

Supporting Information

Mechanism of protonation induced changes in Raman spectra of a trisheteroleptic ruthenium complex revealed by DFT calculations

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Tabelle S1: calculated RuN bond lengths in pm

	Ru	RuH₂
RuN1 (tmbibzim, opposite dppz)	211.5	213.8
RuN1' (tmbibzim, opposite tbbpy)	211.7	214.2
RuN2 (tbbpy, opposite dppz)	208.1	209.1
RuN2' (tbbpy, opposite tmbibzim)	209.5	208.6
RuN3 (dppz, opposite tbbpy)	208.7	210.2
RuN3' (dppz, opposite tmbibzim)	209.9	209.2

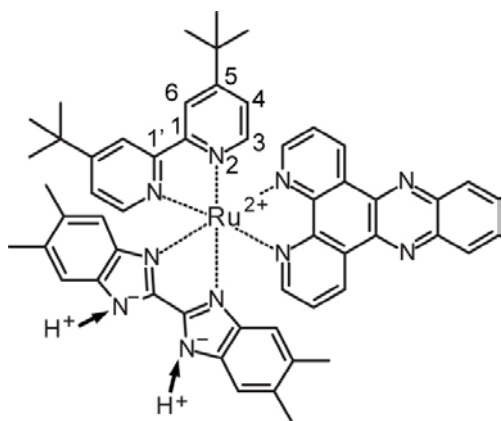


Figure S1: Numbering of the atoms used in table S2.

Tabelle S2: calculated bond lengths in pm and bond angles in degree of tbbpy

	Ru	RuH ₂
C1N2	136.5	136.5
C1C1'	147.6	147.7
N2C3	134.5	134.4
C3C4	139.0	139.0
C4C5	140.1	140.0
C5C6	140.2	140.3
C6C1	139.5	139.4
C6C1N2	121.2°	121.1°
C1N2C3	118.0°	118.1°
N2C3C4	123.0°	123.0°
C3C4C5	120.3°	120.3°
C4C5C6	116.0°	116.1°
C5C6C1	121.4°	121.4°
C1'C1N2	114.8°	114.9°

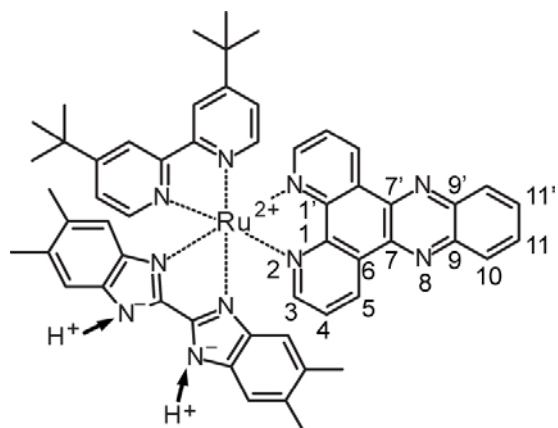


Figure S2: Numbering of the atoms used in table S3.

Tabelle S3: selected bond lengths in pm and bond angles in degree of dppz

	Ru	RuH ₂
C1N2	136.5	136.5
C1C1'	144.6	144.7
N2C3	134.3	134.1
C3C4	139.8	139.9
C4C5	138.8	138.7
C5C6	140.4	140.4
C6C1	140.6	140.6
C6C7	146.5	146.4
C7C7'	143.9	143.7
C7N8	132.7	132.7
N8C9	135.2	135.2
C9C10	142.2	142.2
C9C9'	143.8	143.9
C10C11	137.5	137.5
C11C11'	142.4	142.4

