)	7896(9)	6146(5)	58(3)
C(561)	7477(9)	8295(8)	5572(4)	52(2)
C(611)	6867(7)	9924(6)	4389(4)	40(2)
C(621)	7151(7)	10393(8)	4780(5)	50(2)
C(631)	6660(10)	11412(9)	4862(6)	62(3)
C(641)	5867(9)	11999(8)	4536(6)	66(3)
C(651)	5551(9)	11564(8)	4129(5)	56(3)
C(661)	6074(8)	10532(8)	4044(5)	54(2)
Cl(1)	8530(2)	6908(2)	1290(1)	43(1)
Re(2)	1711(1)	4788(1)	2082(1)	31(1)
O(102)	1221(4)	6111(5)	1986(3)	37(1)
O(202)	2137(5)	3490(5)	2224(3)	41(1)
P(12)	3197(2)	4614(2)	2469(1)	42(1)
C(112)	2801(7)	4533(7)	3364(5)	44(2)
C(122)	3459(8)	4221(8)	3816(5)	50(2)
C(132)	3085(9)	4196(9)	4488(5)	59(3)

C(142)	2083(10)	4490(9)	4728(5)	62(3)
C(152)	1406(8)	4780(8)	4287(4)	49(2)
C(162)	1762(6)	4805(6)	3614(4)	35(2)
N(12)	1063(5)	5086(5)	3146(3)	33(1)
C(312)	3447(8)	5666(9)	2332(5)	54(2)
C(322)	3696(10)	6076(10)	2799(7)	68(3)
C(332)	3847(12)	6915(14)	2645(8)	88(4)
C(342)	3755(12)	7393(12)	2061(9)	88(4)
C(352)	3523(14)	7004(14)	1592(9)	99(5)
C(362)	3359(13)	6168(12)	1724(7)	82(4)
C(412)	4436(7)	3474(7)	2302(4)	45(2)
C(422)	5340(8)	3507(10)	2046(6)	64(3)
C(432)	6242(10)	2611(13)	1950(8)	90(5)
C(442)	6241(10)	1695(12)	2097(7)	85(4)
C(452)	5365(11)	1658(10)	2342(7)	72(3)
C(462)	4437(9)	2552(9)	2438(6)	64(3)
P(22)	2130(2)	4685(2)	866(1)	35(1)
C(22)	995(7)	4856(7)	579(4)	40(2)
C(212)	633(6)	4101(7)	900(4)	37(2)
C(222)	666(7)	3360(8)	526(5)	49(2)
C(232)	354(9)	2675(8)	836(5)	54(2)
C(242)	11(9)	2715(9)	1536(5)	55(2)
C(252)	-11(8)	3419(7)	1893(5)	45(2)
C(262)	268(6)	4133(7)	1587(4)	37(2)
N(22)	205(5)	4914(5)	1965(3)	33(1)
C(512)	2347(7)	5702(7)	453(4)	43(2)
C(522)	1558(8)	6693(7)	519(4)	48(2)
C(532)	1736(10)	7472(9)	242(6)	65(3)

C(542)	2693(12)	7300(10)	-129(7)	82(4)
C(552)	3466(10)	6354(10)	-179(6)	71(3)
C(562)	3331(8)	5527(9)	101(5)	55(2)
C(612)	3179(7)	3555(7)	455(4)	43(2)
C(622)	4060(7)	3026(7)	739(5)	47(2)
C(632)	4912(8)	2212(8)	402(6)	57(3)
C(642)	4898(9)	1956(9)	-209(6)	62(3)
C(652)	4035(10)	2469(9)	-485(6)	68(3)
C(662)	3173(8)	3245(9)	-160(5)	57(3)
CI(2)	8771(2)	5085(2)	3426(1)	49(1)
CI(67)	7641(7)	4370(7)	1260(4)	46(2)
C(68)	7558(15)	5144(15)	1858(9)	6(4)
CI(69)	6304(8)	6023(8)	2132(5)	51(2)
CI(77)	6050(10)	4326(10)	4304(6)	70(3)
C(78)	6310(20)	5160(20)	3831(13)	27(6)
CI(79)	5474(5)	6405(5)	4023(3)	22(1)
CI(87)	3828(3)	774(4)	1322(2)	98(1)
C(88)	2595(11)	1345(10)	1725(8)	83(4)
CI(89)	2292(3)	571(4)	2296(2)	111(2)
CI(97)	3585(3)	327(3)	-962(2)	97(1)
C(98)	2854(13)	890(12)	-216(7)	85(4)
CI(99)	2373(3)	159(3)	278(2)	80(1)

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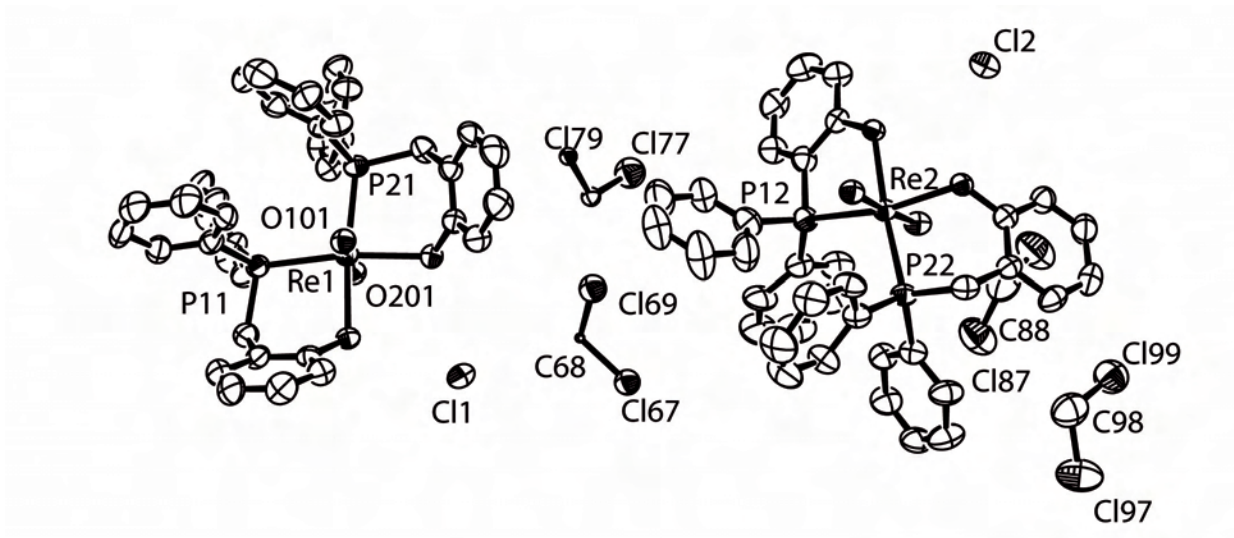


Abbildung 6.7: Ellipsoiddarstellung von  $[\text{ReO}_2(\text{H}_2\text{L}^1)_2]\text{Cl}$ ,  $[\text{ReO}_2(\text{H}_2\text{L}^1)(\text{H}_2\text{L}^{1b})]\text{Cl} \cdot 2.5 \text{CH}_2\text{Cl}_2$ . Die Schwingungsellipsoide repräsentieren 50% der Aufenthaltswahrscheinlichkeit. [121]

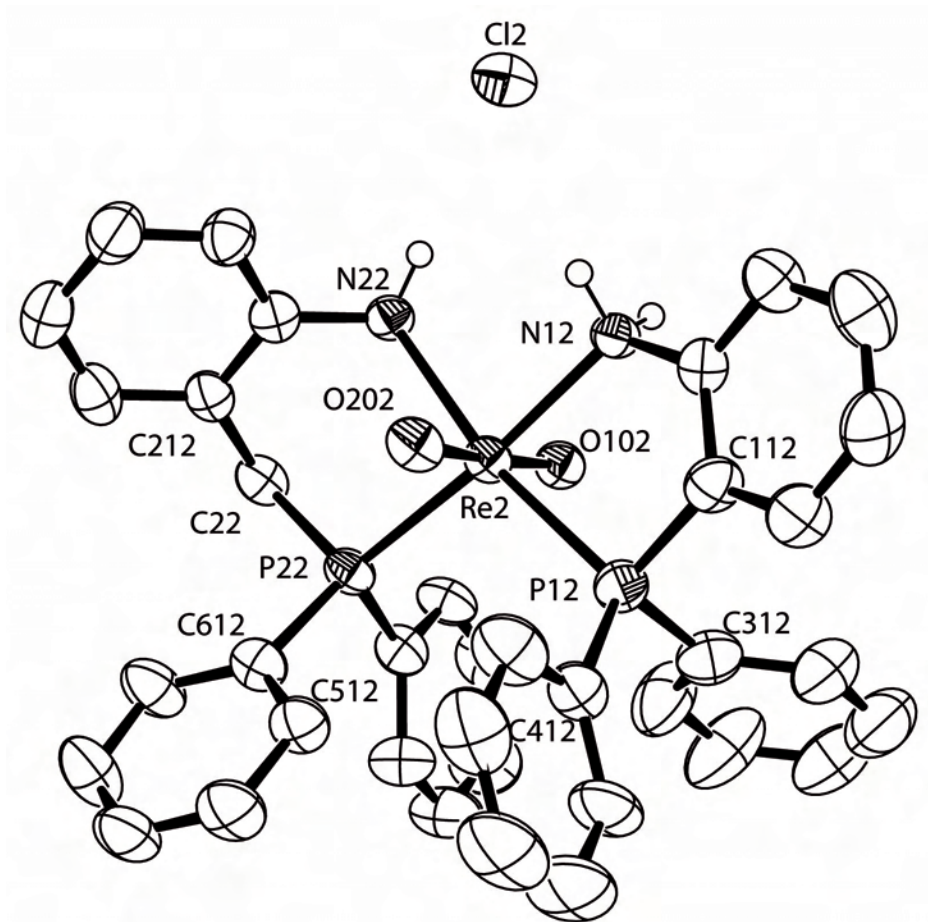


Abbildung 6.8: Ellipsoiddarstellung von  $[\text{ReO}_2(\text{H}_2\text{L}^1)(\text{H}_2\text{L}^{1b})]\text{Cl}$ . Die Schwingungsellipsoide repräsentieren 50% der Aufenthaltswahrscheinlichkeit. [121]



## 6.7 [ReNCl<sub>2</sub>(PPh<sub>3</sub>)(H<sub>2</sub>L<sup>1</sup>)] · 0.5 CH<sub>2</sub>Cl<sub>2</sub>

Tabelle 6.13: Kristallographische Daten und Parameter der Strukturrechnung von [ReNCl<sub>2</sub>(PPh<sub>3</sub>)(H<sub>2</sub>L<sup>1</sup>)] · 0.5 CH<sub>2</sub>Cl<sub>2</sub>

Summenformel	C <sub>37.5</sub> H <sub>34</sub> N <sub>2</sub> Cl <sub>3</sub> P <sub>2</sub> Re	
M (g/mol)	867.16	
Messtemperatur	200(2) K	
Wellenlänge	0.71073 Å	
Kristallsystem, Raumgruppe	monoklin, C 2/c	
Elementarzelle	a = 26.838(1) Å	α = 90°
	b = 15.317(2) Å	β = 95.13(1)°
	c = 17.745(2) Å	γ = 90°
Volumen	7265.4(2) Å <sup>3</sup>	
Z	8	
Berechnete Dichte	1.586 g/cm <sup>3</sup>	
Linearer Absorptionskoeffizient	3.683 mm <sup>-1</sup>	
F(000)	3432	
Kristallgröße	0.26 x 0.12 x 0.11 mm <sup>3</sup>	
Theta-Bereich	1.88 - 27.00°	
Indizes	-34 ≤ h ≤ 36, -19 ≤ k ≤ 19, -22 ≤ l ≤ 22	
Zahl der gemessenen Reflexe	23019	
Zahl der unabhängigen Reflexe	7913 [R(int) = 0.1626]	
Absorptionskorrektur	Integration	
Zahl der verfeinerten Parameter	424	
Goof	0.808	
R <sub>1</sub> / wR <sub>2</sub> [I > 2σ(I)]	R <sub>1</sub> = 0.0560, wR <sub>2</sub> = 0.0986	
R <sub>1</sub> / wR <sub>2</sub> (alle Reflexe)	R <sub>1</sub> = 0.1480, wR <sub>2</sub> = 0.1392	
Restelektronendichte	1.089 und -2.187 e · Å <sup>-3</sup>	
Programm zur Strukturlösung	SHELXS 97 [119]	

Tabelle 6.14: Atomkoordinaten ( $\cdot 10^4$ ) und isotrope Temperaturparameter ( $\text{\AA}^2 \cdot 10^3$ ) von  $[\text{ReNCl}_2(\text{PPh}_3)(\text{H}_2\text{L}^1)] \cdot 0.5 \text{CH}_2\text{Cl}_2$

	x	y	z	E(eq)
Re(1)	2865(1)	3547(1)	1373(1)	30(1)
N(10)	2648(4)	4498(7)	1639(5)	37(3)
Cl(1)	3167(1)	1955(2)	1073(1)	39(1)
Cl(2)	3012(1)	3839(2)	77(1)	43(1)
P(1)	2675(1)	2762(2)	2494(1)	31(1)
C(1)	2161(5)	2012(8)	2205(6)	40(3)
C(11)	1709(5)	2500(8)	1893(6)	37(3)
C(12)	1280(6)	2486(12)	2254(8)	61(4)
C(13)	864(6)	2946(12)	1986(8)	63(5)
C(14)	869(5)	3452(12)	1321(8)	64(4)
C(15)	1295(4)	3453(11)	950(6)	47(3)
C(16)	1715(5)	3000(8)	1223(6)	33(3)
N(1)	2169(3)	3013(7)	830(4)	37(2)
C(21)	2431(5)	3366(8)	3274(5)	33(3)
C(22)	2384(5)	4222(9)	3294(6)	44(3)
C(23)	2231(7)	4668(10)	3926(7)	67(5)
C(24)	2112(6)	4183(11)	4531(7)	60(4)
C(25)	2128(7)	3321(10)	4513(7)	64(5)
C(26)	2295(6)	2890(9)	3894(6)	52(4)
C(31)	3144(4)	2082(8)	3011(5)	31(3)
C(32)	3482(5)	2455(9)	3557(6)	37(3)
C(33)	3843(5)	1943(10)	3940(7)	44(3)
C(34)	3865(6)	1081(12)	3811(8)	61(4)
C(35)	3536(6)	691(9)	3278(8)	58(4)
C(36)	3167(6)	1185(9)	2876(7)	52(4)

P(2)	3723(1)	3983(2)	1718(1)	30(1)
C(41)	3919(4)	4243(8)	2711(5)	32(3)
C(42)	3616(5)	4805(9)	3046(6)	45(3)
C(43)	3735(7)	5088(12)	3780(7)	65(5)
C(44)	4171(6)	4767(10)	4190(7)	54(4)
C(45)	4473(5)	4215(10)	3860(6)	51(4)
C(46)	4351(5)	3930(9)	3101(6)	47(3)
C(51)	3907(5)	5029(8)	1318(6)	36(3)
C(52)	4404(6)	5312(10)	1464(6)	50(4)
C(53)	4552(7)	6122(10)	1210(8)	60(4)
C(54)	4212(7)	6668(10)	838(8)	67(5)
C(55)	3729(6)	6407(11)	686(7)	57(4)
C(56)	3575(5)	5587(8)	927(6)	43(3)
C(61)	4159(5)	3211(9)	1374(7)	42(3)
C(62)	4327(5)	2473(10)	1807(8)	54(4)
C(63)	4631(6)	1870(11)	1501(11)	75(5)
C(64)	4757(6)	1955(13)	758(11)	76(6)
C(65)	4581(6)	2665(12)	332(9)	64(5)
C(66)	4292(5)	3267(9)	642(6)	44(4)
CI(97)	4416(7)	9364(12)	786(8)	168(6)
C(98)	4074(12)	9710(20)	1588(14)	59(8)
CI(99)	4713(6)	9709(11)	2245(9)	160(6)

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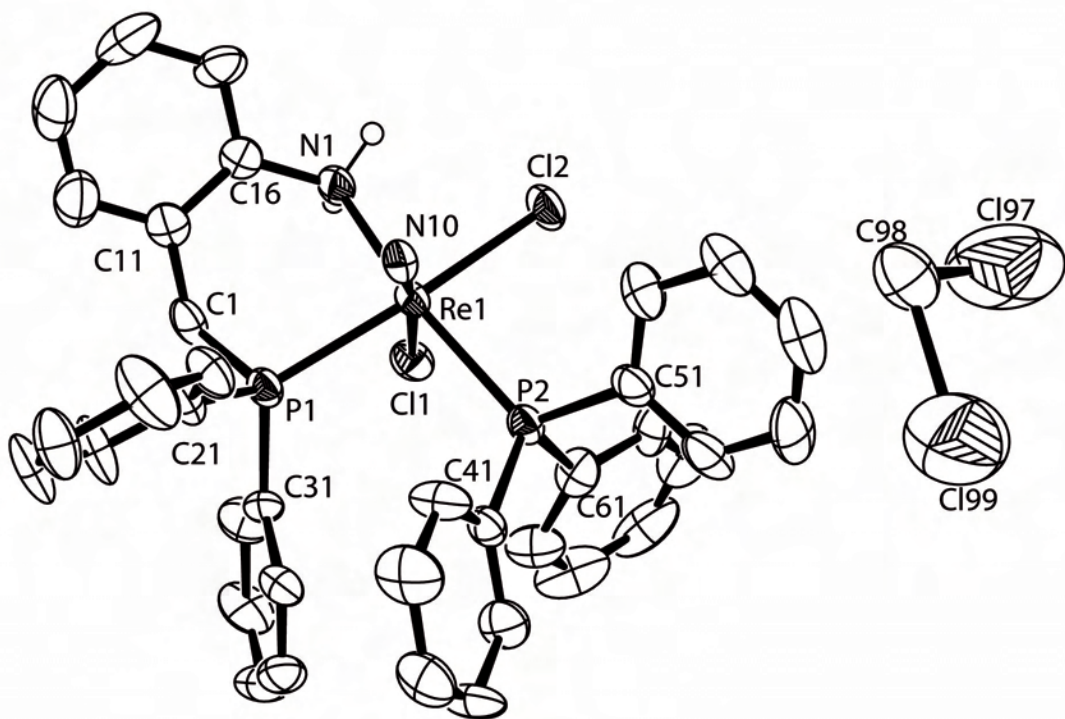


Abbildung 6.9: Ellipsoiddarstellung von  $[\text{ReNCl}_2(\text{PPh}_3)(\text{H}_2\text{L}^1)] \cdot 0.5 \text{CH}_2\text{Cl}_2$ . Die Schwingungsellipsoide repräsentieren 50% der Aufenthaltswahrscheinlichkeit. [121]

## 6.8 [ReNCl(H<sub>2</sub>L<sup>1</sup>)<sub>2</sub>]Cl

Tabelle 6.15: Kristallographische Daten und Parameter der Strukturrechnung von [ReNCl(H<sub>2</sub>L<sup>1</sup>)<sub>2</sub>]Cl

Summenformel	C <sub>38</sub> H <sub>36</sub> N <sub>3</sub> Cl <sub>2</sub> P <sub>2</sub> Re	
M (g/mol)	853.74	
Messtemperatur	200(2) K	
Wellenlänge	0.71073 Å	
Kristallsystem, Raumgruppe	monoklin, P 2 <sub>1</sub> /n	
Elementarzelle	a = 11.006(2) Å	α = 90°
	b = 27.586(2) Å	β = 96.10(1)°
	c = 12.199(2) Å	γ = 90°
Volumen	3676.9(9) Å <sup>3</sup>	
Z	4	
Berechnete Dichte	1.542 g/cm <sup>3</sup>	
Linearer Absorptionskoeffizient	3.568 mm <sup>-1</sup>	
F(000)	1696	
Kristallgröße	0.24 x 0.16 x 0.08 mm <sup>3</sup>	
Theta-Bereich	1.84 - 29.29°	
Indizes	-15 ≤ h ≤ 14, -37 ≤ k ≤ 37, -15 ≤ l ≤ 16	
Zahl der gemessenen Reflexe	28541	
Zahl der unabhängigen Reflexe	9904 [R(int) = 0.1458]	
Absorptionskorrektur	Integration	
Zahl der verfeinerten Parameter	423	
Goof	0.823	
R <sub>1</sub> / wR <sub>2</sub> [I > 2σ(I)]	R <sub>1</sub> = 0.0545, wR <sub>2</sub> = 0.1077	
R <sub>1</sub> / wR <sub>2</sub> (alle Reflexe)	R <sub>1</sub> = 0.1589, wR <sub>2</sub> = 0.1455	
Restelektronendichte	1.122 und -1.363 e · Å <sup>-3</sup>	
Programm zur Strukturlösung	SHELXS 97 [119]	

Tabelle 6.16: Atomkoordinaten ( $\cdot 10^4$ ) und isotrope Temperaturparameter ( $\text{\AA}^2 \cdot 10^3$ ) von  $[\text{ReNCl}(\text{H}_2\text{L}^1)_2]\text{Cl}$

	x	y	z	E(eq)
Re(1)	2016(1)	9063(1)	1591(1)	50(1)
N(10)	1911(7)	9513(3)	2586(6)	67(2)
P(1)	4085(2)	8833(1)	2303(2)	49(1)
C(1)	5081(8)	9099(3)	1353(7)	55(2)
C(11)	4948(8)	9640(3)	1355(7)	53(2)
C(12)	5870(9)	9943(4)	1814(7)	65(3)
C(13)	5746(12)	10441(4)	1825(8)	73(3)
C(14)	4647(13)	10644(4)	1420(8)	82(4)
C(15)	3677(10)	10358(3)	978(8)	61(3)
C(16)	3853(9)	9853(3)	934(7)	53(2)
N(1)	2857(7)	9553(2)	451(6)	53(2)
C(21)	4505(8)	8196(3)	2391(7)	52(2)
C(22)	4675(11)	7965(4)	3411(9)	77(3)
C(23)	4958(13)	7476(4)	3465(11)	96(4)
C(24)	5139(13)	7218(4)	2523(11)	93(4)
C(25)	4966(11)	7444(4)	1540(10)	81(3)
C(26)	4664(9)	7930(4)	1434(8)	65(3)
C(31)	4765(8)	9057(3)	3642(7)	54(2)
C(32)	4075(9)	9262(4)	4410(8)	62(3)
C(33)	4599(12)	9417(4)	5398(8)	83(4)
C(34)	5844(13)	9388(5)	5664(9)	87(4)
C(35)	6551(11)	9170(5)	4937(10)	94(4)
C(36)	6020(10)	9005(5)	3918(8)	81(3)
P(2)	844(2)	8545(1)	2665(2)	65(1)
C(2)	-750(9)	8771(4)	2366(10)	78(3)

C(41)	-1205(9)	8669(4)	1182(11)	76(3)
C(42)	-2136(9)	8322(4)	926(13)	93(4)
C(43)	-2509(13)	8221(5)	-177(16)	111(6)
C(44)	-1981(12)	8436(5)	-1017(15)	106(5)
C(45)	-1057(10)	8779(4)	-763(11)	85(4)
C(46)	-657(9)	8895(4)	353(10)	66(3)
N(2)	280(6)	9244(3)	586(7)	58(2)
C(51)	688(9)	7900(4)	2457(9)	65(3)
C(52)	1310(11)	7647(4)	1728(10)	81(4)
C(53)	1137(13)	7151(4)	1525(11)	94(4)
C(54)	331(16)	6909(5)	2087(13)	106(5)
C(55)	-301(13)	7144(5)	2858(13)	103(5)
C(56)	-122(10)	7639(5)	3031(10)	87(4)
Cl(1)	2280(2)	8508(1)	-77(2)	67(1)
Cl(2)	914(3)	9857(1)	8403(2)	74(1)
C(61)	1370(20)	8510(9)	4170(20)	59(5)
C(62)	2113(19)	8171(8)	4646(18)	72(4)
C(63)	2510(20)	8188(9)	5744(17)	85(4)
C(64)	2120(20)	8549(9)	6401(19)	84(5)
C(65)	1370(20)	8924(11)	5955(19)	85(4)
C(66)	986(19)	8904(8)	4808(17)	72(4)
C(61')	1020(40)	8706(14)	4140(40)	59(5)
C(62')	1740(30)	8393(13)	4840(30)	72(4)
C(63')	1970(40)	8469(18)	5950(30)	85(4)
C(64')	860(30)	9230(13)	5710(20)	84(5)
C(65')	580(30)	9144(13)	4490(20)	85(4)
C(66')	1560(30)	8859(14)	6360(30)	72(4)

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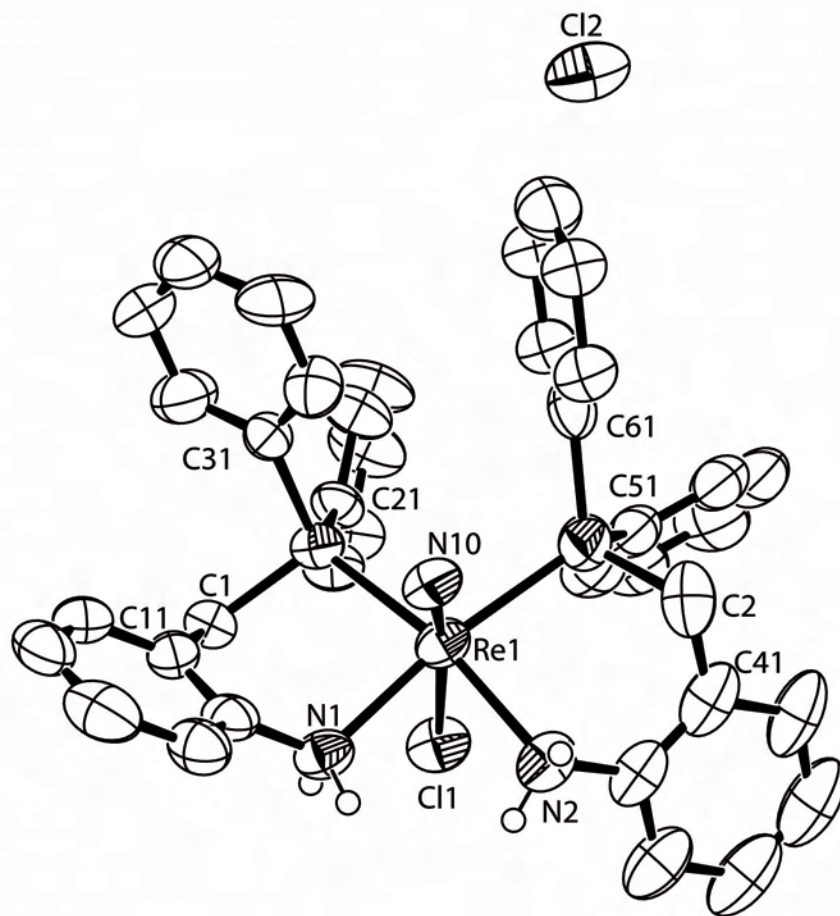


Abbildung 6.10: Ellipsoiddarstellung von  $[\text{ReNCl}(\text{H}_2\text{L}^1)_2]\text{Cl}$ . Die Schwingungsellipsoide repräsentieren 50% der Aufenthaltswahrscheinlichkeit. [121]



## 6.9 [Pd(HL<sup>1</sup>)<sub>2</sub>]Cl<sub>2</sub> · 0.25 MeOH · 0.5 CH<sub>2</sub>Cl<sub>2</sub> · 0.75 H<sub>2</sub>O

Tabelle 6.17: Kristallographische Daten und Parameter der Strukturrechnung von [Pd(HL<sup>1</sup>)<sub>2</sub>]Cl<sub>2</sub> · 0.25 MeOH · 0.5 CH<sub>2</sub>Cl<sub>2</sub> · 0.75 H<sub>2</sub>O

Summenformel	C <sub>38.75</sub> H <sub>38</sub> N <sub>2</sub> Cl <sub>3</sub> OP <sub>2</sub> Pd	
M (g/mol)	822.40	
Messtemperatur	200(2) K	
Wellenlänge	0.71073 Å	
Kristallsystem, Raumgruppe	triklin, P $\bar{1}$	
Elementarzelle	a = 14.262(1) Å	$\alpha = 91.47(1)^\circ$
	b = 15.460(1) Å	$\beta = 93.31(1)^\circ$
	c = 18.343(2) Å	$\gamma = 102.29(1)^\circ$
Volumen	3942.2(7) Å <sup>3</sup>	
Z	4	
Berechnete Dichte	1.386 g/cm <sup>3</sup>	
Linearer Absorptionskoeffizient	0.787 mm <sup>-1</sup>	
F(000)	1678	
Kristallgröße	0.35 x 0.16 x 0.05 mm <sup>3</sup>	
Theta-Bereich	2.39 - 27.00°	
Indizes	-18 ≤ h ≤ 18, -16 ≤ k ≤ 19, -23 ≤ l ≤ 22	
Zahl der gemessenen Reflexe	33805	
Zahl der unabhängigen Reflexe	17001 [R(int) = 0.0774]	
Zahl der verfeinerten Parameter	890	
Goof	0.897	
R <sub>1</sub> / wR <sub>2</sub> [I > 2σ(I)]	R <sub>1</sub> = 0.0624, wR <sub>2</sub> = 0.1494	
R <sub>1</sub> / wR <sub>2</sub> (alle Reflexe)	R <sub>1</sub> = 0.1129, wR <sub>2</sub> = 0.1689	
Restelektronendichte	2.217 und -2.044 e · Å <sup>-3</sup>	
Programm zur Strukturlösung	SHELXS 97 [119]	

Tabelle 6.18: Atomkoordinaten ( $\cdot 10^4$ ) und isotrope Temperaturparameter ( $\text{\AA}^2 \cdot 10^3$ ) von  $[\text{Pd}(\text{HL}^1)_2]\text{Cl}_2 \cdot 0.25 \text{ MeOH} \cdot 0.5 \text{ CH}_2\text{Cl}_2 \cdot 0.75 \text{ H}_2\text{O}$

	x	y	z	E(eq)
Pd(1)	347(1)	1042(1)	6658(1)	33(1)
P(11)	-490(1)	192(1)	7495(1)	34(1)
C(11)	-776(4)	-960(4)	7138(3)	39(1)
C(111)	126(4)	-1260(4)	7009(3)	39(1)
C(121)	434(5)	-1897(4)	7429(3)	46(2)
C(131)	1290(5)	-2141(5)	7320(4)	55(2)
C(141)	1882(5)	-1727(5)	6812(4)	59(2)
C(151)	1609(5)	-1076(5)	6405(4)	52(2)
C(161)	748(4)	-846(4)	6507(3)	36(1)
N(11)	467(4)	-148(3)	6091(3)	39(1)
C(211)	-1640(4)	394(4)	7752(3)	38(1)
C(221)	-2372(4)	318(4)	7204(3)	45(2)
C(231)	-3258(5)	456(5)	7375(4)	53(2)
C(241)	-3430(5)	686(4)	8067(4)	51(2)
C(251)	-2702(5)	764(4)	8613(4)	51(2)
C(261)	-1807(4)	608(4)	8469(3)	44(1)
C(311)	257(4)	141(4)	8313(3)	39(1)
C(321)	-42(5)	-468(4)	8836(3)	44(1)
C(331)	562(5)	-537(5)	9442(4)	54(2)
C(341)	1465(5)	-5(5)	9532(4)	55(2)
C(351)	1768(5)	588(5)	9005(4)	56(2)
C(361)	1182(4)	667(4)	8394(4)	46(2)
P(21)	128(1)	2350(1)	7128(1)	37(1)
C(21)	1042(5)	3236(4)	6766(3)	45(1)
C(411)	874(5)	3223(4)	5958(3)	44(1)

C(421)	545(6)	3901(4)	5605(4)	55(2)
C(431)	325(6)	3835(5)	4867(4)	60(2)
C(441)	414(5)	3096(5)	4459(4)	57(2)
C(451)	742(5)	2438(4)	4792(3)	48(2)
C(461)	968(4)	2480(4)	5539(3)	41(1)
N(21)	1270(4)	1772(3)	5895(3)	41(1)
C(511)	222(5)	2590(4)	8101(3)	43(1)
C(521)	1119(5)	2776(5)	8465(4)	57(2)
C(531)	1206(6)	2899(6)	9218(4)	72(2)
C(541)	398(6)	2851(6)	9606(4)	65(2)
C(551)	-482(6)	2695(6)	9246(4)	65(2)
C(561)	-599(5)	2550(5)	8491(4)	49(2)
C(611)	-984(5)	2592(4)	6746(3)	43(1)
C(621)	-1495(5)	2076(4)	6170(4)	51(2)
C(631)	-2264(6)	2323(6)	5811(4)	66(2)
C(641)	-2565(6)	3077(6)	6040(4)	71(2)
C(651)	-2035(6)	3593(6)	6608(4)	67(2)
C(661)	-1267(5)	3360(5)	6962(4)	55(2)
Cl(1)	6642(1)	5261(1)	630(1)	45(1)
Cl(2)	1807(1)	2642(1)	1487(1)	54(1)
Pd(2)	4428(1)	3801(1)	1425(1)	33(1)
P(12)	5114(1)	4535(1)	2472(1)	38(1)
C(12)	5500(4)	5715(4)	2305(3)	44(1)
C(112)	4676(4)	6095(4)	2033(3)	42(1)
C(122)	4384(5)	6760(4)	2419(4)	49(2)
C(132)	3623(6)	7114(5)	2154(5)	66(2)
C(142)	3158(6)	6812(5)	1493(5)	69(2)
C(152)	3400(5)	6122(5)	1105(4)	59(2)

C(162)	4160(4)	5764(4)	1368(3)	41(1)
N(12)	4425(4)	5064(3)	969(3)	39(1)
C(212)	6187(5)	4280(4)	2910(3)	44(1)
C(222)	7025(5)	4446(5)	2528(4)	58(2)
C(232)	7872(6)	4271(6)	2827(5)	70(2)
C(242)	7895(7)	3938(7)	3519(6)	84(3)
C(252)	7075(9)	3764(7)	3908(5)	89(3)
C(262)	6211(6)	3940(6)	3601(4)	65(2)
C(312)	4242(5)	4507(4)	3162(3)	44(1)
C(322)	3305(5)	4042(5)	3022(4)	55(2)
C(332)	2642(6)	4025(6)	3542(4)	68(2)
C(342)	2926(6)	4481(6)	4219(4)	70(2)
C(352)	3827(6)	4958(6)	4340(4)	69(2)
C(362)	4501(6)	4984(5)	3822(4)	57(2)
P(22)	4636(1)	2454(1)	1763(1)	37(1)
C(22)	3744(5)	1609(4)	1234(3)	43(1)
C(412)	3921(4)	1666(4)	442(3)	41(1)
C(422)	4220(4)	997(4)	58(4)	46(2)
C(432)	4425(5)	1090(5)	-673(4)	52(2)
C(442)	4334(5)	1856(5)	-1022(4)	53(2)
C(452)	4051(4)	2524(4)	-645(3)	44(1)
C(462)	3842(4)	2440(4)	82(3)	37(1)
N(22)	3571(3)	3151(3)	486(2)	37(1)
C(512)	4518(5)	2116(4)	2689(3)	46(2)
C(522)	5289(6)	1949(5)	3124(4)	62(2)
C(532)	5130(9)	1663(7)	3830(5)	83(3)
C(542)	4256(8)	1581(6)	4099(5)	83(3)
C(552)	3507(7)	1745(6)	3684(4)	77(2)

C(562)	3637(6)	2017(5)	2972(4)	58(2)
C(612)	5766(4)	2270(4)	1458(3)	42(1)
C(622)	6325(5)	2885(5)	1049(4)	51(2)
C(632)	7143(5)	2711(6)	750(5)	66(2)
C(642)	7396(5)	1916(6)	855(4)	65(2)
C(652)	6846(5)	1278(5)	1267(4)	59(2)
C(662)	6026(5)	1456(4)	1557(4)	53(2)
Cl(3)	1674(1)	312(1)	4672(1)	46(1)
Cl(4)	7088(1)	7932(2)	2829(1)	69(1)
O(1)	6388(4)	449(4)	4960(4)	27(2)
O(2)	5016(5)	9175(6)	4116(4)	42(2)
O(3)	5849(6)	9590(6)	2659(5)	52(2)
C(98)	483(14)	4169(12)	1536(9)	94(1)
Cl(97)	1502(3)	5042(3)	1491(3)	94(1)
Cl(99)	459(3)	4336(3)	2561(3)	94(1)
C(99)	604(17)	4274(18)	1712(14)	126(2)
Cl(94)	772(5)	5210(6)	1096(4)	126(2)
Cl(96)	-629(5)	3754(6)	1202(4)	126(2)
O(88)	5726(8)	7577(9)	4063(6)	72(3)
C(89)	6237(11)	7107(10)	4535(8)	59(4)

