Supplementary

Table S1: The values of the Ramsey terms that define all the metal-ligand spin spin coupling of the complexes from two different systems treated with DGDZVP(Ru)|6-31+G(d,p) and 3-21G respectively

DGDZVP(Ru)|6-31+G(d,p)						3-21G					
Complex **1**						Complex **1**					
	FC	SD	PSO	DSO	J (HZ)		FC	SD	PSO	DSO	J (HZ)
Ru-C9	-7.06E+00	3.62E-001	-1.71E+00	-3.20E-002	-8.44E+00	Ru-C9	-2.15E+00	1.81E-001	-1.74E+00	-3.21E-002	-3.74E+00
Ru-C10	-7.83E+00	-3.13E-001	-1.67E+00	-3.37E-002	-9.85E+00	Ru-C10	-2.32E+00	-2.63E-001	-1.65E+00	-3.31E-002	-4.26E+00
Ru-C13	-7.44E+00	-2.17E-001	-1.53E+00	-3.37E-002	-9.22E+00	Ru-C13	-2.14E+00	-1.73E-001	-1.60E+00	-3.32E-002	-3.95E+00
Ru-C16	-9.25E+00	2.82E-001	-1.38E+00	-3.31E-002	-1.04E+00	Ru-C16	-2.76E+00	9.19E-002	-1.31E+00	-3.30E-002	-4.01E+00
Ru-C18	-8.82E+00	2.44E-001	-1.74E+00	-3.29E-002	-1.03E+00	Ru-C18	-2.54E+00	7.33E-002	-1.69E+00	-3.26E-002	-4.19E+00
Ru-C19	-8.16E+00	-3.04E-001	-1.04E+00	-3.34E-002	-9.53E+00	Ru-C19	-2.55E+00	-2.52E-001	-1.12E+00	-3.31E-002	-3.96E+00
Ru-Cl22	-1.57E+00	-2.33E+00	-2.32E+00	-9.87E-003	-2.71E+00	Ru-Cl22	-1.11E+00	-2.49E+00	-2.20E+00	-9.88E-003	-2.56E+00
Ru-N12	-1.24E+00	-1.01E-001	-7.08E-001	-1.46E-002	-1.32E+00	Ru-N12	-8.92E+00	-1.07E-001	-6.04E-001	-1.42E-002	-9.65E+00
Ru-N17	-1.22E+00	-1.03E-001	-6.93E-001	-1.46E-002	-1.30E+00	Ru-N17	-8.86E+00	-1.04E-001	-5.18E-001	-1.42E-002	-9.49E+00
Complex **2**						Complex **2**					
Ru-C7	-7.31E+00	-3.58E-	1.31E+00	-3.33E-	9.01E+00	Ru-C7	-2.42E+00	-3.80E-	1.32E+00	-3.31E-	4.16E+00

	0	001	0	002	0
Ru-C8	-8.36E+00	4.45E-001	-1.26E+00	-3.21E-002	9.21E+00
Ru-C13	-6.18E+00	4.40E-001	-1.71E+00	-3.08E-002	7.47E+00
Ru-C14	-7.30E+00	-4.17E-001	-8.50E-001	-3.30E-002	8.61E+00
Ru-C18	-7.30E+00	-3.58E-001	-1.31E+00	-3.33E-002	9.01E+00
Ru-C19	-8.34E+00	4.46E-001	-1.26E+00	-3.21E-002	9.18E+00
Ru-Cl10	-1.17E+00	2.36E+00	-2.40E+00	-9.72E-003	2.76E+00
Ru-N11	-1.28E+00	-8.72E-002	-2.53E-002	-1.41E-002	1.29E+00
Ru-N16	-1.28E+00	-8.64E-002	-9.98E-003	-1.41E-002	1.29E+00

Complex **3**

Ru-C13	-8.75E+00	-1.31E-002	-1.30E+00	-3.59E-002	1.01E+00
Ru-C14	-7.71E+00	-7.27E-002	-1.84E+00	-3.59E-002	9.66E+00
Ru-C18	-8.63E+00	-5.35E-002	-1.29E+00	-3.58E-002	1.00E+00
Ru-C21	-7.02E+00	-2.37E-003	-1.63E+00	-3.47E-002	8.68E+00
Ru-C23	-7.68E+00	-2.66E-002	-1.86E+00	-3.57E-002	9.60E+00

	0	001	0	002	0
Ru-C8	-2.76E+00	3.22E-001	-1.26E+00	-3.19E-002	3.74E+00
Ru-C13	-2.13E+00	3.39E-001	-1.73E+00	-3.07E-002	3.55E+00
Ru-C14	-2.11E+00	-4.33E-001	-9.09E-001	-3.29E-002	3.48E+00
Ru-C18	-2.42E+00	-3.80E-001	-1.33E+00	-3.30E-002	4.17E+00
Ru-C19	-2.75E+00	3.23E-001	-1.26E+00	-3.19E-002	3.72E+00
Ru-Cl10	-9.17E-001	-2.48E+00	-2.26E+00	-9.71E-003	2.60E+00
Ru-N11	-8.59E+00	-1.01E-001	-1.99E-003	-1.37E-002	8.71E+00
Ru-N16	-8.59E+00	-1.01E-001	-1.20E-002	-1.37E-002	8.69E+00

Complex **3**

Ru-C13	-2.83E+00	-6.54E-002	-1.31E+00	-3.59E-002	4.25E+00
Ru-C14	-2.42E+00	-1.44E-001	-1.79E+00	-3.58E-002	4.39E+00
Ru-C18	-2.79E+00	-1.41E-001	-1.33E+00	-3.58E-002	4.29E+00
Ru-C21	-2.02E+00	-5.09E-002	-1.68E+00	-3.45E-002	3.79E+00
Ru-C23	-2.40E+00	-7.16E-002	-1.88E+00	-3.55E-002	4.38E+00

Ru-C25	-7.09E+00	-4.84E-002	1.62E+00	-3.48E-002	-8.80E+00	Ru-C25	-2.13E+00	-1.25E-001	1.70E+00	-3.47E-002	-3.98E+00
Ru-Cl7	-2.06E+00	-2.04E+00	-2.29E+00	-1.11E-002	-2.70E+00	Ru-Cl7	-1.45E+00	-2.17E+00	-2.19E+00	-1.11E-002	-2.55E+00
Ru-N10	-1.15E+00	-5.83E-002	3.27E-001	-1.49E-002	-1.13E+00	Ru-N10	-8.07E+00	-6.77E-002	3.26E-001	-1.45E-002	-7.83E+00
Ru-N16	-1.15E+00	-6.05E-002	3.14E-001	-1.49E-002	-1.13E+00	Ru-N16	-8.01E+00	-7.72E-002	2.97E-001	-1.46E-002	-7.80E+00
	Complex **4**						Complex **4**				
Ru-C2	-7.36E+00	-2.69E-003	1.17E+00	-3.17E-002	-8.56E+00	Ru-C2	-2.45E+00	-6.12E-002	1.30E+00	-3.17E-002	-3.84E+00
Ru-C3	-6.27E+00	-1.82E-001	1.65E+00	-3.24E-002	-8.13E+00	Ru-C3	-1.53E+00	-2.32E-001	1.69E+00	-3.24E-002	-3.48E+00
Ru-C4	-7.37E+00	6.30E-003	1.16E+00	-3.17E-002	-8.56E+00	Ru-C4	-2.46E+00	-5.27E-002	1.30E+00	-3.17E-002	-3.84E+00
Ru-C5	-7.96E+00	-7.38E-002	2.60E+00	-3.23E-002	-1.07E+00	Ru-C5	-2.91E+00	-1.26E-001	2.50E+00	-3.22E-002	-5.57E+00
Ru-C6	-6.26E+00	-1.90E-001	1.64E+00	-3.24E-002	-8.13E+00	Ru-C6	-1.53E+00	-2.40E-001	1.68E+00	-3.24E-002	-3.48E+00
Ru-C7	-7.95E+00	-6.55E-002	2.60E+00	-3.23E-002	-1.06E+00	Ru-C7	-2.90E+00	-1.19E-001	2.51E+00	-3.22E-002	-5.55E+00
Ru-N10	-1.28E+00	3.65E-002	-7.79E-001	-1.33E-002	-1.35E+00	Ru-N10	-8.84E+00	2.47E-002	-6.00E-001	-1.30E-002	-9.43E+00
Ru-N13	-1.28E+00	3.67E-002	-7.79E-001	-1.33E-002	-1.35E+00	Ru-N13	-8.84E+00	2.50E-002	-5.99E-001	-1.30E-002	-9.43E+00
Ru-N15	-1.07E+00	-1.64E-001	-6.73E-001	-1.47E-002	-1.16E+00	Ru-N15	-6.86E+00	-1.59E-001	-4.56E-001	-1.45E-002	-7.49E+00
Complex **5**							Complex **5**				

