

SUPPORTING INFORMATION

Vibrational frequencies for *p*-cymene complex [Ru(*p*-cym)Cl₂(NH₃)]

optimized at B97-D2/def2-TZVP level of theory, with effective core potentials for ruthenium

Frequency [cm ⁻¹]	Intensity
25.3425	3.1442
53.1488	0.1215
90.8029	1.8079
125.6037	0.9088
131.9226	0.8259
140.8728	0.3344
162.4996	2.3723
170.1154	2.9070
183.5082	0.8460
184.7700	1.8761
217.0444	4.2133
225.9295	3.3981
239.0398	10.8455
248.9966	5.9257
259.4935	29.6327
279.2947	7.1521
285.3236	15.9454
318.2556	1.7064
342.0476	0.8949
363.2961	2.9269
376.4640	0.7761
393.3456	0.5812
418.8530	1.0258
438.1215	1.3698
455.7292	1.8458
513.8680	0.6809
562.8973	2.1563
631.7489	0.2985
653.4563	3.8656
674.6067	0.5650

Frequency [cm ⁻¹]	Intensity
714.5251	6.7489
744.9451	9.8435
790.7532	10.0243
855.3992	20.7943
868.4852	1.3103
873.0100	4.9734
908.4309	0.6610
915.9211	0.1149
927.6048	0.5731
940.7334	0.2728
976.7293	1.3599
989.9737	5.4937
1031.424	7.6480
1046.096	8.7990
1075.050	6.7508
1098.494	3.1204
1131.215	0.5164
1140.806	0.5075
1186.990	12.9402
1188.275	120.2354
1199.454	6.2655
1275.560	1.9649
1301.677	6.3212
1315.817	6.7008
1357.355	4.7690
1367.463	3.0996
1378.601	5.1398
1382.121	10.7085
1403.373	1.0793
1431.589	4.9675

Frequency [cm ⁻¹]	Intensity
1443.788	6.6171
1446.755	1.8707
1451.600	0.1524
1456.769	11.4964
1460.675	10.6182
1475.871	6.9363
1491.929	9.0257
1518.840	2.6845
1586.258	17.8547
1631.919	15.4961
2922.266	22.2173
2945.623	29.5103
2947.116	31.3599
2953.406	23.5191
3027.987	4.2815
3028.715	5.0411
3033.184	26.6072
3033.949	38.8867
3043.789	21.9840
3060.528	5.8094
3112.883	11.8723
3143.432	4.6518
3147.085	3.2590
3166.810	2.3247
3328.024	16.4775
3447.370	27.9124
3508.714	14.214

Vibrational frequencies for benzene complex [Ru(benzene)Cl₂(NH₃)]

optimized at B97-D2/def2-TZVP level of theory, with effective core potentials for ruthenium

Frequency [cm ⁻¹]	Intensity
30.5217	1.5923
103.8606	0.3215
134.8129	1.0772
163.2941	0.5762
165.6558	2.5051
194.5458	1.2480
215.6790	9.0716
260.9160	34.699
280.6686	30.1808
341.8412	3.0664
348.2956	4.2784
360.3175	1.0077
383.8218	4.3603
438.8584	0.9951
439.0355	1.6337
590.1515	1.9029
610.1959	0.9957
612.8709	1.8894
731.2547	8.4980
734.8193	6.5003
816.8475	52.4914
863.4510	1.9813
876.8307	1.2925
919.0952	0.2499
927.3307	0.9524
940.9093	0.3495
963.1983	5.2310
981.7028	0.9361
986.6444	2.8121
989.0932	3.1877
1118.079	0.0808
1123.453	0.0701
1131.406	0.0375
1198.353	135.5306
1320.933	0.0045
1396.424	0.0146

Frequency [cm ⁻¹]	Intensity
1423.082	4.0930
1424.179	4.5069
1485.078	0.5263
1488.938	0.9839
1588.262	18.9317
1629.002	17.4196
3117.209	7.2412
3132.461	12.3661
3150.679	0.2868
3154.852	2.5693
3159.115	3.9871
3164.857	3.3414
3328.664	16.3619
3441.472	33.1118
3508.325	10.3512