Electronic Supplementary Information for

Extended π-system and enhanced electronic delocalization on symmetric $[Ru_3O(CH_3COO)_6(L)_3]^n$ complexes combined to azanahthalene ligands

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X-ray diffraction

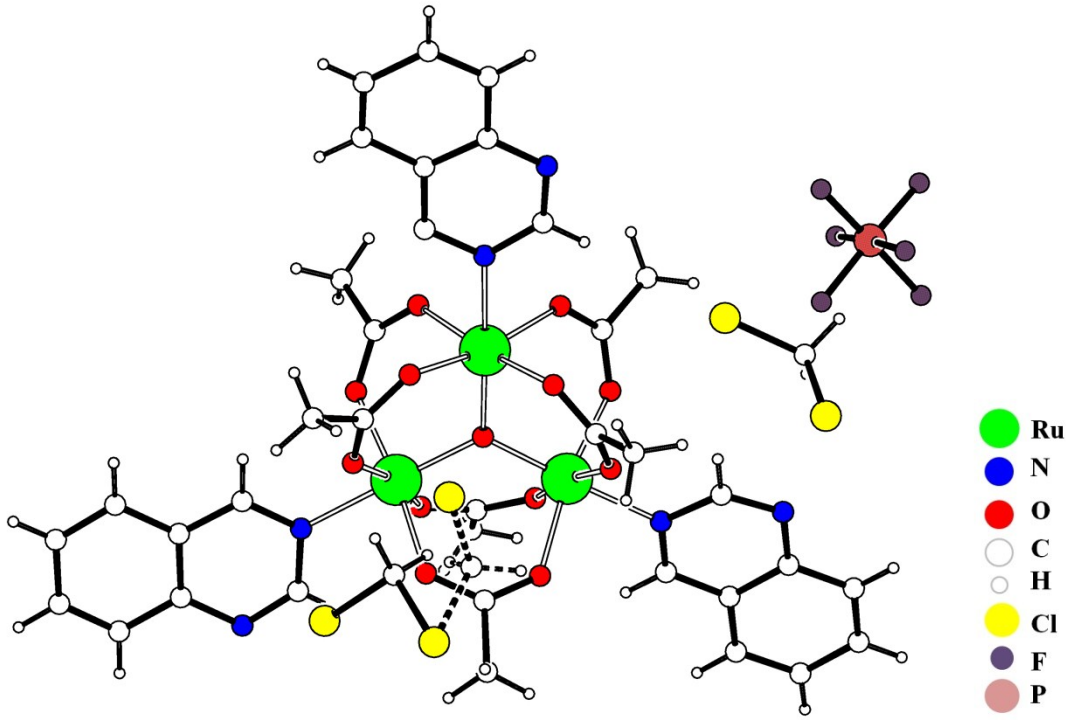


Figure S1. Resolved structure of complex 1 with solvent disorder.

Table S1. Crystal data and structure refinement for mo_snquinaz_0m.

Identification code	shelx	
Empirical formula	C38 H40 Cl4 F6 N6 O13 P Ru3	
Formula weight	1378.74	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C c	
Unit cell dimensions	a = 10.4495(2) Å	α= 90°.
	b = 22.0539(5) Å	β= 94.5290(10)°.
	c = 21.9358(4) Å	γ = 90°.
Volume	5039.37(18) $Å^3$	
Z	4	
Density (calculated)	1.817 Mg/m^3	
Absorption coefficient	1.219 mm^{-1}	
F(000)	2732	
Crystal size	0.120 x 0.120 x 0.120 mm^3	
Theta range for data collection	1.847 to 25.079°.	
Index ranges	-11<=h<=12, -26<=k<=21, -26<=l<=20	
Reflections collected	15553	
Independent reflections	6520 [R(int) = 0.0159]	
Completeness to theta = 25.079°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7452 and 0.7077	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6520 / 8 / 648	
Goodness-of-fit on F^2	1.087	
Final R indices [I>2sigma(I)]	R1 = 0.0300, wR2 = 0.0808	
R indices (all data)	R1 = 0.0310, wR2 = 0.0818	
Absolute structure parameter	0.47(4)	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.204 and -0.668 e.$Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for mo_snquinaz_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

C(1)	6663(8)	503(3)	1292(3)	36(2)
C(2)	7783(10)	251(5)	991(4)	66(3)
C(3)	3155(8)	207(3)	1429(4)	37(2)
C(4)	2202(11)	-249(4)	1218(5)	69(3)
C(5)	6265(7)	2450(3)	1506(3)	36(2)
C(6)	7321(10)	2827(5)	1280(5)	61(3)
C(7)	2606(7)	2312(3)	1613(3)	35(2)
C(8)	1409(10)	2675(5)	1473(4)	63(3)
C(9)	6948(8)	1338(3)	3245(4)	37(2)
C(10)	8036(11)	1348(4)	3729(5)	65(3)
C(11)	5978(7)	-350(3)	3425(3)	34(2)
C(11A)	3323(7)	1117(3)	3226(3)	35(2)
C(12)	6306(7)	-915(3)	3691(3)	36(2)
C(12A)	2216(9)	1020(4)	3609(4)	54(2)
C(13)	6576(8)	-990(4)	4329(4)	47(2)
C(14)	6872(9)	-1558(5)	4554(4)	53(2)
C(15)	6905(9)	-2054(4)	4145(5)	54(2)
C(16)	6643(9)	-1991(3)	3542(4)	49(2)
C(17)	6334(8)	-1418(3)	3296(4)	40(2)
C(18)	5768(8)	-811(3)	2476(3)	38(2)
C(21)	5033(8)	2750(3)	3734(3)	36(2)
C(22)	5082(8)	3268(4)	4122(3)	39(2)
C(23)	5427(9)	3229(5)	4767(4)	53(2)
C(24)	5530(11)	3724(5)	5102(5)	69(3)
C(25)	5257(11)	4297(5)	4825(5)	72(3)
C(26)	4921(10)	4358(4)	4218(5)	60(3)
C(27)	4844(8)	3824(4)	3843(4)	44(2)
C(28)	4516(8)	3376(4)	2915(4)	40(2)
C(31)	3765(7)	1029(3)	-134(3)	32(2)
C(32)	3401(7)	1112(3)	-757(3)	32(2)
C(33)	3143(8)	626(4)	-1169(4)	41(2)
C(34)	2821(8)	748(4)	-1774(4)	46(2)
C(35)	2742(9)	1343(4)	-1981(4)	47(2)
C(36)	2982(8)	1821(4)	-1593(3)	43(2)
C(37)	3314(7)	1711(3)	-968(3)	35(2)
C(38)	3897(9)	2045(3)	-15(4)	43(2)
N(11)	5697(6)	-296(3)	2826(3)	33(1)
N(12)	6065(7)	-1351(3)	2677(3)	41(2)
N(21)	4753(6)	2810(3)	3137(3)	31(1)
N(22)	4533(7)	3869(3)	3235(3)	44(2)
N(31)	4004(6)	1485(3)	240(3)	30(1)
N(32)	3573(7)	2188(3)	-576(3)	43(2)
O(1)	6550(5)	338(2)	1832(2)	42(1)
O(2)	5940(6)	845(2)	974(2)	43(1)
O(3)	3829(6)	86(2)	1910(2)	42(1)

O(4)	3206(6)	680(2)	1116(2)	43(1)
O(5)	5711(6)	2096(2)	1123(2)	43(1)
O(6)	5996(5)	2518(2)	2053(2)	41(1)
O(7)	2912(6)	1944(3)	1228(2)	44(1)
O(8)	3225(5)	2427(2)	2120(2)	39(1)
O(9)	6363(5)	1828(2)	3126(2)	43(1)
O(10)	6664(6)	837(2)	3008(3)	44(1)
O(11)	3576(5)	1664(2)	3121(2)	39(1)
O(12)	3883(6)	657(2)	3051(2)	39(1)
O(13)	4821(4)	1326(2)	2053(2)	25(1)
F(1)	5301(14)	9159(8)	698(4)	207(7)
F(2)	5028(11)	8819(6)	-653(5)	147(4)
F(3)	4031(14)	9450(5)	-86(5)	180(6)
F(4)	6180(11)	8480(6)	128(5)	153(4)
F(5)	6187(15)	9411(6)	-118(6)	175(5)
F(6)	4123(12)	8527(5)	157(8)	199(7)
P(1)	5091(4)	8977(1)	33(1)	75(1)
RU1	5209(1)	550(1)	2422(1)	27(1)
RU2	4796(1)	2045(1)	2563(1)	26(1)
RU3	4461(1)	1393(1)	1187(1)	27(1)
C(1S)	9147(15)	1219(6)	5315(7)	93(4)
CL1S	9276(4)	1367(2)	6087(2)	108(1)
CL2S	10517(4)	1207(3)	4982(2)	131(2)
CL3S	5836(11)	3962(6)	6930(6)	280(5)
CL4A	4515(17)	3047(6)	7536(8)	192(4)
C(2SA)	4210(40)	3581(18)	6940(20)	192(4)
CL4B	4418(16)	4861(6)	7612(7)	192(4)
C(2SB)	4530(40)	4047(16)	7430(20)	192(4)

Table S3. Bond lengths [Å] and angles [°] for mo_snquinaz_0m.

C(1)-O(2)	1.241(9)
C(1)-O(1)	1.253(9)
C(1)-C(2)	1.497(12)
C(2)-H(2A)	0.9600
C(2)-H(2B)	0.9600
C(2)-H(2C)	0.9600
C(3)-O(3)	1.249(9)
C(3)-O(4)	1.253(9)
C(3)-C(4)	1.465(11)
C(4)-H(4A)	0.9600
C(4)-H(4B)	0.9600
C(4)-H(4C)	0.9600
C(5)-O(5)	1.255(9)
C(5)-O(6)	1.263(9)
C(5)-C(6)	1.497(12)
C(6)-H(6A)	0.9600
C(6)-H(6B)	0.9600
C(6)-H(6C)	0.9600
C(7)-O(7)	1.231(9)
C(7)-O(8)	1.267(8)
C(7)-C(8)	1.497(11)
C(8)-H(8A)	0.9600
C(8)-H(8B)	0.9600
C(8)-H(8C)	0.9600
C(9)-O(10)	1.246(9)
C(9)-O(9)	1.259(9)
C(9)-C(10)	1.493(11)
C(10)-H(10A)	0.9600
C(10)-H(10B)	0.9600
C(10)-H(10C)	0.9600
C(11)-N(11)	1.327(9)
C(11)-C(12)	1.407(10)
C(11)-H(11)	0.9300
C(11A)-O(12)	1.248(9)
C(11A)-O(11)	1.259(9)
C(11A)-C(12A)	1.498(11)
C(12)-C(17)	1.409(11)
C(12)-C(13)	1.416(11)
C(12A)-H(12A)	0.9600
C(12A)-H(12B)	0.9600
C(12A)-H(12C)	0.9600
C(13)-C(14)	1.374(13)
C(13)-H(13)	0.9300
C(14)-C(15)	1.416(14)
C(14)-H(14)	0.9300
C(15)-C(16)	1.337(13)
C(15)-H(15)	0.9300
C(16)-C(17)	1.402(11)

C(16)-H(16)	0.9300
C(17)-N(12)	1.372(11)
C(18)-N(12)	1.300(9)
C(18)-N(11)	1.375(9)
C(18)-H(18)	0.9300
C(21)-N(21)	1.325(9)
C(21)-C(22)	1.424(10)
C(21)-H(21)	0.9300
C(22)-C(27)	1.384(12)
C(22)-C(23)	1.433(12)
C(23)-C(24)	1.316(14)
C(23)-H(23)	0.9300
C(24)-C(25)	1.422(17)
C(24)-H(24)	0.9300
C(25)-C(26)	1.356(16)
C(25)-H(25)	0.9300
C(26)-C(27)	1.435(11)
C(26)-H(26)	0.9300
C(27)-N(22)	1.353(11)
C(28)-N(22)	1.294(10)
C(28)-N(21)	1.354(10)
C(28)-H(28)	0.9300
C(31)-N(31)	1.309(9)
C(31)-C(32)	1.402(10)
C(31)-H(31)	0.9300
C(32)-C(37)	1.401(10)
C(32)-C(33)	1.414(10)
C(33)-C(34)	1.369(11)
C(33)-H(33)	0.9300
C(34)-C(35)	1.388(12)
C(34)-H(34)	0.9300
C(35)-C(36)	1.365(12)
C(35)-H(35)	0.9300
C(36)-C(37)	1.409(10)
C(36)-H(36)	0.9300
C(37)-N(32)	1.373(10)
C(38)-N(32)	1.290(10)
C(38)-N(31)	1.355(9)
C(38)-H(38)	0.9300
N(11)-RU1	2.112(6)
N(21)-RU2	2.109(5)
N(31)-RU3	2.106(6)
O(1)-RU1	2.034(6)
O(2)-RU3	2.044(5)
O(3)-RU1	2.032(5)
O(4)-RU3	2.044(5)
O(5)-RU3	2.039(5)
O(6)-RU2	2.032(5)
O(7)-RU3	2.033(5)
O(8)-RU2	2.024(5)

O(9)-RU2	2.029(5)
O(10)-RU1	2.016(5)
O(11)-RU2	2.020(5)
O(12)-RU1	2.045(6)
O(13)-RU3	1.912(4)
O(13)-RU1	1.923(4)
O(13)-RU2	1.941(4)
F(1)-P(1)	1.512(10)
F(2)-P(1)	1.540(10)
F(3)-P(1)	1.528(10)
F(4)-P(1)	1.582(10)
F(5)-P(1)	1.548(13)
F(6)-P(1)	1.458(11)
C(1S)-CL2S	1.657(16)
C(1S)-CL1S	1.719(15)
C(1S)-H(1S1)	0.9700
C(1S)-H(1S2)	0.9700
CL3S-C(2SB)	1.83(3)
CL3S-C(2SA)	1.90(3)
CL4Aa-C(2SA)	1.77(3)
C(2SAa)-H(2S1)	0.9700
C(2SAa)-H(2S2)	0.9700
CL4Bb-C(2SB)	1.85(3)
C(2SBb)-H(2S3)	0.9700
C(2SBb)-H(2S4)	0.9700

O(2)-C(1)-O(1)	127.5(7)
O(2)-C(1)-C(2)	116.0(7)
O(1)-C(1)-C(2)	116.4(7)
C(1)-C(2)-H(2A)	109.5
C(1)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	109.5
C(1)-C(2)-H(2C)	109.5
H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
O(3)-C(3)-O(4)	126.5(7)
O(3)-C(3)-C(4)	116.5(7)
O(4)-C(3)-C(4)	117.1(7)
C(3)-C(4)-H(4A)	109.5
C(3)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(3)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
O(5)-C(5)-O(6)	125.8(7)
O(5)-C(5)-C(6)	115.9(7)
O(6)-C(5)-C(6)	118.3(7)
C(5)-C(6)-H(6A)	109.5
C(5)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5

C(5)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
O(7)-C(7)-O(8)	126.3(7)
O(7)-C(7)-C(8)	118.1(6)
O(8)-C(7)-C(8)	115.6(7)
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
O(10)-C(9)-O(9)	125.3(7)
O(10)-C(9)-C(10)	116.9(7)
O(9)-C(9)-C(10)	117.7(7)
C(9)-C(10)-H(10A)	109.5
C(9)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(9)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
N(11)-C(11)-C(12)	121.1(7)
N(11)-C(11)-H(11)	119.5
C(12)-C(11)-H(11)	119.5
O(12)-C(11A)-O(11)	127.7(7)
O(12)-C(11A)-C(12A)	117.3(7)
O(11)-C(11A)-C(12A)	115.0(7)
C(11)-C(12)-C(17)	117.3(7)
C(11)-C(12)-C(13)	122.4(7)
C(17)-C(12)-C(13)	120.3(7)
C(11A)-C(12A)-H(12A)	109.5
C(11A)-C(12A)-H(12B)	109.5
H(12A)-C(12A)-H(12B)	109.5
C(11A)-C(12A)-H(12C)	109.5
H(12A)-C(12A)-H(12C)	109.5
H(12B)-C(12A)-H(12C)	109.5
C(14)-C(13)-C(12)	118.9(8)
C(14)-C(13)-H(13)	120.6
C(12)-C(13)-H(13)	120.6
C(13)-C(14)-C(15)	119.6(8)
C(13)-C(14)-H(14)	120.2
C(15)-C(14)-H(14)	120.2
C(16)-C(15)-C(14)	122.1(7)
C(16)-C(15)-H(15)	118.9
C(14)-C(15)-H(15)	118.9
C(15)-C(16)-C(17)	119.9(8)
C(15)-C(16)-H(16)	120.0
C(17)-C(16)-H(16)	120.0
N(12)-C(17)-C(16)	120.1(7)
N(12)-C(17)-C(12)	120.7(7)

C(16)-C(17)-C(12)	119.2(8)
N(12)-C(18)-N(11)	126.1(7)
N(12)-C(18)-H(18)	117.0
N(11)-C(18)-H(18)	117.0
N(21)-C(21)-C(22)	120.3(7)
N(21)-C(21)-H(21)	119.9
C(22)-C(21)-H(21)	119.9
C(27)-C(22)-C(21)	116.7(7)
C(27)-C(22)-C(23)	120.7(7)
C(21)-C(22)-C(23)	122.5(8)
C(24)-C(23)-C(22)	120.3(10)
C(24)-C(23)-H(23)	119.8
C(22)-C(23)-H(23)	119.8
C(23)-C(24)-C(25)	119.6(10)
C(23)-C(24)-H(24)	120.2
C(25)-C(24)-H(24)	120.2
C(26)-C(25)-C(24)	122.3(9)
C(26)-C(25)-H(25)	118.8
C(24)-C(25)-H(25)	118.8
C(25)-C(26)-C(27)	118.6(10)
C(25)-C(26)-H(26)	120.7
C(27)-C(26)-H(26)	120.7
N(22)-C(27)-C(22)	121.5(7)
N(22)-C(27)-C(26)	120.2(8)
C(22)-C(27)-C(26)	118.3(8)
N(22)-C(28)-N(21)	125.9(7)
N(22)-C(28)-H(28)	117.1
N(21)-C(28)-H(28)	117.1
N(31)-C(31)-C(32)	122.4(6)
N(31)-C(31)-H(31)	118.8
C(32)-C(31)-H(31)	118.8
C(37)-C(32)-C(31)	116.8(6)
C(37)-C(32)-C(33)	119.9(6)
C(31)-C(32)-C(33)	123.3(7)
C(34)-C(33)-C(32)	119.3(7)
C(34)-C(33)-H(33)	120.3
C(32)-C(33)-H(33)	120.3
C(33)-C(34)-C(35)	120.5(7)
C(33)-C(34)-H(34)	119.8
C(35)-C(34)-H(34)	119.8
C(36)-C(35)-C(34)	121.6(7)
C(36)-C(35)-H(35)	119.2
C(34)-C(35)-H(35)	119.2
C(35)-C(36)-C(37)	119.4(7)
C(35)-C(36)-H(36)	120.3
C(37)-C(36)-H(36)	120.3
N(32)-C(37)-C(32)	120.7(6)
N(32)-C(37)-C(36)	120.0(7)
C(32)-C(37)-C(36)	119.3(7)
N(32)-C(38)-N(31)	128.5(7)

N(32)-C(38)-H(38)	115.7
N(31)-C(38)-H(38)	115.7
C(11)-N(11)-C(18)	117.5(6)
C(11)-N(11)-RU1	121.4(5)
C(18)-N(11)-RU1	121.1(5)
C(18)-N(12)-C(17)	117.3(6)
C(21)-N(21)-C(28)	117.9(6)
C(21)-N(21)-RU2	119.7(5)
C(28)-N(21)-RU2	122.3(5)
C(28)-N(22)-C(27)	117.6(7)
C(31)-N(31)-C(38)	115.9(6)
C(31)-N(31)-RU3	124.1(5)
C(38)-N(31)-RU3	120.0(5)
C(38)-N(32)-C(37)	115.8(6)
C(1)-O(1)-RU1	130.9(5)
C(1)-O(2)-RU3	131.8(5)
C(3)-O(3)-RU1	133.4(5)
C(3)-O(4)-RU3	130.8(5)
C(5)-O(5)-RU3	133.7(5)
C(5)-O(6)-RU2	130.9(5)
C(7)-O(7)-RU3	132.5(5)
C(7)-O(8)-RU2	132.5(5)
C(9)-O(9)-RU2	133.2(5)
C(9)-O(10)-RU1	133.4(5)
C(11A)-O(11)-RU2	131.4(5)
C(11A)-O(12)-RU1	131.3(5)
RU3-O(13)-RU1	120.2(2)
RU3-O(13)-RU2	119.9(2)
RU1-O(13)-RU2	119.8(2)
F(6)-P(1)-F(1)	92.8(10)
F(6)-P(1)-F(3)	89.6(8)
F(1)-P(1)-F(3)	91.8(8)
F(6)-P(1)-F(2)	92.9(9)
F(1)-P(1)-F(2)	173.7(8)
F(3)-P(1)-F(2)	90.8(6)
F(6)-P(1)-F(5)	175.2(8)
F(1)-P(1)-F(5)	89.4(8)
F(3)-P(1)-F(5)	94.6(8)
F(2)-P(1)-F(5)	84.7(7)
F(6)-P(1)-F(4)	90.3(7)
F(1)-P(1)-F(4)	90.4(8)
F(3)-P(1)-F(4)	177.7(7)
F(2)-P(1)-F(4)	87.0(6)
F(5)-P(1)-F(4)	85.4(8)
O(13)-RU1-O(10)	96.41(19)
O(13)-RU1-O(3)	95.70(19)
O(10)-RU1-O(3)	167.9(2)
O(13)-RU1-O(1)	94.0(2)
O(10)-RU1-O(1)	87.4(2)
O(3)-RU1-O(1)	91.6(2)

