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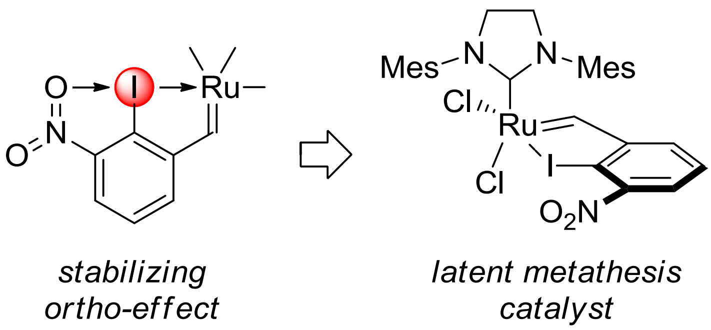

- ruthenium metathesis catalyst incorporating a chelating 2-iodo-3-nitrobenzylidene ligand was synthesized
- the complex displays latent behaviour in model RCM reactions at room temperature
- nitro group present in ortho position to the coordinating iodine atom stabilizes the chelate

Latent Metathesis Catalyst Stabilized with $NO_2 \cdots I$ Interaction

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ABSTRACT A modified Hoveyda-Grubbs metathesis catalyst incorporating a chelating 2-iodo-3-nitrobenzylidene ligand is described. The complex displays very little activity in model metathesis reactions at rt, while easily initiates at slightly elevated temperatures. Latent behavior of the catalyst is attributed to a through-space electron-donating effect of the nitro group, which stabilizes the chelate by the formation of $NO_2 \rightarrow I \rightarrow Ru$ triad.

KEYWORDS (Word Style "BG_Keywords"). Catalysis, metathesis, halogen coordination, ortho effect, donor-acceptor complexes.

MANUSCRIPT TEXT (Word Style "TA_Main_Text"). Coordination of covalently bonded halogen atoms remains largely unexplored area of organometallic chemistry, and only a limited number of examples of stable complexes featured with the rare M···X-R interaction is described in literature.[1] In contrast to the common 'halogen bonding' phenomenon, in which halogens act as acceptors of the electron density, giving highly linear interactions with nucleophilic species,[2] their donor abilities are far less recognized.[3] Due to anisotropic character of the electron density distribution with a torus of negative potential encircling the halogen atoms, their *dative* interactions with electrophiles require side bonding with coordination angles close to 90 degrees.[2a] Moreover, the σ-donor properties are relatively weak, and thus isolable complexes are usually observed for chelate ligands with two different coordinating sites, when one of which is a more powerful donor atom. Recently, we described a family of halogen-chelated Hoveyda-Grubbs type complexes featured with the unique ruthenium-halogen interaction[4] demonstrated on stable bromine and iodine derivatives (**1**-**4**, Chart 1).[5,6]

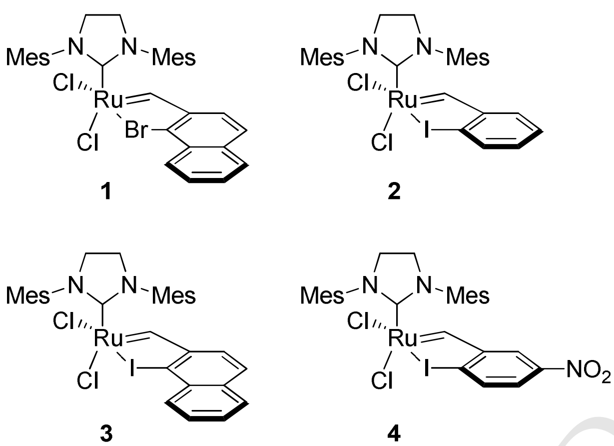
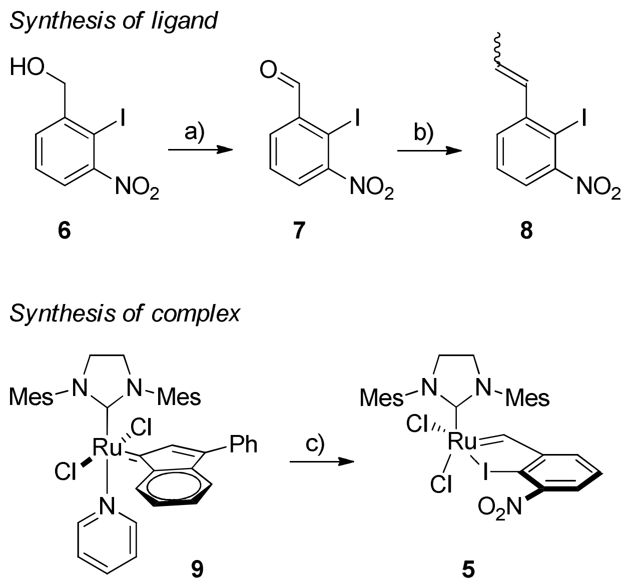


Chart 1. Selected metathesis catalysts bearing chelating halogen atom. Mes = 2,4,6-trimethylphenyl.

The complexes displayed a *cis*-Cl_2 geometry,[7] and were highly active as catalysts in model metathesis reactions at moderate temperatures.[5] Further studies shed more light on their unique structural and electronic characteristics. Particularly, introduction of nitro group in *para* position to the chelating iodine atom (**4**) destabilized the chelate, but also *decreased* its catalytic activity, as compared with **2**. The counterintuitive result was rationalized with different initiation mechanism, in which Ru···I bond is not breaking in the rate-determining step of the initiation process.[6] In our report we present synthesis and properties of isomeric complex **5**, in which interaction between substituents in the benzylidene ring results in unexpected stability and activity in model metathesis reactions.

Synthesis of the ruthenium complex **5** started from preparation of propenylbenzene ligand **8** by oxidation of 2-iodo-3-nitrobenzyl alcohol[6] (**6**), followed by the Wittig reaction (Scheme 1).



Scheme 1. Synthesis of ligand **8** and complex **5**. a) PCC, CH_2Cl_2; **7**, 98%; b) $Ph_3PCH_2CH_3Br$, *t*-PeOK/toluene, THF; **8**, 65%; c) **8**, toluene, 80 °C, 30 min, then rt, filtration; **5**, 78%. PCC = Pyridinium chlorochromate.

Next, ligand **8** was reacted with **9** in toluene at 80 °C for 30 minutes[5] to give complex **5** as a toluene solvate (*ca.* 1:1) in very good yield (78%). The product was characterized with ^{1}H and ^{13}C NMR, MS, IR and elemental analysis, and the data was consistent with the expected formula. Then, crystals suitable for X-ray diffraction studies were obtained by layering of CH_2Cl_2 solution of **5** with methanol, and keeping the sample at -20 °C for few days.

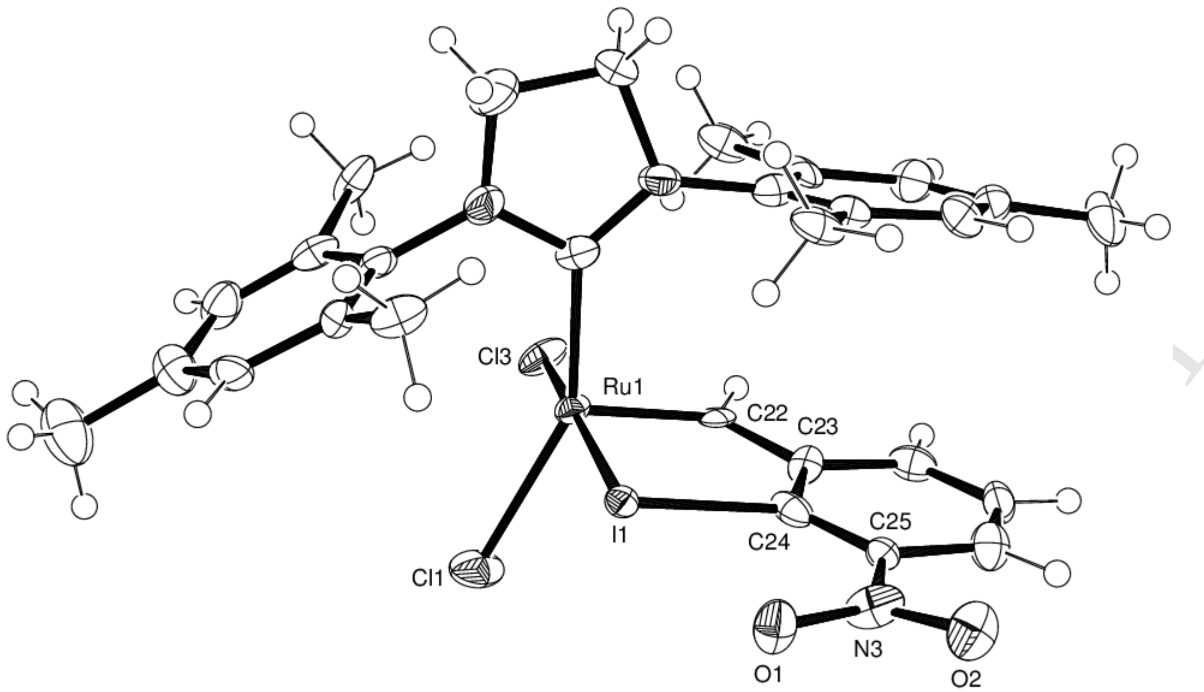


Figure 1. ORTEP[8] drawings of **5**·CH_2Cl_2 represented by thermal ellipsoids drawn at the 50% probability level (solvent molecule omitted for clarity). Selected bond lengths (Å) and angles (deg) are presented in Table 1.

Parameter/ complex	**2**[5]	**4**[6]	**5**
Ru···I	2.646(1)	2.633(1)	2.596(2)
I-C_{Ar}	2.095(4)	2.091(3)	2.10(2)
∠ Ru···I-C_{Ar}	89.48(9)	90.31(7)	90.8(5)
∠ I-C_{Ar}-C_{Ar} a)	114.3(2)/122.3(2)	113.6(2)/122.7(2)	113(1)/126(1)
^{13}C NMR Ru=CH b)	281.5	276.8	279.0
^{13}C NMR I-C_{Ar} c)	100.4	107.6	93.1
^{13}C NMR I-C_{Ar} c) (free ligand)	99.2/100.2	106.7/108.4	90.0/91.6

Table 1. Selected bond lengths (Å), angles (deg) and ^{13}C NMR parameters (δ in ppm) of complexes **2**,[5] **4**,[6] and **5**. a) – values separated with slash correspond to angles I(1)-C(24)-C(23) and I(1)-C(24)-C(25) at Figure 1, respectively; b) - values of ^{1}H NMR chemical shifts of Ru=CH benzylidene protons

varied only slightly within the series (18.10±0.02 ppm); c) – peaks were assigned on the base of abnormal chemical shift values of the aromatic carbons (90-110 ppm range), shielded with 'heavy atom effect'[9] of adjacent iodine atom.

The complex **5** crystallized in the monoclinic P2(1)/n space group, and displayed parameters similar to related *cis*-Cl_2 structures of iodocomplexes **2-4** (Figure 1 and Table 1).[5,6] Interesting exception was surrounding of iodine atom with close proximity of adjacent nitro group. The NO_2 substituent was almost coplanar with the aromatic ring (C(24)-C(25)-N(3)-O(1)=11(3)°), and one of the oxygen atoms was crowded near iodine at distance of 2.91(1)Å.[10] Presence of the O···I interaction was also supported by little tilt of C-I bond (I(1)-C(24)-C(25)=126(1)°), suggesting some repulsion with NO_2 fragment (Table 1).[11]

Next, complex **5** was tested as catalyst in metathesis reactions with model RCM substrates: diethyl diallylmalonate (DEDAM) and diethyl allylmethallylmalonate.[12] Surprisingly, **5** appeared almost inactive at 25 °C,[13] but only little increase of temperature caused upswing in the catalytic activity,[14] and relatively fast conversion of both substrates.[15] (Figure 2).

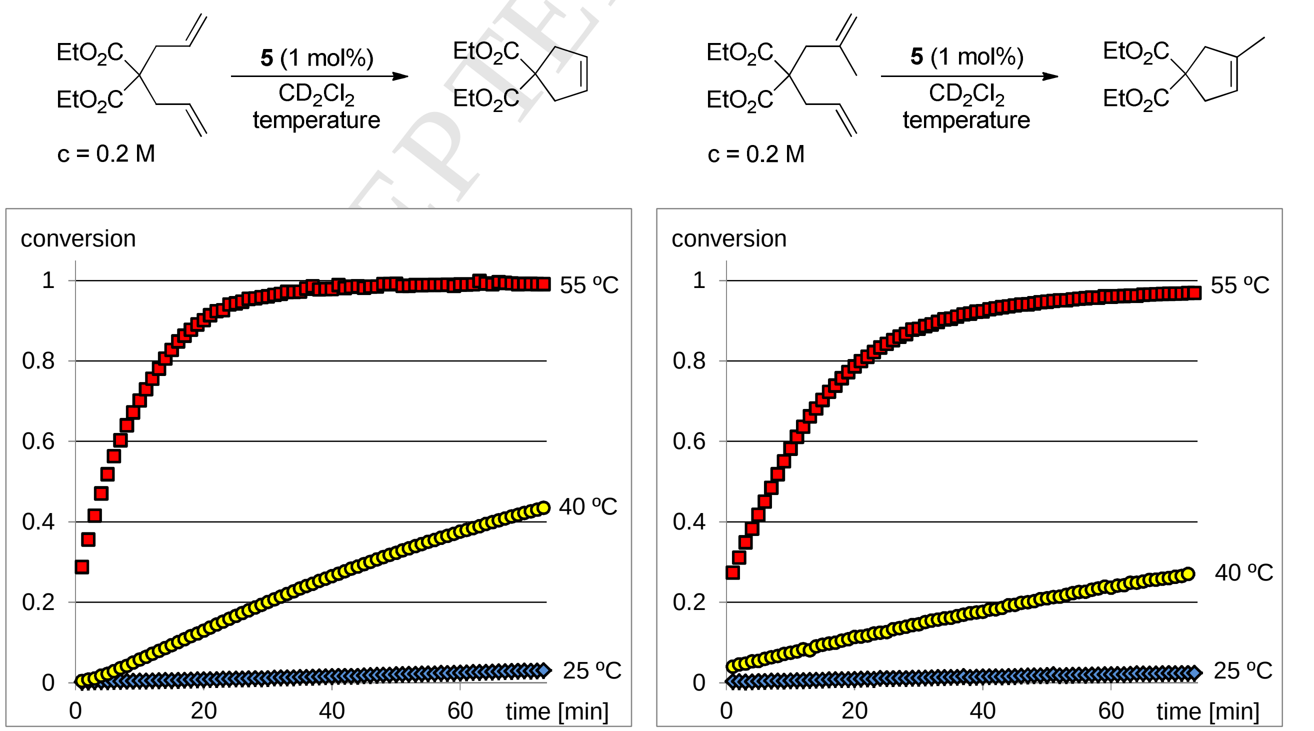


Figure 2. Reaction profiles of the ring-closing metathesis at 25, 40 and 55 °C determined by ^{1}H NMR:[12] (left) diethyl diallylmalonate (1 mol% of **5**, CD_2Cl_2, 0.2 M concentration of substrate); (right) diethyl allylmethallylmalonate (1 mol% of **5**, CD_2Cl_2, 0.2 M concentration of substrate).[14]