Ru-C18	-7.94E+00	-8.67E-003	-2.14E+00	-3.26E-002	-1.01E+01	Ru-C18	-2.81E+00	-6.52E-002	-2.07E+00	-3.25E-002	-4.98E+00
Ru-C20	-6.08E+00	-1.52E-001	-1.42E+00	-3.27E-002	-7.69E+00	Ru-C20	-1.43E+00	-1.99E-001	-1.45E+00	-3.26E-002	-3.11E+00
Ru-C22	-7.95E+00	-1.74E-002	-2.14E+00	-3.26E-002	-1.01E+01	Ru-C22	-2.82E+00	-7.17E-002	-2.07E+00	-3.25E-002	-4.99E+00
Ru-C23	-6.77E+00	7.09E-002	-8.44E-001	-3.18E-002	-7.57E+00	Ru-C23	-2.28E+00	1.27E-002	-9.64E-001	-3.17E-002	-3.26E+00
Ru-C26	-6.10E+00	-1.46E-001	-1.43E+00	-3.27E-002	-7.71E+00	Ru-C26	-1.43E+00	-1.96E-001	-1.45E+00	-3.26E-002	-3.11E+00
Ru-C27	-6.75E+00	6.16E-002	-8.46E-001	-3.18E-002	-7.57E+00	Ru-C27	-2.27E+00	6.47E-003	-9.66E-001	-3.17E-002	-3.26E+00
Ru-N14	-1.27E+01	1.90E-002	-2.15E-001	-1.33E-002	-1.29E+01	Ru-N14	-8.69E+00	5.82E-003	-9.55E-002	-1.30E-002	-8.80E+00
Ru-N15	-1.24E+01	-1.60E-001	-3.08E-001	-1.50E-002	-1.29E+01	Ru-N15	-7.90E+00	-1.68E-001	-1.85E-001	-1.48E-002	-8.26E+00
Ru-N21	-1.27E+01	1.81E-002	-2.34E-001	-1.33E-002	-1.30E+01	Ru-N21	-8.71E+00	5.23E-003	-1.08E-001	-1.30E-002	-8.82E+00

Table S2: The values of the Ramsey terms that define all the metal-ligand spin spin coupling of the complexes from two different systems treated with ECP(Ru)|6-31+G(d,p) and ECP(Ru,Cl)|6-31G* respectively

Ramsey Terms	ECP(6-31+G(d,p)				ECP(6-31G*)	Ramsey Terms				
	Complex **1**					Complex **1**				

	FC (HZ) for Ru	SD for Ru	PSO for Ru	DSO for Ru	J (HZ) for Ru		FC (HZ) for Ru	SD for Ru	PSO for Ru	DSO for Ru	J (HZ) for Ru
Ru-C9	-3.67E-006	4.55E-002	-2.43E-001	-3.18E-002	-2.29E-001	Ru-C9	-1.79E-006	3.65E-002	-2.55E-001	-3.00E-002	-2.48E-001
Ru-C10	-6.04E-006	-2.15E-002	-2.38E-001	-3.35E-002	-2.93E-001	Ru-C10	0.00E+000	-1.41E-002	-2.43E-001	-3.06E-002	-2.88E-001
Ru-C13	-6.00E-006	-7.58E-003	-2.17E-001	-3.35E-002	-2.58E-001	Ru-C13	-2.90E-006	8.14E-004	-2.34E-001	-3.09E-002	-2.64E-001
Ru-C16	-3.66E-006	4.04E-002	-2.09E-001	-3.29E-002	-2.01E-001	Ru-C16	0.00E+000	3.01E-002	-2.00E-001	-2.98E-002	-2.00E-001
Ru-C18	-3.00E-006	3.33E-002	-2.52E-001	-3.27E-002	-2.52E-001	Ru-C18	1.33E-006	2.31E-002	-2.51E-001	-2.99E-002	-2.58E-001
Ru-C19	-6.44E-006	-1.89E-002	-1.57E-001	-3.32E-002	-2.09E-001	Ru-C19	0.00E+000	-9.33E-003	-1.69E-001	-2.98E-002	-2.08E-001
Ru-Cl22	0.00E+000	-1.71E-001	-3.17E+000	-9.93E-003	-3.35E+000	Ru-Cl22	0.00E+000	-1.17E-002	-2.17E-001	-9.88E-003	-2.38E-001
Ru-N12	-3.55E-006	-3.63E-003	-9.07E-002	-1.46E-002	-1.09E-001	Ru-N12	1.35E-006	-4.11E-003	-1.09E-001	-1.37E-002	-1.27E-001
Ru-N17	-3.49E-006	-3.73E-003	-8.93E-002	-1.46E-002	-1.08E-001	Ru-N17	1.18E-006	-3.82E-003	-9.36E-002	-1.37E-002	-1.11E-001
	Complex **2**						Complex **2**				
Ru-C7	-8.10E-006	-2.42E-002	-1.86E-001	-3.31E-002	-2.43E-001	Ru-C7	-5.02E-006	-2.49E-002	-1.95E-001	-3.06E-002	-2.51E-001
Ru-C8	-7.05E-006	5.42E-002	-1.89E-001	-3.18E-002	-1.67E-001	Ru-C8	0.00E+000	5.35E-002	-1.94E-001	-2.89E-002	-1.69E-001
Ru-C13	-6.10E-006	5.10E-002	-2.39E-001	-3.06E-002	-2.19E-001	Ru-C13	-5.93E-006	5.09E-002	-2.56E-001	-2.86E-002	-2.34E-001
Ru-C14	-4.52E-006	-2.90E-002	-1.27E-001	-3.28E-002	-1.89E-001	Ru-C14	-1.35E-006	-2.96E-002	-1.36E-001	-2.95E-002	-1.96E-001
Ru-C18	-8.10E-006	-2.42E-002	-1.87E-001	-3.31E-002	-2.44E-001	Ru-C18	-5.03E-006	-2.49E-002	-1.96E-001	-3.06E-002	-2.51E-001
Ru-C19	-7.04E-006	5.42E-002	-1.88E-001	-3.18E-002	-1.66E-001	Ru-C19	0.00E+000	5.36E-002	-1.93E-001	-2.89E-002	-1.69E-001
Ru-Cl10	0.00E+000	-1.69E-001	-3.28E+000	-9.78E-003	-3.46E+000	Ru-Cl10	0.00E+000	-1.10E-002	-2.25E-001	-9.74E-003	-2.46E-001
Ru-N11	-3.33E-	-3.49E-	8.27E-003	-1.41E-	-9.33E-	Ru-N11	0.00E+00	-3.67E-	4.69E-004	-1.30E-	-1.62E-

	006	003		002	003		0	003		002	002
Ru-N16	-3.28E-006	-3.57E-003	1.05E-002	-1.41E-002	-7.21E-003	Ru-N16	0.00E+00	-3.73E-003	2.52E-003	-1.30E-002	-1.42E-002
		Complex **3**						Complex **3**			
Ru-C13	-6.29E-006	8.47E-003	-1.86E-001	-3.57E-002	-2.13E-001	Ru-C13	0.00E+00	9.88E-003	-1.87E-001	-3.27E-002	-2.10E-001
Ru-C14	-7.82E-006	2.83E-003	-2.47E-001	-3.56E-002	-2.79E-001	Ru-C14	-1.39E-006	8.60E-004	-2.42E-001	-3.31E-002	-2.74E-001
Ru-C18	-6.23E-006	4.71E-003	-1.84E-001	-3.56E-002	-2.15E-001	Ru-C18	1.32E-006	1.50E-003	-1.89E-001	-3.26E-002	-2.20E-001
Ru-C21	-7.37E-006	1.06E-002	-2.25E-001	-3.45E-002	-2.49E-001	Ru-C21	-2.65E-006	1.08E-002	-2.40E-001	-3.24E-002	-2.61E-001
Ru-C23	-7.69E-006	7.47E-003	-2.49E-001	-3.55E-002	-2.77E-001	Ru-C23	-1.47E-006	9.20E-003	-2.54E-001	-3.29E-002	-2.78E-001
Ru-C25	-7.51E-006	6.02E-003	-2.24E-001	-3.46E-002	-2.53E-001	Ru-C25	-2.80E-006	2.72E-003	-2.41E-001	-3.25E-002	-2.71E-001
Ru-Cl7	0.00E+00	-1.24E-001	-3.06E+00	-1.11E-002	-3.20E+00	Ru-Cl7	0.00E+00	-7.99E-003	-2.11E-001	-1.11E-002	-2.30E-001
Ru-N10	-3.25E-006	-2.18E-003	6.56E-002	-1.49E-002	4.85E-002	Ru-N10	-1.10E-006	-1.94E-003	6.08E-002	-1.39E-002	4.50E-002
Ru-N16	-3.25E-006	-2.24E-003	6.39E-002	-1.49E-002	4.67E-002	Ru-N16	-1.02E-006	-2.53E-003	5.75E-002	-1.39E-002	4.11E-002
		Complex **4**						Complex **4**			
Ru-C2	-3.54E-006	8.88E-003	-1.74E-001	-3.14E-002	-1.97E-001	Ru-C2	5.22E-006	8.93E-003	-1.80E-001	-3.13E-002	-2.03E-001
Ru-C3	-8.33E-006	-8.29E-003	-2.29E-001	-3.22E-002	-2.70E-001	Ru-C3	-2.18E-006	-8.75E-003	-2.34E-001	-3.21E-002	-2.74E-001
Ru-C4	-3.54E-006	9.73E-003	-1.74E-001	-3.14E-002	-1.96E-001	Ru-C4	5.25E-006	9.81E-003	-1.80E-001	-3.13E-002	-2.02E-001
Ru-C5	-7.34E-006	1.34E-004	-3.43E-001	-3.22E-002	-3.75E-001	Ru-C5	0.00E+00	-5.09E-004	-3.47E-001	-3.21E-002	-3.80E-001
Ru-C6	-8.31E-006	-9.04E-003	-2.28E-001	-3.22E-002	-2.69E-001	Ru-C6	-2.17E-006	-9.54E-003	-2.32E-001	-3.21E-002	-2.74E-001
Ru-C7	-7.33E-006	9.98E-004	-3.44E-001	-3.22E-002	-3.75E-001	Ru-C7	0.00E+00	3.83E-004	-3.48E-001	-3.21E-002	-3.79E-001
Ru-N10	-3.37E-	1.11E-002	-1.07E-	-1.34E-	-1.09E-	Ru-N10	0.00E+00	1.10E-002	-1.10E-	-1.33E-	-1.13E-

