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Table 1. Crystal Data for $(HBpz_3)ReO(Ph)_2$

Formula	$C_{21}H_{20}BN_6ORe$
Formula Weight	569.44
Unit Cell[a]	monoclinic
a, Å	15.884 (2)
b, Å	17.193 (4)
c, Å	17.245 (3)
β, deg	116.11 (1)
V, Å^3	4227 (3)
Z	8
D(calc), g/cm^3	1.789
Space Group	$P2_1/c$
Crystal Size, mm	0.1 x 0.1 x 0.1
Diffractometer	Enraf-Nonius CAD4
Radiation	Mo Kα (0.71073 Å)
Monochromator	Graphite
Temperature	25 °C
Scan Mode	θ-2θ
Scan Range	$\Delta\theta = 0.65° + 0.347\tan\theta$
Scan Rate, deg/min	1.8
Maximum 2θ, deg	50
Octants collected	*HKL*, *HK*$\bar{L}$
Decay[b]	1.3%
Absorption coefficient[c] μ, cm^{-1}	58.50
Transmission factors	0.853-0.998 (ave = 0.943)
Reflections measured	8595
Reflections after averaging	6783 (R_{int} = 0.047 on F_o)
Unique observed reflections ($I > 2.5\sigma_I$)	3164
Number of parameters refined	311
R[d]	0.073
R_w[e]	0.073
Goodness of fit	1.340
Residual electron density, e/Å^3	±1.6

[a] Calculated from a least-squares fit of the setting angles of 25 reflections from all octants with $24° < 2\theta < 28°$ tuned on Friedel-related pairs ($\pm 2\theta$).

[b] Based on three standard reflections with $2\theta \approx 18°$ measured every 200 reflections. Linear decay correction based on these reflections was applied.

[c] Empirical absorption correction was applied.

[d] $R = \Sigma \mid |F_o| - |F_c| \mid$.

[e] $R_w = [\Sigma w(|F_o| - |F_c|)^2/\Sigma w F_o^2]^{1/2}$, where $w^{-1} = [\sigma^2_{count} + (0.04F^2)^2]/4F^2$.

Table 2. Positional and Equivalent Isotropic Thermal Parameters for $(HBpz_3)ReO(Ph)_2$.

Atom	x	y	z	B (Å2)[a]
Re1	0.10168(7)	0.08740(7)	0.19991(7)	2.98(3)
Re2	0.41534(7)	0.76988(6)	0.81744(7)	2.60(2)
O1	0.118(1)	0.067(1)	0.116(1)	4.3(5)
O2	0.388(1)	0.749(1)	0.8967(9)	3.5(5)
N111	0.209(1)	-0.028(1)	0.350(1)	2.8(5)*
N112	0.219(1)	0.028(1)	0.302(1)	3.5(6)
N121	0.041(1)	-0.060(1)	0.266(1)	4.7(6)*
N122	0.019(1)	-0.011(1)	0.196(1)	5.3(8)
N131	0.090(1)	0.043(1)	0.380(1)	4.6(6)*
N132	0.075(1)	0.100(1)	0.320(1)	4.8(7)
N211	0.338(1)	0.639(1)	0.680(1)	4.0(5)*
N212	0.310(1)	0.697(1)	0.721(1)	4.2(7)
N221	0.506(1)	0.625(1)	0.781(1)	4.5(6)*
N222	0.512(1)	0.677(1)	0.841(1)	3.2(6)
N231	0.457(1)	0.719(1)	0.659(1)	3.2(5)*
N232	0.455(1)	0.785(1)	0.707(1)	3.2(5)
C113	0.311(2)	0.026(2)	0.318(2)	4.5(7)*
C114	0.356(2)	-0.026(2)	0.371(2)	5.4(8)*
C115	0.292(2)	-0.061(2)	0.394(2)	3.8(6)*
C123	-0.056(2)	-0.046(2)	0.128(2)	4.5(7)*
C124	-0.083(2)	-0.115(2)	0.149(2)	4.5(7)*
C125	-0.018(2)	-0.121(2)	0.237(2)	6.4(9)*
C133	0.051(2)	0.162(2)	0.351(2)	4.0(7)*
C134	0.048(2)	0.143(2)	0.428(2)	5.2(8)*
C135	0.069(2)	0.064(2)	0.443(2)	5.5(8)*
C140	-0.022(2)	0.154(1)	0.140(2)	3.6(8)
C141	-0.033(2)	0.206(2)	0.072(2)	4.4(7)*
C142	-0.115(2)	0.248(2)	0.026(2)	5.3(8)*
C143	-0.188(2)	0.242(2)	0.045(2)	5.0(7)*
C144	-0.181(2)	0.191(2)	0.104(2)	4.5(7)*
C145	-0.101(2)	0.146(2)	0.154(2)	4.6(7)*
C150	0.183(2)	0.188(2)	0.248(2)	4.2(8)
C151	0.232(2)	0.216(2)	0.333(2)	4.7(7)*
C152	0.290(2)	0.279(2)	0.355(2)	4.6(7)*
C153	0.303(2)	0.321(2)	0.298(1)	3.2(6)*
C154	0.264(2)	0.303(2)	0.218(2)	5.6(8)*
C155	0.201(2)	0.237(2)	0.184(2)	5.1(7)*
C213	0.220(2)	0.691(2)	0.705(2)	4.2(7)*
C214	0.185(2)	0.627(2)	0.648(2)	3.8(6)*
C215	0.256(2)	0.599(2)	0.639(2)	4.4(7)*
C223	0.580(2)	0.656(2)	0.915(2)	3.6(6)*
C224	0.620(2)	0.584(2)	0.900(2)	3.9(6)*
C225	0.566(2)	0.570(2)	0.810(2)	4.5(7)*
C233	0.477(2)	0.847(2)	0.674(2)	3.5(6)*
C234	0.488(2)	0.821(2)	0.603(2)	5.1(8)*
C235	0.474(2)	0.742(2)	0.593(2)	3.9(6)*
C240	0.526(1)	0.845(1)	0.883(1)	3.4(7)
C241	0.523(2)	0.896(2)	0.945(1)	3.6(6)*