The latent behavior of **5** (*o*-NO_2) at 25 °C clearly contrasted with properties of other halogen-chelated complexes, which under similar conditions gave 55%, and 35% of conversion of DEDAM, for **2**[5] and **4** (*p*-NO_2),[6] respectively. Particular differences were observed also between the two families: halogen-chelated and parent (ether-chelated) Hoveyda-Grubbs complexes. For the latter family presence of electron-withdrawing groups in benzylidene ring is a well-known mode of activation,[16] and also presence of substituents in *ortho* position increases performance by out-of-plane distortion of coordinating O*i*Pr arm.[17] In turn, for the iodocomplexes the *both* effects seem to be reversed: introduction of NO_2 group in *para* position decreases catalytic activity,[6] while for *ortho*-NO_2 substituted complex **5** the inhibiting effect is even stronger. To rationalize the data, we studied relative stability of the chelates in two ligand exchange reactions between complexes **2** and **5** (**2** + **8** ⇆ **5** + 2-iodopropenylbenzene; first reaction starting from **2** and **8**; second reaction starting from **5** + 2-iodopropenylbenzene; equimolar solutions of the reagents in CD_2Cl_2 were equilibrated at 40° C for 40 h; see Supporting Information for details). Although the reactions proceeded exceedingly slow, a clear thermodynamic preference toward formation of *ortho*-substituted complex **5** (**5**:**2** $\geq$ 4:1) was observed in both cases. The result posed an open question about origin of the stabilization. In a simplified picture, proximity of one of oxygen atoms of the nitro group to the covalently bonded iodine atom unavoidably causes repulsion of electron clouds of the latter, and the resulted polarization strengthens I···Ru interaction extended on the opposite side.[18,19] However, consideration of orbital interactions may lead to alternative explanation. The bonding scheme of **5** can be recognized as an example of donor-acceptor (DA) complex, in which central iodine atom is exposed to a push-pull interaction between opposite oxygen and ruthenium centers. Related linear triads involving heavier elements of D$\rightarrow$Ng$\rightarrow$A type (Ng - nobel gas atom, e.g. $H_3N\cdots Kr\text{–}AlF_3$) were studied theoretically,[20] and their chemical bonding was described as 3-center 4-electron system formed by lone pairs of donor and noble gas, and a vacant orbital of acceptor molecule. According to the calculations, interaction with ammonia was *repulsive* and *mostly electrostatic* in character, while orbital interactions with aluminum were strongly *attractive*. Although the both considered systems differ in distinct points, predominant $NO_2{\rightarrow}I{\rightarrow}Ru$ bonding scheme seems to be the most plausible, and agrees with our preliminary DFT calculations with NBO analysis.[21] In turn spectroscopic studies revealed, that the postulated electron-donating effect of NO_2 group goes along with the selected ^{13}C NMR parameters. Aromatic *ipso* carbon atoms (I-C_{Ar}) were shielded more strongly with iodine in **5** and **8**, as compared with complexes **2** and **4** (*p*-NO_2) and their free ligands (Table 1). Accordingly, expected electron densities on the iodine atoms, which influence chemical shift values of adjacent carbon nuclei,[9] follow the same order as thermodynamic stability of the chelates (**5**>**2**>**4**).[6]

In conclusions, we presented synthesis, structure, and properties of *ortho*-NO_2 substituted iodocomplex **5**. The catalyst displays very little activity in model RCM reactions at 25 °C, while easily initiates at elevated temperatures. The latent behavior is attributed to the interaction between nitro group and adjacent iodine atom, which stabilizes the chelate with a through-space electron-donating effect.

Experimental Section

General methods are detailed in the Supporting Information.

Synthesis of **7**. A flask was charged with **6**[6] (1.545 g; 5.54 mmol) and CH_2Cl_2 (100 mL). To the solution was slowly added PCC (1.314 g; 6.09 mmol). The mixture was stirred under air overnight and then filtered through a pad of silica and eluted with CH_2Cl_2. After evaporation **7** was obtained (1.510 g; 5.45 mmol; 98%) as dark yellow crystals.

Data for **7** are as follows. Mp: 112-113 °C. ^1H NMR (400 MHz, $CDCl_3$): δ 10.15 (s, 1H), 8.01 (dd, *J*=7.4, 1.8 Hz, 1H), 7.86 (dd, *J*=7.8, 1.8 Hz, 1H), 7.59 (dd, *J*=7.8, 7.4 Hz, 1H). ^{13}C NMR (100 MHz,

$CDCl_3$): δ 194.7, 155.3, 137.4, 132.8, 129.6, 129.3, 91.7. MS (EI, *m*/*z*, relative intensity): 277 ($M^{+\bullet}$, 100), 260 (10), 230 (13), 149 (19), 103 (45), 76 (63), 50 (28). Anal. Calcd for $C_7H_4INO_3$: C, 30.35; H, 1.46; N, 5.06; I, 45.81. Found: C, 30.54; H, 1.52; N, 4.87; I, 45.68.

Synthesis of **8**. A flask was charged with ethyltriphenylphosphonium bromide (1.641 g; 4.42 mmol) and THF (35 mL), and a solution of potassium tert-amylate (3.2 mL; 5.4 mmol; 1.7 M solution in toluene) was added dropwise with stirring. After 20 min the resulting orange suspension was cooled with an ice−water bath and a solution of **7** (1.116 g; 4.02 mmol) in THF (10 mL) was added dropwise. After 15 min the cooling bath was removed, and after 1 h an aqueous solution of NH_4Cl (25 mL; 5% w/w) was added. The mixture was extracted with ethyl acetate (3 × 50 mL), and the combined organic phases were washed with brine (100 mL) and dried with $MgSO_4$. The mixture was filtered and evaporated, and the residue was separated with two column chromatographies (330 mL of silica; cyclohexane/ethyl acetate 4/1 and 250 mL of silica; *n*-hexane/acetone 6:1) to give **8** (0.751 g; 2.60 mmol; 65%) as a yellowish oil.

Data for **8**, as a mixture of *E*/*Z* isomers (ca. 1.4/1), are as follows. ^{1}H NMR (200 MHz, $CDCl_3$): δ 7.53-7.26 (m, 3H+3H), 6.66-6.56 (m, 1H), 6.39-6.28 (m, 1H), 6.19-6.00 (m, 1H), 5.99-5.81 (m, 1H), 1.91 (dd, *J*=6.6, 1.8 Hz, 3H), 1.67 (dd, *J*=7.1, 1.7 Hz, 3H). ^{13}C NMR (50 MHz, $CDCl_3$): δ 144.6, 144.5, 134.6, 133.5, 132.4, 131.9, 129.4, 129.1, 128.8, 128.3, 122.4, 122.2, 91.6, 90.0, 18.6, 14.1. MS (EI, *m*/*z*, relative intensity): 289 ($M^{+\bullet}$, 63), 272 (5), 242 (3), 145 (6), 132 (11), 115 (100). Anal. Calcd for $C_9H_8INO_2$: C, 37.39; H, 2.79; N, 4.85. Found: C, 37.57; H, 2.86; N, 4.85.

Under the olefination conditions we observed formation of by-product (probably 3-nitropropenyl benzene; 0.050 g), which was separated off by second chromatography (on TLC with *n*-hexane/acetone 6:1 as eluent R_f: **8**, 0.40; by-product, 0.47).

Synthesis of **5**. A Schlenk flask was charged with **8** (0.351 g; 1.21 mmol), **9** ('catalyst M31' Umicore; 0.748 g, 1.00 mmol), and toluene (20 mL). The mixture was stirred at 80°C for 30 min under argon and a precipitate was formed. The reaction mixture was then cooled to rt and filtered through a Schott filter, the crude product was washed with few portions of toluene and dried under vacuum to give **8** as a brownish powder (0.642 g; 0.78 mmol; 78%; toluene solvate ca. 1:1 according to ^{1}H NMR).

Data for **5** are as follows.[22] ^{1}H NMR (500 MHz, CD_2Cl_2): δ 18.12 (s, 1H), 8.41 (dd, *J*=3.2, 0.6 Hz, 1H), 7.52 (dd, *J*=3.2, 3.0 Hz, 1H), 7.20 (dd, *J*=3.0, 0.6 Hz, 1H), 7.16 (s, 1H), 7.08 (s, 1H), 6.96 (s, 1H), 5.97 (s, 1H), 4.25-4.18 (m, 1H), 4.11-3.95 (m, 2H), 3.91-3.84 (m, 1H), 2.69 (s, 3H), 2.51 (s, 3H), 2.47 (s, 3H), 2.39 (s, 3H), 2.14 (s, 3H), 1.62 (s, 3H). ^{13}C NMR (125 MHz, CD_2Cl_2): 279.0, 212.9, 158.7, 150.7, 141.1, 140.4, 139.1, 138.3, 136.1, 135.7, 135.5, 132.2, 131.4, 131.3, 131.1, 130.22, 130.17, 129.1, 125.4, 93.1, 51.9, 51.8, 21.4, 21.1, 20.4, 20.1, 18.8, 18.2. HRMS (ESI, *m*/*z*), calcd for $C_{28}H_{30}N_3O_2ClRuI$: 704.0115; found: 704.0116 (M-Cl$^{+\bullet}$). IR (KBr, cm^{-1}): 2910, 1604, 1582, 1524, 1483, 1439, 1377, 1336, 1292, 1267, 1181, 1020, 959, 850, 837, 733, 696, 629, 577, 468, 419. Anal, calcd for $C_{28}H_{30}N_3O_2ClRuI{\cdot}C_6H_5CH_3$: C, 50.55; H, 4.61; N, 5.05; found: C, 50.65; H, 4.71; N, 4.99.

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SUPPORTING INFORMATION PARAGRAPH **Supporting Information Available**. Spectra reproductions of compounds **5**, **7** and **8**, crystallographic information file (CIF) of compound **5**, and details of DFT calculations.

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[13] However, the very little activity of **5** in RCM of diethyl diallylmalonate resulted in 33% of conversion after 800 minutes (~13.3 h).

[14] Increase of the reaction rate with temperature was reported earlier for complex **3**.[5]

[15] For RCM of diethyl allylmethallylmalonate catalyzed with **5** at 55 °C conversion ≥98% was observed after ca. 1h 45 min.

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[18] The O⋯I⋯Ru system is not ideally linear, however: O(1)-I(1)-Ru(1)=156°; O(1)-I(1)-C(24)=66°.

[19] Crowding of lone pair of adjacent oxygen atom of the nitro group should also increase energy levels of iodine orbitals by a ground-state destabilization, commonly referred as α-effect. In consequence the I⋯Ru bond may become stronger due to decrease of energy gap between the interacting orbitals. For examples of α-effect between neighboring heteroatoms, see: (a) Klopman, G.; Tsuda, K.; Louis, J. B.; Davis, R. E. *Tetrahedron* **1970**, *26*, 4549-4554. (b) Nigst, T. A.; Antipova, A.; Mayr, H. *J. Org. Chem.* **2012**, *77*, 8142-8155. (c) Garver, J. M.; Gronert, S.; Bierbaum, V. M. *J. Am. Chem. Soc.* **2011**, *133*, 13894-13897. (d) Buncel, E.; Um, I.-H. *Tetrahedron* **2004**, *60*, 7801-7825.

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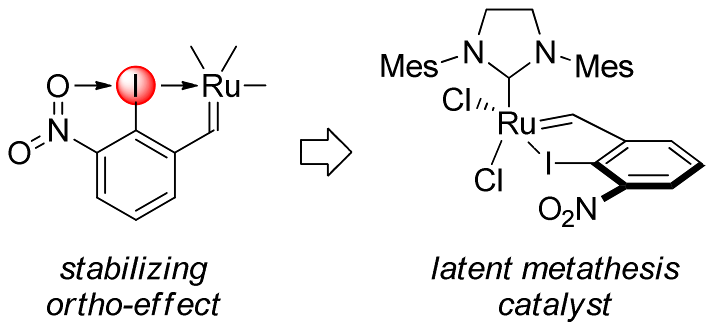
[21] Structure of the complex **5** was optimized with DFT B3LYP method with SDD basis set for Ru and I, and 6-31G(d,p) for all other atoms. Only real values of the analytical harmonic vibrational frequencies confirmed that the geometry under study corresponds to the minimum-energy structure. NBO analysis of the structure revealed, that alternative delocalization paths: n(Ru)$\rightarrow\sigma^*$(C-I) and n(I)$\rightarrow\sigma^*/\pi^*$(N-O) contribute only slightly to the structure (if any). Moreover, also n(O)$\rightarrow\sigma^*$(I-Ru) interaction was weak, supporting electrostatic nature of the O-I interaction.[20] We thank reviewer for valuable suggestions concerning of the issue.

[22] For clarity, peak resonances of toluene, present in equimolar amount in the solution, were omitted at ^{1}H and ^{13}C NMR spectra (^{1}H NMR (500 MHz, CD_2Cl_2): δ 7.26-7.22 (m, 2H), 7.19-7.12 (m, 3H), 2.34 (s, 3H). ^{13}C NMR (125 MHz, CD_2Cl_2): 138.4, 129.4, 128.6, 125.6, 21.5).

