ORGANOMETALLICS
Organometallics, 1996, 15(3), 1023-1032, DOI:10.1021/om950761o

L1032-1

Table S1. Anisotropic displacement parameters ($Å^2 \times 10^4$) for $ReO_2(CH_2CMe_3)_2Ph$.

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Re	134(2)	197(2)	235(2)	-21(1)	65(1)	-31(1)
O(1)	204(27)	338(29)	448(28)	-171(23)	96(24)	-157(24)
O(2)	442(34)	314(31)	284(24)	70(25)	47(24)	13(22)
C(1)	208(36)	256(35)	267(33)	66(29)	132(30)	-19(28)
C(10)	281(42)	255(36)	250(32)	-42(31)	75(30)	-33(29)
C(11)	565(58)	508(57)	242(35)	-122(46)	116(37)	101(38)
C(12)	187(38)	473(47)	232(33)	-67(34)	45(30)	-10(31)
C(13)	365(49)	413(47)	376(42)	-112(38)	117(38)	-184(36)
C(2)	141(33)	218(33)	237(30)	21(28)	44(27)	-16(27)
C(20)	217(39)	239(37)	350(37)	40(31)	116(32)	-75(30)
C(21)	146(38)	419(43)	361(38)	18(32)	98(32)	-24(33)
C(22)	397(48)	346(42)	406(39)	83(39)	167(37)	9(38)
C(23)	286(43)	281(39)	379(39)	23(32)	128(35)	-74(32)
C(3)	106(32)	168(32)	220(32)	-50(24)	53(26)	-78(24)
C(4)	349(42)	214(34)	267(33)	-40(32)	123(31)	-3(28)
C(5)	404(46)	311(40)	232(33)	82(36)	81(33)	20(30)
C(6)	197(41)	377(47)	347(42)	60(34)	-35(35)	-85(35)
C(7)	253(43)	378(47)	354(38)	-120(34)	161(34)	-88(36)
C(8)	250(38)	253(34)	290(33)	-22(32)	146(30)	29(31)

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Table S2. Complete listing of bond lengths (Å) for the non-hydrogen atoms of $ReO_2(CH_2CMe_3)_2Ph$.

Re-O(1)	1.709 (6)	C(20)-C(21)	1.505 (9)
Re-O(2)	1.704 (5)	C(20)-C(22)	1.511 (12)
Re-C(1)	2.163 (8)	C(20)-C(23)	1.553 (10)
Re-C(2)	2.152 (7)	C(3)-C(4)	1.407 (9)
Re-C(3)	2.142 (6)	C(3)-C(8)	1.385 (11)
C(1)-C(10)	1.562 (8)	C(4)-C(5)	1.386 (10)
C(10)-C(11)	1.515 (11)	C(5)-C(6)	1.394 (12)
C(10)-C(12)	1.518 (11)	C(6)-C(7)	1.362 (11)
C(10)-C(13)	1.547 (12)	C(7)-C(8)	1.399 (10)
C(2)-C(20)	1.568 (11)		

Table S3. Complete listing of bond angles (deg) for the non-hydrogen atoms of $ReO_2(CH_2CMe_3)_2Ph$.

O(1)-Re-O(2)	123.8(2)	C(12)-C(10)-C(13)	108.5(6)
O(1)-Re-C(1)	98.6(3)	Re-C(2)-C(20)	114.4(4)
O(2)-Re-C(1)	97.3(3)	C(2)-C(20)-C(21)	113.1(6)
O(1)-Re-C(2)	99.9(3)	C(2)-C(20)-C(22)	110.0(6)
O(2)-Re-C(2)	96.3(2)	C(21)-C(20)-C(22)	111.2(6)
C(1)-Re-C(2)	145.4(2)	C(2)-C(20)-C(23)	104.8(6)
O(1)-Re-C(3)	117.0(2)	C(21)-C(20)-C(23)	109.0(6)
O(2)-Re-C(3)	119.2(3)	C(22)-C(20)-C(23)	108.4(6)
C(1)-Re-C(3)	72.5(2)	Re-C(3)-C(4)	119.2(5)
C(2)-Re-C(3)	73.1(2)	Re-C(3)-C(8)	122.3(4)
Re-C(1)-C(10)	114.0(5)	C(4)-C(3)-C(8)	118.5(6)
C(1)-C(10)-C(11)	110.3(6)	C(3)-C(4)-C(5)	120.7(7)
C(1)-C(10)-C(12)	114.6(6)	C(4)-C(5)-C(6)	119.8(7)
C(11)-C(10)-C(12)	109.9(6)	C(5)-C(6)-C(7)	119.8(7)
C(1)-C(10)-C(13)	104.2(5)	C(6)-C(7)-C(8)	121.1(8)
C(11)-C(10)-C(13)	109.0(7)	C(3)-C(8)-C(7)	120.2(7)

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Table S4. Calculated H-atom coordinates (x 10^4) for $ReO_2(CH_2CMe_3)_2Ph$.

	x	y	z
H(1A)	5969	2155	3466
H(1B)	5431	1060	3881
H(11A)	7756	1063	5992
H(11B)	7558	93	5241
H(11C)	6281	666	5442
H(12A)	9098	2409	5392
H(12B)	9061	1515	4616
H(12C)	8574	2863	4413
H(13A)	6939	3233	5568
H(13B)	6367	3571	4566
H(13C)	5525	2718	5003
H(2A)	6340	-710	1545
H(2B)	6419	-1772	2200
H(21A)	10164	-2113	2599
H(21B)	9576	-1134	3106
H(21C)	9042	-2477	3044
H(22A)	8913	137	1660
H(22B)	9569	-920	1260
H(22C)	8059	-520	795
H(23A)	8617	-3057	1220
H(23B)	7141	-2536	809
H(23C)	7483	-3300	1681
H(4)	5298	1713	1627
H(5)	3003	1808	783
H(6)	1391	505	1105
H(7)	2106	-950	2207
H(8)	4430	-1109	3028