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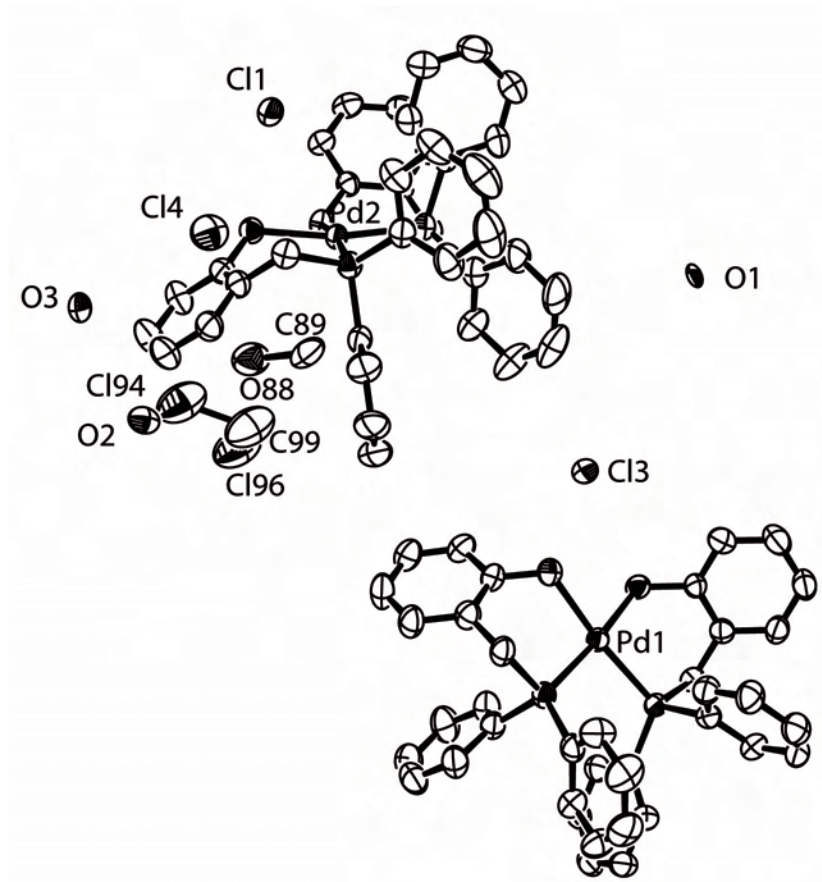


Abbildung 6.11: Ellipsoiddarstellung von  $[\text{Pd}(\text{HL}^1)_2]\text{Cl}_2 \cdot 0.25 \text{ MeOH} \cdot 0.5 \text{ CH}_2\text{Cl}_2 \cdot 0.75 \text{ H}_2\text{O}$ . Die Schwingungsellipsoide repräsentieren 50% der Aufenthaltswahrscheinlichkeit. [121]

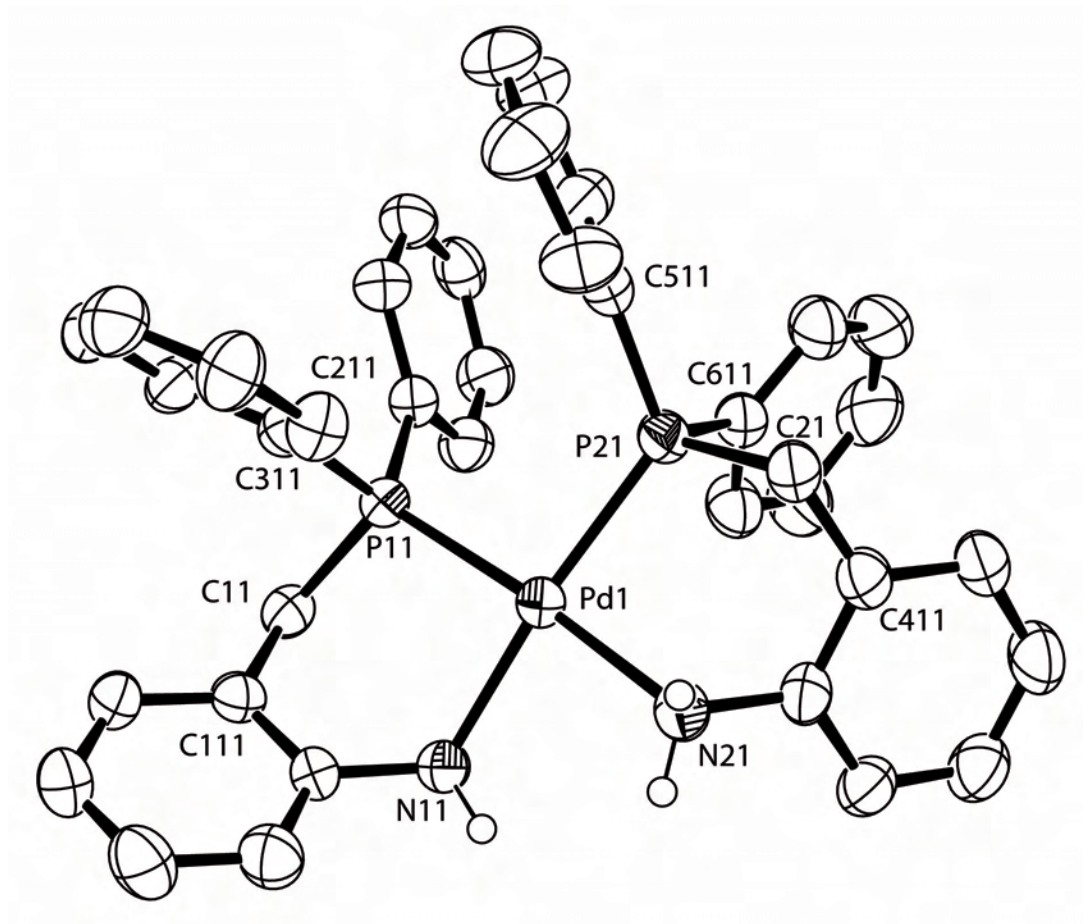


Abbildung 6.12: Ellipsoiddarstellung von  $[Pd(HL^1)_2]^{2+}$ . Die Schwingungsellipsoide repräsentieren 50% der Aufenthaltswahrscheinlichkeit. [121]





## 6.10 [RuCl<sub>2</sub>(CH<sub>3</sub>CN)(H<sub>2</sub>L<sup>1</sup>)(PPh<sub>3</sub>)] · CHCl<sub>3</sub>

Tabelle 6.19: Kristallographische Daten und Parameter der Strukturrechnung von [RuCl<sub>2</sub>(CH<sub>3</sub>CN)(H<sub>2</sub>L<sup>1</sup>)(PPh<sub>3</sub>)] · CHCl<sub>3</sub>

Summenformel	C <sub>40</sub> H <sub>37</sub> N <sub>2</sub> Cl <sub>5</sub> P <sub>1</sub> Ru	
M (g/mol)	885.98	
Messtemperatur	200(2) K	
Wellenlänge	0.71073 Å	
Kristallsystem, Raumgruppe	monoklin, P2 <sub>1</sub> /n	
Elementarzelle	a = 10.393(1) Å	α = 90°
	b = 22.807(1) Å	β = 93.72(1)°
	c = 17.106(1) Å	γ = 90°
Volumen	4046.1(6) Å <sup>3</sup>	
Z	4	
Berechnete Dichte	1.454 g/cm <sup>3</sup>	
Linearer Absorptionskoeffizient	0.828 mm <sup>-1</sup>	
F(000)	1800	
Kristallgröße	0.13 x 0.09 x 0.02 mm <sup>3</sup>	
Theta-Bereich	2.65 - 27.73°	
Indizes	-12 ≤ h ≤ 12, -27 ≤ k ≤ 26, -20 ≤ l ≤ 14	
Zahl der gemessenen Reflexe	19078	
Zahl der unabhängigen Reflexe	7017 [R(int) = 0.1409]	
Zahl der verfeinerten Parameter	453	
Goof	0.864	
R <sub>1</sub> / wR <sub>2</sub> [I > 2σ(I)]	R <sub>1</sub> = 0.0683, wR <sub>2</sub> = 0.0908	
R <sub>1</sub> / wR <sub>2</sub> (alle Reflexe)	R <sub>1</sub> = 0.1584, wR <sub>2</sub> = 0.1116	
Restelektronendichte	0.585 und -0.600 e · Å <sup>-3</sup>	
Programm zur Strukturlösung	SHELXS 97 [119]	

Tabelle 6.20: Atomkoordinaten ( $\cdot 10^4$ ) und isotrope Temperaturparameter ( $\text{\AA}^2 \cdot 10^3$ ) von  $[\text{RuCl}_2(\text{CH}_3\text{CN})(\text{H}_2\text{L}^1)(\text{PPh}_3)] \cdot \text{CHCl}_3$

	x	y	z	E(eq)
Ru(1)	9745(1)	4703(1)	8362(1)	24(1)
Cl(1)	9852(2)	3955(1)	9414(1)	35(1)
Cl(2)	8068(1)	5245(1)	8953(1)	31(1)
N(10)	11325(5)	4309(3)	8007(4)	31(2)
C(9)	12279(7)	4113(4)	7867(5)	37(2)
C(8)	13498(7)	3852(5)	7662(7)	70(3)
P(1)	9944(2)	5489(1)	7551(1)	28(1)
C(1)	10865(6)	6057(3)	8113(5)	33(2)
C(11)	12159(6)	5830(4)	8404(5)	35(2)
C(12)	13339(7)	6034(4)	8128(5)	44(2)
C(13)	14489(6)	5783(5)	8398(7)	55(3)
C(14)	14530(6)	5330(6)	8906(5)	54(3)
C(15)	13402(6)	5122(4)	9195(5)	42(2)
C(16)	12241(6)	5378(4)	8938(4)	30(2)
N(1)	11044(4)	5149(3)	9199(4)	30(2)
C(21)	10845(6)	5409(3)	6683(4)	30(2)
C(22)	10900(6)	4866(3)	6327(5)	30(2)
C(23)	11443(6)	4789(4)	5613(5)	41(2)
C(24)	11955(6)	5255(5)	5246(5)	41(2)
C(25)	11957(7)	5806(5)	5593(5)	48(3)
C(26)	11402(7)	5879(4)	6312(5)	49(2)
C(31)	8594(6)	5926(3)	7137(5)	30(2)
C(32)	8246(6)	5920(4)	6343(6)	45(2)
C(33)	7226(8)	6248(5)	6010(6)	58(3)
C(34)	6560(8)	6610(5)	6485(7)	59(3)

C(35)	6876(7)	6630(4)	7274(6)	49(2)
C(36)	7879(6)	6296(4)	7611(6)	39(2)
P(2)	8354(2)	4063(1)	7662(1)	28(1)
C(41)	9273(6)	3510(3)	7159(5)	32(2)
C(42)	9499(7)	3553(4)	6357(5)	40(2)
C(43)	10329(8)	3161(5)	6016(6)	58(3)
C(44)	10961(9)	2745(5)	6462(8)	64(3)
C(45)	10762(8)	2694(4)	7248(7)	57(3)
C(46)	9935(6)	3089(4)	7587(6)	42(2)
C(51)	7083(6)	4287(4)	6938(5)	32(2)
C(52)	6495(6)	4839(4)	7034(5)	40(2)
C(53)	5441(7)	5002(4)	6549(6)	52(3)
C(54)	4964(7)	4639(5)	5959(6)	57(3)
C(55)	5522(7)	4097(5)	5860(6)	56(3)
C(56)	6564(7)	3926(4)	6351(5)	39(2)
C(61)	7317(6)	3600(3)	8247(5)	31(2)
C(62)	6908(6)	3058(4)	7977(6)	45(2)
C(63)	6066(8)	2720(4)	8413(6)	52(3)
C(64)	5626(8)	2944(5)	9095(7)	60(3)
C(65)	5994(8)	3490(4)	9355(6)	53(3)
C(66)	6835(7)	3821(4)	8931(6)	45(2)
C(6)	3308(10)	7881(5)	4915(8)	91(4)
Cl(3)	3048(4)	7377(2)	5659(3)	153(2)
Cl(4)	1880(4)	8051(3)	4410(3)	200(3)
Cl(5)	4371(5)	7603(2)	4254(4)	174(2)

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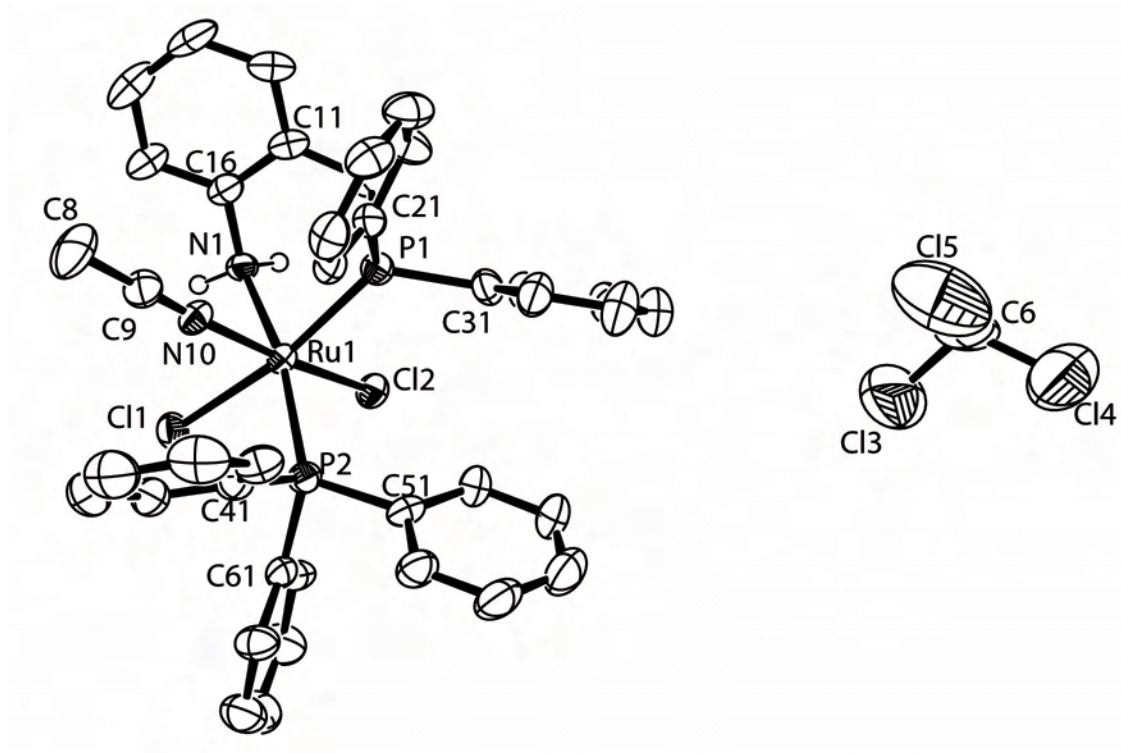


Abbildung 6.13: Ellipsoiddarstellung von  $[\text{RuCl}_2(\text{CH}_3\text{CN})(\text{H}_2\text{L}^1)(\text{PPh}_3)] \cdot \text{CHCl}_3$ . Die Schwingungsellipsoide repräsentieren 50% der Aufenthaltswahrscheinlichkeit. [121]

## 6.11 [RuCl<sub>2</sub>(PPh<sub>3</sub>)(H<sub>2</sub>L<sup>1</sup>)]<sub>2</sub> · 0.5 CH<sub>2</sub>Cl<sub>2</sub>

Tabelle 6.21: Kristallographische Daten und Parameter der Strukturrechnung von [RuCl<sub>2</sub>(PPh<sub>3</sub>)(H<sub>2</sub>L<sup>1</sup>)]<sub>2</sub> · 0.5 CH<sub>2</sub>Cl<sub>2</sub>

Summenformel	C <sub>74.5</sub> H <sub>67</sub> N <sub>2</sub> Cl <sub>5</sub> P <sub>4</sub> Ru <sub>2</sub>	
M (g/mol)	1493.57	
Messtemperatur	200(2) K	
Wellenlänge	0.71073 Å	
Kristallsystem, Raumgruppe	triklin, P $\bar{1}$	
Elementarzelle	a = 13.285(2) Å	$\alpha = 103.83(1)^\circ$
	b = 14.175(2) Å	$\beta = 91.23(1)^\circ$
	c = 18.120(2) Å	$\gamma = 95.86(1)^\circ$
Volumen	3292.3(8) Å <sup>3</sup>	
Z	2	
Berechnete Dichte	1.507 g/cm <sup>3</sup>	
Linearer Absorptionskoeffizient	0.805 mm <sup>-1</sup>	
F(000)	1522	
Kristallgröße	0.20 x 0.09 x 0.02 mm <sup>3</sup>	
Theta-Bereich	2.84 - 29.17°	
Indizes	-16 ≤ h ≤ 16, -15 ≤ k ≤ 17, -22 ≤ l ≤ 21	
Zahl der gemessenen Reflexe	25383	
Zahl der unabhängigen Reflexe	12767 [R(int) = 0.1750]	
Zahl der verfeinerten Parameter	802	
Goof	0.863	
R <sub>1</sub> / wR <sub>2</sub> [I > 2σ(I)]	R <sub>1</sub> = 0.0790, wR <sub>2</sub> = 0.0915	
R <sub>1</sub> / wR <sub>2</sub> (alle Reflexe)	R <sub>1</sub> = 0.2105, wR <sub>2</sub> = 0.1254	
Restelektronendichte	0.515 und -0.477 e · Å <sup>-3</sup>	
Programm zur Strukturlösung	SHELXS 97 [119]	

Tabelle 6.22: Atomkoordinaten ( $\cdot 10^4$ ) und isotrope Temperaturparameter ( $\text{\AA}^2 \cdot 10^3$ ) von  $[\text{RuCl}_2(\text{PPh}_3)(\text{H}_2\text{L}^1)]_2 \cdot 0.5 \text{CH}_2\text{Cl}_2$

	x	y	z	E(eq)
Ru(1)	9646(1)	3805(1)	325(1)	26(1)
P(1)	10378(2)	3322(2)	1287(2)	31(1)
C(1)	11743(7)	3358(7)	1109(5)	36(3)
C(11)	11954(8)	2610(8)	419(6)	37(3)
C(12)	12485(8)	1858(8)	479(6)	41(3)
C(13)	12693(9)	1160(9)	-156(7)	56(3)
C(14)	12333(9)	1210(9)	-867(7)	56(3)
C(15)	11770(8)	1989(8)	-935(6)	44(3)
C(16)	11580(9)	2676(8)	-270(6)	44(3)
N(1)	10998(6)	3464(6)	-319(4)	34(2)
C(21)	10210(8)	2112(7)	1482(5)	33(2)
C(22)	9822(8)	1292(7)	897(6)	35(3)
C(23)	9822(9)	358(8)	1006(6)	49(3)
C(24)	10170(9)	208(8)	1684(7)	45(3)
C(25)	10565(9)	997(9)	2261(7)	48(3)
C(26)	10578(9)	1928(8)	2154(6)	48(3)
C(31)	10382(8)	4128(8)	2235(6)	38(3)
C(32)	9681(8)	3966(8)	2773(6)	40(3)
C(33)	9720(11)	4575(10)	3480(7)	59(4)
C(34)	10510(13)	5336(11)	3699(7)	71(5)
C(35)	11163(11)	5514(9)	3193(7)	56(4)
C(36)	11120(10)	4913(9)	2472(6)	55(3)
P(2)	8079(2)	4046(2)	821(2)	31(1)
C(41)	7934(7)	4852(7)	1769(6)	31(2)
C(42)	7078(8)	4753(7)	2175(6)	43(3)

C(43)	6934(9)	5406(9)	2851(6)	50(3)
C(44)	7657(10)	6176(9)	3143(6)	53(3)
C(45)	8531(8)	6300(7)	2750(6)	40(3)
C(46)	8668(8)	5640(7)	2075(6)	39(3)
C(51)	7222(8)	2944(8)	877(6)	39(3)
C(52)	7619(10)	2296(8)	1250(7)	52(3)
C(53)	7007(10)	1471(9)	1329(8)	55(3)
C(54)	6033(10)	1283(9)	1039(7)	62(4)
C(55)	5650(10)	1941(10)	650(7)	63(4)
C(56)	6255(8)	2751(8)	591(6)	44(3)
C(61)	7242(8)	4568(9)	219(7)	44(3)
C(62)	7076(9)	4040(10)	-545(6)	54(3)
C(63)	6400(11)	4423(17)	-972(9)	99(7)
C(64)	5953(12)	5240(17)	-724(13)	107(8)
C(65)	6143(11)	5746(12)	27(11)	82(5)
C(66)	6797(8)	5413(9)	507(8)	51(3)
Cl(1)	8911(2)	2296(2)	-490(1)	40(1)
Cl(2)	10596(2)	5415(2)	797(1)	33(1)
Ru(2)	5543(1)	8938(1)	5329(1)	27(1)
P(1B)	5362(2)	8568(2)	6471(2)	32(1)
C(1B)	3982(8)	8455(8)	6601(6)	47(3)
C(11B)	3476(8)	7559(8)	6042(6)	40(3)
C(12B)	3080(9)	6726(10)	6256(8)	58(4)
C(13B)	2724(10)	5877(10)	5721(9)	66(4)
C(14B)	2751(9)	5881(9)	4967(8)	59(4)
C(15B)	3138(8)	6699(8)	4745(7)	52(3)
C(16B)	3501(7)	7514(7)	5260(6)	34(2)
N(1B)	3959(6)	8360(6)	5034(5)	37(2)

C(21B)	5625(9)	7415(9)	6719(6)	46(3)
C(22B)	5694(9)	7374(10)	7471(6)	55(3)
C(23B)	5759(12)	6494(12)	7648(9)	79(5)
C(24B)	5796(11)	5662(12)	7084(11)	84(5)
C(25B)	5691(11)	5696(8)	6339(8)	67(4)
C(26B)	5612(9)	6576(9)	6165(7)	52(3)
C(31B)	5816(8)	9495(8)	7326(6)	42(3)
C(32B)	5241(9)	10219(8)	7696(6)	43(3)
C(33B)	5603(9)	10899(9)	8364(7)	55(3)
C(34B)	6526(10)	10864(9)	8689(7)	59(4)
C(35B)	7154(10)	10155(9)	8320(6)	55(3)
C(36B)	6792(8)	9486(8)	7653(6)	45(3)
P(2B)	7271(2)	9402(2)	5392(2)	31(1)
C(41B)	7926(8)	10378(7)	6146(5)	29(2)
C(42B)	7404(8)	11067(8)	6618(6)	44(3)
C(43B)	7907(9)	11828(9)	7198(7)	52(3)
C(44B)	8927(10)	11891(9)	7303(7)	55(4)
C(45B)	9456(9)	11217(9)	6852(7)	51(3)
C(46B)	8965(8)	10488(7)	6294(6)	40(3)
C(51B)	7687(8)	9812(8)	4546(6)	39(3)
C(52B)	7458(8)	9171(8)	3842(6)	39(3)
C(53B)	7750(9)	9403(10)	3166(7)	58(3)
C(54B)	8285(9)	10286(11)	3200(8)	62(4)
C(55B)	8501(9)	10950(11)	3895(7)	57(4)
C(56B)	8237(8)	10688(9)	4559(7)	46(3)
C(61B)	8085(8)	8411(7)	5349(6)	35(3)
C(62B)	7900(8)	7788(9)	5824(6)	45(3)
C(63B)	8492(9)	7016(8)	5822(6)	41(3)



C(64B)	9233(10)	6883(9)	5338(7)	54(3)
C(65B)	9475(8)	7515(8)	4873(7)	52(3)
C(66B)	8885(8)	8269(8)	4881(6)	45(3)
CI(3)	5865(2)	7403(2)	4536(2)	41(1)
CI(4)	5146(2)	9525(2)	4127(1)	32(1)
C(98)	5477(18)	7360(20)	2676(14)	64(8)
CI(99)	4230(5)	7084(5)	2816(4)	64(2)
CI(97)	5961(5)	7286(5)	1878(3)	63(2)

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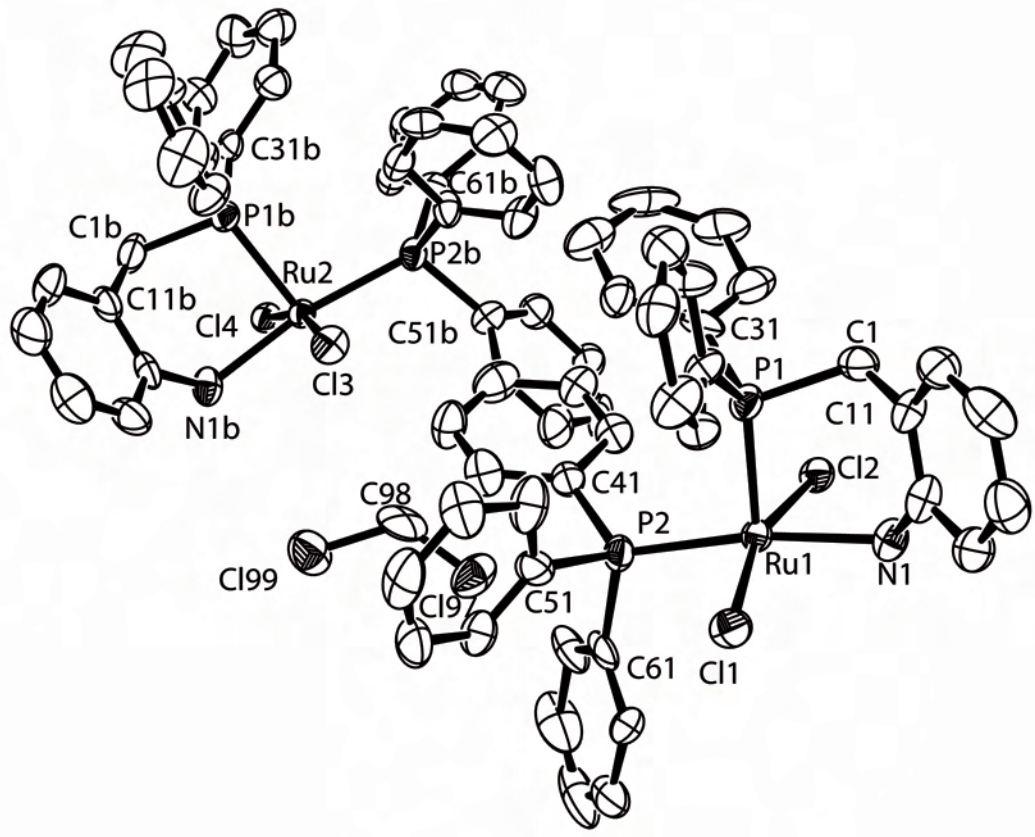


Abbildung 6.14: Ellipsoiddarstellung von der asymmetrischen Einheit von  $[\text{RuCl}_2(\text{PPh}_3)(\text{H}_2\text{L}^1)]_2 \cdot 0.5 \text{CH}_2\text{Cl}_2$ . Die Schwingungsellipsoide repräsentieren 50% der Aufenthaltswahrscheinlichkeit. [121]

## 6.12 [RuCl<sub>2</sub>(H<sub>2</sub>L<sup>1</sup>)<sub>2</sub>]

Tabelle 6.23: Kristallographische Daten und Parameter der Strukturrechnung von [RuCl<sub>2</sub>(H<sub>2</sub>L<sup>1</sup>)<sub>2</sub>]

Summenformel	C <sub>38</sub> H <sub>36</sub> N <sub>2</sub> Cl <sub>2</sub> P <sub>2</sub> Ru	
M (g/mol)	754.60	
Messtemperatur	200(2) K	
Wellenlänge	0.71073 Å	
Kristallsystem, Raumgruppe	monoklin, P2 <sub>1</sub> /c	
Elementarzelle	a = 20.698(2) Å	α = 90°
	b = 16.289(1) Å	β = 103.57(1)°
	c = 10.213(1) Å	γ = 90°
Volumen	3347.2(5) Å <sup>3</sup>	
Z	4	
Berechnete Dichte	1.497 g/cm <sup>3</sup>	
Linearer Absorptionskoeffizient	0.755 mm <sup>-1</sup>	
F(000)	1544	
Kristallgröße	0.18 x 0.10 x 0.02 mm <sup>3</sup>	
Theta-Bereich	2.38 - 28.71°	
Indizes	-26 ≤ h ≤ 26, -20 ≤ k ≤ 20, -13 ≤ l ≤ 8	
Zahl der gemessenen Reflexe	18439	
Zahl der unabhängigen Reflexe	7221 [R(int) = 0.1113]	
Zahl der verfeinerten Parameter	407	
Goof	0.892	
R <sub>1</sub> / wR <sub>2</sub> [I > 2σ(I)]	R <sub>1</sub> = 0.0536, wR <sub>2</sub> = 0.1023	
R <sub>1</sub> / wR <sub>2</sub> (alle Reflexe)	R <sub>1</sub> = 0.1270, wR <sub>2</sub> = 0.1416	
Restelektronendichte	0.578 und -0.760 e · Å <sup>-3</sup>	
Programm zur Strukturlösung	SHELXS 97 [119]	

Tabelle 6.24: Atomkoordinaten ( $\cdot 10^4$ ) und isotrope Temperaturparameter ( $\text{\AA}^2 \cdot 10^3$ ) von  $[\text{RuCl}_2(\text{H}_2\text{L}^1)_2]$

	x	y	z	E(eq)
Ru(1)	2516(1)	-1017(1)	7143(1)	26(1)
Cl(1)	2571(1)	-1893(1)	9084(2)	36(1)
Cl(2)	2422(1)	-542(1)	4885(2)	39(1)
P(1)	1654(1)	-196(1)	7300(2)	29(1)
C(1)	885(3)	-668(4)	6249(8)	40(2)
C(11)	789(3)	-1509(4)	6749(7)	38(2)
C(12)	291(3)	-1698(5)	7394(9)	52(2)
C(13)	220(4)	-2465(6)	7886(9)	61(2)
C(14)	653(4)	-3079(6)	7717(9)	58(2)
C(15)	1165(3)	-2914(5)	7111(8)	45(2)
C(16)	1233(3)	-2129(4)	6625(7)	35(2)
N(1)	1779(2)	-1932(3)	6039(6)	34(1)
C(31)	1384(3)	24(4)	8852(7)	32(1)
C(32)	814(3)	501(4)	8801(8)	40(2)
C(33)	616(3)	691(5)	9953(8)	47(2)
C(34)	999(3)	420(5)	11203(8)	44(2)
C(35)	1553(3)	-43(5)	11261(7)	41(2)
C(36)	1746(3)	-253(4)	10097(7)	35(2)
C(41)	1624(3)	848(4)	6603(7)	35(2)
C(42)	1386(4)	1015(5)	5253(7)	52(2)
C(43)	1382(4)	1816(6)	4787(10)	72(3)
C(44)	1635(4)	2443(5)	5646(10)	60(2)
C(45)	1882(4)	2280(5)	6980(10)	59(2)
C(46)	1874(4)	1489(5)	7453(8)	44(2)
P(2)	3362(1)	-230(1)	8327(2)	29(1)

C(2)	4124(3)	-877(4)	8668(7)	37(2)
C(21)	4303(3)	-1101(4)	7383(7)	34(1)
C(22)	4883(3)	-808(4)	7059(8)	43(2)
C(23)	5016(3)	-978(5)	5843(8)	51(2)
C(24)	4585(3)	-1440(5)	4890(8)	48(2)
C(25)	4014(3)	-1744(4)	5208(7)	39(2)
C(26)	3876(3)	-1588(4)	6429(7)	32(1)
N(2)	3275(2)	-1890(3)	6729(6)	34(1)
C(51)	3667(3)	712(4)	7685(7)	34(1)
C(52)	4236(3)	1104(5)	8432(8)	46(2)
C(53)	4470(4)	1812(5)	7961(10)	55(2)
C(54)	4151(4)	2127(5)	6740(10)	55(2)
C(55)	3594(4)	1756(5)	5971(8)	48(2)
C(56)	3351(3)	1045(5)	6453(7)	39(1)
C(61)	3358(3)	91(4)	10041(7)	34(1)
C(62)	3205(3)	888(5)	10330(7)	41(2)
C(63)	3147(4)	1119(6)	11607(8)	52(2)
C(64)	3238(4)	551(6)	12607(8)	55(2)
C(65)	3406(3)	-239(6)	12362(7)	50(2)
C(66)	3471(3)	-472(5)	11096(7)	42(2)

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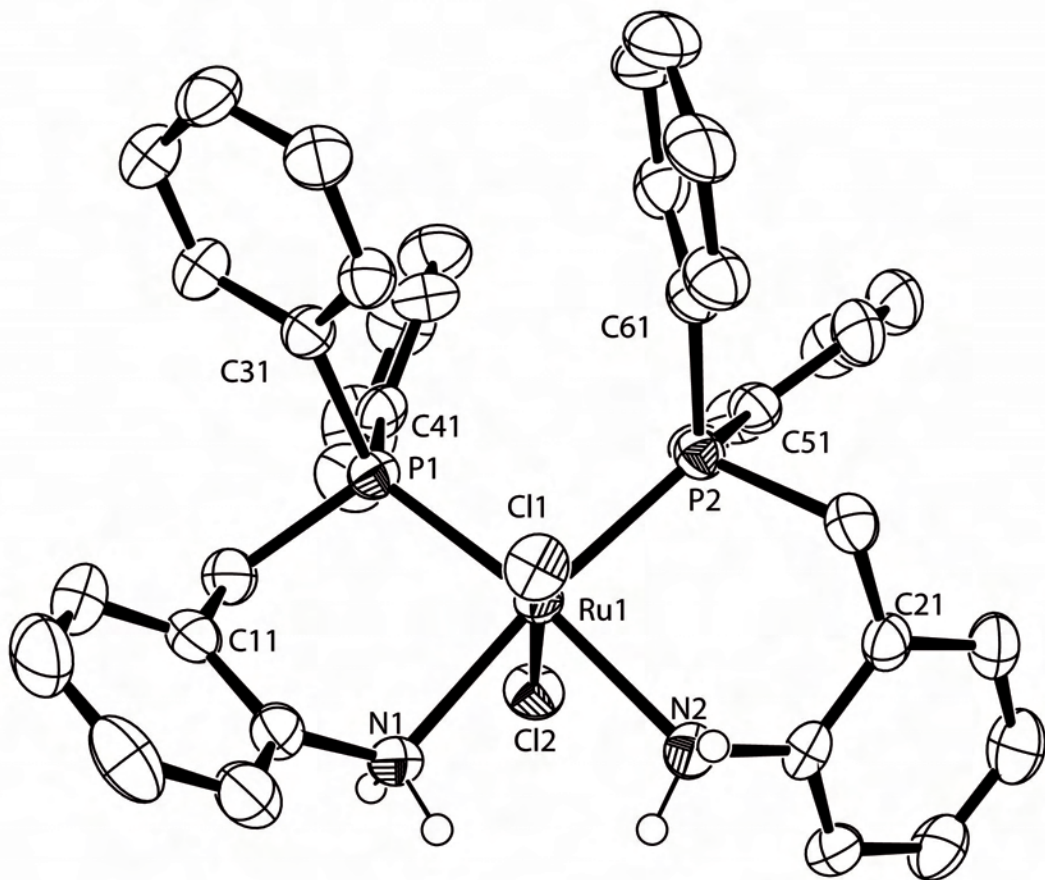


Abbildung 6.15: Ellipsoiddarstellung von  $[\text{RuCl}_2(\text{H}_2\text{L}^1)_2]$ . Die Schwingungsellipsoide repräsentieren 50% der Aufenthaltswahrscheinlichkeit. [121]

## 6.13 [RuCl<sub>2</sub>(DMSO)<sub>2</sub>(H<sub>2</sub>L<sup>1</sup>)]

Tabelle 6.25: Kristallographische Daten und Parameter der Strukturrechnung von [RuCl<sub>2</sub>(DMSO)<sub>2</sub>(H<sub>2</sub>L<sup>1</sup>)]