SYNOPSIS TOC (Word Style "SN_Synopsis_TOC").



Supporting Information for:

Latent Ruthenium Metathesis Catalyst Stabilized with $NO_2 \cdots I$ interaction

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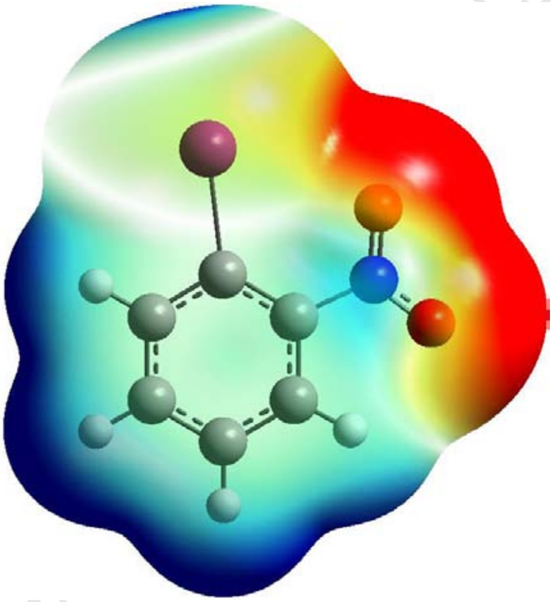


submitted to *Journal of Organometallic Chemistry*

General Informations

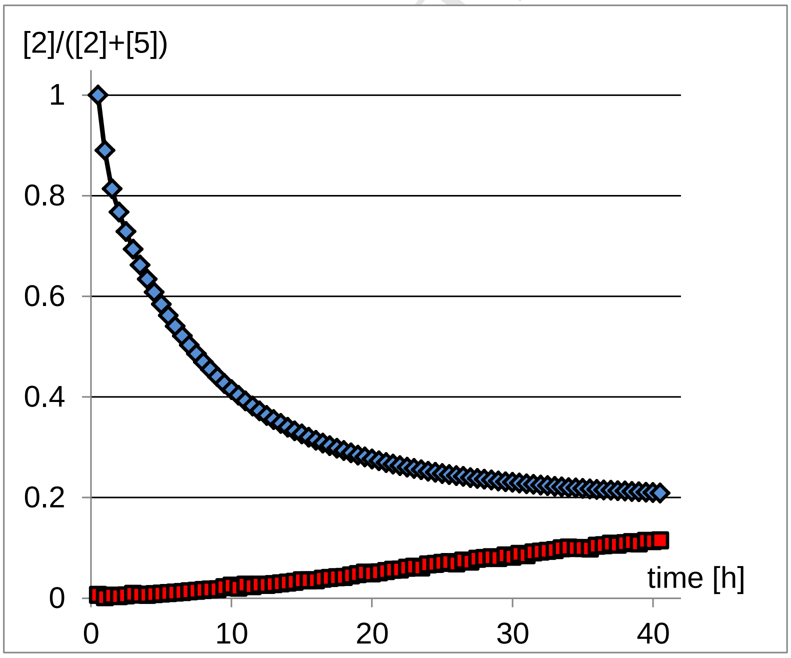
Synthesis of compounds **5** and **8** were performed under argon (oxygen-free) using the Schlenk technique. Tetrahydrofuran (THF) and toluene were dried by standard methods. *c*-Hexane and ethyl acetate used for column chromatography were distilled. Commercially available materials were used without further purification unless stated otherwise. Complex **9** was obtained from Umicore AG & Co. KG. Column chromatography was performed on silica gel 60 (Aldrich, 70-230 mesh). Thin layer chromatography (TLC) was performed on Fluka aluminium backed silica plates with fluorescent UV_{254} indicator. ^{1}H and ^{13}C NMR spectra were recorded with 500, 400 and 200 MHz spectrometers. Activity profiles and ligand exchange experiments were recorded on a 400 MHz spectrometer. Chemical shifts (δ) are given in parts per million (ppm) relative to solvent peaks $CDCl_3$ (7.24 ppm, and 77.0 ppm), and CH_2Cl_2 (5.32 ppm, and 53.84 ppm). Spin multiplicity were abbreviated as follows: s – singlet, d – doublet, t – triplet, sept – septet.

Ligand exchange procedure

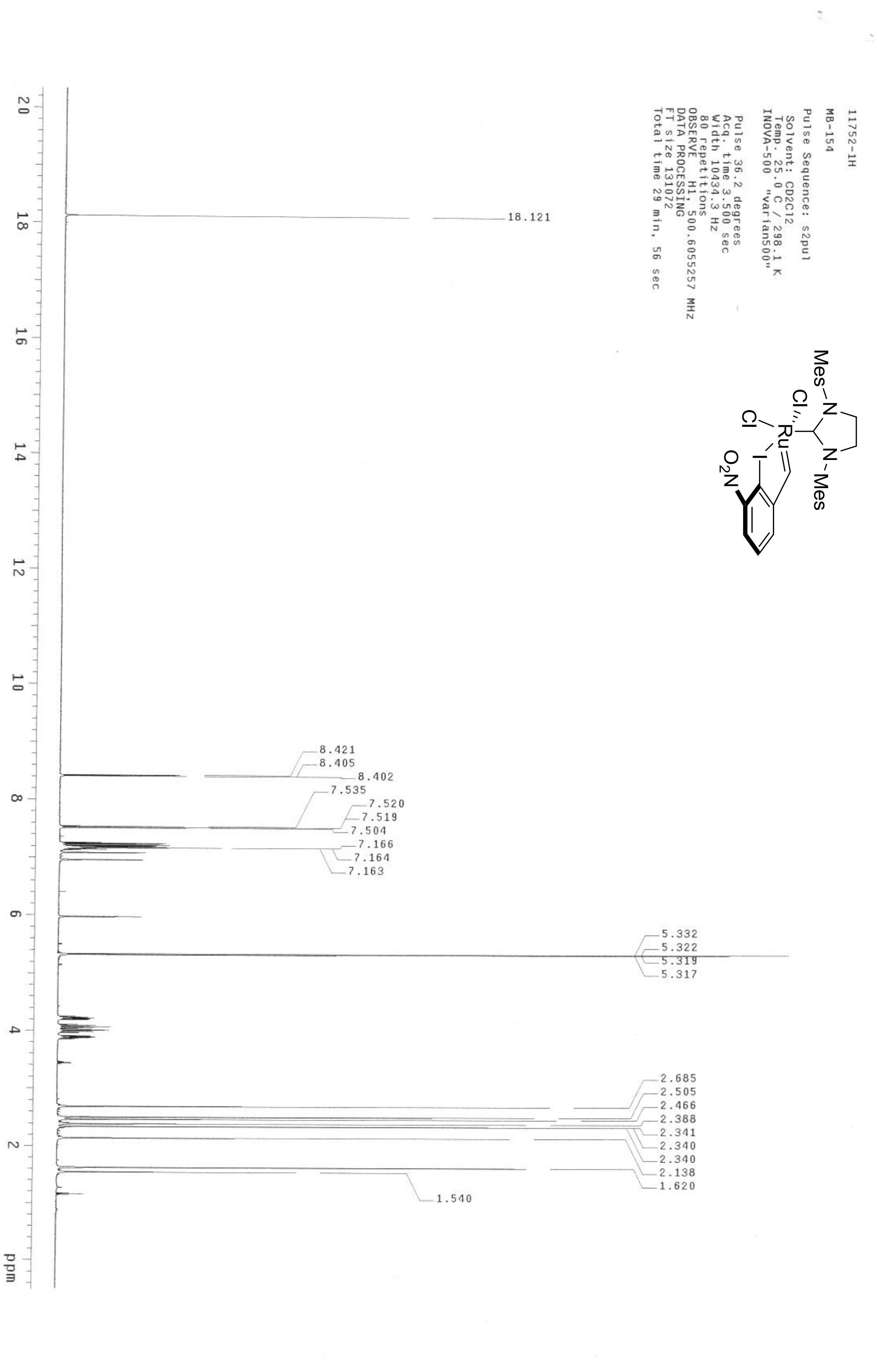
Ligand exchange experiments (**2** + **8** ⇆ **5** + 2-iodopropenylbenzene) were performed according to the procedure described below:

A 20 ml Schlenk flask was charged with catalyst **5** (0.0369 g; 0.05 mmol), 2-iodopropenylbenzene (0.0122 g; 0.05 mmol), CD_2Cl_2 (1 ml), and the mixture was argonated with three freeze-pump-thaw cycles. Ca 0.7 ml of the solution was transferred into Wilmad Young tube under argon and sealed. The tube was kept at 40 °C and ^{1}H NMR spectra (0-20 ppm range) were recorded every 30 minutes. Benzylidene proton resonances (δ=18.06 ppm for **2**, and δ=18.12 ppm for **5**) were integrated and sum of the integrals was normalized to the number of 1 (■).

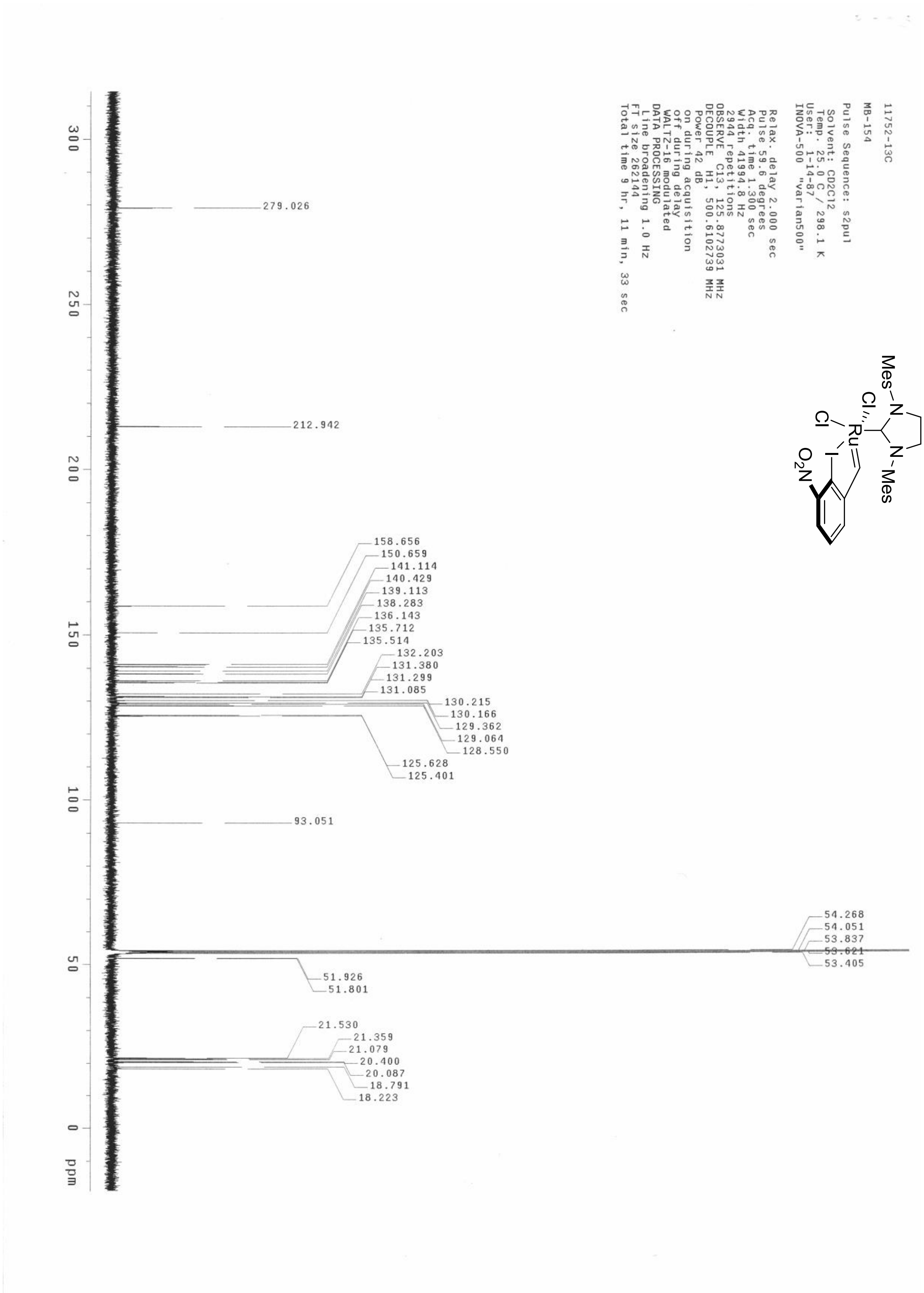
The same procedure was used for a mixture of **2** (0.0346 g; 0.05 mmol), **8** (0.0145 g; 0.05 mmol), and CH_2Cl_2 (1 ml) (■). After 40 h the mixtures did not reached an equilibrium state.