L1032-5

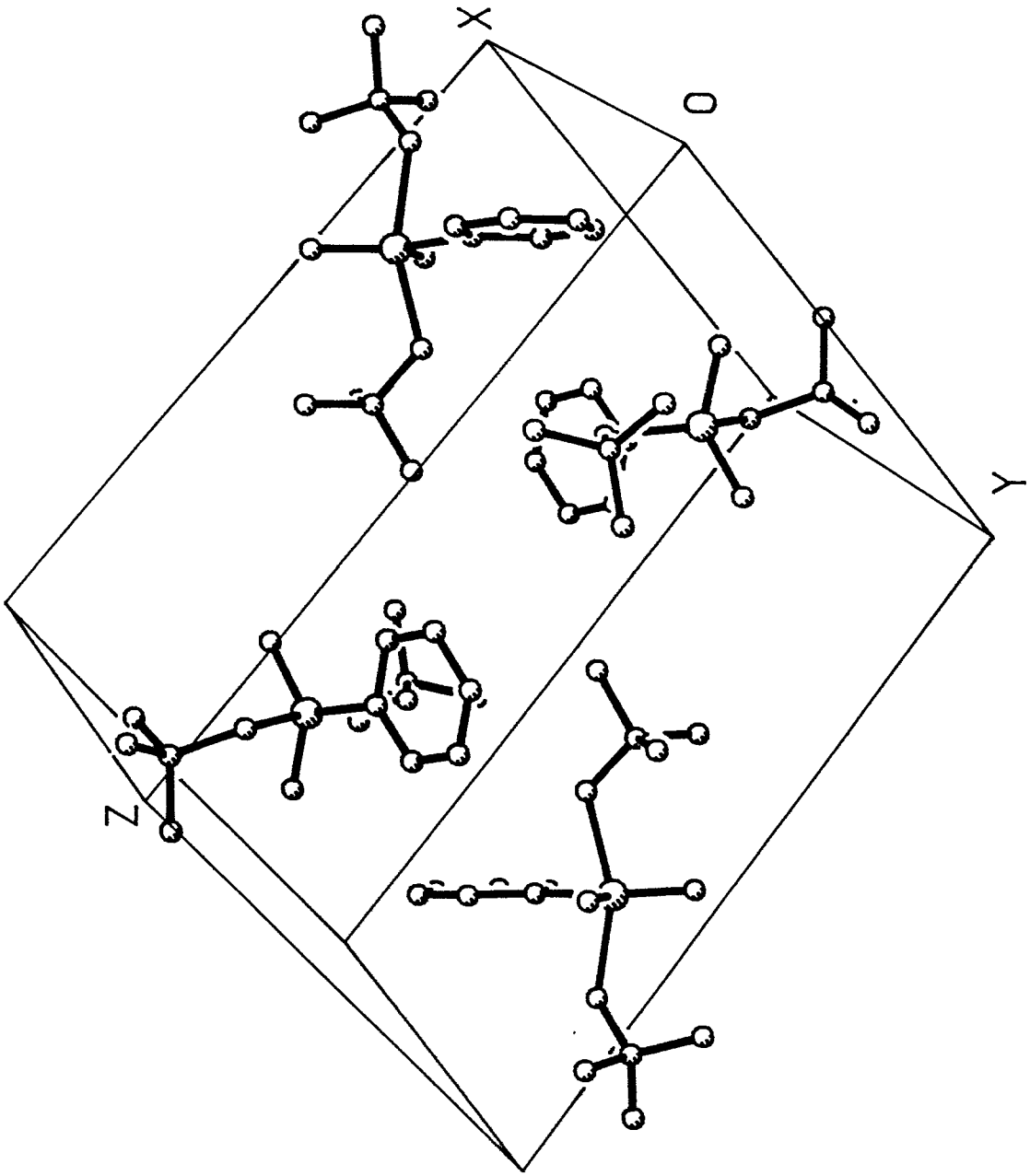

Figure S1. Packing diagram for $ReO_2(CH_2CMe_3)_2Ph$.

L1032-6

Table S5. Anisotropic displacement parameters ($Å^2 \times 10^3$) for $ReO_2(CH_2CMe_3)(py)_3$.[a]

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Re	23(1)	40(1)	27(1)	2(1)	6(1)	-3(1)
O(1)	36(6)	94(9)	24(5)	17(6)	-4(4)	2(5)
O(2)	35(5)	54(6)	38(6)	-5(5)	10(4)	-10(5)
N(1)	28(7)	38(7)	45(8)	7(5)	3(6)	-12(6)
N(2)	21(6)	38(7)	54(9)	5(6)	3(6)	-10(7)
N(3)	20(6)	47(8)	32(7)	-5(6)	11(6)	6(6)
C(11)	49(10)	48(11)	63(12)	17(9)	-3(9)	18(9)
C(12)	59(12)	50(12)	101(17)	-16(10)	-30(12)	31(12)
C(13)	36(11)	43(12)	208(29)	-6(9)	-33(15)	-18(17)
C(14)	58(13)	71(15)	140(22)	1(12)	-15(14)	-76(15)
C(15)	54(11)	51(11)	84(13)	17(9)	-6(10)	-51(11)
C(21)	41(10)	47(10)	66(12)	5(8)	2(9)	-14(9)
C(22)	51(14)	65(14)	118(20)	-7(11)	-34(14)	-31(14)
C(23)	34(13)	41(11)	194(30)	-9(9)	-22(18)	13(16)
C(24)	25(10)	74(14)	144(21)	12(10)	39(12)	40(14)
C(25)	44(10)	30(9)	71(12)	11(7)	14(9)	-9(8)
C(31)	36(9)	49(10)	43(9)	-13(8)	-3(8)	26(8)
C(32)	26(9)	31(9)	98(15)	-2(7)	-15(10)	12(9)
C(33)	12(8)	52(11)	121(17)	16(8)	29(10)	33(12)
C(34)	17(9)	69(12)	82(14)	10(8)	22(9)	26(10)
C(35)	44(10)	56(11)	51(10)	29(8)	13(8)	20(9)
C(4A)	51(14)	35(17)	82(24)	16(13)	30(14)	13(15)
C(4B)	64(30)	63(36)	64(41)	31(27)	-46(28)	-5(29)

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C(40)	51(10)	41(9)	34(9)	11(8)	9(8)	-3(8)
C(41A)	24(15)	57(18)	68(20)	0(13)	6(14)	7(16)
C(41B)	91(44)	91(42)	44(32)	9(35)	-54(32)	10(30)
C(42A)	48(17)	33(15)	101(26)	10(13)	-24(17)	6(16)
C(42B)	38(27)	75(42)	67(40)	15(25)	17(25)	-52(34)
C(43A)	58(18)	81(22)	54(18)	3(16)	2(14)	-1(15)
C(43B)	191(84)	49(36)	44(38)	-54(46)	-31(44)	8(30)

[a] The anisotropic displacement exponent takes the form: $-2\pi^2(h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12})$.

L1032-8

Table S6. Complete listing of bond lengths (Å) between non-hydrogen atoms for $ReO_2(CH_2CMe_3)(py)_3$.

Re-O(1)	1.748(9)	C(31)-C(32)	1.404(20)
Re-O(2)	1.741(9)	C(32)-C(33)	1.375(29)
Re-N(1)	2.348(11)	C(33)-C(34)	1.369(25)
Re-N(2)	2.136(11)	C(34)-C(35)	1.341(22)
Re-N(3)	2.158(11)	C(4A)-C(4B)	0.870(37)
Re-C(4A)	2.171(14)	C(4A)-C(40)	1.488(17)
Re-C(4B)	2.187(19)	C(4A)-C(41B)	1.827(38)
N(1)-C(11)	1.337(20)	C(4B)-C(40)	1.514(22)
N(1)-C(15)	1.301(22)	C(4B)-C(43A)	1.877(31)
N(2)-C(21)	1.328(20)	C(40)-C(41A)	1.517(20)
N(2)-C(25)	1.354(22)	C(40)-C(41B)	1.534(31)
N(3)-C(31)	1.319(18)	C(40)-C(42A)	1.511(20)
N(3)-C(35)	1.376(20)	C(40)-C(42B)	1.503(24)
C(11)-C(12)	1.375(25)	C(40)-C(43A)	1.542(23)
C(12)-C(13)	1.383(37)	C(40)-C(43B)	1.508(27)
C(13)-C(14)	1.311(39)	C(41A)-C(41B)	1.853(36)
C(14)-C(15)	1.354(27)	C(41A)-C(42B)	0.882(36)
C(21)-C(22)	1.372(26)	C(41B)-C(42A)	1.678(37)
C(22)-C(23)	1.378(43)	C(42A)-C(43B)	1.075(39)
C(23)-C(24)	1.332(37)	C(42B)-C(43A)	1.812(37)
C(24)-C(25)	1.359(24)	C(43A)-C(43B)	1.661(41)

L1032-9

Table S7. Complete listing of non-hydrogen atom bond angles (deg) for $ReO_2(CH_2CMe_3)(py)_3$.