O(13)-RU1-O(12)	92.9(2)
O(10)-RU1-O(12)	92.9(2)
O(3)-RU1-O(12)	86.7(2)
O(1)-RU1-O(12)	173.0(2)
O(13)-RU1-N(11)	178.2(2)
O(10)-RU1-N(11)	82.2(2)
O(3)-RU1-N(11)	85.7(2)
O(1)-RU1-N(11)	84.8(2)
O(12)-RU1-N(11)	88.4(2)
O(13)-RU2-O(11)	92.7(2)
O(13)-RU2-O(8)	96.38(19)
O(11)-RU2-O(8)	86.5(2)
O(13)-RU2-O(9)	96.32(19)
O(11)-RU2-O(9)	92.8(2)
O(8)-RU2-O(9)	167.3(2)
O(13)-RU2-O(6)	93.8(2)
O(11)-RU2-O(6)	173.5(2)
O(8)-RU2-O(6)	92.0(2)
O(9)-RU2-O(6)	87.3(2)
O(13)-RU2-N(21)	178.3(2)
O(11)-RU2-N(21)	85.8(2)
O(8)-RU2-N(21)	84.2(2)
O(9)-RU2-N(21)	83.1(2)
O(6)-RU2-N(21)	87.8(2)
O(13)-RU3-O(7)	95.6(2)
O(13)-RU3-O(5)	92.87(19)
O(7)-RU3-O(5)	93.7(2)
O(13)-RU3-O(2)	95.1(2)
O(7)-RU3-O(2)	169.3(2)
O(5)-RU3-O(2)	86.2(2)
O(13)-RU3-O(4)	95.28(19)
O(7)-RU3-O(4)	87.4(3)
O(5)-RU3-O(4)	171.6(2)
O(2)-RU3-O(4)	91.2(2)
O(13)-RU3-N(31)	177.8(2)
O(7)-RU3-N(31)	82.3(2)
O(5)-RU3-N(31)	87.4(2)
O(2)-RU3-N(31)	87.0(2)
O(4)-RU3-N(31)	84.5(2)
CL2S-C(1S)-CL1S	115.7(8)
CL2S-C(1S)-H(1S1)	108.3
CL1S-C(1S)-H(1S1)	108.3
CL2S-C(1S)-H(1S2)	108.3
CL1S-C(1S)-H(1S2)	108.3
H(1S1)-C(1S)-H(1S2)	107.4
CL4Aa-C(2SAa)-CL3S	101(2)
CL4Aa-C(2SAa)-H(2S1)	111.5
CL3S-C(2SAa)-H(2S1)	111.5
CL4Aa-C(2SAa)-H(2S2)	111.5
CL3S-C(2SAa)-H(2S2)	111.5

H(2S1a)-C(2SAa)-H(2S2)109.4
CL3S-C(2SBb)-CL4B 107(2)
CL3S-C(2SBb)-H(2S3) 110.3
CL4Bb-C(2SBb)-H(2S3) 110.3
CL3S-C(2SBb)-H(2S4) 110.3
CL4Bb-C(2SBb)-H(2S4) 110.3
H(2S3b)-C(2SBb)-H(2S4)108.6

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for mo_snquinaz_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	39(4)	34(4)	35(4)	-5(3)	6(3)	2(3)
C(2)	64(6)	92(8)	44(5)	5(5)	22(5)	30(6)
C(3)	38(4)	36(4)	37(4)	-2(3)	1(3)	-8(3)
C(4)	92(8)	59(6)	52(6)	13(5)	-27(5)	-40(6)
C(5)	35(4)	38(4)	33(4)	2(3)	2(3)	-3(3)
C(6)	70(7)	63(6)	53(6)	4(5)	11(5)	-32(5)
C(7)	32(4)	37(4)	34(4)	0(3)	-3(3)	2(3)
C(8)	61(6)	83(7)	42(5)	-16(5)	-16(4)	43(6)
C(9)	39(4)	35(4)	35(4)	1(3)	-8(3)	1(3)
C(10)	70(7)	54(6)	64(6)	-10(4)	-39(6)	12(5)
C(11)	39(4)	26(4)	37(4)	0(3)	5(3)	0(3)
C(11A)	32(4)	37(4)	34(4)	2(3)	2(3)	-1(3)
C(12)	37(4)	36(4)	35(4)	4(3)	5(3)	2(3)
C(12A)	59(6)	55(5)	53(5)	3(4)	27(4)	-4(4)
C(13)	46(5)	55(5)	42(5)	5(4)	8(4)	8(4)
C(14)	48(5)	66(6)	44(5)	23(4)	2(4)	8(4)
C(15)	56(6)	40(5)	67(6)	26(4)	11(5)	8(4)
C(16)	59(6)	28(4)	61(6)	8(4)	5(4)	5(4)
C(17)	44(5)	31(4)	47(5)	2(3)	7(4)	4(3)
C(18)	48(5)	31(4)	34(4)	7(3)	4(3)	5(3)
C(21)	40(4)	32(4)	35(4)	-4(3)	0(3)	0(3)
C(22)	40(4)	43(4)	34(4)	-17(3)	5(3)	-3(4)
C(23)	52(5)	69(6)	38(5)	-6(4)	2(4)	-1(5)
C(24)	69(7)	91(8)	46(6)	-28(5)	1(5)	-2(6)
C(25)	68(7)	81(7)	66(7)	-46(6)	3(5)	-7(6)
C(26)	56(6)	43(5)	80(7)	-29(5)	10(5)	-4(4)
C(27)	34(4)	44(4)	53(5)	-21(4)	4(4)	3(4)
C(28)	41(5)	41(4)	39(4)	-8(3)	-2(3)	0(4)
C(31)	43(4)	25(3)	29(4)	1(3)	0(3)	3(3)
C(32)	35(4)	34(4)	26(4)	-1(3)	1(3)	4(3)
C(33)	53(5)	37(4)	33(4)	-9(3)	-4(4)	4(4)
C(34)	48(5)	53(5)	35(4)	-10(4)	-2(3)	11(4)
C(35)	53(5)	67(6)	20(4)	0(3)	0(3)	15(4)
C(36)	54(5)	43(4)	32(4)	8(3)	0(3)	16(4)
C(37)	39(4)	37(4)	27(4)	-3(3)	3(3)	13(3)
C(38)	64(6)	26(4)	37(5)	-7(3)	-8(4)	6(4)
N(11)	46(4)	23(3)	29(3)	-1(2)	5(3)	3(3)
N(12)	55(4)	32(3)	37(4)	-2(3)	7(3)	4(3)
N(21)	39(4)	26(3)	28(3)	-6(2)	0(3)	1(3)
N(22)	47(4)	26(3)	57(4)	-6(3)	-2(3)	0(3)
N(31)	41(4)	24(3)	27(3)	-2(2)	6(3)	5(3)
N(32)	65(5)	33(3)	32(3)	3(3)	6(3)	9(3)
O(1)	47(3)	42(3)	38(3)	4(2)	11(3)	14(3)

O(2)	52(3)	49(3)	29(3)	-1(2)	9(2)	21(3)
O(3)	55(4)	35(3)	35(3)	0(2)	-8(2)	-11(3)
O(4)	59(4)	35(3)	31(3)	5(2)	-11(2)	-15(3)
O(5)	57(4)	42(3)	30(3)	0(2)	5(2)	-18(3)
O(6)	50(3)	39(3)	36(3)	-5(2)	11(2)	-19(3)
O(7)	53(4)	50(3)	28(3)	-10(2)	-7(2)	20(3)
O(8)	40(3)	42(3)	35(3)	-12(2)	-10(2)	13(2)
O(9)	49(3)	37(3)	41(3)	-11(2)	-17(3)	5(3)
O(10)	54(3)	28(3)	46(3)	-6(2)	-14(3)	4(2)
O(11)	52(3)	27(3)	42(3)	-4(2)	18(2)	-4(2)
O(12)	53(3)	28(3)	38(3)	4(2)	14(2)	3(2)
O(13)	29(3)	21(2)	24(2)	0(2)	2(2)	1(2)
F(1)	252(17)	292(17)	68(6)	-42(8)	-35(8)	13(13)
F(2)	137(9)	209(11)	90(6)	-31(7)	-20(6)	48(8)
F(3)	257(16)	133(9)	140(9)	-17(7)	-39(10)	108(10)
F(4)	116(8)	198(11)	144(9)	63(8)	8(7)	48(8)
F(5)	208(14)	156(10)	162(12)	9(8)	21(10)	-67(10)
F(6)	129(10)	131(9)	340(20)	58(10)	63(11)	-36(8)
P(1)	93(2)	70(2)	59(2)	9(1)	-12(2)	8(2)
RU1	34(1)	23(1)	23(1)	-1(1)	2(1)	0(1)
RU2	32(1)	23(1)	23(1)	-3(1)	0(1)	0(1)
RU3	35(1)	24(1)	21(1)	-2(1)	2(1)	0(1)
C(1S)	95(10)	79(8)	102(10)	-21(7)	-12(8)	-6(7)
CL1S	109(3)	122(3)	95(3)	-31(2)	20(2)	-26(2)
CL2S	100(3)	209(5)	84(3)	16(3)	8(2)	26(3)
CL3S	202(9)	356(13)	289(13)	70(11)	69(8)	-16(10)
CL4A	218(11)	169(7)	186(8)	-12(6)	4(8)	-28(7)
C(2SA)	218(11)	169(7)	186(8)	-12(6)	4(8)	-28(7)
CL4B	218(11)	169(7)	186(8)	-12(6)	4(8)	-28(7)
C(2SB)	218(11)	169(7)	186(8)	-12(6)	4(8)	-28(7)

Table S5. Hydrogen bonds for mo_snquinaz_0m [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(6)-H(6C)...CL2S$1#1	0.96	2.97	3.919(12)	170.8
C(8)-H(8A)...F4$2#2	0.96	2.52	3.436(14)	160.3
C(8)-H(8B)...N12$3#3	0.96	2.50	3.445(11)	167.8
C(10)-H(10C)...CL4Aa$4#4	0.96	2.66	3.41(2)	136.2
C(12A)-H(12A)...F3$5#5	0.96	2.55	3.466(15)	159.1
C(31)-H(31)...F3$6#6	0.93	2.64	3.494(12)	153.8
C(38)-H(38)...O(5)	0.93	2.53	3.014(9)	112.6
C(1S)-H(1S2)...F4$5#5	0.97	2.53	3.17(2)	123.5

Symmetry transformations used to generate equivalent atoms:
#1 x-1/2,-y+1/2,z-1/2 #2 x-1/2,y-1/2,z #3 x-1/2,y+1/2,z
#4 x+1/2,-y+1/2,z-1/2 #5 x,-y+1,z+1/2 #6 x,y-1,z

Distance X..Y
3.3434 (0.0007) _ RU1 - RU2
3.3252 (0.0007) _ RU1 - RU3
3.3360 (0.0007) _ RU2 - RU3

Angle ANG
59.71 (0.01) _ RU1 - RU2 - RU3
60.25 (0.02) _ RU2 - RU3 - RU1
60.03 (0.01) _ RU3 - RU1 - RU2

Least-squares planes (x,y,z in crystal coordinates) and deviations from them
(* indicates atom used to define plane)

10.2780 (0.0005) x + 3.2162 (0.0051) y - 4.0266 (0.0053) z = 4.5551 (0.0018)

* 0.0000 (0.0012) RU1
* 0.0000 (0.0012) RU2
* 0.0000 (0.0012) RU3
* -0.0001 (0.0035) O13

Rms deviation of fitted atoms = 0.0001

10.2222 (0.0038) x + 3.9114 (0.0482) y - 4.0476 (0.0429) z = 4.5804 (0.0145)

Angle to previous plane (with approximate esd) = 1.834 (0.074)

* 0.0070 (0.0064) C11
* 0.0136 (0.0074) C12
* 0.0023 (0.0071) C13
* -0.0088 (0.0072) C14

* -0.0037 (0.0078) C15
* -0.0028 (0.0077) C16
*   0.0053 (0.0080) C17
* -0.0032 (0.0066) C18
* -0.0169 (0.0058) N11
*   0.0071 (0.0064) N12

Rms deviation of fitted atoms =   0.0084

10.2780 (0.0005) x + 3.2162 (0.0051) y - 4.0266 (0.0053) z = 4.5551 (0.0018)

Angle to previous plane (with approximate esd) = 1.834 (0.074)

*   0.0000 (0.0012) RU1
*   0.0000 (0.0012) RU2
*   0.0000 (0.0012) RU3
* -0.0001 (0.0035) O13

Rms deviation of fitted atoms =   0.0001

10.2705 (0.0049) x + 2.2280 (0.0571) y - 5.0729 (0.0422) z = 3.8915 (0.0210)

Angle to previous plane (with approximate esd) = 3.759 (0.089)

* -0.0034 (0.0067) C21
* -0.0354 (0.0076) C22
* -0.0165 (0.0078) C23
*   0.0293 (0.0091) C24
*   0.0174 (0.0090) C25
* -0.0067 (0.0080) C26
* -0.0146 (0.0080) C27
*   0.0198 (0.0064) C28
*   0.0248 (0.0059) N21
* -0.0147 (0.0065) N22

Rms deviation of fitted atoms =   0.0204

10.2780 (0.0005) x + 3.2162 (0.0051) y - 4.0266 (0.0053) z = 4.5551 (0.0018)

Angle to previous plane (with approximate esd) = 3.759 (0.089)

*   0.0000 (0.0012) RU1
*   0.0000 (0.0012) RU2
*   0.0000 (0.0012) RU3
* -0.0001 (0.0035) O13

Rms deviation of fitted atoms = 0.0001

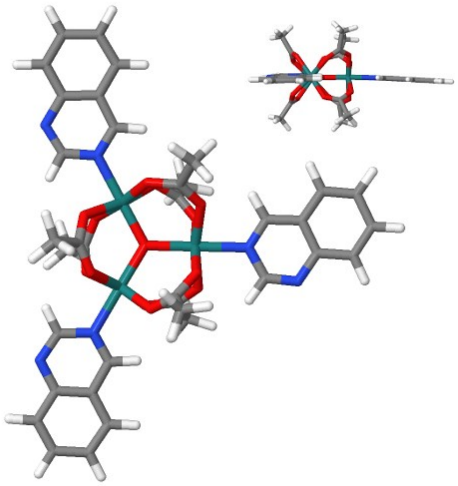
10.2593 (0.0032) x - 0.6096 (0.0557) y - 5.8099 (0.0355) z = 3.8724 (0.0091)

Angle to previous plane (with approximate esd) = 11.004 (0.066)

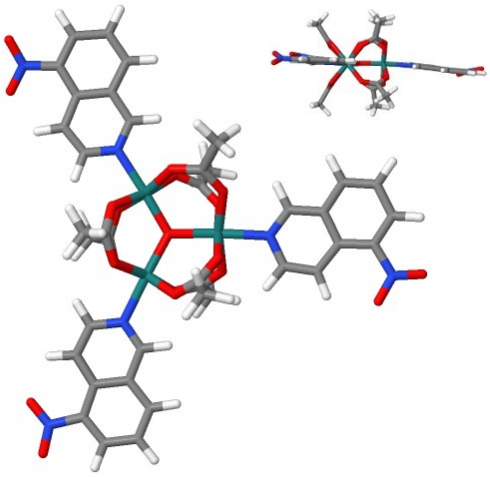
* 0.0048 (0.0065) C31
* -0.0112 (0.0070) C32
* -0.0063 (0.0071) C33
* 0.0062 (0.0072) C34
* 0.0100 (0.0072) C35
* 0.0014 (0.0073) C36
* -0.0139 (0.0074) C37
* 0.0094 (0.0079) C38
* 0.0053 (0.0059) N31
* -0.0057 (0.0067) N32

Rms deviation of fitted atoms = 0.0082

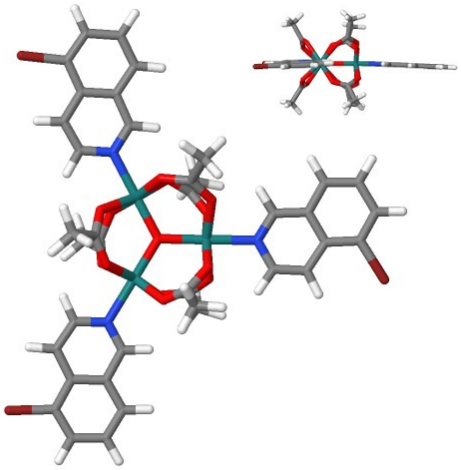
DFT calculations



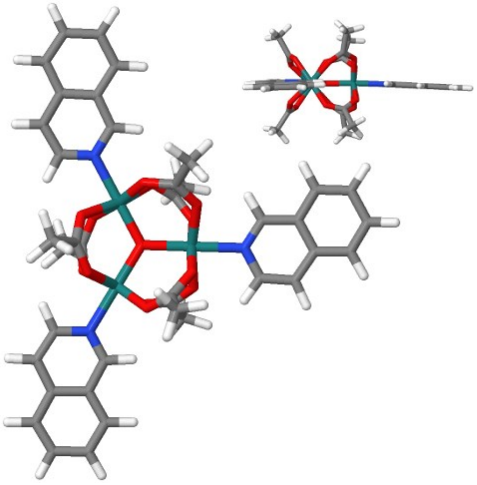
(1) qui



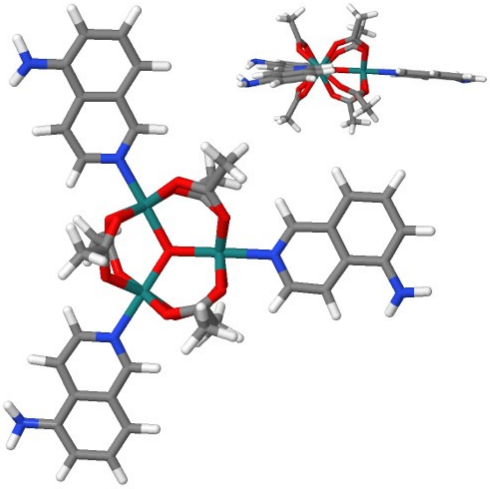
(2) nitroiq



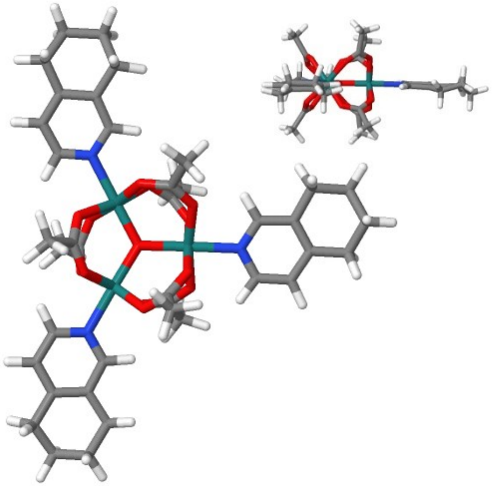
(3) briq



(4) iq



(5) amiq



(6) thiq

Figure S2. Up and side views of the equilibrium geometries obtained with DFT using PBE0/def2-TZVP. Color labels: Ru (green), O (red), N (blue), C (dark gray), H (white).

Table S6. Cartesian coordinates for complex (1) qui obtained with DFT using PBE0/def2-TZVP.