Summenformel	C <sub>23</sub> H <sub>30</sub> NCl <sub>2</sub> PO <sub>2</sub> S <sub>2</sub> Ru	
M (g/mol)	619.58	
Messtemperatur	200(2) K	
Wellenlänge	0.71073 Å	
Kristallsystem, Raumgruppe	triklin, P $\bar{1}$	
Elementarzelle	a = 9.205(2) Å	$\alpha = 61.31(2)^\circ$
	b = 13.615(3) Å	$\beta = 84.53(2)^\circ$
	c = 14.031(3) Å	$\gamma = 87.41(2)^\circ$
Volumen	1535.5(6) Å <sup>3</sup>	
Z	2	
Berechnete Dichte	1.340 g/cm <sup>3</sup>	
Linearer Absorptionskoeffizient	0.891 mm <sup>-1</sup>	
F(000)	632	
Kristallgröße	0.50 x 0.10 x 0.04 mm <sup>3</sup>	
Theta-Bereich	2.22 - 29.48°	
Indizes	-12 ≤ h ≤ 12, -18 ≤ k ≤ 18, -19 ≤ l ≤ 19	
Zahl der gemessenen Reflexe	13064	
Zahl der unabhängigen Reflexe	8179 [R(int) = 0.0871]	
Zahl der verfeinerten Parameter	290	
Goof	0.845	
R <sub>1</sub> / wR <sub>2</sub> [I > 2σ(I)]	R <sub>1</sub> = 0.0544, wR <sub>2</sub> = 0.1306	
R <sub>1</sub> / wR <sub>2</sub> (alle Reflexe)	R <sub>1</sub> = 0.0900, wR <sub>2</sub> = 0.1426	
Restelektronendichte	0.856 und -1.228 e · Å <sup>-3</sup>	
Programm zur Strukturlösung	SHELXS 97 [119]	

Tabelle 6.26: Atomkoordinaten ( $\cdot 10^4$ ) und isotrope Temperaturparameter ( $\text{\AA}^2 \cdot 10^3$ ) von  $[\text{RuCl}_2(\text{DMSO})_2(\text{H}_2\text{L}^1)]$

	x	y	z	E(eq)
Ru(1)	771(1)	2376(1)	3694(1)	26(1)
P(1)	3251(1)	2683(1)	3365(1)	29(1)
O(4)	964(4)	4765(3)	1371(3)	39(1)
S(4)	122(1)	3714(1)	2000(1)	32(1)
C(41)	-1724(6)	4156(5)	2003(5)	49(1)
C(42)	30(7)	3110(5)	1127(4)	49(1)
O(5)	-274(5)	4674(3)	3702(3)	45(1)
S(5)	207(1)	3519(1)	4436(1)	33(1)
C(51)	-1208(7)	2928(5)	5514(5)	47(1)
C(52)	1521(6)	3672(4)	5228(4)	40(1)
Cl(1)	-1758(1)	1673(1)	4137(1)	37(1)
Cl(2)	1361(1)	1002(1)	3071(1)	34(1)
C(1)	4109(5)	1474(4)	4476(4)	34(1)
C(11)	3563(5)	1259(4)	5595(4)	33(1)
C(12)	4473(7)	1343(5)	6290(5)	48(1)
C(13)	3946(8)	1148(5)	7330(5)	57(2)
C(14)	2521(8)	841(5)	7690(5)	51(2)
C(15)	1587(7)	733(4)	7028(4)	40(1)
C(16)	2095(6)	969(4)	5977(4)	32(1)
N(1)	1140(4)	934(3)	5247(3)	29(1)
C(21)	4026(5)	3933(4)	3313(4)	33(1)
C(22)	5262(6)	3883(4)	3836(5)	41(1)
C(23)	5757(6)	4824(5)	3819(5)	48(1)
C(24)	5057(7)	5836(5)	3289(5)	49(1)
C(25)	3868(7)	5907(4)	2747(5)	45(1)



C(26)	3341(6)	4967(4)	2752(4)	39(1)
C(31)	4243(5)	2710(4)	2152(4)	35(1)
C(32)	5321(7)	1929(5)	2230(5)	53(2)
C(33)	6120(8)	2019(5)	1312(5)	63(2)
C(34)	5806(9)	2875(6)	283(5)	67(2)
C(35)	4773(7)	3654(5)	193(5)	53(2)
C(36)	3984(7)	3577(5)	1123(4)	45(1)

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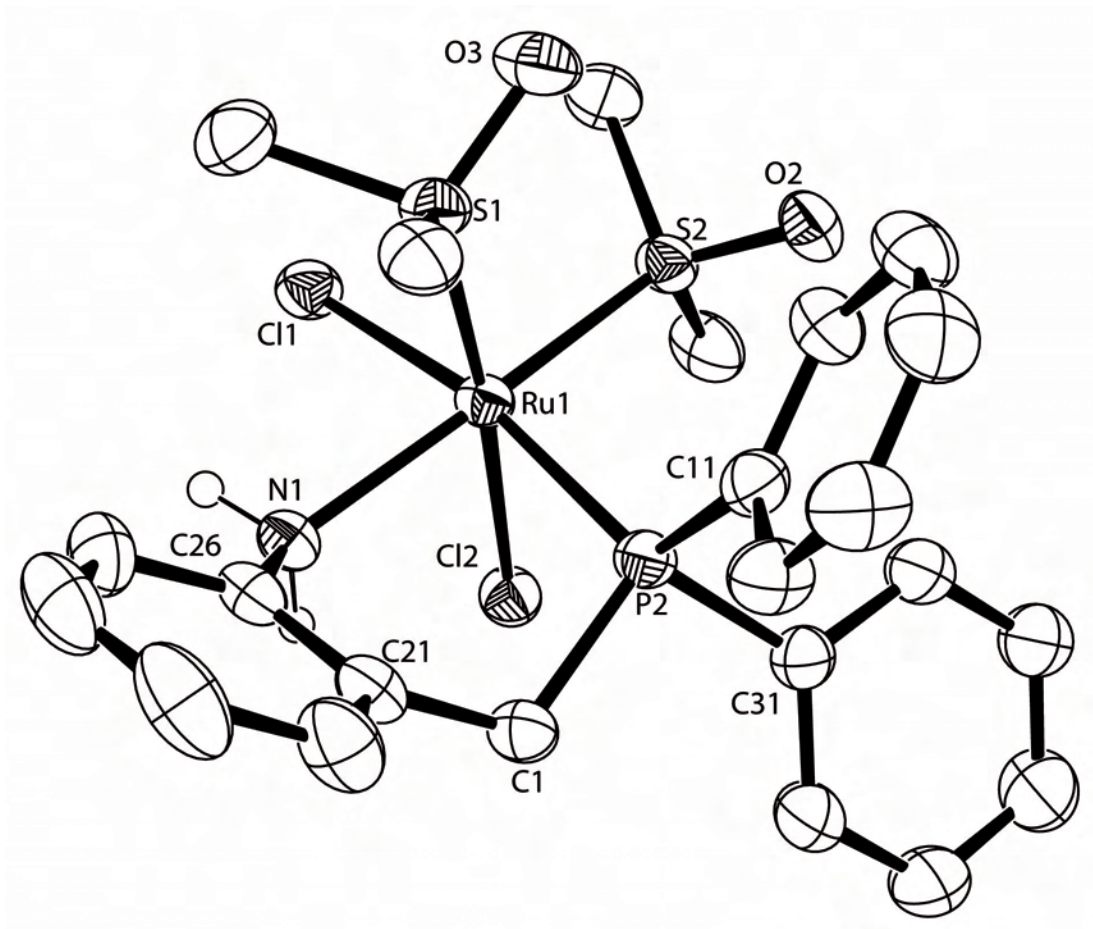


Abbildung 6.16: Ellipsoiddarstellung von  $[\text{RuCl}_2(\text{DMSO})_2(\text{H}_2\text{L}^1)]$ . Die Schwingungsellipsoide repräsentieren 50% der Aufenthaltswahrscheinlichkeit. [121]

## 6.14 [ReCl<sub>3</sub>(H<sub>2</sub>L<sup>2</sup>)]

Tabelle 6.27: Kristallographische Daten und Parameter der Strukturrechnung von [ReCl<sub>3</sub>(H<sub>2</sub>L<sup>2</sup>)]

Summenformel	C <sub>20</sub> H <sub>19</sub> N <sub>2</sub> PCl <sub>3</sub> Re	
M (g/mol)	610.89	
Messtemperatur	200(2) K	
Wellenlänge	0.71073 Å	
Kristallsystem, Raumgruppe	triklin, P $\bar{1}$	
Elementarzelle	a = 14.941(1) Å	$\alpha = 103.90(1)^\circ$
	b = 15.669(1) Å	$\beta = 103.94(1)^\circ$
	c = 19.179(1) Å	$\gamma = 90.69(1)^\circ$
Volumen	4218.5(4) Å <sup>3</sup>	
Z	8	
Berechnete Dichte	1.924 g/cm <sup>3</sup>	
Linearer Absorptionskoeffizient	6.225 mm <sup>-1</sup>	
F(000)	2352	
Kristallgröße	0.18 x 0.14 x 0.08 mm <sup>3</sup>	
Theta-Bereich	2.18 - 29.61°	
Indizes	$-19 \leq h \leq 20, -21 \leq k \leq 21, -26 \leq l \leq 26$	
Zahl der gemessenen Reflexe	44497	
Zahl der unabhängigen Reflexe	22508 [R(int) = 0.0716]	
Absorptionskorrektur	Integration	
Zahl der verfeinerten Parameter	974	
Goof	0.926	
R <sub>1</sub> / wR <sub>2</sub> [I > 2σ(I)]	R <sub>1</sub> = 0.0476, wR <sub>2</sub> = 0.1067	
R <sub>1</sub> / wR <sub>2</sub> (alle Reflexe)	R <sub>1</sub> = 0.0848, wR <sub>2</sub> = 0.1296	
Restelektronendichte	1.550 und -2.304 e · Å <sup>-3</sup>	
Programm zur Strukturlösung	SHELXS 97 [119]	

Tabelle 6.28: Atomkoordinaten ( $\cdot 10^4$ ) und isotrope Temperaturparameter ( $\text{\AA}^2 \cdot 10^3$ ) von  $[\text{ReCl}_3(\text{H}_2\text{L}^2)]$

	x	y	z	E(eq)
Re(1)	798(1)	3501(1)	483(1)	34(1)
P(11)	1916(2)	2965(1)	-175(1)	37(1)
C(11)	2423(7)	3878(6)	-423(5)	48(2)
C(111)	2783(7)	4630(6)	254(5)	46(2)
C(121)	3717(7)	4871(7)	506(6)	56(2)
C(131)	4055(8)	5545(7)	1158(7)	62(3)
C(141)	3479(7)	5952(7)	1544(6)	58(3)
C(151)	2551(7)	5727(6)	1308(6)	51(2)
C(161)	2194(6)	5079(6)	663(5)	43(2)
N(11)	1207(5)	4817(4)	434(4)	42(2)
C(21)	2884(7)	2585(6)	425(5)	46(2)
C(211)	3241(6)	3170(6)	1196(4)	39(2)
C(221)	4187(7)	3327(6)	1536(5)	50(2)
C(231)	4509(7)	3860(7)	2231(5)	51(2)
C(241)	3898(6)	4266(7)	2627(5)	48(2)
C(251)	2958(6)	4132(6)	2310(5)	45(2)
C(261)	2637(6)	3595(5)	1597(4)	37(2)
N(21)	1704(5)	3545(5)	1239(4)	41(2)
C(311)	1569(6)	2068(6)	-1006(5)	45(2)
C(321)	1399(10)	2246(9)	-1704(6)	75(4)
C(331)	1029(14)	1539(11)	-2323(7)	109(6)
C(341)	860(13)	733(10)	-2247(8)	98(5)
C(351)	1008(11)	566(8)	-1566(8)	82(4)
C(361)	1343(9)	1244(7)	-941(6)	67(3)
Cl(11)	-482(2)	4161(2)	913(1)	51(1)

Cl(21)	64(2)	2101(1)	373(1)	46(1)
Cl(31)	-56(2)	3444(1)	-781(1)	44(1)
Re(2)	6607(1)	4228(1)	4504(1)	32(1)
P(12)	7204(2)	3263(1)	5262(1)	35(1)
C(12)	6241(6)	2867(6)	5578(5)	46(2)
C(112)	5488(6)	2432(6)	4924(5)	39(2)
C(122)	5275(7)	1517(6)	4741(6)	49(2)
C(132)	4631(8)	1089(6)	4099(7)	59(3)
C(142)	4176(8)	1578(7)	3637(6)	59(3)
C(152)	4345(6)	2478(6)	3790(5)	46(2)
C(162)	5001(6)	2897(5)	4428(5)	40(2)
N(12)	5232(4)	3828(4)	4587(4)	36(1)
C(22)	7562(6)	2262(5)	4724(4)	39(2)
C(212)	7008(5)	1885(5)	3939(4)	35(2)
C(222)	6940(7)	984(5)	3637(5)	42(2)
C(232)	6524(7)	623(6)	2891(5)	51(2)
C(242)	6171(8)	1160(6)	2441(5)	57(3)
C(252)	6178(7)	2056(6)	2728(5)	50(2)
C(262)	6595(6)	2414(5)	3483(4)	35(2)
N(22)	6583(5)	3302(4)	3797(4)	35(1)
C(312)	8175(6)	3587(6)	6085(4)	42(2)
C(322)	8334(9)	3103(8)	6616(6)	67(3)
C(332)	9079(12)	3333(11)	7220(7)	93(5)
C(342)	9675(10)	4035(9)	7296(7)	86(4)
C(352)	9551(10)	4493(9)	6757(9)	90(5)
C(362)	8796(8)	4259(8)	6146(7)	75(4)
Cl(12)	5848(2)	5385(1)	4024(1)	43(1)
Cl(22)	8019(2)	4953(1)	4489(1)	46(1)

Cl(32)	6676(1)	5143(1)	5732(1)	42(1)
Re(3)	8418(1)	-624(1)	5383(1)	32(1)
P(13)	7979(1)	-2125(1)	4745(1)	34(1)
C(13)	8995(6)	-2643(5)	4513(5)	40(2)
C(113)	9754(6)	-2553(5)	5213(5)	38(2)
C(123)	10055(7)	-3291(6)	5458(6)	48(2)
C(133)	10705(7)	-3203(6)	6125(6)	53(2)
C(143)	11057(6)	-2368(6)	6563(5)	46(2)
C(153)	10783(6)	-1632(6)	6321(4)	39(2)
C(163)	10137(5)	-1719(5)	5651(4)	34(2)
N(13)	9839(4)	-940(4)	5417(4)	32(1)
C(23)	7645(7)	-2735(6)	5359(5)	46(2)
C(213)	8209(6)	-2520(5)	6152(5)	41(2)
C(223)	8419(7)	-3183(6)	6532(5)	50(2)
C(233)	8913(8)	-2978(7)	7257(6)	54(2)
C(243)	9220(7)	-2116(6)	7641(5)	48(2)
C(253)	9036(6)	-1451(6)	7293(4)	41(2)
C(263)	8539(6)	-1665(5)	6541(4)	37(2)
N(23)	8443(5)	-1016(4)	6150(4)	38(2)
C(313)	7058(6)	-2387(6)	3899(5)	41(2)
C(323)	7218(8)	-2713(8)	3217(6)	62(3)
C(333)	6527(9)	-2808(10)	2580(6)	84(4)
C(343)	5658(9)	-2554(9)	2627(6)	70(3)
C(353)	5476(7)	-2270(9)	3308(7)	70(3)
C(363)	6178(7)	-2157(8)	3941(6)	60(3)
Cl(13)	9025(2)	900(1)	5843(1)	42(1)
Cl(23)	6923(2)	-91(2)	5182(1)	48(1)
Cl(33)	8440(1)	-587(1)	4129(1)	37(1)

Re(4)	5443(1)	1496(1)	-552(1)	33(1)
P(14)	6966(1)	2099(1)	108(1)	34(1)
C(14)	7611(6)	1217(5)	442(5)	42(2)
C(114)	7589(6)	449(5)	-211(5)	40(2)
C(124)	8410(7)	213(6)	-408(6)	49(2)
C(134)	8401(7)	-470(6)	-1021(6)	53(2)
C(144)	7584(7)	-921(6)	-1431(6)	53(2)
C(154)	6746(7)	-701(5)	-1243(5)	44(2)
C(164)	6773(6)	-17(5)	-630(5)	40(2)
N(14)	5915(5)	221(4)	-439(4)	37(1)
C(24)	7600(6)	2413(5)	-509(5)	41(2)
C(214)	7443(6)	1829(5)	-1286(4)	38(2)
C(224)	8164(7)	1722(7)	-1647(5)	49(2)
C(234)	8001(8)	1261(7)	-2373(6)	64(3)
C(244)	7134(8)	842(7)	-2778(6)	60(3)
C(254)	6420(7)	923(6)	-2415(5)	50(2)
C(264)	6584(6)	1404(5)	-1680(4)	38(2)
N(24)	5886(5)	1423(4)	-1317(4)	38(2)
C(314)	7132(6)	3036(5)	899(5)	41(2)
C(324)	7579(15)	3019(10)	1593(7)	124(8)
C(334)	7649(17)	3755(9)	2185(7)	143(10)
C(344)	7227(11)	4466(7)	2086(7)	78(4)
C(354)	6773(11)	4523(8)	1387(8)	88(4)
C(364)	6724(10)	3787(7)	799(8)	81(4)
Cl(14)	3913(2)	766(1)	-942(1)	44(1)
Cl(24)	4725(2)	2847(1)	-546(1)	45(1)
Cl(34)	5362(2)	1624(1)	718(1)	40(1)

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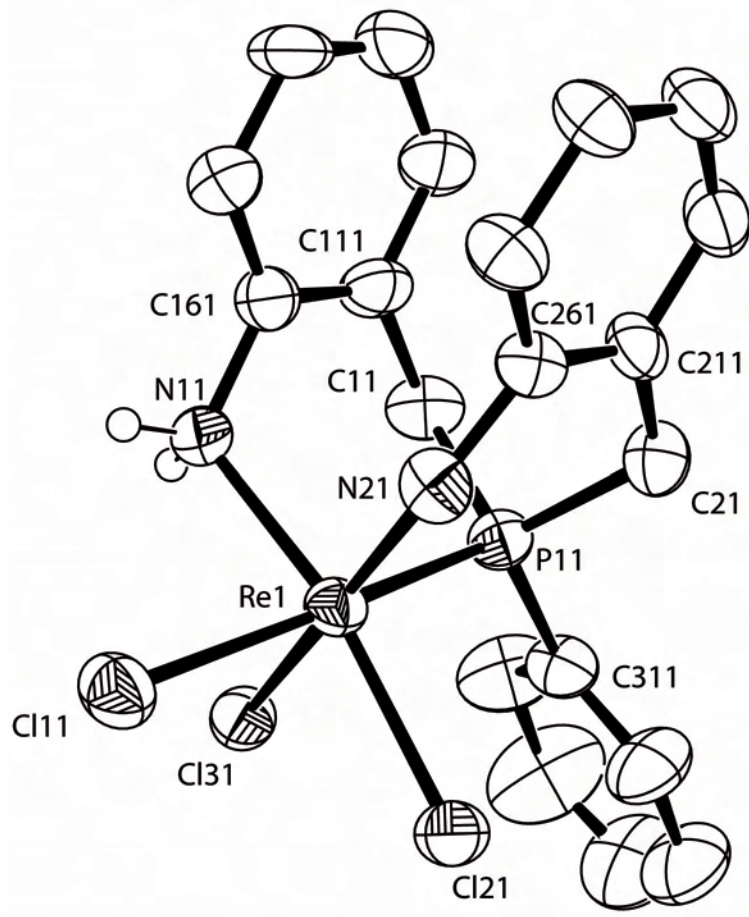


Abbildung 6.17: Ellipsoiddarstellung von  $[\text{ReCl}_3(\text{H}_2\text{L}^2)]$ . Die Schwingungsellipsoide repräsentieren 50% der Aufenthaltswahrscheinlichkeit. [121]



## 6.15 [ReOCl<sub>2</sub>(L<sup>13,Diethyl</sup>)]

Tabelle 6.29: Kristallographische Daten und Parameter der Strukturrechnung von [ReOCl<sub>2</sub>(L<sup>13,Diethyl</sup>)]

Summenformel	C <sub>31</sub> H <sub>31</sub> N <sub>3</sub> POCl <sub>2</sub> SRe	
M (g/mol)	781.49	
Messtemperatur	200(2) K	
Wellenlänge	0.71073 Å	
Kristallsystem, Raumgruppe	orthorombisch, Fdd2	
Elementarzelle	a = 33.318(2) Å	α = 90°
	b = 30.267(2) Å	β = 90°
	c = 12.376(1) Å	γ = 90°
Volumen	12480(2) Å <sup>3</sup>	
Z	16	
Berechnete Dichte	1.664 g/cm <sup>3</sup>	
Linearer Absorptionskoeffizient	4.213 mm <sup>-1</sup>	
F(000)	6175	
Kristallgröße	0.3 x 0.3 x 0.2 mm <sup>3</sup>	
Theta-Bereich	2.45 - 29.58°	
Indizes	-45 ≤ h ≤ 45, -41 ≤ k ≤ 41, -16 ≤ l ≤ 16	
Zahl der gemessenen Reflexe	33869	
Zahl der unabhängigen Reflexe	8393 [R(int) = 0.0920]	
Absorptionskorrektur	Integration	
Zahl der verfeinerten Parameter	361	
Goof	1.108	
R <sub>1</sub> / wR <sub>2</sub> [I > 2σ(I)]	R <sub>1</sub> = 0.0347, wR <sub>2</sub> = 0.0766	
R <sub>1</sub> / wR <sub>2</sub> (alle Reflexe)	R <sub>1</sub> = 0.0408, wR <sub>2</sub> = 0.0906	
Restelektronendichte	0.831 und -2.217 e · Å <sup>-3</sup>	
Programm zur Strukturlösung	SHELXS 97 [119]	

Tabelle 6.30: Atomkoordinaten ( $\cdot 10^4$ ) und isotrope Temperaturparameter ( $\text{\AA}^2 \cdot 10^3$ ) von  $[\text{ReOCl}_2(\text{L}^{13, \text{Diethyl}})]$

	x	y	z	E(eq)
Re(1)	728(1)	6928(1)	2500(1)	22(1)
O(10)	312(1)	7203(2)	2886(3)	30(1)
Cl(1)	687(1)	6343(1)	3805(1)	36(1)
Cl(2)	1423(1)	6693(1)	2132(1)	28(1)
S(1)	499(1)	6372(1)	1335(1)	29(1)
P(1)	1136(1)	7378(1)	3740(1)	22(1)
N(3)	747(2)	6912(2)	-297(4)	31(1)
N(5)	852(1)	7371(2)	1252(4)	23(1)
N(51)	192(2)	6500(2)	-631(4)	34(1)
C(1)	1389(2)	7794(2)	2903(4)	25(1)
C(2)	476(2)	6625(2)	59(6)	30(1)
C(4)	922(2)	7239(2)	222(4)	26(1)
C(11)	1085(2)	8045(2)	2231(4)	27(1)
C(12)	1044(2)	8500(2)	2363(5)	34(1)
C(13)	784(2)	8749(2)	1748(6)	41(2)
C(14)	554(2)	8541(2)	968(6)	39(1)
C(15)	589(2)	8094(2)	805(5)	31(1)
C(16)	852(2)	7835(2)	1436(4)	25(1)
C(21)	1525(2)	7107(2)	4522(4)	27(1)
C(22)	1931(2)	7163(3)	4303(6)	41(2)
C(23)	2219(2)	6946(3)	4917(8)	54(2)
C(24)	2106(2)	6669(4)	5741(7)	56(2)
C(25)	1703(3)	6604(4)	5957(7)	55(2)
C(26)	1416(2)	6827(3)	5367(6)	42(2)
C(31)	854(2)	7669(2)	4779(4)	25(1)

C(32)	1002(2)	8056(2)	5220(5)	31(1)
C(33)	807(2)	8249(2)	6094(5)	35(1)
C(34)	468(2)	8051(2)	6534(5)	34(1)
C(35)	325(2)	7661(2)	6090(5)	35(1)
C(36)	511(2)	7469(2)	5204(5)	31(1)
C(41)	1237(2)	7458(2)	-440(5)	31(1)
C(42)	1180(3)	7534(4)	-1541(6)	61(3)
C(43)	1489(3)	7698(5)	-2172(7)	83(4)
C(44)	1858(3)	7782(4)	-1747(7)	62(3)
C(45)	1921(2)	7701(3)	-659(7)	52(2)
C(46)	1613(2)	7543(2)	-11(6)	38(1)
C(52)	-97(2)	6148(2)	-394(6)	38(1)
C(53)	32(3)	5694(3)	-747(10)	69(3)
C(54)	167(2)	6708(3)	-1707(6)	46(2)
C(55)	454(4)	6509(3)	-2523(8)	69(3)

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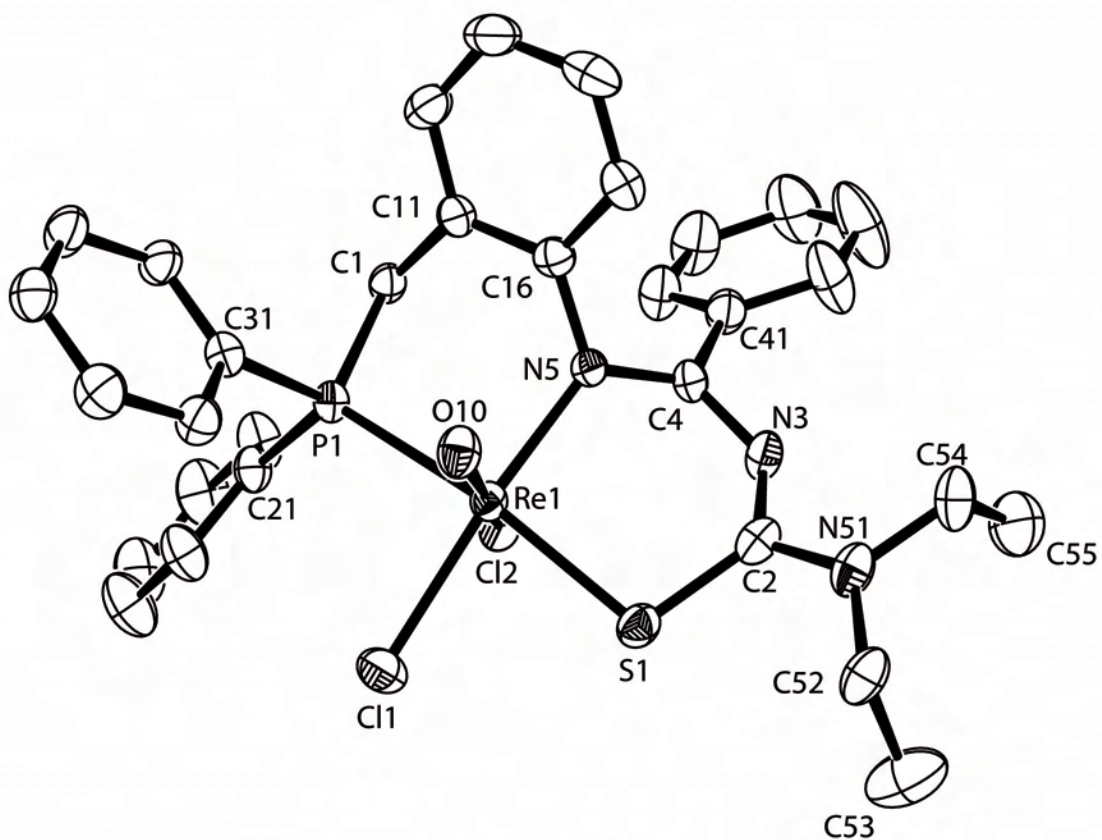


Abbildung 6.18: Ellipsoiddarstellung von  $[\text{ReOCl}_2(\text{L}^{13,\text{Diethyl}})]$ . Die Schwingungsellipsoide repräsentieren 50% der Aufenthaltswahrscheinlichkeit. [121]

## 6.16 [ReOCl<sub>2</sub>(L<sup>13,Morph</sup>)] · 2 Aceton

Tabelle 6.31: Kristallographische Daten und Parameter der Strukturrechnung von [ReOCl<sub>2</sub>(L<sup>13,Morph</sup>)] · 2 Aceton

Summenformel	C <sub>37</sub> H <sub>41</sub> N <sub>2</sub> PO <sub>4</sub> Cl <sub>2</sub> Re	
M (g/mol)	911.86	
Messtemperatur	200(2) K	
Wellenlänge	0.71073 Å	
Kristallsystem, Raumgruppe	monoklin, P2 <sub>1</sub> /c	
Elementarzelle	a = 15.281(2) Å	α = 90°
	b = 15.252(1) Å	β = 107.46(1)°
	c = 16.642(2) Å	γ = 90°
Volumen	3700.0(2) Å <sup>3</sup>	
Z	4	
Berechnete Dichte	1.637 g/cm <sup>3</sup>	
Linearer Absorptionskoeffizient	3.572 mm <sup>-1</sup>	
F(000)	1824	
Kristallgröße	0.26 x 0.07 x 0.04 mm <sup>3</sup>	
Theta-Bereich	2.52 - 27.15°	
Indizes	-19 ≤ h ≤ 19, -17 ≤ k ≤ 19, -21 ≤ l ≤ 20	
Zahl der gemessenen Reflexe	18348	
Zahl der unabhängigen Reflexe	7792 [R(int) = 0.0843]	
Absorptionskorrektur	Integration	
Zahl der verfeinerten Parameter	447	
Goof	1.088	
R <sub>1</sub> / wR <sub>2</sub> [I > 2σ(I)]	R <sub>1</sub> = 0.0534, wR <sub>2</sub> = 0.1230	
R <sub>1</sub> / wR <sub>2</sub> (alle Reflexe)	R <sub>1</sub> = 0.1005, wR <sub>2</sub> = 0.1459	
Restelektronendichte	1.220 und -1.295 e · Å <sup>-3</sup>	
Programm zur Strukturlösung	SHELXS 97 [119]	

Tabelle 6.32: Atomkoordinaten ( $\cdot 10^4$ ) und isotrope Temperaturparameter ( $\text{\AA}^2 \cdot 10^3$ ) von  $[\text{ReOCl}_2(\text{L}^{13, \text{Morph}})] \cdot 2 \text{ Aceton}$

	x	y	z	E(eq)
Re(1)	4733(1)	537(1)	7948(1)	35(1)
O(10)	4560(4)	-171(4)	7149(4)	40(1)
Cl(1)	6228(2)	23(2)	8734(2)	51(1)
Cl(2)	5022(2)	1838(2)	8888(2)	45(1)
P(1)	5431(2)	1579(2)	7201(1)	35(1)
C(1)	4574(7)	2433(6)	6788(6)	40(2)
C(11)	3697(6)	2046(6)	6255(6)	40(2)
C(12)	3357(7)	2289(7)	5419(7)	47(2)
C(13)	2527(7)	1954(7)	4885(7)	51(3)
C(14)	2043(8)	1359(6)	5194(6)	48(2)
C(15)	2375(6)	1115(6)	6051(6)	41(2)
C(16)	3188(6)	1446(6)	6578(6)	38(2)
C(21)	6499(6)	2154(6)	7746(6)	38(2)
C(22)	7322(7)	1698(7)	7923(6)	45(2)
C(23)	8141(8)	2127(8)	8275(7)	54(3)
C(24)	8151(7)	3018(7)	8447(7)	52(3)
C(25)	7319(8)	3459(7)	8291(7)	54(3)
C(26)	6521(7)	3032(6)	7944(6)	43(2)
C(31)	5697(6)	1062(6)	6316(6)	35(2)
C(32)	5569(6)	1512(6)	5543(6)	41(2)
C(33)	5814(7)	1102(7)	4903(6)	45(2)
C(34)	6188(7)	267(7)	5014(6)	46(2)
C(35)	6326(7)	-162(6)	5762(7)	48(2)
C(36)	6071(7)	242(6)	6404(6)	39(2)
N(5)	3462(5)	1141(5)	7433(5)	34(2)

C(4)	2823(6)	1209(6)	7845(6)	39(2)
C(41)	2222(6)	1994(6)	7721(6)	38(2)
C(42)	1328(6)	1918(7)	7762(7)	47(2)
C(43)	788(7)	2632(8)	7690(8)	57(3)
C(44)	1108(7)	3456(7)	7591(7)	56(3)
C(45)	1987(7)	3548(7)	7554(7)	49(2)
C(46)	2548(7)	2817(6)	7619(7)	46(2)
N(3)	2673(5)	626(5)	8376(5)	41(2)
N(51)	2615(5)	-790(5)	8815(5)	42(2)
C(52)	2994(7)	-1634(6)	9149(7)	49(2)
C(53)	2490(7)	-2010(7)	9696(7)	50(2)
O(54)	1535(5)	-2079(5)	9282(6)	61(2)
C(55)	1189(8)	-1222(7)	9068(8)	59(3)
C(56)	1583(7)	-777(8)	8457(8)	57(3)
C(2)	3102(6)	-118(6)	8667(6)	36(2)
S(1)	4295(2)	-236(2)	8975(2)	43(1)
C(86)	1608(12)	4099(12)	5232(12)	119(7)
C(87)	703(9)	3804(10)	4744(9)	71(3)
C(88)	367(11)	2951(9)	4990(10)	84(4)
O(89)	247(8)	4203(9)	4129(8)	112(4)
C(96)	-1043(10)	4171(9)	1822(9)	72(4)
C(97)	-538(9)	4495(7)	1257(8)	62(3)
C(98)	-869(14)	4149(9)	372(10)	101(6)
O(99)	81(8)	5023(7)	1473(7)	92(3)

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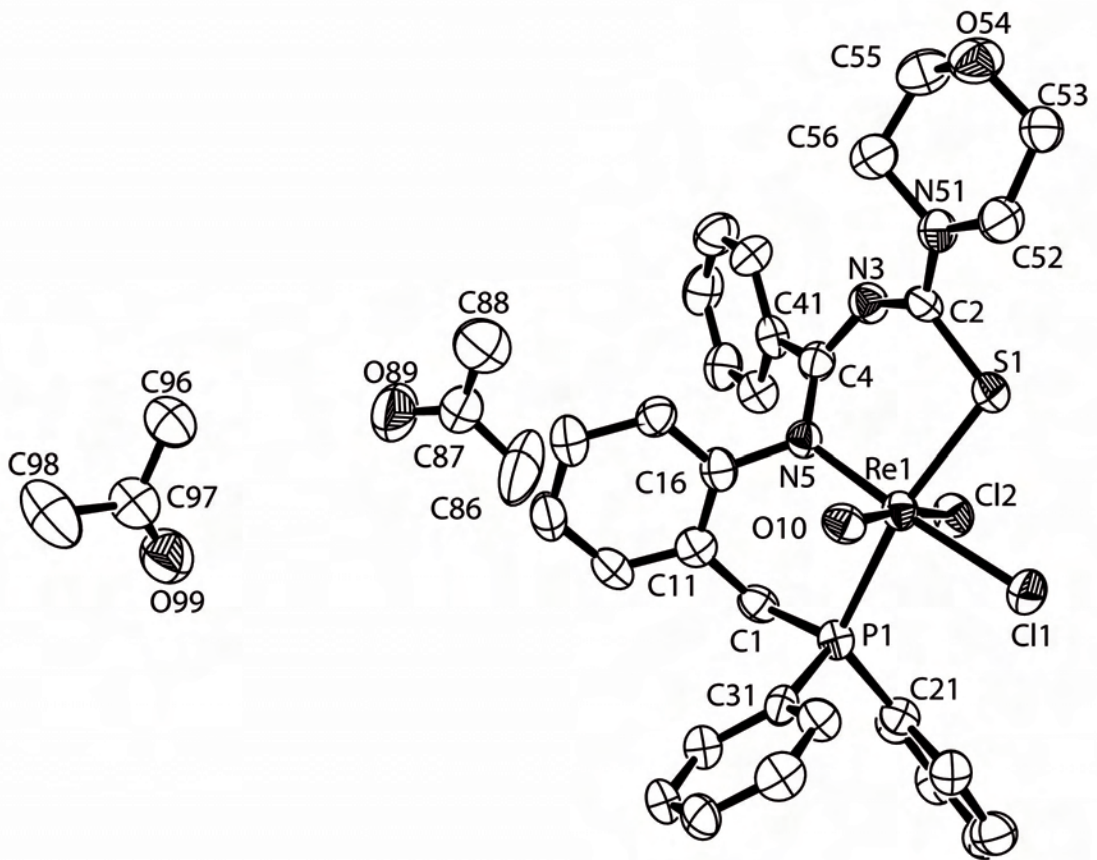


Abbildung 6.19: Ellipsoiddarstellung von  $[\text{ReOCl}_2(\text{L}^{13,\text{Morph}})] \cdot 2 \text{ Aceton}$ . Die Schwingungsellipsoide repräsentieren 50% der Aufenthaltswahrscheinlichkeit. [121]