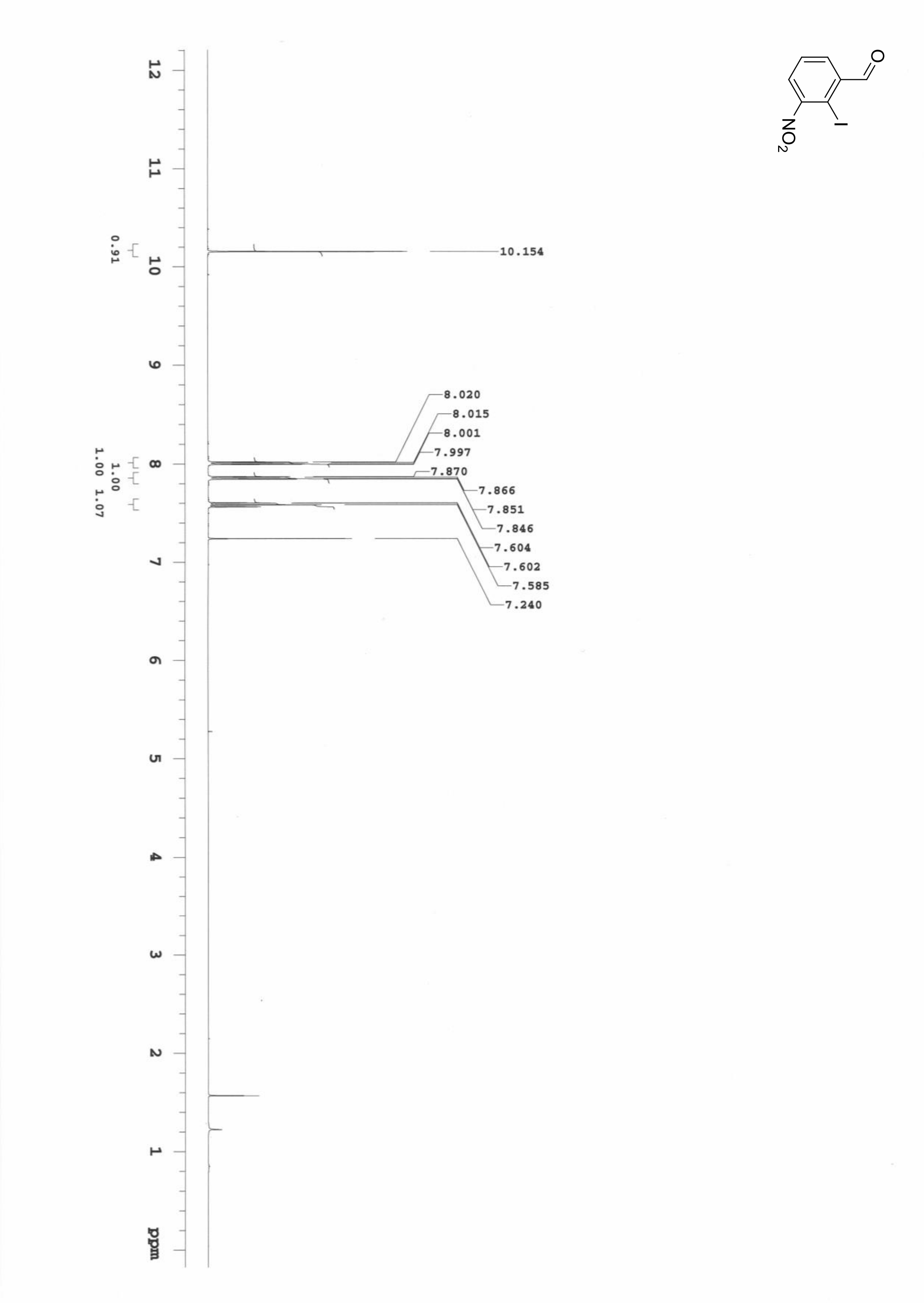
Reproduction of ^{1}H NMR spectrum of complex **5**.



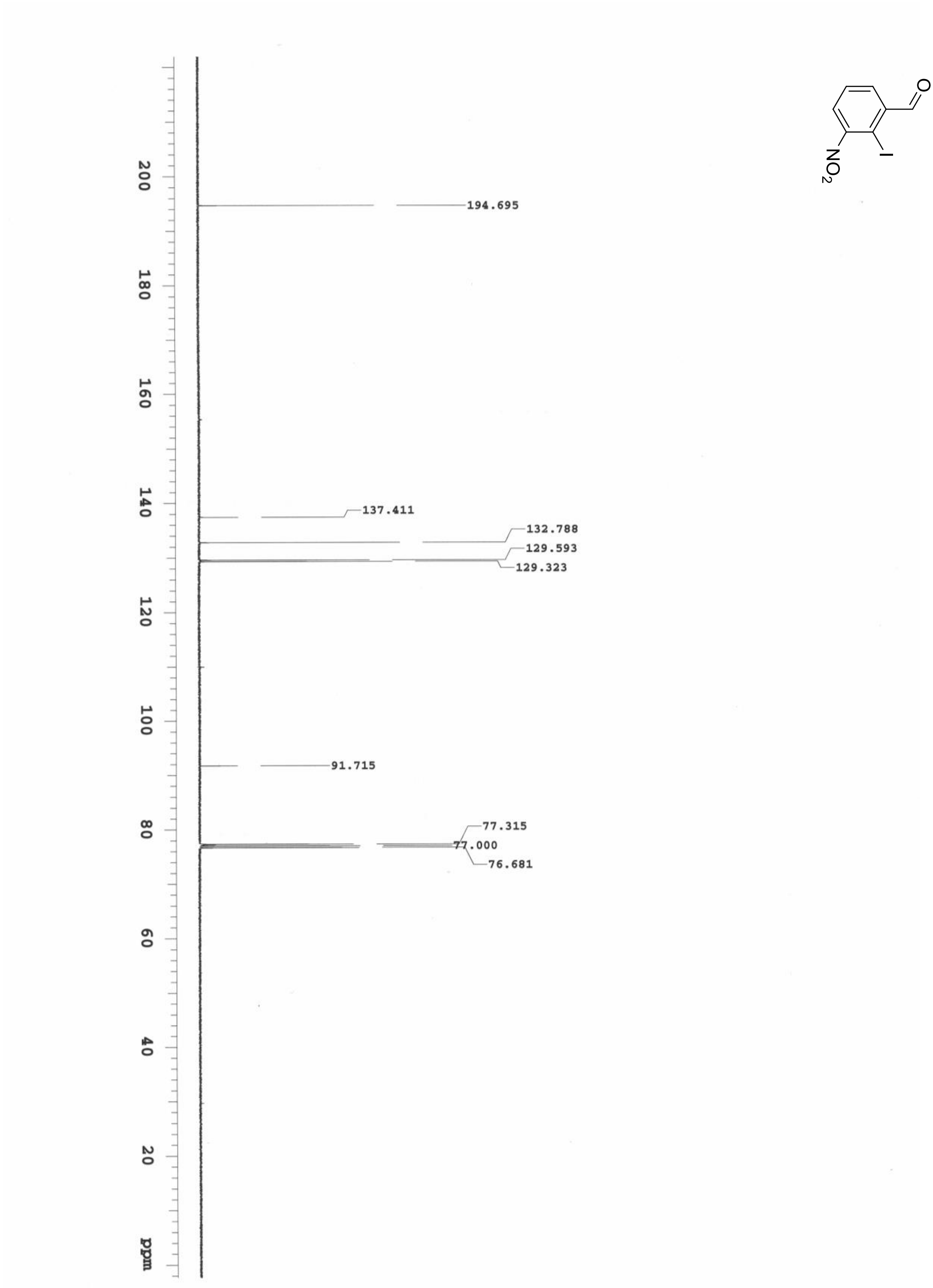
Reproduction of [13]C NMR spectrum of complex **5**.



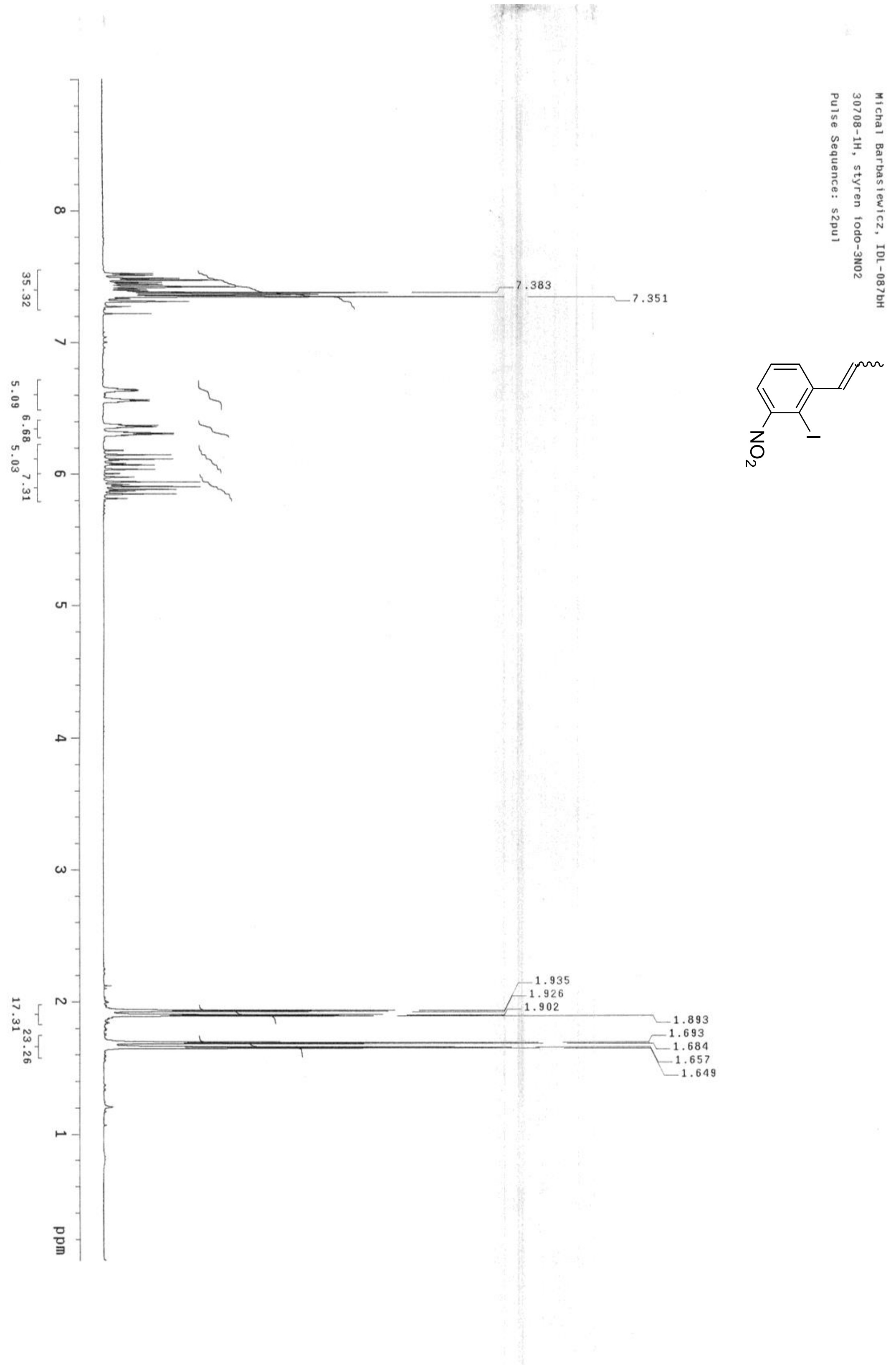
Reproduction of [1]H NMR spectrum of compound **7**.



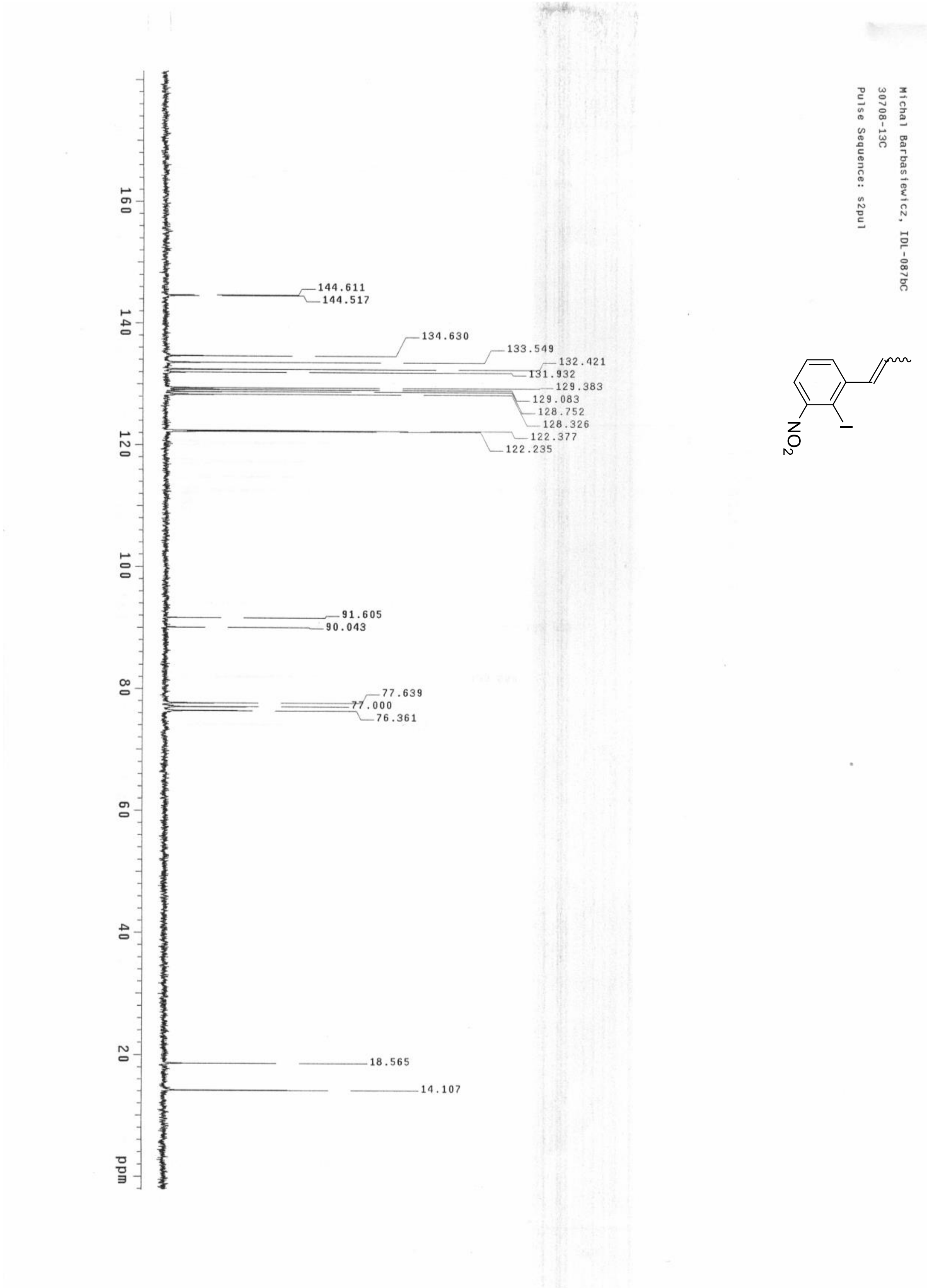
Reproduction of ^{13}C NMR spectrum of compound **7**.