O	-0.044913	0.020847	-0.016789
Ru	1.931002	-0.026692	-0.028966
Ru	-0.956311	1.703676	-0.083972
Ru	-1.027546	-1.611475	0.066193
N	4.026938	-0.070297	0.014845
N	5.985523	-1.401936	0.118711
C	4.744624	1.031867	0.039115
H	4.204336	1.970556	0.011022
C	6.144017	1.001833	0.114281
C	6.941215	2.164823	0.160018
H	6.465012	3.138840	0.138841
C	8.300927	2.044962	0.231920
H	8.926075	2.928770	0.270582
C	8.902998	0.769705	0.262684
H	9.983098	0.699267	0.323096
C	8.149824	-0.374481	0.224448
H	8.600869	-1.358747	0.253781
C	6.746878	-0.279149	0.151208
C	4.699226	-1.256939	0.057739
H	4.075671	-2.141184	0.027139
N	-1.940001	3.568659	-0.102808
N	-3.984737	4.758387	-0.020902
C	-1.252917	4.689251	-0.063968
H	-0.172624	4.604383	-0.097065
C	-1.880024	5.938131	0.018394
C	-1.173968	7.157912	0.090008
H	-0.089311	7.150387	0.077158
C	-1.870245	8.330261	0.180082
H	-1.341832	9.274045	0.239144
C	-3.281779	8.321080	0.199390
H	-3.812737	9.263176	0.271911
C	-3.988911	7.149431	0.132475
H	-5.071387	7.130387	0.151089
C	-3.297265	5.927019	0.040675
C	-3.300182	3.659837	-0.084248
H	-3.827397	2.714978	-0.121718
N	-2.096150	-3.429014	0.142565
N	-4.198330	-4.515681	0.156644
C	-1.467079	-4.579694	0.057064
H	-0.383486	-4.546642	0.028314
C	-2.159598	-5.794997	-0.004395

C	-1.518935	-7.045414	-0.125988
H	-0.435886	-7.089493	-0.166460
C	-2.275702	-8.180929	-0.198607
H	-1.797526	-9.148030	-0.294588
C	-3.684445	-8.103247	-0.155442
H	-4.264071	-9.016765	-0.219531
C	-4.329256	-6.900114	-0.037580
H	-5.409283	-6.827719	-0.005301
C	-3.574112	-5.715008	0.042489
C	-3.457996	-3.452994	0.195272
H	-3.934149	-2.483607	0.271709
O	2.028133	-1.665648	-1.208130
O	-0.068367	-2.384456	-1.547934
C	1.140328	-2.287433	-1.859969
C	1.558374	-2.953404	-3.135074
H	1.471511	-2.212066	-3.934847
H	0.896625	-3.783958	-3.371123
H	2.596073	-3.279440	-3.088374
O	1.986129	-1.052518	1.702184
O	0.230133	-2.443956	1.471958
C	1.183787	-1.944534	2.111404
C	1.392299	-2.406053	3.521727
H	2.423931	-2.258677	3.834657
H	1.076756	-3.441043	3.644668
H	0.752374	-1.790318	4.160406
O	-2.441562	-1.033566	-1.290975
O	-2.080782	1.147154	-1.680183
C	-2.560975	0.020222	-1.966385
C	-3.315441	-0.091475	-3.259649
H	-2.628389	-0.499050	-4.006941
H	-3.667272	0.880808	-3.598708
H	-4.143145	-0.791802	-3.161355
O	-2.109625	-1.029585	1.669428
O	-2.374714	1.171669	1.305731
C	-2.563061	0.111507	1.951328
C	-3.390353	0.182597	3.202186
H	-4.247447	-0.487419	3.114969
H	-3.727124	1.197305	3.399658
H	-2.784825	-0.179963	4.035269
O	0.307885	2.504717	-1.489717
O	1.987116	1.037790	-1.740389
C	1.234641	1.964910	-2.143922
C	1.464930	2.444471	-3.544925
H	2.491847	2.263631	-3.856920

H	1.192355	3.493985	-3.646544
H	0.804221	1.869827	-4.199806
O	0.097139	2.464772	1.480567
O	2.157101	1.637478	1.119373
C	1.324465	2.372121	1.720243
C	1.876998	3.215137	2.831240
H	2.592303	3.927710	2.414099
H	2.424024	2.579425	3.529163
H	1.085445	3.752317	3.348069

Table S7. Cartesian coordinates for complex (2) nitroiq obtained with DFT using PBE0/def2-TZVP.

O	-1.952413	5.815146	-0.520188
Ru	-0.965430	7.546368	-0.531700
Ru	-0.980036	4.175020	-0.418433
Ru	-3.865602	5.830408	-0.642928
N	-0.031205	9.420030	-0.658769
C	1.268843	9.589771	-0.717175
H	1.880284	8.698622	-0.649521
C	1.877190	10.850360	-0.876160
C	3.283084	10.954787	-0.929786
H	3.879395	10.051694	-0.859979
C	3.878775	12.176985	-1.063582
H	4.956773	12.267066	-1.106109
C	3.086553	13.332025	-1.147690
H	3.542208	14.309234	-1.241443
C	1.719011	13.249829	-1.122454
C	1.051769	12.004739	-0.981667
C	-0.340740	11.785362	-0.905785
H	-1.032005	12.608172	-0.983222
C	-0.822197	10.521159	-0.748982
H	-1.884608	10.339742	-0.680953
N	0.986323	14.522073	-1.249474
O	1.603657	15.537739	-1.029715
O	-0.180929	14.479354	-1.579551
N	0.003356	2.312862	-0.236845
C	-0.756882	1.188999	-0.229217
H	-1.818025	1.345182	-0.354583
C	-0.242350	-0.061661	-0.074784
H	-0.906041	-0.910153	-0.061136
C	1.151247	-0.232395	0.071575
C	1.849139	-1.460019	0.205336
C	3.216473	-1.505413	0.276066

H	3.696329	-2.472228	0.355629
C	3.977245	-0.326146	0.258209
H	5.055163	-0.387125	0.337382
C	3.350706	0.882866	0.148873
H	3.922008	1.804580	0.138604
C	1.945723	0.948537	0.042390
C	1.301608	2.191659	-0.103819
H	1.881025	3.107576	-0.111960
N	1.146050	-2.752243	0.272914
O	1.792297	-3.742417	0.023945
O	-0.025504	-2.748999	0.589688
N	-5.985603	5.930819	-0.732696
C	-6.570711	7.102325	-0.818870
H	-5.923246	7.965939	-0.916641
C	-7.965845	7.274810	-0.795780
C	-8.507607	8.572758	-0.900782
H	-7.832864	9.415990	-0.997915
C	-9.859793	8.756159	-0.886896
H	-10.290439	9.745041	-0.978814
C	-10.703806	7.648089	-0.737167
H	-11.777957	7.773652	-0.705452
C	-10.199193	6.380139	-0.606314
C	-8.799229	6.127925	-0.655775
C	-8.134877	4.880990	-0.593040
H	-8.697713	3.967210	-0.501832
C	-6.771077	4.829391	-0.635514
H	-6.243040	3.888438	-0.577209
N	-11.199545	5.319405	-0.380277
O	-12.363764	5.646231	-0.391470
O	-10.803716	4.191369	-0.177673
O	0.441052	4.673597	-1.790938
C	1.011257	5.769226	-1.991570
O	0.648536	6.899061	-1.560271
C	2.267261	5.769530	-2.814521
H	3.083054	6.161505	-2.202897
H	2.149209	6.442192	-3.665174
H	2.512892	4.768923	-3.162125
O	-1.776450	8.037971	-2.308129
C	-2.927580	7.777004	-2.767257
O	-3.868998	7.228877	-2.150002
C	-3.152916	8.154041	-4.200503
H	-2.838006	9.181842	-4.384180
H	-4.190938	8.000410	-4.485582
H	-2.517996	7.513691	-4.817914

O	-3.922417	4.479509	-2.162007
C	-3.079029	3.623997	-2.536748
O	-2.007247	3.313685	-1.955477
C	-3.354632	2.933155	-3.842986
H	-4.422952	2.782077	-3.990939
H	-2.814630	1.991028	-3.906440
H	-2.994222	3.586781	-4.642359
O	-2.175279	3.430702	1.040634
C	-3.361965	3.660229	1.380272
O	-4.173655	4.413894	0.788376
C	-3.834691	2.995270	2.639306
H	-3.673390	3.696667	3.462676
H	-3.258765	2.094897	2.841665
H	-4.899939	2.774913	2.591015
O	0.006289	7.082522	1.189426
C	0.351356	5.960942	1.654061
O	0.221455	4.842961	1.098080
C	0.975113	5.957820	3.019931
H	1.307373	6.952318	3.309580
H	1.799932	5.247687	3.060712
H	0.220521	5.611039	3.731402
O	-2.298696	8.475043	0.651681
C	-3.275444	8.012769	1.311992
O	-4.043451	7.104446	0.931699
C	-3.510673	8.580245	2.676480
H	-2.866265	8.029664	3.367917
H	-4.543468	8.432814	2.985787
H	-3.220682	9.628961	2.723815

Table S8. Cartesian coordinates for complex (3) briq obtained with DFT using PBE0/def2-TZVP.

O	-0.064018	-0.003109	-0.008650
Ru	1.913965	-0.053556	-0.006058
Ru	-0.967751	1.688364	-0.087395
Ru	-1.056537	-1.632099	0.050979
N	4.008441	-0.079177	0.041183
C	4.697421	1.040036	0.066887
H	4.128591	1.960937	0.044985
C	6.101653	1.084030	0.136886
C	6.797214	2.310609	0.185292
H	6.236665	3.238078	0.170752
C	8.161879	2.314623	0.251729
H	8.710343	3.247763	0.293647

C	8.878869	1.103510	0.270514
H	9.960313	1.117567	0.323944
C	8.219225	-0.094796	0.226880
C	6.806803	-0.147743	0.165462
C	4.681173	-1.259324	0.075767
H	4.065063	-2.146134	0.043370
N	-1.945400	3.560389	-0.117772
C	-1.243685	4.671603	-0.105942
H	-0.166907	4.565251	-0.161696
C	-1.820053	5.951144	-0.024355
C	-1.025861	7.117950	0.009361
H	0.053525	7.030004	-0.040636
C	-1.624960	8.341225	0.106949
H	-1.029260	9.245363	0.136575
C	-3.027476	8.445248	0.171389
H	-3.489591	9.421024	0.250562
C	-3.812913	7.324190	0.138987
C	-3.236956	6.036356	0.037739
C	-3.300452	3.640372	-0.077549
H	-3.823226	2.694905	-0.093141
N	-2.156958	-3.436293	0.112782
C	-1.543846	-4.596300	0.068468
H	-0.460239	-4.571994	0.063630
C	-2.223423	-5.826663	0.024054
C	-1.525591	-7.050775	-0.042661
H	-0.441578	-7.045758	-0.051919
C	-2.223826	-8.223411	-0.099345
H	-1.702569	-9.171200	-0.153316
C	-3.631892	-8.218560	-0.091821
H	-4.173378	-9.154757	-0.140432
C	-4.324525	-7.039395	-0.025931
C	-3.643693	-5.801368	0.034721
C	-3.514507	-3.408976	0.135466
H	-3.958983	-2.424901	0.170437
O	2.011774	-1.678949	-1.209319
O	-0.086076	-2.393558	-1.559828
C	1.124621	-2.297588	-1.864373
C	1.545843	-2.963438	-3.139221
H	1.447729	-2.226356	-3.941514
H	0.892028	-3.801914	-3.369670
H	2.587065	-3.278090	-3.095233
O	1.986292	-1.151722	1.683859
O	0.188908	-2.490108	1.444240
C	1.187176	-2.059096	2.064616

C	1.462374	-2.643998	3.420088
H	2.532652	-2.730978	3.602275
H	0.962939	-3.602939	3.538878
H	1.054690	-1.952511	4.162807
O	-2.458727	-1.037487	-1.314705
O	-2.073478	1.138966	-1.701845
C	-2.558613	0.016143	-1.993215
C	-3.294503	-0.091600	-3.298206
H	-2.594459	-0.491212	-4.037705
H	-3.645274	0.881018	-3.637649
H	-4.119817	-0.796816	-3.217208
O	-2.137451	-1.052729	1.654844
O	-2.392251	1.151779	1.299417
C	-2.575166	0.091407	1.946403
C	-3.370855	0.164978	3.218187
H	-4.209174	-0.531906	3.174068
H	-3.727553	1.174281	3.408310
H	-2.727211	-0.162081	4.037872
O	0.303575	2.488884	-1.484477
O	1.988711	1.025869	-1.706713
C	1.238510	1.947399	-2.125159
C	1.481274	2.417920	-3.527318
H	2.510074	2.232475	-3.830230
H	1.211584	3.467216	-3.638297
H	0.823902	1.840456	-4.183127
O	0.065707	2.445391	1.488411
O	2.120161	1.579174	1.188285
C	1.284232	2.332402	1.760160
C	1.822701	3.178350	2.876339
H	2.527956	3.901938	2.460578
H	2.377227	2.550167	3.574617
H	1.022601	3.706409	3.389412
C	-4.269911	-4.541115	0.101398
C	6.040322	-1.329827	0.131907
C	-3.962453	4.828436	-0.004155
H	-5.349304	-4.471972	0.117459
H	-5.043393	4.844191	0.032404
H	6.529944	-2.293929	0.155020
Br	-6.207915	-7.077407	-0.021081
Br	-5.685247	7.514534	0.234690
Br	9.222512	-1.687817	0.254375

Table S9. Cartesian coordinates for complex (4) iq obtained with DFT using PBE0/def2-TZVP.

O	-0.064908	0.005135	-0.026148
Ru	1.908611	-0.049238	-0.030762
Ru	-0.970357	1.698937	-0.094532
Ru	-1.059852	-1.625618	0.049158
N	4.009456	-0.113600	0.021898
C	4.725751	0.989743	0.042341
H	4.177582	1.923089	0.010977
C	6.130388	0.995179	0.117683
C	6.872274	2.195986	0.157681
H	6.346102	3.143757	0.133648
C	8.236964	2.153350	0.227386
H	8.811321	3.071374	0.261254
C	8.909702	0.914390	0.261453
H	9.992055	0.900277	0.318783
C	8.213805	-0.264158	0.230281
H	8.734751	-1.214611	0.263723
C	6.804940	-0.250875	0.161002
C	4.651970	-1.312000	0.069650
H	4.012311	-2.182067	0.040292
N	-1.957977	3.563497	-0.118234
C	-1.266494	4.681751	-0.079182
H	-0.188092	4.584809	-0.121622
C	-1.860837	5.951541	0.017051
C	-1.094830	7.137108	0.084745
H	-0.012543	7.074431	0.051219
C	-1.720998	8.346832	0.195524
H	-1.138622	9.258580	0.250902
C	-3.129088	8.416970	0.241540
H	-3.608694	9.384618	0.332391
C	-3.893732	7.283552	0.177357
H	-4.975361	7.343983	0.218899
C	-3.276955	6.021199	0.061752
C	-3.315786	3.625840	-0.094130
H	-3.824863	2.673617	-0.133082
N	-2.152530	-3.433297	0.121757
C	-1.526148	-4.587330	0.066458
H	-0.442903	-4.549447	0.059363
C	-2.195388	-5.821992	0.011139
C	-1.498905	-7.047530	-0.071638
H	-0.414422	-7.042659	-0.082688
C	-2.195017	-8.221540	-0.142156

H	-1.666243	-9.164561	-0.208160
C	-3.605603	-8.214454	-0.134032
H	-4.140808	-9.154798	-0.195184
C	-4.304245	-7.040164	-0.052726
H	-5.388360	-7.040617	-0.049695
C	-3.613744	-5.813216	0.023680
C	-3.511563	-3.418349	0.150444
H	-3.963174	-2.437848	0.197792
O	1.998631	-1.692371	-1.212073
O	-0.101820	-2.393388	-1.566274
C	1.109923	-2.303989	-1.869722
C	1.527169	-2.969355	-3.146343
H	1.430328	-2.230103	-3.946800
H	0.870168	-3.805173	-3.377432
H	2.567402	-3.287514	-3.104375
O	1.948509	-1.075949	1.702889
O	0.190156	-2.463252	1.458652
C	1.140730	-1.965056	2.103954
C	1.335082	-2.426607	3.517069
H	2.362935	-2.276348	3.840986
H	1.020095	-3.462215	3.636783
H	0.687118	-1.812220	4.148766
O	-2.464870	-1.033645	-1.314243
O	-2.085041	1.144818	-1.701237
C	-2.568059	0.020751	-1.990816
C	-3.307944	-0.087318	-3.293851
H	-2.609652	-0.485676	-4.035592
H	-3.660754	0.885238	-3.631469
H	-4.132191	-0.793556	-3.210531
O	-2.136286	-1.039738	1.655683
O	-2.391156	1.164127	1.297587
C	-2.575474	0.104369	1.944303
C	-3.379306	0.179272	3.211702
H	-4.225061	-0.507950	3.155979
H	-3.727290	1.191287	3.403794
H	-2.747611	-0.159434	4.035665
O	0.304902	2.493012	-1.491478
O	1.971970	1.012239	-1.745895
C	1.228700	1.946973	-2.145531
C	1.463398	2.430142	-3.545128
H	2.490844	2.248180	-3.854836
H	1.193000	3.480440	-3.644162
H	0.803261	1.858143	-4.202867
O	0.075634	2.448841	1.476135

O	2.134199	1.613521	1.123260
C	1.303770	2.354534	1.715838
C	1.856270	3.207849	2.819685
H	2.563012	3.923357	2.393005
H	2.412201	2.581097	3.518448
H	1.063369	3.743215	3.336394
C	-4.254150	-4.558838	0.107764
C	6.008553	-1.414878	0.133444
C	-3.990203	4.805569	-0.009684
H	-5.335755	-4.499353	0.130212
H	-5.073316	4.807300	0.011513
H	6.473013	-2.393034	0.167030

Table S10. Cartesian coordinates for complex (5) amiq obtained with DFT using PBE0/def2-TZVP.

O	-2.031928	5.919579	-0.430101
Ru	-1.029788	7.565234	-0.522168
Ru	-1.086692	4.191040	-0.181670
Ru	-3.939983	5.919954	-0.602572
N	0.041870	9.387473	-0.663585
C	1.352310	9.422276	-0.575353
H	1.848337	8.477523	-0.388825
C	2.114290	10.597226	-0.710950
C	3.520936	10.568599	-0.631992
H	4.030420	9.629353	-0.453080
C	4.214356	11.738979	-0.777331
H	5.296025	11.743305	-0.713344
C	3.546238	12.951488	-0.995158
H	4.125841	13.863445	-1.096477
C	2.169053	13.020359	-1.087447
C	1.420786	11.814123	-0.943675
C	0.014303	11.742898	-1.027023
H	-0.583818	12.622208	-1.229774
C	-0.626354	10.547849	-0.889623
H	-1.700293	10.462429	-0.966345
N	1.536040	14.209995	-1.372064
H	2.100719	15.036733	-1.267646
H	0.603305	14.332871	-1.016164
N	-0.107306	2.337440	-0.001405
C	-0.816971	1.184787	-0.124260
H	-1.891904	1.295284	-0.135812
C	-0.215323	-0.033132	-0.239200
H	-0.848241	-0.902023	-0.368372

C	1.191833	-0.141238	-0.229940
C	1.904452	-1.365835	-0.400471
C	3.286019	-1.329003	-0.373557
H	3.838246	-2.254497	-0.501621
C	3.992527	-0.132377	-0.193934
H	5.075653	-0.161587	-0.184109
C	3.334285	1.055759	-0.029871
H	3.872937	1.985290	0.109694
C	1.925192	1.060334	-0.049163
C	1.203286	2.262606	0.062756
H	1.735870	3.198160	0.173132
N	1.233569	-2.541370	-0.653617
H	1.780427	-3.381700	-0.565465
H	0.308533	-2.639013	-0.271410
N	-6.061207	5.903254	-0.741521
C	-6.742871	7.025469	-0.816510
H	-6.163865	7.936502	-0.903550
C	-8.147930	7.092468	-0.760563
C	-8.822321	8.328622	-0.812638
H	-8.255371	9.245664	-0.915528
C	-10.188471	8.339145	-0.731936
H	-10.731624	9.275810	-0.777359
C	-10.912911	7.148031	-0.589018
H	-11.995406	7.192470	-0.525204
C	-10.287893	5.918116	-0.512744
C	-8.865220	5.875935	-0.614337
C	-8.105548	4.688111	-0.570173
H	-8.579041	3.721310	-0.458966
C	-6.744549	4.734173	-0.635640
H	-6.137806	3.840777	-0.602148
N	-11.009441	4.769704	-0.274357
H	-12.004132	4.844145	-0.411204
H	-10.635314	3.907465	-0.632204
O	0.560867	4.661628	-1.272407
C	0.951649	5.721464	-1.827115
O	0.395216	6.843202	-1.772589
C	2.233847	5.645610	-2.606420
H	3.047295	5.948174	-1.940266
H	2.212885	6.343611	-3.441521
H	2.427057	4.632160	-2.951739
O	-1.997424	8.206955	-2.204858
C	-2.999432	7.743882	-2.808422
O	-3.859997	6.943771	-2.360395
C	-3.162215	8.158644	-4.242207

H	-2.866350	9.198037	-4.381622
H	-4.179953	7.982350	-4.584088
H	-2.485387	7.547119	-4.844311
O	-3.972790	4.247314	-1.800332
C	-3.056514	3.569192	-2.319657
O	-1.884511	3.413225	-1.869755
C	-3.343156	2.886759	-3.627188
H	-4.404933	2.672742	-3.737038
H	-2.746380	1.983231	-3.735323
H	-3.051831	3.578501	-4.423065
O	-2.505043	3.426924	1.039502
C	-3.469604	3.996495	1.627040
O	-4.166209	4.926875	1.162680
C	-3.785120	3.536919	3.018215
H	-3.143060	4.102927	3.699034
H	-3.545991	2.481978	3.143866
H	-4.821362	3.749323	3.274907
O	0.058466	7.107200	1.153950
C	0.162175	6.053532	1.829387
O	-0.172406	4.889724	1.478302
C	0.753450	6.160354	3.206777
H	1.069392	7.177512	3.424910
H	1.594004	5.472364	3.305661
H	0.000294	5.843046	3.931489
O	-2.252833	8.562948	0.741447
C	-3.468846	8.431908	1.022644
O	-4.263266	7.596395	0.528918
C	-4.004893	9.380635	2.055930
H	-3.413175	9.277171	2.966649
H	-5.052080	9.181444	2.271593
H	-3.880810	10.406500	1.703381

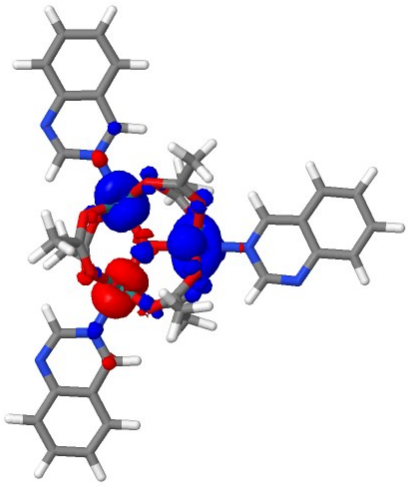
Table S11. Cartesian coordinates for complex (6) thiq obtained with DFT using PBE0/def2-TZVP.