## 6.17 [ReN(L<sup>13,Diethyl</sup>)(PPh<sub>3</sub>)(ReO<sub>4</sub>)] · 0.5 CH<sub>2</sub>Cl<sub>2</sub>

Tabelle 6.33: Kristallographische Daten und Parameter der Strukturrechnung von [ReN(L<sup>13,Diethyl</sup>)(PPh<sub>3</sub>)(ReO<sub>4</sub>)] · 0.5 CH<sub>2</sub>Cl<sub>2</sub>

Summenformel	C <sub>49.5</sub> H <sub>47</sub> N <sub>4</sub> P <sub>2</sub> O <sub>4</sub> ClRe <sub>2</sub>	
M (g/mol)	1263.76	
Messtemperatur	200(2) K	
Wellenlänge	0.71073 Å	
Kristallsystem, Raumgruppe	triklin, P $\bar{1}$	
Elementarzelle	a = 12.049(1) Å	$\alpha = 98.2(1)^\circ$
	b = 12.274(1) Å	$\beta = 101.54(1)^\circ$
	c = 19.040(2) Å	$\gamma = 112.39(1)^\circ$
Volumen	2475.4(4) Å <sup>3</sup>	
Z	2	
Berechnete Dichte	1.696 g/cm <sup>3</sup>	
Linearer Absorptionskoeffizient	5.093 mm <sup>-1</sup>	
F(000)	1234	
Kristallgröße	0.23 x 0.15 x 0.10 mm <sup>3</sup>	
Theta-Bereich	1.85 - 29.28°	
Indizes	-16 ≤ h ≤ 15, -16 ≤ k ≤ 16, -26 ≤ l ≤ 25	
Zahl der gemessenen Reflexe	25981	
Zahl der unabhängigen Reflexe	13220 [R(int) = 0.0789]	
Absorptionskorrektur	Integration	
Zahl der verfeinerten Parameter	594	
Goof	0.999	
R <sub>1</sub> / wR <sub>2</sub> [I > 2σ(I)]	R <sub>1</sub> = 0.0500, wR <sub>2</sub> = 0.1243	
R <sub>1</sub> / wR <sub>2</sub> (alle Reflexe)	R <sub>1</sub> = 0.0764, wR <sub>2</sub> = 0.1462	
Restelektronendichte	2.020 und -1.901 e · Å <sup>-3</sup>	
Programm zur Strukturlösung	SHELXS 97 [119]	

Tabelle 6.34: Atomkoordinaten ( $\cdot 10^4$ ) und isotrope Temperaturparameter ( $\text{\AA}^2 \cdot 10^3$ ) von  $[\text{ReN}(\text{L}^{13, \text{Diethyl}})(\text{PPh}_3)(\text{ReO}_4)] \cdot 0.5 \text{CH}_2\text{Cl}_2$

	x	y	z	E(eq)
Re(1)	8247(1)	4001(1)	2896(1)	31(1)
N(10)	9520(6)	3837(5)	3268(3)	42(1)
P(1)	9184(2)	5542(2)	2244(1)	34(1)
C(1)	9144(7)	6924(6)	2735(4)	40(1)
C(11)	9994(7)	7225(6)	3496(4)	41(1)
C(12)	11164(8)	8197(7)	3714(5)	50(2)
C(13)	12012(9)	8437(8)	4389(6)	60(2)
C(14)	11694(8)	7655(8)	4842(5)	57(2)
C(15)	10538(7)	6677(7)	4637(4)	46(2)
C(16)	9678(6)	6466(6)	3966(4)	36(1)
C(21)	10858(7)	6105(6)	2297(4)	39(1)
C(22)	11336(8)	6938(7)	1901(5)	52(2)
C(23)	12588(9)	7417(9)	1940(6)	68(3)
C(24)	13390(9)	7058(10)	2383(6)	73(3)
C(25)	12912(8)	6220(10)	2781(6)	62(2)
C(26)	11649(7)	5749(7)	2741(5)	48(2)
C(31)	8454(7)	5317(6)	1266(4)	40(1)
C(32)	8879(7)	4802(7)	734(4)	43(2)
C(33)	8323(9)	4598(8)	-19(4)	55(2)
C(34)	7349(10)	4906(9)	-238(5)	61(2)
C(35)	6925(8)	5437(8)	284(5)	56(2)
C(36)	7484(8)	5638(7)	1031(4)	46(2)
N(5)	8465(5)	5454(5)	3765(3)	33(1)
C(4)	7758(7)	5464(6)	4213(4)	37(1)
C(41)	8110(7)	6623(6)	4776(4)	39(1)

C(42)	8184(8)	7676(6)	4559(4)	45(2)
C(43)	8552(9)	8749(7)	5095(5)	56(2)
C(44)	8820(8)	8740(8)	5824(5)	58(2)
C(45)	8739(9)	7714(8)	6043(5)	55(2)
C(46)	8356(8)	6626(7)	5514(4)	45(2)
N(3)	6725(6)	4592(5)	4260(3)	40(1)
C(2)	6202(7)	3414(6)	3932(4)	39(1)
N(51)	5203(7)	2728(6)	4120(5)	59(2)
C(52)	4709(9)	3267(9)	4650(6)	70(3)
C(53)	5278(16)	3349(19)	5403(8)	124(6)
C(54)	4330(40)	1380(30)	3690(20)	70(7)
C(55)	4820(20)	600(20)	3998(15)	104(7)
C(56)	4580(50)	1560(40)	3900(20)	70(7)
C(57)	3590(30)	990(30)	3234(19)	104(7)
S(1)	6682(2)	2627(2)	3317(1)	47(1)
P(2)	7563(2)	2240(2)	1877(1)	37(1)
C(71)	6042(7)	1909(7)	1264(4)	45(2)
C(72)	4972(8)	1230(8)	1449(5)	58(2)
C(73)	3798(10)	1082(11)	1055(7)	80(3)
C(74)	3713(10)	1608(11)	457(7)	83(4)
C(75)	4751(11)	2275(9)	271(6)	74(3)
C(76)	5936(8)	2448(7)	671(5)	53(2)
C(81)	8619(7)	2260(6)	1301(4)	41(2)
C(82)	8212(10)	1667(8)	554(5)	59(2)
C(83)	9087(11)	1714(10)	172(6)	73(3)
C(84)	10349(12)	2330(10)	514(7)	80(3)
C(85)	10764(9)	2894(8)	1259(6)	65(3)
C(86)	9893(8)	2849(7)	1656(5)	48(2)

C(91)	7350(7)	832(6)	2171(4)	41(2)
C(92)	6599(9)	-300(7)	1672(5)	57(2)
C(93)	6450(10)	-1368(7)	1898(6)	67(3)
C(94)	7015(10)	-1325(8)	2598(6)	65(3)
C(95)	7806(10)	-214(8)	3093(7)	68(3)
C(96)	7964(8)	865(7)	2877(5)	49(2)
Re(2)	5282(1)	4679(1)	2305(1)	48(1)
O(1)	6580(5)	4387(4)	2300(3)	43(1)
O(2)	4146(7)	3514(7)	2500(6)	100(3)
O(3)	4750(10)	4925(12)	1480(5)	125(4)
O(4)	5728(7)	5966(6)	2976(5)	71(2)
C(99')	9820(20)	9991(14)	1709(14)	72(6)
Cl(1')	9017(5)	8532(4)	1173(2)	53(1)
Cl(2')	11338(6)	10414(6)	2145(4)	88(2)

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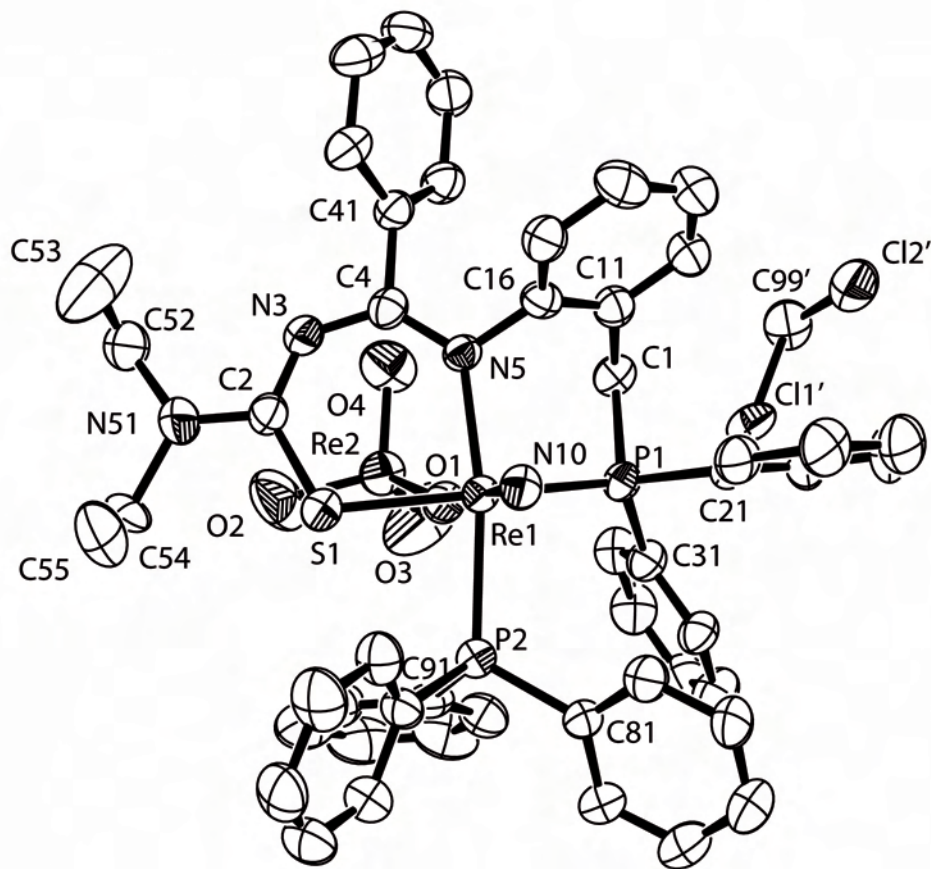


Abbildung 6.20: Ellipsoiddarstellung von  $[\text{ReN}(\text{L}^{13,\text{Diethyl}})(\text{PPh}_3)(\text{ReO}_4)] \cdot 0.5 \text{CH}_2\text{Cl}_2$ . Die Schwingungsellipsoide repräsentieren 50% der Aufenthaltswahrscheinlichkeit. [121]



## 6.18 [PdCl(L<sup>15</sup>)]

Tabelle 6.35: Kristallographische Daten und Parameter der Strukturrechnung von [PdCl(L<sup>15</sup>)]

Summenformel	C <sub>38</sub> H <sub>32</sub> NCIP <sub>2</sub> Pd	
M (g/mol)	706.44	
Messtemperatur	200(2) K	
Wellenlänge	0.71073 Å	
Kristallsystem, Raumgruppe	triklin, P $\bar{1}$	
Elementarzelle	a = 9.412(1) Å	$\alpha = 86.00(1)^\circ$
	b = 9.747(1) Å	$\beta = 80.07(1)^\circ$
	c = 18.48(2) Å	$\gamma = 67.93(1)^\circ$
Volumen	1547.3(3) Å <sup>3</sup>	
Z	2	
Berechnete Dichte	1.516 g/cm <sup>3</sup>	
Linearer Absorptionskoeffizient	0.819 mm <sup>-1</sup>	
F(000)	720	
Kristallgröße	0.17 x 0.17 x 0.05 mm <sup>3</sup>	
Theta-Bereich	2.77 - 27.00°	
Indizes	-12 ≤ h ≤ 11, -12 ≤ k ≤ 11, -23 ≤ l ≤ 23	
Zahl der gemessenen Reflexe	12574	
Zahl der unabhängigen Reflexe	6609 [R(int) = 0.0742]	
Zahl der verfeinerten Parameter	388	
Goof	0.857	
R <sub>1</sub> / wR <sub>2</sub> [I > 2σ(I)]	R <sub>1</sub> = 0.0562, wR <sub>2</sub> = 0.1253	
R <sub>1</sub> / wR <sub>2</sub> (alle Reflexe)	R <sub>1</sub> = 0.1092, wR <sub>2</sub> = 0.1541	
Restelektronendichte	0.564 und -0.698 e · Å <sup>-3</sup>	
Programm zur Strukturlösung	SHELXS 97 [119]	

Tabelle 6.36: Atomkoordinaten ( $\cdot 10^4$ ) und isotrope Temperaturparameter ( $\text{\AA}^2 \cdot 10^3$ ) von [PdCl(L<sup>15</sup>)]

	x	y	z	E(eq)
Pd(1)	9365(1)	2811(1)	7362(1)	20(1)
Cl(1)	6660(2)	3765(2)	7678(1)	36(1)
P(1)	9198(2)	2093(2)	6223(1)	24(1)
C(1)	11142(8)	844(7)	5828(3)	28(1)
C(11)	11969(7)	-216(7)	6385(3)	28(1)
C(12)	12459(8)	-1735(7)	6308(4)	33(1)
C(13)	13307(9)	-2707(8)	6793(4)	37(2)
C(14)	13650(8)	-2136(7)	7382(4)	35(2)
C(15)	13143(8)	-628(7)	7481(3)	28(1)
C(16)	12257(7)	387(7)	6994(3)	24(1)
C(21)	11549(7)	2810(6)	8712(3)	22(1)
C(22)	11776(8)	2641(7)	9443(3)	25(1)
C(23)	13253(8)	2096(7)	9620(4)	33(2)
C(24)	14538(9)	1729(8)	9070(4)	38(2)
C(25)	14323(8)	1872(7)	8341(4)	31(1)
C(26)	12829(7)	2403(6)	8148(3)	21(1)
C(31)	8589(8)	3554(7)	5554(3)	26(1)
C(32)	7239(8)	4786(8)	5745(4)	34(2)
C(33)	6699(9)	5875(8)	5219(4)	40(2)
C(34)	7495(10)	5741(8)	4514(4)	40(2)
C(35)	8856(10)	4543(9)	4326(4)	41(2)
C(36)	9416(9)	3439(8)	4834(3)	35(2)
N(1)	11702(6)	1942(6)	7044(3)	23(1)
C(2)	12665(7)	2577(7)	7335(3)	26(1)
C(41)	7947(7)	1058(7)	6184(3)	26(1)



C(42)	8255(9)	-293(8)	6547(4)	36(2)
C(43)	7407(9)	-1160(8)	6502(4)	39(2)
C(44)	6166(9)	-644(8)	6110(4)	38(2)
C(45)	5830(9)	700(8)	5757(4)	38(2)
C(46)	6694(8)	1558(8)	5796(4)	35(2)
C(51)	8430(7)	3168(7)	9271(3)	24(1)
C(52)	8645(9)	1683(7)	9388(4)	33(1)
C(53)	7852(10)	1253(9)	10001(4)	43(2)
C(54)	6843(9)	2270(10)	10505(4)	47(2)
C(55)	6618(9)	3757(9)	10397(4)	41(2)
C(56)	7404(9)	4206(8)	9785(3)	33(2)
C(61)	9122(7)	5585(6)	8465(3)	24(1)
C(62)	7643(8)	6526(7)	8350(3)	31(1)
C(63)	7273(9)	8043(7)	8310(4)	38(2)
C(64)	8357(9)	8646(7)	8372(4)	35(2)
C(65)	9837(9)	7726(8)	8477(4)	39(2)
C(66)	10216(8)	6205(7)	8526(3)	30(1)
P(2)	9611(2)	3596(2)	8469(1)	21(1)

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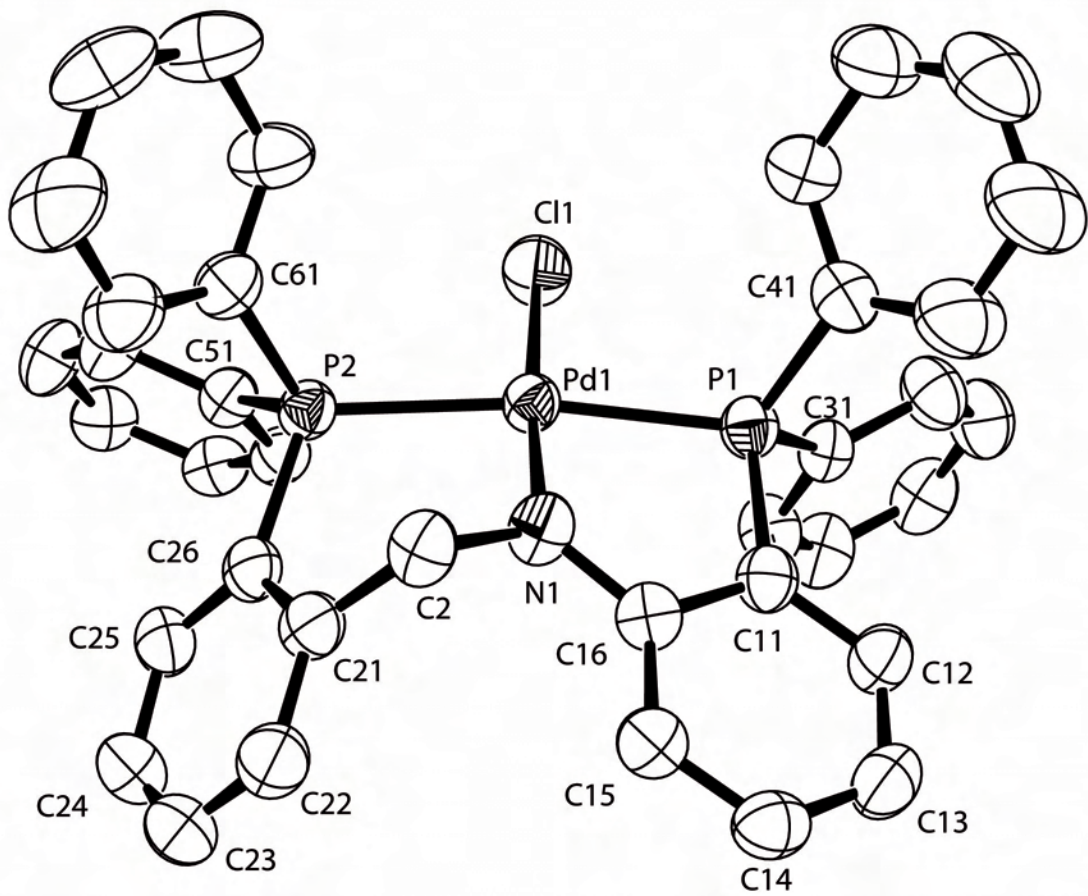


Abbildung 6.21: Ellipsoiddarstellung von  $[\text{PdCl}(\text{L}^{15})]$ . Die Schwingungsellipsoide repräsentieren 50% der Aufenthaltswahrscheinlichkeit. [121]

## 6.19 [PdCl(L<sup>17</sup>)]

Tabelle 6.37: Kristallographische Daten und Parameter der Strukturrechnung von [PdCl(L<sup>17</sup>)]

Summenformel	C <sub>37</sub> H <sub>30</sub> NCIP <sub>2</sub> Pd	
M (g/mol)	692.41	
Messtemperatur	200(2) K	
Wellenlänge	0.71073 Å	
Kristallsystem, Raumgruppe	triklin, P $\bar{1}$	
Elementarzelle	a = 9.765(1) Å	$\alpha = 99.74(1)^\circ$
	b = 12.050(1) Å	$\beta = 96.48(1)^\circ$
	c = 15.078(2) Å	$\gamma = 103.33)^\circ$
Volumen	1680.0(3) Å <sup>3</sup>	
Z	2	
Berechnete Dichte	1.369 g/cm <sup>3</sup>	
Linearer Absorptionskoeffizient	0.753 mm <sup>-1</sup>	
F(000)	704	
Kristallgröße	0.25 x 0.19 x 0.12 mm <sup>3</sup>	
Theta-Bereich	2.17 - 29.66°	
Indizes	-13 ≤ h ≤ 13, -16 ≤ k ≤ 16, -19 ≤ l ≤ 20	
Zahl der gemessenen Reflexe	18435	
Zahl der unabhängigen Reflexe	8977 [R(int) = 0.0614]	
Zahl der verfeinerten Parameter	380	
Goof	0.945	
R <sub>1</sub> / wR <sub>2</sub> [I > 2σ(I)]	R <sub>1</sub> = 0.0582, wR <sub>2</sub> = 0.1558	
R <sub>1</sub> / wR <sub>2</sub> (alle Reflexe)	R <sub>1</sub> = 0.0717, wR <sub>2</sub> = 0.1638	
Restelektronendichte	0.801 und -0.899 e · Å <sup>-3</sup>	
Programm zur Strukturlösung	SHELXS 97 [119]	

Tabelle 6.38: Atomkoordinaten ( $\cdot 10^4$ ) und isotrope Temperaturparameter ( $\text{\AA}^2 \cdot 10^3$ ) von  $[\text{PdCl}(\text{L}^{17})]$

	x	y	z	E(eq)
Pd(1)	9326(1)	8243(1)	7521(1)	38(1)
Cl(1)	6979(1)	8284(1)	7591(1)	59(1)
P(1)	8866(1)	6272(1)	7296(1)	40(1)
C(11)	10621(4)	6102(3)	7620(3)	43(1)
C(12)	10929(5)	5097(3)	7820(3)	51(1)
C(13)	12332(5)	5061(4)	8051(3)	57(1)
C(14)	13409(5)	6052(4)	8107(3)	53(1)
C(15)	13130(4)	7067(3)	7906(3)	48(1)
C(16)	11726(4)	7127(3)	7658(2)	41(1)
N(1)	11331(3)	8079(3)	7429(2)	45(1)
C(2)	12422(4)	9045(3)	7278(3)	48(1)
C(21)	12930(4)	10008(3)	8102(3)	46(1)
C(22)	14320(4)	10265(4)	8588(3)	58(1)
C(23)	14721(5)	11104(4)	9398(4)	70(1)
C(24)	13782(5)	11683(4)	9727(3)	65(1)
C(25)	12429(4)	11474(3)	9250(3)	51(1)
C(26)	11990(4)	10644(3)	8442(3)	43(1)
P(2)	10168(1)	10256(1)	7845(1)	39(1)
C(31)	7699(4)	5513(3)	7981(3)	42(1)
C(32)	6654(5)	4501(4)	7633(3)	58(1)
C(33)	5831(5)	3945(4)	8212(4)	67(1)
C(34)	6050(5)	4414(4)	9121(4)	61(1)
C(35)	7079(5)	5435(4)	9476(3)	60(1)
C(36)	7899(5)	5985(4)	8909(3)	54(1)
C(41)	8196(4)	5495(3)	6122(3)	49(1)

C(42)	8622(7)	4548(5)	5727(4)	81(2)
C(43)	8025(8)	3983(6)	4849(4)	99(2)
C(44)	7042(8)	4376(6)	4364(4)	88(2)
C(45)	6629(7)	5304(5)	4745(4)	81(2)
C(46)	7196(6)	5888(4)	5628(3)	66(1)
C(51)	9311(4)	11131(3)	8585(3)	42(1)
C(52)	8856(4)	10735(3)	9346(3)	45(1)
C(53)	8445(4)	11478(4)	10017(3)	51(1)
C(54)	8447(4)	12599(4)	9915(3)	54(1)
C(55)	8843(5)	12974(4)	9151(3)	59(1)
C(56)	9282(5)	12239(3)	8473(3)	54(1)
C(61)	10230(4)	10881(3)	6828(3)	46(1)
C(62)	9000(5)	10554(4)	6188(3)	62(1)
C(63)	8964(6)	11038(6)	5405(4)	80(2)
C(64)	10149(7)	11798(6)	5264(4)	81(2)
C(65)	11378(7)	12119(6)	5896(5)	89(2)
C(66)	11422(5)	11655(5)	6681(4)	69(1)

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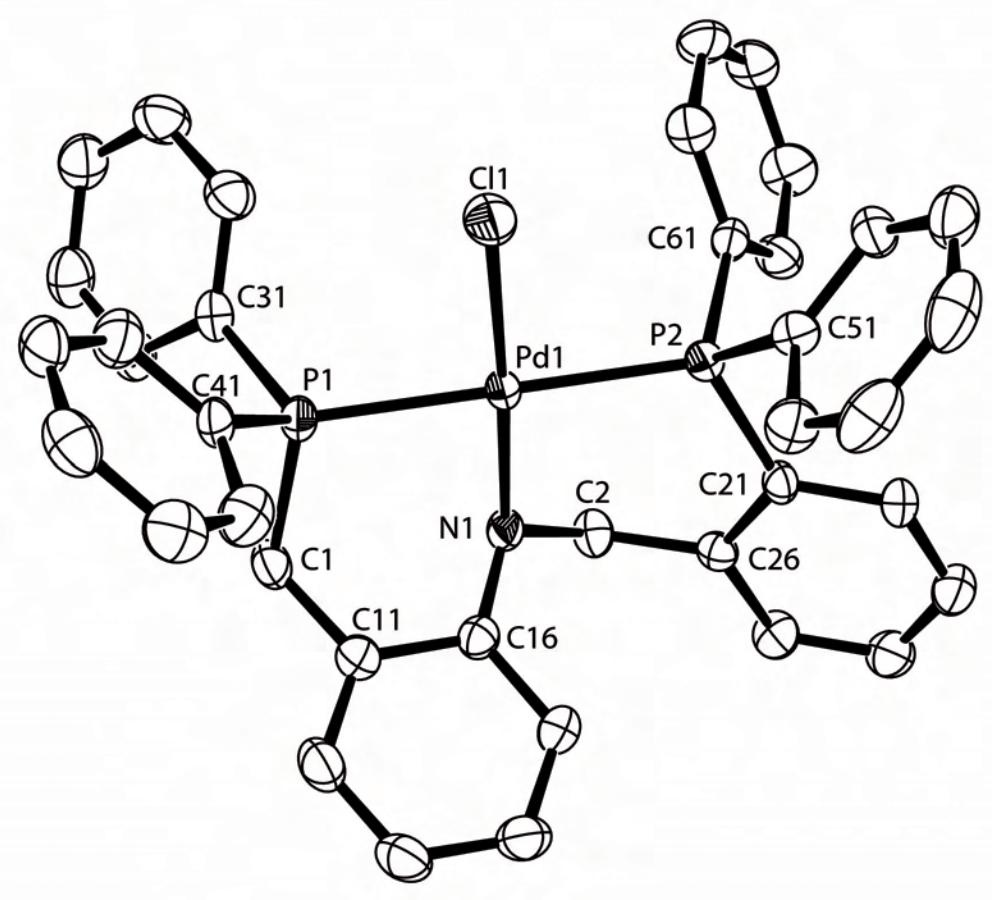


Abbildung 6.22: Ellipsoiddarstellung von [PdCl(L<sup>17</sup>)]. Die Schwingungsellipsoide repräsentieren 50% der Aufenthaltswahrscheinlichkeit. [121]

## 6.20 [RuCl<sub>2</sub>(PPh<sub>3</sub>)(HL<sup>15</sup>)] · CH<sub>2</sub>Cl<sub>2</sub>

Tabelle 6.39: Kristallographische Daten und Parameter der Strukturrechnung von [RuCl<sub>2</sub>(PPh<sub>3</sub>)(HL<sup>15</sup>)] · CH<sub>2</sub>Cl<sub>2</sub>

Summenformel	C <sub>57</sub> H <sub>50</sub> NCl <sub>4</sub> P <sub>3</sub> Ru	
M (g/mol)	1084.76	
Messtemperatur	200(2) K	
Wellenlänge	0.71073 Å	
Kristallsystem, Raumgruppe	monoklin, P2 <sub>1</sub> /n	
Elementarzelle	a = 12.484(1) Å	α = 90°
	b = 10.582(1) Å	β = 96.81(1)°
	c = 39.596(3) Å	γ = 90°
Volumen	5194.0(8) Å <sup>3</sup>	
Z	4	
Berechnete Dichte	1.387 g/cm <sup>3</sup>	
Linearer Absorptionskoeffizient	0.638 mm <sup>-1</sup>	
F(000)	2224	
Kristallgröße	0.25 x 0.2 x 0.14 mm <sup>3</sup>	
Theta-Bereich	2.18 - 27.00°	
Indizes	-15 ≤ h ≤ 15, -13 ≤ k ≤ 13, -50 ≤ l ≤ 42	
Zahl der gemessenen Reflexe	29905	
Zahl der unabhängigen Reflexe	10892 [R(int) = 0.0844]	
Zahl der verfeinerten Parameter	611	
Goof	0.926	
R <sub>1</sub> / wR <sub>2</sub> [I > 2σ(I)]	R <sub>1</sub> = 0.0648, wR <sub>2</sub> = 0.1656	
R <sub>1</sub> / wR <sub>2</sub> (alle Reflexe)	R <sub>1</sub> = 0.1050, wR <sub>2</sub> = 0.1823	
Restelektronendichte	1.508 und -0.990 e · Å <sup>-3</sup>	
Programm zur Strukturlösung	SHELXS 97 [119]	

Tabelle 6.40: Atomkoordinaten ( $\cdot 10^4$ ) und isotrope Temperaturparameter ( $\text{\AA}^2 \cdot 10^3$ ) von  $[\text{RuCl}_2(\text{PPh}_3)(\text{HL}^{15})] \cdot \text{CH}_2\text{Cl}_2$

	x	y	z	E(eq)
Ru(1)	4888(1)	649(1)	1196(1)	40(1)
Cl(1)	5638(1)	2511(1)	962(1)	47(1)
Cl(2)	3938(1)	-1325(1)	1271(1)	48(1)
P(1)	3275(1)	1539(1)	1375(1)	42(1)
C(1)	2155(5)	1080(5)	1045(1)	49(1)
C(11)	2322(5)	1803(5)	730(1)	47(1)
C(12)	1637(5)	2784(6)	616(2)	61(2)
C(13)	1861(6)	3576(6)	353(2)	63(2)
C(14)	2814(6)	3418(6)	216(2)	65(2)
C(15)	3517(5)	2434(5)	320(1)	52(1)
C(16)	3254(4)	1599(5)	572(1)	44(1)
C(31)	2940(4)	3228(5)	1404(1)	47(1)
C(32)	2191(5)	3670(5)	1608(2)	50(1)
C(33)	1948(6)	4949(6)	1622(2)	65(2)
C(34)	2441(6)	5796(6)	1427(2)	67(2)
C(35)	3155(6)	5368(6)	1215(2)	63(2)
C(36)	3417(5)	4083(5)	1201(2)	52(1)
C(41)	2830(4)	885(5)	1760(2)	47(1)
C(42)	2230(5)	-234(5)	1758(2)	51(1)
C(43)	1971(5)	-778(6)	2054(2)	63(2)
C(44)	2318(5)	-220(7)	2364(2)	69(2)
C(45)	2889(5)	918(7)	2375(2)	64(2)
C(46)	3150(5)	1449(6)	2076(2)	53(1)
N(1)	3914(4)	523(4)	674(1)	44(1)
C(2)	4527(5)	50(5)	393(1)	48(1)



C(21)	4695(5)	-1342(5)	425(1)	48(1)
C(22)	4112(5)	-2138(6)	191(2)	59(2)
C(23)	4235(6)	-3443(6)	215(2)	67(2)
C(24)	4937(6)	-3960(6)	479(2)	66(2)
C(25)	5528(5)	-3177(5)	713(2)	56(2)
C(26)	5424(5)	-1861(5)	688(1)	48(1)
C(51)	7195(5)	-193(5)	712(1)	49(1)
C(52)	7446(5)	-893(6)	432(2)	54(1)
C(53)	8268(5)	-520(6)	252(2)	63(2)
C(54)	8871(6)	523(6)	348(2)	67(2)
C(55)	8624(6)	1226(7)	622(2)	70(2)
C(56)	7783(5)	871(6)	801(2)	60(2)
C(61)	7006(5)	-1833(5)	1267(2)	50(1)
C(62)	6546(5)	-2457(5)	1522(2)	56(2)
C(63)	7161(6)	-3253(6)	1752(2)	63(2)
C(64)	8232(6)	-3456(6)	1714(2)	68(2)
C(65)	8699(6)	-2856(6)	1463(2)	65(2)
C(66)	8094(5)	-2058(6)	1239(2)	55(1)
P(2)	6180(1)	-754(1)	981(1)	45(1)
P(3)	5922(1)	981(1)	1714(1)	43(1)
C(71)	5603(4)	2385(5)	1963(1)	43(1)
C(72)	5323(4)	3517(5)	1798(2)	50(1)
C(73)	5095(5)	4594(6)	1978(2)	58(2)
C(74)	5151(5)	4553(6)	2325(2)	60(2)
C(75)	5431(5)	3443(6)	2494(2)	57(2)
C(76)	5650(5)	2380(6)	2316(1)	51(1)
C(81)	5975(4)	-220(5)	2047(1)	47(1)
C(82)	5069(5)	-953(5)	2069(2)	49(1)

C(83)	5032(6)	-1823(6)	2333(2)	61(2)
C(84)	5910(6)	-1929(6)	2579(2)	64(2)
C(85)	6788(5)	-1200(6)	2571(2)	59(2)
C(86)	6829(5)	-329(6)	2309(2)	52(1)
C(91)	7361(5)	1317(5)	1679(1)	47(1)
C(92)	8140(5)	380(6)	1718(1)	51(1)
C(93)	9203(5)	643(7)	1665(2)	52(2)
C(94)	9499(5)	1837(7)	1571(2)	68(2)
C(95)	8726(5)	2778(7)	1532(2)	63(2)
C(96)	7667(5)	2537(6)	1588(1)	52(1)
C(98)	-1400(12)	5386(12)	636(3)	64(4)
Cl(3)	-228(3)	4976(3)	890(1)	64(1)
Cl(4)	-2462(3)	4431(3)	680(1)	82(1)
C(99)	1503(18)	7255(16)	542(6)	114(1)
Cl(5)	833(5)	6824(4)	170(2)	114(1)
Cl(6)	766(5)	8168(4)	808(2)	114(1)

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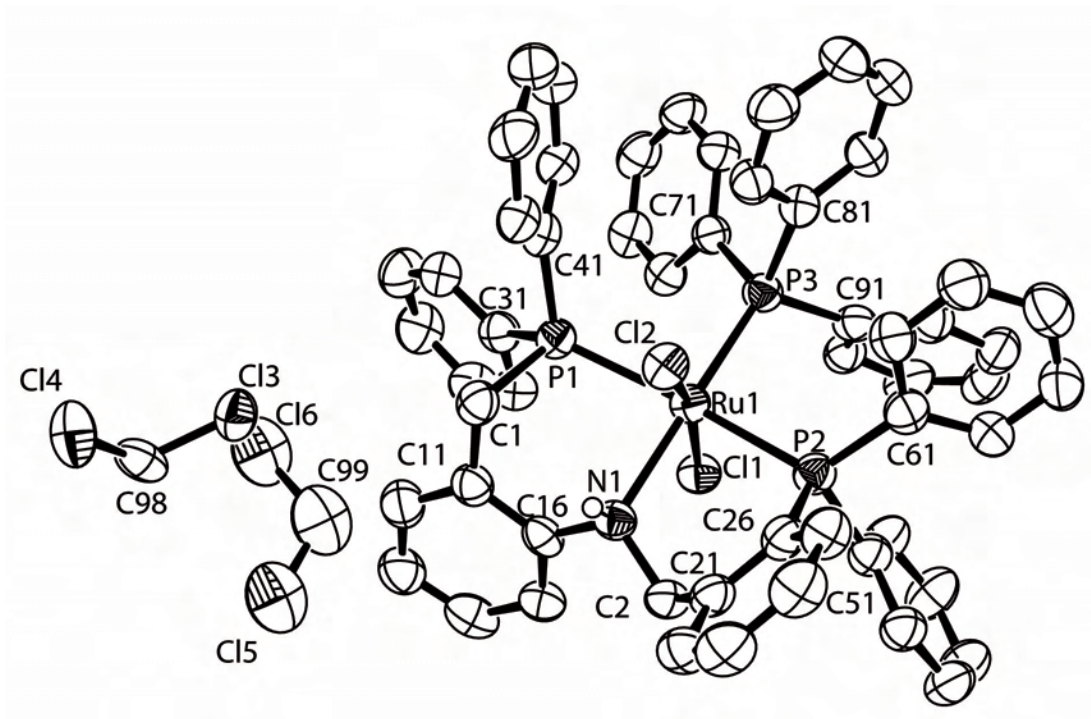


Abbildung 6.23: Ellipsoiddarstellung von  $[\text{RuCl}_2(\text{PPh}_3)(\text{HL}^{15})] \cdot \text{CH}_2\text{Cl}_2$ . Die Schwingungsellipsoide repräsentieren 50% der Aufenthaltswahrscheinlichkeit. [121]