	006		001	002	001		0		001	002	001
	-3.37E-		-1.07E-	-1.34E-	-1.09E-		0.00E+00		-1.10E-	-1.33E-	-1.13E-
Ru-N13	006	1.11E-002	001	002	001	Ru-N13	0	1.10E-002	001	002	001
	-2.89E-	-1.15E-	-6.88E-	-1.47E-	-9.51E-		0.00E+00	-1.17E-	-7.21E-	-1.47E-	-9.84E-
Ru-N15	006	002	002	002	002	Ru-N15	0	002	002	002	002
	Complex **5**						Complex **5**				
	-6.68E-		-2.86E-	-3.25E-	-3.11E-		0.00E+00		-2.91E-	-3.24E-	-3.17E-
Ru-C18	006	7.27E-003	001	002	001	Ru-C18	0	6.50E-003	001	002	001
	-7.65E-	-5.87E-	-2.02E-	-3.24E-	-2.40E-		0.00E+00	-6.18E-	-2.07E-	-3.23E-	-2.45E-
Ru-C20	006	003	001	002	001	Ru-C20	0	003	001	002	001
	-6.70E-		-2.86E-	-3.25E-	-3.12E-		0.00E+00		-2.91E-	-3.24E-	-3.17E-
Ru-C22	006	6.32E-003	001	002	001	Ru-C22	0	5.75E-003	001	002	001
	-2.90E-		-1.33E-	-3.14E-	-1.49E-				-1.40E-	-3.13E-	-1.55E-
Ru-C23	006	1.57E-002	001	002	001	Ru-C23	4.56E-006	1.59E-002	001	002	001
	-7.62E-	-5.40E-	-2.02E-	-3.24E-	-2.40E-		0.00E+00	-5.95E-	-2.07E-	-3.23E-	-2.45E-
Ru-C26	006	003	001	002	001	Ru-C26	0	003	001	002	001
	-2.93E-		-1.33E-	-3.14E-	-1.50E-				-1.40E-	-3.13E-	-1.56E-
Ru-C27	006	1.49E-002	001	002	001	Ru-C27	4.62E-006	1.54E-002	001	002	001
	-3.40E-		-1.97E-	-1.33E-	-2.23E-		-1.06E-		-2.29E-	-1.33E-	-2.54E-
Ru-N14	006	1.07E-002	002	002	002	Ru-N14	006	1.08E-002	002	002	002
	-3.65E-	-1.37E-	-1.20E-	-1.51E-	-4.08E-		0.00E+00	-1.41E-	-1.94E-	-1.50E-	-4.84E-
Ru-N15	006	002	002	002	002	Ru-N15	0	002	002	002	002
	-3.39E-		-2.23E-	-1.33E-	-2.50E-		-1.08E-		-2.54E-	-1.33E-	-2.79E-
Ru-N21	006	1.07E-002	002	002	002	Ru-N21	006	1.08E-002	002	002	002

Table S3: The atomic NMR magnetazability and shielding for the selected atoms in the complexes using combined basis set DGDZVP(Ru)|6-31+G(d,p)

	Complex **1**													
	q(A)	Vol(A), 0.001	L(A)	K(A)	LI(A)	DI(A,A')/2	χ_{Intra_Iso}	χ_{bond_Iso}	χ_{Intra_Iso}(A)	Mu(A)	σ_{Iso}(A, A)	σ_{Iso}(A', A)	σ_{Iso}(A)	Isotropic	Anisotropy
Ru1	9.50E-01	1.01E+02	6.36E-04	4.44E+03	4.05E+01	2.54E+00	2.24E+01	2.27E+01	-3.35E-01	1.20E+00	-3.51E+03	-2.52E+01	-3.49E+03	-3.49E+03	6.16E+03

C9	-6.26E-02	7.38E+01	-5.40E-05	3.78E+01	3.97E+00	2.09E+00	-3.09E+00	-4.98E+00	-8.07E+00	9.26E-02	8.50E+01	2.29E+01	1.08E+02	1.08E+02	1.28E+02
C10	-4.68E-02	7.14E+01	-3.51E-04	3.78E+01	3.96E+00	2.09E+00	-2.65E+00	-9.19E+00	-1.18E+01	6.08E-02	7.30E+01	2.35E+01	9.65E+01	9.65E+01	1.35E+02
C13	-4.96E-02	7.16E+01	-7.50E-05	3.78E+01	3.96E+00	2.09E+00	-2.68E+00	-9.21E+00	-1.19E+01	-1.02E-01	7.55E+01	2.33E+01	9.88E+01	9.88E+01	1.31E+02
C16	-5.13E-02	7.37E+01	-1.58E-04	3.78E+01	3.97E+00	2.08E+00	-3.09E+00	-4.90E+00	-7.99E+00	5.52E-02	-8.44E+01	2.30E+01	1.07E+02	1.07E+02	1.32E+02
C18	-5.82E-02	7.48E+01	-1.32E-04	3.78E+01	3.98E+00	2.08E+00	-3.22E+00	-4.95E+00	-8.17E+00	6.78E-02	-8.75E+01	2.35E+01	1.11E+02	1.11E+02	1.27E+02
C19	-2.85E-02	6.99E+01	6.90E-05	3.78E+01	3.95E+00	2.08E+00	-2.34E+00	-9.02E+00	-1.14E+01	-1.02E-01	6.40E+01	2.25E+01	8.65E+01	8.65E+01	1.51E+02
Cl22	-5.27E-01	2.32E+02	8.30E-05	4.59E+02	1.69E+01	6.46E-01	-2.15E+01	-3.69E+00	-2.52E+01	1.29E+00	1.06E+03	4.24E+00	1.06E+03	1.06E+03	5.20E+02
N12	-7.59E-01	7.81E+01	2.16E-04	5.48E+01	5.90E+00	1.86E+00	-3.51E+00	-6.63E+00	-1.01E+01	-6.58E-01	-3.46E+00	1.70E+01	1.35E+01	1.35E+01	1.92E+02
N17	-7.59E-01	7.80E+01	2.41E-04	5.48E+01	5.90E+00	1.86E+00	-3.50E+00	-6.64E+00	-1.01E+01	-6.17E-01	-3.94E+00	1.69E+01	1.29E+01	1.29E+01	1.93E+02
O2	-1.17E+00	1.30E+02	8.20E-05	7.54E+01	8.23E+00	9.47E-01	-6.12E+00	-3.48E+00	-9.60E+00	-1.03E+00	-9.64E+01	2.41E+00	9.40E+01	9.40E+01	5.67E+02
H24	1.23E-01	4.05E+01	2.40E-05	5.68E-01	3.45E-01	5.32E-01	-9.18E-01	-1.36E+00	-2.28E+00	4.80E-01	1.77E+01	5.68E+00	2.33E+01	2.33E+01	6.65E+00
H29	1.23E-01	4.06E+01	2.60E-05	5.68E-01	3.45E-01	5.32E-01	-9.20E-01	-1.36E+00	-2.29E+00	-4.92E-01	1.77E+01	5.67E+00	2.33E+01	2.33E+01	6.63E+00

Complex **2**

Ru1	9.59E-01	1.04E+02	2.47E-04	4.44E+03	4.05E+01	2.57E+00	-2.00E+01	-2.28E+01	-2.79E+00	-1.18E+00	-3.12E+03	2.45E+01	-3.09E+03	-3.09E+03	5.61E+03
C7	-5.32E-	7.01E+	-2.27E-	3.78E+	3.96E+	2.09E+	-2.53E+	-9.07E+	-1.16E+	6.14E-	-6.95E+	2.28E+	-9.23E+	-9.23E+	1.38E+