C242	0.602(2)	0.942(2)	0.999(2)	3.9(6)*
C243	0.685(2)	0.943(2)	0.995(2)	4.1(7)*
C244	0.690(2)	0.895(2)	0.934(2)	5.3(8)*
C245	0.612(2)	0.846(2)	0.876(2)	3.7(6)*
C250	0.329(1)	0.866(1)	0.761(1)	2.7(6)
C251	0.276(2)	0.873(2)	0.670(2)	3.6(6)*
C252	0.214(2)	0.931(2)	0.630(2)	5.3(8)*
C253	0.194(2)	0.985(2)	0.679(2)	4.6(7)*
C254	0.241(2)	0.978(2)	0.771(2)	5.1(8)*
C255	0.305(2)	0.917(2)	0.805(2)	4.1(6)*
B1	0.113(2)	-0.037(2)	0.356(2)	3.9(8)*
B2	0.434(2)	0.635(2)	0.685(2)	5.3(9)*

[a] Isotropically refined atoms are indicated with an asterisk. Anisotropically refined atoms given in the form of the isotropic equivalent thermal parameter defined as:

$4/3\ [a^2\beta_{11} + b^2\beta_{22} + c^2\beta_{33} + ab(\cos\gamma)\beta_{12} + ac(\cos\beta)\beta_{13} + bc(\cos\alpha)\beta_{23}]$

Table 3. Anisotropic Thermal Parameters for $(HBpz_3)ReO(Ph)_2$

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Re1	0.0364(5)	0.0287(6)	0.0504(5)	0.0032(6)	0.0213(4)	0.0042(6)
Re2	0.0383(5)	0.0292(5)	0.0336(4)	-0.0031(6)	0.0179(3)	-0.0048(6)
O1	0.05(1)	0.03(1)	0.08(1)	-0.007(9)	0.027(8)	0.01(1)
O2	0.059(9)	0.04(1)	0.031(8)	-0.015(9)	0.020(7)	0.008(8)
N112	0.06(1)	0.04(1)	0.05(1)	0.02(1)	0.043(7)	0.01(1)
N122	0.07(1)	0.03(1)	0.10(2)	-0.01(1)	0.04(1)	0.02(1)
N132	0.05(1)	0.08(2)	0.05(1)	-0.01(1)	0.028(9)	-0.03(1)
N212	0.05(1)	0.05(2)	0.07(1)	-0.01(1)	0.032(9)	-0.01(1)
N222	0.04(1)	0.05(1)	0.04(1)	-0.00(1)	0.027(7)	0.01(1)
N232	0.03(1)	0.03(1)	0.06(1)	-0.02(1)	0.019(8)	-0.03(1)
C140	0.07(2)	0.01(1)	0.06(2)	-0.01(1)	0.03(1)	-0.01(1)
C150	0.05(1)	0.04(2)	0.08(2)	-0.01(1)	0.03(1)	-0.01(2)
C240	0.04(1)	0.03(2)	0.08(1)	0.01(1)	0.054(8)	0.01(1)
C250	0.04(1)	0.01(1)	0.06(1)	0.01(1)	0.02(1)	0.01(1)

The form of the anisotropic thermal parameter is:

$$\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2hka^*b^*U_{12} + 2hla^*c^*U_{13} + 2klb^*c^*U_{23})]$$

