Supplementary Information for:

# Synthesis, Crystallographic Structure, Theoretical Analysis, Molecular Docking Studies, and Biological Activity Evaluation of Binuclear Ru(II)-1-Naphthylhydrazine Complex

**Thomas Eichhorn [1], Franz Kolbe [1], Stefan Mišić [1,2], Dušan Dimić [2], Ibrahim Morgan [3], Mohamad Saoud [3], Dejan Milenković [4], Zoran Marković [4], Tobias Rüffer [5], Jasmina Dimitrić Marković [2,*] and Goran N. Kaluđerović [1,*]**

[1] Department of Engineering and Natural Sciences, University of Applied Sciences Merseburg, Eberhard-Leibnitz-Straße 2, 06217 Merseburg, Germany
[2] Faculty of Physical Chemistry, University of Belgrade, Studentski trg 12-16, 11000 Belgrade, Serbia
[3] Department of Bioorganic Chemistry, Leibniz Institute of Plant Biochemistry, Weinberg 3, 06120 Halle (Saale), Germany
[4] Department of Science, Institute for Information Technologies, University of Kragujevac, Jovana Cvijića bb, 34000 Kragujevac, Serbia
[5] Institute of Chemistry, Chemnitz University of Technology, Straße der Nationen 62, D-09111 Chemnitz, Germany
* Correspondence: markovich@ffh.bg.ac.rs (J.D.M.); goran.kaluderovic@hs-merseburg.de (G.N.K.)