Reproduction of ^{1}H NMR spectrum of compound **8**.

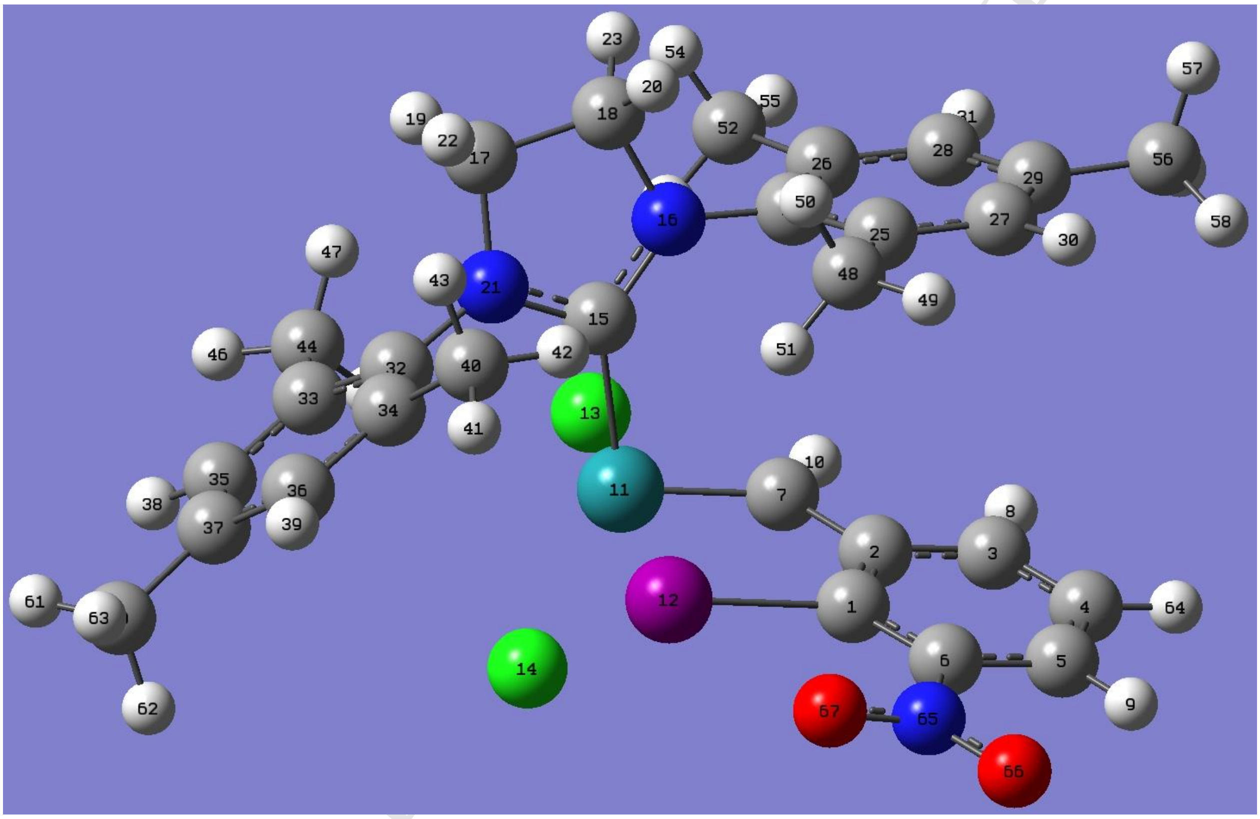


Reproduction of ^{13}C NMR spectrum of compound **8**.



DFT Calculations of complex 5

Structure of complex **5** was optimized with DFT B3LYP method with SDD basis set for Ru and I, and 6-31G(d,p) for other atoms as implemented in Gaussian 03 program (gen, pseudo=read). Only real values of the analytical harmonic vibrational frequencies confirmed that the geometry under study corresponds to the minimum-energy structure. NBO analysis (NBO 3.1 program implemented in the Gaussian package) of the structure revealed, that alternative delocalization paths: n(Ru)$\rightarrow\sigma^*$(C-I) and n(I)$\rightarrow\sigma^*/\pi^*$(N-O) contribute only slightly to the structure, if any (the latter interaction was not listed in the analysis at all). Moreover, also n(O)$\rightarrow\sigma^*$(I-Ru) interaction was weak, suppoorting electrostatic nature of the O-I interaction.



Coordinates of the structure

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.737249	2.146478	0.333433
2	6	0	2.161071	0.992837	1.022791
3	6	0	3.510533	0.923751	1.427806
4	6	0	4.405580	1.955152	1.164793
5	6	0	3.972366	3.089413	0.488047
6	6	0	2.638923	3.180776	0.072443
7	6	0	1.270648	-0.128090	1.353015
8	1	0	3.838663	0.036123	1.960331

9	1	0	4.636236	3.915497	0.268648
10	1	0	1.757292	-0.908552	1.945872
11	44	0	-0.540098	-0.287523	1.117269
12	53	0	-0.341515	2.117817	-0.170498
13	17	0	-0.587000	-2.250100	2.475763
14	17	0	-1.739026	0.845180	2.811856
15	6	0	-0.620146	-1.506025	-0.530822
16	7	0	0.276687	-2.339753	-1.111227
17	6	0	-1.799835	-2.764782	-2.148166
18	6	0	-0.304901	-3.099826	-2.241408
19	1	0	-2.399688	-3.612611	-1.798434
20	1	0	0.144602	-2.769212	-3.185052
21	7	0	-1.816650	-1.682729	-1.146192
22	1	0	-2.219468	-2.417762	-3.096241
23	1	0	-0.102686	-4.167315	-2.126015
24	6	0	1.692270	-2.445681	-0.881487
25	6	0	2.560676	-1.546260	-1.530280
26	6	0	2.192969	-3.516495	-0.114930
27	6	0	3.938113	-1.691906	-1.337450
28	6	0	3.579661	-3.618033	0.045395
29	6	0	4.468410	-2.717399	-0.548839
30	1	0	4.611194	-0.991165	-1.826155
31	1	0	3.972636	-4.432294	0.649610
32	6	0	-3.001927	-0.898184	-0.913189
33	6	0	-3.928266	-1.282358	0.077065
34	6	0	-3.251676	0.207643	-1.756388
35	6	0	-5.052234	-0.470433	0.272001
36	6	0	-4.386524	0.985357	-1.514066
37	6	0	-5.287914	0.676034	-0.489010
38	1	0	-5.763029	-0.750173	1.045457
39	1	0	-4.578384	1.845774	-2.151191
40	6	0	-2.371300	0.525692	-2.944802
41	1	0	-2.490238	1.569157	-3.248183
42	1	0	-1.312276	0.350975	-2.744813
43	1	0	-2.646880	-0.091569	-3.810177
44	6	0	-3.761638	-2.531445	0.906996
45	1	0	-3.062083	-2.379312	1.734786
46	1	0	-4.724951	-2.833319	1.326281
47	1	0	-3.372361	-3.366419	0.316950
48	6	0	2.040901	-0.462500	-2.444656
49	1	0	2.849306	0.207159	-2.748670
50	1	0	1.607811	-0.884440	-3.360232
51	1	0	1.263307	0.138843	-1.968973
52	6	0	1.284651	-4.545935	0.509432
53	1	0	0.530647	-4.073077	1.144668
54	1	0	0.761613	-5.135678	-0.254140
55	1	0	1.863004	-5.245357	1.118312
56	6	0	5.961389	-2.879948	-0.385029

57	1	0	6.375563	-3.526338	-1.169203
58	1	0	6.479923	-1.918949	-0.451286
59	1	0	6.211165	-3.337913	0.576479
60	6	0	-6.481165	1.558286	-0.212686
61	1	0	-7.338046	0.974819	0.137130
62	1	0	-6.246934	2.291616	0.568320
63	1	0	-6.785905	2.114177	-1.104288
64	1	0	5.437998	1.881885	1.490323
65	7	0	2.267368	4.412664	-0.650899
66	8	0	3.112729	5.299678	-0.734430
67	8	0	1.138508	4.482546	-1.137430

NBO output data

Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis
Threshold for printing: 0.50 kcal/mol

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
====================	====================	======	======	======
1. BD (1) C 1 - C 2	/132. LP*(3)Ru 11	1.15	0.94	0.030
1. BD (1) C 1 - C 2	/168. RY*(2) C 3	0.65	1.50	0.028
1. BD (1) C 1 - C 2	/194. RY*(1) C 6	2.57	1.78	0.061
1. BD (1) C 1 - C 2	/204. RY*(2) C 7	0.87	2.97	0.046
1. BD (1) C 1 - C 2	/224. RY*(1)Ru 11	0.52	1.48	0.025
1. BD (1) C 1 - C 2	/616. BD*(1) C 1 - C 6	4.28	1.28	0.066
1. BD (1) C 1 - C 2	/618. BD*(1) C 2 - C 3	3.23	1.28	0.058
1. BD (1) C 1 - C 2	/619. BD*(1) C 2 - C 7	3.19	1.20	0.055
1. BD (1) C 1 - C 2	/622. BD*(1) C 3 - H 8	1.53	1.20	0.038
1. BD (1) C 1 - C 2	/628. BD*(1) C 6 - N 65	4.85	1.01	0.064
1. BD (1) C 1 - C 2	/630. BD*(1) C 7 -Ru 11	0.52	1.09	0.022
2. BD (2) C 1 - C 2	/170. RY*(4) C 3	0.90	1.00	0.030
2. BD (2) C 1 - C 2	/197. RY*(4) C 6	1.09	1.29	0.037
2. BD (2) C 1 - C 2	/615. BD*(2) C 1 - C 2	1.02	0.28	0.015
2. BD (2) C 1 - C 2	/621. BD*(2) C 3 - C 4	17.87	0.29	0.066
2. BD (2) C 1 - C 2	/626. BD*(2) C 5 - C 6	20.12	0.28	0.067
2. BD (2) C 1 - C 2	/631. BD*(2) C 7 -Ru 11	12.36	0.30	0.057
3. BD (1) C 1 - C 6	/158. RY*(1) C 2	0.97	2.20	0.041
3. BD (1) C 1 - C 6	/159. RY*(2) C 2	1.42	1.98	0.048
3. BD (1) C 1 - C 6	/185. RY*(1) C 5	0.71	1.95	0.033
3. BD (1) C 1 - C 6	/587. RY*(1) N 65	0.95	1.80	0.037
3. BD (1) C 1 - C 6	/614. BD*(1) C 1 - C 2	3.72	1.30	0.062
3. BD (1) C 1 - C 6	/619. BD*(1) C 2 - C 7	2.52	1.23	0.050
3. BD (1) C 1 - C 6	/625. BD*(1) C 5 - C 6	4.89	1.31	0.071
3. BD (1) C 1 - C 6	/627. BD*(1) C 5 - H 9	1.37	1.24	0.037
3. BD (1) C 1 - C 6	/628. BD*(1) C 6 - N 65	0.94	1.04	0.029
3. BD (1) C 1 - C 6	/693. BD*(1) N 65 - O 66	1.46	1.19	0.038

4. BD (1) C 1 - I 12	/132. LP*(3)Ru 11	1.51	0.72	0.030
4. BD (1) C 1 - I 12	/158. RY*(1) C 2	2.00	1.95	0.056
4. BD (1) C 1 - I 12	/194. RY*(1) C 6	0.70	1.56	0.030
4. BD (1) C 1 - I 12	/195. RY*(2) C 6	2.20	1.67	0.054
4. BD (1) C 1 - I 12	/196. RY*(3) C 6	0.77	1.51	0.031
4. BD (1) C 1 - I 12	/618. BD*(1) C 2 - C 3	4.29	1.06	0.060
4. BD (1) C 1 - I 12	/619. BD*(1) C 2 - C 7	0.55	0.98	0.021
4. BD (1) C 1 - I 12	/625. BD*(1) C 5 - C 6	3.71	1.06	0.056
4. BD (1) C 1 - I 12	/628. BD*(1) C 6 - N 65	1.21	0.79	0.028
4. BD (1) C 1 - I 12	/632. BD*(1)Ru 11 - I 12	0.72	0.95	0.024
5. BD (1) C 2 - C 3	/132. LP*(3)Ru 11	0.84	0.91	0.026
5. BD (1) C 2 - C 3	/150. RY*(2) C 1	1.23	1.99	0.045
5. BD (1) C 2 - C 3	/176. RY*(1) C 4	0.77	1.96	0.035
5. BD (1) C 2 - C 3	/177. RY*(2) C 4	1.43	1.39	0.040
5. BD (1) C 2 - C 3	/203. RY*(1) C 7	0.61	1.89	0.030
5. BD (1) C 2 - C 3	/614. BD*(1) C 1 - C 2	4.14	1.24	0.064
5. BD (1) C 2 - C 3	/617. BD*(1) C 1 - I 12	3.28	0.77	0.045
5. BD (1) C 2 - C 3	/619. BD*(1) C 2 - C 7	2.68	1.18	0.050
5. BD (1) C 2 - C 3	/620. BD*(1) C 3 - C 4	2.59	1.28	0.052
5. BD (1) C 2 - C 3	/622. BD*(1) C 3 - H 8	1.17	1.17	0.033
5. BD (1) C 2 - C 3	/624. BD*(1) C 4 - H 64	2.04	1.17	0.044
5. BD (1) C 2 - C 3	/630. BD*(1) C 7 -Ru 11	2.07	1.06	0.043
6. BD (1) C 2 - C 7	/132. LP*(3)Ru 11	13.16	0.87	0.098
6. BD (1) C 2 - C 7	/149. RY*(1) C 1	0.83	1.80	0.035
6. BD (1) C 2 - C 7	/167. RY*(1) C 3	1.34	1.94	0.046
6. BD (1) C 2 - C 7	/204. RY*(2) C 7	0.71	2.90	0.041
6. BD (1) C 2 - C 7	/224. RY*(1)Ru 11	0.94	1.41	0.033
6. BD (1) C 2 - C 7	/225. RY*(2)Ru 11	0.60	1.31	0.025
6. BD (1) C 2 - C 7	/241. RY*(18)Ru 11	0.66	4.37	0.048
6. BD (1) C 2 - C 7	/243. RY*(20)Ru 11	0.78	33.84	0.146
6. BD (1) C 2 - C 7	/614. BD*(1) C 1 - C 2	3.69	1.20	0.059
6. BD (1) C 2 - C 7	/616. BD*(1) C 1 - C 6	2.13	1.21	0.045
6. BD (1) C 2 - C 7	/618. BD*(1) C 2 - C 3	2.43	1.21	0.049
6. BD (1) C 2 - C 7	/620. BD*(1) C 3 - C 4	1.98	1.24	0.044
6. BD (1) C 2 - C 7	/630. BD*(1) C 7 -Ru 11	1.92	1.02	0.040
7. BD (1) C 3 - C 4	/158. RY*(1) C 2	0.90	2.15	0.039
7. BD (1) C 3 - C 4	/159. RY*(2) C 2	1.48	1.94	0.048
7. BD (1) C 3 - C 4	/186. RY*(2) C 5	1.99	1.49	0.049
7. BD (1) C 3 - C 4	/618. BD*(1) C 2 - C 3	2.88	1.27	0.054
7. BD (1) C 3 - C 4	/619. BD*(1) C 2 - C 7	2.73	1.19	0.051
7. BD (1) C 3 - C 4	/622. BD*(1) C 3 - H 8	1.42	1.19	0.037
7. BD (1) C 3 - C 4	/623. BD*(1) C 4 - C 5	2.83	1.30	0.054
7. BD (1) C 3 - C 4	/624. BD*(1) C 4 - H 64	1.43	1.19	0.037
7. BD (1) C 3 - C 4	/627. BD*(1) C 5 - H 9	2.29	1.19	0.047
8. BD (2) C 3 - C 4	/188. RY*(4) C 5	1.14	1.78	0.045
8. BD (2) C 3 - C 4	/615. BD*(2) C 1 - C 2	19.34	0.27	0.065
8. BD (2) C 3 - C 4	/626. BD*(2) C 5 - C 6	25.31	0.27	0.074
9. BD (1) C 3 - H 8	/158. RY*(1) C 2	1.34	1.97	0.046