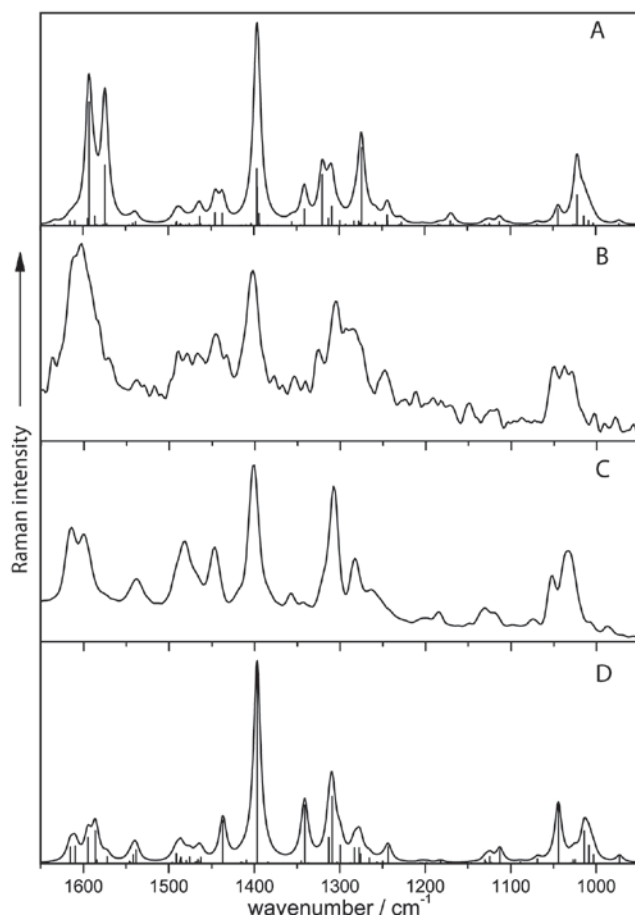


Figure S3: Comparison of experimental Raman spectra of **RuH₂** (B) and **[(tbbpy)₂Ru(dppz)](PF₆)₂** (C) in the solid state at 1064 nm excitation with the calculated Raman spectrum of **RuH₂** (A) and the spectrum of **RuH₂** without tmbibzim modes (D), which is very similar to the Raman spectrum of and **[(tbbpy)₂Ru(dppz)](PF₆)₂**. The poor quality of the spectrum of **RuH₂** is due to the strong background.

Table S4: Signal positions of the experimental and calculated Raman bands and their respective Raman activity for **Ru** and **RuH₂**. tmbibzim modes are marked red and phz centered dppz modes are marked in green corresponding to Figure 2 in the main text. Mixed modes involving more than one ligand are marked yellow.

Ru Freq. (Calc.) / cm ⁻¹	Raman activity	RuH₂ Freq. (Calc.) / cm ⁻¹	Raman activity	Assignment ^a
		1633	197.7	v _{sym} -ring, tmbibzim
		1632	34.8	v _{asym} -ring, tmbibzim
1622	20.5	1622	17.1	v _{asym} -ring, dppz phenaz
1618	635.23			v _{sym} -ring, tmbibzim
1617	148.6			v _{asym} -ring, tmbibzim
1613	1515.5	1615	824.3	v _{asym} -ring, tbbpy
1609	861.0	1610	852.1	v _{sym} -ring, tbbpy
1591	2086.0	1595	1239.0	v _{asym} -ring, dppz phen
		1593	20710.0	v _{sym} -ring, tmbibzim
1584	1123.9	1586	1546.2	v _{sym} -ring, dppz phen
1580	416.2	1584	166.3	v _{asym} -ring, dppz phen
		1576	161.2	v _{asym} -ring, tmbibzim
		1574	9867.4	v _{sym} -ring, tmbibzim
		1572	321.5	v _{sym} -ring, dppz phen
1569	11377.0			v _{sym} -ring, tmbibzim, v _{sym} -ring, dppz phen
1567	363.2			v _{sym} -ring, dppz phen, v _{sym} -ring, tmbibzim
		1546	107.1	v _{sym} -ring, dppz phz; v _{asym} -ring, tbbpy
1546	73.9			v _{sym} -ring, dppz phz
		1545	46.9	v _{asym} -ring, tbbpy; v _{sym} -ring, dppz phz
1543	7.2			v _{asym} -ring, tmbibzim
1542	55.8			v _{asym} -ring, tbbpy; v _{asym} -ring, dppz phz
1542	190.6			v _{asym} -ring, dppz phz; v _{asym} -ring, tbbpy
		1542	385.2	v _{asym} -ring, dppz phz
1534	593.4	1538	589.5	v _{sym} -ring, tbbpy
1519	4616.3			v _{sym} -ring, tmbibzim
		1496	52.5	v _{asym} -ring, tmbibzim; v-tb, tbbpy
		1496	35.7	v-tb, tbbpy; v _{asym} -ring, tmbibzim
1496	6.9			v-tb, tbbpy