Table 4. Hydrogen Atoms for $(HBpz_3)ReO(Ph)_2$

Atom	x	y	z	B(Å^2)
H1	0.1158	-0.0779	0.4014	4
H2	0.4386	0.5926	0.6443	5
H141	0.0199	0.2135	0.0581	4
H142	-0.1191	0.2825	-0.0200	5
H143	-0.2437	0.2728	0.0157	5
H144	-0.2362	0.1838	0.1138	5
H145	-0.1011	0.1108	0.1984	4
H151	0.2258	0.1894	0.3800	4
H152	0.3220	0.2947	0.4150	4
H153	0.3452	0.3652	0.3165	3
H154	0.2759	0.3348	0.1776	5
H155	0.1708	0.2249	0.1228	5
H241	0.4646	0.8999	0.9520	4
H242	0.5971	0.9749	1.0425	4
H243	0.7381	0.9751	1.0338	4
H244	0.7487	0.8929	0.9272	5
H245	0.6176	0.8131	0.8320	3
H251	0.2832	0.8325	0.6334	3
H252	0.1855	0.9355	0.5680	5
H253	0.1489	1.0268	0.6512	4
H254	0.2279	1.0143	0.8083	5
H255	0.3350	0.9126	0.8680	4
H113	0.3404	0.0602	0.2911	4
H114	0.4216	-0.0387	0.3919	5
H115	0.3062	-0.1032	0.4371	4
H123	-0.0868	-0.0245	0.0699	5
H124	-0.1345	-0.1494	0.1131	4
H125	-0.0169	-0.1652	0.2725	6
H133	0.0370	0.2134	0.3230	4
H134	0.0347	0.1776	0.4658	5
H135	0.0682	0.0319	0.4891	5
H213	0.1838	0.7235	0.7279	4
H214	0.1215	0.6076	0.6207	4
H215	0.2510	0.5502	0.6050	4
H223	0.6000	0.6823	0.9710	3
H224	0.6718	0.5528	0.9412	3
H225	0.5729	0.5265	0.7764	4
H233	0.4855	0.8999	0.6957	3
H234	0.5028	0.8544	0.5653	5
H235	0.4764	0.7111	0.5476	4

Isotropic hydrogen atoms were fixed in calculated positions.

Table 5. Bond Distances (Å) for $(HBpz_3)ReO(Ph)_2$

Atom	Atom	Distance	Atom	Atom	Distance	Atom	Atom	Distance
Re1	O1	1.61(2)	N211	N212	1.41(3)	C150	C151	1.41(3)
Re1	N112	2.17(2)	N211	C215	1.36(3)	C150	C155	1.52(4)
Re1	N122	2.13(2)	N211	B2	1.50(4)	C151	C152	1.36(3)
Re1	N132	2.30(2)	N212	C213	1.35(3)	C152	C153	1.30(3)
Re1	C140	2.10(2)	N221	N222	1.34(3)	C153	C154	1.28(3)
Re1	C150	2.10(2)	N221	C225	1.27(3)	C154	C155	1.44(4)
Re2	O2	1.647(14)	N221	B2	1.56(4)	C213	C214	1.42(3)
Re2	N212	2.16(2)	N222	C223	1.31(3)	C214	C215	1.29(3)
Re2	N222	2.13(2)	N231	N232	1.41(2)	C223	C224	1.46(3)
Re2	N232	2.27(2)	N231	C235	1.33(3)	C224	C225	1.43(3)
Re2	C240	2.06(2)	N231	B2	1.61(4)	C233	C234	1.37(3)
Re2	C250	2.09(2)	N232	C233	1.33(3)	C234	C235	1.37(3)
N111	N112	1.33(2)	C113	C114	1.26(3)	C240	C241	1.40(3)
N111	C115	1.33(3)	C114	C115	1.37(3)	C240	C245	1.43(3)
N111	B1	1.57(3)	C123	C124	1.36(3)	C241	C242	1.43(3)
N112	C113	1.35(3)	C124	C125	1.41(3)	C242	C243	1.35(3)
N121	N122	1.39(3)	C133	C134	1.40(3)	C243	C244	1.37(3)
N121	C125	1.35(3)	C134	C135	1.39(4)	C244	C245	1.47(3)
N121	B1	1.53(3)	C140	C141	1.43(3)	C250	C251	1.42(3)
N122	C123	1.38(3)	C140	C145	1.39(3)	C250	C255	1.33(3)
N131	N132	1.37(3)	C141	C142	1.38(3)	C251	C252	1.36(3)
N131	C135	1.32(3)	C142	C143	1.34(3)	C252	C253	1.38(3)
N131	B1	1.53(4)	C143	C144	1.31(3)	C253	C254	1.44(3)
N132	C133	1.33(3)	C144	C145	1.41(3)	C254	C255	1.39(3)