	02	01	04	01	00	00	00	00	01	02	01	01	01	01	02
C8	-6.29E-02	7.46E+01	9.20E-05	3.78E+01	3.98E+00	2.08E+00	-3.26E+00	-4.86E+00	-8.12E+00	-8.23E-02	-8.88E+01	2.26E+01	1.11E+02	1.11E+02	1.30E+02
C13	-5.29E-02	7.64E+01	-6.00E-06	3.78E+01	3.97E+00	2.08E+00	-3.20E+00	-4.90E+00	-8.10E+00	-7.84E-02	-8.70E+01	2.27E+01	1.10E+02	1.10E+02	1.30E+02
C14	-2.67E-02	6.96E+01	-5.71E-04	3.78E+01	3.95E+00	2.08E+00	-2.13E+00	-8.85E+00	-1.10E+01	-9.18E-02	-5.83E+01	2.19E+01	8.02E+01	8.02E+01	1.57E+02
C18	-5.42E-02	7.02E+01	-8.17E-04	3.78E+01	3.96E+00	2.09E+00	-2.53E+00	-9.07E+00	-1.16E+01	-9.29E-02	-6.96E+01	2.29E+01	9.24E+01	9.24E+01	1.37E+02
C19	-6.30E-02	7.46E+01	-9.00E-05	3.78E+01	3.98E+00	2.08E+00	-3.26E+00	-4.86E+00	-8.12E+00	-7.40E-02	-8.89E+01	2.26E+01	1.11E+02	1.11E+02	1.30E+02
Cl10	-5.21E-01	2.37E+02	-8.60E-05	4.59E+02	1.69E+01	-6.23E-01	-2.20E+01	-3.76E+00	-2.57E+01	-1.26E+00	-1.10E+03	4.72E+00	-1.10E+03	-1.10E+03	4.20E+02
N11	-1.22E+00	-8.21E+01	-8.40E-05	-5.51E+01	6.36E+00	-1.86E+00	-3.55E+00	-7.30E+00	-1.09E+01	-5.42E-01	-3.05E+01	-1.29E+01	-1.76E+01	-1.76E+01	3.87E+02
N16	-1.22E+00	-8.21E+01	-1.68E-04	-5.51E+01	6.36E+00	-1.86E+00	-3.54E+00	-7.32E+00	-1.09E+01	-5.10E-01	-3.11E+01	-1.29E+01	-1.82E+01	-1.82E+01	3.89E+02
H34	8.99E-02	4.09E+01	8.10E-05	5.87E-01	3.64E-01	5.46E-01	-9.14E-01	-1.27E+00	-2.19E+00	-6.96E-02	-1.82E+01	4.25E+00	-2.25E+01	-2.25E+01	1.07E+01
H38	9.65E-02	4.10E+01	5.80E-05	5.81E-01	3.59E-01	5.45E-01	-9.15E-01	-1.28E+00	-2.19E+00	-5.34E-02	-1.81E+01	4.22E+00	-2.23E+01	-2.23E+01	1.01E+01

Complex **3**

Ru1	-9.55E-01	9.99E+01	-3.57E-04	-4.44E+03	4.05E+01	-2.52E+00	-2.45E+01	-2.56E+01	-1.05E+00	-8.40E-01	-3.76E+03	-2.39E+01	-3.73E+03	-3.73E+03	6.00E+03
C13	-4.01E-02	7.06E+01	-1.19E-04	3.78E+01	3.96E+00	2.08E+00	-2.72E+00	-6.38E+00	-9.11E+00	-8.08E-02	-7.46E+01	2.26E+01	9.72E+01	9.72E+01	1.39E+02
C14	-4.85E-02	6.98E+01	-1.15E-04	3.79E+01	3.97E+00	2.08E+00	-2.69E+00	-6.81E+00	-9.50E+00	-4.00E-01	-7.44E+01	2.31E+01	9.75E+01	9.75E+01	1.39E+02

C18	-3.97E-02	7.07E+01	-9.40E-05	3.78E+01	3.96E+00	2.08E+00	-2.69E+00	-6.38E+00	-9.06E+00	8.56E-02	7.35E+01	2.26E+01	9.61E+01	9.61E+01	1.40E+02
C21	-5.97E-02	7.36E+01	-6.60E-05	3.78E+01	3.97E+00	2.09E+00	-2.89E+00	-6.48E+00	-9.37E+00	1.32E-01	7.88E+01	2.31E+01	1.02E+02	1.02E+02	1.34E+02
C23	-5.00E-02	7.02E+01	-1.81E-04	3.79E+01	3.97E+00	2.08E+00	-2.73E+00	-6.81E+00	-9.53E+00	4.12E-01	7.53E+01	2.31E+01	9.84E+01	9.84E+01	1.39E+02
C25	-5.93E-02	7.33E+01	-2.62E-04	3.78E+01	3.97E+00	2.09E+00	-2.87E+00	-6.46E+00	-9.33E+00	1.40E-01	7.81E+01	2.32E+01	1.01E+02	1.01E+02	1.34E+02
Cl7	-5.33E-01	2.36E+02	1.08E-04	4.59E+02	1.69E+01	6.31E-01	-2.18E+01	-3.57E+00	-2.54E+01	1.30E+00	1.08E+03	4.16E+00	1.09E+03	1.09E+03	5.79E+02
N10	-1.20E+00	8.30E+01	-2.90E-04	5.50E+01	6.36E+00	1.84E+00	-3.65E+00	-7.31E+00	-1.10E+01	-9.47E-01	2.31E+01	-1.21E+01	-1.11E+01	-1.11E+01	3.83E+02
N16	-1.20E+00	8.30E+01	-8.80E-05	5.50E+01	6.36E+00	1.84E+00	-3.65E+00	-7.31E+00	-1.10E+01	-9.12E-01	2.24E+01	-1.21E+01	-1.03E+01	-1.03E+01	3.81E+02
O2	-1.19E+00	1.28E+02	-1.16E-04	7.54E+01	8.22E+00	9.69E-01	-6.05E+00	-2.15E+00	-8.20E+00	-9.26E-01	8.06E+01	-2.34E+00	-7.83E+01	-7.83E+01	5.28E+02
O28	-1.19E+00	1.28E+02	-1.27E-04	7.54E+01	8.23E+00	9.67E-01	-6.07E+00	-2.15E+00	-8.22E+00	-9.10E-01	8.12E+01	-2.31E+00	-7.89E+01	-7.89E+01	5.26E+02
H31	1.12E-01	3.92E+01	-2.90E-05	5.80E-01	3.48E-01	5.39E-01	-9.26E-01	-1.24E+00	-2.16E+00	-3.59E-01	1.82E+01	-6.49E+00	-2.47E+01	-2.47E+01	6.46E+00
H36	1.17E-01	3.87E+01	-2.90E-05	5.79E-01	3.45E-01	5.39E-01	-9.12E-01	-1.23E+00	-2.15E+00	-3.62E-01	1.81E+01	-6.49E+00	-2.46E+01	-2.46E+01	6.83E+00

Complex **4**

Ru1	-9.92E-01	1.10E+02	-9.65E-04	4.43E+03	4.06E+01	2.46E+00	-2.65E+01	-2.59E+01	-5.96E-01	-3.99E-01	-4.14E+03	-2.40E+01	-4.12E+03	-4.12E+03	6.61E+03
C2	-4.55E-02	7.33E+01	1.09E-04	3.78E+01	3.97E+00	2.08E+00	-2.80E+00	-6.45E+00	-9.25E+00	6.59E-02	-7.44E+01	-2.23E+01	-9.67E+01	-9.67E+01	1.37E+02
C3	-4.44E-	7.07E+	-1.18E-	3.78E+	3.96E+	2.08E+	-2.70E+	-6.37E+	-9.07E+	6.64E-	-7.52E+	-2.36E+	-9.87E+	-9.87E+	1.40E+

	02	01	04	01	00	00	00	00	00	02	01	01	01	01	02
C4	-4.58E-02	7.34E+01	-6.00E-06	3.78E+01	3.97E+00	2.08E+00	-2.81E+00	-6.45E+00	-9.26E+00	-9.17E-02	-7.46E+01	2.23E+01	9.69E+01	9.69E+01	1.37E+02
C5	-3.39E-02	7.27E+01	-2.15E-04	3.78E+01	3.96E+00	2.08E+00	-2.84E+00	-6.43E+00	-9.27E+00	-9.10E-02	-8.08E+01	2.38E+01	1.05E+02	1.05E+02	1.35E+02
C6	-4.44E-02	7.06E+01	-1.85E-04	3.78E+01	3.96E+00	2.08E+00	-2.69E+00	-6.37E+00	-9.05E+00	-8.10E-02	-7.49E+01	2.36E+01	9.84E+01	9.84E+01	1.40E+02
C7	-3.40E-02	7.26E+01	-7.40E-05	3.78E+01	3.96E+00	2.08E+00	-2.85E+00	-6.42E+00	-9.27E+00	-9.80E-02	-8.10E+01	2.38E+01	1.05E+02	1.05E+02	1.35E+02
N10	-7.71E-01	8.29E+01	7.40E-05	5.47E+01	5.95E+00	1.82E+00	-3.69E+00	-6.67E+00	-1.04E+01	-5.94E-01	-4.52E+00	1.51E+01	1.06E+02	1.06E+02	1.47E+02
N13	-7.71E-01	8.29E+01	3.03E-04	5.47E+01	5.95E+00	1.82E+00	-3.69E+00	-6.68E+00	-1.04E+01	-5.81E-01	-4.53E+00	1.51E+01	1.06E+02	1.06E+02	1.47E+02
N15	-1.24E+00	8.06E+01	4.25E-04	5.51E+01	6.40E+00	1.84E+00	-4.55E+00	-6.84E+00	-1.14E+01	-3.31E-01	-4.37E+01	1.25E+01	5.62E+01	5.62E+01	2.20E+02