1495	48.3	1496	38.2	v-tb, tbbpy
		1491	405.5	v _{sym} -ring, dppz; v _{sym} -ring, tmbibzim
		1490	546.4	v _{sym} -ring, tmbibzim; v _{sym} -ring, dppz
1489	433.6			v _{sym} -ring, dppz
1485	45.9	1487	134.1	v _{asym} -ring, tbbpy
		1486	256.6	v _{asym} -ring, dppz; v _{sym} -ring, tbbpy; v _{asym} -ring, tmbibzim
		1486	132.5	v _{sym} -ring, tbbpy; v _{asym} -ring, tmbibzim; v _{asym} -ring, dppz;
1485	22.8			v _{asym} -ring, tbbpy; v-tb, tbbpy; v _{asym} -ring, dppz
1485	57.9			v _{asym} -ring, dppz; v _{asym} -ring, tbbpy; v-tb, tbbpy
		1485	63.0	v-tb, tbbpy
		1485	50.8	v-tb, tbbpy
1484	92.4			v _{asym} -ring, dppz; v _{asym} -ring, tbbpy; v-tb, tbbpy
		1484	126.6	v _{asym} -ring, tmbibzim; v _{sym} -ring, tbbpy; v _{asym} -ring, dppz
1482	340.1			v _{sym} -ring, tbbpy
1481	23.2			v _{asym} -ring, tmbibzim
1480	43.6			v _{sym} -ring, tmbibzim
1478	273.0	1480	112.6	v _{sym} -ring, tbbpy
		1476	275.0	v _{asym} -ring, tbbpy; v _{asym} -ring, tmbibzim
		1475	73.9	v _{asym} -ring, tmbibzim; v _{asym} -ring, tbbpy
		1474	37.4	v _{sym} -ring, tmbibzim
1474	12.6			v _{asym} -ring, tmbibzim
1472	760.5			v _{asym} -ring, tbbpy, v _{sym} -ring, tmbibzim
1472	1009.2			v _{sym} -ring, tmbibzim, v _{asym} -ring, tbbpy
1468	148.3	1469	65.9	v _{asym} -ring, tbbpy
		1468	123.9	v _{asym} -ring, tmbibzim, v _{sym} -ring, dppz
1467	43.5	1467	41.3	v-ch3, tmbibzim
1467	46.4	1467	56.2	v-ch3, tmbibzim
1466	92.8	1466	68.8	v _{sym} -ring, tbbpy
		1466	153.6	v _{sym} -ring, dppz; v _{asym} -ring, tmbibzim
1465	4.5	1465	4.8	v-tb, tbbpy
1465	11.1	1465	3.5	v-tb, tbbpy
		1464	1252.0	v _{sym} -ring, tmbibzim; v _{asym} -ring, dppz;
1463	54.5	1463	87.3	v-tb, tbbpy
1463	49.6	1463	48.6	v-tb, tbbpy
		1462	245.7	v _{asym} -ring, dppz; v _{sym} -ring,