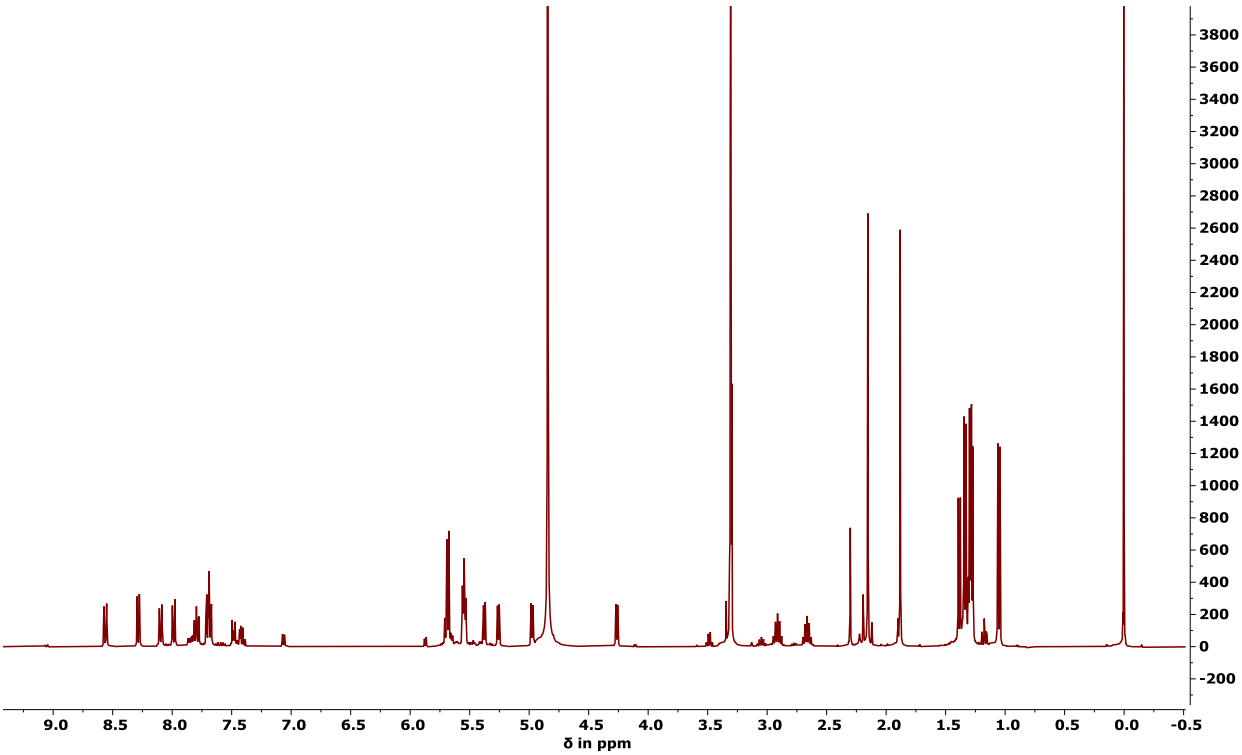


Figure S1. $^{1}$H NMR spectrum of **1**

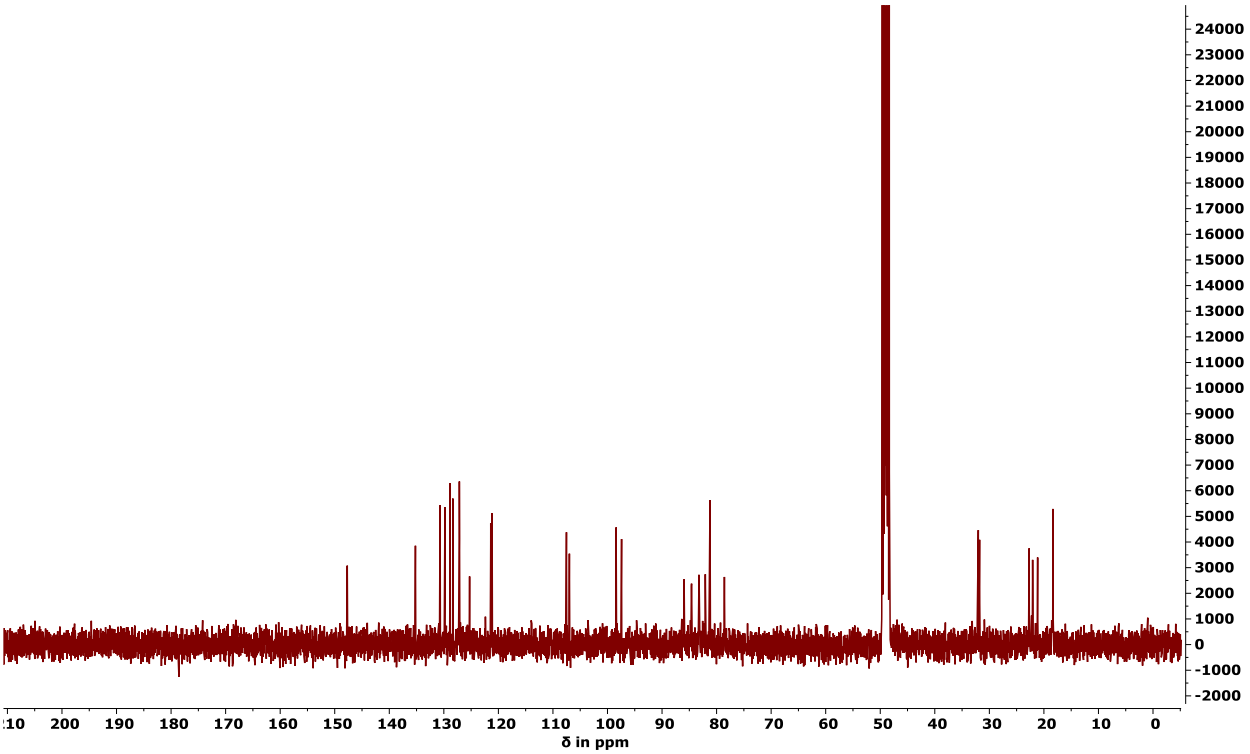


Figure S2. $^{13}C$ NMR spectrum of **1**

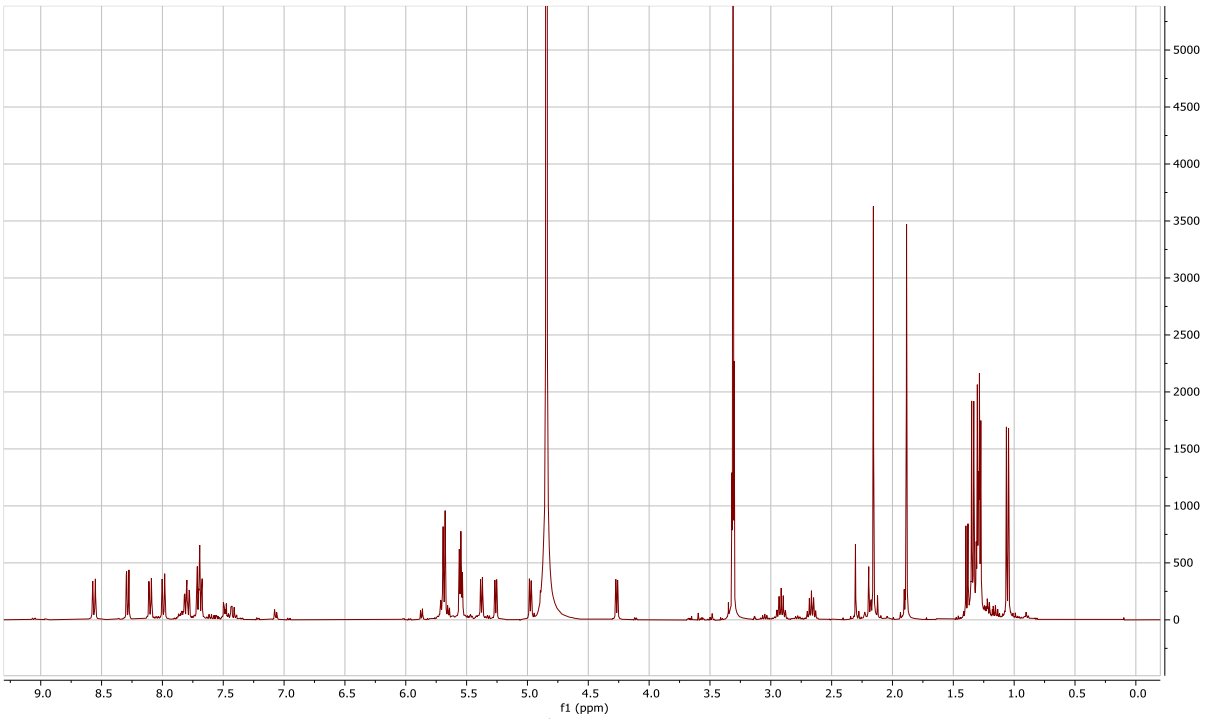