## 6.21 [ReOCl<sub>2</sub>(HL<sup>12</sup>)]

Tabelle 6.41: Kristallographische Daten und Parameter der Strukturrechnung von [ReOCl<sub>2</sub>HL<sup>12</sup>]

Summenformel	C <sub>26</sub> H <sub>23</sub> NCl <sub>2</sub> PO <sub>2</sub> Re	
M (g/mol)	669.56	
Messtemperatur	200(2) K	
Wellenlänge	0.71073 Å	
Kristallsystem, Raumgruppe	triklin, P $\bar{1}$	
Elementarzelle	a = 10.052(5) Å	$\alpha = 81.99(1)^\circ$
	b = 11.136(1) Å	$\beta = 83.70(1)^\circ$
	c = 12.050 Å	$\gamma = 63.25(1)^\circ$
Volumen	1191.1(6) Å <sup>3</sup>	
Z	2	
Berechnete Dichte	1.867 g/cm <sup>3</sup>	
Linearer Absorptionskoeffizient	5.418 mm <sup>-1</sup>	
F(000)	652	
Kristallgröße	0.300 x 0.200 x 0.050 mm <sup>3</sup>	
Theta-Bereich	2.77 - 29.16°	
Indizes	-13 ≤ h ≤ 13, -15 ≤ k ≤ 15, -16 ≤ l ≤ 16	
Zahl der gemessenen Reflexe	11911	
Zahl der unabhängigen Reflexe	6293 [R(int) = 0.0549]	
Absorptionskorrektur	Integration	
Zahl der verfeinerten Parameter	298	
Goof	1.073	
R <sub>1</sub> / wR <sub>2</sub> [I > 2σ(I)]	R <sub>1</sub> = 0.0370, wR <sub>2</sub> = 0.0923	
R <sub>1</sub> / wR <sub>2</sub> (alle Reflexe)	R <sub>1</sub> = 0.0425, wR <sub>2</sub> = 0.0958	
Restelektronendichte	2.218 und -3.453 e · Å <sup>-3</sup>	
Programm zur Strukturlösung	SHELXS 97 [119]	

Tabelle 6.42: Atomkoordinaten ( $\cdot 10^4$ ) und isotrope Temperaturparameter ( $\text{\AA}^2 \cdot 10^3$ ) von  $[\text{ReOCl}_2(\text{HL}^{12})]$

	x	y	z	E(eq)
Re(1)	2081(1)	3484(1)	3143(1)	21(1)
O(10)	2980(4)	2966(4)	4349(3)	31(1)
Cl(1)	2048(1)	1456(1)	2830(1)	31(1)
Cl(2)	-479(1)	4203(2)	3887(1)	37(1)
P(1)	4398(1)	2959(1)	2066(1)	22(1)
C(1)	4537(5)	4546(4)	1669(3)	23(1)
C(11)	4394(5)	5316(4)	2649(4)	25(1)
C(12)	5572(6)	5632(5)	2765(4)	30(1)
C(13)	5550(6)	6364(6)	3605(5)	35(1)
C(14)	4335(6)	6809(6)	4369(5)	36(1)
C(15)	3156(6)	6511(5)	4273(4)	33(1)
C(16)	3185(5)	5754(5)	3426(4)	25(1)
C(21)	6011(5)	1801(5)	2851(4)	25(1)
C(22)	7254(5)	2028(5)	2882(4)	32(1)
C(23)	8456(6)	1107(6)	3516(5)	38(1)
C(24)	8406(6)	-1(6)	4097(5)	40(1)
C(25)	7175(7)	-256(6)	4075(5)	42(1)
C(26)	5976(6)	651(5)	3445(5)	34(1)
C(31)	4661(5)	2273(5)	734(4)	25(1)
C(32)	6042(6)	1888(6)	146(4)	36(1)
C(33)	6267(7)	1398(7)	-890(5)	44(1)
C(34)	5168(7)	1272(6)	-1344(4)	38(1)
C(35)	3769(6)	1656(5)	-773(4)	34(1)
C(36)	3514(6)	2161(5)	268(4)	30(1)
N(1)	1870(4)	5487(4)	3444(3)	27(1)

C(2)	554(6)	6695(5)	2917(5)	35(1)
C(41)	643(5)	6799(5)	1662(5)	32(1)
C(42)	239(7)	8045(6)	1026(6)	48(2)
C(43)	226(8)	8146(7)	-130(6)	54(2)
C(44)	629(7)	7011(7)	-670(5)	49(2)
C(45)	1033(6)	5754(6)	-59(5)	37(1)
C(46)	998(5)	5660(5)	1107(4)	31(1)
O(1)	1282(4)	4476(3)	1705(3)	28(1)

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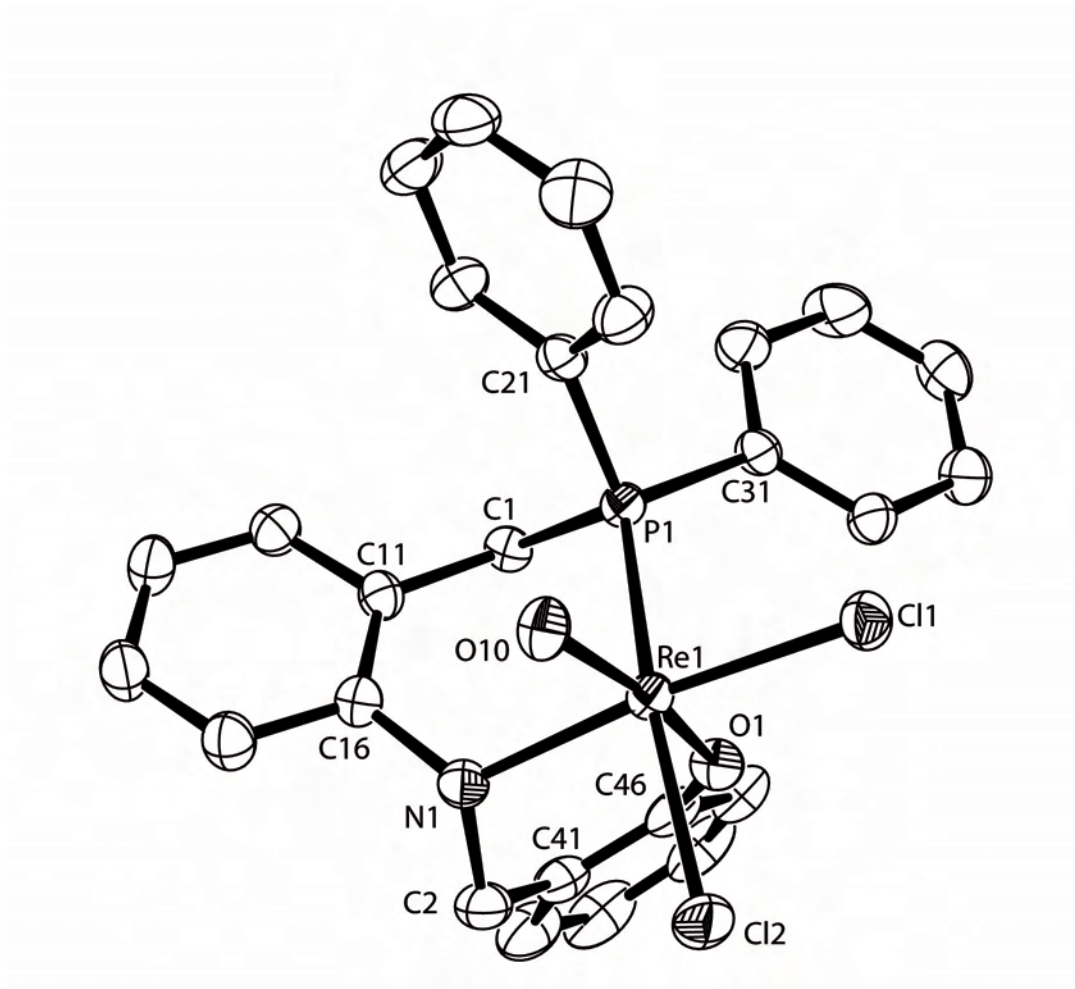


Abbildung 6.24: Ellipsoiddarstellung von  $[\text{ReOCl}_2(\text{HL}^{12})]$ . Die Schwingungsellipsoide repräsentieren 50% der Aufenthaltswahrscheinlichkeit. [121]



## 6.22 [ReO(L<sup>12</sup>)(malt)]

Tabelle 6.43: Kristallographische Daten und Parameter der Strukturrechnung von [ReO(L<sup>12</sup>)(malt)]

Summenformel	C <sub>32</sub> H <sub>27</sub> NPO <sub>5</sub> Re	
M (g/mol)	722.75	
Messtemperatur	200(2) K	
Wellenlänge	0.71073 Å	
Kristallsystem, Raumgruppe	monoklin, P <sub>2</sub> <sub>1</sub> /n	
Elementarzelle	a = 11.594(6) Å	α = 90°
	b = 16.624(6) Å	β = 101.70(4)°
	c = 14.760(6) Å	γ = 90°
Volumen	2786(2) Å <sup>3</sup>	
Z	4	
Berechnete Dichte	1.723 g/cm <sup>3</sup>	
Linearer Absorptionskoeffizient	4.462 mm <sup>-1</sup>	
F(000)	1424	
Kristallgröße	0.400 x 0.300 x 0.200 mm <sup>3</sup>	
Theta-Bereich	2.78 - 29.24°	
Indizes	-15 ≤ h ≤ 15, -22 ≤ k ≤ 22, -19 ≤ l ≤ 20	
Zahl der gemessenen Reflexe	20686	
Zahl der unabhängigen Reflexe	7461 [R(int) = 0.0520]	
Absorptionskorrektur	Integration	
Zahl der verfeinerten Parameter	361	
Goof	1.088	
R <sub>1</sub> / wR <sub>2</sub> [I > 2σ(I)]	R <sub>1</sub> = 0.0329, wR <sub>2</sub> = 0.0794	
R <sub>1</sub> / wR <sub>2</sub> (alle Reflexe)	R <sub>1</sub> = 0.0380, wR <sub>2</sub> = 0.0817	
Restelektronendichte	2.218 und -3.453 e · Å <sup>-3</sup>	
Programm zur Strukturlösung	SHELXS 97 [119]	

Tabelle 6.44: Atomkoordinaten ( $\cdot 10^4$ ) und isotrope Temperaturparameter ( $\text{\AA}^2 \cdot 10^3$ ) von [ReO(L<sup>12</sup>)(malt)]

	x	y	z	E(eq)
Re(1)	1545(1)	2417(1)	3091(1)	23(1)
O(10)	2773(2)	2746(2)	2749(2)	34(1)
P(1)	364(1)	2162(1)	1577(1)	23(1)
C(1)	-943(3)	2771(2)	1560(2)	28(1)
C(11)	-566(2)	3638(2)	1634(2)	26(1)
C(12)	-1000(3)	4152(2)	893(2)	29(1)
C(13)	-684(3)	4955(2)	913(3)	35(1)
C(14)	100(3)	5245(2)	1672(3)	35(1)
C(15)	545(3)	4749(2)	2415(2)	32(1)
C(16)	222(3)	3930(2)	2417(2)	26(1)
C(21)	-142(3)	1135(2)	1354(2)	28(1)
C(22)	-1331(3)	935(2)	1252(3)	38(1)
C(23)	-1680(4)	130(3)	1121(3)	51(1)
C(24)	-858(5)	-460(3)	1084(3)	56(1)
C(25)	318(4)	-267(2)	1179(3)	50(1)
C(26)	675(3)	531(2)	1300(3)	38(1)
C(31)	894(3)	2424(2)	539(2)	27(1)
C(32)	2093(3)	2445(2)	552(3)	37(1)
C(33)	2492(4)	2576(2)	-277(3)	39(1)
C(34)	1690(3)	2692(2)	-1092(2)	36(1)
C(35)	493(3)	2665(2)	-1110(2)	34(1)
C(36)	89(3)	2531(2)	-295(3)	32(1)
N(1)	703(2)	3431(2)	3178(2)	26(1)
C(2)	987(3)	3879(2)	4071(2)	34(1)
C(41)	784(3)	3396(2)	4879(2)	31(1)

C(42)	151(3)	3704(2)	5506(3)	40(1)
C(43)	6(4)	3260(3)	6278(3)	44(1)
C(44)	464(4)	2499(2)	6407(3)	40(1)
C(45)	1097(3)	2173(2)	5785(2)	32(1)
C(46)	1284(3)	2634(2)	5034(2)	29(1)
O(1)	1974(2)	2331(1)	4476(2)	30(1)
C(51)	1150(4)	-648(2)	3813(3)	45(1)
C(52)	1964(3)	-132(2)	3644(3)	37(1)
C(53)	1639(3)	685(2)	3455(2)	28(1)
C(54)	454(3)	916(2)	3492(2)	27(1)
C(55)	-320(3)	342(2)	3661(3)	36(1)
C(56)	-1584(3)	469(3)	3667(4)	52(1)
O(2)	2310(2)	1221(1)	3230(2)	29(1)
O(3)	167(2)	1677(1)	3310(2)	26(1)
O(4)	32(2)	-435(2)	3827(2)	47(1)

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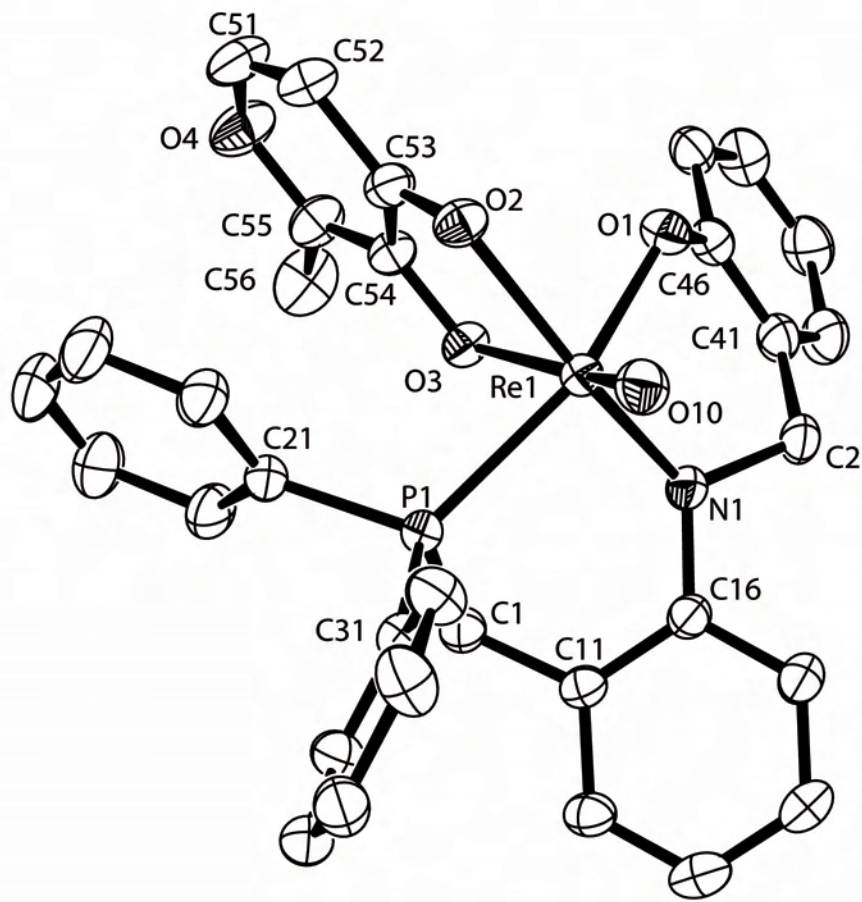


Abbildung 6.25: Ellipsoiddarstellung von  $[\text{ReO}(\text{L}^{12})(\text{malt})]$ . Die Schwingungsellipsoide repräsentieren 50% der Aufenthaltswahrscheinlichkeit. [121]

## 6.23 [ReO(HL<sup>22</sup>)] · 0.5 Toluol

Tabelle 6.45: Kristallographische Daten und Parameter der Strukturrechnung von [ReO(HL<sup>22</sup>)Cl] · 0.5 Toluol

Summenformel	C <sub>37.5</sub> H <sub>34</sub> N <sub>2</sub> PO <sub>3</sub> Re	
M (g/mol)	777.84	
Messtemperatur	200(2) K	
Wellenlänge	0.71073 Å	
Kristallsystem, Raumgruppe	triklin, P $\bar{1}$	
Elementarzelle	a = 12.088(1) Å	$\alpha = 107.10(1)^\circ$
	b = 12.739(1) Å	$\beta = 100.37(1)^\circ$
	c = 14.180(1) Å	$\gamma = 116.84(1)^\circ$
Volumen	1732.4(2) Å <sup>3</sup>	
Z	2	
Berechnete Dichte	1.491 g/cm <sup>3</sup>	
Linearer Absorptionskoeffizient	3.590 mm <sup>-1</sup>	
F(000)	774	
Kristallgröße	0.20 x 0.15 x 0.05 mm <sup>3</sup>	
Theta-Bereich	2.98 - 29.58°	
Indizes	-16 ≤ h ≤ 16, -15 ≤ k ≤ 17, -19 ≤ l ≤ 19	
Zahl der gemessenen Reflexe	18024	
Zahl der unabhängigen Reflexe	9243 [R(int) = 0.0511]	
Absorptionskorrektur	Integration	
Zahl der verfeinerten Parameter	386	
Goof	1.008	
R <sub>1</sub> / wR <sub>2</sub> [I > 2σ(I)]	R <sub>1</sub> = 0.0431, wR <sub>2</sub> = 0.1177	
R <sub>1</sub> / wR <sub>2</sub> (alle Reflexe)	R <sub>1</sub> = 0.0551, wR <sub>2</sub> = 0.1219	
Restelektronendichte	2.116 und -2.700 e · Å <sup>-3</sup>	
Programm zur Strukturlösung	SHELXS 97 [119]	

Tabelle 6.46: Atomkoordinaten ( $\cdot 10^4$ ) und isotrope Temperaturparameter ( $\text{\AA}^2 \cdot 10^3$ ) von  $[\text{ReO}(\text{HL}^{22})] \cdot 0.5 \text{ Toluol}$

	x	y	z	E(eq)
Re(1)	7022(1)	6240(1)	6880(1)	27(1)
O(10)	5808(4)	4828(4)	6805(3)	38(1)
P(1)	7724(1)	7423(1)	8726(1)	30(1)
C(1)	7274(5)	8637(5)	8963(4)	33(1)
C(11)	5777(5)	7991(5)	8498(4)	33(1)
C(12)	5192(6)	8287(7)	9217(5)	45(1)
C(13)	3807(7)	7736(8)	8886(6)	54(2)
C(14)	3019(7)	6925(7)	7848(7)	53(2)
C(15)	3591(6)	6615(6)	7118(6)	44(1)
C(16)	4960(5)	7136(5)	7432(5)	34(1)
N(1)	5438(4)	6730(4)	6605(4)	33(1)
C(3)	5582(6)	7477(6)	5950(5)	38(1)
C(31)	6785(6)	8849(6)	6512(5)	37(1)
C(32)	6711(8)	9900(7)	6528(6)	49(2)
C(33)	7845(9)	11152(7)	6994(7)	59(2)
C(34)	9073(8)	11351(7)	7441(6)	54(2)
C(35)	9174(7)	10301(6)	7448(5)	45(1)
C(36)	8029(6)	9029(6)	6981(4)	37(1)
O(1)	8154(4)	8067(4)	7032(3)	33(1)
C(2)	9535(5)	8265(5)	9195(4)	35(1)
C(21)	9879(5)	7239(6)	9015(4)	33(1)
C(22)	10699(6)	7306(7)	9887(5)	42(1)
C(23)	11030(7)	6403(8)	9837(5)	47(2)
C(24)	10489(7)	5343(7)	8861(5)	46(1)
C(25)	9671(6)	5240(6)	7987(5)	40(1)

C(26)	9366(5)	6188(5)	8016(4)	32(1)
N(2)	8569(4)	6054(4)	7065(4)	32(1)
C(4)	8758(6)	5430(6)	6104(4)	36(1)
C(41)	8816(6)	6068(5)	5368(4)	35(1)
C(42)	9881(6)	6510(7)	5030(5)	45(1)
C(43)	9892(8)	7046(8)	4310(6)	53(2)
C(44)	8793(8)	7121(8)	3905(6)	56(2)
C(45)	7742(7)	6708(7)	4253(5)	47(1)
C(46)	7746(5)	6185(5)	4980(4)	34(1)
O(2)	6694(4)	5733(4)	5284(3)	35(1)
C(51)	7214(5)	6599(6)	9564(4)	34(1)
C(52)	6859(6)	5319(6)	9252(5)	43(1)
C(53)	6543(7)	4726(7)	9926(6)	51(2)
C(54)	6563(7)	5387(8)	10893(6)	49(2)
C(55)	6877(8)	6629(7)	11194(5)	50(2)
C(56)	7229(7)	7265(7)	10548(5)	44(1)
C(61)	7350(9)	10136(9)	2684(8)	53(3)
C(62)	5969(9)	9492(10)	2275(7)	42(3)
C(63)	5210(8)	8676(12)	2680(10)	104(8)
C(64)	5833(12)	8503(13)	3494(11)	95(7)
C(65)	7214(12)	9147(12)	3902(8)	71(4)
C(66)	7973(8)	9963(11)	3497(8)	64(4)
C(67)	8100(20)	10850(20)	2358(18)	81(5)

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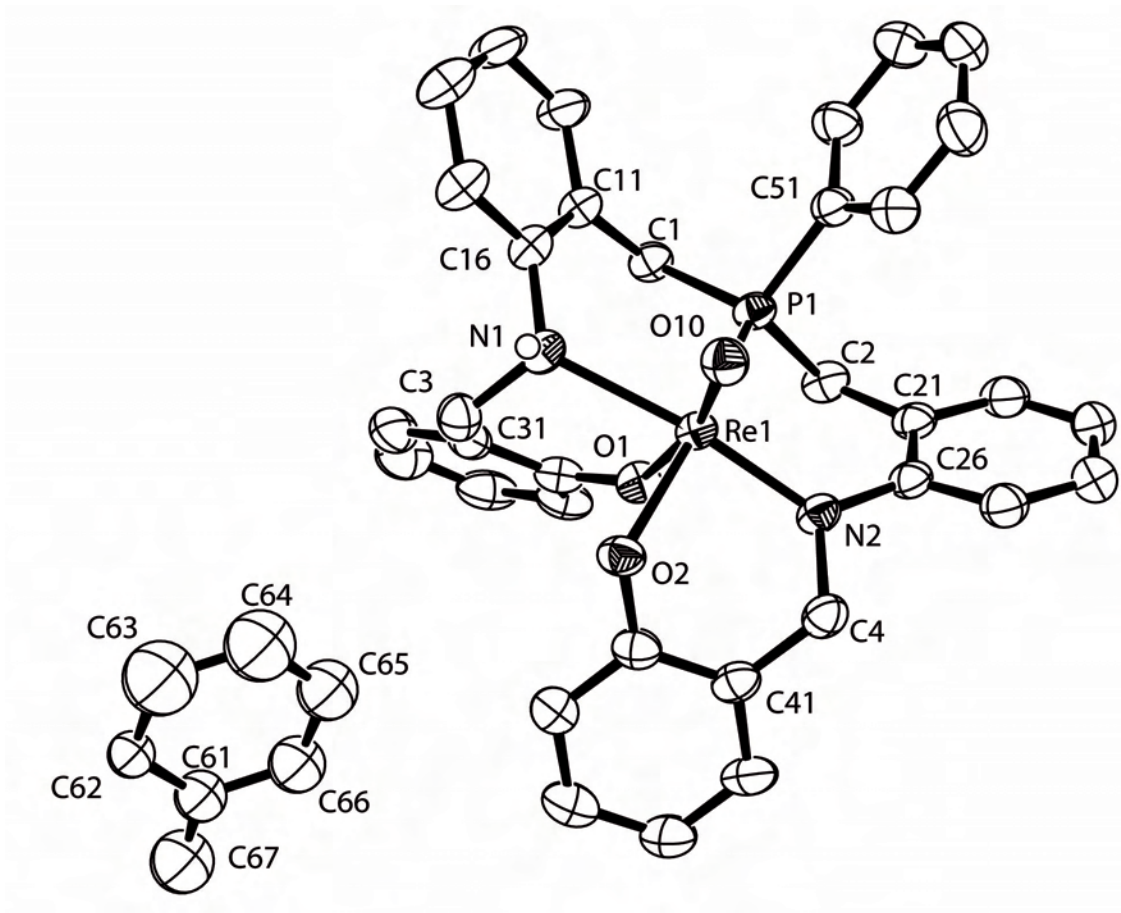


Abbildung 6.26: Ellipsoiddarstellung von  $[\text{ReO}(\text{HL}^{22})] \cdot 0.5 \text{ Toluol}$ . Die Schwingungsellipsoide repräsentieren 50% der Aufenthaltswahrscheinlichkeit. [121]



## 6.24 [ReOCl{ $\mu_2$ -(OL<sup>3</sup>)}ReOCl<sub>3</sub>] · 0.25 CH<sub>2</sub>Cl<sub>2</sub>

Tabelle 6.47: Kristallographische Daten und Parameter der Strukturrechnung von [ReOCl{ $\mu_2$ -(OL<sup>3</sup>)}ReOCl<sub>3</sub>] · 0.25 CH<sub>2</sub>Cl<sub>2</sub>

Summenformel	C <sub>43.25</sub> H <sub>31.5</sub> N <sub>3</sub> O <sub>5</sub> Cl <sub>4.5</sub> P <sub>2</sub> Re <sub>2</sub>	
M (g/mol)	1267.08	
Messtemperatur	200(2) K	
Wellenlänge	0.71073 Å	
Kristallsystem, Raumgruppe	triklin, P $\bar{1}$	
Elementarzelle	a = 12.615(2) Å	$\alpha = 100.59(1)^\circ$
	b = 14.186(2) Å	$\beta = 105.15(1)^\circ$
	c = 16.108(2) Å	$\gamma = 93.21(1)^\circ$
Volumen	2718.6(7) Å <sup>3</sup>	
Z	2	
Berechnete Dichte	1.548 g/cm <sup>3</sup>	
Linearer Absorptionskoeffizient	4.768 mm <sup>-1</sup>	
F(000)	1217	
Kristallgröße	0.140 x 0.073 x 0.030 mm <sup>3</sup>	
Theta-Bereich	2.29 - 27.75°	
Indizes	-13 ≤ h ≤ 16, -18 ≤ k ≤ 18, -20 ≤ l ≤ 20	
Zahl der gemessenen Reflexe	23.821	
Zahl der unabhängigen Reflexe	11704 [R(int) = 0.1127]	
Zahl der verfeinerten Parameter	542	
Goof	1.119	
R <sub>1</sub> / wR <sub>2</sub> [I > 2σ(I)]	R <sub>1</sub> = 0.0579, wR <sub>2</sub> = 0.0988	
R <sub>1</sub> / wR <sub>2</sub> (alle Reflexe)	R <sub>1</sub> = 0.1438, wR <sub>2</sub> = 0.1186	
Restelektronendichte	1.349 und -0.964 e · Å <sup>-3</sup>	
Programm zur Strukturlösung	SHELXS 97 [119]	

Tabelle 6.48: Atomkoordinaten ( $\cdot 10^4$ ) und isotrope Temperaturparameter ( $\text{\AA}^2 \cdot 10^3$ ) von  $[\text{ReOCl}\{\mu_2\text{-(OL}^3)\}\text{ReOCl}_3] \cdot 0.25 \text{CH}_2\text{Cl}_2$

	x	y	z	E(eq)
Re(1)	6917(1)	1763(1)	2329(1)	33(1)
O(10)	5565(6)	2049(6)	2253(4)	41(2)
Cl(1)	6513(2)	72(2)	2142(2)	41(1)
O(11)	8578(6)	1357(5)	2417(4)	33(2)
P(1)	8999(2)	945(2)	1645(2)	32(1)
C(11)	7916(9)	440(8)	668(6)	36(3)
C(12)	7949(10)	-439(8)	121(6)	39(3)
C(13)	7065(12)	-759(9)	-661(8)	51(3)
C(14)	6220(10)	-231(9)	-850(7)	45(3)
C(15)	6156(10)	633(10)	-319(7)	51(3)
C(16)	7005(9)	954(8)	454(6)	33(3)
N(1)	6995(7)	1806(6)	1090(5)	35(2)
C(41)	9803(8)	1861(7)	1402(6)	29(2)
C(42)	9891(10)	1814(8)	564(7)	42(3)
C(43)	10559(12)	2532(9)	395(8)	57(3)
C(44)	11123(12)	3276(10)	1047(9)	61(4)
C(45)	11023(11)	3336(10)	1883(8)	60(4)
C(46)	10362(10)	2615(8)	2058(7)	43(3)
C(51)	9837(10)	9(7)	1897(6)	34(3)
C(52)	9404(12)	-725(9)	2257(8)	52(3)
C(53)	9993(12)	-1478(9)	2414(8)	52(3)
C(54)	10983(12)	-1542(9)	2191(8)	53(3)
C(55)	11389(10)	-872(9)	1844(7)	45(3)
C(56)	10800(10)	-93(8)	1685(6)	38(3)
C(17)	7279(10)	2689(8)	942(7)	40(3)

O(17)	7306(8)	2884(6)	231(5)	55(2)
C(21)	7643(10)	3457(9)	1766(7)	42(3)
C(22)	8077(11)	4429(9)	1876(8)	48(3)
C(23)	8497(11)	4930(10)	2710(8)	54(3)
C(24)	8481(10)	4570(8)	3437(8)	40(3)
C(25)	8030(9)	3644(8)	3305(7)	34(2)
N(26)	7645(7)	3118(6)	2493(5)	33(2)
Re(2)	7494(1)	4210(1)	5683(1)	40(1)
O(20)	6691(8)	4595(6)	6312(6)	58(2)
Cl(2)	8895(3)	3649(2)	6715(2)	55(1)
Cl(3)	8782(3)	5557(2)	5861(2)	58(1)
Cl(4)	6436(3)	4705(2)	4427(2)	52(1)
P(2)	6432(2)	2584(2)	5288(2)	32(1)
C(31)	7282(9)	1625(7)	5042(6)	36(3)
C(32)	7472(9)	965(7)	5592(7)	36(3)
C(33)	8091(11)	195(9)	5422(8)	50(3)
C(34)	8510(10)	99(8)	4708(7)	43(3)
C(35)	8312(9)	752(8)	4155(7)	38(3)
C(36)	7727(8)	1506(7)	4317(6)	28(2)
N(3)	7596(7)	2154(6)	3718(5)	31(2)
C(37)	7980(9)	3071(7)	4006(7)	30(2)
O(37)	8318(7)	3475(5)	4797(5)	42(2)
C(61)	5938(10)	2297(8)	6186(7)	38(3)
C(62)	6469(11)	2726(9)	7055(7)	48(3)
C(63)	6093(12)	2433(9)	7720(8)	54(3)
C(64)	5229(11)	1762(9)	7555(8)	51(3)
C(65)	4686(12)	1357(9)	6691(8)	56(3)
C(66)	5046(11)	1619(9)	6019(7)	49(3)

C(71)	5178(9)	2301(8)	4382(6)	34(3)
C(72)	4906(9)	1422(8)	3831(7)	39(3)
C(73)	3860(11)	1209(10)	3238(8)	55(4)
C(74)	3106(11)	1841(11)	3173(9)	60(4)
C(75)	3409(11)	2767(10)	3744(9)	62(4)
C(76)	4428(10)	3006(9)	4338(7)	42(3)
Cl(97)	1980(11)	2574(7)	6346(8)	50(2)
C(98)	980(30)	2610(30)	5465(13)	50(2)
Cl(99)	741(11)	2094(8)	4449(8)	50(2)

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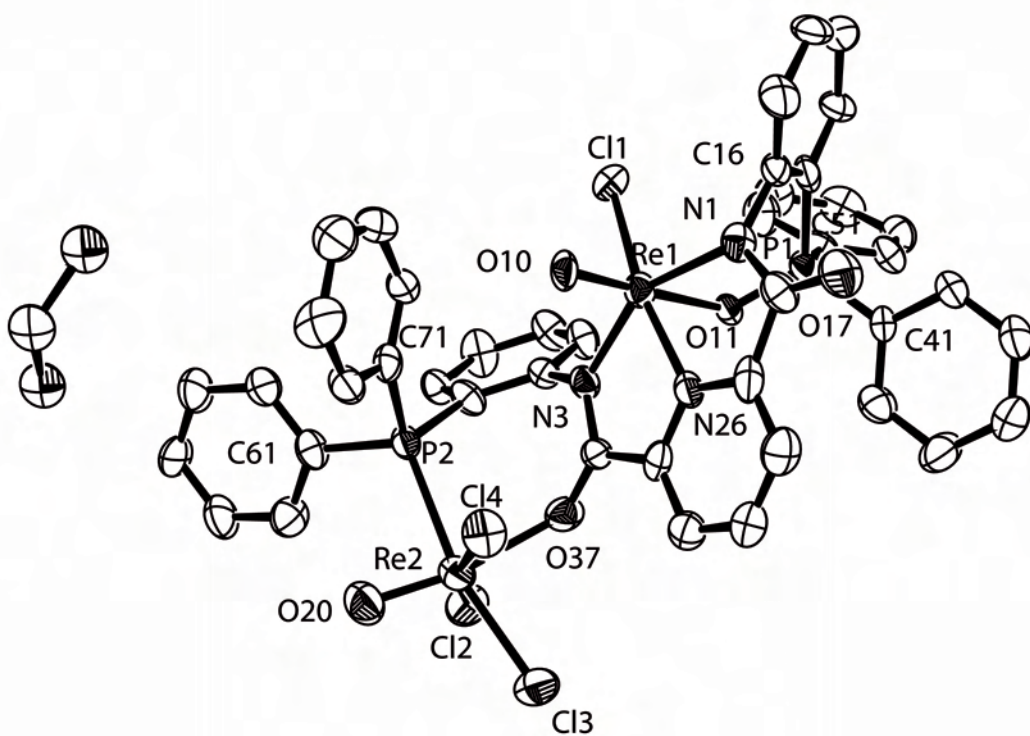


Abbildung 6.27: Ellipsoiddarstellung von  $[\text{ReOCl}\{\mu_2\text{-(OL}^3)\}\text{ReOCl}_3] \cdot 0.25 \text{CH}_2\text{Cl}_2$ . Die Schwingungsellipsoide repräsentieren 50% der Aufenthaltswahrscheinlichkeit. [121]



## 6.25 [ReCl{ $\mu_2$ -(O<sub>2</sub>L<sup>3</sup>)}( $\mu_2$ -Cl)( $\mu_2$ -O)ReCl<sub>3</sub>] · 0.25 CH<sub>2</sub>Cl<sub>2</sub>

Tabelle 6.49: Kristallographische Daten und Parameter der Strukturrechnung von [ReCl{ $\mu_2$ -(O<sub>2</sub>L<sup>3</sup>)}( $\mu_2$ -Cl)( $\mu_2$ -O)ReCl<sub>3</sub>] · 0.25 CH<sub>2</sub>Cl<sub>2</sub>

Summenformel	C <sub>43.25</sub> H <sub>31.5</sub> N <sub>3</sub> O <sub>5</sub> Cl <sub>4.5</sub> P <sub>2</sub> Re <sub>2</sub>	
M (g/mol)	1267.08	
Messtemperatur	200(2) K	
Wellenlänge	0.71073 Å	
Kristallsystem, Raumgruppe	monoklin, P2 <sub>1</sub> /c	
Elementarzelle	a = 11.7090(1) Å	$\alpha = 90.00^\circ$
	b = 16.240(1) Å	$\beta = 97.27(1)^\circ$
	c = 24.725(2) Å	$\gamma = 90.00^\circ$
Volumen	4663.8(6) Å <sup>3</sup>	
Z	4	
Berechnete Dichte	1.805 g/cm <sup>3</sup>	
Linearer Absorptionskoeffizient	5.559 mm <sup>-1</sup>	
F(000)	2434	
Kristallgröße	0.20 x 0.13 x 0.06 mm <sup>3</sup>	
Theta-Bereich	2.25 - 28.68°	
Indizes	-14 ≤ h ≤ 14, -19 ≤ k ≤ 20, -31 ≤ l ≤ 31	
Zahl der gemessenen Reflexe	27097	
Zahl der unabhängigen Reflexe	10069 [R(int) = 0.1152]	
Zahl der verfeinerten Parameter	555	
Goof	0.924	
R <sub>1</sub> / wR <sub>2</sub> [I > 2σ(I)]	R <sub>1</sub> = 0.0582, wR <sub>2</sub> = 0.1170	
R <sub>1</sub> / wR <sub>2</sub> (alle Reflexe)	R <sub>1</sub> = 0.1068, wR <sub>2</sub> = 0.1327	
Restelektronendichte	1.790 und -1.515 e · Å <sup>-3</sup>	
Programm zur Strukturlösung	SHELXS 97 [119]	