O	-0.116832	0.009243	-0.073999
Ru	1.854171	-0.040648	-0.060243
Ru	-1.018966	1.709331	-0.138292
Ru	-1.100375	-1.629567	-0.013410
N	3.957234	-0.107469	0.015769
C	4.691038	1.000941	0.127627
H	4.135992	1.928780	0.175523
C	6.076322	1.004150	0.204690
C	6.816204	2.298266	0.409315

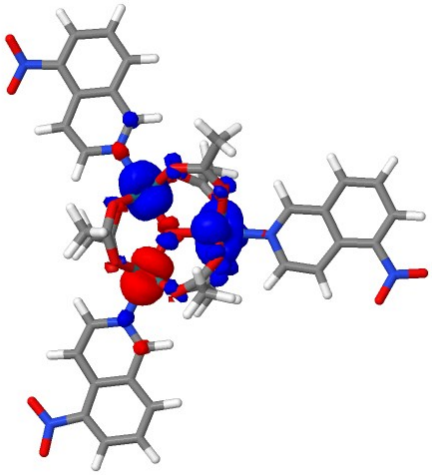
C	8.284737	2.211177	0.014042
C	8.931296	0.962698	0.595391
H	9.989115	0.923691	0.324211
C	8.240230	-0.303597	0.108359
C	6.742335	-0.219338	0.118919
C	4.593963	-1.283291	-0.024706
H	3.968924	-2.160756	-0.112534
N	-1.981844	3.592666	-0.127869
C	-1.258282	4.705154	0.037920
H	-0.183476	4.580830	-0.002471
C	-1.822365	5.944610	0.276654
C	-1.016962	7.162040	0.603560
C	-1.558687	8.441192	-0.049255
C	-3.096600	8.525949	-0.094430
C	-3.811626	7.374173	0.617163
C	-3.215388	6.043956	0.296948
C	-3.313432	3.691173	-0.128976
H	-3.857827	2.767184	-0.271040
N	-2.162203	-3.456469	0.051247
C	-1.519241	-4.619129	-0.059025
H	-0.440203	-4.554326	-0.132926
C	-2.155008	-5.851497	-0.087031
C	-1.356654	-7.112021	-0.288156
C	-2.112202	-8.372492	0.109425
C	-3.532098	-8.357949	-0.438671
C	-4.312282	-7.159267	0.081089
C	-3.545145	-5.870904	0.040999
C	-3.494754	-3.472964	0.152692
H	-3.978671	-2.508604	0.228026
O	1.962754	-1.692395	-1.236638
O	-0.131792	-2.388882	-1.624301
C	1.086186	-2.307230	-1.904654
C	1.525756	-2.989188	-3.165030
H	1.457513	-2.257504	-3.975118
H	0.865394	-3.820383	-3.402928
H	2.560639	-3.319718	-3.093429
O	1.875718	-1.052893	1.682695
O	0.142275	-2.463003	1.405051
C	1.074455	-1.954061	2.067622
C	1.250986	-2.415244	3.483485
H	2.274894	-2.264720	3.819752
H	0.934749	-3.450794	3.599605
H	0.596113	-1.799898	4.107054
O	-2.498259	-1.031825	-1.380954

O	-2.119530	1.152029	-1.755429
C	-2.598157	0.027194	-2.051224
C	-3.331286	-0.076639	-3.359070
H	-2.630634	-0.478020	-4.096962
H	-3.678418	0.897295	-3.698510
H	-4.158851	-0.779594	-3.280605
O	-2.196843	-1.044274	1.583389
O	-2.456843	1.161892	1.229512
C	-2.644147	0.097798	1.868089
C	-3.467655	0.165653	3.123668
H	-4.316203	-0.516281	3.047514
H	-3.814644	1.177694	3.317747
H	-2.851414	-0.182754	3.955072
O	0.272325	2.508344	-1.514974
O	1.919618	1.009423	-1.783634
C	1.186859	1.954229	-2.176056
C	1.420212	2.438346	-3.575784
H	2.447003	2.254186	-3.886755
H	1.152144	3.489275	-3.673436
H	0.758581	1.867416	-4.232985
O	0.003549	2.433105	1.460667
O	2.068092	1.626711	1.090543
C	1.234660	2.353532	1.692271
C	1.784599	3.209996	2.795423
H	2.492178	3.924160	2.367696
H	2.338459	2.584972	3.497448
H	0.990425	3.745978	3.309605
C	-4.206196	-4.650566	0.159885
C	5.966899	-1.370459	0.014887
C	-3.960431	4.896506	0.059234
H	-5.285570	-4.620220	0.255784
H	-5.043521	4.929335	0.048837
H	6.439073	-2.344948	-0.035812
H	-2.140685	-8.458468	1.201514
H	-1.573460	-9.248873	-0.258584
H	-0.413251	-7.040586	0.260204
H	-1.082472	-7.177871	-1.348838
H	-4.604121	-7.336063	1.124344
H	-5.249226	-7.034572	-0.469154
H	-4.054960	-9.276137	-0.161559
H	-3.502825	-8.332021	-1.533750
H	-4.876965	7.383128	0.376025
H	-3.735718	7.518291	1.703361
H	-3.428526	8.540270	-1.135215

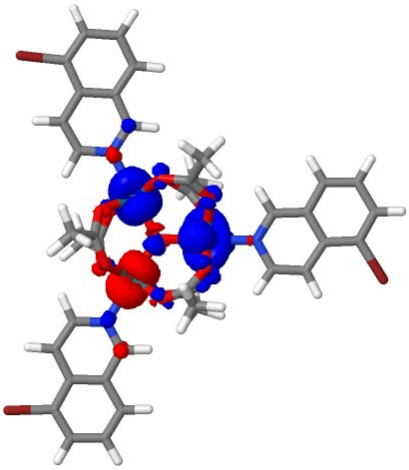
H	-3.438330	9.465399	0.344780
H	-1.166421	8.508588	-1.066376
H	-1.146925	9.298163	0.487728
H	0.030431	7.013895	0.329112
H	-1.034422	7.286270	1.694004
H	8.810790	3.102219	0.364774
H	8.377858	2.199473	-1.077630
H	6.746172	2.567707	1.471194
H	6.311985	3.100229	-0.136238
H	8.887569	1.008385	1.689474
H	8.548726	-0.520474	-0.922375
H	8.557932	-1.169890	0.695527



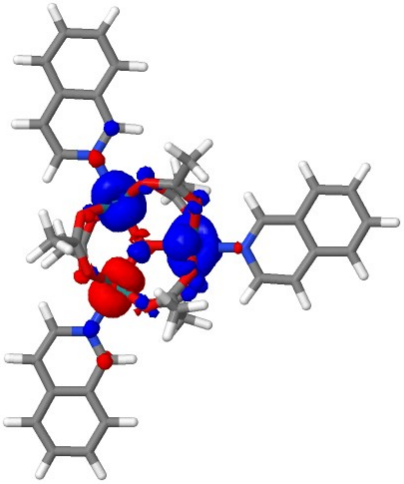
(1) qui



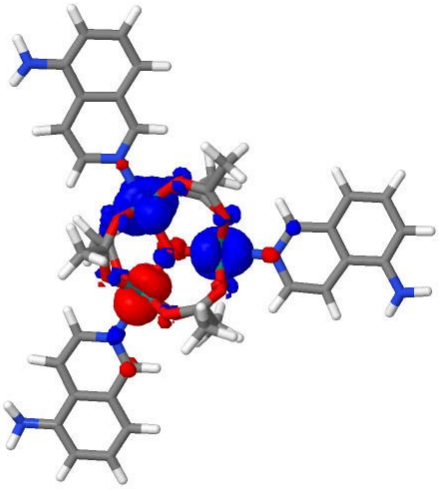
(2) nitro



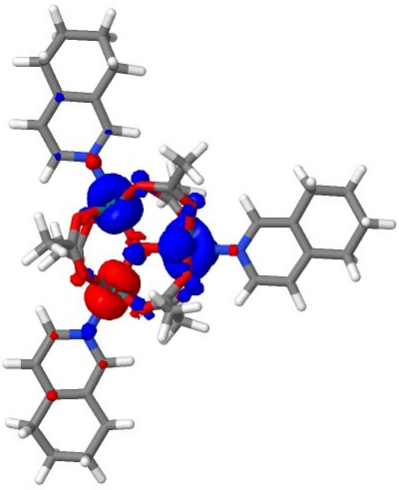
(3) briq



(4) iq

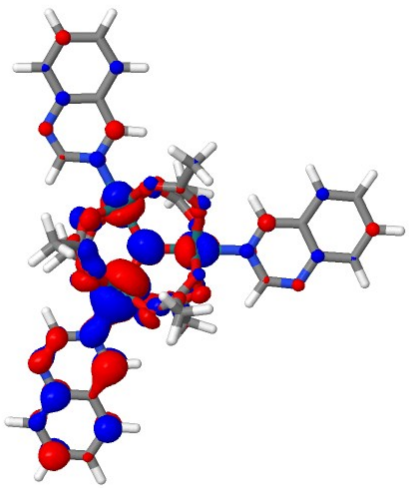


(5) amiq

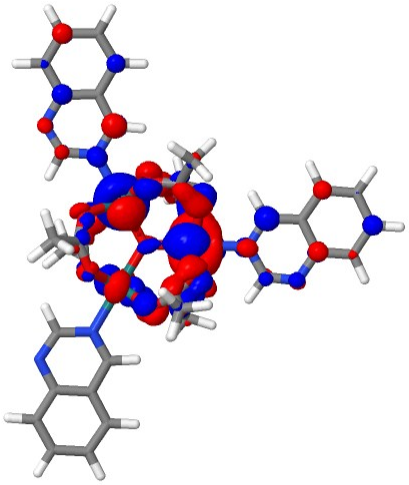


(6) thiq

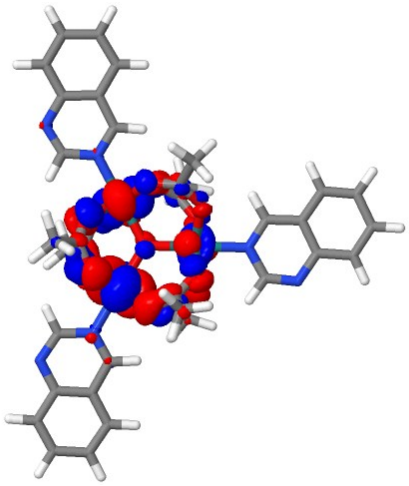
Figure S3. Plots of the spin densities calculated for all complexes obtained with DFT using PBE0/def2-TZVP. Color labels: positive (blue) and negative (red) spin densities (cutoff = 0.0025 au).



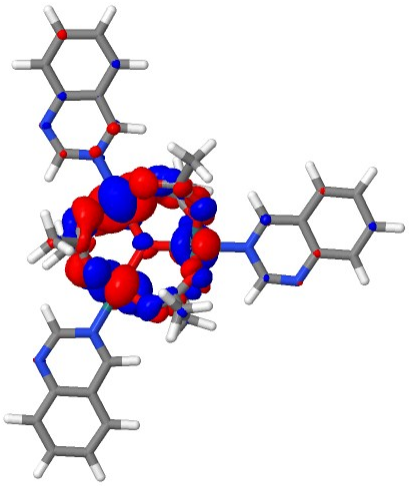
α–LUMO



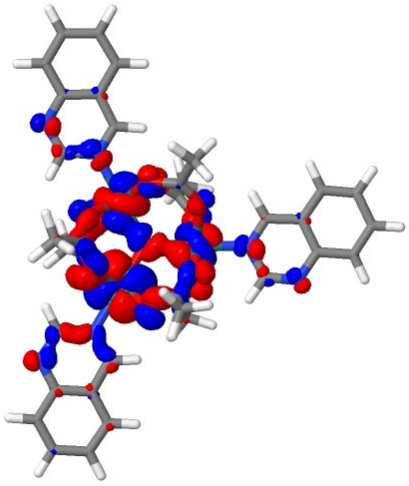
β–LUMO



α–HOMO



β–HOMO



α–HOMO-1

Figure S4. Plots of the frontier Kohn-Sham orbitals obtained with DFT using PBE0/def2-TZVP for the complex (1).

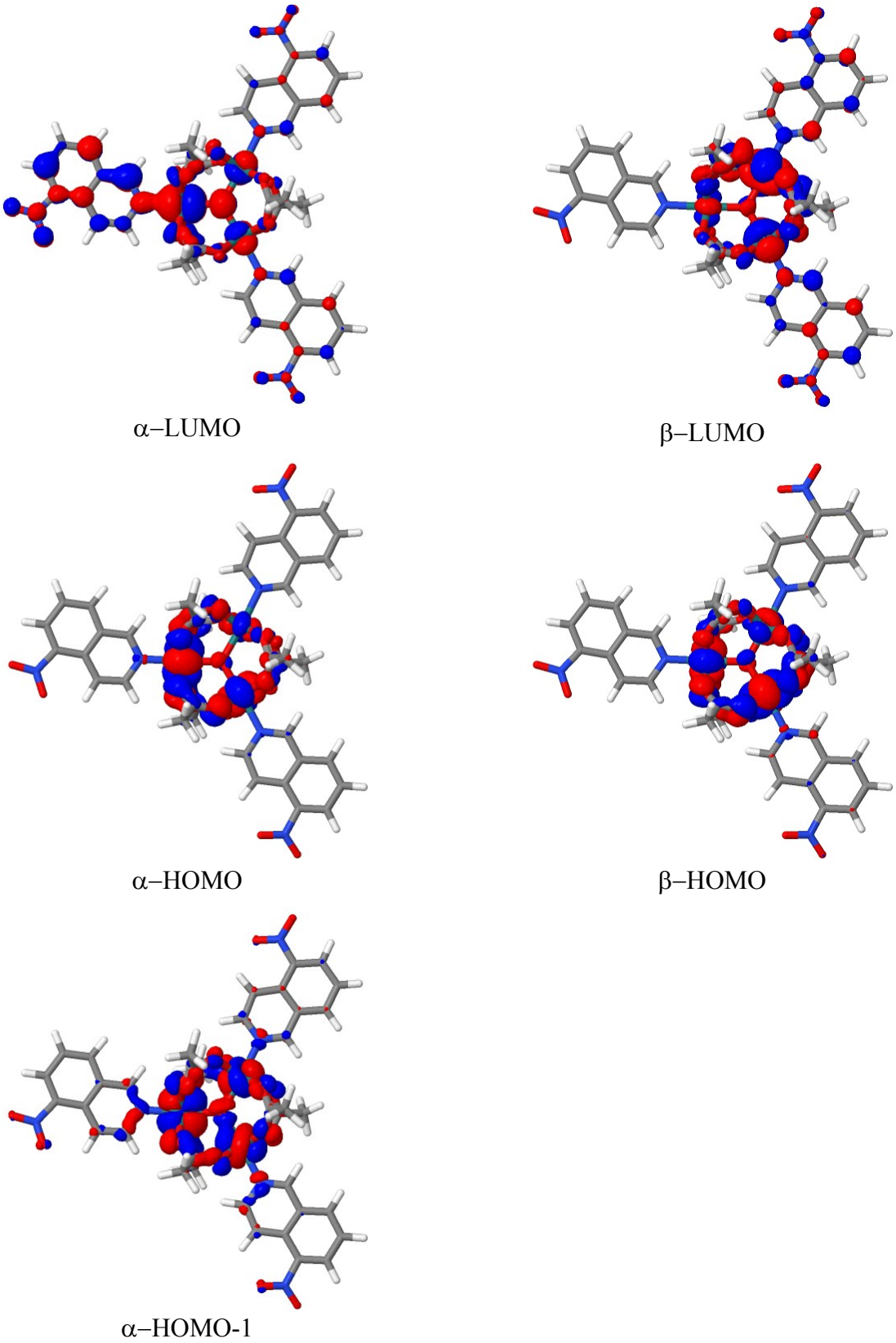
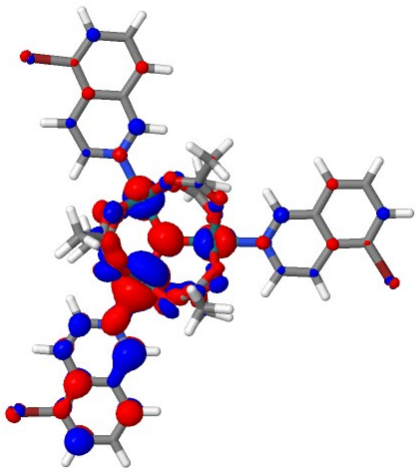
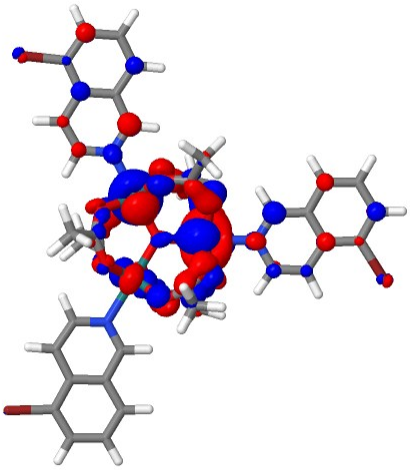


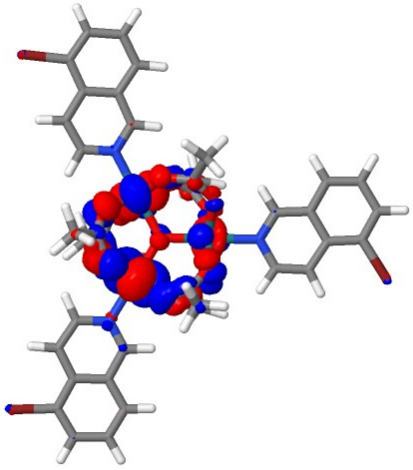
Figure S5. Plots of the frontier Kohn-Sham orbitals obtained with DFT using PBE0/def2-TZVP for the complex (2).



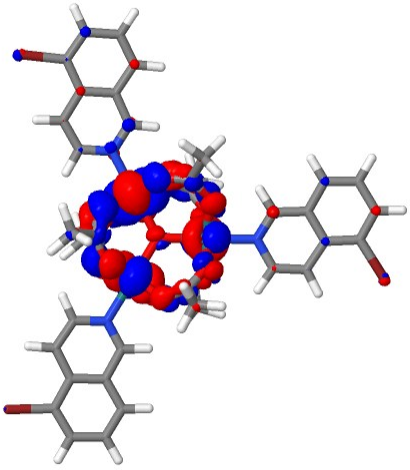
α–LUMO



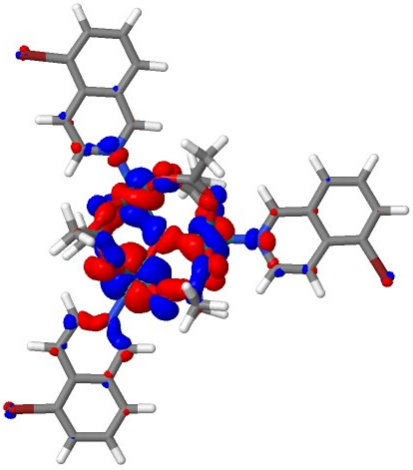
β–LUMO



α–HOMO

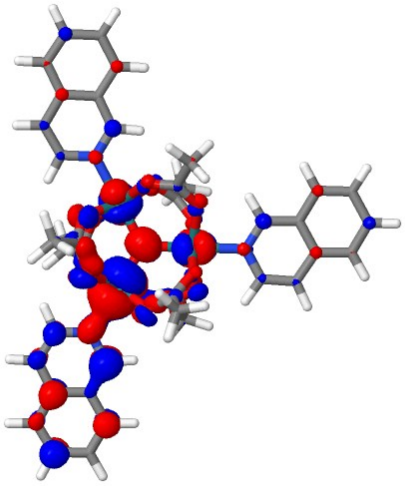


β–HOMO

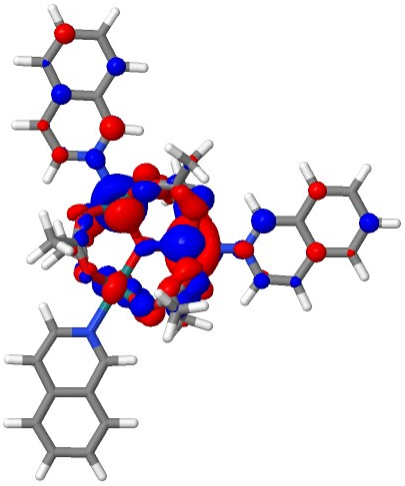


α–HOMO-1

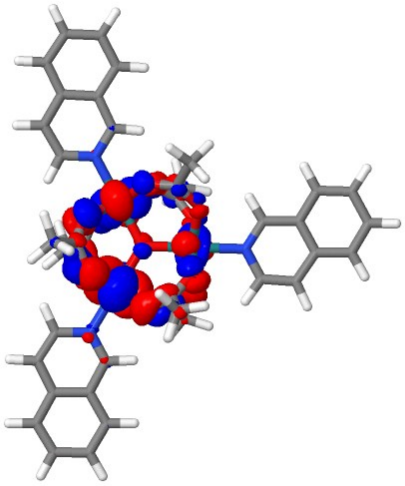
Figure S6. Plots of the frontier Kohn-Sham orbitals obtained with DFT using PBE0/def2-TZVP for the complex (3).