Figure S3. $^{1}H$ NMR spectrum of **2**

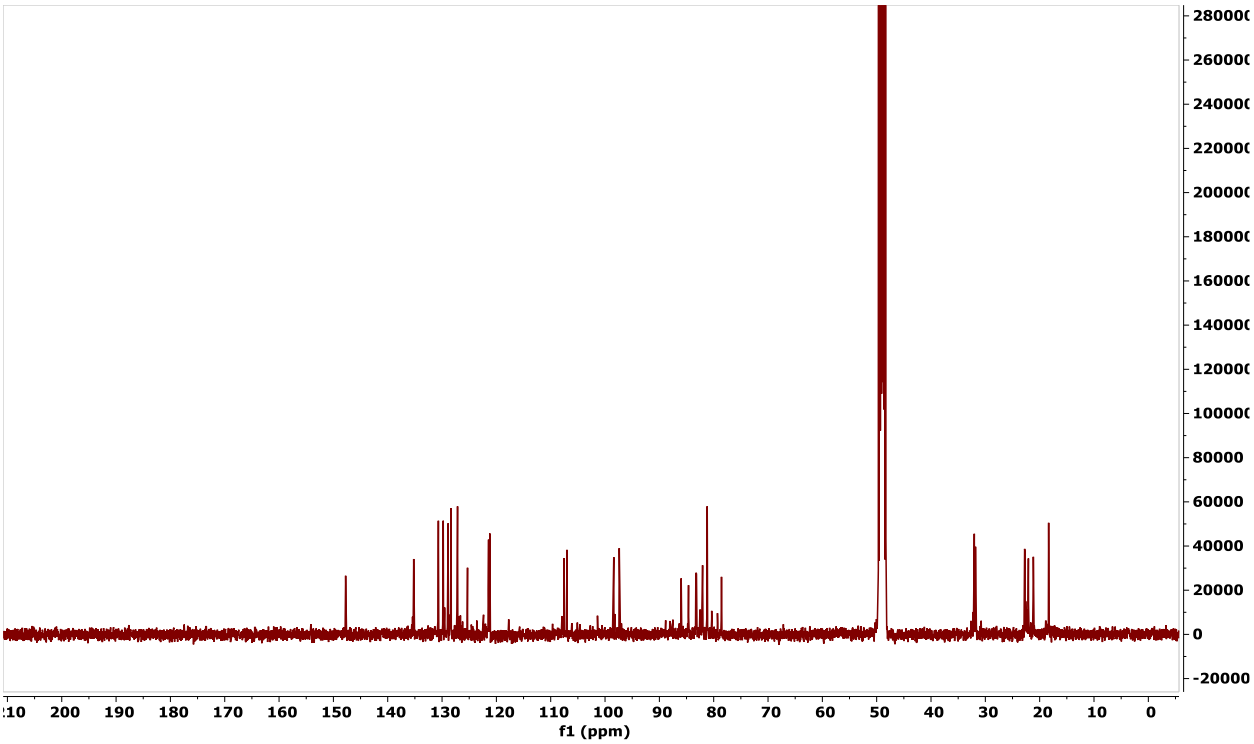


Figure S4. $^{13}$C NMR spectrum of **2**

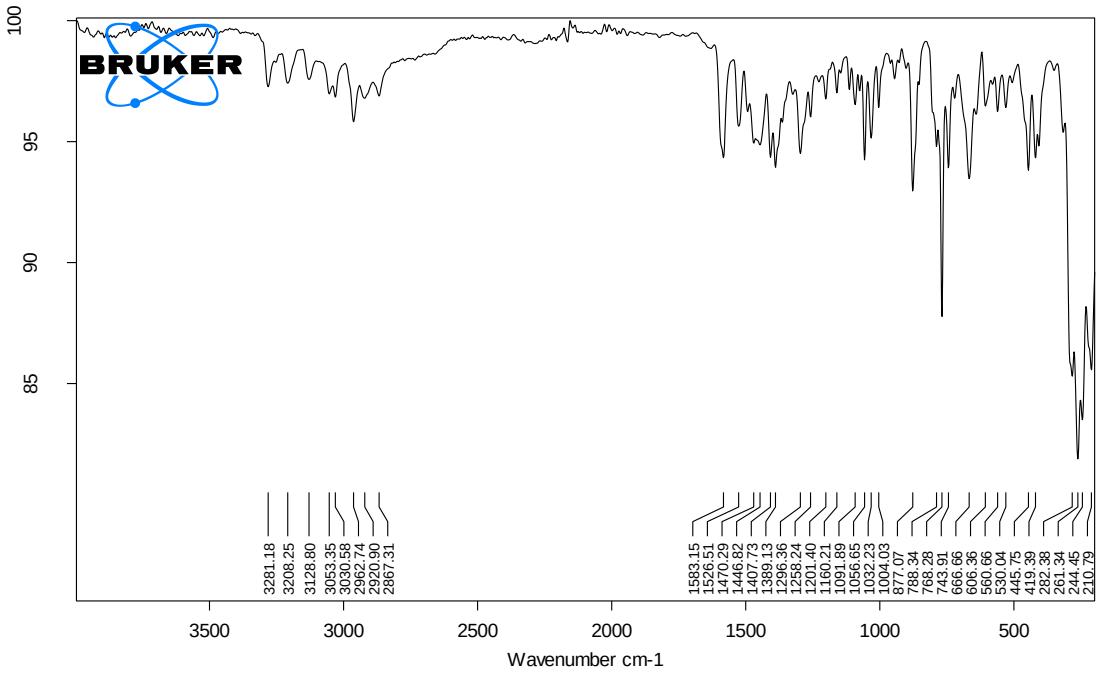


Figure S5. IR spectrum of **2**

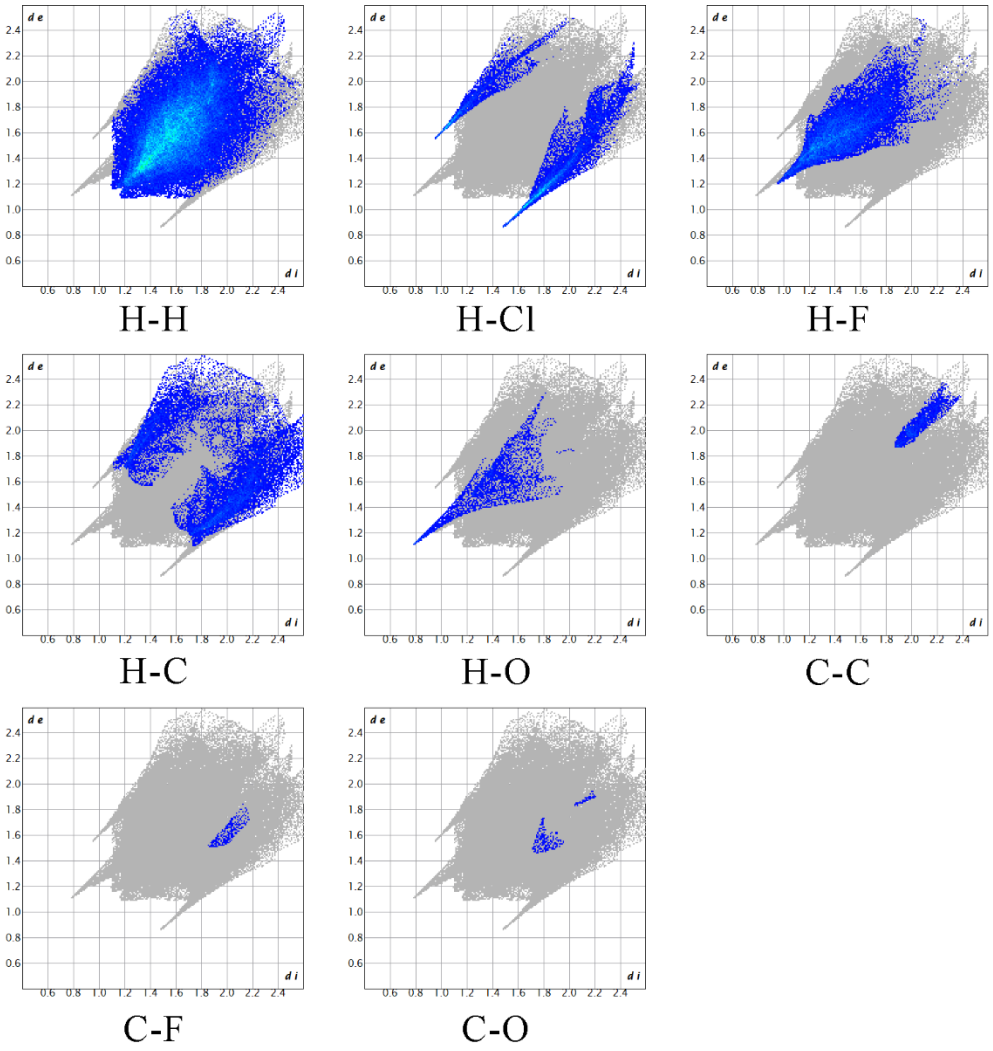