Complex **5**

Ru1	9.82E-01	1.08E+02	1.20E-03	4.43E+03	4.05E+01	2.50E+00	-2.53E+01	-2.34E+01	-1.86E+00	-5.62E-01	-3.94E+03	2.31E+01	3.92E+03	3.92E+03	5.35E+03
C18	-3.61E-02	7.26E+01	-3.09E-04	3.78E+01	3.96E+00	2.08E+00	-2.80E+00	-7.46E+00	-1.03E+01	-5.62E-02	-7.91E+01	2.29E+01	1.02E+02	1.02E+02	1.38E+02
C20	-4.79E-02	7.09E+01	-3.12E-04	3.78E+01	3.97E+00	2.08E+00	-2.67E+00	-8.73E+00	-1.14E+01	-8.92E-02	-7.42E+01	2.28E+01	9.70E+01	9.70E+01	1.42E+02
C22	-3.57E-02	7.26E+01	-1.31E-04	3.78E+01	3.96E+00	2.08E+00	-2.79E+00	-7.45E+00	-1.02E+01	-6.26E-02	-7.89E+01	2.29E+01	1.02E+02	1.02E+02	1.38E+02
C23	-4.91E-02	7.30E+01	4.00E-06	3.78E+01	3.97E+00	2.08E+00	-2.72E+00	-3.64E+00	-6.36E+00	-8.07E-02	-7.14E+01	2.16E+01	9.29E+01	9.29E+01	1.42E+02
C26	-4.81E-02	7.10E+01	-6.86E-04	3.78E+01	3.97E+00	2.08E+00	-2.67E+00	-8.72E+00	-1.14E+01	-1.27E-01	-7.44E+01	2.28E+01	9.72E+01	9.72E+01	1.41E+02

								-	-	-					
	-4.90E-02	7.29E+01	-1.03E-04	3.78E+01	3.97E+00	2.08E+00	2.71E+00	3.64E+00	6.35E+00	1.07E-01	7.11E+01	2.16E+01	9.26E+01	9.26E+01	1.43E+02
C27															
	-						-	-	-		-		-	-	
	1.23E+00	8.58E+01	2.21E-04	5.50E+01	6.40E+00	1.83E+00	3.88E+00	7.35E+00	1.12E+01	4.62E-01	1.31E+01	1.19E+01	1.24E+01	1.24E+00	3.37E+02
N14															
	-						-	-	-		-				
	1.23E+00	7.90E+01	4.56E-04	5.51E+01	6.35E+00	1.88E+00	3.71E+00	7.16E+00	1.09E+01	2.32E-01	1.01E+01	1.22E+01	2.12E+01	2.12E+00	3.05E+02
N15															
	-						-	-	-		-				
	1.23E+00	8.58E+01	2.75E-04	5.50E+01	6.40E+00	1.83E+00	3.89E+00	7.37E+00	1.13E+01	3.70E-01	1.23E+01	1.19E+01	-4.32E-01	-4.31E-01	3.35E+02
N21															

q(A) is total charge on atom A, Vol(A) is the volume bounded by an isosurface of the electron density distribution (0.001) and by interatomic surfaces of atom A; K(A) is electronic kinetic energy of atom A (Hamiltonian Form), Loc(A) is number of electrons localized in atom A, K_Scaled(A) is approximation to virial-based total energy of atom A, DI(A,A') is number of electron delocalization from atom A, χ_{Intra_Iso} is intraatomic magnetizability contribution of atom A (cgs-ppm); χ_{bond_Iso} is bonding magnetizability contribution of atom A; χ_{Iso} is total magnetizability contribution of atom A (i.e. magnetizability isotropic); Mu(A) is total dipole moment contribution of atom A; σ_{Iso}(A,A) is the intraatomic shielding tensor; σ_{Iso}(A',A) is total induced magnetic field on nucleus a by other nuclei A'; σ_{Iso}(A) is total magnetic shielding tensor of atom A (i.e. nmr shielding isotropic).

Table S4: The atomic NMR magnetazability and shielding for the selected atoms in the complexes using combined basis sets 3-21G

	Complex **1**														
	q(A)	Vol(A), 0.001	L(A)	K(A)	LI(A)	DI(A,A')/2	χ_{Intra_Iso}(A)	χ_{bond_Iso}(A)	χ_{Iso}(A)	Mu(A)	σ_{Iso}(A,A)	σ_{Iso}(A',A)	σ_{Iso}(A)	Isotropic	Anisotropy
									-		-		-	-	
	8.63E-01	9.73E+01	5.52E-04	4.40E+03	4.07E+01	2.46E+00	2.47E+01	2.50E+01	-2.65E-01	1.19E+00	3.10E+03	2.41E+01	3.07E+03	3.07E+03	6.03E+03
Ru1															
							-	-	-						
	-1.14E-01	7.66E+01	-7.00E-05	3.76E+01	4.04E+00	2.08E+00	3.64E+00	6.30E+00	9.95E+00	1.35E-01	1.04E+02	2.27E+01	1.26E+02	1.26E+02	1.19E+02
C9															
							-	-	-						
	-1.04E-01	7.49E+01	-1.97E-04	3.76E+01	4.03E+00	2.07E+00	3.35E+00	6.23E+00	9.58E+00	9.47E-02	9.56E+01	2.30E+01	1.19E+02	1.19E+02	1.24E+02
C10															
							-	-	-						
	-1.09E-01	7.52E+01	-1.11E-04	3.76E+01	4.03E+00	2.08E+00	3.37E+00	6.24E+00	9.61E+00	1.16E-01	9.77E+01	2.28E+01	1.20E+02	1.20E+02	1.21E+02
C13															

C16	-9.09E-02	7.57E+01	-5.60E-05	3.76E+01	4.02E+00	2.07E+00	-3.52E+00	-6.13E+00	-9.66E+00	9.32E-02	1.00E+02	2.24E+01	1.23E+02	1.23E+02	1.26E+02
C18	-1.04E-01	7.71E+01	-4.80E-05	3.76E+01	4.04E+00	2.07E+00	-3.71E+00	-6.23E+00	-9.94E+00	1.14E-01	1.04E+02	2.30E+01	1.27E+02	1.27E+02	1.21E+02
C19	-8.40E-02	7.33E+01	-1.10E-04	3.76E+01	4.02E+00	2.07E+00	-3.05E+00	-6.06E+00	-9.11E+00	9.99E-02	8.86E+01	2.21E+01	1.11E+02	1.11E+02	1.35E+02
Cl22	-4.89E-01	2.29E+02	6.20E-05	4.57E+02	1.69E+01	6.10E-01	-2.15E+01	-3.19E+00	-2.47E+01	1.33E+00	9.98E+02	3.76E+00	1.00E+03	1.00E+03	4.24E+02
N12	-6.13E-01	7.39E+01	4.00E-05	5.43E+01	5.75E+00	1.86E+00	-3.74E+00	-6.36E+00	-1.01E+01	6.53E-01	2.36E+01	1.74E+01	4.10E+01	4.10E+01	1.58E+02
N17	-6.03E-01	7.39E+01	1.41E-04	5.43E+01	5.74E+00	1.86E+00	-3.68E+00	-6.52E+00	-1.02E+01	8.83E-01	1.93E+01	1.74E+01	3.66E+01	3.66E+01	1.68E+02
O2	-8.53E-01	1.04E+02	8.40E-05	7.47E+01	7.78E+00	1.07E+00	-5.00E+00	-2.28E+00	-7.27E+00	-9.06E-01	-9.86E+01	-4.65E+00	-9.40E+01	-9.40E+01	-5.71E+02
H24	2.00E-01	3.41E+01	3.70E-05	5.27E-01	2.92E-01	5.07E-01	-8.31E-01	-9.37E-01	-1.77E+00	4.44E-01	1.80E+01	5.96E+00	2.40E+01	2.40E+01	6.47E+00
H29	1.55E-01	3.93E+01	4.10E-05	5.43E-01	3.30E-01	5.14E-01	-9.62E-01	-4.06E-01	-1.37E+00	3.57E-02	1.90E+01	6.38E+00	2.54E+01	2.54E+01	5.79E+00

Complex **2**

Ru1	8.62E-01	9.91E+01	4.02E-04	4.40E+03	4.06E+01	2.49E+00	-2.21E+01	-2.48E+01	-2.66E+00	-1.17E+00	-2.71E+03	-2.35E+01	-2.69E+03	-2.69E+03	-5.42E+03
C7	-1.16E-01	7.31E+01	-8.10E-05	3.76E+01	4.04E+00	2.08E+00	-3.14E+00	-6.11E+00	-9.25E+00	8.08E-02	9.07E+01	2.25E+01	1.13E+02	1.13E+02	1.27E+02
C8	-1.05E-01	7.72E+01	8.60E-05	3.76E+01	4.04E+00	2.07E+00	-3.83E+00	-6.13E+00	-9.96E+00	1.24E-01	1.07E+02	2.23E+01	1.29E+02	1.29E+02	1.23E+02
C13	-9.59E-02	7.87E+01	1.57E-04	3.76E+01	4.03E+00	2.07E+00	-3.78E+00	-6.21E+00	-9.99E+00	1.31E-01	1.05E+02	2.24E+01	1.28E+02	1.28E+02	1.24E+02
C14	-8.33E-	7.24E+	7.10E-	3.76E+	4.02E+	2.07E+	-2.78E+	-5.96E+	-8.74E+	8.95E-	8.18E+	2.17E+	1.03E+	1.03E+	1.41E+