Tabelle 6.50: Atomkoordinaten ( $\cdot 10^4$ ) und isotrope Temperaturparameter ( $\text{\AA}^2 \cdot 10^3$ ) von  $[\text{ReCl}\{\mu_2\text{-(O}_2\text{L}^3)\}(\mu_2\text{-Cl})(\mu_2\text{-O})\text{ReCl}_3] \cdot 0.25 \text{CH}_2\text{Cl}_2$

	x	y	z	E(eq)
Re(1)	4083(1)	5154(1)	1467(1)	35(1)
Cl(1)	4740(3)	5264(2)	631(1)	49(1)
Cl(2)	6046(2)	5159(2)	1886(1)	45(1)
Cl(3)	4333(3)	3702(2)	1399(1)	53(1)
Cl(4)	2154(2)	4957(2)	1042(1)	47(1)
O(30)	4242(6)	6260(5)	1649(3)	36(2)
O(10)	3663(6)	4837(5)	2223(3)	42(2)
P(1)	2925(2)	4885(2)	2674(1)	39(1)
C(41)	3453(10)	5660(8)	3143(5)	44(3)
C(42)	2825(11)	5933(9)	3556(6)	56(3)
C(43)	3280(12)	6526(9)	3932(5)	62(4)
C(44)	4327(13)	6860(10)	3895(6)	71(4)
C(45)	4952(11)	6623(9)	3466(6)	58(4)
C(46)	4516(10)	6012(8)	3107(6)	53(3)
C(51)	3023(10)	3892(8)	3003(5)	46(3)
C(52)	3391(11)	3235(8)	2731(5)	55(3)
C(53)	3516(14)	2482(9)	2975(7)	69(4)
C(54)	3320(13)	2374(10)	3503(7)	70(4)
C(55)	2998(16)	3004(10)	3778(7)	83(5)
C(56)	2846(15)	3789(10)	3547(7)	77(5)
C(11)	1429(8)	5085(7)	2449(4)	35(2)
C(12)	560(10)	4524(9)	2540(5)	55(3)
C(13)	-564(11)	4713(12)	2377(6)	68(5)
C(14)	-882(11)	5475(11)	2142(6)	63(4)
C(15)	-44(9)	6036(9)	2050(5)	51(3)



C(16)	1113(9)	5838(8)	2196(4)	42(3)
N(1)	1997(7)	6391(6)	2058(3)	36(2)
C(17)	2111(9)	7129(8)	2322(5)	42(3)
O(17)	1649(7)	7329(6)	2717(3)	55(2)
C(21)	2839(9)	7737(7)	2057(4)	38(2)
C(22)	3255(10)	8485(7)	2270(5)	45(3)
C(23)	3854(11)	8982(9)	1942(6)	58(4)
C(24)	4014(11)	8728(8)	1419(6)	56(3)
C(25)	3619(9)	7970(7)	1242(5)	40(3)
N(26)	3040(7)	7515(6)	1565(3)	36(2)
C(27)	3618(9)	7618(8)	671(5)	43(3)
O(27)	4026(8)	7998(6)	317(3)	56(2)
N(3)	3056(7)	6886(6)	611(3)	39(2)
C(31)	1377(10)	6663(8)	-44(5)	47(3)
C(32)	846(10)	6383(10)	-554(5)	58(4)
C(33)	1512(12)	6158(10)	-943(5)	62(4)
C(34)	2678(10)	6175(9)	-838(5)	54(3)
C(35)	3229(10)	6387(8)	-325(5)	49(3)
C(36)	2580(9)	6627(7)	79(4)	37(2)
Re(2)	2693(1)	6320(1)	1326(1)	32(1)
P(2)	604(2)	7052(2)	481(1)	43(1)
O(20)	986(6)	6651(6)	1037(3)	43(2)
C(61)	831(9)	8151(8)	518(5)	48(3)
C(62)	1207(13)	8573(11)	98(7)	72(4)
C(63)	1398(17)	9405(13)	158(10)	99(6)
C(64)	1230(20)	9822(12)	628(10)	107(7)
C(65)	817(18)	9395(12)	1047(8)	94(6)
C(66)	614(13)	8542(9)	1001(6)	60(4)

C(71)	-904(9)	6863(10)	301(5)	53(3)
C(72)	-1377(10)	6154(10)	506(6)	60(4)
C(73)	-2524(12)	5996(11)	345(7)	72(4)
C(74)	-3171(11)	6536(11)	-12(6)	70(5)
C(75)	-2713(12)	7220(12)	-205(6)	74(4)
C(76)	-1563(10)	7419(11)	-38(5)	64(4)
Cl(97)	1540(8)	2943(7)	1548(4)	39(2)
C(98)	710(30)	2209(16)	1768(11)	29(8)
Cl(99)	224(12)	1454(7)	1339(6)	59(3)

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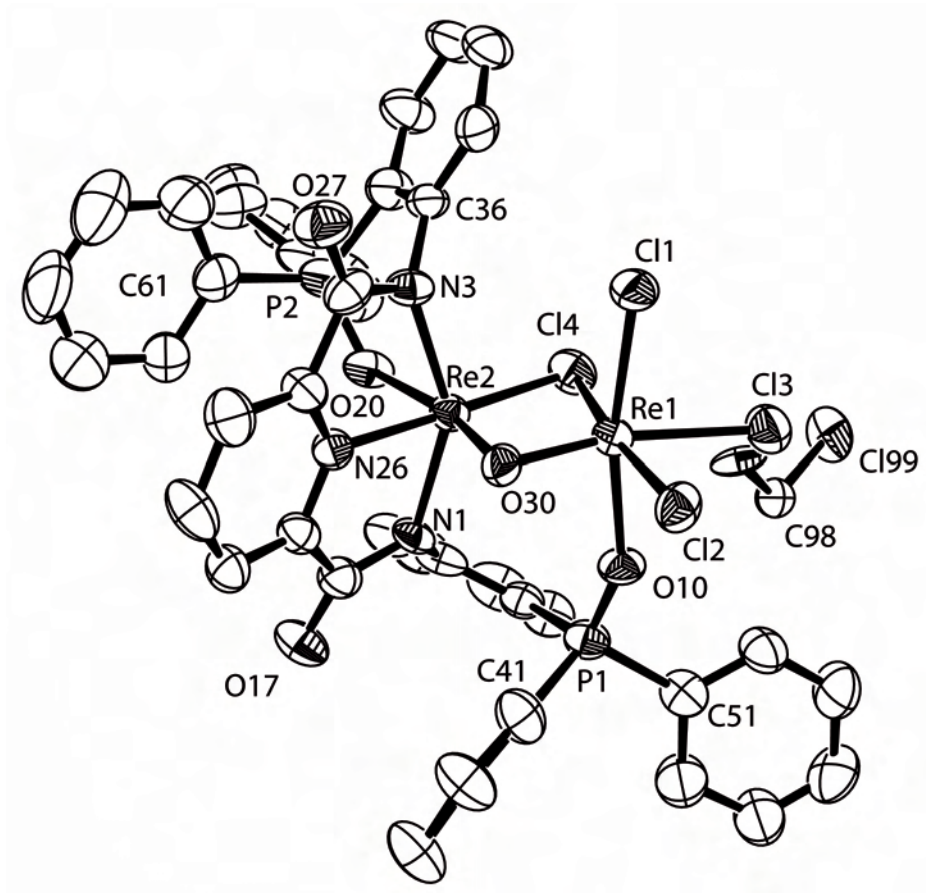


Abbildung 6.28: Ellipsoiddarstellung von  $[\text{ReCl}\{\mu_2\text{-(O}_2\text{L}^3)\}(\mu_2\text{-Cl})(\mu_2\text{-O})\text{ReCl}_3] \cdot 0.25 \text{CH}_2\text{Cl}_2$ . Die Schwingungsellipsoide repräsentieren 50% der Aufenthaltswahrscheinlichkeit. [121]



## 6.26 [ReO{OL<sub>3</sub>(OP,N,N,N,P)}][ReO<sub>4</sub>]

Tabelle 6.51: Kristallographische Daten und Parameter der Strukturrechnung von [ReO{OL<sub>3</sub>(OP,N,N,N,P)}][ReO<sub>4</sub>]

Summenformel	C <sub>43</sub> H <sub>31</sub> N <sub>3</sub> O <sub>8</sub> P <sub>2</sub> Re <sub>2</sub>	
M (g/mol)	1152.05	
Messtemperatur	200(2) K	
Wellenlänge	0.71073 Å	
Kristallsystem, Raumgruppe	monoklin, P2 <sub>1</sub> /c	
Elementarzelle	a = 15.573(2) Å	α = 90.00°
	b = 14.403(1) Å	β = 93.10(1)°
	c = 17.410(2) Å	γ = 90.00°
Volumen	3899.3(7) Å <sup>3</sup>	
Z	4	
Berechnete Dichte	1.962 g/cm <sup>3</sup>	
Linearer Absorptionskoeffizient	6.345 mm <sup>-1</sup>	
F(000)	2216	
Kristallgröße	0.45 x 0.05 x 0.05 mm <sup>3</sup>	
Theta-Bereich	2.22 - 28.11°	
Indizes	-21 ≤ h ≤ 21, -19 ≤ k ≤ 19, -16 ≤ l ≤ 23	
Zahl der gemessenen Reflexe	27775	
Zahl der unabhängigen Reflexe	10468 [R(int) = 0.0973]	
Zahl der verfeinerten Parameter	524	
Goof	0.845	
R <sub>1</sub> / wR <sub>2</sub> [I > 2σ(I)]	R <sub>1</sub> = 0.0441, wR <sub>2</sub> = 0.840	
R <sub>1</sub> / wR <sub>2</sub> (alle Reflexe)	R <sub>1</sub> = 0.0961, wR <sub>2</sub> = 0.0983	
Restelektronendichte	1.154 und -1.481 e · Å <sup>-3</sup>	
Programm zur Strukturlösung	SHELXS 86 [118]	

Tabelle 6.52: Atomkoordinaten ( $\cdot 10^4$ ) und isotrope Temperaturparameter ( $\text{\AA}^2 \cdot 10^3$ ) von  $[\text{ReO}\{\text{OL}_3(\text{OP},\text{N},\text{N},\text{N},\text{P})\}][\text{ReO}_4]$

	x	y	z	E(eq)
Re(1)	-1(1)	3089(1)	1557(1)	39(1)
O(10)	489(3)	2613(3)	841(3)	53(1)
P(1)	-1364(1)	2601(1)	912(1)	44(1)
C(11)	-1663(4)	3693(5)	470(4)	46(2)
C(12)	-2360(5)	3779(6)	-64(4)	53(2)
C(13)	-2587(6)	4614(6)	-378(5)	66(2)
C(14)	-2135(6)	5396(6)	-162(5)	64(2)
C(15)	-1425(6)	5344(5)	329(4)	56(2)
C(16)	-1157(5)	4491(5)	650(4)	46(2)
N(1)	-382(4)	4354(4)	1119(3)	44(1)
C(17)	184(5)	5074(5)	1295(4)	48(2)
O(17)	125(4)	5878(4)	1062(4)	73(2)
C(21)	910(5)	4818(5)	1845(4)	45(2)
C(22)	1561(5)	5397(6)	2138(5)	56(2)
C(23)	2154(5)	5033(6)	2674(5)	59(2)
C(24)	2105(5)	4117(6)	2926(5)	55(2)
C(25)	1449(4)	3574(5)	2618(4)	46(2)
N(26)	884(4)	3944(4)	2093(3)	43(1)
C(27)	1233(5)	2606(5)	2847(4)	45(2)
O(27)	1660(4)	2172(4)	3319(3)	62(1)
N(3)	448(4)	2321(4)	2498(3)	40(1)
C(31)	-714(5)	1947(5)	3283(4)	45(2)
C(32)	-1186(6)	1322(5)	3710(5)	61(2)
C(33)	-941(7)	392(6)	3756(6)	79(3)
C(34)	-218(6)	102(5)	3389(6)	72(3)

C(35)	237(6)	714(5)	2956(5)	59(2)
C(36)	-11(5)	1629(5)	2902(4)	45(2)
P(2)	-936(1)	3166(1)	3221(1)	39(1)
O(20)	-928(3)	3513(3)	2398(2)	40(1)
C(41)	-1237(5)	1815(5)	109(4)	45(2)
C(42)	-1384(6)	862(5)	154(5)	64(2)
C(43)	-1174(7)	310(6)	-452(5)	77(3)
C(44)	-882(6)	662(6)	-1106(5)	64(2)
C(45)	-762(5)	1598(6)	-1169(4)	54(2)
C(46)	-924(5)	2165(5)	-558(4)	49(2)
C(51)	-2277(5)	2198(5)	1438(4)	50(2)
C(52)	-3067(5)	2656(6)	1402(5)	59(2)
C(53)	-3742(6)	2333(8)	1770(6)	80(3)
C(54)	-3638(7)	1558(7)	2261(6)	80(3)
C(55)	-2859(7)	1109(7)	2318(6)	79(3)
C(56)	-2171(6)	1426(6)	1908(5)	62(2)
C(61)	-1959(4)	3363(4)	3604(4)	39(1)
C(62)	-2645(5)	3647(5)	3127(4)	50(2)
C(63)	-3458(5)	3716(6)	3426(5)	67(2)
C(64)	-3577(5)	3476(6)	4181(5)	61(2)
C(65)	-2893(5)	3220(5)	4656(4)	53(2)
C(66)	-2085(5)	3168(5)	4365(4)	48(2)
C(71)	-137(4)	3757(4)	3820(4)	40(2)
C(72)	-11(5)	4696(5)	3683(4)	45(2)
C(73)	611(5)	5173(5)	4118(5)	54(2)
C(74)	1111(5)	4727(6)	4665(5)	58(2)
C(75)	976(6)	3804(6)	4814(5)	63(2)
C(76)	361(5)	3309(5)	4388(4)	48(2)

Re(2)	3586(1)	2829(1)	1594(1)	50(1)
O(30)	4013(5)	2894(5)	724(4)	84(2)
O(40)	2551(4)	2413(5)	1523(4)	88(2)
O(50)	3601(4)	3889(4)	2002(4)	76(2)
O(60)	4222(5)	2107(4)	2156(4)	84(2)

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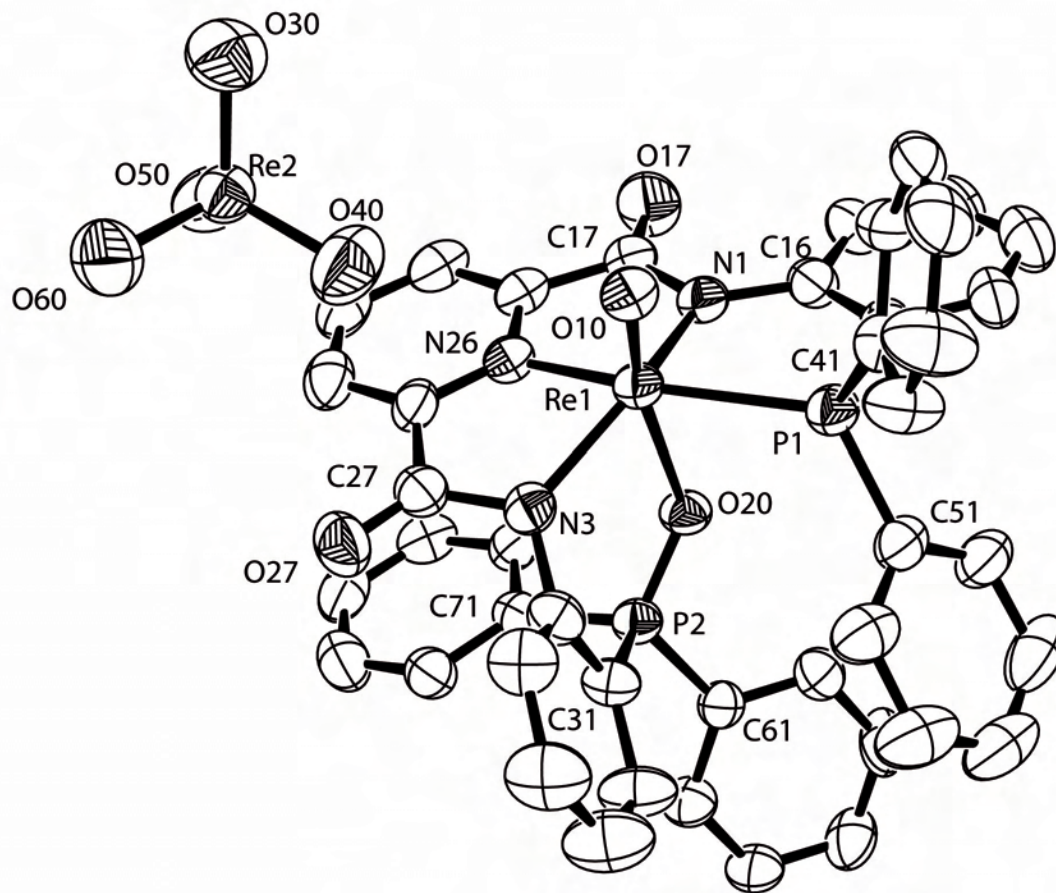


Abbildung 6.29: Ellipsoiddarstellung von  $[\text{ReO}\{\text{OL}_3(\text{OP},\text{N},\text{N},\text{N},\text{P})\}][\text{ReO}_4]$ . Die Schwingungsellipsoide repräsentieren 50% der Aufenthaltswahrscheinlichkeit. [121]



## 6.27 [ReO{O<sub>2</sub>L<sub>3</sub>(OP,N,N,N)}Cl]

Tabelle 6.53: Kristallographische Daten und Parameter der Strukturrechnung von [ReO{O<sub>2</sub>L<sub>3</sub>(OP,N,N,N)}Cl]

Summenformel	C <sub>43</sub> H <sub>31</sub> N <sub>3</sub> O <sub>5</sub> ClP <sub>2</sub> Re	
M (g/mol)	953.30	
Messtemperatur	200(2) K	
Wellenlänge	0.71073 Å	
Kristallsystem, Raumgruppe	triklin, P $\bar{1}$	
Elementarzelle	a = 11.987(1) Å	$\alpha = 68.17(1)^\circ$
	b = 14.832(2) Å	$\beta = 89.40(1)^\circ$
	c = 15.059(2) Å	$\gamma = 74.86(1)^\circ$
Volumen	2387.9(5) Å <sup>3</sup>	
Z	2	
Berechnete Dichte	1.326 g/cm <sup>3</sup>	
Linearer Absorptionskoeffizient	2.708 mm <sup>-1</sup>	
F(000)	944	
Kristallgröße	0.400 x 0.207 x 0.020 mm <sup>3</sup>	
Theta-Bereich	2.21 - 29.34°	
Indizes	-15 ≤ h ≤ 13, -18 ≤ k ≤ 18, -18 ≤ l ≤ 19	
Zahl der gemessenen Reflexe	20099	
Zahl der unabhängigen Reflexe	10220 [R(int) = 0.1185]	
Zahl der verfeinerten Parameter	579	
Goof	0.865	
R <sub>1</sub> / wR <sub>2</sub> [I > 2σ(I)]	R <sub>1</sub> = 0.0579, wR <sub>2</sub> = 0.1278	
R <sub>1</sub> / wR <sub>2</sub> (alle Reflexe)	R <sub>1</sub> = 0.0967, wR <sub>2</sub> = 0.1393	
Restelektronendichte	1.480 und -2.073 e · Å <sup>-3</sup>	
Programm zur Strukturlösung	SHELXS 97 [119]	

Tabelle 6.54: Atomkoordinaten ( $\cdot 10^4$ ) und isotrope Temperaturparameter ( $\text{\AA}^2 \cdot 10^3$ ) von  $[\text{ReO}\{\text{O}_2\text{L}_3(\text{OP},\text{N},\text{N},\text{N})\}\text{Cl}]$

	x	y	z	E(eq)
Re(1)	8045(1)	7639(1)	6800(1)	38(1)
O(30)	7780(5)	8482(4)	7320(4)	51(1)
Cl(1)	8252(2)	8830(1)	5266(2)	50(1)
P(1)	7486(2)	6578(1)	5299(2)	42(1)
O(10)	8334(5)	6647(3)	5981(4)	42(1)
C(41)	7081(7)	5419(5)	5866(6)	48(2)
C(42)	7908(9)	4601(7)	6470(9)	81(4)
C(43)	7611(12)	3709(7)	6999(11)	106(5)
C(44)	6524(11)	3644(7)	6876(9)	77(3)
C(45)	5709(11)	4469(9)	6313(10)	92(4)
C(46)	5971(9)	5358(7)	5807(9)	74(3)
C(51)	8147(8)	6582(6)	4212(6)	50(2)
C(52)	8798(9)	7272(7)	3819(7)	65(3)
C(53)	9218(11)	7378(9)	2953(9)	87(3)
C(54)	9080(10)	6775(9)	2508(8)	77(3)
C(55)	8438(10)	6072(8)	2904(7)	71(3)
C(56)	7986(8)	5985(6)	3753(7)	60(2)
C(11)	6158(7)	7605(5)	4928(6)	43(2)
C(12)	5584(8)	7961(6)	4042(6)	51(2)
C(13)	4557(7)	8743(6)	3802(7)	52(2)
C(14)	4148(8)	9151(6)	4458(7)	54(2)
C(15)	4732(7)	8810(5)	5364(7)	50(2)
C(16)	5739(6)	8015(5)	5602(6)	41(2)
N(1)	6397(5)	7589(4)	6538(4)	38(1)
C(17)	5986(8)	6904(6)	7255(6)	50(2)

O(17)	5028(5)	6760(4)	7240(5)	63(2)
C(21)	6899(8)	6228(6)	8072(6)	50(2)
C(22)	6772(9)	5455(7)	8881(7)	66(3)
C(23)	7775(9)	4807(7)	9495(7)	71(3)
C(24)	8869(8)	4937(6)	9261(7)	58(2)
C(25)	8927(7)	5738(6)	8459(6)	49(2)
N(26)	7953(6)	6384(5)	7894(5)	47(2)
C(27)	10009(7)	6015(5)	8056(6)	44(2)
O(28)	10960(5)	5427(4)	8413(4)	51(1)
N(3)	9768(6)	6889(4)	7255(5)	42(2)
C(31)	11524(7)	7528(5)	6939(6)	46(2)
C(32)	12505(7)	7579(6)	6435(6)	48(2)
C(33)	12753(8)	7170(6)	5765(6)	50(2)
C(34)	11981(8)	6683(6)	5554(6)	50(2)
C(35)	11015(7)	6634(5)	6016(6)	46(2)
C(36)	10767(7)	7029(5)	6739(6)	41(2)
P(2)	11264(2)	8049(1)	7865(2)	45(1)
O(20)	11006(5)	7356(4)	8796(4)	53(1)
C(61)	10125(8)	9211(5)	7372(6)	46(2)
C(62)	9976(8)	9804(6)	6387(7)	52(2)
C(63)	9139(9)	10729(6)	6040(7)	60(2)
C(64)	8489(9)	11075(6)	6660(8)	62(2)
C(65)	8632(10)	10495(7)	7626(8)	76(3)
C(66)	9452(9)	9564(7)	7976(7)	64(3)
C(71)	12548(8)	8413(6)	8004(6)	50(2)
C(72)	12739(10)	9302(8)	7416(8)	74(3)
C(73)	13800(13)	9502(12)	7575(11)	96(4)
C(74)	14617(12)	8862(13)	8262(13)	100(4)

C(75)	14467(12)	8003(12)	8804(12)	104(5)
C(76)	13438(10)	7733(9)	8713(10)	84(4)

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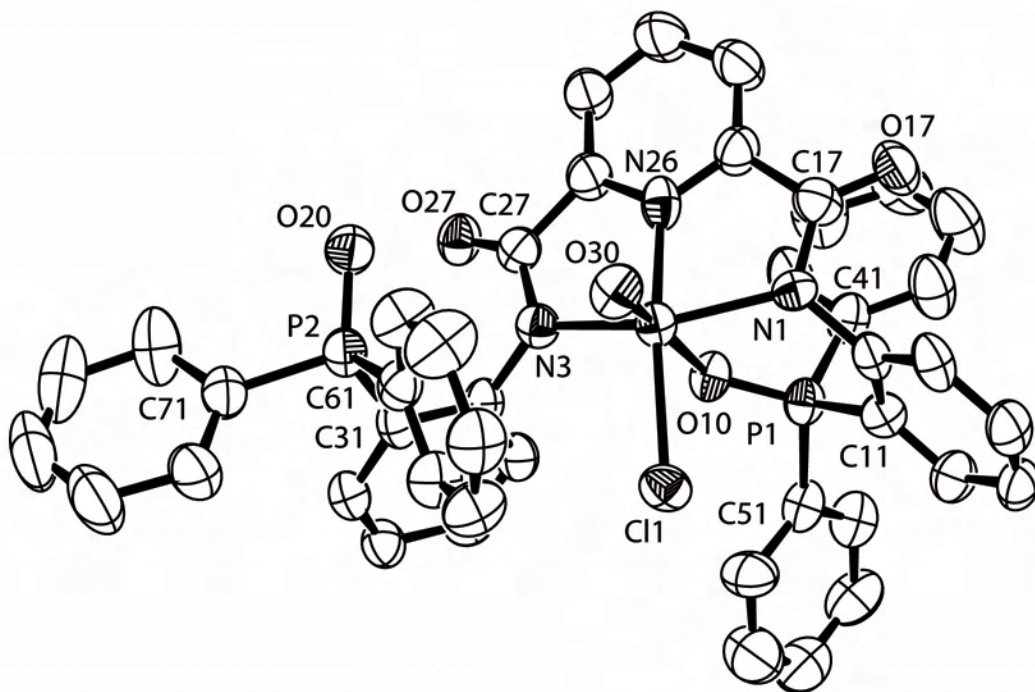


Abbildung 6.30: Ellipsoiddarstellung von  $[\text{ReO}\{\text{O}_2\text{L}_3(\text{OP},\text{N},\text{N},\text{N})\}\text{Cl}]$ . Die Schwingungselipsoide repräsentieren 50% der Aufenthaltswahrscheinlichkeit. [121]





## 6.28 [ReNCl<sub>2</sub>{H<sub>2</sub>L<sup>3</sup>(P,P)}] · CH<sub>2</sub>Cl<sub>2</sub>

Tabelle 6.55: Kristallographische Daten und Parameter der Strukturrechnung von [ReNCl<sub>2</sub>{H<sub>2</sub>L<sup>3</sup>(P,P)}] · CH<sub>2</sub>Cl<sub>2</sub>

Summenformel	C <sub>44</sub> H <sub>35</sub> N <sub>4</sub> O <sub>2</sub> Cl <sub>4</sub> P <sub>2</sub> Re	
M (g/mol)	1041.70	
Messtemperatur	200(2) K	
Wellenlänge	0.71073 Å	
Kristallsystem, Raumgruppe	triklin, P $\bar{1}$	
Elementarzelle	a = 13.484(2) Å	$\alpha = 82.66(1)^\circ$
	b = 13.558(2) Å	$\beta = 64.01(1)^\circ$
	c = 14.114(2) Å	$\gamma = 77.88(1)^\circ$
Volumen	2265.8(6) Å <sup>3</sup>	
Z	2	
Berechnete Dichte	1.527 g/cm <sup>3</sup>	
Linearer Absorptionskoeffizient	3.028 mm <sup>-1</sup>	
F(000)	1032	
Kristallgröße	0.500 x 0.253 x 0.090 mm <sup>3</sup>	
Theta-Bereich	2.09 - 29.65°	
Indizes	-18 ≤ h ≤ 18, -15 ≤ k ≤ 18, -19 ≤ l ≤ 19	
Zahl der gemessenen Reflexe	31074	
Zahl der unabhängigen Reflexe	12098 [R(int) = 0.0808]	
Zahl der verfeinerten Parameter	542	
Goof	1.119	
R <sub>1</sub> / wR <sub>2</sub> [I > 2σ(I)]	R <sub>1</sub> = 0.0560, wR <sub>2</sub> = 0.1600	
R <sub>1</sub> / wR <sub>2</sub> (alle Reflexe)	R <sub>1</sub> = 0.0610, wR <sub>2</sub> = 0.1669	
Restelektronendichte	3.050 und -2.377 e · Å <sup>-3</sup>	
Programm zur Strukturlösung	SHELXS 97 [119]	

Tabelle 6.56: Atomkoordinaten ( $\cdot 10^4$ ) und isotrope Temperaturparameter ( $\text{\AA}^2 \cdot 10^3$ ) von  $[\text{ReNCl}_2\{\text{H}_2\text{L}^3(\text{P},\text{P})\}] \cdot \text{CH}_2\text{Cl}_2$

	x	y	z	E(eq)
N(10)	6718(4)	1651(4)	1343(4)	36(1)
Re(1)	6448(1)	2875(1)	1137(1)	28(1)
Cl(1)	7355(1)	3658(1)	1872(1)	43(1)
Cl(2)	5284(1)	3276(1)	223(1)	35(1)
P(1)	8079(1)	2963(1)	-568(1)	29(1)
C(41)	9340(4)	2079(4)	-665(4)	33(1)
C(42)	9548(5)	1825(5)	227(5)	45(1)
C(43)	10518(6)	1155(5)	149(6)	51(1)
C(44)	11230(5)	710(5)	-785(7)	54(2)
C(45)	11037(5)	952(6)	-1665(6)	55(2)
C(46)	10093(5)	1644(5)	-1621(5)	48(1)
C(51)	8395(4)	4235(4)	-741(4)	32(1)
C(52)	9424(5)	4418(4)	-895(5)	42(1)
C(53)	9606(6)	5409(5)	-1001(6)	51(2)
C(54)	8765(6)	6200(5)	-930(6)	50(1)
C(55)	7711(5)	6017(4)	-769(5)	44(1)
C(56)	7535(4)	5042(4)	-673(5)	37(1)
C(11)	8018(4)	2782(4)	-1804(4)	33(1)
C(12)	8517(5)	3425(4)	-2704(5)	40(1)
C(13)	8679(5)	3208(5)	-3681(5)	47(1)
C(14)	8365(5)	2362(5)	-3830(5)	46(1)
C(15)	7851(5)	1727(5)	-2967(4)	39(1)
C(16)	7684(4)	1946(4)	-1967(4)	33(1)
N(1)	7124(4)	1308(3)	-1083(3)	33(1)
C(17)	7346(4)	284(4)	-1080(4)	32(1)

O(17)	8124(4)	-202(3)	-1781(3)	43(1)
C(21)	6562(4)	-226(4)	-121(4)	32(1)
C(22)	6771(5)	-1273(4)	-22(5)	40(1)
C(23)	6075(6)	-1740(4)	869(5)	46(1)
C(24)	5204(5)	-1149(4)	1653(5)	42(1)
C(25)	5047(4)	-113(4)	1484(4)	35(1)
N(26)	5701(3)	354(3)	607(3)	30(1)
C(27)	4085(4)	524(4)	2319(4)	34(1)
O(27)	3435(4)	145(3)	3106(4)	45(1)
N(3)	4041(4)	1527(3)	2081(4)	35(1)
C(31)	3364(4)	3154(4)	2904(4)	31(1)
C(32)	2457(4)	3931(4)	3382(5)	38(1)
C(33)	1356(5)	3809(5)	3635(5)	44(1)
C(34)	1158(5)	2933(5)	3416(5)	44(1)
C(35)	2042(4)	2166(4)	2920(5)	38(1)
C(36)	3142(4)	2283(4)	2641(4)	32(1)
P(2)	4749(1)	3215(1)	2798(1)	29(1)
C(61)	4571(4)	4513(4)	3131(4)	33(1)
C(62)	4330(6)	4782(5)	4126(5)	45(1)
C(63)	4151(7)	5783(5)	4356(6)	55(2)
C(64)	4237(6)	6534(5)	3555(6)	50(1)
C(65)	4464(5)	6266(5)	2563(6)	47(1)
C(66)	4650(5)	5260(4)	2336(5)	40(1)
C(71)	4799(4)	2397(4)	3911(4)	35(1)
C(72)	5803(5)	2025(5)	3967(5)	47(1)
C(73)	5857(7)	1387(6)	4801(6)	57(2)
C(74)	4902(7)	1117(6)	5580(6)	62(2)
C(75)	3893(8)	1500(9)	5536(8)	81(3)

C(76)	3838(6)	2134(7)	4717(6)	59(2)
Cl(97)	8680(2)	9820(3)	4698(3)	54(1)
C(98)	9640(8)	10414(12)	3640(10)	49(3)
Cl(99)	9008(2)	11535(3)	3208(2)	46(1)
Cl(87)	8381(5)	5782(7)	3631(4)	115(3)
C(88)	7504(17)	5789(14)	2995(14)	129(13)
Cl(89)	7644(4)	6708(6)	2050(5)	113(2)

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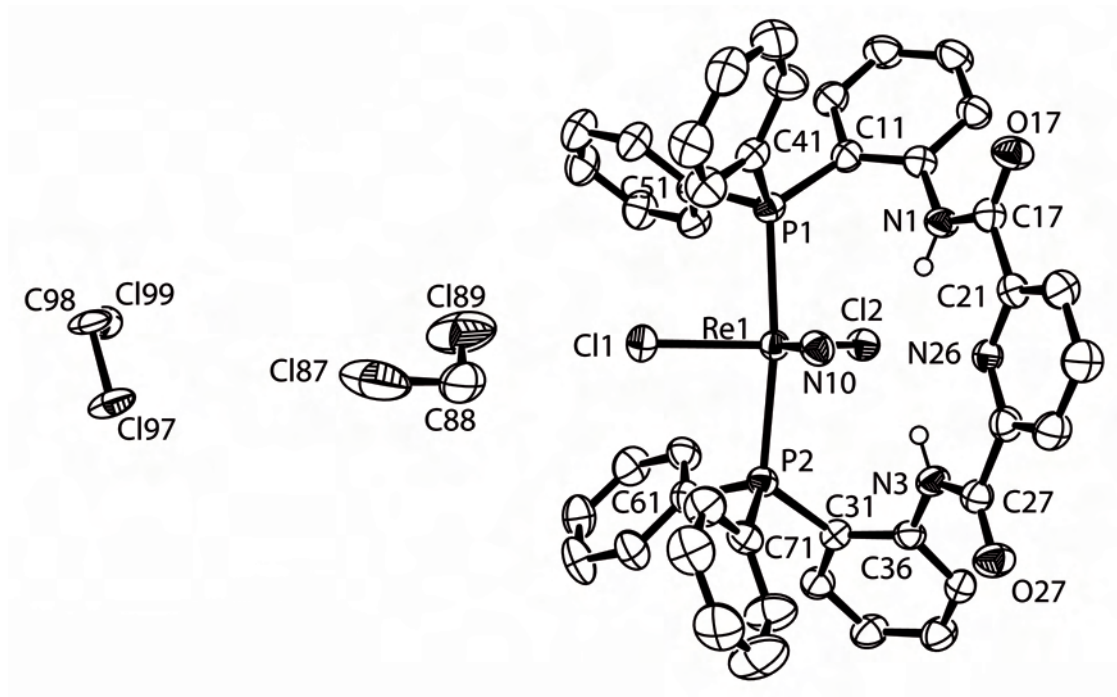


Abbildung 6.31: Ellipsoiddarstellung von  $[\text{ReNCl}_2\{\text{H}_2\text{L}^3(\text{P},\text{P})\}] \cdot \text{CH}_2\text{Cl}_2$ . Die Schwingungsellipsoide repräsentieren 50% der Aufenthaltswahrscheinlichkeit. [121]



## 6.29 [TcNCl<sub>2</sub>{H<sub>2</sub>L<sup>3</sup>(P,P)}] · CH<sub>2</sub>Cl<sub>2</sub>

Tabelle 6.57: Kristallographische Daten und Parameter der Strukturrechnung von [TcNCl<sub>2</sub>{H<sub>2</sub>L<sup>3</sup>(P,P)}] · CH<sub>2</sub>Cl<sub>2</sub>