Figure S6. The fingerprint plots for the most abundant contacts in crystal structure of **2·2MeOH**.

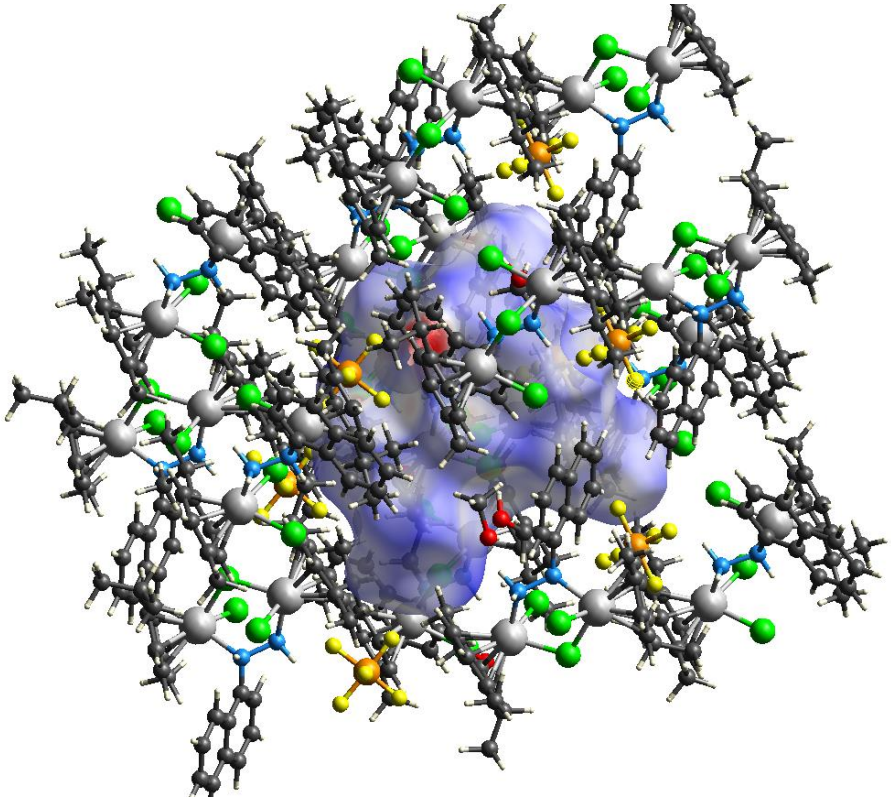

Figure S7. Hirshfeld surface of **2a** with surrounding units.