O(1)-Re-O(2)	165.9(5)	C(4A)-C(40)-C(41A)	111.5(13)
O(1)-Re-N(1)	82.7(5)	C(4B)-C(40)-C(41B)	108.0(19)
O(2)-Re-N(1)	83.3(4)	C(4A)-C(40)-C(42A)	111.7(11)
O(1)-Re-N(2)	89.6(5)	C(41A)-C(40)-C(42A)	109.4(13)
O(2)-Re-N(2)	90.3(5)	C(4B)-C(40)-C(42B)	110.7(19)
N(1)-Re-N(2)	92.4(4)	C(41B)-C(40)-C(42B)	108.7(18)
O(1)-Re-N(3)	89.9(4)	C(4A)-C(40)-C(43A)	109.5(14)
O(2)-Re-N(3)	89.4(4)	C(41A)-C(40)-C(43A)	106.9(12)
N(1)-Re-N(3)	84.1(4)	C(42A)-C(40)-C(43A)	107.6(13)
N(2)-Re-N(3)	176.6(4)	C(4B)-C(40)-C(43B)	110.1(15)
O(1)-Re-C(4A)	103.1(7)	C(41B)-C(40)-C(43B)	108.6(19)
O(2)-Re-C(4A)	90.8(7)	C(42B)-C(40)-C(43B)	110.6(19)
N(1)-Re-C(4A)	171.6(7)	C(11)-C(12)-C(13)	119.2(20)
N(2)-Re-C(4A)	81.5(5)	C(12)-C(13)-C(14)	116.3(19)
N(3)-Re-C(4A)	101.9(5)	C(13)-C(14)-C(15)	122.9(23)
O(1)-Re-C(4B)	84.9(7)	N(1)-C(15)-C(14)	122.3(18)
O(2)-Re-C(4B)	109.1(7)	N(2)-C(21)-C(22)	123.8(18)
N(1)-Re-C(4B)	165.2(8)	C(21)-C(22)-C(23)	117.8(21)
N(2)-Re-C(4B)	95.4(9)	C(22)-C(23)-C(24)	119.7(20)
N(3)-Re-C(4B)	87.9(9)	C(23)-C(24)-C(25)	119.5(23)
Re-N(1)-C(11)	120.1(10)	N(2)-C(25)-C(24)	123.1(17)
Re-N(1)-C(15)	122.8(10)	N(3)-C(31)-C(32)	121.4(15)
C(11)-N(1)-C(15)	117.2(13)	C(31)-C(32)-C(33)	119.9(16)
Re-N(2)-C(21)	122.5(11)	C(32)-C(33)-C(34)	117.1(14)

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Re-N(2)-C(25)	121.5(10)	C(33)-C(34)-C(35)	121.9(17)
C(21)-N(2)-C(25)	115.9(13)	N(3)-C(35)-C(34)	121.3(15)
Re-N(3)-C(31)	121.1(10)	Re-C(4A)-C(40)	129.9(11)
Re-N(3)-C(35)	120.3(9)	Re-C(4B)-C(40)	127.2(15)
C(31)-N(3)-C(35)	118.3(12)		
N(1)-C(11)-C(12)	122.1(16)		

L1032-11

Table S8. Calculated H-atom coordinates (x 10^4) for $ReO_2(CH_2CMe_3)(py)_3$.

	x	y	z
H(11A)	-648	4201	706
H(12A)	-1902	5263	361
H(13A)	-2275	6013	1990
H(14A)	-1335	5666	3814
H(15A)	-171	4605	4108
H(21A)	3180	3805	4403
H(22A)	5391	4278	4390
H(23A)	6276	4473	2559
H(24A)	4973	4158	830
H(25A)	2831	3616	933
H(31A)	-1684	2714	1057
H(32A)	-3966	2288	1095
H(33A)	-4963	2238	2915
H(34A)	-3520	2455	4651
H(35A)	-1290	2839	4573
H(4AA)	2550	2251	3574
H(4AB)	2674	2279	2238
H(4BA)	1147	2068	4155
H(4BB)	2533	2245	3657
H(41D)	939	1419	940
H(41E)	386	803	1711
H(41F)	-254	1573	1748
H(41A)	2010	1905	1175

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H(41B)	3335	1719	2019
H(41C)	2511	1109	1310
H(42D)	3367	1034	2175
H(42E)	3326	984	3554
H(42F)	2380	483	2713
H(42A)	-450	1184	2950
H(42B)	-277	1612	1782
H(42C)	182	808	1886
H(43D)	1337	1388	4591
H(43E)	-67	1560	3844
H(43F)	573	790	3807
H(43A)	1781	759	4264
H(43B)	2307	461	3092
H(43C)	3131	1070	3801