				tmbibzim
1462	79.5			v _{sym} -ring, dppz
1459	95.1			v _{asym} -ring, dppz
1458	27.4			v _{asym} -ring, tmbibzim
1455	2800.2			v _{sym} -ring, tmbibzim
1454	126.7	1453	54.0	v-ch3, tmbibzim
1454	87.6	1452	55.9	v-ch3, tmbibzim
		1448	4.1	v _{asym} -ring, tmbibzim
		1445	1724.4	v _{sym} -ring, tmbibzim
1442	17.1			v _{asym} -ring, tmbibzim
1434	2013.3	1436	1624.0	v _{sym} -ring, dppz phen
1429	310.4			v _{sym} -ring, tmbibzim
1419	12.6			v _{asym} -ring, tmbibzim
		1415	36.0	v _{asym} -ring, dppz phen; v _{sym} -ring, tbbpy
1415	47.4			v _{sym} -ring, tbbpy;
		1415	42.1	v _{sym} -ring, tbbpy; v _{asym} -ring, dppz phen
1414	12.4			v _{asym} -ring, dppz phen
1413	45.1	1414	25.0	v _{asym} -ring, tbbpy
1412	6.9	1413	3.6	v _{asym} -ring, tbbpy
1408	84.9	1409	110.4	v _{sym} -ring, tbbpy
1401	566.6	1404	26.5	v-ch3, tmbibzim
1401	17.9	1403	257.9	v-ch3, tmbibzim
		1401	7.7	v _{asym} -ring, tmbibzim
		1397	7086.7	v _{sym} -ring, dppz phz; v _{sym} -ring, tmbibzim
		1396	4752.1	v _{sym} -ring, tmbibzim; v _{sym} -ring, dppz phz
1395	8354.6			v _{sym} -ring, dppz phz
		1394	1486.3	v-ch3, tmbibzim; v _{sym} -ring, tmbibzim
		1393	321.8	v-ch3, tmbibzim; v _{asym} -ring, tmbibzim
1391	29.2			v-ch3, tmbibzim
1390	173.2			v-ch3, tmbibzim
1384	43.9	1384	37.1	v-tb, tbbpy
1383	9.0	1384	10.7	v-tb, tbbpy
1383	25.8	1383	4.6	v-tb, tbbpy
1383	4.5	1383	29.1	v-tb, tbbpy
		1356	462.7	v _{sym} -ring, tmbibzim
1344	26.9	1345	85.8	v _{sym} -ring, dppz phz
		1341	1896.3	v _{sym} -ring, dppz phen
1339	1929.2			v _{sym} -ring, dppz phen; v _{sym} -ring, tmbibzim
		1338	3.1	v _{asym} -ring, tmbibzim
1336	49.9	1337	13.1	v _{asym} -ring, dppz phz

1335	898.3			$v_{\text{sym}}\text{-ring, tmbibzim}; v_{\text{sym}}\text{-ring, dppz phen}$
1332	142.5			$v_{\text{asym}}\text{-ring, tmbibzim}$
		1319	5573.5	$v_{\text{sym}}\text{-ring, tmbibzim}$
1318	1338.6			$v_{\text{sym}}\text{-ring, tmbibzim}$
1311	1100.1	1313	796.1	$v_{\text{sym}}\text{-ring, tbbpy}$
		1308	2050.5	$v_{\text{sym}}\text{-ring, dppz phen}$
1304	1878.9			$v_{\text{sym}}\text{-ring, dppz phen}; v_{\text{asym}}\text{-ring, tmbibzim}$
		1303	38.2	$v_{\text{asym}}\text{-ring, tbbpy}$
1301	872.1			$v_{\text{asym}}\text{-ring, tmbibzim}; v_{\text{sym}}\text{-ring, dppz phen}; v_{\text{asym}}\text{-ring, tbbpy};$
1300	1418.7			$v_{\text{asym}}\text{-ring, tbbpy}; v_{\text{asym}}\text{-ring, tmbibzim}$
1298	9076.0			$v_{\text{sym}}\text{-ring, tmbibzim}; v_{\text{asym}}\text{-ring, tbbpy};$
1298	477.9	1300	556.2	$v_{\text{asym}}\text{-ring, dppz phen}$
		1293	123.8	$v_{\text{asym}}\text{-ring, tmbibzim}$
1286	2.9	1287	14.7	$v_{\text{asym}}\text{-ring, dppz phen}$
1278	682.5	1283	456.4	$v_{\text{sym}}\text{-ring, tbbpy};$
1276	352.3	1277	449.2	$v_{\text{sym}}\text{-ring, dppz phen}; v_{\text{sym}}\text{-ring, tbbpy};$
1273	564.8	1275	277.3	$v_{\text{sym}}\text{-ring, tbbpy}; v_{\text{sym}}\text{-ring, dppz phen}$
		1274	7890.2	$v_{\text{sym}}\text{-ring, tmbibzim}$
1265	230.2	1266	156.3	$v_{\text{asym}}\text{-ring, tbbpy}$
1260	8.8			$v_{\text{asym}}\text{-ring, tmbibzim}$
		1258	337.8	$v_{\text{asym}}\text{-ring, tmbibzim}$
1256	64.6	1257	35.8	$v_{\text{asym}}\text{-ring, tbbpy}$
1248	77.9	1250	62.3	$v_{\text{sym}}\text{-ring, dppz phz}$
1245	62.6			$v_{\text{asym}}\text{-ring, tmbibzim}; v_{\text{sym}}\text{-ring, tbbpy}$
		1244	1011.0	$v_{\text{sym}}\text{-ring, tmbibzim}; v_{\text{sym}}\text{-ring, tbbpy}$
		1243	459.3	$v_{\text{sym}}\text{-ring, tbbpy}; v_{\text{sym}}\text{-ring, tmbibzim};$
1244	194.0			$v_{\text{sym}}\text{-ring, tmbibzim}$
1243	213.9			$v_{\text{sym}}\text{-ring, tbbpy}, v_{\text{asym}}\text{-ring, tmbibzim}$
1230	1.2	1230	1.7	$v_{\text{asym}}\text{-ring, dppz phz}$
		1230	85.39	$v_{\text{asym}}\text{-ring, tmbibzim}$
		1227	319.6	$v_{\text{sym}}\text{-ring, tmbibzim}$
1227	188.5			$v_{\text{sym}}\text{-ring, tmbibzim}$
1213	7.6			$v_{\text{asym}}\text{-ring, tmbibzim}$
1205	30.1	1206	22.8	$v_{\text{sym}}\text{-ring, tbbpy}$
1200	18.0	1205	1.8	$v_{\text{asym}}\text{-ring, dppz phen}$
1203	24.8	1203	21.2	$v_{\text{asym}}\text{-ring, tbbpy}$
1199	18.1	1199	17.5	$v\text{-tb, tbbpy}$