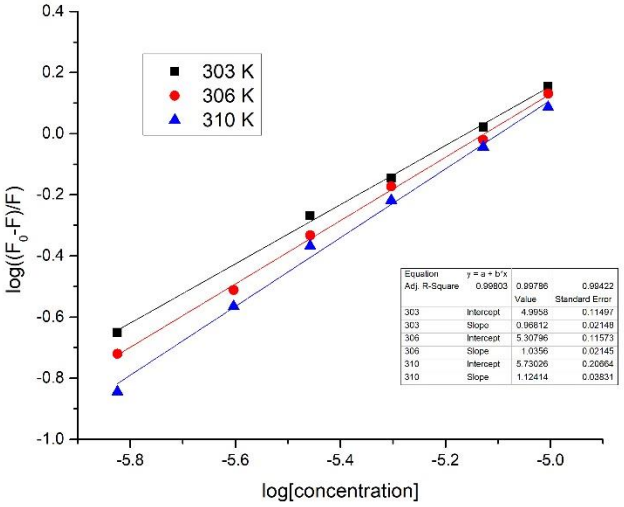


Figure S8. Stern-Volmer plots for the binding of **1** to BSA.

Table S1. The experimental and theoretical bond lengths of **2a** (in Å), the notations follow Figure 1.

| Bond | Experimental | Theoretical |
|---|---|---|
| C1−C2 | 1.402(5) | 1.440 |
| C1−C6 | 1.434(5) | 1.414 |
| C1−C7 | 1.508(5) | 1.502 |
| C2−C3 | 1.425(4) | 1.406 |
| C3−C4 | 1.404(4) | 1.443 |
| C4−C5 | 1.435(4) | 1.410 |
| C4−C8 | 1.523(4) | 1.517 |
| C5−C6 | 1.392(5) | 1.436 |
| C8−C9 | 1.513(5) | 1.533 |
| C9−C10 | 1.555(5) | 1.547 |
| C11−C16 | 1.404(5) | 1.413 |
| C11−C12 | 1.430(5) | 1.440 |
| C11−C17 | 1.508(5) | 1.501 |
| C12−C13 | 1.401(5) | 1.406 |
| C13−C14 | 1.431(4) | 1.443 |
| C14−C15 | 1.413(4) | 1.411 |
| C14−C18 | 1.516(4) | 1.517 |
| C15−C16 | 1.422(4) | 1.411 |
| C18−C20 | 1.519(4) | 1.533 |
| C18−C19 | 1.544(4) | 1.546 |
| C21−C22 | 1.371(4) | 1.382 |
| C21−C30 | 1.425(4) | 1.433 |
| C21−N2 | 1.465(3) | 1.460 |
| C22−C23 | 1.410(4) | 1.412 |
| C23−C24 | 1.369(4) | 1.375 |
| C24−C25 | 1.422(4) | 1.420 |
| C25−C26 | 1.411(4) | 1.421 |
| C25−C30 | 1.435(4) | 1.439 |
| C26−C27 | 1.366(4) | 1.375 |
| C27−C28 | 1.416(4) | 1.414 |
| C28−C29 | 1.373(4) | 1.379 |
| C29−C30 | 1.423(4) | 1.425 |
| N1−N2 | 1.467(3) | 1.465 |
| N1−Ru1 | 2.138(2) | 2.189 |
| N2−Ru2 | 2.193(2) | 2.238 |
| Cl1−Ru1 | 2.4063(7) | 2.444 |
| Cl2−Ru2 | 2.4172(7) | 2.482 |
| Cl2−Ru1 | 2.4287(7) | 2.487 |

| | | |
|---|---|---|
| Cl3−Ru2 | 2.4150(7) | 2.462 |
| C1−Ru1 | 2.196(3) | 2.274 |
| C2−Ru1 | 2.161(3) | 2.229 |
| C3−Ru1 | 2.178(3) | 2.241 |
| C4−Ru1 | 2.216(3) | 2.321 |
| C5−Ru1 | 2.171(3) | 2.279 |
| C6−Ru1 | 2.171(3) | 2.239 |
| C11−Ru2 | 2.203(3) | 2.276 |
| C12−Ru2 | 2.165(3) | 2.247 |
| C13−Ru2 | 2.184(3) | 2.275 |
| C14−Ru2 | 2.226(3) | 2.311 |
| C15−Ru | 2.198(3) | 2.238 |
| C16−Ru | 2.175(3) | 2.230 |
| R | | 0.999 |
| MAE [Å] | | 0.031 |

Table S2. The experimental and theoretical bond angles of **2a** (in $^{o}$), the notations follow Figure 1.