L1032-13

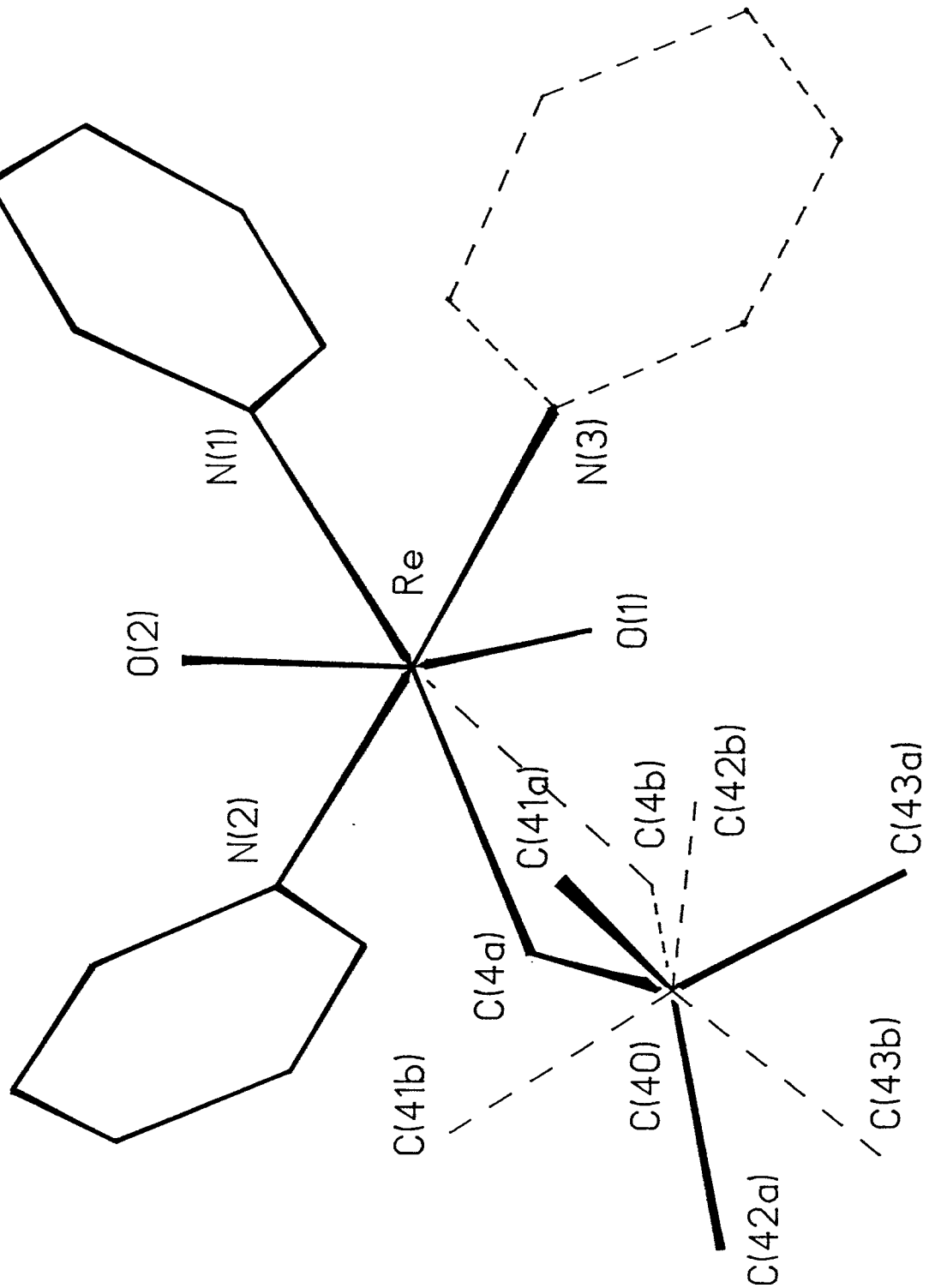

Figure S2. Stick drawing illustrating the disorder in the neopentyl ligand of $ReO_2(CH_2CMe_3)(py)_3$.

L1032-14

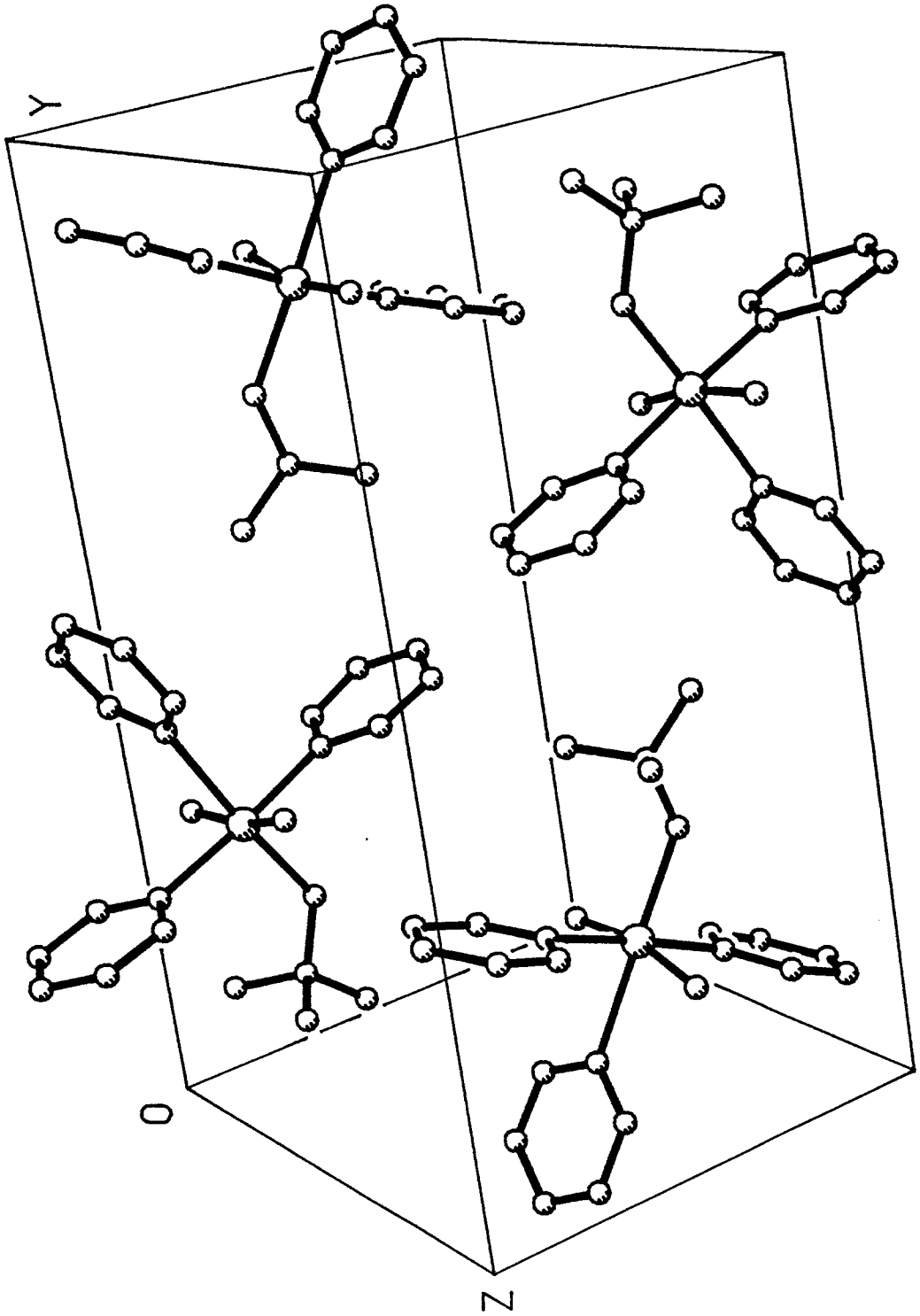

Figure S3. Packing diagram for $ReO_2(CH_2CMe_3)(py)_3$.

L1032-15

Table S9. Anisotropic displacement parameters ($Å^2 \times 10^3$) for $ReO_2(CHCMe_3)(CH_2CMe_3)$.[a]

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Re	33(1)	21(1)	19(1)	-1(1)	-1(1)	-2(1)
O(1)	45(5)	35(4)	32(4)	-3(4)	-16(4)	-1(3)
O(2)	37(5)	38(4)	40(5)	1(4)	9(4)	-8(4)
C(1)	24(6)	17(5)	20(6)	2(4)	-4(5)	-17(4)
C(10)	32(7)	13(5)	33(7)	1(4)	-7(5)	2(5)
C(11)	82(11)	35(7)	20(7)	2(7)	-12(7)	-3(5)
C(12)	90(13)	22(6)	36(8)	-14(7)	-10(8)	4(5)
C(13)	53(9)	53(9)	60(10)	11(8)	9(8)	28(8)
C(2)	23(6)	26(5)	16(5)	2(5)	-3(5)	6(4)
C(20)	30(6)	20(5)	26(6)	-6(4)	-8(6)	1(5)
C(21)	31(7)	34(6)	24(6)	-8(5)	2(5)	5(5)
C(22)	42(8)	26(6)	36(7)	1(5)	-10(7)	14(6)
C(23)	55(9)	28(6)	28(7)	-14(6)	3(6)	-1(5)

[a] The anisotropic displacement exponent takes the form: $-2\pi^2(h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12})$.