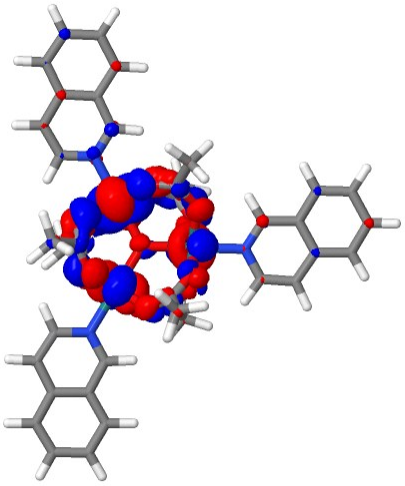
α–LUMO



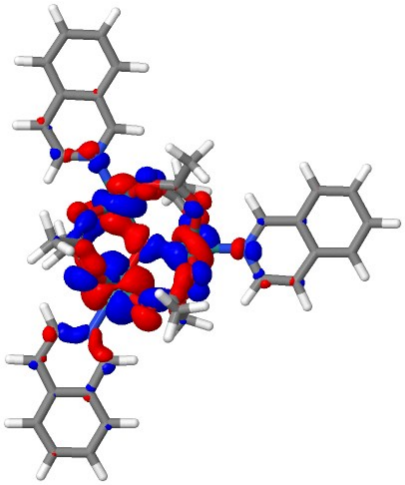
β–LUMO



α–HOMO

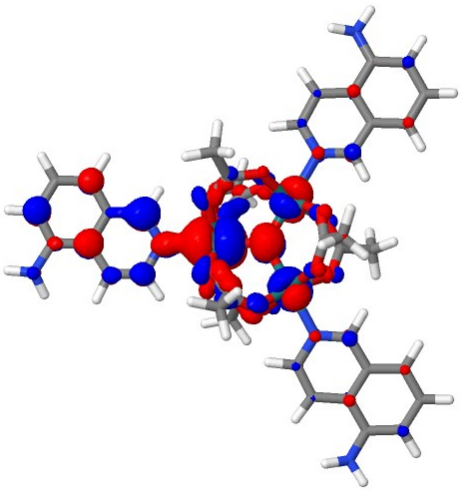


β–HOMO

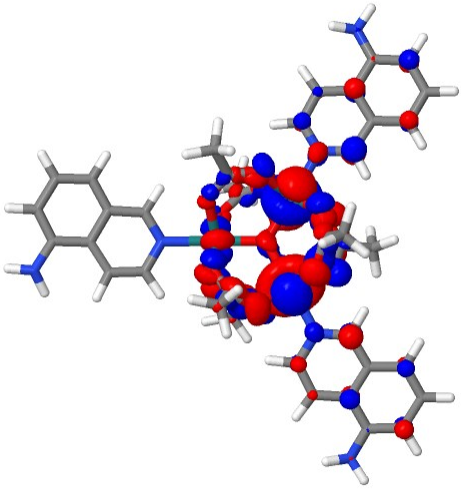


α–HOMO-1

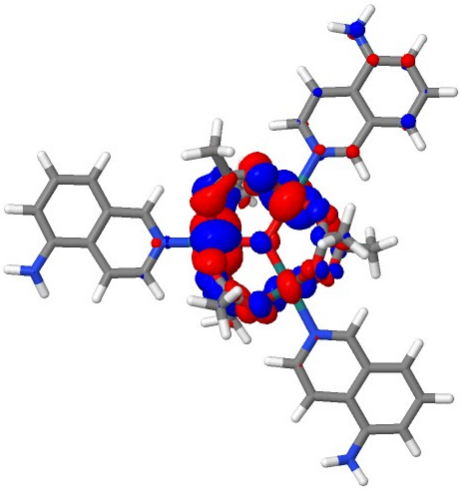
Figure S7. Plots of the frontier Kohn-Sham orbitals obtained with DFT using PBE0/def2-TZVP for the complex (4).



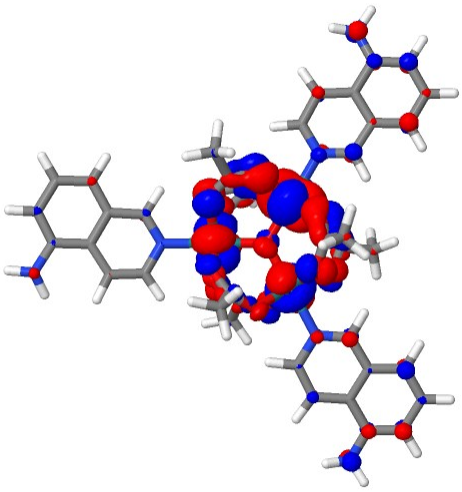
α–LUMO



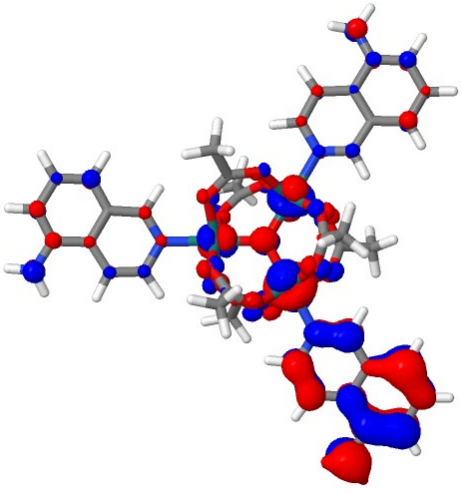
β–LUMO



α–HOMO



β–HOMO



α–HOMO-1

Figure S8. Plots of the frontier Kohn-Sham orbitals obtained with DFT using PBE0/def2-TZVP for the complex (5).

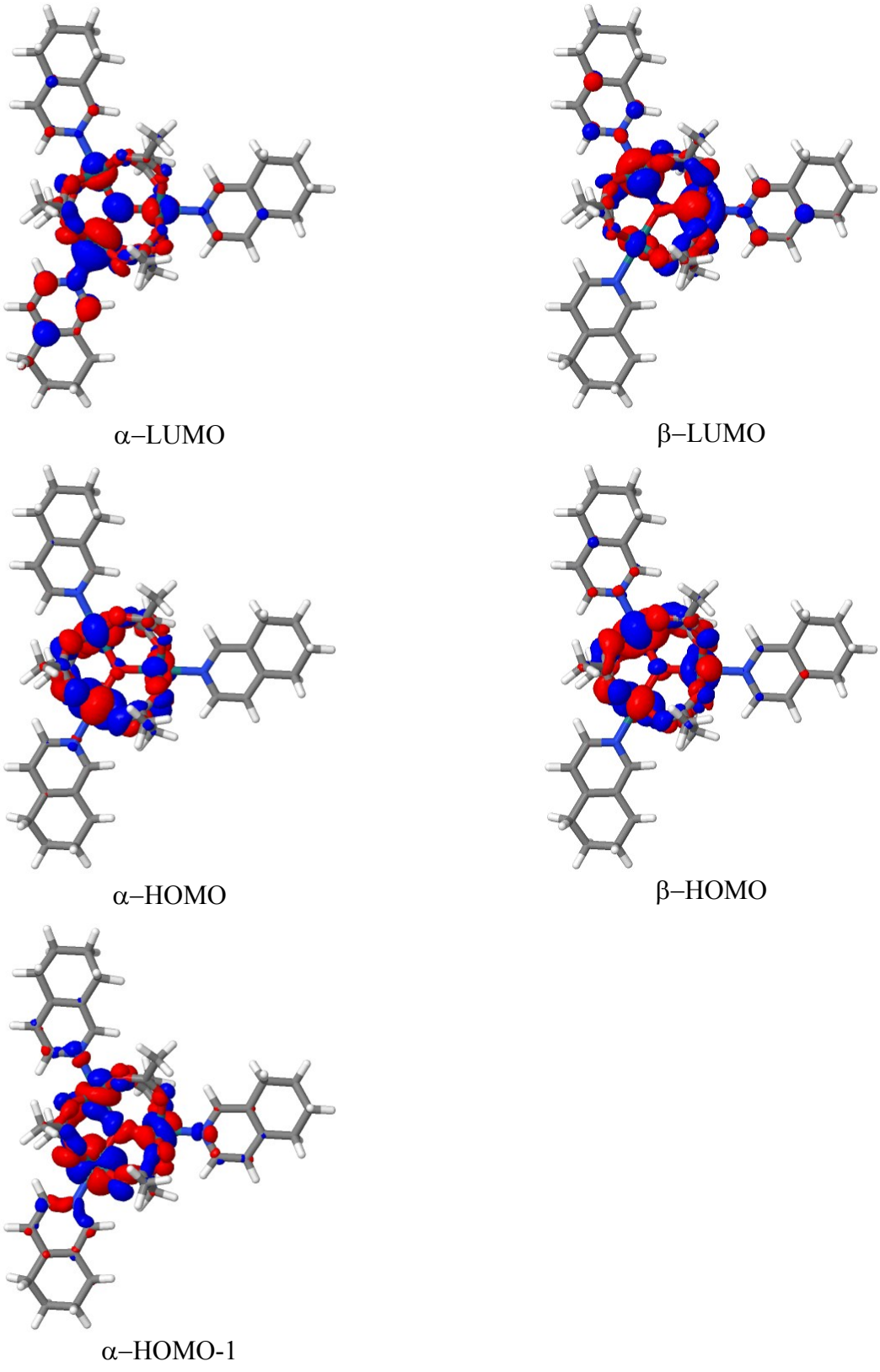


Figure S9. Plots of the frontier Kohn-Sham orbitals obtained with DFT using PBE0/def2-TZVP for the complex (6).

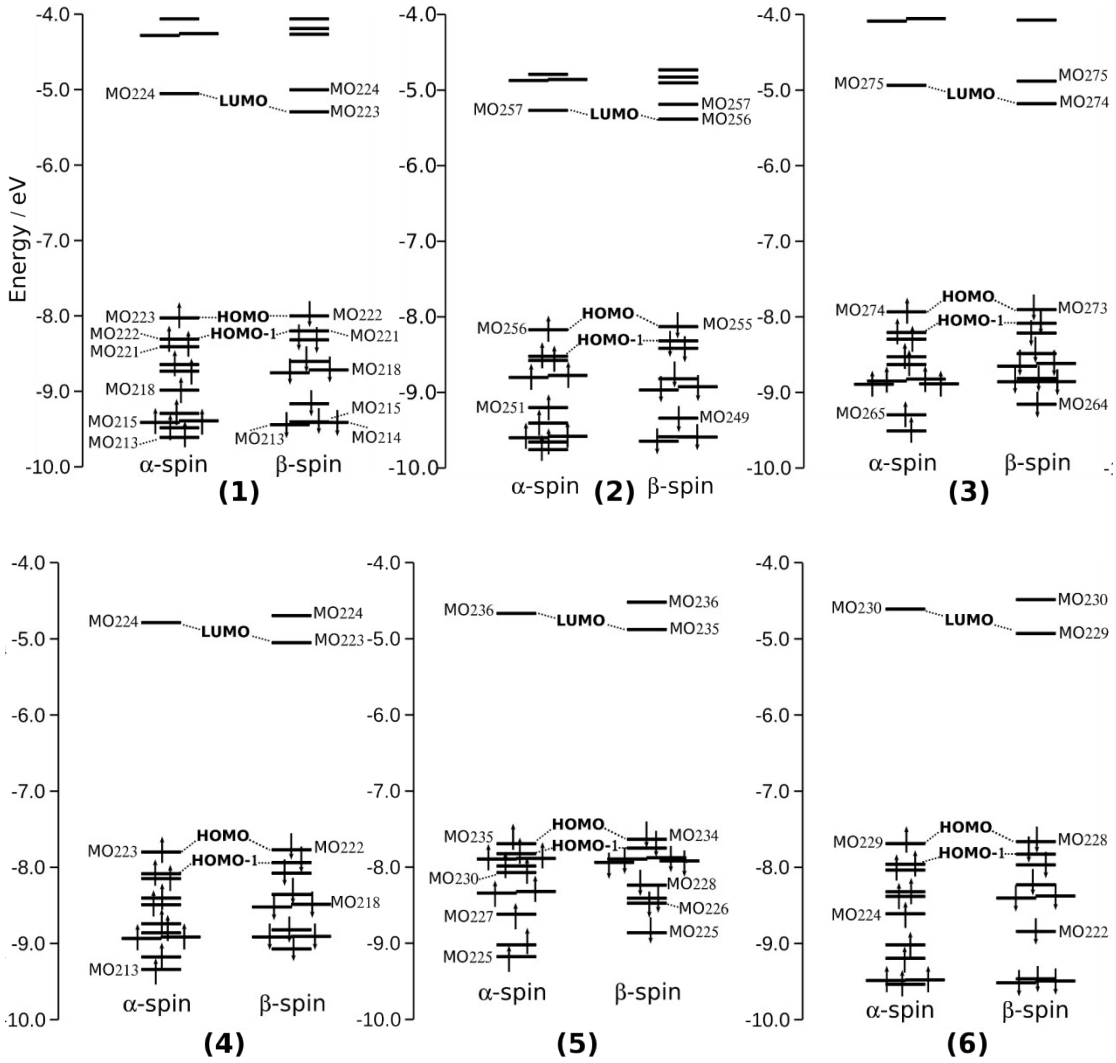


Figure S10. MO energy level obtained with DFT for complexes **(1)-(6)** using PBE0/def2-TZVP. The diagram highlights the two sets of orbitals and the numbers of the orbitals can be compared with the compositions in Tables S12-S17.

Table S12. Composition (%) of selected Kohn-Sham orbitals obtained for complex (1) with DFT using PBE0/def2-TZVP. Alpha (spin up) and beta (spin down) frontier KS orbitals are highlighted in bold.

Alpha orbitals						Beta orbitals					
Orb. Nr.	Energy (a.u.)	Oxo	Ru_3	L	OAc	Orb. Nr.	Energy (a.u.)	Oxo	Ru_3	L	OAc
213	-0.353	1.2	63.2	9.2	26.5	213	-0.347	1.3	13.3	79.6	5.9
214	-0.349	1.2	28.3	57.9	12.7	214	-0.346	0.1	0.5	98.3	1.1
215	-0.346	0.1	8.3	88.4	3.3	215	-0.346	0.2	0.9	97.8	1.2
216	-0.345	0.0	1.2	97.7	1.0	216	-0.337	4.4	59.5	18.2	18.0
217	-0.342	1.2	45.5	38.5	14.9	217	-0.322	7.1	68.0	12.7	12.3
218	-0.330	6.0	60.0	21.7	12.4	218	-0.320	4.0	71.3	6.7	18.0
219	-0.321	7.1	71.4	9.0	12.4	219	-0.316	5.7	65.7	16.8	11.7
220	-0.318	6.7	68.6	7.0	17.8	220	-0.306	2.5	77.4	6.4	13.7
221	-0.309	6.0	63.7	11.3	19.1	221	-0.301	5.3	69.6	7.9	17.3
222	-0.305	3.1	75.8	8.1	12.9	**222 HOMO**	**-0.294**	**0.5**	**72.5**	**3.2**	**23.8**
223 HOMO	**-0.295**	**0.5**	**71.2**	**4.5**	**23.8**	**223 LUMO**	**-0.195**	**0.1**	**69.0**	**14.1**	**16.8**
224 LUMO	**-0.186**	**11.8**	**55.1**	**24.8**	**8.3**	224	-0.184	12.9	49.6	27.8	9.7
225	-0.157	0.1	2.3	94.8	2.7	225	-0.157	0.1	2.3	94.3	3.3
226	-0.157	0.1	2.5	94.7	2.6	226	-0.154	0.1	7.4	89.5	2.9
227	-0.149	2.8	14.3	78.2	4.6	227	-0.149	3.8	15.7	75.3	5.1
228	-0.121	0.0	3.2	89.3	7.5	228	-0.120	0.0	1.7	93.0	5.2
229	-0.121	0.1	1.7	93.4	4.8	229	-0.120	0.1	3.0	90.9	6.1
230	-0.118	0.7	5.0	87.2	7.1	230	-0.118	0.9	4.9	88.4	5.8
231	-0.112	0.3	38.8	13.5	47.5	231	-0.106	0.2	40.4	11.7	47.7
232	-0.101	1.3	36.3	7.1	55.3	232	-0.095	0.9	34.8	5.3	59.1
233	-0.097	9.6	38.7	26.2	25.5	233	-0.090	6.3	34.7	26.1	32.9
234	-0.089	1.2	29.8	8.4	60.6	234	-0.089	4.3	33.9	11.8	50.0

Table S13. Composition (%) of selected Kohn-Sham orbitals obtained for complex (2) with DFT using PBE0/def2-TZVP. Alpha (spin up) and beta (spin down) frontier KS orbitals are highlighted in bold.

Alpha orbitals						Beta orbitals					
Orb. Nr.	Energy (a.u.)	Oxo	Ru_3	L	OAc	Orb. Nr.	Energy (a.u.)	Oxo	Ru_3	L	OAc
246	-0.359	1.0	57.6	17.6	23.8	246	-0.355	1.8	15.3	75.1	7.8
247	-0.355	1.0	21.2	66.7	11.1	247	-0.353	0.3	0.8	97.6	1.3
248	-0.353	0.2	8.2	87.9	3.7	248	-0.352	0.0	1.0	97.0	2.0
249	-0.352	0.1	1.4	96.9	1.6	249	-0.343	5.6	55.6	20.7	18.1
250	-0.346	1.6	52.1	28.3	17.9	250	-0.330	2.9	65.6	15.7	15.8
251	-0.338	6.8	70.1	9.7	13.5	251	-0.328	6.3	66.2	16.3	11.1
252	-0.324	8.7	67.5	11.3	12.5	252	-0.324	5.7	70.9	10.6	12.9
253	-0.323	4.8	67.9	9.3	18.0	253	-0.309	4.9	74.7	6.5	14.0
254	-0.315	7.4	63.5	11.3	17.8	254	-0.306	4.7	66.7	13.7	14.9
255	-0.313	1.9	71.6	13.9	12.6	**255 HOMO**	**-0.299**	**0.6**	**69.9**	**6.2**	**23.4**
256 HOMO	**-0.300**	**0.5**	**65.4**	**11.8**	**22.3**	**256 LUMO**	**-0.198**	**0.3**	**62.8**	**19.6**	**17.3**
257 LUMO	**-0.194**	**11.1**	**49.3**	**32.6**	**6.9**	257	-0.191	9.2	38.4	44.4	8.0
258	-0.179	0.0	0.6	98.9	0.5	258	-0.180	0.1	0.7	98.5	0.7
259	-0.179	0.0	0.7	98.5	0.7	259	-0.177	0.1	3.4	95.3	1.2
260	-0.176	2.4	10.9	85.0	1.6	260	-0.174	2.9	12.0	83.1	1.9
261	-0.144	0.1	2.1	93.1	4.7	261	-0.143	0.1	2.7	93.5	3.7
262	-0.143	0.1	4.5	91.5	3.7	262	-0.142	0.1	6.6	89.3	3.9
263	-0.137	2.0	11.6	80.2	6.3	263	-0.136	2.5	12.3	77.9	7.4
264	-0.124	0.0	0.4	97.6	1.9	264	-0.124	0.0	0.2	98.1	1.7
265	-0.123	0.0	1.6	95.6	2.9	265	-0.123	0.0	1.3	96.9	1.9
266	-0.121	0.0	2.7	91.9	5.4	266	-0.122	0.0	0.9	95.6	3.5
267	-0.116	0.3	37.3	15.4	47.1	267	-0.110	0.4	40.0	11.8	47.8
268	-0.105	8.1	31.6	44.1	16.2	268	-0.104	1.0	31.6	13.4	54.0
269	-0.103	0.2	30.5	21.8	47.4	269	-0.100	7.4	30.4	43.4	18.8
270	-0.095	0.3	25.0	19.6	55.0	270	-0.090	0.0	22.3	43.4	34.3

Table S14. Composition (%) of selected Kohn-Sham orbitals obtained for complex (3) with DFT using PBE0/def2-TZVP. Alpha (spin up) and beta (spin down) frontier KS orbitals are highlighted in bold.