| Angle | Experimental | Theoretical |
|---|---|---|
| C2−C1−C6 | 117.2(3) | 116.9 |
| C2−C1−C7 | 121.7(3) | 120.6 |
| C6−C1−C7 | 121.1(3) | 122.4 |
| C2−C1−Ru1 | 69.91(17) | 69.7 |
| C6−C1−Ru | 69.89(17) | 70.4 |
| C7−C1−Ru1 | 128.5(2) | 128.7 |
| C1−C2−C3 | 121.7(3) | 121.2 |
| C1−C2−Ru1 | 72.57(18) | 73.07 |
| C3−C2−Ru1 | 71.47(16) | 72.11 |
| C4−C3−C2 | 121.2(3) | 121.7 |
| C4−C3−Ru1 | 72.82(16) | 74.60 |
| C2−C3−Ru1 | 70.18(16) | 71.21 |
| C3−C4−C5 | 116.9(3) | 117.1 |
| C3−C4−C8 | 123.1(3) | 119.1 |
| C5−C4−C8 | 120.0(3) | 123.8 |
| C3−C4−Ru1 | 69.93(15) | 68.57 |
| C5−C4−Ru1 | 69.22(15) | 70.53 |
| C8−C4−Ru1 | 129.3(2) | 131.5 |
| C6−C5−C4 | 122.0(3) | 121.0 |

| | | |
|---|---|---|
| C6−C5−Ru1 | 71.29(16) | 69.99 |
| C4−C5−Ru1 | 72.60(15) | 73.77 |
| C5−C6−C1 | 121.0(3) | 121.9 |
| C5−C6−Ru1 | 71.31(16) | 72.96 |
| C1−C6−Ru1 | 71.78(16) | 73.08 |
| C9−C8−C4 | 113.7(3) | 114.5 |
| C9−C8−C10 | 110.0(3) | 111.2 |
| C4−C8−C10 | 108.5(3) | 108.6 |
| C16−C11−C12 | 116.8(3) | 117.0 |
| C16−C11−C17 | 121.7(3) | 120.8 |
| C12−C11−C17 | 121.5(3) | 122.1 |
| C16−C11−Ru2 | 70.19(16) | 70.67 |
| C12−C11−Ru2 | 69.45(17) | 69.61 |
| C17−C11−Ru2 | 129.3(2) | 128.8 |
| C13−C12−C11 | 121.6(3) | 121.1 |
| C13−C12−Ru2 | 71.93(17) | 71.98 |
| C11−C12−Ru2 | 72.35(17) | 73.13 |
| C12−C13−C14 | 121.0(3) | 121.8 |
| C12−C13−Ru2 | 70.49(17) | 71.33 |
| C14−C13−Ru2 | 72.70(16) | 74.29 |
| C15−C14−C13 | 117.9(3) | 117.0 |
| C15−C14−C18 | 123.3(3) | 123.9 |
| C13−C14−C18 | 118.8(3) | 119.1 |
| C15−C14−Ru2 | 70.29(16) | 70.66 |
| C13−C14−Ru2 | 69.46(16) | 68.78 |
| C18−C14−Ru2 | 131.3(2) | 131.3 |
| C14−C15−C16 | 120.2(3) | 121.2 |
| C14−C15−Ru2 | 72.47(16) | 73.51 |
| C16−C15−Ru2 | 70.13(16) | 70.46 |
| C11−C16−C15 | 122.4(3) | 121.8 |
| C11−C16−Ru2 | 72.41(17) | 72.94 |
| C15−C16−Ru2 | 71.93(16) | 72.55 |
| C14−C18−C20 | 113.9(3) | 114.5 |
| C14−C18−C19 | 107.3(3) | 108.6 |
| C20−C18−C19 | 111.4(3) | 111.3 |
| C22−C21−C30 | 121.9(2) | 121.3 |
| C22−C21−N2 | 119.0(2) | 119.0 |
| C30−C21−N2 | 119.1(2) | 119.6 |
| C21−C22−C23 | 120.1(3) | 120.4 |
| C24−C23−C22 | 120.5(3) | 120.2 |
| C23−C24−C25 | 120.6(3) | 120.8 |

| | | |
|---|---|---|
| C26−C25−C24 | 121.3(2) | 120.9 |
| C26−C25−C30 | 119.0(3) | 119.2 |
| C24−C25−C30 | 119.7(2) | 119.9 |
| C27−C26−C25 | 121.3(3) | 121.1 |
| C26−C27−C28 | 120.1(3) | 119.8 |
| C29−C28−C27 | 120.4(3) | 120.9 |
| C28−C29−C30 | 120.7(3) | 120.8 |
| C29−C30−C21 | 124.3(2) | 124.5 |
| C29−C30−C25 | 118.5(2) | 118.2 |
| C21−C30−C25 | 117.2(2) | 117.3 |
| N2−N1−Ru1 | 116.16(16) | 116.3 |
| C21−N2−N1 | 111.6(2) | 112.7 |
| C21−N2−Ru2 | 112.84(16) | 115.4 |
| N1−N2−Ru2 | 115.98(15) | 110.5 |
| Ru2−Cl2−Ru1 | 110.47(3) | 109.72 |
| N1−Ru1−C2 | 91.60(10) | 95.74 |
| N1−Ru1−C6 | 153.87(12) | 155.69 |
| C2−Ru1−C6 | 67.92(12) | 65.97 |
| N1−Ru1−C5 | 158.36(10) | 159.11 |
| C2−Ru1−C5 | 80.26(12) | 77.66 |
| C6−Ru1−C5 | 37.40(12) | 36.68 |
| N1−Ru1−C3 | 93.63(10) | 97.57 |
| C2−Ru1−C3 | 38.35(11) | 37.04 |
| C6−Ru1−C3 | 80.40(11) | 77.66 |
| C5−Ru1−C3 | 67.58(11) | 65.18 |
| N1−Ru1−C1 | 115.85(11) | 118.90 |
| C2−Ru1−C1 | 37.52(12) | 36.51 |
| C6−Ru1−C1 | 38.33(13) | 37.28 |
| C5−Ru1−C1 | 68.56(13) | 66.61 |
| C3−Ru1−C1 | 68.73(12) | 66.36 |
| N1−Ru1−C4 | 120.19(10) | 122.40 |
| C2−Ru1−C4 | 68.55(11) | 65.79 |
| C6−Ru1−C4 | 68.61(11) | 66.29 |
| C5−Ru1−C4 | 38.18(11) | 36.83 |
| C3−Ru1−C4 | 37.25(10) | 35.70 |
| C1−Ru1−C4 | 81.87(11) | 78.60 |
| N1−Ru1−Cl1 | 83.98(6) | 84.86 |
| C2−Ru1−Cl1 | 118.71(9) | 119.47 |
| C6−Ru1−Cl1 | 91.70(8) | 90.47 |
| C5−Ru1−Cl1 | 117.53(8) | 115.73 |
| C3−Ru−Cl1 | 157.00(8) | 156.45 |