L1032-16

Table S10. Hydrogen atom coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for $ReO_2(CHCMe_3)(CH_2CMe_3)$.

atom	x	y	z	U
H(1A)	3026(132)	6358(62)	6869(100)	63(39)
H(11A)	1585(75)	6547(51)	4832(81)	19(23)
H(11B)	1562(102)	7332(64)	4488(108)	49(36)
H(11C)	2936(107)	6877(51)	4804(96)	35(30)
H(12A)	2643(100)	8052(47)	7267(102)	36(31)
H(12B)	3379(142)	7715(79)	6146(156)	91(57)
H(12C)	2351(143)	8179(72)	5979(126)	81(48)
H(13A)	306(138)	7453(63)	7312(152)	84(48)
H(13B)	53(97)	7036(58)	6214(102)	37(36)
H(13C)	125(127)	7751(67)	5750(126)	85(46)
H(2A)*	1643	5282	6563	26
H(2B)*	349	5601	6512	26
H(21A)*	-420	5190	9021	36
H(21B)*	-1035	4521	8651	36
H(21C)*	-1266	5165	7906	36
H(22A)	1122(88)	4020(49)	8588(80)	14(25)
H(22B)	2243(153)	4288(68)	7625(148)	104(49)
H(22C)	1643(81)	4605(45)	9025(96)	20(25)
H(23A)	686(144)	4247(70)	6019(140)	86(50)
H(23B)	-270(105)	3996(55)	6922(87)	30(31)
H(23C)	-612(79)	4615(38)	6052(79)	6(21)

*These hydrogens were fixed in idealized positions.

L1032-17

Table S11. Complete listing of bond lengths (Å) between non-hydrogen atoms for $ReO_2(CHCMe_3)(CH_2CMe_3)$.

Re-O(2)	1.696(7)	C(10)-C(12)	1.547(17)
Re-O(1)	1.706(7)	C(10)-C(13)	1.508(18)
Re-C(2)	2.114(9)	C(2)-C(20)	1.558(13)
Re-C(1)	1.869(9)	C(20)-C(21)	1.536(15)
C(1)-C(10)	1.501(13)	C(20)-C(22)	1.542(16)
C(10)-C(11)	1.533(16)	C(20)-C(23)	1.519(16)

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Table S12. Complete listing of bond lengths (Å) between non-hydrogen and hydrogen atoms for $ReO_2(C(H)CMe_3)(CH_2CMe_3)$.

C(1)-H(1A)	1.140(138)	C(13)-H(13A)	1.053(172)
C(2)-H(2A)*	0.960	C(21)-H(21A)*	0.960
C(2)-H(2B)*	0.960	C(21)-H(21B)*	0.960
C(11)-H(11C)	1.062(119)	C(21)-H(21C)*	0.960
C(11)-H(11B)	1.001(125)	C(22)-H(22C)	1.007(101)
C(11)-H(11A)	1.041(103)	C(22)-H(22B)	1.216(169)
C(12)-H(12A)	0.965(110)	C(22)-H(22A)	0.864(99)
C(12)-H(12B)	1.019(167)	C(23)-H(23C)	1.007(88)
C(12)-H(12C)	0.900(149)	C(23)-H(23B)	0.867(111)
C(13)-H(13C)	1.091(143)	C(23)-H(23A)	0.991(161)
C(13)-H(13B)	0.881(121)		

*These hydrogen atoms were fixed in idealized positions.

L1032-19

Table S13. Complete listing of non-hydrogen atom bond angles (deg) for $ReO_2(CHCMe_3)(CH_2CMe_3)$.

O(2)-Re-O(1)	124.6(4)	C(2)-C(20)-C(23)	107.0(9)
O(2)-Re-C(2)	105.0(4)	C(22)-C(20)-C(23)	109.8(9)
O(1)-Re-C(2)	106.9(3)	C(21)-C(20)-C(23)	109.1(9)
O(2)-Re-C(1)	111.7(4)	C(1)-C(10)-C(13)	113.0(10)
O(1)-Re-C(1)	109.3(4)	C(1)-C(10)-C(11)	107.1(8)
C(2)-Re-C(1)	94.8(4)	C(13)-C(10)-C(11)	109.4(11)
Re-C(2)-C(20)	117.4(6)	C(1)-C(10)-C(12)	108.3(9)
Re-C(1)-C(10)	136.6(8)	C(13)-C(10)-C(12)	109.9(10)
C(2)-C(20)-C(22)	110.4(9)	C(11)-C(10)-C(12)	109.1(10)
C(2)-C(20)-C(21)	110.6(8)		
C(22)-C(20)-C(21)	109.9(9)		

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Table S14. Bond angles (deg) involving the hydrogen atoms of $ReO_2(CHCMe_3)(CH_2CMe_3)$.

Re-C(1)-H(1A)	96.2(60)	H(2A)-C(2)-H(2B)	109.5(1)
C(10)-C(1)-H(1A)	124.2(57)	H(2A)-C(2)-C(20)	107.1(5)
C(10)-C(11)-H(11C)	113.4(59)	H(2B)-C(2)-C(20)	107.8(5)
C(10)-C(11)-H(11B)	102.9(69)	C(20)-C(21)-H(21A)	110.1(5)
H(11C)-C(11)-H(11B)	122.5(85)	C(20)-C(21)-H(21B)	109.9(5)
C(10)-C(11)-H(11A)	109.8(50)	H(21A)-C(21)-H(21B)	109.5(1)
H(11C)-C(11)-H(11A)	101.8(73)	C(20)-C(21)-H(21C)	108.4(6)
H(11B)-C(11)-H(11A)	105.9(88)	H(21A)-C(21)-H(21C)	109.5(1)
C(10)-C(12)-H(12A)	122.7(66)	H(21B)-C(21)-H(21C)	109.5(1)
C(10)-C(12)-H(12B)	101.0(89)	C(20)-C(22)-H(22C)	115.1(55)
H(12A)-C(12)-H(12B)	112.6(115)	C(20)-C(22)-H(22B)	108.3(75)
C(10)-C(12)-H(12C)	109.0(99)	H(22C)-C(22)-H(22B)	110.4(95)
H(12A)-C(12)-H(12C)	108.3(112)	C(20)-C(22)-H(22A)	114.2(64)
H(12B)-C(12)-H(12C)	101.1(129)	H(22C)-C(22)-H(22A)	96.7(86)
C(10)-C(13)-H(13C)	113.6(71)	H(22B)-C(22)-H(22A)	111.8(89)
C(10)-C(13)-H(13B)	107.2(68)	C(20)-C(23)-H(23C)	107.6(48)
H(13C)-C(13)-H(13B)	101.8(103)	C(20)-C(23)-H(23B)	98.8(69)
C(10)-C(13)-H(13A)	107.3(82)	H(23C)-C(23)-H(23B)	120.9(88)
H(13C)-C(13)-H(13A)	121.8(104)	C(20)-C(23)-H(23A)	107.6(90)
H(13B)-C(13)-H(13A)	103.6(104)	H(23C)-C(23)-H(23A)	107.7(99)
Re-C(2)-H(2A)	107.2(3)	H(23B)-C(23)-H(23A)	113.0(107)
Re-C(2)-H(2B)	107.7(3)		