Table 6. Bond Angles (deg) for $(HBpz_3)ReO(Ph)_2$

Atom	Atom	Atom	Angle	Atom	Atom	Atom	Angle
O1	Re1	N112	101.7(7)	N232	N231	B2	119. (2)
O1	Re1	N122	97.7(8)	C235	N231	B2	131. (2)
O1	Re1	N132	172.6(8)	Re2	N232	N231	119.8(14)
O1	Re1	C140	99.2(9)	Re2	N232	C233	132.6(16)
O1	Re1	C150	102.9(9)	N231	N232	C233	108. (2)
N112	Re1	N122	87.3(8)	N112	C113	C114	112. (3)
N112	Re1	N132	75.4(7)	C113	C114	C115	106. (3)
N112	Re1	C140	159.1(8)	N111	C115	C114	109. (2)
N112	Re1	C150	84.5(9)	N122	C123	C124	114. (2)
N122	Re1	N132	75.5(9)	C123	C124	C125	101. (2)
N122	Re1	C140	89.1(9)	N121	C125	C124	114. (3)
N122	Re1	C150	159. (1)	N132	C133	C134	109. (3)
N132	Re1	C140	83.8(9)	C133	C134	C135	107. (3)
N132	Re1	C150	83.6(9)	N131	C135	C134	104. (3)
C140	Re1	C150	91.6(9)	Re1	C140	C141	120. (2)
O2	Re2	N212	96.7(7)	Re1	C140	C145	126. (2)
O2	Re2	N222	96.3(7)	C141	C140	C145	113. (2)
O2	Re2	N232	173.9(7)	C140	C141	C142	123. (3)
O2	Re2	C240	98.9(8)	C141	C142	C143	121. (3)
O2	Re2	C250	101.2(8)	C142	C143	C144	117. (3)
N212	Re2	N222	87.7(8)	C143	C144	C145	125. (3)
N212	Re2	N232	79.9(7)	C140	C145	C144	120. (3)
N212	Re2	C240	164.5(8)	Re1	C150	C151	131. (2)
N212	Re2	C250	88.4(8)	Re1	C150	C155	117. (2)
N222	Re2	N232	78.6(7)	C151	C150	C155	112. (2)
N222	Re2	C240	90.0(8)	C150	C151	C152	124. (3)
N222	Re2	C250	162.4(8)	C151	C152	C153	123. (3)
N232	Re2	C240	84.6(8)	C152	C153	C154	121. (3)
N232	Re2	C250	83.9(8)	C153	C154	C155	123. (3)
C240	Re2	C250	89.2(9)	C150	C155	C154	117. (2)
N112	N111	C115	107. (2)	N212	C213	C214	105. (2)
N112	N111	B1	121. (2)	C213	C214	C215	107. (2)
C115	N111	B1	132. (2)	N211	C215	C214	115. (3)
Re1	N112	N111	122.9(15)	N222	C223	C224	108. (2)
Re1	N112	C113	130. (2)	C223	C224	C225	103. (2)
N111	N112	C113	106. (2)	N221	C225	C224	107. (2)
N122	N121	C125	106. (2)	N232	C233	C234	107. (2)
N122	N121	B1	121. (2)	C233	C234	C235	111. (3)
C125	N121	B1	132. (3)	N231	C235	C234	106. (2)
Re1	N122	N121	122. (2)	Re2	C240	C241	121. (2)
Re1	N122	C123	132. (2)	Re2	C240	C245	125. (2)
N121	N122	C123	105. (2)	C241	C240	C245	114. (2)
N132	N131	C135	114. (2)	C240	C241	C242	123. (2)
N132	N131	B1	115. (2)	C241	C242	C243	125. (3)
C135	N131	B1	130. (3)	C242	C243	C244	115. (2)
Re1	N132	N131	125. (2)	C243	C244	C245	124. (3)
Re1	N132	C133	130. (2)	C240	C245	C244	120. (2)
N131	N132	C133	105. (2)	Re2	C250	C251	122. (2)
N212	N211	C215	101. (2)	Re2	C250	C255	124. (2)

N212	N211	B2	122. (2)	C251	C250	C255	113. (2)
C215	N211	B2	136. (3)	C250	C251	C252	124. (2)
Re2	N212	N211	120.0(15)	C251	C252	C253	120. (3)
Re2	N212	C213	127. (2)	C252	C253	C254	118. (3)
N211	N212	C213	112. (2)	C253	C254	C255	117. (3)
N222	N221	C225	114. (2)	C250	C255	C254	127. (3)
N222	N221	B2	121. (2)	N111	B1	N121	105. (2)
C225	N221	B2	125. (3)	N111	B1	N131	107. (2)
Re2	N222	N221	123.6(16)	N121	B1	N131	110. (2)
Re2	N222	C223	128. (2)	N211	B2	N221	108. (2)
N221	N222	C223	108. (2)	N211	B2	N231	107. (2)
N232	N231	C235	109. (2)	N221	B2	N231	105. (2)