1199	18.3	1198	18.9	v-tb, tbbpy
		1184	87.8	$v_{\text{asym}}\text{-ring}$, tmbibzim
1177	142.1	1182	59.9	$v_{\text{sym}}\text{-ring}$, dppz phen
1165	253.8	1170	382.5	$v_{\text{sym}}\text{-ring}$, tmbibzim
1161	11.0	1167	123.3	$v_{\text{asym}}\text{-ring}$, tmbibzim
1150	1.1	1152	2.8	$v_{\text{asym}}\text{-ring}$, tbbpy
1145	27.8	1146	11.7	$v_{\text{sym}}\text{-ring}$, dppz phz
1128	64.5	1130	80.4	$v_{\text{sym}}\text{-ring}$, tbbpy; $v_{\text{asym}}\text{-ring}$, dppz phz
1127	10.2	1129	22.1	$v_{\text{asym}}\text{-ring}$, dppz phz; $v_{\text{sym}}\text{-ring}$, tbbpy
1122	180.3	1124	153.45	$v_{\text{sym}}\text{-ring}$, tbbpy
1120	33.4	1123	16.4	$v_{\text{asym}}\text{-ring}$, dppz
1115	2.9	1116	3.2	$v_{\text{asym}}\text{-ring}$, tbbpy
1109	276.6	1113	296.9	$v_{\text{sym}}\text{-ring}$, dppz
		1102	44.3	$v_{\text{sym}}\text{-ring}$, tmbibzim
1101	10.3	1099	4.6	$v_{\text{asym}}\text{-ring}$, tmbibzim
1100	167.8			$v_{\text{sym}}\text{-ring}$, tmbibzim
1086	38.1	1089	30.6	$v_{\text{asym}}\text{-ring}$, dppz phen
1071	11.9	1075	5.6	$v_{\text{sym}}\text{-ring}$, dppz; $v_{\text{asym}}\text{-ring}$, tbbpy;
1066	114.1	1069	89.89	$v_{\text{asym}}\text{-ring}$, tbbpy; $v_{\text{sym}}\text{-ring}$, dppz
1048	1.7	1050	1.4	$\delta_{\text{asym}}\text{-ch}$, tmbibzim
1048	1.9	1050	1.6	$\delta_{\text{asym}}\text{-ch}$, tmbibzim
1042	1240.3	1044	1098.5	$v_{\text{sym}}\text{-ring}$, dppz phen
1029	7.9	1029	7.0	v-tb, tbbpy
1029	6.5	1029	7.3	v-tb, tbbpy
1026	1.6	1028	0.5	$\delta_{\text{asym}}\text{-ch}$, tmbibzim
1026	2.7	1028	0.7	$\delta_{\text{asym}}\text{-ch}$, tmbibzim
1026	36.8	1027	67.4	v-tb, tbbpy
1023	42.8	1025	18.0	$v_{\text{asym}}\text{-ring}$, dppz phen; $v_{\text{sym}}\text{-ring}$, tbbpy
1024	22.7	1024	75.5	v-tb, tbbpy
1020	1048.2	1022	1910.3	$v_{\text{sym}}\text{-ring}$, tmbibzim; $v_{\text{sym}}\text{-ring}$, tbbpy; $v_{\text{sym}}\text{-ring}$, dppz
1010	887.4	1014	567.0	$v_{\text{sym}}\text{-ring}$, tbbpy; $v_{\text{sym}}\text{-ring}$, tmbibzim; $v_{\text{sym}}\text{-ring}$, dppz
1007	6.6	1014	20.1	$v_{\text{asym}}\text{-ring}$, tmbibzim
1006	19.9	1013	4.4	$v_{\text{sym}}\text{-ring}$, tmbibzim
1004	541.5	1008	314.3	$v_{\text{asym}}\text{-ring}$, tbbpy
		1003	1.9	$v_{\text{sym}}\text{-ring}$, tmbibzim
1003	102.4	1003	152.0	$v_{\text{sym}}\text{-ring}$, dppz phz
		1002	6.9	$v_{\text{asym}}\text{-ring}$, tmbibzim
999	14.9			$v_{\text{sym}}\text{-ring}$, tmbibzim
997	1.4			$v_{\text{asym}}\text{-ring}$, tmbibzim
979	1.0	987	0.22	$\delta_{\text{asym}}\text{-ch}$, dppz phen
984	0.1	986	0.22	$\delta_{\text{asym}}\text{-ch}$, dppz phz