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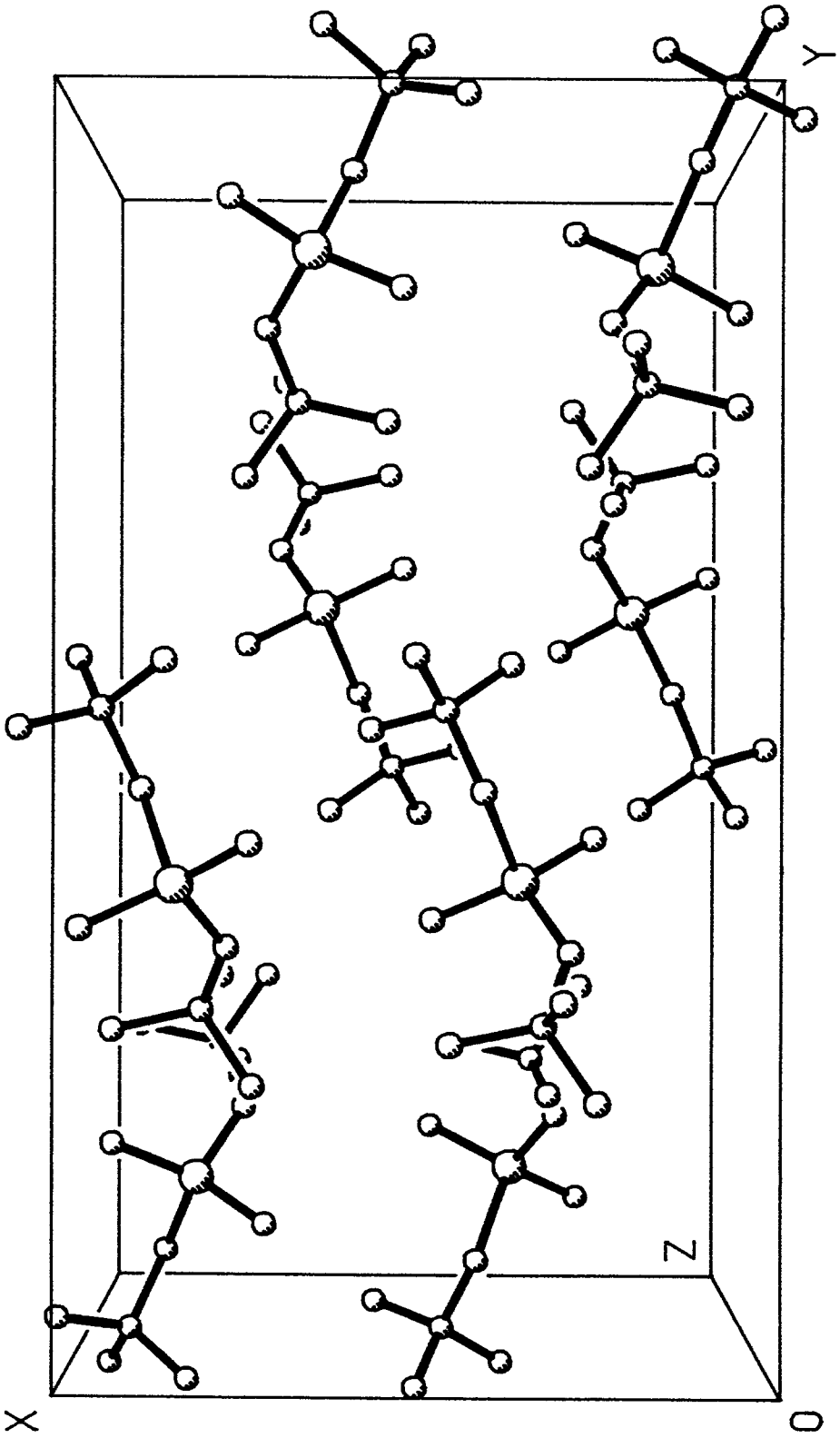

Figure S4. Packing diagram for $ReO_2(C(H)CMe_3)(CH_2CMe_3)$.

L 1032-22

Table S15. Anisotropic displacement parameters ($Å^2$ x 10^3) for $ReO_2(CHCMe_3)$-(CH_2CMe_3)(quin).[a]

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Re	18(1)	18(1)	22(1)	-1(1)	-4(1)	-1(1)
O(1)	32(2)	25(2)	26(2)	-2(2)	-2(2)	-2(2)
O(2)	20(2)	32(2)	30(2)	-4(2)	-5(2)	2(2)
C(1)	20(3)	31(3)	22(3)	-6(2)	-1(2)	-5(2)
C(10)	22(3)	30(3)	28(3)	-2(2)	-4(2)	2(2)
C(11)	47(5)	51(5)	29(4)	0(4)	-16(4)	1(4)
C(12)	31(4)	34(4)	47(4)	3(3)	-2(3)	12(3)
C(13)	26(3)	27(3)	33(3)	7(3)	-5(3)	0(3)
C(2)	30(3)	28(3)	25(3)	-10(2)	-5(3)	4(3)
C(20)	34(3)	23(3)	35(3)	-9(3)	-5(3)	0(3)
C(21)	42(5)	51(6)	168(12)	-43(6)	-32(6)	15(4)
C(22)	128(9)	27(4)	52(5)	0(3)	12(6)	31(5)
C(23)	95(8)	48(5)	51(5)	-34(4)	-12(5)	30(5)
N	21(2)	14(2)	31(3)	0(2)	-5(2)	1(2)
C(31)	23(3)	23(3)	37(3)	0(3)	-10(3)	6(3)
C(32)	35(4)	28(3)	30(3)	0(3)	-10(3)	2(3)
C(33)	41(4)	25(3)	27(3)	-9(2)	-4(3)	1(3)
C(34)	41(4)	24(3)	35(3)	-7(3)	-2(3)	-4(3)
C(35)	34(3)	23(3)	25(3)	0(2)	4(3)	-9(3)
C(36)	31(3)	29(3)	30(3)	-5(3)	3(3)	6(3)
C(37)	20(3)	27(3)	31(3)	-4(3)	-2(3)	0(3)

[a] The anisotropic displacement exponent takes the form: $-2\pi^2(h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12})$.