Alpha orbitals						Beta orbitals					
Orb. Nr.	Energy (a.u.)	Oxo	Ru_3	L	OAc	Orb. Nr.	Energy (a.u.)	Oxo	Ru_3	L	OAc
264	-0.350	1.1	66.1	5.5	27.3	264	-0.337	5.0	59.4	15.7	20.0
265	-0.342	2.1	63.8	10.3	23.9	265	-0.326	0.3	4.4	93.4	1.8
266	-0.327	5.4	52.4	31.9	10.3	266	-0.326	0.0	0.8	98.0	1.2
267	-0.327	3.3	29.1	61.0	6.6	267	-0.324	0.5	12.1	83.9	3.6
268	-0.325	0.2	2.7	95.7	1.4	268	-0.318	7.5	69.0	11.9	11.6
269	-0.324	0.7	8.0	88.9	2.3	269	-0.317	3.6	68.7	10.0	17.7
270	-0.317	6.7	72.8	7.8	12.6	270	-0.312	6.5	71.0	10.3	12.1
271	-0.313	6.1	64.0	12.9	17.0	271	-0.302	2.0	77.1	7.3	13.5
272	-0.305	6.0	63.3	11.7	18.9	272	-0.297	5.2	68.4	9.3	17.2
273	-0.302	3.0	72.2	12.7	12.1	**273 HOMO**	**-0.291**	**0.4**	**66.5**	**11.5**	**21.6**
274 HOMO	**-0.292**	**0.5**	**66.7**	**10.9**	**22.0**	**274 LUMO**	**-0.190**	**0.1**	**69.2**	**14.1**	**16.5**
275 LUMO	**-0.181**	**11.9**	**55.4**	**24.3**	**8.4**	275	-0.179	13.0	49.7	27.7	9.6
276	-0.150	0.1	2.2	95.6	2.2	276	-0.150	0.1	2.1	95.3	2.5
277	-0.149	0.1	2.3	95.8	1.8	277	-0.147	0.1	6.5	91.3	2.2
278	-0.143	2.3	12.1	82.2	3.4	278	-0.143	3.1	12.9	80.3	3.8
279	-0.121	0.0	1.8	93.3	4.8	279	-0.121	0.1	1.2	93.9	4.9
280	-0.121	0.1	1.2	94.3	4.4	280	-0.120	0.1	2.1	93.1	4.8
281	-0.118	0.8	4.6	87.8	6.8	281	-0.118	1.0	5.1	88.3	5.6
282	-0.108	0.2	38.1	14.8	46.8	282	-0.101	0.2	40.4	11.1	48.3
283	-0.097	1.2	32.0	14.7	52.0	283	-0.090	1.0	32.5	9.6	56.9
284	-0.093	7.2	28.6	45.9	18.3	284	-0.087	3.3	22.8	45.9	28.0
285	-0.083	0.7	26.3	16.6	56.4	285	-0.085	4.5	26.9	33.2	35.4

Table S15. Composition (%) of selected Kohn-Sham orbitals obtained for complex (4) with DFT using PBE0/def2-TZVP. Alpha (spin up) and beta (spin down) frontier KS orbitals are highlighted in bold.

Alpha orbitals						Beta orbitals					
Orb. Nr.	Energy (a.u.)	Oxo	Ru_3	L	OAc	Orb. Nr.	Energy (a.u.)	Oxo	Ru_3	L	OAc
213	-0.343	1.2	63.6	8.5	26.7	213	-0.333	4.3	44.0	36.2	15.6
214	-0.337	2.2	58.8	17.4	21.7	214	-0.328	0.1	1.3	97.2	1.4
215	-0.328	0.7	9.0	87.2	3.1	215	-0.327	0.1	3.3	94.3	2.4
216	-0.328	0.1	1.0	97.5	1.4	216	-0.324	2.2	33.9	54.4	9.6
217	-0.326	0.6	14.1	81.0	4.3	217	-0.313	6.5	67.9	12.8	12.7
218	-0.321	7.1	69.4	9.9	13.5	218	-0.312	4.9	68.9	9.8	16.3
219	-0.312	6.8	72.3	8.1	12.8	219	-0.307	6.3	71.6	9.9	12.3
220	-0.309	6.6	66.0	10.4	17.0	220	-0.297	2.1	78.6	5.4	13.9
221	-0.299	5.8	64.1	10.7	19.4	221	-0.292	4.7	69.9	7.0	18.4
222	-0.297	2.9	73.3	11.5	12.2	**222 HOMO**	**-0.286**	**0.5**	**70.0**	**6.9**	**22.6**
223 HOMO	**-0.287**	**0.4**	**69.3**	**7.3**	**22.9**	**223 LUMO**	**-0.186**	**0.1**	**70.2**	**13.6**	**16.2**
224 LUMO	**-0.176**	**12.2**	**57.5**	**21.8**	**8.5**	224	-0.173	13.1	50.6	26.5	9.8
225	-0.141	0.1	2.3	94.9	2.6	225	-0.141	0.1	2.3	94.5	3.0
226	-0.140	0.1	2.5	95.4	2.0	226	-0.137	0.0	6.7	90.9	2.4
227	-0.134	2.1	11.4	82.6	3.9	227	-0.134	3.0	12.7	80.0	4.3
228	-0.112	0.0	2.9	89.8	7.2	228	-0.112	0.1	1.4	92.1	6.3
229	-0.111	0.1	1.6	93.6	4.7	229	-0.110	0.0	2.7	91.8	5.4
230	-0.109	0.6	4.6	86.8	8.1	230	-0.109	0.8	4.5	88.6	6.1
231	-0.103	0.3	37.8	15.6	46.4	231	-0.097	0.3	39.5	12.1	48.1
232	-0.092	1.2	33.7	9.7	55.4	232	-0.086	1.0	32.0	10.2	57.0
233	-0.088	8.4	35.3	32.0	24.2	233	-0.082	6.0	29.6	37.3	27.1
234	-0.081	1.3	27.2	15.4	56.1	234	-0.081	3.0	31.0	15.1	50.9

Table S16. Composition (%) of selected Kohn-Sham orbitals obtained for complex (5) with DFT using PBE0/def2-TZVP. Alpha (spin up) and beta (spin down) frontier KS orbitals are highlighted in bold.

Alpha orbitals						Beta orbitals					
Orb. Nr.	Energy (a.u.)	Oxo	Ru_3	L	OAc	Orb. Nr.	Energy (a.u.)	Oxo	Ru_3	L	OAc
225	-0.337	1.0	63.2	9.8	26.0	225	-0.326	6.3	62.9	10.7	20.2
226	-0.332	2.5	66.0	8.6	22.9	226	-0.311	2.9	71.2	7.8	18.1
227	-0.317	6.2	58.6	24.3	10.8	227	-0.309	7.5	65.8	16.7	10.0
228	-0.307	5.0	60.6	22.6	11.8	228	-0.303	5.5	59.6	24.6	10.2
229	-0.306	9.7	61.3	15.4	13.6	229	-0.292	2.6	41.6	46.1	9.7
230	-0.297	3.1	57.4	19.4	20.1	230	-0.291	0.8	32.5	60.1	6.6
231	-0.294	2.7	77.2	7.3	12.7	231	-0.290	0.3	10.4	87.1	2.2
232	-0.290	0.1	2.4	96.5	1.0	232	-0.290	0.6	18.0	77.4	3.9
233	-0.290	0.3	0.9	98.2	0.6	233	-0.285	2.9	42.7	42.5	11.8
234	-0.288	1.1	7.6	89.1	2.2	**234 HOMO**	**-0.281**	**0.6**	**56.8**	**24.3**	**18.3**
235 HOMO	**-0.283**	**0.5**	**57.2**	**23.6**	**18.7**	**235 LUMO**	**-0.179**	**0.3**	**68.2**	**15.4**	**16.1**
236 LUMO	**-0.172**	**12.8**	**58.6**	**20.3**	**8.4**	236	-0.166	12.9	52.8	24.0	10.3
237	-0.131	0.1	2.9	95.2	1.9	237	-0.131	0.1	2.7	94.6	2.5
238	-0.129	0.1	4.1	93.0	2.8	238	-0.127	0.0	7.8	89.9	2.3
239	-0.124	1.4	9.4	86.8	2.5	239	-0.124	1.8	9.8	85.7	2.8
240	-0.105	0.0	1.0	94.8	4.1	240	-0.105	0.1	0.9	95.9	3.2
241	-0.103	0.1	1.4	95.1	3.3	241	-0.103	0.1	1.7	94.8	3.5
242	-0.103	0.3	3.4	90.7	5.4	242	-0.102	0.5	2.4	92.1	4.9
243	-0.096	0.3	37.5	17.3	45.0	243	-0.092	0.2	38.6	12.8	48.4
244	-0.086	7.2	25.8	56.3	10.8	244	-0.082	2.9	28.7	34.0	34.4
245	-0.084	0.2	29.0	18.4	52.4	245	-0.079	4.8	24.8	46.8	23.6
246	-0.075	0.3	30.7	6.1	62.9	246	-0.072	0.1	24.2	26.7	49.1

Table S17. Composition (%) of selected Kohn-Sham orbitals obtained for complex (6) with DFT using PBE0/def2-TZVP. Alpha (spin up) and beta (spin down) frontier KS orbitals are highlighted in bold.

Alpha orbitals						Beta orbitals					
Orb. Nr.	Energy (a.u.)	Oxo	Ru_3	L	OAc	Orb. Nr.	Energy (a.u.)	Oxo	Ru_3	L	OAc
219	-0.350	0.1	3.4	93.0	3.5	219	-0.350	0.2	0.8	96.7	2.2
220	-0.349	0.0	0.9	96.4	2.7	220	-0.349	0.0	0.4	96.1	3.5
221	-0.348	0.1	1.1	95.6	3.2	221	-0.348	0.1	0.6	97.2	2.1
222	-0.338	1.2	63.6	9.0	26.3	222	-0.325	5.5	66.1	8.7	19.7
223	-0.331	2.2	66.9	8.3	22.7	223	-0.309	5.4	72.4	5.9	16.3
224	-0.316	7.4	70.7	8.3	13.6	224	-0.308	7.0	71.6	7.4	14.0
225	-0.308	6.9	72.8	7.3	13.0	225	-0.302	6.5	73.2	7.9	12.4
226	-0.306	7.9	69.5	6.1	16.6	226	-0.293	1.9	78.8	5.0	14.3
227	-0.295	5.1	68.7	4.4	21.8	227	-0.288	4.0	72.0	4.4	19.6
228	-0.293	3.2	77.4	6.6	12.9	**228 HOMO**	**-0.282**	**0.6**	**72.5**	**3.5**	**23.3**
229 HOMO	**-0.283**	**0.4**	**72.5**	**3.2**	**23.9**	**229 LUMO**	**-0.181**	**0.1**	**71.9**	**12.2**	**15.9**
230 LUMO	**-0.169**	**12.6**	**60.2**	**18.5**	**8.8**	230	-0.165	14.3	54.7	20.6	10.4
231	-0.114	0.2	3.6	91.2	5.0	231	-0.114	0.1	3.8	89.0	7.1
232	-0.113	0.1	5.9	90.1	4.0	232	-0.110	0.1	7.8	88.1	4.0
233	-0.107	1.0	8.2	80.6	10.2	233	-0.106	1.5	9.1	81.5	7.9
234	-0.101	0.2	32.8	24.4	42.6	234	-0.096	0.1	20.8	49.7	29.4
235	-0.093	0.1	3.1	89.0	7.9	235	-0.094	0.1	4.7	86.5	8.7
236	-0.093	0.1	2.9	86.3	10.7	236	-0.092	0.1	4.0	86.0	9.9
237	-0.091	0.2	5.4	85.6	8.9	237	-0.090	0.2	14.7	65.1	20.0
238	-0.088	1.2	33.5	9.0	56.3	238	-0.081	1.0	31.4	7.8	59.8
239	-0.084	8.2	35.2	33.7	22.9	239	-0.078	5.7	30.1	31.1	33.1
240	-0.077	1.4	30.1	6.8	61.8	240	-0.077	3.7	32.7	15.3	48.3

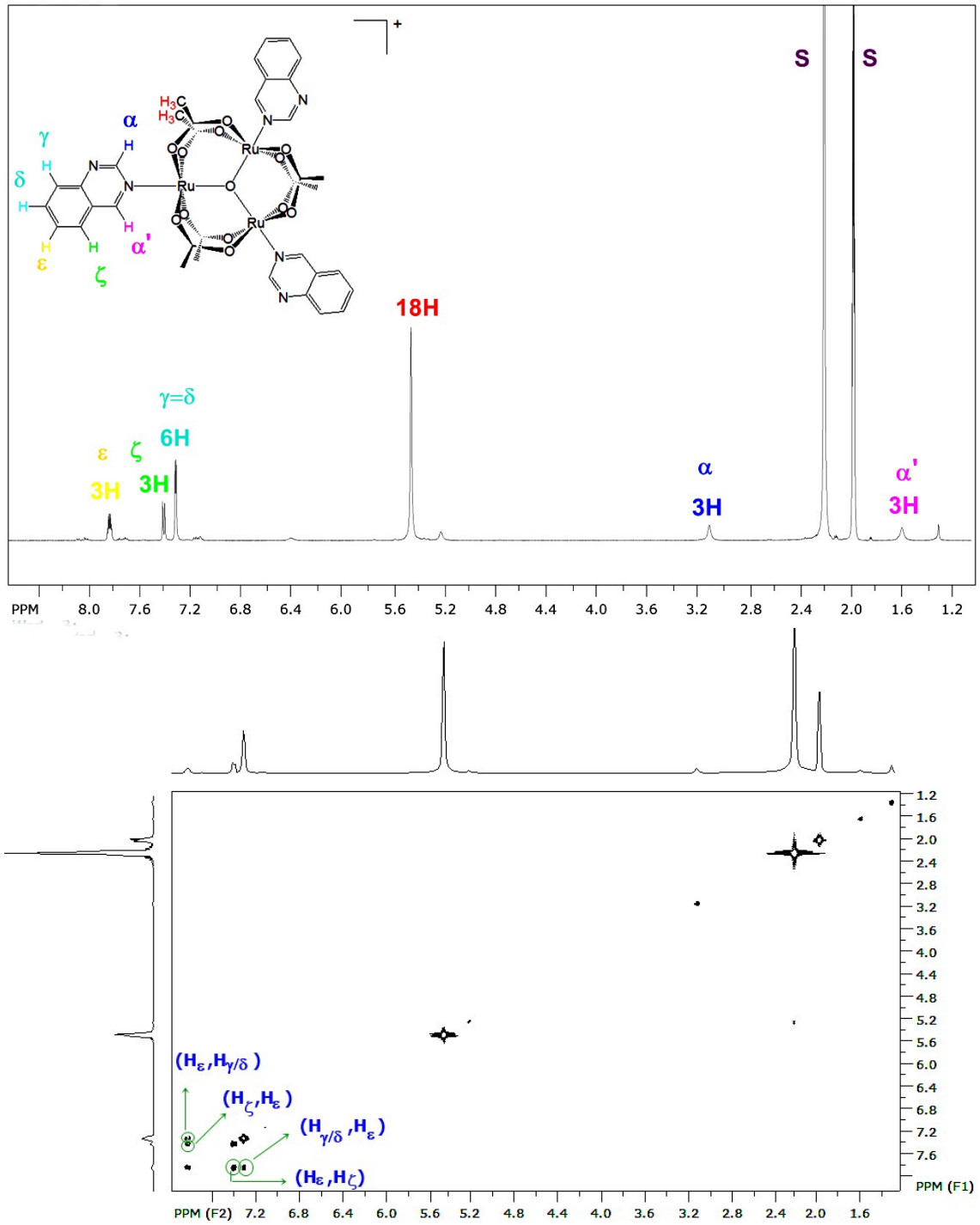


Figure S11. ^{1}H-NMR and COSY spectra of complex **1**, obtained from 10 mM acetonitrile-d_3 solution.

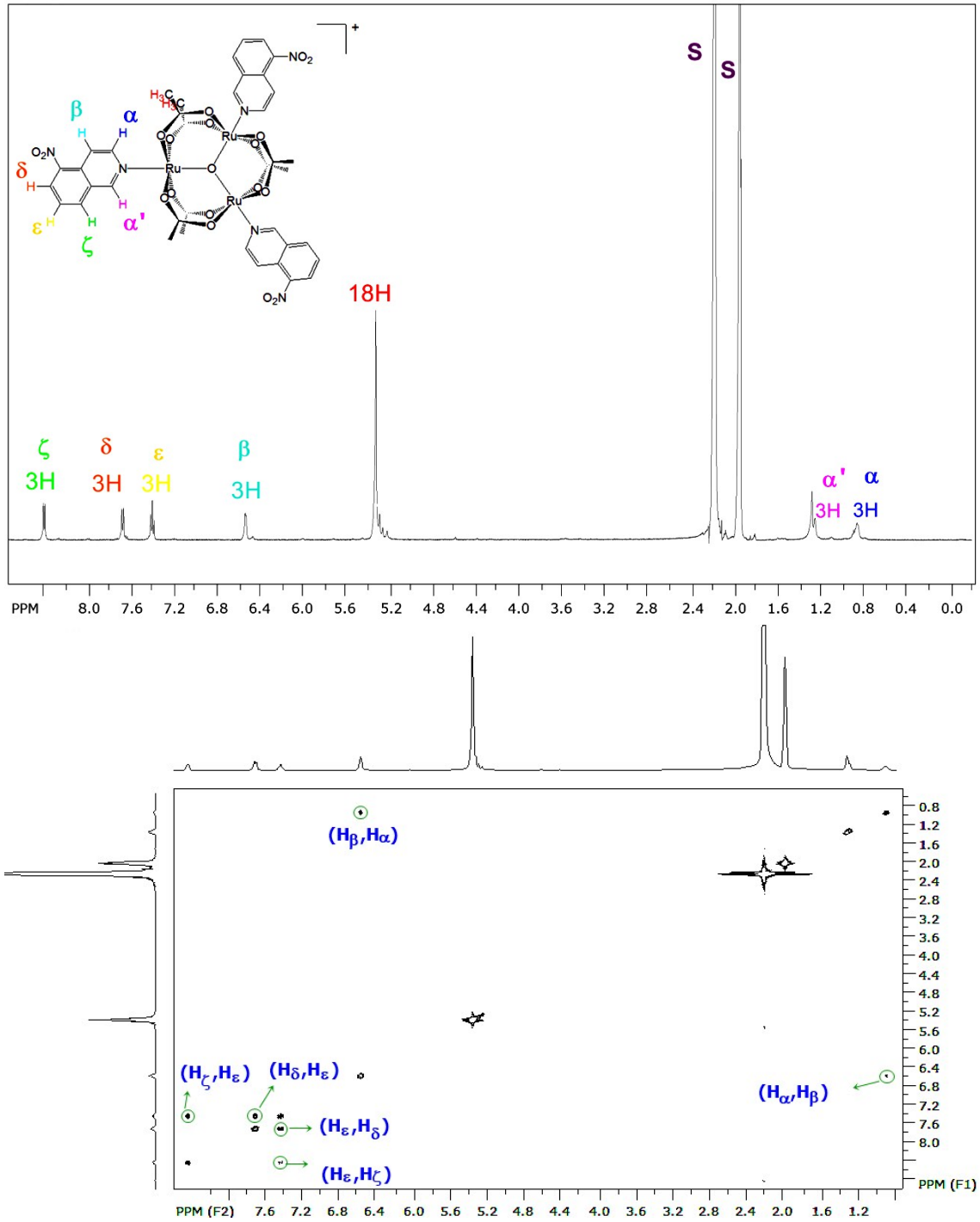


Figure S12. ^{1}H-NMR and COSY spectra of complex **2**, obtained from a 1 mM acetonitrile-d_3 solution.

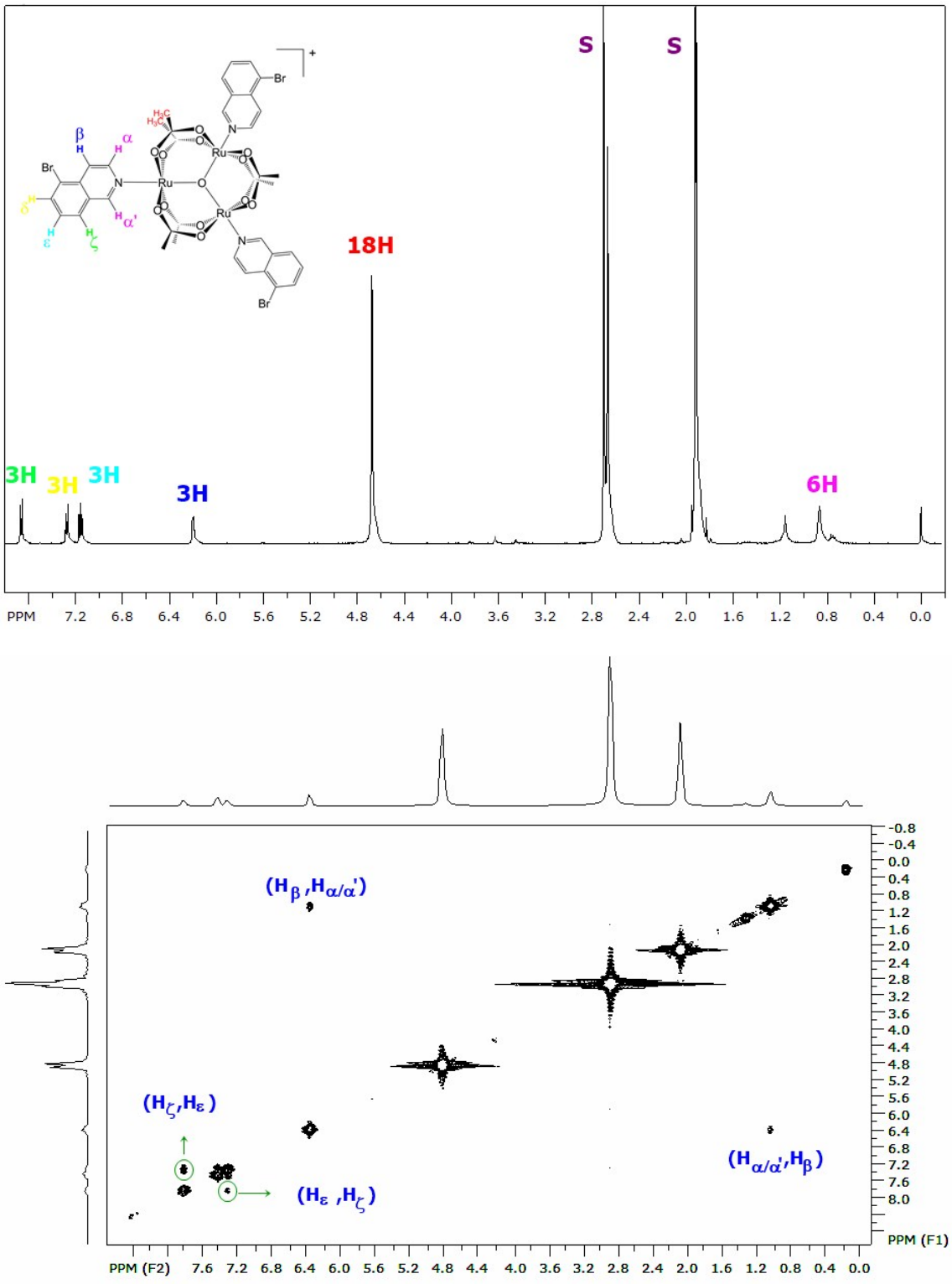


Figure S13. [1]H-NMR and COSY spectra of complex **3** obtained from a 10 mM chloroform-d solution.