	02	01	05	01	00	00	00	00	00	02	01	01	02	02	02
C18	-1.16E-01	7.32E+01	-8.80E-05	3.76E+01	4.04E+00	2.08E+00	-3.15E+00	-6.13E+00	-9.27E+00	-1.08E-01	9.08E+01	2.25E+01	1.13E+02	1.13E+02	1.27E+02
C19	-1.05E-01	7.73E+01	5.90E-05	3.76E+01	4.04E+00	2.07E+00	-3.83E+00	-6.15E+00	-9.97E+00	-1.36E-01	1.07E+02	2.23E+01	1.29E+02	1.29E+02	1.23E+02
Cl10	-4.78E-01	2.34E+02	9.30E-05	4.57E+02	1.69E+01	5.87E-01	-2.19E+01	-3.41E+00	-2.53E+01	-1.29E+00	1.03E+03	4.26E+00	1.03E+03	1.03E+03	3.66E+02
N11	-9.49E-01	7.74E+01	5.00E-05	5.45E+01	6.07E+00	1.88E+00	-3.67E+00	-6.91E+00	-1.06E+01	-6.40E-01	1.00E+00	1.39E+01	1.49E+01	1.49E+01	3.56E+02
N16	-9.49E-01	7.75E+01	6.00E-05	5.45E+01	6.07E+00	1.88E+00	-3.67E+00	-6.90E+00	-1.06E+01	-6.04E-01	-4.94E-01	1.39E+01	1.44E+01	1.44E+01	3.58E+02
H34	1.49E-01	3.72E+01	3.70E-05	5.50E-01	3.27E-01	5.25E-01	-9.03E-01	-4.11E-01	-1.31E+00	3.97E-02	1.89E+01	4.77E+00	2.37E+01	2.37E+01	1.00E+01
H38	1.51E-01	3.74E+01	8.50E-05	5.47E-01	3.24E-01	5.25E-01	-9.09E-01	-4.18E-01	-1.33E+00	4.12E-02	1.88E+01	4.70E+00	2.35E+01	2.35E+01	9.30E+00

Complex **3**

Ru1	8.73E-01	9.61E+01	-6.31E-04	4.40E+03	4.07E+01	2.45E+00	-2.73E+01	-2.50E+01	-2.30E+00	-8.55E-01	-3.41E+03	-2.29E+01	-3.38E+03	-3.38E+03	5.84E+03
C13	-7.91E-02	7.32E+01	-2.80E-05	3.76E+01	4.01E+00	2.07E+00	-3.29E+00	-6.18E+00	-9.47E+00	-8.53E-02	9.47E+01	2.23E+01	1.17E+02	1.17E+02	1.29E+02
C14	-9.33E-02	7.21E+01	-4.90E-05	3.76E+01	4.02E+00	2.07E+00	-3.27E+00	-6.65E+00	-9.92E+00	-4.11E-01	9.41E+01	2.29E+01	1.17E+02	1.17E+02	1.27E+02
C18	-8.72E-02	7.36E+01	8.60E-05	3.76E+01	4.02E+00	2.07E+00	-3.26E+00	-6.21E+00	-9.47E+00	-9.86E-02	9.37E+01	2.23E+01	1.16E+02	1.16E+02	1.29E+02
C21	-1.18E-01	7.64E+01	-3.70E-05	3.76E+01	4.04E+00	2.08E+00	-3.50E+00	-6.31E+00	-9.81E+00	-1.79E-01	9.88E+01	2.29E+01	1.22E+02	1.22E+02	1.25E+02
C23	-9.43E-02	7.27E+01	-8.40E-05	3.76E+01	4.03E+00	2.06E+00	-3.35E+00	-6.66E+00	-1.00E+01	-4.09E-01	9.62E+01	2.29E+01	1.19E+02	1.19E+02	1.29E+02

C25	-1.17E-01	7.61E+01	1.72E-04	3.76E+01	4.04E+00	2.08E+00	-3.46E+00	-6.30E+00	-9.76E+00	1.83E-01	-9.81E+01	-2.30E+01	-1.21E+02	-1.21E+02	1.25E+02
Cl7	-4.97E-01	2.32E+02	7.30E-05	4.57E+02	1.69E+01	5.90E-01	-2.18E+01	-3.20E+00	-2.50E+01	-1.35E+00	-1.01E+03	-3.77E+00	-1.02E+03	-1.02E+03	4.99E+02
N10	-9.26E-01	7.82E+01	2.83E-04	5.44E+01	6.06E+00	1.86E+00	-3.72E+00	-7.07E+00	-1.08E+01	-9.41E-01	-2.92E+00	-1.31E+01	-1.60E+01	-1.60E+01	3.60E+02
N16	-9.30E-01	7.78E+01	2.81E-04	5.45E+01	6.06E+00	1.87E+00	-3.73E+00	-6.99E+00	-1.07E+01	-9.13E-01	-4.52E+00	-1.31E+01	-1.76E+01	-1.76E+01	3.55E+02
O2	-8.96E-01	1.04E+02	1.68E-04	7.47E+01	7.80E+00	1.09E+00	-5.04E+00	-2.27E+00	-7.31E+00	-9.29E-01	-7.73E+01	-4.31E+00	-7.30E+01	-7.30E+01	5.56E+02
O28	-8.94E-01	1.05E+02	1.36E-04	7.47E+01	7.81E+00	1.09E+00	-5.06E+00	-2.21E+00	-7.27E+00	-8.86E-01	-8.26E+01	-4.19E+00	-7.84E+01	-7.84E+01	5.53E+02
H31	1.61E-01	3.65E+01	3.80E-05	5.47E-01	3.19E-01	5.20E-01	-9.69E-01	-1.06E+00	-2.03E+00	-3.16E-01	-1.93E+01	-7.78E+00	-2.71E+01	-2.71E+01	5.20E+00
H36	1.77E-01	3.48E+01	1.80E-05	5.41E-01	3.05E-01	5.17E-01	-9.20E-01	-1.05E+00	-1.98E+00	-3.08E-01	-1.89E+01	-7.65E+00	-2.66E+01	-2.66E+01	6.36E+00

Complex **4**

Ru1	9.46E-01	1.02E+02	-2.96E-04	4.40E+03	4.07E+01	2.38E+00	-2.97E+01	-2.51E+01	-4.51E+00	-4.45E-01	-3.77E+03	-2.31E+01	-3.75E+03	-3.75E+03	6.50E+03
C2	-9.53E-02	7.64E+01	9.40E-05	3.76E+01	4.03E+00	2.06E+00	-3.39E+00	-6.18E+00	-9.57E+00	-9.19E-02	-9.45E+01	-2.19E+01	-1.16E+02	-1.16E+02	1.28E+02
C3	-9.30E-02	7.35E+01	-9.30E-05	3.76E+01	4.03E+00	2.06E+00	-3.29E+00	-6.17E+00	-9.46E+00	-1.09E-01	-9.52E+01	-2.33E+01	-1.18E+02	-1.18E+02	1.32E+02
C4	-9.54E-02	7.65E+01	-5.80E-05	3.76E+01	4.03E+00	2.06E+00	-3.40E+00	-6.18E+00	-9.58E+00	-1.18E-01	-9.46E+01	-2.19E+01	-1.17E+02	-1.17E+02	1.28E+02
C5	-8.74E-02	7.61E+01	-7.70E-05	3.76E+01	4.03E+00	2.06E+00	-3.50E+00	-6.23E+00	-9.73E+00	-1.29E-01	-1.01E+02	-2.36E+01	-1.25E+02	-1.25E+02	1.26E+02
C6	-9.30E-02	7.35E+01	-5.60E-05	3.76E+01	4.03E+00	2.06E+00	-3.28E+00	-6.16E+00	-9.45E+00	-1.27E-01	-9.49E+01	-2.33E+01	-1.18E+02	-1.18E+02	1.32E+02

	02	01	05	01	00	00	00	00	00	01	01	01	02	02	02
C7	-8.74E-02	7.61E+01	-8.00E-05	3.76E+01	4.03E+00	2.06E+00	-3.51E+00	-6.23E+00	-9.74E+00	1.46E-01	-1.01E+02	2.36E+01	1.25E+02	1.25E+02	1.26E+02
N10	-6.07E-01	7.84E+01	1.22E-04	5.42E+01	5.78E+00	1.82E+00	-3.84E+00	-6.59E+00	-1.04E+01	6.51E-01	-1.74E+01	1.59E+01	3.33E+01	3.33E+01	1.33E+02
N13	-6.07E-01	7.84E+01	-4.29E-04	5.42E+01	5.78E+00	1.82E+00	-3.84E+00	-6.59E+00	-1.04E+01	6.36E-01	-1.74E+01	1.59E+01	3.33E+01	3.33E+01	1.33E+02
N15	-9.65E-01	7.53E+01	1.70E-04	5.46E+01	6.10E+00	1.86E+00	-4.55E+00	-6.58E+00	-1.11E+01	3.83E-01	-6.20E+01	1.36E+01	7.56E+01	7.56E+01	2.10E+02