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Table S16. Hydrogen atom coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for $ReO_2(CHCMe_3)(CH_2CMe_3)$(quin).

atom	x	y	z	U
H(1)	5867(133)	-1681(76)	2739(47)	44(21)
H(11A)	4476(163)	-2103(92)	4517(56)	59(30)
H(11B)	7152(121)	-2259(69)	4134(43)	34(18)
H(11C)	5499(169)	-3003(98)	4614(58)	36(35)
H(12A)	5423(165)	-4572(95)	2844(64)	75(30)
H(12B)	5763(178)	-5349(108)	3759(66)	92(34)
H(12C)	7357(131)	-3945(73)	3104(48)	41(20)
H(13A)	1124(121)	-2889(74)	4120(44)	40(19)
H(13B)	2026(132)	-4341(82)	4436(52)	47(22)
H(13C)	1478(110)	-3923(65)	3452(43)	28(17)
H(2A)	3648(122)	673(71)	3403(44)	38(19)
H(2B)	1319(140)	-215(83)	3869(53)	54(23)
H(21A)*	-2706	2100	3062	94
H(21B)*	-1801	886	2632	94
H(21C)*	-2453	671	3629	94
H(22A)*	445	3514	2386	98
H(22B)*	2802	3018	2543	98
H(22C)*	1523	2360	1937	98
H(23A)	-328(239)	3018(141)	3968(88)	126(50)
H(23B)	1742(199)	2544(115)	4212(73)	93(40)
H(23C)	-941(205)	1299(127)	4582(78)	115(43)
H(31A)	1741(91)	-452(60)	520(33)	9(13)

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H(31B)	-387(102)	-1314(58)	860(37)	19(15)
H(32A)	2109(110)	-1463(68)	-716(42)	22(17)
H(32B)	130(120)	-1964(67)	-472(42)	28(17)
H(33A)	2628(106)	-3722(63)	-623(41)	26(16)
H(34A)	1844(111)	-5082(70)	738(41)	30(17)
H(34B)	-409(140)	-4183(78)	697(49)	51(23)
H(35A)*	173	-3412	1810	34
H(35B)*	2504	-4016	1816	34
H(36A)	5641(116)	-3941(74)	230(43)	33(18)
H(36B)	5848(117)	-2650(70)	-436(46)	32(18)
H(37A)	5437(101)	-1367(65)	551(38)	18(15)
H(37B)	5681(115)	-2553(67)	1191(43)	30(17)

*These hydrogens were fixed in idealized positions.

L1032-25

Table S17. Complete listing of bond lengths (Å) between non-hydrogen atoms for $ReO_2(CHCMe_3)(CH_2CMe_3)$(quin).

Re-O(1)	1.718(4)	C(20)-C(22)	1.513(10)
Re-O(2)	1.722(4)	C(20)-C(23)	1.534(12)
Re-C(1)	1.893(6)	N-C(31)	1.494(8)
Re-C(2)	2.144(7)	N-C(35)	1.500(7)
Re-N	2.425(5)	N-C(37)	1.480(7)
C(1)-C(10)	1.494(8)	C(31)-C(32)	1.541(10)
C(10)-C(11)	1.546(13)	C(32)-C(33)	1.541(9)
C(10)-C(12)	1.528(10)	C(33)-C(34)	1.530(8)
C(10)-C(13)	1.517(8)	C(33)-C(36)	1.532(10)
C(2)-C(20)	1.540(9)	C(34)-C(35)	1.521(10)
C(20)-C(21)	1.516(12)	C(36)-C(37)	1.543(10)

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Table S18. Complete listing of bond lengths (Å) between non-hydrogen and hydrogen atoms for $ReO_2(CHCMe_3)(CH_2CMe_3)$(quin).

C(1)-H(1)	0.891(77)	C(22)-H(22C)	0.960*
C(11)-H(11A)	0.842(96)	C(23)-H(23A)	0.842(144)
C(11)-H(11B)	1.137(71)	C(23)-H(23B)	0.932(124)
C(11)-H(11C)	0.493(87)	C(23)-H(23C)	1.457(117)
C(12)-H(12A)	0.973(116)	C(31)-H(31A)	0.892(60)
C(12)-H(12B)	1.183(99)	C(31)-H(31B)	1.051(59)
C(12)-H(12C)	0.946(76)	C(32)-H(32A)	0.802(59)
C(13)-H(13A)	1.101(75)	C(32)-H(32B)	0.935(79)
C(13)-H(13B)	0.898(76)	C(33)-H(33A)	1.006(72)
C(13)-H(13C)	0.985(77)	C(34)-H(34A)	1.041(70)
C(2)-H(2A)	1.088(76)	C(34)-H(34B)	1.040(88)
C(2)-H(2B)	1.028(75)	C(35)-H(35A)	0.960*
C(21)-H(21A)	0.960*	C(35)-H(35B)	0.960*
C(21)-H(21B)	0.960*	C(36)-H(36A)	1.007(71)
C(21)-H(21C)	0.960*	C(36)-H(36B)	0.949(64)
C(22)-H(22A)	0.960*	C(37)-H(37A)	0.885(60)
C(22)-H(22B)	0.960*	C(37)-H(37B)	0.941(69)

*These hydrogen atoms were fixed in idealized positions.

L1032-27

Table S19. Complete listing of non-hydrogen atom bond angles (deg) for $ReO_2(CHCMe_3)(CH_2CMe_3)(quin)$.

O(1)-Re-O(2)	133.3(2)	C(2)-C(20)-C(23)	107.5(6)
O(1)-Re-C(1)	110.8(2)	C(21)-C(20)-C(23)	109.2(8)
O(2)-Re-C(1)	113.9(2)	C(22)-C(20)-C(23)	106.6(6)
O(1)-Re-C(2)	95.6(2)	Re-N-C(31)	107.6(4)
O(2)-Re-C(2)	94.5(2)	Re-N-C(35)	112.8(3)
C(1)-Re-C(2)	93.8(3)	C(31)-N-C(35)	107.2(5)
O(1)-Re-N	81.5(2)	Re-N-C(37)	111.9(4)
O(2)-Re-N	82.3(2)	C(31)-N-C(37)	108.4(4)
C(1)-Re-N	94.2(2)	C(35)-N-C(37)	108.6(5)
C(2)-Re-N	172.0(2)	N-C(31)-C(32)	111.5(5)
Re-C(1)-C(10)	136.8(4)	C(31)-C(32)-C(33)	108.6(5)
C(1)-C(10)-C(11)	105.1(6)	C(32)-C(33)-C(34)	106.6(5)
C(1)-C(10)-C(12)	109.2(5)	C(32)-C(33)-C(36)	107.9(5)
C(11)-C(10)-C(12)	108.6(6)	C(34)-C(33)-C(36)	109.2(5)
C(1)-C(10)-C(13)	112.9(5)	C(33)-C(34)-C(35)	109.3(5)
C(11)-C(10)-C(13)	110.9(6)	N-C(35)-C(34)	111.5(5)
C(12)-C(10)-C(13)	109.9(5)	C(33)-C(36)-C(37)	108.7(5)
Re-C(2)-C(20)	120.5(4)	N-C(37)-C(36)	111.8(5)
C(2)-C(20)-C(21)	112.1(6)	C(21)-C(20)-C(22)	109.6(8)
C(2)-C(20)-C(22)	111.6(6)		

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Table S20. Bond angles (deg) involving the hydrogen atoms of $ReO_2(CHCMe_3)(CH_2CMe_3)$(quin).