| | | |
|---|---|---|
| C1−Ru1−Cl1 | 91.68(9) | 91.87 |
| C4−Ru1−Cl1 | 155.43(7) | 152.48 |
| N1−Ru1−Cl2 | 85.57(7) | 82.88 |
| C2−Ru1−Cl2 | 154.54(9) | 152.28 |
| C6−Ru1−Cl2 | 119.94(10) | 120.86 |
| C5−Ru−Cl2 | 93.21(9) | 93.79 |
| C3−Ru1−Cl2 | 116.50(8) | 115.47 |
| C1−Ru1−Cl2 | 158.17(10) | 158.14 |
| C4−Ru1−Cl2 | 91.09(8) | 91.49 |
| Cl1−Ru1−Cl2 | 86.19(2) | 88.08 |
| C12−Ru2−C16 | 67.60(12) | 65.86 |
| C12−Ru2−C13 | 37.58(12) | 36.69 |
| C16−Ru2−C13 | 79.90(12) | 77.58 |
| C12−Ru2−N2 | 150.19(11) | 157.52 |
| C16−Ru2−N2 | 92.39(10) | 96.80 |
| C13−Ru2−N2 | 163.77(10) | 157.74 |
| C16−Ru2−C15 | 37.95(11) | 36.99 |
| C13−Ru2−C15 | 67.55(11) | 65.25 |
| N2−Ru2−C15 | 97.62(9) | 97.21 |
| C12−Ru2−C11 | 38.20(13) | 37.27 |
| C16−Ru2−C11 | 37.40(12) | 36.40 |
| C13−Ru2−C11 | 68.57(13) | 66.60 |
| N2−Ru2−C11 | 113.25(11) | 120.59 |
| C15−Ru2−C11 | 68.49(12) | 66.29 |
| C12−Ru2−C14 | 68.25(12) | 66.46 |
| C16−Ru2−C14 | 67.89(11) | 65.87 |
| C13−Ru2−C14 | 37.84(10) | 36.93 |
| N2−Ru2−C14 | 125.96(9) | 121.10 |
| C15−Ru2−C14 | 37.24(10) | 35.83 |
| C11−Ru2−C14 | 81.33(12) | 78.74 |
| C12−Ru2−Cl3 | 88.23(9) | 90.46 |
| C16−Ru2−Cl3 | 125.23(9) | 118.32 |
| C13−Ru2−Cl3 | 110.26(8) | 116.31 |
| N2−Ru2−Cl3 | 85.87(6) | 85.45 |
| C15−Ru2−Cl3 | 162.65(8) | 155.28 |
| C11−Ru2−Cl3 | 94.47(9) | 91.13 |
| C14−Ru2−Cl3 | 147.01(7) | 153.20 |
| C12−Ru2−Cl2 | 124.60(10) | 118.51 |
| C16−Ru2−Cl2 | 148.68(9) | 153.66 |
| C13−Ru2−Cl2 | 95.10(9) | 92.19 |
| N2−Ru2−Cl2 | 84.06(6) | 83.49 |

| | | |
|---|---|---|
| C15−Ru2−Cl2 | 111.58(8) | 116.71 |
| C11−Ru2−Cl2 | 162.67(10) | 155.77 |
| C14−Ru2−Cl2 | 89.14(8) | 91.33 |
| Cl3−Ru2−Cl2 | 85.65(2) | 88.00 |
| R | | 0.994 |
| MAE [°] | | 1.66 |

Table S3. Experimental and calculated chemical shifts (the numbering scheme follows Figure 2)

| H atom | Experimental [ppm] | Theoretical [ppm] |
|---|---|---|
| $CH_3$ (isopropyl) | 1.05 | 1.34 |
| $CH_3$ (isopropyl) | 1.28 | 1.47 |
| $CH_3$ (isopropyl) | 1.29 | 1.20 |
| $CH_3$ (isopropyl) | 1.34 | 1.37 |
| $CH_3$ (methyl) | 1.88 | 1.95 |
| $CH_3$ (methyl) | 2.15 | 1.73 |
| CH (isopropyl) | 2.66 | 2.86 |
| CH (isopropyl) | 2.91 | 2.97 |
| C(15)H | 4.26 | 4.42 |
| C(16)H | 4.98 | 4.77 |
| C(3)H | 5.26 | 4.77 |
| C(2)H | 5.38 | 4.77 |
| C(12)H | 5.52 | 5.06 |
| C(13)H | 5.52 | 5.34 |
| C(5)H | 5.68 | 5.19 |
| C(6)H | 5.68 | 5.47 |
| C(23)H | 7.72 | 7.79 |
| C(27)H | 7.67 | 7.94 |
| C(22)H | 7.8 | 8.09 |
| C(28)H | 8.29 | 8.09 |
| C(24)h | 7.99 | 8.26 |
| C(26)H | 8.1 | 8.32 |
| C(29)H | 8.56 | 8.57 |
| R | | 0.994 |
| MAE [ppm] | | 0.24 |