9. BD (1) C 3 - H 8	/176. RY*(1) C 4	0.98	1.80	0.038
9. BD (1) C 3 - H 8	/614. BD*(1) C 1 - C 2	4.29	1.07	0.061
9. BD (1) C 3 - H 8	/618. BD*(1) C 2 - C 3	1.04	1.09	0.030
9. BD (1) C 3 - H 8	/620. BD*(1) C 3 - C 4	0.97	1.11	0.029
9. BD (1) C 3 - H 8	/623. BD*(1) C 4 - C 5	3.46	1.11	0.056
10. BD (1) C 4 - C 5	/167. RY*(1) C 3	0.73	2.00	0.034
10. BD (1) C 4 - C 5	/168. RY*(2) C 3	1.36	1.49	0.040
10. BD (1) C 4 - C 5	/195. RY*(2) C 6	2.20	1.88	0.058
10. BD (1) C 4 - C 5	/620. BD*(1) C 3 - C 4	2.80	1.30	0.054
10. BD (1) C 4 - C 5	/622. BD*(1) C 3 - H 8	2.23	1.19	0.046
10. BD (1) C 4 - C 5	/624. BD*(1) C 4 - H 64	1.31	1.19	0.035
10. BD (1) C 4 - C 5	/625. BD*(1) C 5 - C 6	3.03	1.27	0.055
10. BD (1) C 4 - C 5	/627. BD*(1) C 5 - H 9	1.69	1.20	0.040
10. BD (1) C 4 - C 5	/628. BD*(1) C 6 - N 65	3.94	0.99	0.057
11. BD (1) C 4 - H 64	/167. RY*(1) C 3	1.00	1.82	0.038
11. BD (1) C 4 - H 64	/185. RY*(1) C 5	0.78	1.72	0.033
11. BD (1) C 4 - H 64	/618. BD*(1) C 2 - C 3	3.75	1.09	0.057
11. BD (1) C 4 - H 64	/620. BD*(1) C 3 - C 4	1.08	1.12	0.031
11. BD (1) C 4 - H 64	/623. BD*(1) C 4 - C 5	1.04	1.12	0.031
11. BD (1) C 4 - H 64	/625. BD*(1) C 5 - C 6	3.70	1.09	0.057
12. BD (1) C 5 - C 6	/149. RY*(1) C 1	1.03	1.87	0.039
12. BD (1) C 5 - C 6	/176. RY*(1) C 4	0.82	1.99	0.036
12. BD (1) C 5 - C 6	/177. RY*(2) C 4	1.41	1.41	0.040
12. BD (1) C 5 - C 6	/587. RY*(1) N 65	0.77	1.77	0.033
12. BD (1) C 5 - C 6	/616. BD*(1) C 1 - C 6	6.17	1.28	0.079
12. BD (1) C 5 - C 6	/617. BD*(1) C 1 - I 12	4.33	0.79	0.053
12. BD (1) C 5 - C 6	/623. BD*(1) C 4 - C 5	2.48	1.30	0.051
12. BD (1) C 5 - C 6	/624. BD*(1) C 4 - H 64	2.07	1.20	0.045
12. BD (1) C 5 - C 6	/627. BD*(1) C 5 - H 9	1.39	1.20	0.037
12. BD (1) C 5 - C 6	/695. BD*(1) N 65 - O 67	2.00	1.15	0.043
13. BD (2) C 5 - C 6	/151. RY*(3) C 1	1.22	1.15	0.037
13. BD (2) C 5 - C 6	/179. RY*(4) C 4	0.84	1.00	0.029
13. BD (2) C 5 - C 6	/197. RY*(4) C 6	0.53	1.29	0.026
13. BD (2) C 5 - C 6	/592. RY*(6) N 65	0.87	1.93	0.041
13. BD (2) C 5 - C 6	/615. BD*(2) C 1 - C 2	21.12	0.28	0.070
13. BD (2) C 5 - C 6	/621. BD*(2) C 3 - C 4	15.53	0.30	0.062
13. BD (2) C 5 - C 6	/694. BD*(2) N 65 - O 66	25.58	0.15	0.059
14. BD (1) C 5 - H 9	/176. RY*(1) C 4	0.96	1.80	0.037
14. BD (1) C 5 - H 9	/195. RY*(2) C 6	1.06	1.70	0.038
14. BD (1) C 5 - H 9	/616. BD*(1) C 1 - C 6	4.66	1.09	0.064
14. BD (1) C 5 - H 9	/620. BD*(1) C 3 - C 4	3.29	1.12	0.054
14. BD (1) C 5 - H 9	/623. BD*(1) C 4 - C 5	1.26	1.12	0.034
14. BD (1) C 5 - H 9	/625. BD*(1) C 5 - C 6	1.00	1.09	0.030
14. BD (1) C 5 - H 9	/628. BD*(1) C 6 - N 65	1.01	0.82	0.026
15. BD (1) C 6 - N 65	/149. RY*(1) C 1	0.75	1.96	0.034
15. BD (1) C 6 - N 65	/185. RY*(1) C 5	0.79	2.01	0.036
15. BD (1) C 6 - N 65	/596. RY*(1) O 66	1.43	1.90	0.047
15. BD (1) C 6 - N 65	/605. RY*(1) O 67	1.42	1.97	0.047

15. BD (1) C 6 - N 65	/614. BD*(1) C 1 - C 2	1.23	1.36	0.037
15. BD (1) C 6 - N 65	/616. BD*(1) C 1 - C 6	0.96	1.37	0.033
15. BD (1) C 6 - N 65	/623. BD*(1) C 4 - C 5	1.38	1.40	0.039
15. BD (1) C 6 - N 65	/625. BD*(1) C 5 - C 6	0.68	1.37	0.027
16. BD (1) C 7 - H 10	/132. LP*(3)Ru 11	18.92	0.70	0.106
16. BD (1) C 7 - H 10	/159. RY*(2) C 2	1.08	1.72	0.039
16. BD (1) C 7 - H 10	/204. RY*(2) C 7	1.16	2.74	0.051
16. BD (1) C 7 - H 10	/228. RY*(5)Ru 11	0.77	1.34	0.029
16. BD (1) C 7 - H 10	/237. RY*(14)Ru 11	1.19	2.08	0.045
16. BD (1) C 7 - H 10	/241. RY*(18)Ru 11	1.11	4.21	0.062
16. BD (1) C 7 - H 10	/243. RY*(20)Ru 11	1.77	33.68	0.220
16. BD (1) C 7 - H 10	/273. RY*(2) C 15	0.61	1.56	0.028
16. BD (1) C 7 - H 10	/614. BD*(1) C 1 - C 2	5.44	1.03	0.067
16. BD (1) C 7 - H 10	/630. BD*(1) C 7 -Ru 11	2.30	0.86	0.040
16. BD (1) C 7 - H 10	/633. BD*(1)Ru 11 -Cl 13	0.90	0.80	0.025
16. BD (1) C 7 - H 10	/635. BD*(1)Ru 11 - C 15	1.20	0.88	0.030
17. BD (1) C 7 -Ru 11	/149. RY*(1) C 1	0.79	1.59	0.032
17. BD (1) C 7 -Ru 11	/153. RY*(5) C 1	0.62	1.74	0.030
17. BD (1) C 7 -Ru 11	/158. RY*(1) C 2	3.32	1.89	0.072
17. BD (1) C 7 -Ru 11	/159. RY*(2) C 2	4.98	1.68	0.084
17. BD (1) C 7 -Ru 11	/160. RY*(3) C 2	2.32	1.55	0.055
17. BD (1) C 7 -Ru 11	/204. RY*(2) C 7	24.45	2.69	0.235
17. BD (1) C 7 -Ru 11	/206. RY*(4) C 7	3.49	1.88	0.074
17. BD (1) C 7 -Ru 11	/220. RY*(1) H 10	3.21	1.34	0.060
17. BD (1) C 7 -Ru 11	/226. RY*(3)Ru 11	2.92	1.12	0.052
17. BD (1) C 7 -Ru 11	/227. RY*(4)Ru 11	16.49	2.19	0.174
17. BD (1) C 7 -Ru 11	/228. RY*(5)Ru 11	3.59	1.30	0.062
17. BD (1) C 7 -Ru 11	/229. RY*(6)Ru 11	7.33	1.50	0.096
17. BD (1) C 7 -Ru 11	/230. RY*(7)Ru 11	1.92	1.24	0.045
17. BD (1) C 7 -Ru 11	/232. RY*(9)Ru 11	7.67	1.55	0.100
17. BD (1) C 7 -Ru 11	/233. RY*(10)Ru 11	3.50	1.42	0.065
17. BD (1) C 7 -Ru 11	/234. RY*(11)Ru 11	2.88	1.46	0.059
17. BD (1) C 7 -Ru 11	/235. RY*(12)Ru 11	3.51	1.17	0.059
17. BD (1) C 7 -Ru 11	/236. RY*(13)Ru 11	15.89	2.27	0.174
17. BD (1) C 7 -Ru 11	/237. RY*(14)Ru 11	18.48	2.04	0.178
17. BD (1) C 7 -Ru 11	/239. RY*(16)Ru 11	13.45	1.88	0.146
17. BD (1) C 7 -Ru 11	/240. RY*(17)Ru 11	3.83	1.39	0.067
17. BD (1) C 7 -Ru 11	/241. RY*(18)Ru 11	25.30	4.16	0.297
17. BD (1) C 7 -Ru 11	/242. RY*(19)Ru 11	2.82	2.21	0.072
17. BD (1) C 7 -Ru 11	/243. RY*(20)Ru 11	37.18	33.64	1.025
17. BD (1) C 7 -Ru 11	/247. RY*(1) I 12	3.02	1.02	0.051
17. BD (1) C 7 -Ru 11	/253. RY*(7) I 12	0.66	11.98	0.082
17. BD (1) C 7 -Ru 11	/254. RY*(1)Cl 13	1.51	1.28	0.040
17. BD (1) C 7 -Ru 11	/256. RY*(3)Cl 13	1.15	1.29	0.035
17. BD (1) C 7 -Ru 11	/263. RY*(1)Cl 14	0.51	1.31	0.024
17. BD (1) C 7 -Ru 11	/265. RY*(3)Cl 14	0.76	1.31	0.029
17. BD (1) C 7 -Ru 11	/266. RY*(4)Cl 14	1.26	1.40	0.038
17. BD (1) C 7 -Ru 11	/268. RY*(6)Cl 14	3.01	1.66	0.065