Re-C(1)-H(1)	112.9(48)	H(21A)-C(21)-H(21B)	109.5(1)
H(1)-C(1)-C(10)	110.2(48)	H(21A)-C(21)-H(21C)	109.5(1)
C(10)-C(11)-H(11A)	103.2(71)	H(21B)-C(21)-H(21C)	109.5(1)
C(10)-C(11)-H(11B)	111.1(38)	C(20)-C(22)-H(22A)	111.1(5)
C(10)-C(11)-H(11C)	115.9(129)	C(20)-C(22)-H(22B)	107.7(5)
H(11A)-C(11)-H(11B)	117.2(75)	C(20)-C(22)-H(22C)	109.7(4)
H(11A)-C(11)-H(11C)	107.3(133)	H(22A)-C(22)-H(22B)	109.5(1)
H(11B)-C(11)-H(11C)	102.7(129)	H(22A)-C(22)-H(22C)	109.5(1)
C(10)-C(12)-H(12A)	112.3(56)	H(22B)-C(22)-H(22C)	109.5(1)
C(10)-C(12)-H(12B)	117.0(52)	C(20)-C(23)-H(23A)	110.1(104)
C(10)-C(12)-H(12C)	113.8(47)	C(20)-C(23)-H(23B)	123.0(80)
H(12A)-C(12)-H(12B)	92.6(76)	C(20)-C(23)-H(23C)	95.6(55)
H(12A)-C(12)-H(12C)	102.5(73)	H(23A)-C(23)-H(23B)	107.8(130)
H(12B)-C(12)-H(12C)	115.5(69)	H(23A)-C(23)-H(23C)	102.8(99)
C(10)-C(13)-H(13A)	106.7(38)	H(23B)-C(23)-H(23C)	115.5(86)
C(10)-C(13)-H(13B)	114.1(53)	N-C(31)-H(31A)	100.3(37)
C(10)-C(13)-H(13C)	108.9(35)	N-C(31)-H(31B)	106.2(32)
H(13A)-C(13)-H(13B)	103.3(64)	H(31A)-C(31)-H(31B)	106.3(49)
H(13A)-C(13)-H(13C)	101.5(56)	H(31A)-C(31)-C(32)	117.9(34)
H(13B)-C(13)-H(13C)	120.4(68)	H(31B)-C(31)-C(32)	113.4(37)
Re-C(2)-H(2A)	103.5(40)	C(31)-C(32)-H(32A)	120.6(53)
Re-C(2)-H(2B)	103.7(51)	C(31)-C(32)-H(32B)	112.0(41)
H(2A)-C(2)-H(2B)	107.4(61)	H(32A)-C(32)-H(32B)	97.3(63)
H(2A)-C(2)-C(20)	113.6(38)	H(32A)-C(32)-C(33)	107.2(50)

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H(2B)-C(2)-C(20)	107.0(46)	H(32B)-C(32)-C(33)	110.5(41)
C(20)-C(21)-H(21A)	109.5(4)	C(32)-C(33)-H(33A)	110.2(35)
C(20)-C(21)-H(21B)	108.5(6)	H(33A)-C(33)-C(34)	113.0(33)
C(20)-C(21)-H(21C)	110.3(5)	H(33A)-C(33)-C(36)	109.7(37)
C(34)-C(35)-H(35B)	109.3(3)	C(33)-C(34)-H(34A)	105.5(34)
H(35A)-C(35)-H(35B)	108.0(1)	C(33)-C(34)-H(34B)	116.6(39)
C(33)-C(36)-H(36A)	110.1(44)	H(34A)-C(34)-H(34B)	104.8(58)
C(33)-C(36)-H(36B)	112.4(48)	H(34A)-C(34)-C(35)	114.2(39)
H(36A)-C(36)-H(36B)	101.3(57)	H(34B)-C(34)-C(35)	106.5(45)
H(36A)-C(36)-C(37)	112.7(43)	N-C(35)-H(35A)	109.4(3)
H(36B)-C(36)-C(37)	111.7(47)	C(34)-C(35)-H(35A)	109.4(4)
N-C(37)-H(37A)	112.5(42)	N-C(35)-H(35B)	109.1(3)
C(36)-C(37)-H(37A)	110.0(42)	C(36)-C(37)-H(37B)	110.1(45)
N-C(37)-H(37B)	108.0(42)	H(37A)-C(37)-H(37B)	104.1(59)

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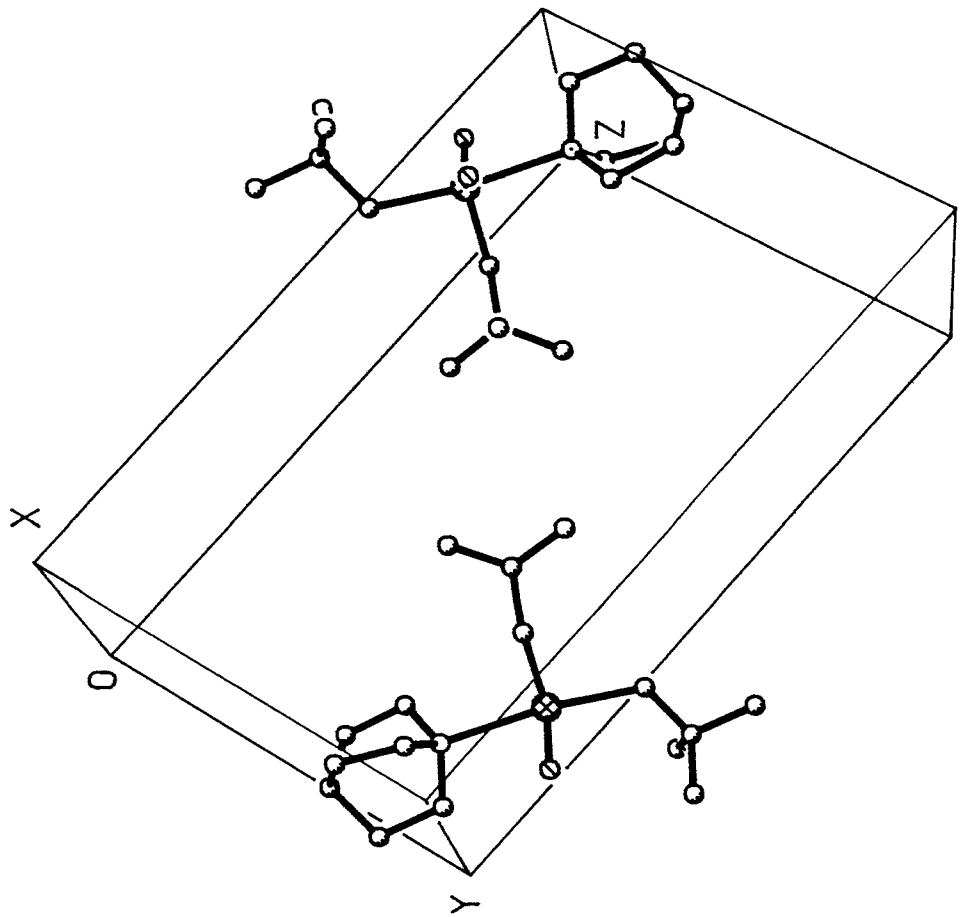

Figure S5. Packing diagram for $ReO_2(C(H)CMe_3)(CH_2CMe_3)(quin)$.