| C atom | Experimental [ppm] | Theoretical [ppm] |
|---|---|---|
| C10 | 18.35 | 18.13 |
| C17 | 18.46 | 19.08 |
| C19 | 21.15 | 19.24 |
| C7 | 22.07 | 19.59 |
| C9 | 22.71 | 26.85 |
| C20 | 22.75 | 27.30 |
| C18 | 31.79 | 34.65 |
| C8 | 32.02 | 35.47 |
| C17 | 78.57 | 76.20 |
| C3 | 81.20 | 78.00 |
| C2 | 82.07 | 83.02 |
| C16 | 83.16 | 83.66 |
| C5 | 83.20 | 84.97 |
| C13 | 84.59 | 87.90 |
| C15 | 84.62 | 88.21 |
| C6 | 85.95 | 89.96 |
| C11 | 97.42 | 99.47 |
| C1 | 98.42 | 101.30 |
| C14 | 106.98 | 114.48 |
| C22 | 107.52 | 114.61 |
| C4 | 121.16 | 115.57 |
| C29 | 121.40 | 116.66 |
| C30 | 125.27 | 119.85 |
| C23 | 127.15 | 121.22 |
| C27 | 128.35 | 123.51 |
| C28 | 128.89 | 123.98 |
| C24 | 129.80 | 126.65 |
| C26 | 130.69 | 126.65 |
| C25 | 135.21 | 131.01 |
| C21 | 147.70 | 143.60 |
| R | | 0.996 |
| MAE [ppm] | | 3.54 |

Table S4. Calculated chemical shifts at PBE0/6-31+G(d,p)(H,C,N,Cl)/LanL2DZ(Ru) (lev.1) and PBE0/6-311++G(d,p)(H, C, N, Cl)/LanL2DZ(Ru) (lev.2) (the numbering scheme follows Figure 2)

| H atom | lev.1 [ppm] | lev.2 [ppm] |
|---|---|---|
| $CH_3$ (isopropyl) | 1.18 | 1.12 |
| $CH_3$ (isopropyl) | 1.20 | 1.24 |
| $CH_3$ (isopropyl) | 1.31 | 1.27 |
| $CH_3$ (isopropyl) | 1.37 | 1.34 |
| $CH_3$ (methyl) | 1.73 | 2.02 |
| $CH_3$ (methyl) | 2.06 | 2.30 |
| CH (isopropyl) | 2.99 | 3.10 |
| CH (isopropyl) | 2.99 | 3.10 |
| C(16)H | 4.88 | 4.99 |
| C(3)H | 4.81 | 4.96 |
| C(2)H | 4.74 | 8.86 |
| C(12)H | 4.93 | 4.99 |
| C(13)H | 4.93 | 4.99 |
| C(5)H | 5.22 | 5.36 |
| C(6)H | 5.13 | 5.20 |
| C(23)H | 7.78 | 8.01 |
| C(27)H | 7.93 | 8.13 |
| C(22)H | 8.13 | 8.37 |
| C(28)H | 8.01 | 8.17 |
| C(24)h | 8.13 | 8.37 |
| C(26)H | 8.21 | 8.44 |
| C(29)H | 8.45 | 8.75 |
| R | 0.994 | 0.993 |
| MAE [ppm] | 0.26 | 0.23 |

| C atom | lev.l [ppm] | lev.2 [ppm] |
|---|---|---|
| C10 | 19.03 | 18.28 |
| C17 | 20.80 | 19.51 |
| C19 | 19.07 | 18.67 |
| C7 | 21.57 | 20.06 |
| C9 | 27.81 | 26.92 |
| C20 | 27.97 | 27.03 |
| C18 | 38.80 | 37.47 |
| C8 | 38.89 | 37.24 |
| C17 | 78.45 | 79.88 |
| C3 | 80.56 | 80.64 |
| C2 | 84.24 | 84.28 |
| C16 | 83.54 | 84.46 |
| C5 | 85.77 | 86.58 |
| C13 | 89.70 | 89.59 |
| C15 | 87.92 | 88.30 |
| C6 | 89.77 | 90.11 |
| C11 | 89.77 | 101.43 |
| C1 | 103.25 | 101.93 |
| C14 | 115.39 | 115.00 |
| C22 | 118.22 | 118.16 |
| C4 | 117.68 | 116.21 |
| C29 | 120.27 | 119.52 |
| C30 | 122.36 | 121.43 |
| C23 | 125.74 | 125.83 |
| C27 | 127.78 | 127.52 |
| C28 | 127.93 | 127.56 |
| C24 | 131.03 | 129.91 |
| C26 | 130.63 | 129.82 |
| C25 | 134.00 | 132.32 |
| C21 | 147.65 | 146.71 |
| R | 0.996 | 0.996 |
| MAE [ppm] | 3.08 | 3.05 |