978	1.2	986	0.6	$\delta_{\text{sym}}\text{-ch}$, dppz phen
971	179.0	972	108.7	$\nu_{\text{asym}}\text{-ring}$, dppz
959	2.5	961	0.4	$\delta_{\text{asym}}\text{-ch}$, tbbpy
956	0.5	960	1.1	$\delta_{\text{asym}}\text{-ch}$, tbbpy
953	1.0	955	1.0	$\delta_{\text{sym}}\text{-ch}$, dppz phz
950	4.0			$\nu_{\text{asym}}\text{-ring}$, tmbibzim
948	0.1	949	0.1	$\delta_{\text{asym}}\text{-ch}$, tbbpy
948	0.1	949	0.1	$\delta_{\text{asym}}\text{-ch}$, tbbpy
942	2.3	944	2.5	$\delta_{\text{asym}}\text{-ch}$, dppz phen
		943	3.2	$\nu_{\text{asym}}\text{-ring}$, tmbibzim; $\delta_{\text{asym}}\text{-ch}$, dppz phen
		942	2.9	$\delta_{\text{asym}}\text{-ch}$, dppz phen; $\nu_{\text{asym}}\text{-ring}$, tmbibzim
938	3.3			$\delta_{\text{asym}}\text{-ch}$, dppz phen
923	11.7	924	10.4	$\delta_{\text{asym}}\text{-ch}$, tbbpy
923	17.5	924	15.4	$\delta_{\text{asym}}\text{-ch}$, tbbpy
913	21.9	914	21.2	$\delta_{\text{sym}}\text{-ch}$, tbbpy
913	9.9	914	9.2	$\delta_{\text{asym}}\text{-ch}$, tbbpy
888	61.1			$\nu_{\text{asym}}\text{-ring}$, dppz phz; $\nu_{\text{sym}}\text{-ring}$, tbbpy
887	4.3	891	2.2	$\delta_{\text{sym}}\text{-ch}$, tbbpy
		888	35.7	$\nu_{\text{asym}}\text{-ring}$, dppz phz; $\nu_{\text{sym}}\text{-ring}$, tbbpy; $\nu_{\text{sym}}\text{-ring}$, tmbibzim
		887	64.5	$\nu_{\text{sym}}\text{-ring}$, tbbpy, $\nu_{\text{sym}}\text{-ring}$, tmbibzim; $\nu_{\text{asym}}\text{-ring}$, dppz phz
886	71.2			$\nu_{\text{sym}}\text{-ring}$, tbbpy; $\nu_{\text{asym}}\text{-ring}$, dppz phz
		883	98.8	$\nu_{\text{sym}}\text{-ring}$, tmbibzim; $\nu_{\text{sym}}\text{-ring}$, tbbpy; $\nu_{\text{asym}}\text{-ring}$, dppz phz
882	212.6			$\nu_{\text{sym}}\text{-ring}$, tmbibzim
876	2.3	883	3.4	$\delta_{\text{asym}}\text{-ch}$, tbbpy
868	5.7	869	5.5	$\delta_{\text{asym}}\text{-ch}$, dppz phz
859	2.7	855	1.2	$\delta_{\text{asym}}\text{-ch}$, tmbibzim
858	1.4	854	0.8	$\delta_{\text{asym}}\text{-ch}$, tmbibzim
		843	2.3	$\delta_{\text{asym}}\text{-ch}$, tmbibzim
		842	3.7	$\delta_{\text{asym}}\text{-ch}$, tmbibzim
838	12.6	840	5.8	$\delta_{\text{asym}}\text{-ch}$, tbbpy
		838	7.4	$\delta_{\text{sym}}\text{-ch}$, tbbpy
		838	64.6	$\nu_{\text{sym}}\text{-ring}$, dppz; $\delta_{\text{sym}}\text{-ch}$, tbbpy; $\nu_{\text{asym}}\text{-ring}$, tmbibzim;
837	60.7			$\nu_{\text{sym}}\text{-ring}$, dppz; $\nu_{\text{asym}}\text{-ring}$, tmbibzim; $\delta_{\text{sym}}\text{-ch}$, tbbpy
835	32.9			$\nu_{\text{sym}}\text{-ring}$, dppz, $\nu_{\text{asym}}\text{-ring}$, tmbibzim; $\delta_{\text{sym}}\text{-ch}$, tbbpy;
		834	3.8	$\nu_{\text{asym}}\text{-ring}$, tmbibzim; $\delta_{\text{asym}}\text{-ch}$, dppz; $\nu_{\text{sym}}\text{-ring}$, tbbpy
		834	1.3	$\nu_{\text{asym}}\text{-ring}$, tbbpy; $\delta_{\text{asym}}\text{-ch}$, dppz; $\nu_{\text{asym}}\text{-ring}$, tmbibzim
834	2.1			$\nu_{\text{asym}}\text{-ring}$, tmbibzim; $\delta_{\text{asym}}\text{-ch}$,