Summenformel	C <sub>44</sub> H <sub>35</sub> N <sub>4</sub> O <sub>2</sub> Cl <sub>4</sub> P <sub>2</sub> Tc	
M (g/mol)	953.50	
Messtemperatur	200(2) K	
Wellenlänge	0.71073 Å	
Kristallsystem, Raumgruppe	triklin, P $\bar{1}$	
Elementarzelle	a = 13.447(2) Å	$\alpha = 82.87(2)^\circ$
	b = 13.548(2) Å	$\beta = 64.04(1)^\circ$
	c = 14.156(2) Å	$\gamma = 77.30(1)^\circ$
Volumen	2268.7(6) Å <sup>3</sup>	
Z	2	
Berechnete Dichte	1.396 g/cm <sup>3</sup>	
Linearer Absorptionskoeffizient	0.663 mm <sup>-1</sup>	
F(000)	968	
Kristallgröße	0.27 x 0.07 x 0.06 mm <sup>3</sup>	
Theta-Bereich	2.12 - 29.07°	
Indizes	-16 ≤ h ≤ 16, -16 ≤ k ≤ 12, -17 ≤ l ≤ 17	
Zahl der gemessenen Reflexe	11276	
Zahl der unabhängigen Reflexe	8734 [R(int) = 0.1284]	
Zahl der verfeinerten Parameter	541	
Goof	0.898	
R <sub>1</sub> / wR <sub>2</sub> [I > 2σ(I)]	R <sub>1</sub> = 0.0671, wR <sub>2</sub> = 0.1452	
R <sub>1</sub> / wR <sub>2</sub> (alle Reflexe)	R <sub>1</sub> = 0.1274, wR <sub>2</sub> = 0.1680	
Restelektronendichte	0.989 und -0.965 e · Å <sup>-3</sup>	
Programm zur Strukturlösung	SHELXS 97 [119]	

Tabelle 6.58: Atomkoordinaten ( $\cdot 10^4$ ) und isotrope Temperaturparameter ( $\text{\AA}^2 \cdot 10^3$ ) von  $[\text{TcNCl}_2\{\text{H}_2\text{L}^3(\text{P},\text{P})\}] \cdot \text{CH}_2\text{Cl}_2$

	x	y	z	E(eq)
Tc(1)	6450(1)	7864(1)	6133(1)	32(1)
N(10)	6698(4)	6687(4)	6334(4)	37(1)
Cl(1)	7360(1)	8663(1)	6861(1)	47(1)
Cl(2)	5276(1)	8254(1)	5221(1)	37(1)
P(1)	8089(1)	7974(1)	4414(1)	33(1)
C(41)	9354(6)	7091(5)	4305(5)	41(2)
C(42)	9563(6)	6843(6)	5199(6)	48(2)
C(43)	10503(6)	6163(6)	5138(7)	58(2)
C(44)	11224(6)	5709(6)	4205(7)	57(2)
C(45)	11023(6)	5949(6)	3330(7)	59(2)
C(46)	10084(6)	6647(6)	3385(6)	51(2)
C(51)	8401(5)	9239(5)	4241(5)	37(2)
C(52)	7558(6)	10048(5)	4325(5)	40(2)
C(53)	7735(6)	11023(5)	4221(6)	47(2)
C(54)	8772(7)	11220(6)	4064(6)	51(2)
C(55)	9617(7)	10430(6)	3991(6)	53(2)
C(56)	9438(6)	9432(6)	4082(6)	48(2)
C(11)	8021(5)	7811(5)	3184(5)	37(2)
C(12)	8503(6)	8440(5)	2306(5)	45(2)
C(13)	8656(7)	8214(6)	1315(6)	54(2)
C(14)	8353(6)	7365(6)	1175(5)	50(2)
C(15)	7837(6)	6750(5)	2017(5)	43(2)
C(16)	7669(5)	6966(5)	3028(5)	35(1)
N(1)	7125(4)	6321(4)	3892(4)	36(1)
C(17)	7339(5)	5309(5)	3918(5)	34(1)



O(17)	8137(4)	4813(4)	3222(4)	47(1)
C(21)	6574(5)	4779(5)	4868(5)	35(1)
C(22)	6761(6)	3745(5)	4979(5)	42(2)
C(23)	6073(6)	3273(5)	5874(6)	49(2)
C(24)	5202(6)	3858(5)	6643(6)	43(2)
C(25)	5042(5)	4894(5)	6471(5)	35(1)
N(26)	5703(4)	5359(4)	5605(4)	32(1)
C(27)	4100(5)	5532(5)	7307(5)	34(1)
O(27)	3439(4)	5147(4)	8108(4)	49(1)
N(3)	4025(5)	6532(4)	7084(4)	39(1)
C(31)	3355(5)	8154(5)	7902(5)	33(1)
C(32)	2433(6)	8900(5)	8391(5)	44(2)
C(33)	1358(6)	8797(6)	8640(5)	46(2)
C(34)	1152(6)	7907(6)	8415(5)	45(2)
C(35)	2041(6)	7165(5)	7897(5)	44(2)
C(36)	3123(5)	7276(5)	7643(5)	33(1)
P(2)	4737(1)	8217(1)	7796(1)	33(1)
C(61)	4785(6)	7405(5)	8911(5)	39(2)
C(62)	3840(7)	7131(7)	9708(6)	60(2)
C(63)	3911(9)	6488(8)	10542(7)	81(3)
C(64)	4910(8)	6122(6)	10558(7)	59(2)
C(65)	5851(8)	6405(7)	9798(6)	61(2)
C(66)	5809(6)	7052(6)	8955(6)	50(2)
C(71)	4571(5)	9511(5)	8119(5)	36(1)
C(72)	4303(6)	9788(5)	9132(5)	46(2)
C(73)	4172(8)	10789(6)	9331(6)	60(2)
C(74)	4255(7)	11518(6)	8541(6)	53(2)
C(75)	4476(6)	11258(6)	7561(6)	49(2)

C(76)	4641(6)	10269(5)	7352(5)	43(2)
Cl(87)	1640(4)	9242(6)	1359(4)	108(2)
C(88)	2567(17)	9157(13)	1998(12)	102(9)
Cl(89)	2381(4)	8250(5)	2926(4)	97(2)
Cl(97)	1333(3)	5191(3)	303(3)	55(1)
C(98)	341(10)	4615(11)	1346(10)	45(4)
Cl(99)	988(3)	3489(3)	1805(3)	44(1)

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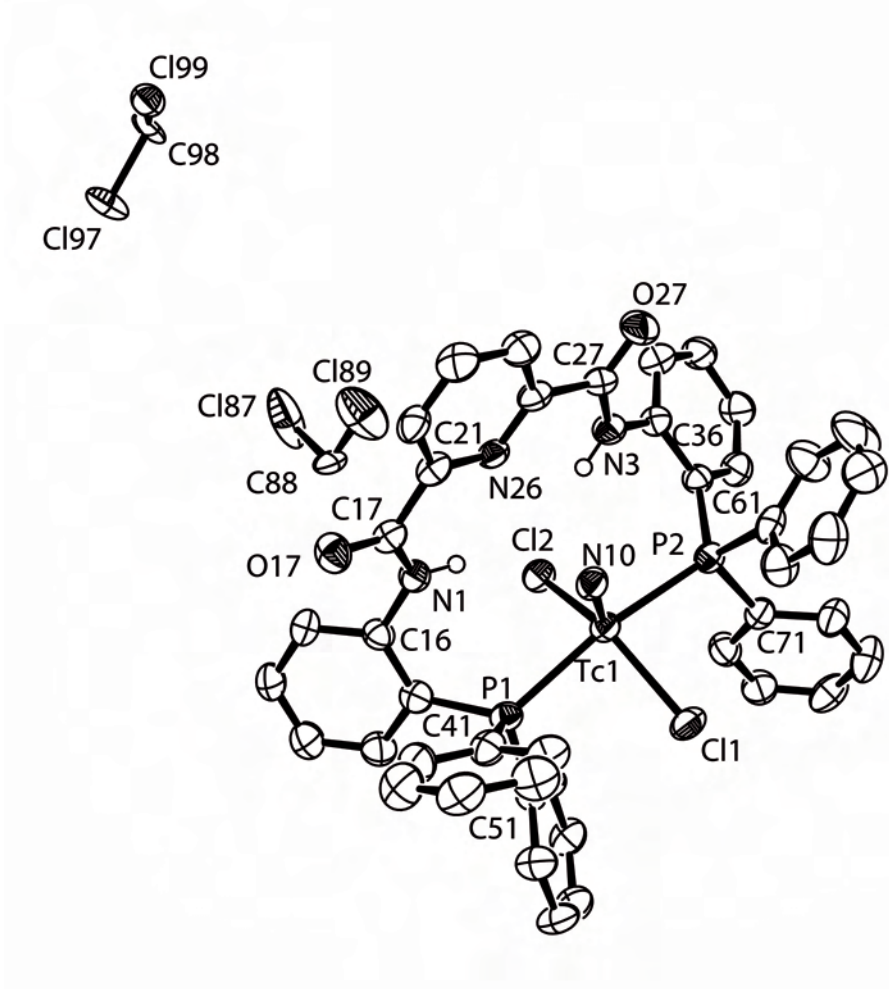


Abbildung 6.32: Ellipsoiddarstellung von  $[\text{TcNCl}_2\{\text{H}_2\text{L}^3(\text{P},\text{P})\}] \cdot \text{CH}_2\text{Cl}_2$ . Die Schwingungsellipsoide repräsentieren 50% der Aufenthaltswahrscheinlichkeit. [121]



## 6.30 [Ni{L<sub>3</sub>(P,N,N,N)}]

Tabelle 6.59: Kristallographische Daten und Parameter der Strukturrechnung von [Ni{L<sub>3</sub>(P,N,N,N)}]

Summenformel	C <sub>43</sub> H <sub>31</sub> N <sub>3</sub> O <sub>2</sub> P <sub>2</sub> Ni	
M (g/mol)	742.36	
Messtemperatur	200(2) K	
Wellenlänge	0.71073 Å	
Kristallsystem, Raumgruppe	monoklin, P2 <sub>1</sub> /c	
Elementarzelle	a = 19.272(2) Å	α = 90°
	b = 16.533(2) Å	β = 100.27(1)°
	c = 11.601(1) Å	γ = 90°
Volumen	3637.1(7) Å <sup>3</sup>	
Z	4	
Berechnete Dichte	1.356 g/cm <sup>3</sup>	
Linearer Absorptionskoeffizient	0.663 mm <sup>-1</sup>	
F(000)	1536	
Kristallgröße	0.25 x 0.10 x 0.05 mm <sup>3</sup>	
Theta-Bereich	2.17 - 28.69°	
Indizes	-22 ≤ h ≤ 22, -19 ≤ k ≤ 19, -13 ≤ l ≤ 13	
Zahl der gemessenen Reflexe	18439	
Zahl der unabhängigen Reflexe	6330 [R(int) = 0.1270]	
Zahl der verfeinerten Parameter	460	
Goof	0.939	
R <sub>1</sub> / wR <sub>2</sub> [I > 2σ(I)]	R <sub>1</sub> = 0.0661, wR <sub>2</sub> = 0.1182	
R <sub>1</sub> / wR <sub>2</sub> (alle Reflexe)	R <sub>1</sub> = 0.1309, wR <sub>2</sub> = 0.1401	
Restelektronendichte	0.957 und -0.404 e · Å <sup>-3</sup>	
Programm zur Strukturlösung	SHELXS 97 [119]	

Tabelle 6.60: Atomkoordinaten ( $\cdot 10^4$ ) und isotrope Temperaturparameter ( $\text{\AA}^2 \cdot 10^3$ ) von  $[\text{Ni}\{\text{L}_3(\text{P},\text{N},\text{N},\text{N})\}]$

	x	y	z	E(eq)
Ni(1)	3378(1)	5190(1)	-72(1)	27(1)
P(1)	3115(1)	5082(1)	1668(1)	26(1)
C(41)	2269(3)	5292(3)	2075(4)	27(1)
C(42)	1802(3)	4663(4)	2187(6)	47(2)
C(43)	1149(3)	4835(4)	2440(6)	60(2)
C(44)	941(3)	5611(4)	2592(6)	50(2)
C(45)	1389(3)	6238(4)	2477(5)	43(2)
C(46)	2051(3)	6077(3)	2209(5)	34(1)
C(51)	3349(3)	4107(3)	2324(5)	35(1)
C(52)	3332(4)	3436(3)	1642(5)	50(2)
C(53)	3462(5)	2678(4)	2140(7)	68(2)
C(54)	3622(4)	2582(4)	3301(7)	55(2)
C(55)	3670(6)	3243(4)	3989(7)	105(4)
C(56)	3542(7)	3999(4)	3505(7)	109(4)
C(11)	3726(3)	5814(3)	2434(5)	31(1)
C(12)	3740(3)	6073(3)	3581(5)	36(1)
C(13)	4228(3)	6645(4)	4081(6)	50(2)
C(14)	4679(3)	6981(4)	3423(6)	47(2)
C(15)	4682(3)	6738(3)	2286(5)	36(1)
C(16)	4201(3)	6145(3)	1772(5)	30(1)
C(17)	4631(3)	6021(3)	-78(5)	34(1)
O(17)	5184(2)	6401(2)	174(4)	45(1)
N(1)	4138(2)	5863(2)	607(4)	29(1)
C(21)	4426(3)	5633(3)	-1249(5)	31(1)
C(22)	4780(3)	5662(4)	-2188(6)	47(2)

C(23)	4507(3)	5225(4)	-3192(5)	50(2)
C(24)	3895(3)	4787(4)	-3248(5)	45(1)
C(25)	3549(3)	4796(3)	-2293(4)	35(1)
N(26)	3829(2)	5216(3)	-1345(3)	30(1)
C(27)	2875(3)	4400(3)	-2169(5)	34(1)
O(27)	2527(2)	4009(2)	-2969(3)	47(1)
N(3)	2710(2)	4569(2)	-1092(4)	30(1)
P(2)	1874(1)	6040(1)	-871(1)	33(1)
C(31)	1538(3)	5003(3)	-891(4)	33(1)
C(32)	863(3)	4813(4)	-694(5)	42(1)
C(33)	672(3)	4019(4)	-541(6)	47(2)
C(34)	1146(3)	3406(4)	-587(6)	50(2)
C(35)	1811(3)	3571(3)	-793(6)	46(2)
C(36)	2014(3)	4372(3)	-932(5)	33(1)
C(61)	2141(3)	6182(3)	-2298(5)	35(1)
C(62)	2663(3)	6760(3)	-2334(6)	46(2)
C(63)	2866(4)	6944(4)	-3387(7)	61(2)
C(64)	2580(4)	6557(4)	-4398(7)	62(2)
C(65)	2077(4)	5966(4)	-4370(6)	59(2)
C(66)	1860(3)	5772(4)	-3324(5)	45(2)
C(71)	1064(3)	6654(3)	-1072(5)	37(1)
C(72)	993(3)	7243(3)	-267(5)	41(1)
C(73)	421(4)	7754(4)	-415(6)	52(2)
C(74)	-108(4)	7682(4)	-1389(7)	57(2)
C(75)	-53(3)	7096(4)	-2213(6)	51(2)
C(76)	521(3)	6591(3)	-2066(5)	43(1)

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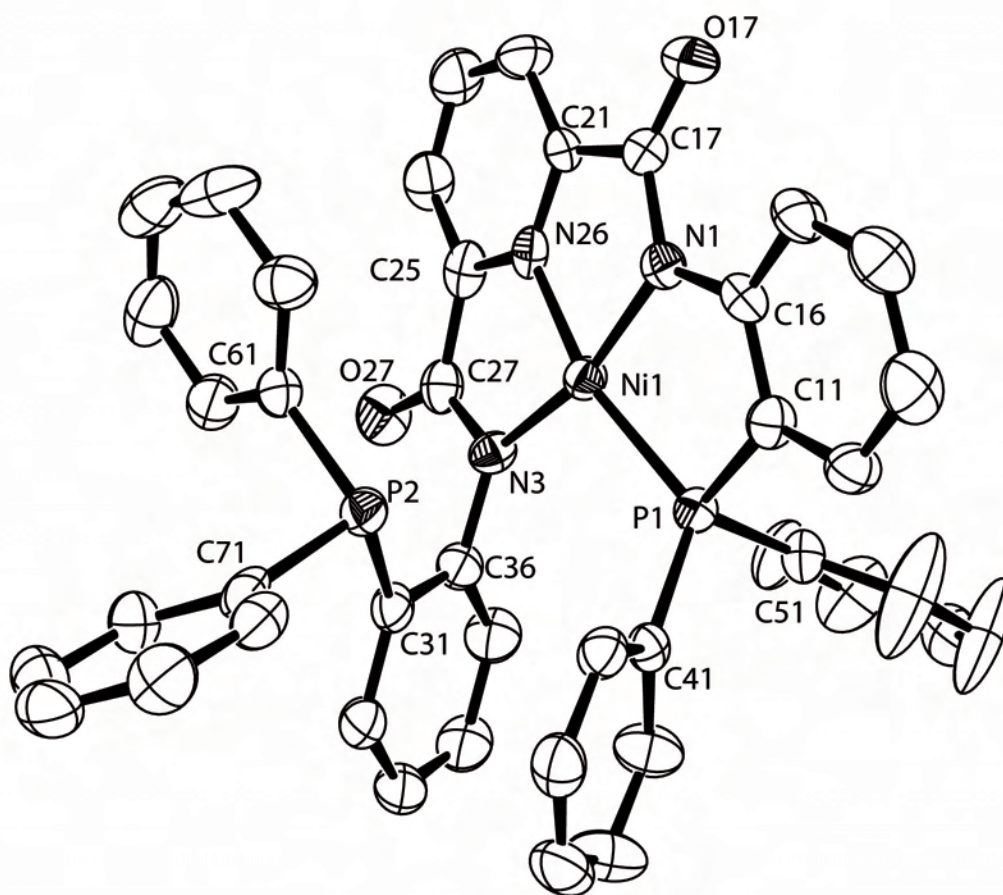


Abbildung 6.33: Ellipsoiddarstellung von  $[\text{Ni}\{\text{L}_3(\text{P},\text{N},\text{N},\text{N})\}]$ . Die Schwingungsellipsoide repräsentieren 50% der Aufenthaltswahrscheinlichkeit. [121]



## 6.31 [Pd{H<sub>2</sub>L<sup>3</sup>(P,P)}] · MeOH · CH<sub>2</sub>Cl<sub>2</sub>

Tabelle 6.61: Kristallographische Daten und Parameter der Strukturrechnung von [Pd{H<sub>2</sub>L<sup>3</sup>(P,P)}] · MeOH · CH<sub>2</sub>Cl<sub>2</sub>

Summenformel	C <sub>45</sub> H <sub>39</sub> N <sub>3</sub> O <sub>3</sub> P <sub>2</sub> Cl <sub>4</sub> Pd	
M (g/mol)	979.93	
Messtemperatur	200(2) K	
Wellenlänge	0.71073 Å	
Kristallsystem, Raumgruppe	triklin, P $\bar{1}$	
Elementarzelle	a = 11.360(1) Å	$\alpha = 114.08(1)^\circ$
	b = 13.778(1) Å	$\beta = 95.77(1)^\circ$
	c = 15.451(1) Å	$\gamma = 101.13(1)^\circ$
Volumen	3794.9(7) Å <sup>3</sup>	
Z	2	
Berechnete Dichte	1.533 g/cm <sup>3</sup>	
Linearer Absorptionskoeffizient	0.809 mm <sup>-1</sup>	
F(000)	996	
Kristallgröße	0.250 x 0.100 x 0.015 mm <sup>3</sup>	
Theta-Bereich	2.16 - 29.57°	
Indizes	-15 ≤ h ≤ 15, -18 ≤ k ≤ 16, -21 ≤ l ≤ 21	
Zahl der gemessenen Reflexe	23825	
Zahl der unabhängigen Reflexe	11351 [R(int) = 0.1042]	
Zahl der verfeinerten Parameter	525	
Goof	0.963	
R <sub>1</sub> / wR <sub>2</sub> [I > 2σ(I)]	R <sub>1</sub> = 0.0513, wR <sub>2</sub> = 0.1179	
R <sub>1</sub> / wR <sub>2</sub> (alle Reflexe)	R <sub>1</sub> = 0.0810, wR <sub>2</sub> = 0.1339	
Restelektronendichte	1.963 und -1.994 e · Å <sup>-3</sup>	
Programm zur Strukturlösung	SHELXS 86 [118]	

Tabelle 6.62: Atomkoordinaten ( $\cdot 10^4$ ) und isotrope Temperaturparameter ( $\text{\AA}^2 \cdot 10^3$ ) von  $[\text{Pd}\{\text{H}_2\text{L}^3(\text{P},\text{P})\}] \cdot \text{MeOH} \cdot \text{CH}_2\text{Cl}_2$

	x	y	z	E(eq)
Pd(1)	7587(1)	7461(1)	5463(1)	24(1)
Cl(1)	5479(1)	6885(1)	5181(1)	33(1)
Cl(2)	9660(1)	8028(1)	5661(1)	43(1)
C(41)	9015(4)	9102(3)	7990(2)	31(1)
C(42)	10213(4)	8991(4)	7970(3)	44(1)
C(43)	11181(5)	9825(5)	8639(3)	57(1)
C(44)	10995(5)	10756(4)	9336(3)	56(1)
C(45)	9823(5)	10878(4)	9363(3)	52(1)
C(46)	8835(4)	10061(3)	8701(3)	39(1)
C(51)	7884(3)	6789(3)	7298(2)	27(1)
C(52)	8668(4)	6862(3)	8093(3)	39(1)
C(53)	8743(4)	5923(4)	8194(3)	46(1)
C(54)	8036(4)	4915(4)	7516(4)	46(1)
C(55)	7240(4)	4833(4)	6739(3)	45(1)
C(56)	7177(4)	5763(3)	6623(3)	38(1)
P(1)	7735(1)	7994(1)	7131(1)	25(1)
C(11)	6433(3)	8356(3)	7679(2)	28(1)
C(12)	6073(4)	7980(3)	8351(3)	35(1)
C(13)	5209(4)	8373(4)	8877(3)	45(1)
C(14)	4682(4)	9134(4)	8727(3)	46(1)
C(15)	4998(4)	9487(4)	8041(3)	39(1)
C(16)	5875(4)	9106(3)	7523(2)	30(1)
N(26)	6429(3)	9768(2)	5240(2)	27(1)
C(17)	6531(3)	10518(3)	6970(2)	30(1)
O(17)	6705(3)	11314(2)	7759(2)	40(1)

C(21)	6712(3)	10671(3)	6075(3)	30(1)
C(22)	7158(4)	11710(3)	6147(3)	39(1)
C(23)	7336(5)	11822(4)	5315(3)	46(1)
C(24)	7030(4)	10897(3)	4445(3)	40(1)
C(25)	6585(3)	9889(3)	4437(3)	29(1)
N(1)	6187(3)	9463(3)	6815(2)	31(1)
C(27)	6243(3)	8857(3)	3503(3)	30(1)
O(27)	6280(3)	8903(2)	2726(2)	42(1)
P(2)	7581(1)	6543(1)	3828(1)	25(1)
C(31)	6213(3)	6083(3)	2883(2)	27(1)
C(32)	5876(4)	5030(3)	2129(3)	35(1)
C(33)	4964(4)	4749(3)	1341(3)	38(1)
C(34)	4361(4)	5516(3)	1303(3)	39(1)
C(35)	4668(4)	6560(3)	2047(3)	34(1)
C(36)	5592(3)	6850(3)	2837(2)	27(1)
N(2)	5926(3)	7926(2)	3601(2)	30(1)
C(61)	7903(3)	5284(3)	3765(2)	28(1)
C(62)	6960(4)	4497(3)	3798(3)	35(1)
C(63)	7165(4)	3537(4)	3785(3)	41(1)
C(64)	8329(4)	3374(4)	3768(3)	45(1)
C(65)	9275(4)	4157(4)	3768(3)	43(1)
C(66)	9075(4)	5126(3)	3767(3)	34(1)
C(71)	8690(3)	7170(3)	3318(3)	31(1)
C(72)	9078(4)	6514(4)	2498(3)	44(1)
C(73)	9859(5)	7006(6)	2080(4)	67(2)
C(74)	10224(5)	8118(7)	2440(5)	74(2)
C(75)	9828(5)	8791(5)	3246(5)	68(2)
C(76)	9057(4)	8299(4)	3682(4)	44(1)

Cl(97)	8376(2)	4099(2)	9946(1)	85(1)
C(98)	7348(6)	3000(6)	9988(4)	77(2)
Cl(99)	7848(2)	2817(2)	11001(1)	90(1)
O(88)	3854(4)	2364(3)	9275(2)	56(1)
C(89)	2932(5)	2892(5)	9143(4)	56(1)

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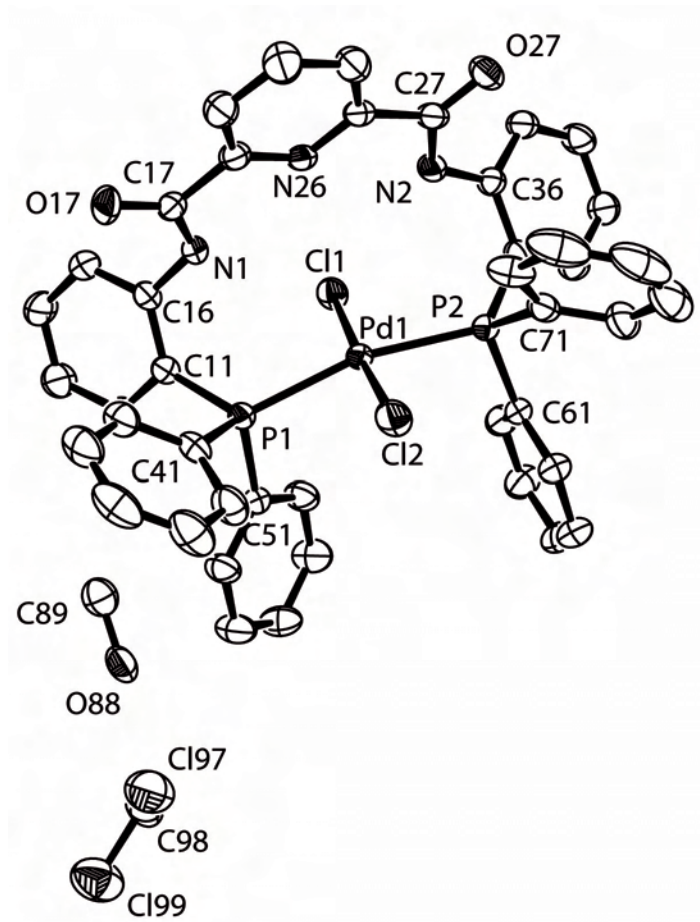


Abbildung 6.34: Ellipsoiddarstellung von  $[\text{Pd}\{\text{H}_2\text{L}^3(\text{P},\text{P})\}] \cdot \text{MeOH} \cdot \text{CH}_2\text{Cl}_2$ . Die Schwingungsellipsoide repräsentieren 50% der Aufenthaltswahrscheinlichkeit. [121]



## 6.32 [Pd{L<sup>3</sup>(P,N,N,N)}] · 0.5 MeOH · CH<sub>2</sub>Cl<sub>2</sub>

Tabelle 6.63: Kristallographische Daten und Parameter der Strukturrechnung von [Pd{L<sup>3</sup>(P,N,N,N)}] · 0.5 MeOH · CH<sub>2</sub>Cl<sub>2</sub>

Summenformel	C <sub>44.5</sub> H <sub>35</sub> N <sub>3</sub> O <sub>2.5</sub> P <sub>2</sub> Pd	
M (g/mol)	891.00	
Messtemperatur	200(2) K	
Wellenlänge	0.71073 Å	
Kristallsystem, Raumgruppe	monoklin, P2 <sub>1</sub> /n	
Elementarzelle	a = 12.883(1) Å	α = 90°
	b = 20.403(2) Å	β = 90.62(1)°
	c = 15.089(1) Å	γ = 90°
Volumen	3965.9(6) Å <sup>3</sup>	
Z	4	
Berechnete Dichte	1.492 g/cm <sup>3</sup>	
Linearer Absorptionskoeffizient	0.727 mm <sup>-1</sup>	
F(000)	1812	
Kristallgröße	0.59 x 0.32 x 0.27 mm <sup>3</sup>	
Theta-Bereich	2.70 - 29.56°	
Indizes	-12 ≤ h ≤ 15, -24 ≤ k ≤ 22, -17 ≤ l ≤ 17	
Zahl der gemessenen Reflexe	17297	
Zahl der unabhängigen Reflexe	6799 [R(int) = 0.0372]	
Zahl der verfeinerten Parameter	505	
Goof	1.057	
R <sub>1</sub> / wR <sub>2</sub> [I > 2σ(I)]	R <sub>1</sub> = 0.0684, wR <sub>2</sub> = 0.1991	
R <sub>1</sub> / wR <sub>2</sub> (alle Reflexe)	R <sub>1</sub> = 0.0781, wR <sub>2</sub> = 0.2066	
Restelektronendichte	1.188 und -1.601 e · Å <sup>-3</sup>	
Programm zur Strukturlösung	SHELXS 86 [118]	

Tabelle 6.64: Atomkoordinaten ( $\cdot 10^4$ ) und isotrope Temperaturparameter ( $\text{\AA}^2 \cdot 10^3$ ) von  $[\text{Pd}\{\text{L}^3(\text{P},\text{N},\text{N},\text{N})\}] \cdot 0.5 \text{ MeOH} \cdot \text{CH}_2\text{Cl}_2$

	x	y	z	E(eq)
Pd(1)	1547(1)	743(1)	4640(1)	32(1)
P(1)	1309(1)	1501(1)	3548(1)	23(1)
C(41)	461(4)	2183(2)	3802(3)	24(1)
C(42)	761(5)	2583(3)	4511(4)	36(1)
C(43)	188(5)	3133(3)	4717(4)	40(1)
C(44)	-706(5)	3286(3)	4236(4)	38(1)
C(45)	-1020(4)	2886(3)	3541(4)	35(1)
C(46)	-440(4)	2335(3)	3323(4)	29(1)
C(51)	2334(4)	1876(3)	2906(3)	26(1)
C(52)	3177(5)	1501(3)	2677(5)	41(1)
C(53)	3929(5)	1762(3)	2117(5)	46(2)
C(54)	3841(5)	2403(3)	1803(4)	42(1)
C(55)	3028(5)	2776(3)	2051(4)	36(1)
C(56)	2258(4)	2529(3)	2602(4)	31(1)
C(11)	666(4)	985(2)	2724(3)	24(1)
C(12)	403(5)	1212(3)	1879(4)	35(1)
C(13)	-107(5)	803(3)	1285(4)	40(1)
C(14)	-367(5)	175(3)	1533(4)	40(1)
C(15)	-110(5)	-73(3)	2364(4)	36(1)
C(16)	443(4)	332(2)	2962(3)	24(1)
N(1)	812(3)	114(2)	3794(3)	25(1)
C(17)	819(4)	-527(2)	4063(3)	25(1)
O(17)	466(4)	-1003(2)	3667(3)	41(1)
C(21)	1374(4)	-618(3)	4934(4)	27(1)
C(22)	1609(5)	-1218(3)	5320(4)	37(1)



C(23)	2170(5)	-1221(3)	6107(4)	41(1)
C(24)	2439(5)	-640(3)	6527(4)	39(1)
C(25)	2179(4)	-52(3)	6109(3)	29(1)
N(26)	1667(3)	-63(2)	5336(3)	25(1)
C(27)	2424(4)	627(3)	6432(3)	29(1)
O(27)	2746(4)	724(2)	7194(3)	44(1)
N(3)	2288(3)	1087(2)	5806(3)	26(1)
C(31)	3281(4)	2104(2)	5706(3)	22(1)
C(32)	3349(4)	2775(3)	5920(3)	27(1)
C(33)	2625(5)	3079(3)	6459(4)	33(1)
C(34)	1825(5)	2715(3)	6814(4)	36(1)
C(35)	1734(4)	2057(3)	6604(4)	32(1)
C(36)	2434(4)	1759(2)	6053(3)	23(1)
P(2)	4176(1)	1672(1)	4980(1)	23(1)
C(61)	4968(4)	1199(3)	5766(3)	24(1)
C(62)	5538(5)	683(3)	5436(4)	36(1)
C(63)	6200(5)	315(3)	5967(5)	46(2)
C(64)	6295(5)	466(3)	6856(5)	43(2)
C(65)	5713(5)	969(3)	7204(4)	40(1)
C(66)	5044(4)	1336(3)	6662(4)	32(1)
C(71)	5072(4)	2332(3)	4698(3)	25(1)
C(72)	6010(4)	2457(3)	5134(4)	35(1)
C(73)	6635(5)	2980(3)	4870(5)	47(2)
C(74)	6334(5)	3374(3)	4167(5)	46(2)
C(75)	5412(6)	3257(3)	3745(4)	45(2)
C(76)	4783(5)	2745(3)	3998(4)	37(1)
C(89)	5793(11)	173(5)	1353(8)	39(3)
O(88)	6863(6)	77(5)	1408(5)	40(2)

Cl(95)	2166(7)	-970(3)	1022(5)	88(1)
C(94)	2180(30)	-152(10)	450(17)	88(1)
Cl(96)	2993(8)	408(4)	903(6)	88(1)
Cl(97)	2527(11)	-961(6)	759(8)	88(1)
C(98)	2090(40)	-299(17)	500(30)	88(1)
Cl(99)	2694(12)	359(8)	1021(9)	88(1)

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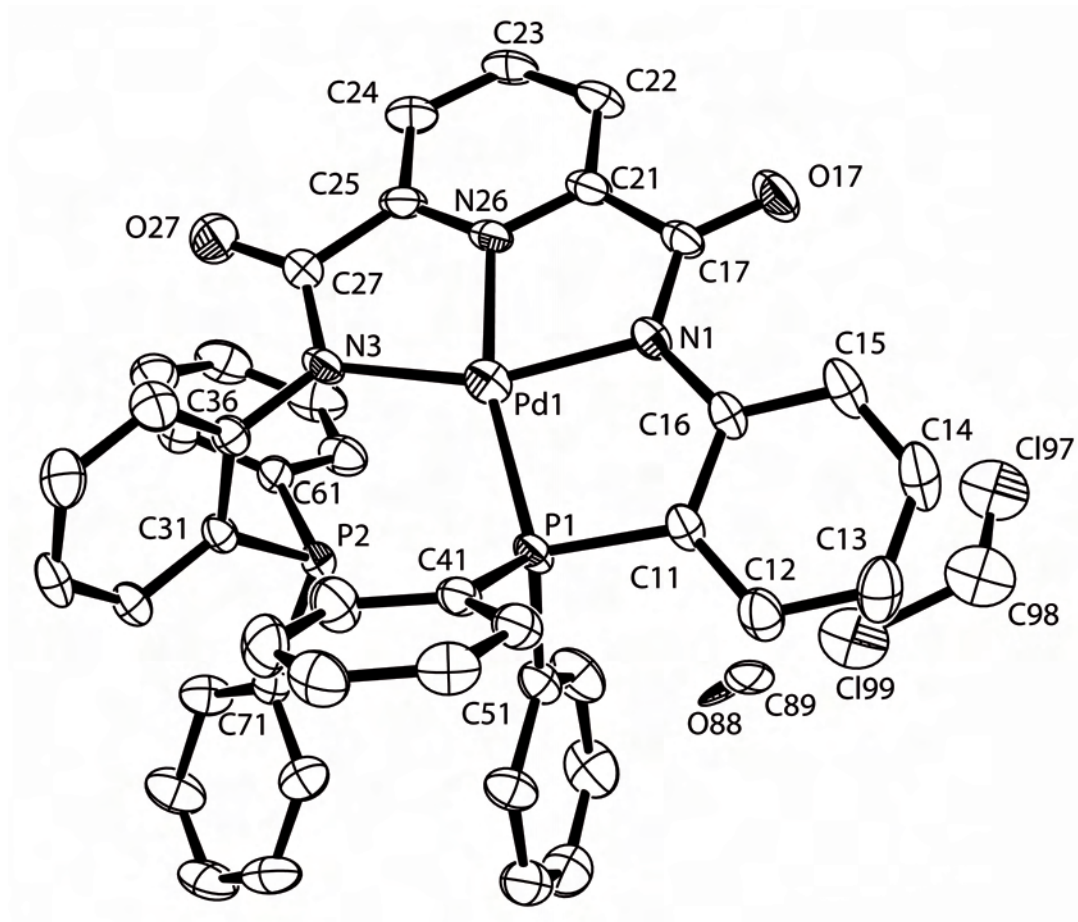