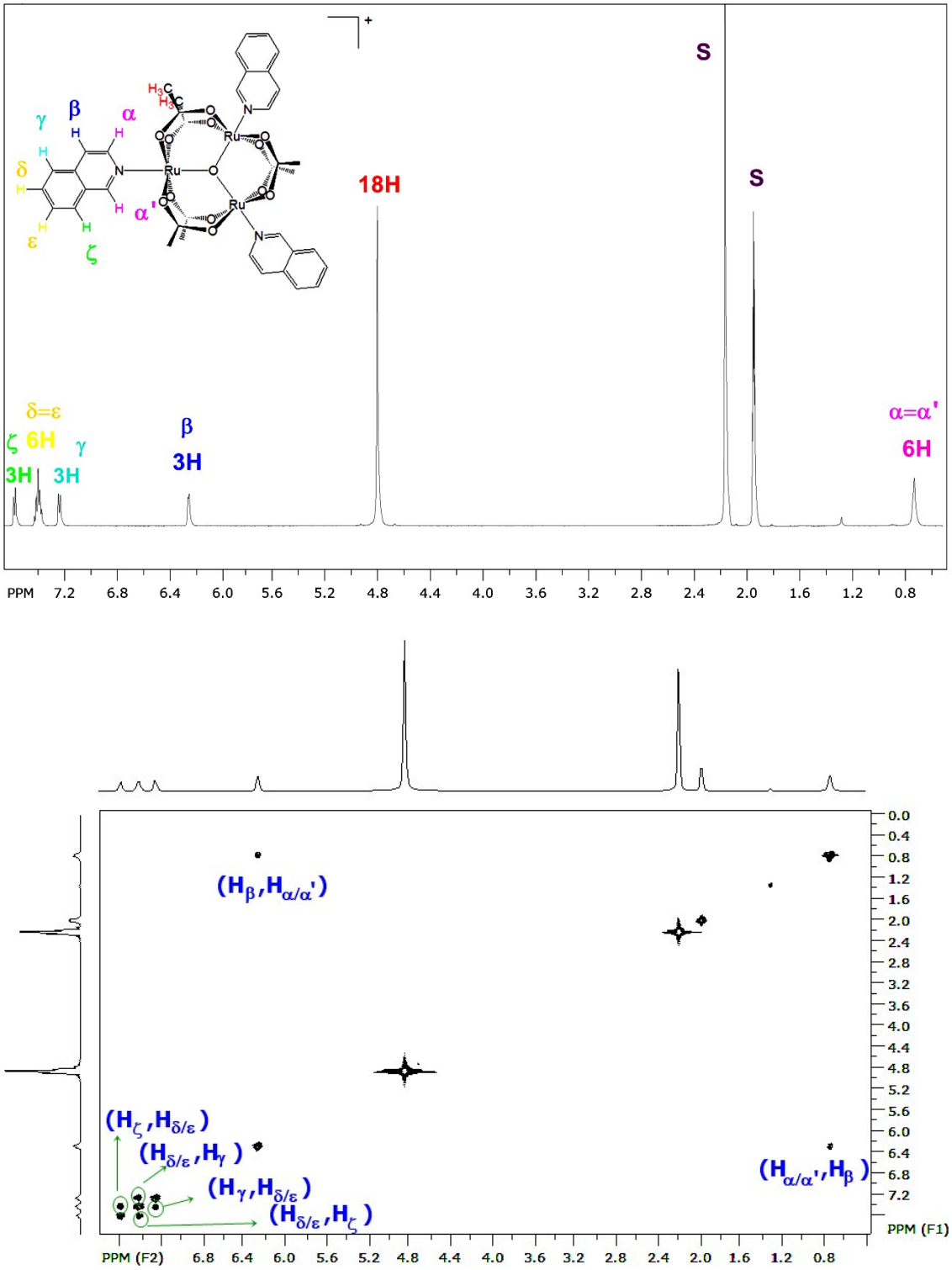


Figure S14. ^{1}H-NMR and COSY spectra of complex **4**, obtained from a 10 mM acetonitrile-d_3 solution.

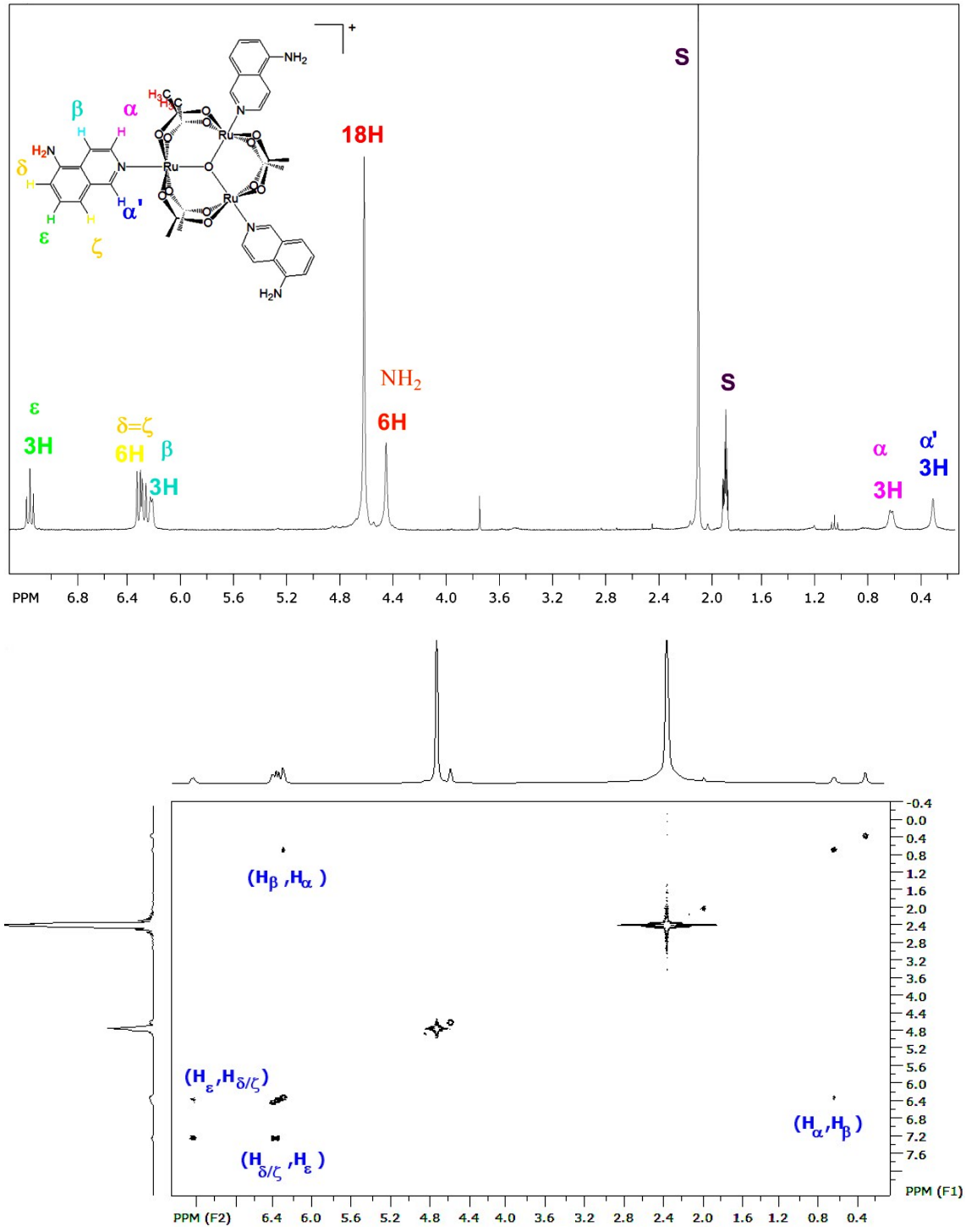


Figure S15. ^{1}H-NMR and COSY spectra of complex **5**, obtained from a 10 mM acetonitrile-d_3 solution.

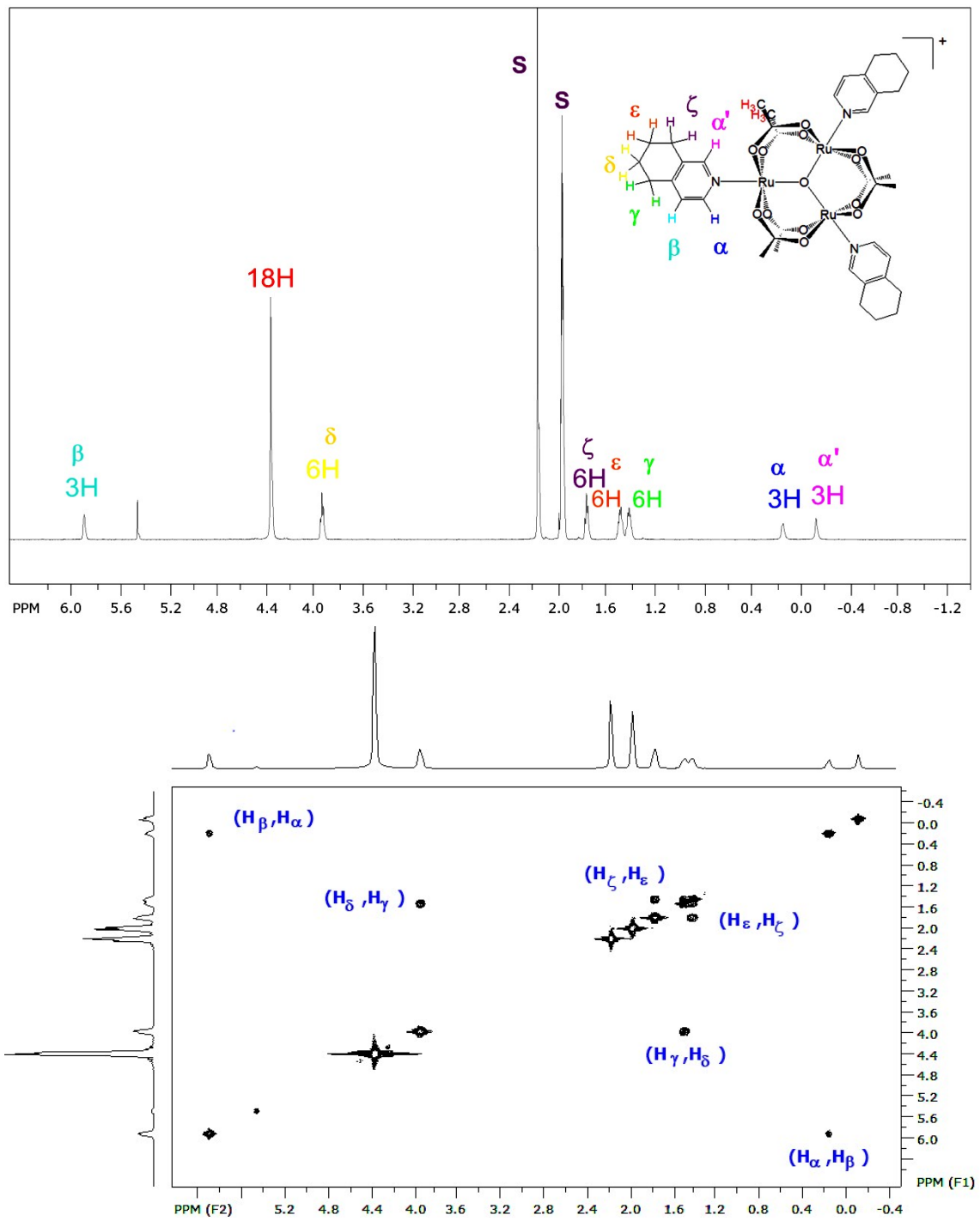


Figure S16. ^{1}H-NMR and COSY spectra of complex **6**, obtained from a 10 mM acetonitrile-d_3 solution.

Table S18. ^{1}H NMR chemical shifts (δ) and Δδ observed for free ligands **1-6**. Data collected from Aldrich Library of ^{13}C and ^{1}H FT-NMR Spectra

δ (ppm) (free ligands)						
Hydrogen	**1**, qui	**2,** 5-nitro	**3**, 5-briq*	**4**, iq	**5**, 5-amino	**6**, THIQ
α'	9.40	9.50	9.37	9.22	9.25	8.25
α	9.35	8.75	8.66	8.48	8.40	α=α'
β	-	8.55	7.91	7.60	8.05	6.93
γ	8.05	-	-	7.90	-	2.76
δ	7.90	8.65	8.19	7.54	6.95	1.79
ε	7.50	7.85	7.62	7.64	7.40	ε=δ
ζ	δ= ζ	8.40	8.15	7.76	7.35	ζ= γ
NH_2	-	-	-	-	6.05	-
Δδ (ppm)						
Hydrogen	**1**, qui	**2,** 5-nitro	**3**, 5-briq*	**4**, iq	**5**, 5-amino	**6**, THIQ
α	6.28	7.9	7.69	7.76	7.79	8.28
α'	7.85	8.26	8.40	8.5	8.94	8.41
β	-	2.01	1.59	1.34	1.82	1.04
γ	0.76	-	-	0.65	-	1.37
δ	0.61	1.05	0.78	0.15	0.63	-2.14
ε	0.11	0.44	0.34	0.25	0.23	0.33
ζ	0.09	-0.02	0.36	0.19	1.03	1.02
NH_2	-	-	-	-	1.6	-

UV-vis absorption spectroscopy

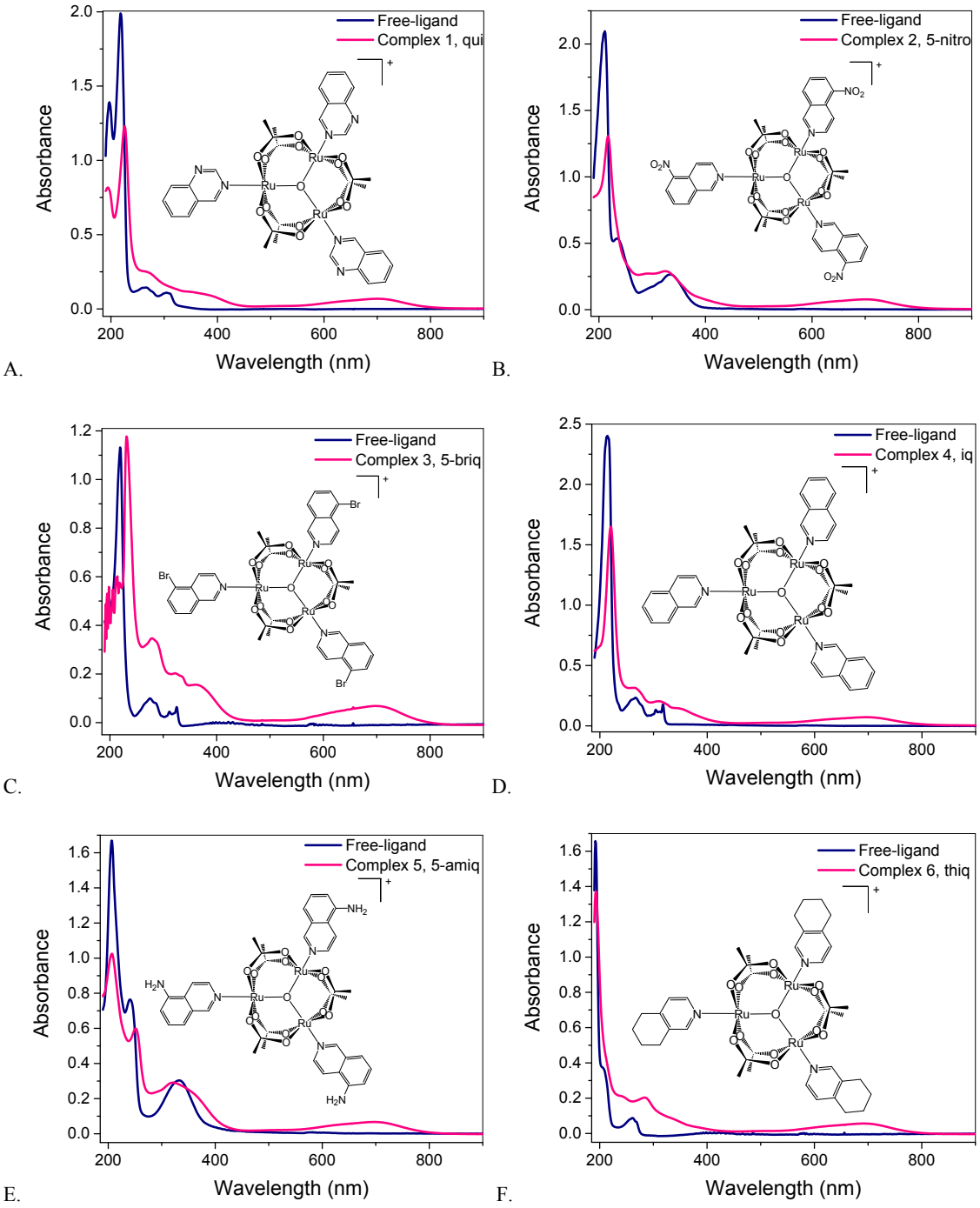
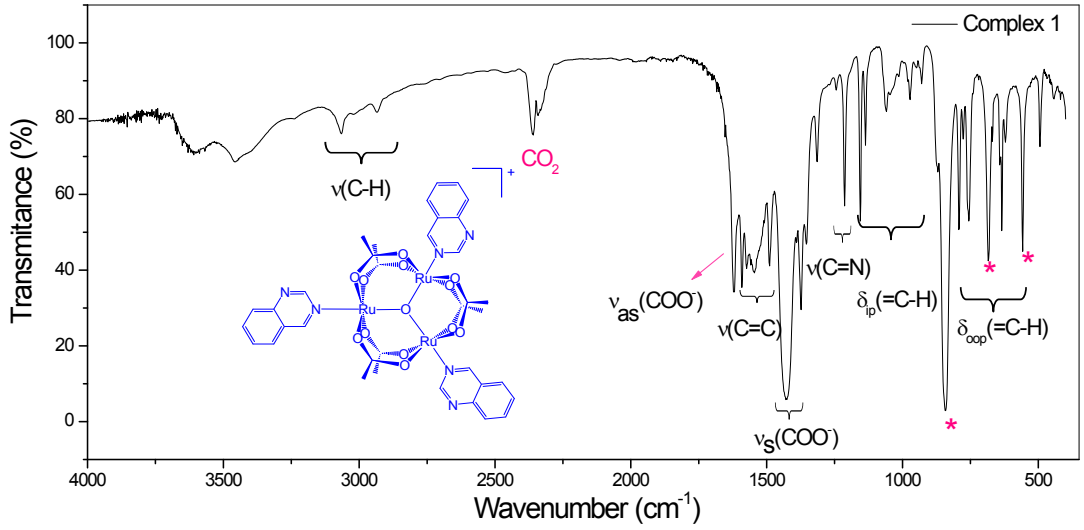
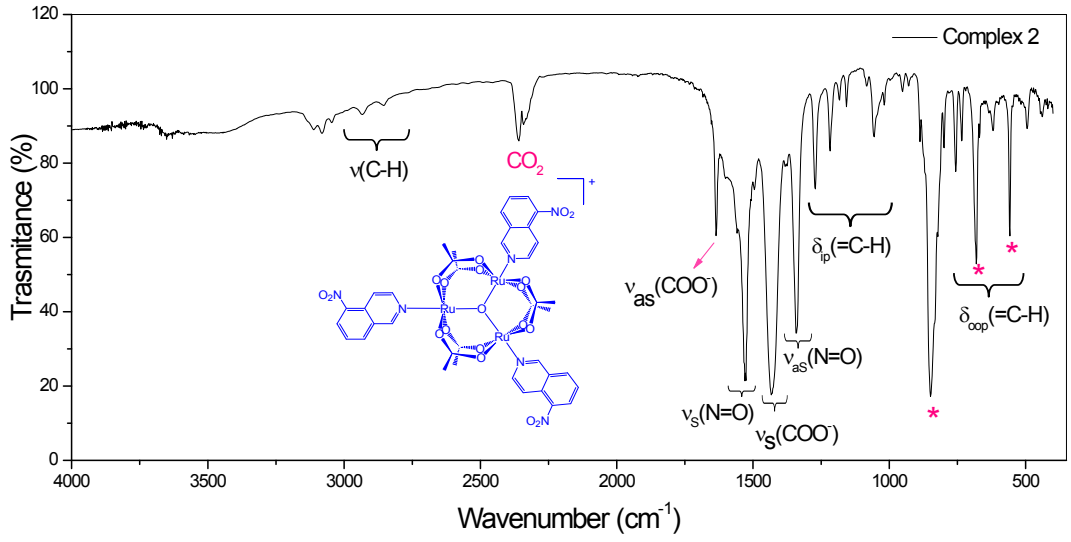


Figure S17 A-F. Absorption spectra complexes **1-6** ($1x10^{-5}$ mol L^{-1}) and the respective free ligands ($5x10^{-5}$ mol L^{-1}), collected from acetonitrile solutions.