				tbbpy; $v_{\text{sym}}\text{-ring}$, dppz
834	1.6			$v_{\text{asym}}\text{-ring}$, tbbpy
		833	0.6	$v_{\text{asym}}\text{-ring}$, tmbibzim; $\delta_{\text{asym}}\text{-ch}$, dppz; $v_{\text{asym}}\text{-ring}$, tbbpy
832	2.9			$\delta_{\text{sym}}\text{-ch}$, tmbibzim
831	1.8			$\delta_{\text{asym}}\text{-ch}$, tmbibzim
830	0.8			$\delta_{\text{asym}}\text{-ch}$, dppz
807	6.3	809	8.0	$\delta_{\text{sym}}\text{-ch}$, dppz phen
791	3.0	793	2.72	$\delta_{\text{asym}}\text{-ch}$, dppz
785	3.4	788	0.24	$\delta_{\text{asym}}\text{-ch}$, dppz phen
786	39.4	786	30.2	$v_{\text{sym}}\text{-ring}$, tbbpy
		783	46.6	$v_{\text{sym}}\text{-ring}$, tmbibzim
780	2.4			$v_{\text{sym}}\text{-ring}$, tmbibzim
		778	18.2	$v_{\text{asym}}\text{-ring}$, tmbibzim

a) The nominated symmetry is referred to the ligand mirror plane containing the Ru atom.