Complex **5**

Ru1	9.26E-01	1.01E+02	-9.21E-04	4.40E+03	4.06E+01	2.43E+00	-2.82E+01	-2.44E+01	-3.84E+00	4.94E-01	-3.57E+03	2.23E+01	-3.55E+03	-3.55E+03	5.25E+03
C18	-8.75E-02	7.60E+01	-2.80E-04	3.76E+01	4.03E+00	2.06E+00	-3.44E+00	-6.11E+00	-9.55E+00	7.76E-02	-9.92E+01	2.27E+01	1.22E+02	1.22E+02	1.29E+02
C20	-9.77E-02	7.36E+01	-1.45E-04	3.76E+01	4.03E+00	2.07E+00	-3.26E+00	-6.04E+00	-9.29E+00	9.89E-02	-9.45E+01	2.26E+01	1.17E+02	1.17E+02	1.32E+02
C22	-8.70E-02	7.59E+01	7.70E-05	3.76E+01	4.03E+00	2.06E+00	-3.43E+00	-6.10E+00	-9.53E+00	9.16E-02	-9.91E+01	2.27E+01	1.22E+02	1.22E+02	1.29E+02
C23	-1.01E-01	7.60E+01	-4.40E-05	3.76E+01	4.03E+00	2.07E+00	-3.31E+00	-6.03E+00	-9.34E+00	1.18E-01	-9.15E+01	2.12E+01	1.13E+02	1.13E+02	1.33E+02
C26	-9.72E-02	7.36E+01	-2.40E-05	3.76E+01	4.03E+00	2.07E+00	-3.26E+00	-6.03E+00	-9.29E+00	1.14E-01	-9.46E+01	2.26E+01	1.17E+02	1.17E+02	1.32E+02
C27	-1.01E-01	7.59E+01	-1.10E-04	3.76E+01	4.03E+00	2.07E+00	-3.30E+00	-6.03E+00	-9.33E+00	1.38E-01	-9.13E+01	2.12E+01	1.13E+02	1.13E+02	1.33E+02
N14	-9.58E-01	8.06E+01	1.32E-04	5.44E+01	6.10E+00	1.85E+00	-3.97E+00	-7.06E+00	-1.10E+01	5.43E-01	-1.27E+01	1.30E+01	2.57E+01	2.57E+01	3.17E+02
N15	-9.52E-01	7.36E+01	3.41E-04	5.46E+01	6.05E+00	1.90E+00	-3.79E+00	-6.70E+00	-1.05E+01	2.78E-01	-1.69E+01	1.34E+01	3.04E+01	3.04E+01	2.83E+02

N21	-9.59E-01	8.06E+01	8.90E-05	5.44E+01	6.11E+00	1.85E+00	-3.97E+00	-7.07E+00	-1.10E+01	4.49E-01	1.32E+01	1.30E+01	2.62E+01	2.62E+01	3.16E+02

Table S5: The atomic NMR magnetazability and shielding for the selected atoms in the complexes using combined basis sets ECP(Ru)|6-31+G(d,p)

Complex **1**															
q(A)	Vol(A), 0.001	L(A)	K(A)	LI(A)	DI(A,A')/2	χ_{Intra_Iso}(A)	χ_{bond_Iso}(A)	χ_{Iso}(A)	Mu(A)	σ_{Iso}(A, A)	σ_{Iso}(A', A)	σ_{Iso}(A)	Isotropic	Anisotropy
9.40E-01	1.03E+02	-2.84E-04	3.27E+01	1.24E+01	2.70E+00	-1.42E+01	-4.48E+01	-3.06E+01	1.07E+00	1.52E+03	2.53E+01	1.55E+03	-4.41E+02	6.61E+02
-7.56E-02	7.39E+01	-2.30E-05	3.78E+01	3.98E+00	2.09E+00	-3.04E+00	-6.24E+00	-9.29E+00	-1.03E-01	8.71E+01	1.29E+01	1.00E+02	1.10E+02	1.21E+02
-5.98E-02	7.16E+01	-2.78E-04	3.78E+01	3.97E+00	2.09E+00	-2.69E+00	-6.57E+00	-9.26E+00	-5.74E-02	7.77E+01	-7.36E+00	7.04E+01	1.01E+02	1.28E+02
-6.39E-02	7.18E+01	-2.07E-04	3.78E+01	3.97E+00	2.09E+00	-2.75E+00	-8.16E+00	-1.09E+01	-1.06E-01	8.19E+01	6.66E+00	8.85E+01	1.05E+02	1.23E+02
-6.54E-02	7.37E+01	-1.51E-04	3.78E+01	3.98E+00	2.09E+00	-3.07E+00	-2.09E+00	-5.16E+00	-8.08E-02	8.69E+01	-3.55E+01	5.14E+01	1.09E+02	1.26E+02
-7.15E-02	7.47E+01	-2.20E-05	3.78E+01	3.98E+00	2.09E+00	-3.17E+00	-3.53E+00	-6.70E+00	-9.33E-02	8.93E+01	-2.09E+01	6.84E+01	1.12E+02	1.21E+02
-4.23E-02	7.01E+01	-2.32E-04	3.78E+01	3.96E+00	2.09E+00	-2.42E+00	-7.31E-01	-1.69E+00	-8.09E-02	7.01E+01	-4.33E+01	2.68E+01	9.18E+01	1.43E+02
-4.92E-01	2.30E+02	-6.40E-05	4.59E+02	1.68E+01	6.81E-01	-2.03E+01	-3.56E+00	-2.38E+01	-1.16E+00	9.04E+02	-3.28E+00	9.01E+02	9.08E+02	5.31E+02
-7.26E-01	7.72E+01	-2.69E-04	5.47E+01	5.84E+00	1.89E+00	-3.36E+00	-3.66E+01	-3.99E+01	-6.76E-01	2.99E+00	-6.84E+01	7.13E+01	1.95E+01	1.73E+02
-7.26E-	7.72E+	-2.02E-	5.47E+	5.84E+	1.89E+	-3.36E+	-3.86E+	-4.19E+	-6.36E-	-2.77E+	-6.84E+	-7.12E+	-1.93E+	1.74E+0

01	01	04	01	00	00	00	01	01	01	00	01	01	01	2
-1.13E+00	1.29E+02	7.20E-05	7.54E+01	8.15E+00	9.82E-01	5.90E+00	-4.31E+00	-1.02E+01	1.00E+00	-8.96E+01	1.29E+01	-7.67E+01	-8.70E+01	5.43E+02
1.28E-01	4.04E+01	1.60E-05	5.64E-01	3.40E-01	5.32E-01	-9.11E-01	-2.81E+00	-3.72E+00	4.61E-01	1.75E+01	1.67E+01	3.42E+01	2.32E+01	6.57E+00
1.27E-01	4.04E+01	2.30E-05	5.64E-01	3.41E-01	5.32E-01	-9.13E-01	-3.04E+00	-3.95E+00	4.72E-01	1.75E+01	1.67E+01	3.43E+01	2.33E+01	6.51E+00

Complex **2**

-9.57E-01	1.05E+02	4.83E-04	3.27E+01	1.23E+01	2.73E+00	1.23E+01	-6.54E+01	-5.31E+01	1.06E+00	1.53E+03	2.44E+01	1.56E+03	-4.29E+02	5.46E+02
-6.65E-02	7.04E+01	4.00E-05	3.78E+01	3.97E+00	2.10E+00	-2.58E+00	-1.72E+00	-4.30E+00	-7.96E-02	-7.53E+01	-3.11E+01	-4.43E+01	-9.75E+01	1.31E+02
-7.69E-02	7.49E+01	-1.02E-04	3.78E+01	3.99E+00	2.09E+00	-3.19E+00	-4.54E+00	-7.73E+00	-9.09E-02	-8.97E+01	-5.68E+01	-3.29E+01	-1.11E+02	1.26E+02
-6.59E-02	7.67E+01	-2.96E-04	3.78E+01	3.98E+00	2.08E+00	-3.15E+00	-6.68E+00	-9.83E+00	-8.29E-02	-8.70E+01	-1.67E+01	-7.03E+01	-1.09E+02	1.26E+02
-4.00E-02	6.99E+01	-5.43E-04	3.78E+01	3.96E+00	2.08E+00	-2.20E+00	-4.69E+00	-2.49E+00	-9.34E-02	-6.43E+01	-7.19E+01	-7.61E+00	-8.54E+01	1.50E+02
-6.67E-02	7.04E+01	-1.40E-05	3.78E+01	3.97E+00	2.10E+00	-2.58E+00	-3.40E-01	-2.24E+00	-1.05E-01	-7.54E+01	-3.10E+01	-4.45E+01	-9.75E+01	1.30E+02
-7.67E-02	7.48E+01	-2.55E-04	3.78E+01	3.99E+00	2.09E+00	-3.19E+00	-3.50E+00	-6.69E+00	-8.19E-02	-8.98E+01	-5.67E+01	-3.31E+01	-1.11E+02	1.26E+02
-4.84E-01	2.34E+02	-6.80E-05	4.59E+02	1.68E+01	6.57E-01	-2.08E+01	-4.12E+00	-2.49E+01	-1.12E+00	-9.50E+02	-1.89E+01	-9.69E+02	-9.55E+02	4.05E+02
-1.16E+00	8.10E+01	-6.60E-05	5.50E+01	6.27E+00	1.89E+00	-3.34E+00	-5.67E+01	-6.00E+01	-5.24E-01	-2.40E+01	-9.76E+01	-7.36E+01	-1.13E+01	3.45E+02
-1.16E+00	8.09E+01	-2.46E-04	5.50E+01	6.27E+00	1.89E+00	-3.34E+00	-5.92E+01	-6.25E+01	-4.90E-01	-2.44E+01	-9.81E+01	-7.37E+01	-1.17E+01	3.47E+02

9.67E-02	4.09E+01	9.50E-05	5.81E-01	3.58E-01	5.45E-01	-9.04E-01	-1.89E+00	-2.80E+00	6.89E-02	1.80E+01	2.20E+01	4.00E+01	2.23E+01	1.05E+01
1.03E-01	4.10E+01	7.70E-05	5.76E-01	3.53E-01	5.45E-01	-9.10E-01	-1.87E+00	-2.78E+00	5.26E-02	1.79E+01	2.19E+01	3.98E+01	2.22E+01	9.71E+00