17. BD (1) C 7 -Ru 11	/270. RY*(8)Cl 14	1.83	1.57	0.049
17. BD (1) C 7 -Ru 11	/272. RY*(1) C 15	18.00	2.01	0.174
17. BD (1) C 7 -Ru 11	/273. RY*(2) C 15	6.20	1.52	0.089
17. BD (1) C 7 -Ru 11	/282. RY*(2) N 16	1.65	2.16	0.055
17. BD (1) C 7 -Ru 11	/317. RY*(2) N 21	0.74	2.15	0.037
17. BD (1) C 7 -Ru 11	/336. RY*(4) C 24	0.55	1.93	0.030
17. BD (1) C 7 -Ru 11	/516. RY*(1) H 51	1.59	1.42	0.044
17. BD (1) C 7 -Ru 11	/617. BD*(1) C 1 - I 12	1.21	0.51	0.022
17. BD (1) C 7 -Ru 11	/618. BD*(1) C 2 - C 3	3.94	1.01	0.057
17. BD (1) C 7 -Ru 11	/630. BD*(1) C 7 -Ru 11	32.32	0.81	0.145
17. BD (1) C 7 -Ru 11	/631. BD*(2) C 7 -Ru 11	3.37	0.48	0.037
17. BD (1) C 7 -Ru 11	/632. BD*(1)Ru 11 - I 12	15.35	0.89	0.106
17. BD (1) C 7 -Ru 11	/633. BD*(1)Ru 11 -Cl 13	20.37	0.76	0.112
17. BD (1) C 7 -Ru 11	/634. BD*(1)Ru 11 -Cl 14	6.00	0.59	0.055
17. BD (1) C 7 -Ru 11	/635. BD*(1)Ru 11 - C 15	46.24	0.84	0.180
18. BD (2) C 7 -Ru 11	/132. LP*(3)Ru 11	2.05	0.41	0.027
18. BD (2) C 7 -Ru 11	/141. LP*(1) C 15	1.72	0.10	0.013
18. BD (2) C 7 -Ru 11	/158. RY*(1) C 2	0.65	1.64	0.031
18. BD (2) C 7 -Ru 11	/204. RY*(2) C 7	5.96	2.45	0.115
18. BD (2) C 7 -Ru 11	/205. RY*(3) C 7	0.71	0.99	0.025
18. BD (2) C 7 -Ru 11	/206. RY*(4) C 7	0.96	1.63	0.038
18. BD (2) C 7 -Ru 11	/220. RY*(1) H 10	0.64	1.09	0.025
18. BD (2) C 7 -Ru 11	/226. RY*(3)Ru 11	1.76	0.87	0.038
18. BD (2) C 7 -Ru 11	/227. RY*(4)Ru 11	6.54	1.95	0.108
18. BD (2) C 7 -Ru 11	/228. RY*(5)Ru 11	1.16	1.05	0.033
18. BD (2) C 7 -Ru 11	/229. RY*(6)Ru 11	3.69	1.25	0.065
18. BD (2) C 7 -Ru 11	/230. RY*(7)Ru 11	1.57	1.00	0.038
18. BD (2) C 7 -Ru 11	/231. RY*(8)Ru 11	1.59	0.94	0.037
18. BD (2) C 7 -Ru 11	/232. RY*(9)Ru 11	1.67	1.30	0.045
18. BD (2) C 7 -Ru 11	/233. RY*(10)Ru 11	1.60	1.17	0.042
18. BD (2) C 7 -Ru 11	/234. RY*(11)Ru 11	0.83	1.22	0.030
18. BD (2) C 7 -Ru 11	/235. RY*(12)Ru 11	0.76	0.93	0.025
18. BD (2) C 7 -Ru 11	/236. RY*(13)Ru 11	5.14	2.02	0.098
18. BD (2) C 7 -Ru 11	/237. RY*(14)Ru 11	4.37	1.79	0.085
18. BD (2) C 7 -Ru 11	/239. RY*(16)Ru 11	4.48	1.63	0.082
18. BD (2) C 7 -Ru 11	/241. RY*(18)Ru 11	6.99	3.92	0.159
18. BD (2) C 7 -Ru 11	/242. RY*(19)Ru 11	0.77	1.96	0.037
18. BD (2) C 7 -Ru 11	/243. RY*(20)Ru 11	10.93	33.39	0.578
18. BD (2) C 7 -Ru 11	/247. RY*(1) I 12	1.39	0.77	0.031
18. BD (2) C 7 -Ru 11	/254. RY*(1)Cl 13	0.90	1.03	0.029
18. BD (2) C 7 -Ru 11	/265. RY*(3)Cl 14	1.17	1.06	0.034
18. BD (2) C 7 -Ru 11	/266. RY*(4)Cl 14	0.61	1.15	0.025
18. BD (2) C 7 -Ru 11	/268. RY*(6)Cl 14	1.37	1.42	0.042
18. BD (2) C 7 -Ru 11	/270. RY*(8)Cl 14	0.73	1.32	0.030
18. BD (2) C 7 -Ru 11	/272. RY*(1) C 15	5.04	1.76	0.090
18. BD (2) C 7 -Ru 11	/273. RY*(2) C 15	5.34	1.27	0.079
18. BD (2) C 7 -Ru 11	/274. RY*(3) C 15	0.65	1.28	0.028
18. BD (2) C 7 -Ru 11	/282. RY*(2) N 16	0.87	1.92	0.039

18. BD (2) C 7 -Ru 11	/516. RY*(1) H 51	0.52	1.18	0.024
18. BD (2) C 7 -Ru 11	/615. BD*(2) C 1 - C 2	17.09	0.20	0.055
18. BD (2) C 7 -Ru 11	/630. BD*(1) C 7 -Ru 11	9.40	0.57	0.068
18. BD (2) C 7 -Ru 11	/631. BD*(2) C 7 -Ru 11	6.05	0.23	0.034
18. BD (2) C 7 -Ru 11	/632. BD*(1)Ru 11 - I 12	3.26	0.65	0.042
18. BD (2) C 7 -Ru 11	/633. BD*(1)Ru 11 -Cl 13	0.96	0.51	0.020
18. BD (2) C 7 -Ru 11	/634. BD*(1)Ru 11 -Cl 14	29.10	0.35	0.091
18. BD (2) C 7 -Ru 11	/635. BD*(1)Ru 11 - C 15	38.79	0.59	0.137
18. BD (2) C 7 -Ru 11	/636. BD*(1) C 15 - N 16	1.56	0.71	0.032
18. BD (2) C 7 -Ru 11	/637. BD*(1) C 15 - N 21	1.95	0.71	0.035
19. BD (1)Ru 11 - I 12	/141. LP*(1) C 15	0.80	0.30	0.017
19. BD (1)Ru 11 - I 12	/149. RY*(1) C 1	1.32	1.54	0.041
19. BD (1)Ru 11 - I 12	/150. RY*(2) C 1	0.64	1.69	0.030
19. BD (1)Ru 11 - I 12	/158. RY*(1) C 2	0.51	1.84	0.028
19. BD (1)Ru 11 - I 12	/203. RY*(1) C 7	1.42	1.59	0.043
19. BD (1)Ru 11 - I 12	/204. RY*(2) C 7	0.99	2.64	0.046
19. BD (1)Ru 11 - I 12	/224. RY*(1)Ru 11	1.07	1.15	0.032
19. BD (1)Ru 11 - I 12	/236. RY*(13)Ru 11	0.75	2.22	0.037
19. BD (1)Ru 11 - I 12	/238. RY*(15)Ru 11	0.86	1.25	0.030
19. BD (1)Ru 11 - I 12	/243. RY*(20)Ru 11	0.82	33.58	0.152
19. BD (1)Ru 11 - I 12	/247. RY*(1) I 12	0.90	0.97	0.027
19. BD (1)Ru 11 - I 12	/249. RY*(3) I 12	1.99	2.17	0.060
19. BD (1)Ru 11 - I 12	/252. RY*(6) I 12	1.74	1.99	0.054
19. BD (1)Ru 11 - I 12	/253. RY*(7) I 12	3.94	11.93	0.198
19. BD (1)Ru 11 - I 12	/273. RY*(2) C 15	0.60	1.46	0.027
19. BD (1)Ru 11 - I 12	/605. RY*(1) O 67	0.66	1.56	0.029
19. BD (1)Ru 11 - I 12	/614. BD*(1) C 1 - C 2	0.56	0.94	0.021
19. BD (1)Ru 11 - I 12	/616. BD*(1) C 1 - C 6	2.42	0.95	0.043
19. BD (1)Ru 11 - I 12	/617. BD*(1) C 1 - I 12	0.68	0.46	0.016
19. BD (1)Ru 11 - I 12	/629. BD*(1) C 7 - H 10	1.05	0.87	0.027
19. BD (1)Ru 11 - I 12	/630. BD*(1) C 7 -Ru 11	4.50	0.76	0.053
19. BD (1)Ru 11 - I 12	/632. BD*(1)Ru 11 - I 12	3.67	0.84	0.050
19. BD (1)Ru 11 - I 12	/633. BD*(1)Ru 11 -Cl 13	9.61	0.71	0.075
19. BD (1)Ru 11 - I 12	/635. BD*(1)Ru 11 - C 15	1.77	0.79	0.034
20. BD (1)Ru 11 -Cl 13	/141. LP*(1) C 15	1.87	0.39	0.029
20. BD (1)Ru 11 -Cl 13	/149. RY*(1) C 1	0.97	1.64	0.036
20. BD (1)Ru 11 -Cl 13	/150. RY*(2) C 1	1.56	1.79	0.048
20. BD (1)Ru 11 -Cl 13	/159. RY*(2) C 2	1.21	1.72	0.042
20. BD (1)Ru 11 -Cl 13	/195. RY*(2) C 6	0.51	1.66	0.027
20. BD (1)Ru 11 -Cl 13	/203. RY*(1) C 7	1.41	1.68	0.045
20. BD (1)Ru 11 -Cl 13	/204. RY*(2) C 7	4.20	2.74	0.098
20. BD (1)Ru 11 -Cl 13	/224. RY*(1)Ru 11	3.00	1.25	0.056
20. BD (1)Ru 11 -Cl 13	/227. RY*(4)Ru 11	5.62	2.24	0.103
20. BD (1)Ru 11 -Cl 13	/230. RY*(7)Ru 11	2.34	1.29	0.050
20. BD (1)Ru 11 -Cl 13	/231. RY*(8)Ru 11	1.01	1.23	0.032
20. BD (1)Ru 11 -Cl 13	/232. RY*(9)Ru 11	4.33	1.59	0.076
20. BD (1)Ru 11 -Cl 13	/233. RY*(10)Ru 11	2.58	1.46	0.056
20. BD (1)Ru 11 -Cl 13	/236. RY*(13)Ru 11	1.28	2.31	0.050

20. BD (1)Ru 11 -Cl 13	/237. RY*(14)Ru 11	3.28	2.08	0.076
20. BD (1)Ru 11 -Cl 13	/238. RY*(15)Ru 11	2.50	1.35	0.053
20. BD (1)Ru 11 -Cl 13	/239. RY*(16)Ru 11	2.81	1.92	0.067
20. BD (1)Ru 11 -Cl 13	/240. RY*(17)Ru 11	4.11	1.43	0.070
20. BD (1)Ru 11 -Cl 13	/241. RY*(18)Ru 11	6.06	4.21	0.146
20. BD (1)Ru 11 -Cl 13	/242. RY*(19)Ru 11	1.72	2.25	0.057
20. BD (1)Ru 11 -Cl 13	/243. RY*(20)Ru 11	6.27	33.68	0.421
20. BD (1)Ru 11 -Cl 13	/248. RY*(2) I 12	1.79	0.92	0.037
20. BD (1)Ru 11 -Cl 13	/249. RY*(3) I 12	3.51	2.26	0.082
20. BD (1)Ru 11 -Cl 13	/252. RY*(6) I 12	4.60	2.08	0.090
20. BD (1)Ru 11 -Cl 13	/253. RY*(7) I 12	8.01	12.02	0.284
20. BD (1)Ru 11 -Cl 13	/254. RY*(1)Cl 13	1.10	1.32	0.035
20. BD (1)Ru 11 -Cl 13	/256. RY*(3)Cl 13	1.10	1.34	0.035
20. BD (1)Ru 11 -Cl 13	/266. RY*(4)Cl 14	0.63	1.44	0.028
20. BD (1)Ru 11 -Cl 13	/272. RY*(1) C 15	3.17	2.05	0.074
20. BD (1)Ru 11 -Cl 13	/273. RY*(2) C 15	0.53	1.56	0.026
20. BD (1)Ru 11 -Cl 13	/274. RY*(3) C 15	0.61	1.57	0.028
20. BD (1)Ru 11 -Cl 13	/617. BD*(1) C 1 - I 12	0.96	0.56	0.021
20. BD (1)Ru 11 -Cl 13	/619. BD*(1) C 2 - C 7	1.35	0.97	0.033
20. BD (1)Ru 11 -Cl 13	/630. BD*(1) C 7 -Ru 11	8.33	0.86	0.076
20. BD (1)Ru 11 -Cl 13	/632. BD*(1)Ru 11 - I 12	7.12	0.94	0.074
20. BD (1)Ru 11 -Cl 13	/633. BD*(1)Ru 11 -Cl 13	4.68	0.80	0.055
20. BD (1)Ru 11 -Cl 13	/634. BD*(1)Ru 11 -Cl 14	1.17	0.64	0.025
20. BD (1)Ru 11 -Cl 13	/635. BD*(1)Ru 11 - C 15	6.26	0.88	0.068
20. BD (1)Ru 11 -Cl 13	/678. BD*(1) C 44 - H 45	0.60	1.01	0.023
21. BD (1)Ru 11 -Cl 14	/204. RY*(2) C 7	0.85	2.79	0.044
21. BD (1)Ru 11 -Cl 14	/205. RY*(3) C 7	0.58	1.33	0.025
21. BD (1)Ru 11 -Cl 14	/226. RY*(3)Ru 11	0.92	1.22	0.030
21. BD (1)Ru 11 -Cl 14	/227. RY*(4)Ru 11	1.80	2.29	0.058
21. BD (1)Ru 11 -Cl 14	/228. RY*(5)Ru 11	0.56	1.39	0.025
21. BD (1)Ru 11 -Cl 14	/236. RY*(13)Ru 11	1.07	2.36	0.046
21. BD (1)Ru 11 -Cl 14	/237. RY*(14)Ru 11	0.89	2.13	0.040
21. BD (1)Ru 11 -Cl 14	/239. RY*(16)Ru 11	1.03	1.97	0.041
21. BD (1)Ru 11 -Cl 14	/241. RY*(18)Ru 11	1.35	4.26	0.069
21. BD (1)Ru 11 -Cl 14	/243. RY*(20)Ru 11	2.26	33.73	0.252
21. BD (1)Ru 11 -Cl 14	/272. RY*(1) C 15	3.08	2.10	0.073
21. BD (1)Ru 11 -Cl 14	/631. BD*(2) C 7 -Ru 11	1.89	0.57	0.030
21. BD (1)Ru 11 -Cl 14	/635. BD*(1)Ru 11 - C 15	4.85	0.93	0.062
22. BD (1)Ru 11 - C 15	/132. LP*(3)Ru 11	6.94	0.63	0.059
22. BD (1)Ru 11 - C 15	/158. RY*(1) C 2	1.17	1.86	0.043
22. BD (1)Ru 11 - C 15	/160. RY*(3) C 2	1.06	1.52	0.037
22. BD (1)Ru 11 - C 15	/204. RY*(2) C 7	15.11	2.67	0.185
22. BD (1)Ru 11 - C 15	/206. RY*(4) C 7	2.18	1.85	0.059
22. BD (1)Ru 11 - C 15	/220. RY*(1) H 10	2.12	1.31	0.049
22. BD (1)Ru 11 - C 15	/226. RY*(3)Ru 11	2.57	1.09	0.049
22. BD (1)Ru 11 - C 15	/227. RY*(4)Ru 11	12.46	2.17	0.152
22. BD (1)Ru 11 - C 15	/228. RY*(5)Ru 11	2.54	1.27	0.052
22. BD (1)Ru 11 - C 15	/229. RY*(6)Ru 11	5.35	1.48	0.082

