

Table S1 Energy of molecular orbitals in cm^{-1} for $[\text{Ru}(\text{x},\text{x}'\text{-dmb})(\text{CN}-\text{H}_2\text{O})_4]^{2-}$ in water.

	3,3'-dmb	4,4'-dmb	5,5'-dmb	6,6'-dmb
HOMO - 12	-66669.8	-66715.9	-66680.8	-66788.3
HOMO - 11	-66630.3	-66617.1	-66272.6	-65745.8
HOMO - 10	-65947.7	-65912.6	-65844.6	-65691
HOMO - 9	-65706.3	-65701.9	-65638.3	-65456.1
HOMO - 8	-65625.1	-65583.4	-65552.7	-65238.8
HOMO - 7	-64266.6	-64835	-65238.8	-64936
HOMO - 6	-63992.2	-63985.6	-65094	-63430.4
HOMO - 5	-63298.7	-63783.7	-63946.1	-62262.8
HOMO - 4	-60803.3	-61446.3	-61854.5	-61810.6
HOMO - 3	-55421.7	-55880.4	-54054.4	-53696.7
HOMO - 2	-45958	-45747.3	-45990.9	-46186.2
HOMO - 1	-45795.6	-45742.9	-45903.1	-45569.5
HOMO	-45286.4	-45128.4	-45306.1	-45014.2
LUMO	-16623	-17389	-16886.4	-17112.4
LUMO + 1	-10798.2	-10177	-10512.8	-9944.4
LUMO + 2	-8838.24	-7874.75	-8969.93	-8346.62
LUMO + 3	-1483.65	-1560.46	-1591.19	-1499.01
LUMO + 4	-713.293	-94.3741	-296.291	245.8116
LUMO + 5	-142.659	39.50543	704.5136	305.0697
LUMO + 6	539.9076	471.8705	884.4828	919.5987
LUMO + 7	959.1041	1233.447	1121.515	1086.399
LUMO + 8	2280.341	1964.298	2085.009	2286.926
LUMO + 9	2708.317	2352.768	2194.746	2921.207
LUMO + 10	3932.985	4253.418	3750.821	3700.342
LUMO + 11	4007.607	4832.831	3856.169	4231.471
LUMO + 12	4938.179	5879.725	6437.191	5835.83
LUMO + 13	6608.381	6053.11	6503.033	6215.522
LUMO + 14	7378.737	6296.727	6740.066	6788.35
LUMO + 15	7547.733	7701.365	7427.021	7782.57