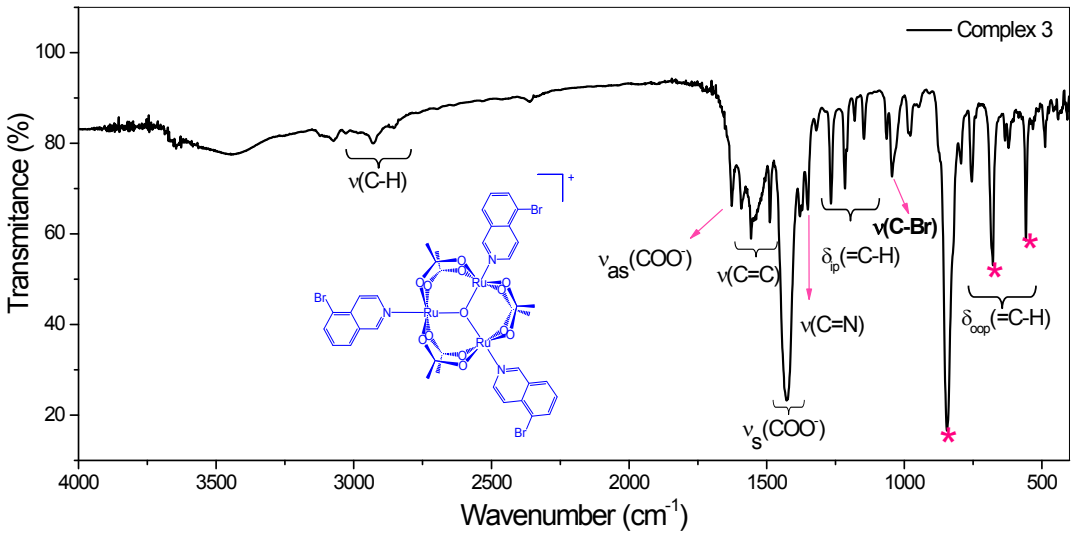
Infrared vibrational spectroscopy



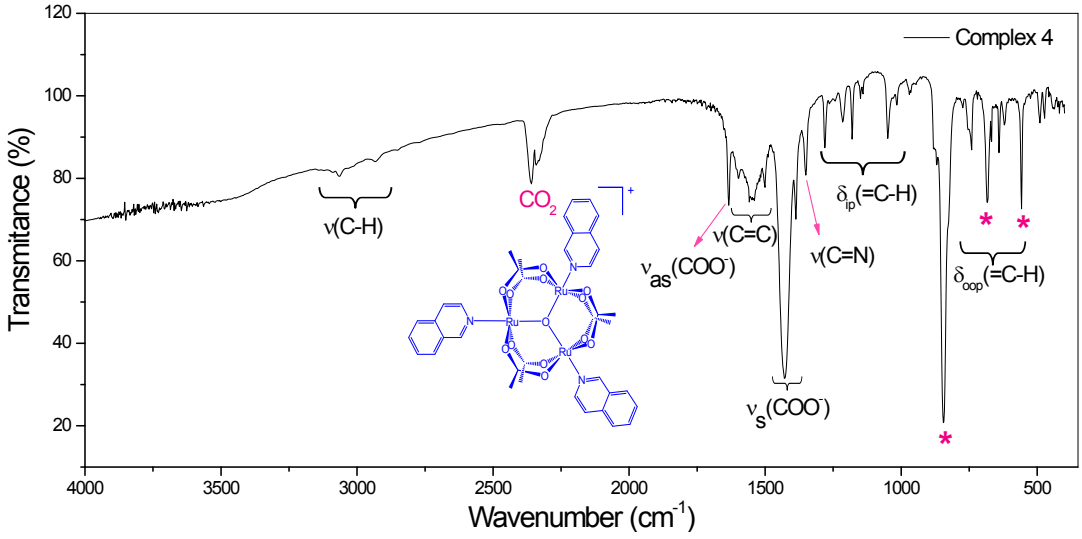
A.



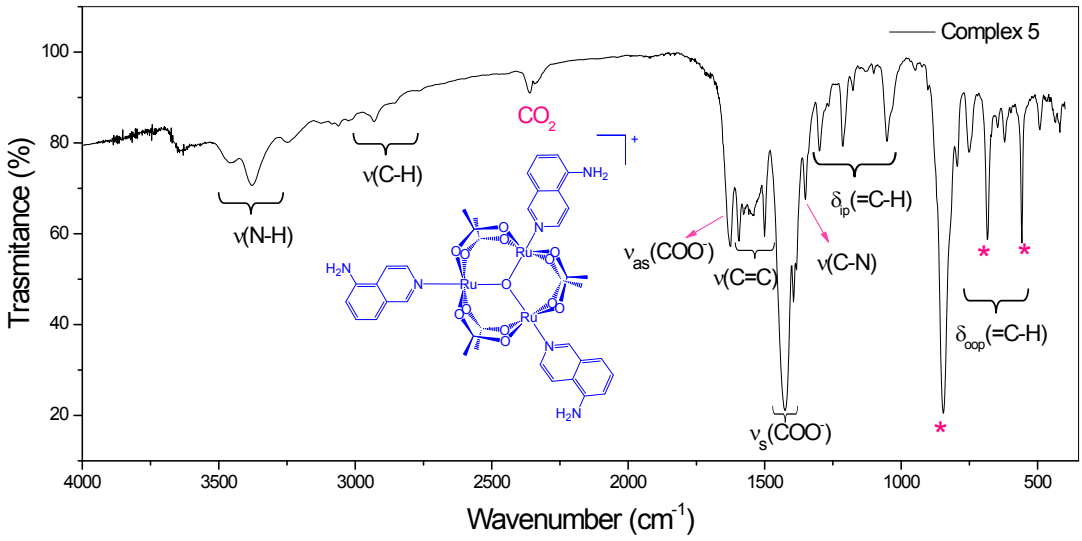
B.



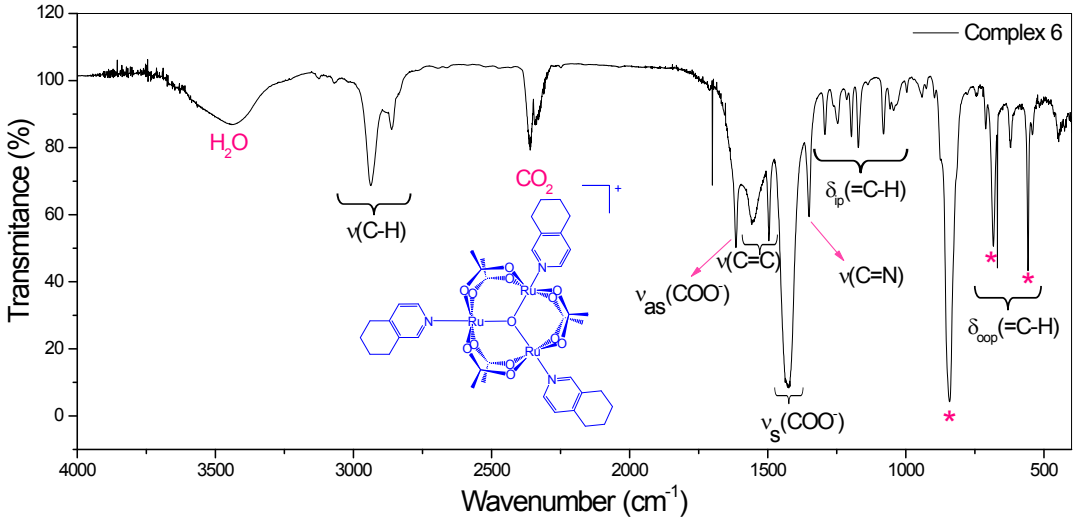
C.



D.



E.



F.

Figure S18 A-F. Infrared spectra of complexes **1 - 6** recorded from KBr pellets (the bands marked by * correspond to PF_6^- vibrations).

Table S19. Tentative assignment of the main vibrational transitions observed in the IR spectra of complexes **1** to **6**, collected from KBr pellets.

Complex	Wavenumber (cm^{-1})	Assignment
(**1**), qui	1591m, 1556br and 1489m	ν(C=C) aromatic ring
	1620m	$\nu_{as}(COO^-)$ from bridged acetate
	1427s	ν(COO) from μ-acetate bridge
	1216m	ν(C=N) fused aromatic ring
	790w, 752w, 685w, 635w	δ_{oop}(=C-H) aromatic ring
(**2**), 5-nitro	1635m	$\nu_{as}(COO^-)$ from bridged acetate
	1527s and 1341s	ν_s(N=O) and ν_{as}(N=O)
	1429s	ν_s(COO) from μ-acetate bridge
	1271w, 1217w, 1182w	δ_{ip}(=C-H) aromatic ring
	756w, 680w	δ_{oop}(=C-H) aromatic ring
(**3**), 5-briq	1592m, 1556br and 1488m	ν(C=C) aromatic ring
	1628m	$\nu_{as}(COO^-)$ from bridged acetate
	1427s	ν(COO) from μ-acetate bridge
	1266m, 1215m, 1146w	δ_{ip}(=C-H) aromatic ring
	1044m	ν(C-Br) linked to aromatic ring
	758w, 620w, 487w	δ_{oop}(=C-H) aromatic ring
(**4**), iq	1598m, 1556br and 1501m	ν(C=C) aromatic ring
	1633m	$\nu_{as}(COO^-)$ from bridged acetate
	1427s	ν_s(COO) from μ-acetate bridge
	1274w, 1215w, 1180w	δ_{ip}(=C-H) aromatic ring
	741w, 683w, 639w	δ_{oop}(=C-H) aromatic ring
(**5**), 5-amino	3458w, 3377w	ν_s(N-H) and ν_{as}(N-H)
	2937w	ν(C-H)
	1594m, 1556br and 1500m	ν(C=C) aromatic ring
	1626m	$\nu_{as}(COO^-)$ from bridged acetate
	1425s	$\nu_s(COO^-)$ from bridged acetate
	1298w, 1213w, 1176w	δ_{ip}(=C-H) aromatic ring
	751w, 621w, 491w	δ_{oop}(=C-H) aromatic ring
(**6**), THIQ	2936m and 2862m	ν(C-H)
	1556br and 1496m	ν(C=C) aromatic ring
	1616m	$\nu_{as}(COO^-)$ from bridged acetate
	1427s	$\nu_s(COO^-)$ from bridged acetate
	1290w, 1244w, 1200w, 1170w, 1080w	δ_{ip}(=C-H) aromatic ring
	708w, 620w	δ_{oop}(=C-H) aromatic ring

Cyclic Voltammetry

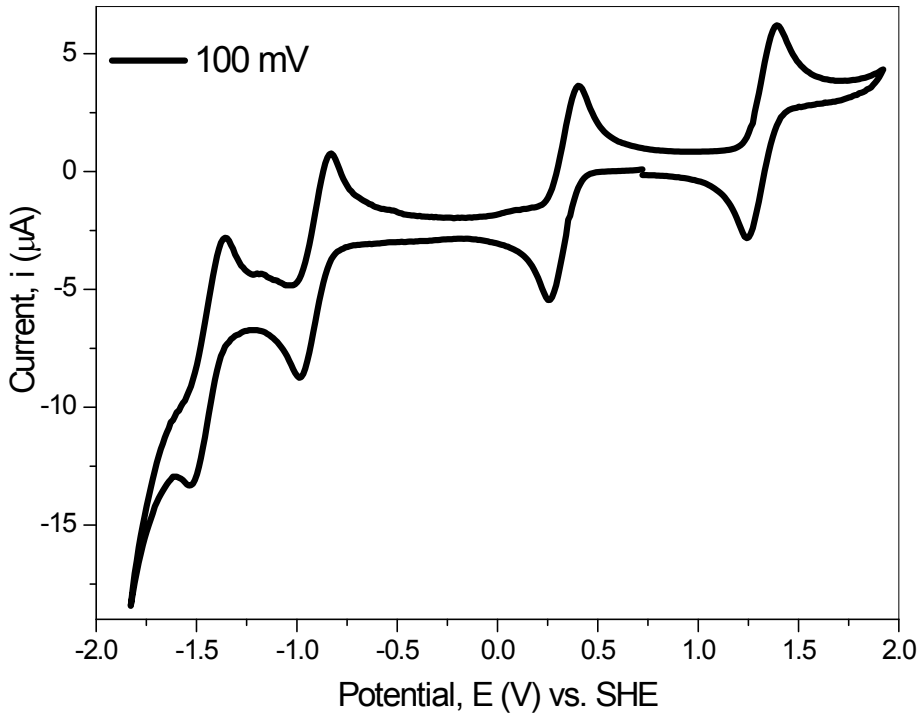


Figure S19. Cyclic voltammogram of **1**, [complex]= 0,001 mol L^{-1}, [$TBABF_4$]=0,1 mol L^{-1} in benzonitrile.

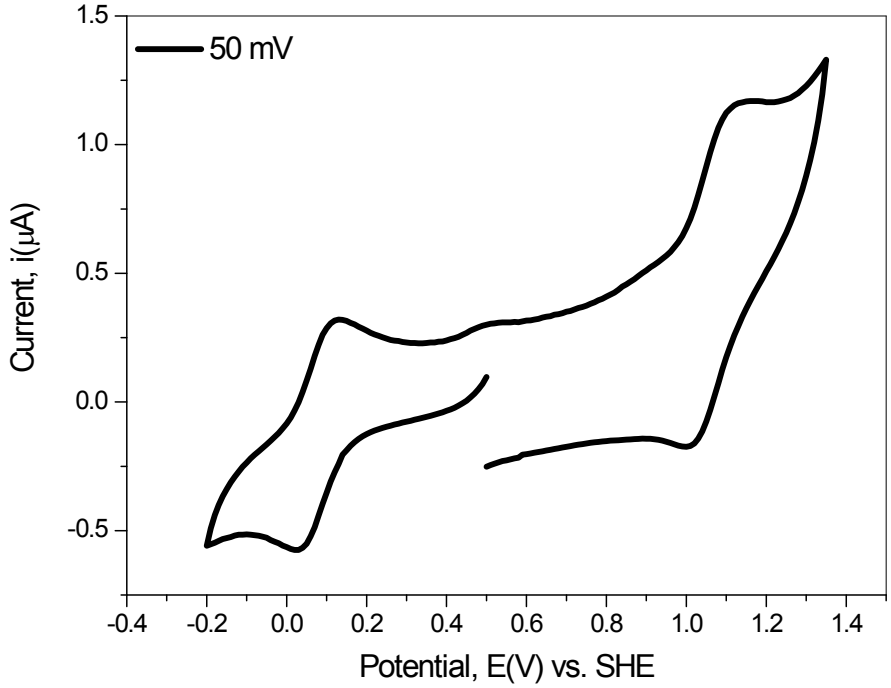


Figure S20. Cyclic voltammogram of complex **2**, [complex]= 0,0001 mol L^{-1}, [$TBABF_4$]=0,1 mol L^{-1} in benzonitrile.

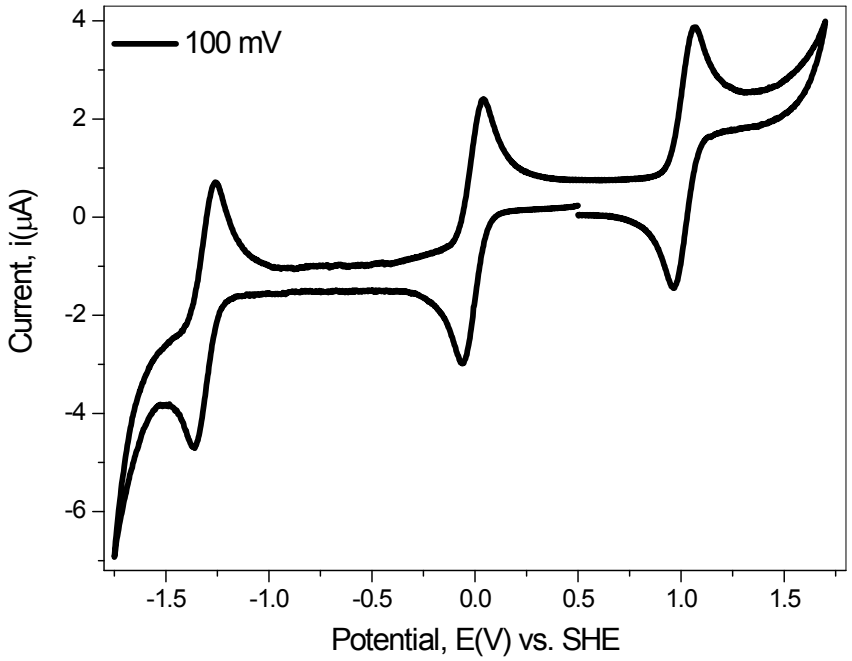


Figure S21. Cyclic voltammogram of complex **4**, [complex]= 0,001 mol L^{-1}, [$TBABF_4$]=0,1 mol L^{-1} in benzonitrile.

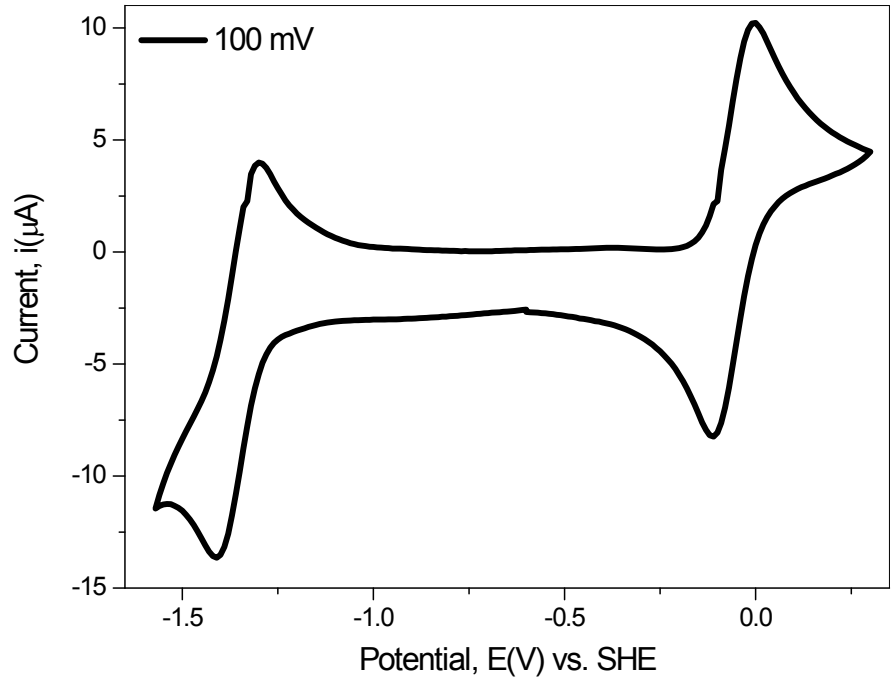


Figure S22. Cyclic voltammogram of complex **5** [complex]= 0,001 mol L^{-1}, [$TBABF_4$]= 0,1 mol L^{-1} in benzonitrile.

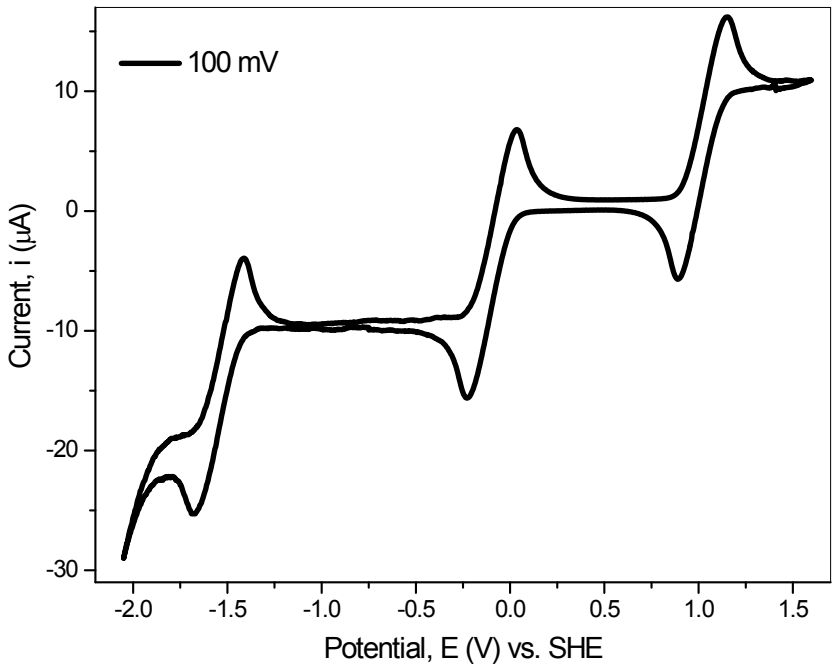


Figure S23. Cyclic voltammogram of complex **6** [complex]= 0,01 mol L^{-1}, [$TBABF_4$]= 0,1 mol L^{-1} in benzonitrile.