Abbildung 6.35: Ellipsoiddarstellung von  $[\text{Pd}\{\text{L}^3(\text{P},\text{N},\text{N},\text{N})\}] \cdot 0.5 \text{ MeOH} \cdot \text{CH}_2\text{Cl}_2$ . Die Schwingungsellipsoide repräsentieren 50% der Aufenthaltswahrscheinlichkeit. [121]



### 6.33 [CoCl{L<sup>3</sup>(P,N,N,N,P)}]

Tabelle 6.65: Kristallographische Daten und Parameter der Strukturrechnung von [CoCl{L<sup>3</sup>(P,N,N,N,P)}]

Summenformel	C <sub>43</sub> H <sub>31</sub> N <sub>3</sub> O <sub>2</sub> ClP <sub>2</sub> Co	
M (g/mol)	779.04	
Messtemperatur	200(2) K	
Wellenlänge	0.71073 Å	
Kristallsystem, Raumgruppe	monoklin, P <sub>2</sub> <sub>1</sub> /c	
Elementarzelle	a = 21.053(3) Å	α = 90°
	b = 9.865(1) Å	β = 111.88(1)°
	c = 18.258(2) Å	γ = 90°
Volumen	36518.9(7) Å <sup>3</sup>	
Z	4	
Berechnete Dichte	1.471 g/cm <sup>3</sup>	
Linearer Absorptionskoeffizient	0.699 mm <sup>-1</sup>	
F(000)	1604	
Kristallgröße	0.150 x 0.105 x 0.010 mm <sup>3</sup>	
Theta-Bereich	2.24 - 29.57°	
Indizes	-26 ≤ h ≤ 24, -11 ≤ k ≤ 12, -21 ≤ l ≤ 23	
Zahl der gemessenen Reflexe	18188	
Zahl der unabhängigen Reflexe	7579 [R(int) = 0.1128]	
Zahl der verfeinerten Parameter	470	
Goof	0.915	
R <sub>1</sub> / wR <sub>2</sub> [I > 2σ(I)]	R <sub>1</sub> = 0.0528, wR <sub>2</sub> = 0.0906	
R <sub>1</sub> / wR <sub>2</sub> (alle Reflexe)	R <sub>1</sub> = 0.1141, wR <sub>2</sub> = 0.1072	
Restelektronendichte	0.356 und -0.532 e · Å <sup>-3</sup>	
Programm zur Strukturlösung	SHELXS 97 [119]	

Tabelle 6.66: Atomkoordinaten ( $\cdot 10^4$ ) und isotrope Temperaturparameter ( $\text{\AA}^2 \cdot 10^3$ ) von  $[\text{CoCl}\{\text{L}^3(\text{P},\text{N},\text{N},\text{N},\text{P})\}]$

	x	y	z	E(eq)
Co(1)	2653(1)	7677(1)	2237(1)	24(1)
Cl(1)	2157(1)	6896(1)	3074(1)	34(1)
P(1)	1626(1)	8524(1)	1518(1)	27(1)
C(41)	896(2)	7689(4)	1628(2)	32(1)
C(42)	774(2)	6322(4)	1420(2)	43(1)
C(43)	199(2)	5701(5)	1455(3)	51(1)
C(44)	-237(2)	6381(6)	1730(3)	54(1)
C(45)	-111(2)	7697(5)	1958(2)	47(1)
C(46)	443(2)	8354(5)	1899(2)	38(1)
C(51)	1323(2)	8846(4)	459(2)	32(1)
C(52)	1524(2)	10013(4)	170(2)	35(1)
C(53)	1351(2)	10194(4)	-634(2)	41(1)
C(54)	971(2)	9239(5)	-1164(2)	44(1)
C(55)	753(2)	8101(5)	-884(2)	46(1)
C(56)	926(2)	7897(4)	-86(2)	42(1)
C(11)	1731(2)	10184(4)	1964(2)	31(1)
C(12)	1233(2)	11192(4)	1699(2)	38(1)
C(13)	1352(2)	12462(4)	2044(2)	44(1)
C(14)	1972(2)	12733(4)	2657(2)	47(1)
C(15)	2468(2)	11758(4)	2918(2)	39(1)
C(16)	2362(2)	10457(4)	2581(2)	30(1)
N(1)	2848(2)	9403(3)	2791(2)	30(1)
C(17)	3420(2)	9411(4)	3469(2)	36(1)
O(17)	3628(2)	10332(3)	3965(2)	49(1)
C(21)	3794(2)	8111(4)	3586(2)	31(1)

C(22)	4390(2)	7741(4)	4209(2)	39(1)
C(23)	4642(2)	6455(5)	4229(2)	47(1)
C(24)	4293(2)	5512(4)	3660(2)	41(1)
C(25)	3697(2)	5911(4)	3061(2)	29(1)
N(26)	3485(2)	7189(3)	3026(1)	28(1)
C(27)	3242(2)	5079(4)	2374(2)	28(1)
O(27)	3378(2)	3900(3)	2277(2)	41(1)
N(3)	2715(2)	5840(3)	1891(2)	27(1)
C(31)	2438(2)	5542(4)	1067(2)	25(1)
C(32)	2100(2)	4366(4)	728(2)	33(1)
C(33)	1864(2)	4261(4)	-95(2)	42(1)
C(34)	1963(2)	5276(5)	-550(2)	43(1)
C(35)	2301(2)	6458(4)	-213(2)	35(1)
C(36)	2537(2)	6593(4)	605(2)	26(1)
P(2)	3054(1)	7894(1)	1267(1)	25(1)
C(61)	3929(2)	7297(4)	1546(2)	28(1)
C(62)	4445(2)	8059(4)	2095(2)	37(1)
C(63)	5124(2)	7733(5)	2296(2)	48(1)
C(64)	5300(2)	6663(5)	1934(3)	55(1)
C(65)	4790(2)	5876(5)	1385(3)	56(1)
C(66)	4108(2)	6193(4)	1198(2)	41(1)
C(71)	3112(2)	9463(4)	781(2)	28(1)
C(72)	3161(2)	9471(4)	38(2)	34(1)
C(73)	3252(2)	10692(4)	-289(2)	41(1)
C(74)	3319(2)	11882(4)	113(2)	41(1)
C(75)	3292(2)	11887(4)	858(2)	36(1)
C(76)	3184(2)	10689(4)	1184(2)	32(1)

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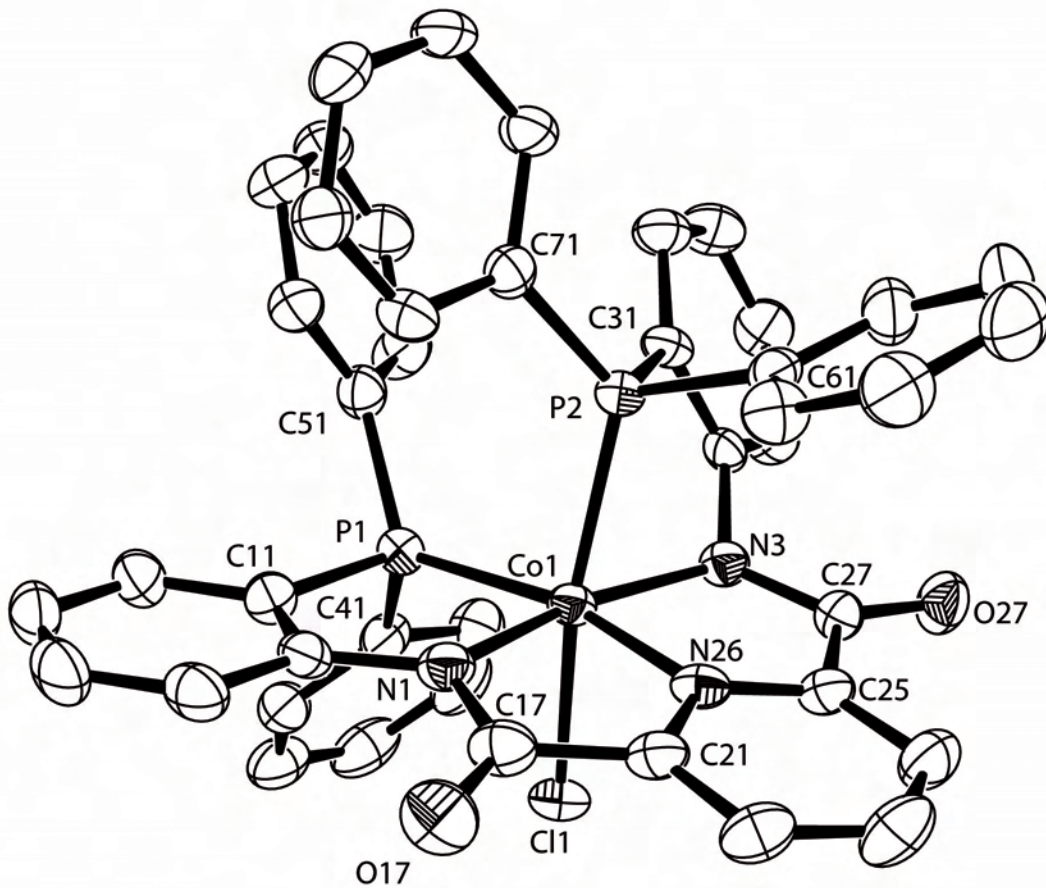


Abbildung 6.36: Ellipsoiddarstellung von  $[\text{CoCl}\{\text{L}^3(\text{P},\text{N},\text{N},\text{N},\text{P})\}]$ . Die Schwingungsellipsoide repräsentieren 50% der Aufenthaltswahrscheinlichkeit. [121]



### 6.34 [CuCl{H<sub>2</sub>L<sup>3</sup>(P,P)}] · CH<sub>2</sub>Cl<sub>2</sub>

Tabelle 6.67: Kristallographische Daten und Parameter der Strukturrechnung von [CuClH<sub>2</sub>L<sup>3</sup>(P,P)] · CH<sub>2</sub>Cl<sub>2</sub>

Summenformel	C <sub>44</sub> H <sub>35</sub> N <sub>3</sub> O <sub>2</sub> P <sub>2</sub> Cl <sub>3</sub> Cu	
M (g/mol)	869.58	
Messtemperatur	200(2) K	
Wellenlänge	0.71073 Å	
Kristallsystem, Raumgruppe	monoklin, P2 <sub>1</sub> /c	
Elementarzelle	a = 13.523(1) Å	α = 90°
	b = 13.004(1) Å	β = 99.23(1)°
	c = 24.949(2) Å	γ = 90°
Volumen	4330.6(6) Å <sup>3</sup>	
Z	4	
Berechnete Dichte	1.334 g/cm <sup>3</sup>	
Linearer Absorptionskoeffizient	0.802 mm <sup>-1</sup>	
F(000)	10506	
Kristallgröße	0.30 x 0.21 x 0.21 mm <sup>3</sup>	
Theta-Bereich	2.06-28.82°	
Indizes	-15 ≤ h ≤ 16, -14 ≤ k ≤ 15, -29 ≤ l ≤ 29	
Zahl der gemessenen Reflexe	17228	
Zahl der unabhängigen Reflexe	7462 [R(int) = 0.0666]	
Zahl der verfeinerten Parameter	508	
Goof	0.985	
R <sub>1</sub> / wR <sub>2</sub> [I > 2σ(I)]	R <sub>1</sub> = 0.0801, wR <sub>2</sub> = 0.2090	
R <sub>1</sub> / wR <sub>2</sub> (alle Reflexe)	R <sub>1</sub> = 0.1216, wR <sub>2</sub> = 0.2339	
Restelektronendichte	2.334 und -0.485 e · Å <sup>-3</sup>	
Programm zur Strukturlösung	SHELXS 86 [118]	

Tabelle 6.68: Atomkoordinaten ( $\cdot 10^4$ ) und isotrope Temperaturparameter ( $\text{\AA}^2 \cdot 10^3$ ) von  $[\text{CuCl}\{\text{H}_2\text{L}^3(\text{P},\text{P})\}] \cdot \text{CH}_2\text{Cl}_2$

	x	y	z	E(eq)
Cu(1)	1931(1)	1054(1)	1801(1)	31(1)
Cl(1)	615(1)	-12(1)	1764(1)	39(1)
P(1)	1381(1)	2689(1)	1719(1)	28(1)
C(41)	1579(5)	3432(5)	1124(3)	35(2)
C(42)	2382(6)	3182(8)	860(3)	58(2)
C(43)	2582(8)	3789(11)	429(4)	80(4)
C(44)	1971(9)	4621(9)	251(4)	75(3)
C(45)	1167(8)	4861(7)	504(3)	67(3)
C(46)	978(6)	4252(6)	926(3)	44(2)
C(51)	1905(5)	3500(5)	2281(2)	30(1)
C(52)	1670(6)	4540(6)	2301(3)	44(2)
C(53)	2075(6)	5152(7)	2751(3)	54(2)
C(54)	2715(6)	4730(8)	3162(3)	55(2)
C(55)	2972(6)	3719(8)	3149(3)	59(2)
C(56)	2578(5)	3092(6)	2708(3)	43(2)
C(11)	21(4)	2782(5)	1697(2)	28(1)
C(12)	-418(5)	3254(5)	2104(3)	36(2)
C(13)	-1445(6)	3327(6)	2057(3)	48(2)
C(14)	-2034(6)	2948(6)	1597(4)	53(2)
C(15)	-1627(5)	2463(6)	1197(3)	41(2)
C(16)	-593(5)	2367(5)	1253(2)	30(1)
N(1)	-148(4)	1818(4)	857(2)	31(1)
C(17)	-208(5)	2102(5)	330(3)	32(1)
O(17)	-726(4)	2808(4)	120(2)	45(1)
C(21)	1633(5)	215(5)	31(2)	32(1)

C(22)	1706(5)	400(6)	-516(3)	42(2)
C(23)	1108(6)	1163(6)	-785(3)	47(2)
C(24)	480(6)	1708(6)	-518(3)	43(2)
C(25)	457(5)	1489(5)	22(2)	30(1)
N(26)	1011(4)	743(4)	293(2)	31(1)
C(27)	2248(5)	-613(5)	338(3)	32(1)
O(27)	2834(4)	-1129(4)	125(2)	45(1)
N(3)	2091(4)	-725(4)	852(2)	31(1)
C(31)	3124(5)	-1253(4)	1706(2)	28(1)
C(32)	3490(5)	-2033(5)	2052(3)	38(2)
C(33)	3293(6)	-3064(5)	1918(3)	46(2)
C(34)	2759(6)	-3307(6)	1429(3)	47(2)
C(35)	2366(5)	-2539(5)	1064(3)	37(2)
C(36)	2533(5)	-1516(5)	1208(2)	30(1)
P(2)	3342(1)	112(1)	1876(1)	27(1)
C(61)	4249(5)	538(5)	1462(3)	32(1)
C(62)	4610(5)	-76(6)	1073(3)	39(2)
C(63)	5261(6)	316(7)	757(3)	49(2)
C(64)	5570(6)	1329(7)	818(3)	56(2)
C(65)	5229(6)	1950(7)	1190(4)	60(2)
C(66)	4565(6)	1557(5)	1523(3)	45(2)
C(71)	4071(5)	32(5)	2560(3)	31(1)
C(72)	5068(5)	-294(5)	2636(3)	38(2)
C(73)	5569(5)	-427(6)	3164(3)	43(2)
C(74)	5105(6)	-242(6)	3603(3)	50(2)
C(75)	4118(6)	85(6)	3516(3)	49(2)
C(76)	3607(6)	224(6)	3003(3)	41(2)
Cl(87)	4177(3)	8828(3)	4923(2)	60(1)

C(88)	4489(9)	7902(10)	5454(5)	30(2)
Cl(89)	5724(3)	7548(3)	5501(2)	61(1)
Cl(97)	387(2)	6774(2)	1720(1)	28(1)
C(98)	-724(9)	6231(10)	1847(5)	33(3)
Cl(99)	-1552(4)	6002(5)	1259(2)	82(2)

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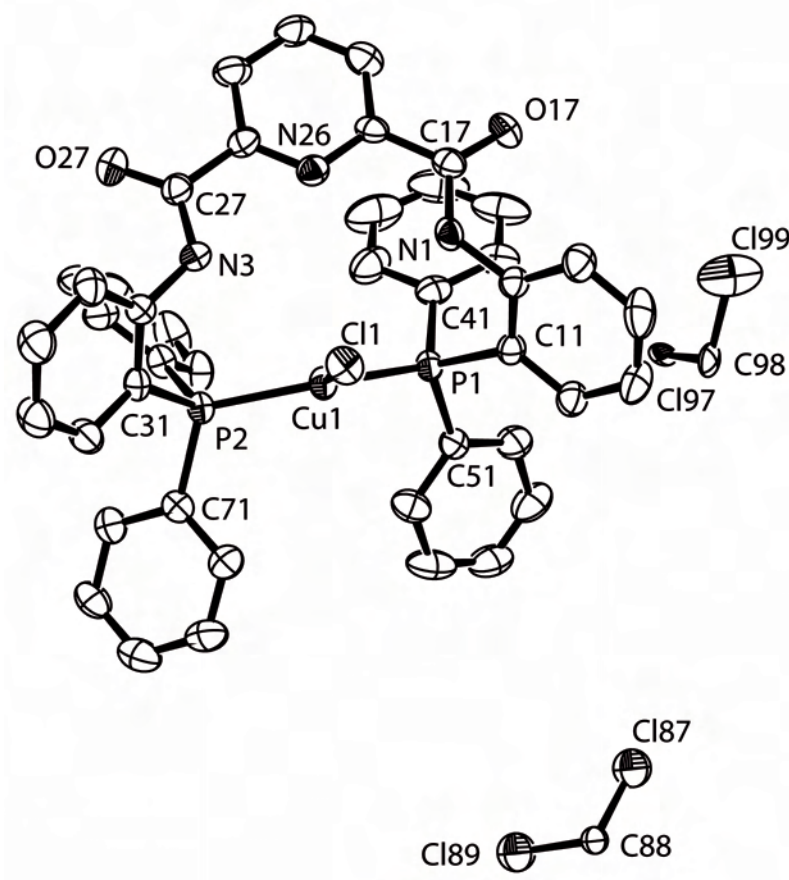


Abbildung 6.37: Ellipsoiddarstellung von  $[\text{CuCl}\{\text{H}_2\text{L}^3(\text{P},\text{P})\}] \cdot \text{CH}_2\text{Cl}_2$ . Die Schwingungselipsoide repräsentieren 50% der Aufenthaltswahrscheinlichkeit. [121]



## 6.35 [Cu{OL<sup>3</sup>(P,N,N,N,P-O)}] · 0.5 MeOH

Tabelle 6.69: Kristallographische Daten und Parameter der Strukturrechnung von [Cu{OL<sup>3</sup>(P,N,N,N,P-O)}] · 0.5 MeOH

Summenformel	C <sub>43.5</sub> H <sub>33</sub> N <sub>3</sub> O <sub>3.5</sub> P <sub>2</sub> Cu	
M (g/mol)	779.21	
Messtemperatur	200(2) K	
Wellenlänge	0.71073 Å	
Kristallsystem, Raumgruppe	monoklin, P <sub>2</sub> <sub>1</sub> /c	
Elementarzelle	a = 19.181(2) Å	α = 90°
	b = 16.765(2) Å	β = 98.43(1)°
	c = 11.930(1) Å	γ = 90°
Volumen	3794.9(7) Å <sup>3</sup>	
Z	4	
Berechnete Dichte	1.364 g/cm <sup>3</sup>	
Linearer Absorptionskoeffizient	0.706 mm <sup>-1</sup>	
F(000)	6279	
Kristallgröße	0.40 x 0.10 x 0.05 mm <sup>3</sup>	
Theta-Bereich	2.11 - 25.56°	
Indizes	-21 ≤ h ≤ 23, -19 ≤ k ≤ 20, -14 ≤ l ≤ 14	
Zahl der gemessenen Reflexe	17046	
Zahl der unabhängigen Reflexe	7351 [R(int) = 0.1134]	
Zahl der verfeinerten Parameter	480	
Goof	0.805	
R <sub>1</sub> / wR <sub>2</sub> [I > 2σ(I)]	R <sub>1</sub> = 0.0607, wR <sub>2</sub> = 0.1163	
R <sub>1</sub> / wR <sub>2</sub> (alle Reflexe)	R <sub>1</sub> = 0.1523, wR <sub>2</sub> = 0.1406	
Restelektronendichte	1.712 und -0.505 e · Å <sup>-3</sup>	
Programm zur Strukturlösung	SHELXS 97 [119]	

Tabelle 6.70: Atomkoordinaten ( $\cdot 10^4$ ) und isotrope Temperaturparameter ( $\text{\AA}^2 \cdot 10^3$ ) von  $[\text{Cu}\{\text{OL}^3(\text{P},\text{N},\text{N},\text{N},\text{P}-\text{O})\}] \cdot 0.5 \text{ MeOH}$

	x	y	z	E(eq)
Cu(1)	3364(1)	4724(1)	4970(1)	35(1)
P(1)	3123(1)	4914(1)	6790(1)	35(1)
C(41)	2267(3)	4664(3)	7157(4)	36(1)
C(42)	2079(3)	3878(3)	7356(4)	42(1)
C(43)	1417(3)	3695(4)	7563(5)	50(2)
C(44)	912(3)	4281(4)	7545(5)	54(2)
C(45)	1077(3)	5048(4)	7334(6)	58(2)
C(46)	1748(3)	5251(4)	7136(5)	48(2)
C(51)	3329(3)	5878(3)	7430(4)	38(1)
C(52)	3237(3)	6537(4)	6746(6)	56(2)
C(53)	3362(4)	7301(4)	7165(7)	70(2)
C(54)	3587(3)	7403(4)	8280(7)	64(2)
C(55)	3684(4)	6756(5)	8980(7)	83(3)
C(56)	3546(4)	5989(4)	8566(5)	64(2)
C(11)	3736(3)	4189(3)	7486(4)	36(1)
C(12)	3754(3)	3964(3)	8608(5)	44(2)
C(13)	4229(3)	3397(4)	9090(5)	53(2)
C(14)	4682(3)	3047(4)	8462(5)	53(2)
C(15)	4689(3)	3256(4)	7348(5)	48(2)
C(16)	4218(3)	3837(3)	6824(4)	37(1)
N(1)	4172(2)	4078(3)	5692(4)	37(1)
C(17)	4683(3)	3913(3)	5044(5)	39(1)
O(17)	5235(2)	3548(3)	5277(3)	54(1)
C(21)	4507(3)	4275(3)	3877(5)	36(1)
C(22)	4892(3)	4218(4)	3005(5)	49(2)



C(23)	4667(3)	4621(4)	2014(5)	56(2)
C(24)	4059(3)	5079(4)	1897(5)	48(2)
C(25)	3685(3)	5100(3)	2798(5)	40(1)
N(26)	3909(2)	4700(3)	3745(3)	36(1)
C(27)	2993(3)	5518(3)	2854(5)	41(2)
O(27)	2719(2)	5899(2)	2009(3)	53(1)
N(3)	2749(2)	5380(3)	3830(4)	38(1)
C(31)	1567(3)	5002(3)	4003(4)	35(1)
C(32)	890(3)	5199(4)	4213(5)	45(1)
C(33)	699(3)	5990(4)	4351(5)	50(2)
C(34)	1187(3)	6586(4)	4253(5)	53(2)
C(35)	1863(3)	6403(4)	4051(5)	49(2)
C(36)	2055(3)	5619(3)	3945(4)	38(1)
P(2)	1874(1)	3990(1)	3919(1)	32(1)
O(2)	2452(2)	3769(2)	4842(3)	36(1)
C(61)	1107(3)	3372(3)	3923(4)	33(1)
C(62)	1076(3)	2845(3)	4809(5)	43(1)
C(63)	508(3)	2342(4)	4786(5)	52(2)
C(64)	-35(3)	2364(4)	3920(6)	56(2)
C(65)	-30(3)	2897(4)	3035(6)	52(2)
C(66)	551(3)	3397(3)	3020(5)	43(2)
C(71)	2154(3)	3828(3)	2573(4)	35(1)
C(72)	2666(3)	3262(3)	2505(5)	45(2)
C(73)	2874(4)	3055(4)	1488(6)	57(2)
C(74)	2559(4)	3410(4)	511(6)	62(2)
C(75)	2077(4)	3985(4)	552(5)	59(2)
C(76)	1850(3)	4208(4)	1575(5)	47(2)
C(99)	1748(6)	8697(7)	4818(9)	40(3)

O(99)

1489(4)

8712(5)

5719(7)

52(2)

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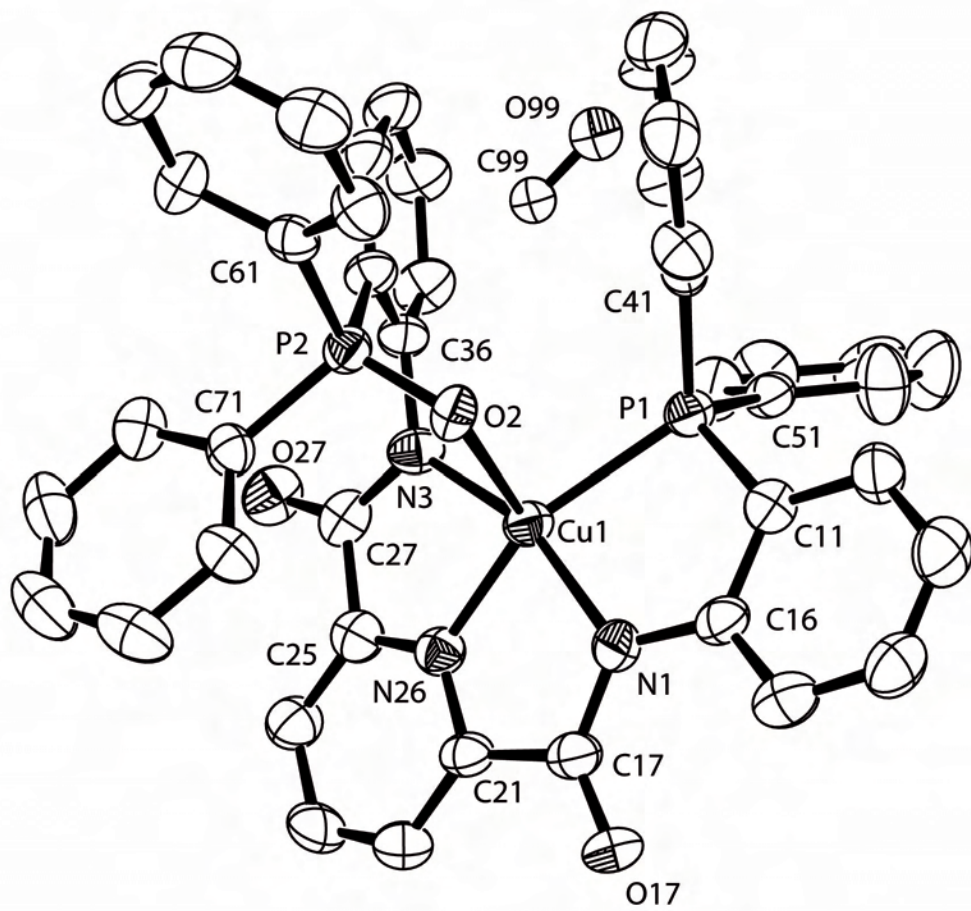


Abbildung 6.38: Ellipsoiddarstellung von  $[\text{Cu}\{\text{OL}^3(\text{P},\text{N},\text{N},\text{N},\text{P}-\text{O})\}] \cdot 0.5 \text{ MeOH}$ . Die Schwingungsellipsoide repräsentieren 50% der Aufenthaltswahrscheinlichkeit. [121]



## 6.36 [Cu{O<sub>2</sub>L<sup>3</sup>(P-O,N,N,N,P-O)}] · 3 MeOH

Tabelle 6.71: Kristallographische Daten und Parameter der Strukturrechnung von [Cu{O<sub>2</sub>L<sup>3</sup>(O,N,N,N,O)}] · 3 MeOH

Summenformel	C <sub>46</sub> H <sub>43</sub> N <sub>3</sub> O <sub>7</sub> P <sub>2</sub> Cu	
M (g/mol)	875.31	
Messtemperatur	200(2) K	
Wellenlänge	0.71073 Å	
Kristallsystem, Raumgruppe	monoklin, P2 <sub>1</sub> /c	
Elementarzelle	a = 22.069(2) Å	α = 90°
	b = 9.380(1) Å	β = 93.15(1)°
	c = 20.228(2) Å	γ = 90°
Volumen	4181.0(7) Å <sup>3</sup>	
Z	4	
Berechnete Dichte	1.391 g/cm <sup>3</sup>	
Linearer Absorptionskoeffizient	0.655 mm <sup>-1</sup>	
F(000)	1820	
Kristallgröße	0.17 x 0.13 x 0.10 mm <sup>3</sup>	
Theta-Bereich	2.17 - 29.12°	
Indizes	-26 ≤ h ≤ 26, -9 ≤ k ≤ 11, -24 ≤ l ≤ 24	
Zahl der gemessenen Reflexe	28191	
Zahl der unabhängigen Reflexe	7264 [R(int) = 0.1485]	
Zahl der verfeinerten Parameter	480	
Goof	0.975	
R <sub>1</sub> / wR <sub>2</sub> [I > 2σ(I)]	R <sub>1</sub> = 0.0724, wR <sub>2</sub> = 0.1496	
R <sub>1</sub> / wR <sub>2</sub> (alle Reflexe)	R <sub>1</sub> = 0.1285, wR <sub>2</sub> = 0.1720	
Restelektronendichte	0.507 und -0.795 e · Å <sup>-3</sup>	
Programm zur Strukturlösung	SHELXS 97 [119]	

Tabelle 6.72: Atomkoordinaten ( $\cdot 10^4$ ) und isotrope Temperaturparameter ( $\text{\AA}^2 \cdot 10^3$ ) von  $[\text{Cu}\{\text{O}_2\text{L}^3(\text{P-O},\text{N},\text{N},\text{N},\text{P-O})\}] \cdot 3 \text{ MeOH}$

	x	y	z	E(eq)
Cu(1)	2403(1)	5908(1)	1457(1)	35(1)
P(1)	1414(1)	4600(2)	470(1)	21(1)
O(10)	2076(2)	4471(4)	691(2)	24(1)
C(41)	1266(2)	3604(6)	-284(2)	25(1)
C(42)	1732(3)	3434(7)	-700(3)	35(1)
C(43)	1624(3)	2672(9)	-1291(3)	52(2)
C(44)	1065(3)	2126(7)	-1458(3)	45(2)
C(45)	594(3)	2291(7)	-1042(3)	38(2)
C(46)	695(3)	3034(7)	-451(3)	32(1)
C(51)	918(2)	3903(6)	1073(2)	23(1)
C(52)	1026(3)	2511(6)	1289(3)	32(1)
C(53)	653(3)	1908(7)	1751(3)	39(2)
C(54)	188(3)	2664(7)	1996(3)	34(1)
C(55)	85(2)	4043(7)	1775(3)	36(1)
C(56)	449(2)	4665(6)	1322(3)	28(1)
C(11)	1191(2)	6410(6)	312(3)	24(1)
C(12)	893(2)	6825(6)	-293(3)	29(1)
C(13)	710(3)	8210(7)	-387(3)	37(2)
C(14)	834(3)	9220(7)	107(3)	39(2)
C(15)	1130(3)	8827(6)	694(3)	33(1)
C(16)	1303(2)	7437(6)	807(3)	24(1)
N(1)	1613(2)	6990(5)	1402(2)	25(1)
C(17)	1390(2)	7332(6)	1983(3)	25(1)
O(17)	928(2)	8026(5)	2083(2)	38(1)
C(21)	1760(2)	6672(6)	2553(2)	25(1)

C(22)	1652(3)	6791(8)	3218(3)	40(2)
C(23)	2045(3)	6136(9)	3669(3)	47(2)
C(24)	2538(3)	5360(7)	3473(3)	37(1)
C(25)	2621(2)	5294(6)	2801(3)	26(1)
N(26)	2235(2)	5934(5)	2367(2)	24(1)
C(27)	3141(2)	4594(6)	2483(3)	28(1)
O(27)	3526(2)	3908(5)	2829(2)	39(1)
N(3)	3145(2)	4845(5)	1828(2)	27(1)
C(31)	3831(2)	5181(6)	943(2)	25(1)
C(32)	4292(2)	4661(7)	573(3)	32(1)
C(33)	4537(3)	3328(7)	681(3)	37(2)
C(34)	4308(3)	2485(7)	1158(3)	36(1)
C(35)	3856(3)	2955(6)	1538(3)	32(1)
C(36)	3609(2)	4326(6)	1447(3)	26(1)
P(2)	3571(1)	6993(2)	849(1)	24(1)
O(20)	2899(2)	7183(4)	892(2)	32(1)
C(61)	4006(3)	7967(6)	1476(3)	31(1)
C(62)	3724(3)	8902(7)	1884(3)	41(2)
C(63)	4055(4)	9606(8)	2387(3)	59(2)
C(64)	4673(4)	9391(9)	2462(4)	63(2)
C(65)	4960(3)	8499(9)	2063(4)	53(2)
C(66)	4633(3)	7764(7)	1563(3)	39(2)
C(71)	3790(2)	7618(6)	59(3)	28(1)
C(72)	3566(3)	6869(8)	-506(3)	44(2)
C(73)	3715(4)	7351(10)	-1126(3)	60(2)
C(74)	4062(3)	8547(10)	-1190(4)	58(2)
C(75)	4267(3)	9271(8)	-662(4)	50(2)
C(76)	4135(3)	8819(7)	-21(3)	36(1)

O(79)	2460(3)	1713(6)	992(3)	67(2)
C(79)	2681(4)	907(11)	471(4)	73(2)
O(89)	2583(3)	1376(7)	2365(3)	77(2)
C(89)	2243(4)	151(10)	2462(5)	73(2)
O(99)	3183(3)	1404(9)	3700(3)	98(2)
C(99)	3632(5)	1905(11)	4094(5)	92(3)

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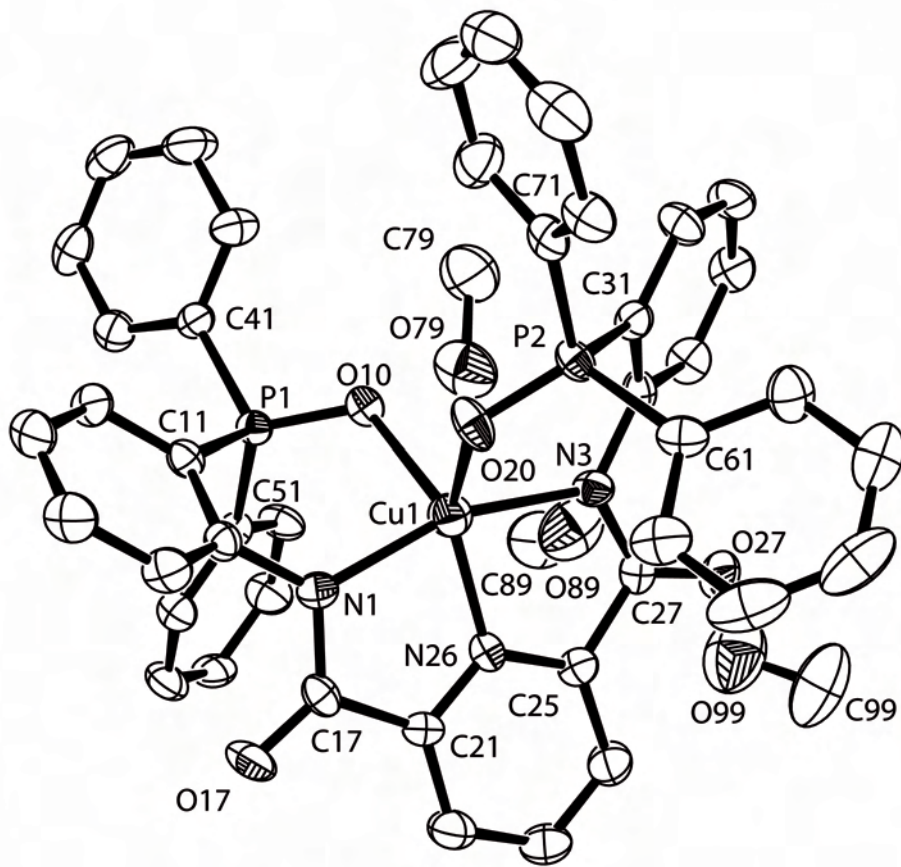


Abbildung 6.39: Ellipsoiddarstellung von  $[\text{Cu}\{\text{O}_2\text{L}^3(\text{P-O,N,N,N,P-O})\}] \cdot 3 \text{MeOH}$ . Die Schwingungsellipsoide repräsentieren 50% der Aufenthaltswahrscheinlichkeit. [121]



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