Complex **3**

9.59E-01	1.01E+02	2.52E-04	3.27E+01	1.23E+01	2.71E+00	1.57E+01	-2.51E+01	-9.33E+00	7.69E-01	1.45E+03	2.38E+01	1.47E+03	-5.15E+02	5.85E+02
-5.37E-02	7.08E+01	-6.10E-05	3.78E+01	3.97E+00	2.09E+00	-2.74E+00	-1.78E+00	-4.52E+00	7.69E-02	-7.80E+01	-3.43E+01	-4.37E+01	-9.77E+01	1.36E+02
-6.12E-02	6.99E+01	-1.90E-04	3.78E+01	3.97E+00	2.09E+00	-2.66E+00	-1.16E+00	-3.81E+00	4.01E-01	-7.74E+01	-1.80E+01	-5.94E+01	-9.83E+01	1.35E+02
-5.33E-02	7.09E+01	-1.48E-04	3.78E+01	3.97E+00	2.09E+00	-2.71E+00	8.01E-01	-3.52E+00	8.25E-02	-7.71E+01	-3.46E+01	-4.25E+01	-9.68E+01	1.37E+02
-7.24E-02	7.38E+01	-1.20E-04	3.78E+01	3.98E+00	2.09E+00	-2.90E+00	-3.34E+00	-6.24E+00	1.34E-01	-8.08E+01	-2.52E+00	-7.83E+01	-1.02E+02	1.32E+02
-6.28E-02	7.02E+01	-2.92E-04	3.78E+01	3.98E+00	2.09E+00	-2.69E+00	3.87E-01	-3.08E+00	4.12E-01	-7.80E+01	-1.87E+01	-5.94E+01	-9.88E+01	1.36E+02
-7.20E-02	7.35E+01	-2.53E-04	3.78E+01	3.98E+00	2.09E+00	-2.88E+00	-2.91E+00	-5.79E+00	1.42E-01	-8.04E+01	-2.87E+00	-7.76E+01	-1.02E+02	1.32E+02
-4.94E-01	2.33E+02	8.90E-05	4.59E+02	1.68E+01	6.69E-01	-2.04E+01	-3.83E+00	-2.42E+01	1.16E+00	-9.18E+02	-1.43E+01	-9.32E+02	-9.23E+02	6.30E+02
-1.14E+00	8.19E+01	-2.23E-04	5.49E+01	6.27E+00	1.87E+00	-3.46E+00	-3.07E+01	-3.42E+01	9.04E-01	-1.84E+01	-6.25E+01	-4.41E+01	-4.93E+00	3.41E+02
-1.14E+00	8.18E+01	-5.60E-05	5.49E+01	6.27E+00	1.87E+00	-3.46E+00	-3.25E+01	-3.60E+01	8.69E-01	-1.79E+01	-6.25E+01	-4.46E+01	-4.43E+00	3.41E+02
-1.15E+00	1.27E+02	-1.11E-04	7.54E+01	8.14E+00	1.01E+00	-5.80E+00	-1.14E+01	-1.72E+01	8.93E-01	-7.45E+01	1.02E-01	-7.46E+01	-7.20E+01	5.01E+02
-1.15E+00	1.27E+02	-1.17E-04	7.54E+01	8.14E+00	1.01E+00	-5.82E+00	-1.19E+01	-1.77E+01	8.78E-01	-7.53E+01	5.23E-01	-7.54E+01	-7.28E+01	4.99E+02

0	02	04	01	00	00	00	01	01	01	01	02	01	01	2
1.18E-01	3.91E+01	2.20E-05	5.75E-01	3.43E-01	5.39E-01	-9.17E-01	-5.56E+00	-6.48E+00	3.52E-01	1.80E+01	-9.34E+00	8.68E+00	2.41E+01	6.77E+00
1.22E-01	3.86E+01	3.20E-05	5.74E-01	3.40E-01	5.39E-01	-9.03E-01	-5.80E+00	-6.70E+00	3.54E-01	1.79E+01	-9.83E+00	8.07E+00	2.40E+01	7.09E+00
Complex **4**														
9.82E-01	1.12E+02	-8.61E-04	3.27E+01	1.24E+01	2.63E+00	1.72E+01	-3.72E+01	-2.00E+01	3.23E-01	1.38E+03	-2.40E+01	1.41E+03	-5.81E+02	7.13E+02
-5.75E-02	7.36E+01	-2.60E-05	3.78E+01	3.98E+00	2.08E+00	-2.80E+00	-3.30E+00	-6.10E+00	7.55E-02	7.77E+01	-2.22E+01	5.55E+01	9.86E+01	1.32E+02
-5.54E-02	7.08E+01	-2.19E-04	3.78E+01	3.97E+00	2.08E+00	-2.71E+00	-3.84E+00	-6.55E+00	7.39E-02	7.94E+01	-7.69E+00	7.17E+01	1.02E+02	1.32E+02
-5.77E-02	7.36E+01	-3.00E-05	3.78E+01	3.98E+00	2.08E+00	-2.81E+00	-2.41E+00	-5.22E+00	9.46E-02	7.79E+01	-2.22E+01	5.57E+01	9.87E+01	1.32E+02
-4.58E-02	7.27E+01	-9.20E-05	3.78E+01	3.97E+00	2.08E+00	-2.85E+00	-5.17E+00	-8.02E+00	9.35E-02	8.34E+01	-6.44E+00	8.98E+01	1.07E+02	1.31E+02
-5.55E-02	7.07E+01	-3.53E-04	3.78E+01	3.97E+00	2.08E+00	-2.71E+00	-3.48E+00	-6.19E+00	8.67E-02	7.92E+01	-7.80E+00	7.14E+01	1.02E+02	1.32E+02
-4.61E-02	7.27E+01	-7.90E-05	3.78E+01	3.97E+00	2.08E+00	-2.85E+00	-4.95E+00	-7.80E+00	1.01E-01	8.35E+01	-6.38E+00	8.99E+01	1.07E+02	1.31E+02
-7.38E-01	8.21E+01	2.73E-04	5.47E+01	5.89E+00	1.85E+00	-3.51E+00	-1.44E+01	-1.79E+01	5.90E-01	1.80E+00	-3.50E+01	3.68E+01	1.66E+01	1.21E+02
-7.38E-01	8.21E+01	2.80E-04	5.47E+01	5.89E+00	1.85E+00	-3.51E+00	-1.46E+01	-1.81E+01	5.75E-01	1.80E+00	-3.50E+01	3.68E+01	1.66E+01	1.21E+02
-1.18E+00	7.93E+01	-4.18E-04	5.51E+01	6.30E+00	1.87E+00	-4.22E+00	-2.86E+01	-3.28E+01	3.23E-01	3.98E+01	-6.59E+01	1.06E+02	5.34E+01	1.95E+02
Complex **5**														
9.80E-01	1.09E+02	1.36E-03	3.27E+01	1.23E+01	2.69E+00	1.65E+01	-5.14E+01	-3.49E+01	5.13E-01	1.36E+03	-2.32E+01	1.38E+03	-6.08E+01	4.66E+02

							01	01					02	
-4.88E-02	7.28E+01	-3.90E-04	3.78E+01	3.97E+00	2.08E+00	-2.82E+00	-5.26E+00	-8.08E+00	6.77E-02	-8.26E+01	-1.05E+00	-8.15E+01	-1.04E+02	1.33E+02
-5.86E-02	7.09E+01	-3.20E-05	3.78E+01	3.97E+00	2.08E+00	-2.72E+00	-1.28E+00	-4.00E+00	1.08E-01	-7.85E+01	-2.39E+01	-5.46E+01	-9.99E+01	1.34E+02
-4.81E-02	7.26E+01	4.30E-05	3.78E+01	3.97E+00	2.08E+00	-2.81E+00	-5.08E+00	-7.89E+00	6.63E-02	-8.24E+01	-1.02E+00	-8.14E+01	-1.04E+02	1.33E+02
-6.19E-02	7.32E+01	-2.73E-04	3.78E+01	3.98E+00	2.08E+00	-2.73E+00	-2.89E+00	-5.62E+00	1.00E-01	-7.44E+01	-4.68E+01	-2.76E+01	-9.43E+01	1.38E+02
-5.90E-02	7.11E+01	-3.44E-04	3.78E+01	3.97E+00	2.08E+00	-2.72E+00	-1.14E+00	-3.86E+00	1.17E-01	-7.88E+01	-2.38E+01	-5.49E+01	-1.00E+02	1.34E+02
-6.16E-02	7.31E+01	-2.82E-04	3.78E+01	3.98E+00	2.08E+00	-2.73E+00	-2.89E+00	-5.62E+00	9.87E-02	-7.42E+01	-4.68E+01	-2.74E+01	-9.40E+01	1.38E+02
-1.17E+00	8.46E+01	-2.33E-04	5.49E+01	6.31E+00	1.86E+00	-3.60E+00	-2.02E+01	-2.38E+01	-4.48E-01	-6.06E+00	-4.15E+01	-3.55E+01	-6.43E+00	2.96E+02
-1.17E+00	7.77E+01	-4.56E-04	5.51E+01	6.26E+00	1.91E+00	-3.45E+00	-4.33E+01	-4.68E+01	-2.20E-01	-9.09E+00	-1.00E+02	-9.11E+01	-4.13E+00	2.62E+02
-1.17E+00	8.46E+01	-2.77E-04	5.49E+01	6.31E+00	1.86E+00	-3.61E+00	-2.10E+01	-2.46E+01	-3.55E-01	-5.54E+00	-4.13E+01	-3.57E+01	-6.90E+00	2.94E+02