22. BD (1)Ru 11 - C 15	/230. RY*(7)Ru 11	2.31	1.22	0.049
22. BD (1)Ru 11 - C 15	/231. RY*(8)Ru 11	1.24	1.16	0.035
22. BD (1)Ru 11 - C 15	/232. RY*(9)Ru 11	4.16	1.52	0.074
22. BD (1)Ru 11 - C 15	/233. RY*(10)Ru 11	2.71	1.39	0.057
22. BD (1)Ru 11 - C 15	/234. RY*(11)Ru 11	1.91	1.44	0.048
22. BD (1)Ru 11 - C 15	/235. RY*(12)Ru 11	1.84	1.15	0.042
22. BD (1)Ru 11 - C 15	/236. RY*(13)Ru 11	10.69	2.24	0.143
22. BD (1)Ru 11 - C 15	/237. RY*(14)Ru 11	9.76	2.01	0.130
22. BD (1)Ru 11 - C 15	/239. RY*(16)Ru 11	8.58	1.85	0.117
22. BD (1)Ru 11 - C 15	/240. RY*(17)Ru 11	1.94	1.36	0.048
22. BD (1)Ru 11 - C 15	/241. RY*(18)Ru 11	15.80	4.14	0.237
22. BD (1)Ru 11 - C 15	/242. RY*(19)Ru 11	1.34	2.18	0.050
22. BD (1)Ru 11 - C 15	/243. RY*(20)Ru 11	23.09	33.61	0.815
22. BD (1)Ru 11 - C 15	/247. RY*(1) I 12	2.04	0.99	0.042
22. BD (1)Ru 11 - C 15	/254. RY*(1)Cl 13	1.28	1.25	0.037
22. BD (1)Ru 11 - C 15	/256. RY*(3)Cl 13	0.67	1.27	0.027
22. BD (1)Ru 11 - C 15	/266. RY*(4)Cl 14	0.84	1.37	0.031
22. BD (1)Ru 11 - C 15	/268. RY*(6)Cl 14	2.10	1.64	0.054
22. BD (1)Ru 11 - C 15	/270. RY*(8)Cl 14	1.24	1.54	0.040
22. BD (1)Ru 11 - C 15	/272. RY*(1) C 15	10.63	1.98	0.134
22. BD (1)Ru 11 - C 15	/273. RY*(2) C 15	4.19	1.49	0.073
22. BD (1)Ru 11 - C 15	/274. RY*(3) C 15	0.60	1.50	0.028
22. BD (1)Ru 11 - C 15	/282. RY*(2) N 16	5.49	2.14	0.100
22. BD (1)Ru 11 - C 15	/317. RY*(2) N 21	2.89	2.12	0.072
22. BD (1)Ru 11 - C 15	/516. RY*(1) H 51	0.94	1.40	0.033
22. BD (1)Ru 11 - C 15	/630. BD*(1) C 7 -Ru 11	33.24	0.79	0.145
22. BD (1)Ru 11 - C 15	/631. BD*(2) C 7 -Ru 11	10.55	0.45	0.062
22. BD (1)Ru 11 - C 15	/632. BD*(1)Ru 11 - I 12	5.63	0.87	0.063
22. BD (1)Ru 11 - C 15	/633. BD*(1)Ru 11 -Cl 13	11.39	0.73	0.081
22. BD (1)Ru 11 - C 15	/634. BD*(1)Ru 11 -Cl 14	5.58	0.57	0.051
22. BD (1)Ru 11 - C 15	/635. BD*(1)Ru 11 - C 15	14.55	0.81	0.098
22. BD (1)Ru 11 - C 15	/638. BD*(1) N 16 - C 18	4.63	0.74	0.053
22. BD (1)Ru 11 - C 15	/642. BD*(1) C 17 - N 21	6.28	0.74	0.063
23. BD (1) C 15 - N 16	/273. RY*(2) C 15	0.65	1.89	0.031
23. BD (1) C 15 - N 16	/317. RY*(2) N 21	0.69	2.52	0.037
23. BD (1) C 15 - N 16	/334. RY*(2) C 24	1.42	1.74	0.045
23. BD (1) C 15 - N 16	/631. BD*(2) C 7 -Ru 11	1.25	0.85	0.030
23. BD (1) C 15 - N 16	/635. BD*(1)Ru 11 - C 15	2.99	1.21	0.056
23. BD (1) C 15 - N 16	/638. BD*(1) N 16 - C 18	1.13	1.14	0.032
23. BD (1) C 15 - N 16	/639. BD*(1) N 16 - C 24	2.97	1.23	0.054
23. BD (1) C 15 - N 16	/646. BD*(1) N 21 - C 32	3.58	1.23	0.059
23. BD (1) C 15 - N 16	/648. BD*(2) C 24 - C 25	0.57	0.87	0.022
23. BD (1) C 15 - N 16	/649. BD*(1) C 24 - C 26	0.53	1.42	0.024
24. BD (1) C 15 - N 21	/132. LP*(3)Ru 11	1.17	1.03	0.032
24. BD (1) C 15 - N 21	/282. RY*(2) N 16	0.56	2.53	0.034
24. BD (1) C 15 - N 21	/396. RY*(2) C 32	0.58	1.74	0.029
24. BD (1) C 15 - N 21	/630. BD*(1) C 7 -Ru 11	0.53	1.18	0.023
24. BD (1) C 15 - N 21	/635. BD*(1)Ru 11 - C 15	2.95	1.21	0.056

24. BD (1) C 15 - N 21	/639. BD*(1) N 16 - C 24	3.96	1.22	0.062
24. BD (1) C 15 - N 21	/642. BD*(1) C 17 - N 21	1.26	1.14	0.034
24. BD (1) C 15 - N 21	/643. BD*(1) C 17 - H 22	0.51	1.27	0.023
24. BD (1) C 15 - N 21	/646. BD*(1) N 21 - C 32	2.73	1.22	0.052
24. BD (1) C 15 - N 21	/662. BD*(2) C 32 - C 33	0.75	0.86	0.025
25. BD (1) N 16 - C 18	/273. RY*(2) C 15	1.29	1.77	0.043
25. BD (1) N 16 - C 18	/334. RY*(2) C 24	1.46	1.62	0.044
25. BD (1) N 16 - C 18	/635. BD*(1)Ru 11 - C 15	3.44	1.10	0.057
25. BD (1) N 16 - C 18	/636. BD*(1) C 15 - N 16	1.25	1.21	0.035
25. BD (1) N 16 - C 18	/637. BD*(1) C 15 - N 21	1.10	1.21	0.033
25. BD (1) N 16 - C 18	/639. BD*(1) N 16 - C 24	1.20	1.11	0.033
25. BD (1) N 16 - C 18	/642. BD*(1) C 17 - N 21	1.29	1.03	0.033
25. BD (1) N 16 - C 18	/643. BD*(1) C 17 - H 22	0.78	1.16	0.027
25. BD (1) N 16 - C 18	/648. BD*(2) C 24 - C 25	2.01	0.75	0.038
26. BD (1) N 16 - C 24	/272. RY*(1) C 15	0.66	2.32	0.035
26. BD (1) N 16 - C 24	/300. RY*(2) C 18	0.61	1.60	0.028
26. BD (1) N 16 - C 24	/342. RY*(1) C 25	1.08	2.06	0.042
26. BD (1) N 16 - C 24	/351. RY*(1) C 26	1.19	2.06	0.044
26. BD (1) N 16 - C 24	/636. BD*(1) C 15 - N 16	2.91	1.27	0.054
26. BD (1) N 16 - C 24	/637. BD*(1) C 15 - N 21	1.21	1.26	0.035
26. BD (1) N 16 - C 24	/638. BD*(1) N 16 - C 18	0.82	1.07	0.027
26. BD (1) N 16 - C 24	/640. BD*(1) C 17 - C 18	0.74	1.12	0.026
26. BD (1) N 16 - C 24	/647. BD*(1) C 24 - C 25	1.41	1.35	0.039
26. BD (1) N 16 - C 24	/649. BD*(1) C 24 - C 26	1.52	1.35	0.041
26. BD (1) N 16 - C 24	/650. BD*(1) C 25 - C 27	1.60	1.36	0.042
26. BD (1) N 16 - C 24	/652. BD*(1) C 26 - C 28	1.50	1.37	0.040
27. BD (1) C 17 - C 18	/639. BD*(1) N 16 - C 24	2.68	1.03	0.047
27. BD (1) C 17 - C 18	/641. BD*(1) C 17 - H 19	0.55	1.08	0.022
27. BD (1) C 17 - C 18	/643. BD*(1) C 17 - H 22	0.55	1.07	0.022
27. BD (1) C 17 - C 18	/644. BD*(1) C 18 - H 20	0.54	1.07	0.021
27. BD (1) C 17 - C 18	/645. BD*(1) C 18 - H 23	0.59	1.08	0.022
27. BD (1) C 17 - C 18	/646. BD*(1) N 21 - C 32	3.03	1.02	0.050
28. BD (1) C 17 - H 19	/299. RY*(1) C 18	0.78	1.58	0.031
28. BD (1) C 17 - H 19	/316. RY*(1) N 21	0.90	1.57	0.034
28. BD (1) C 17 - H 19	/637. BD*(1) C 15 - N 21	1.02	1.03	0.029
28. BD (1) C 17 - H 19	/644. BD*(1) C 18 - H 20	1.38	0.97	0.033
29. BD (1) C 17 - N 21	/273. RY*(2) C 15	1.52	1.78	0.047
29. BD (1) C 17 - N 21	/396. RY*(2) C 32	1.45	1.64	0.044
29. BD (1) C 17 - N 21	/635. BD*(1)Ru 11 - C 15	2.44	1.10	0.048
29. BD (1) C 17 - N 21	/636. BD*(1) C 15 - N 16	0.91	1.22	0.030
29. BD (1) C 17 - N 21	/637. BD*(1) C 15 - N 21	1.29	1.22	0.035
29. BD (1) C 17 - N 21	/638. BD*(1) N 16 - C 18	1.28	1.03	0.032
29. BD (1) C 17 - N 21	/645. BD*(1) C 18 - H 23	0.80	1.17	0.027
29. BD (1) C 17 - N 21	/646. BD*(1) N 21 - C 32	1.27	1.12	0.034
29. BD (1) C 17 - N 21	/662. BD*(2) C 32 - C 33	1.52	0.76	0.033
30. BD (1) C 17 - H 22	/300. RY*(2) C 18	0.51	1.37	0.024
30. BD (1) C 17 - H 22	/316. RY*(1) N 21	0.62	1.57	0.028
30. BD (1) C 17 - H 22	/637. BD*(1) C 15 - N 21	1.74	1.03	0.038

30. BD (1) C 17 - H 22	/638. BD*(1) N 16 - C 18	0.78	0.84	0.023
30. BD (1) C 17 - H 22	/645. BD*(1) C 18 - H 23	0.58	0.99	0.021
31. BD (1) C 18 - H 20	/281. RY*(1) N 16	0.82	1.58	0.032
31. BD (1) C 18 - H 20	/290. RY*(1) C 17	0.88	1.56	0.033
31. BD (1) C 18 - H 20	/636. BD*(1) C 15 - N 16	1.09	1.03	0.030
31. BD (1) C 18 - H 20	/641. BD*(1) C 17 - H 19	1.33	0.98	0.032
32. BD (1) C 18 - H 23	/281. RY*(1) N 16	0.76	1.58	0.031
32. BD (1) C 18 - H 23	/291. RY*(2) C 17	0.54	1.40	0.025
32. BD (1) C 18 - H 23	/636. BD*(1) C 15 - N 16	1.64	1.04	0.037
32. BD (1) C 18 - H 23	/642. BD*(1) C 17 - N 21	0.75	0.85	0.023
32. BD (1) C 18 - H 23	/643. BD*(1) C 17 - H 22	0.60	0.98	0.022
33. BD (1) N 21 - C 32	/132. LP*(3)Ru 11	1.14	0.97	0.031
33. BD (1) N 21 - C 32	/272. RY*(1) C 15	0.94	2.32	0.042
33. BD (1) N 21 - C 32	/404. RY*(1) C 33	1.23	2.06	0.045
33. BD (1) N 21 - C 32	/413. RY*(1) C 34	1.19	2.04	0.044
33. BD (1) N 21 - C 32	/635. BD*(1)Ru 11 - C 15	0.61	1.15	0.025
33. BD (1) N 21 - C 32	/636. BD*(1) C 15 - N 16	1.32	1.26	0.037
33. BD (1) N 21 - C 32	/637. BD*(1) C 15 - N 21	2.75	1.26	0.053
33. BD (1) N 21 - C 32	/640. BD*(1) C 17 - C 18	0.64	1.11	0.024
33. BD (1) N 21 - C 32	/642. BD*(1) C 17 - N 21	0.93	1.08	0.028
33. BD (1) N 21 - C 32	/661. BD*(1) C 32 - C 33	1.49	1.35	0.040
33. BD (1) N 21 - C 32	/663. BD*(1) C 32 - C 34	1.32	1.34	0.038
33. BD (1) N 21 - C 32	/664. BD*(1) C 33 - C 35	1.45	1.37	0.040
33. BD (1) N 21 - C 32	/666. BD*(1) C 34 - C 36	1.56	1.36	0.041
34. BD (1) C 24 - C 25	/281. RY*(1) N 16	1.04	1.73	0.038
34. BD (1) C 24 - C 25	/351. RY*(1) C 26	0.93	1.99	0.039
34. BD (1) C 24 - C 25	/352. RY*(2) C 26	0.98	1.69	0.037
34. BD (1) C 24 - C 25	/360. RY*(1) C 27	0.63	1.97	0.032
34. BD (1) C 24 - C 25	/361. RY*(2) C 27	0.75	1.49	0.030
34. BD (1) C 24 - C 25	/499. RY*(1) C 48	0.63	1.53	0.028
34. BD (1) C 24 - C 25	/636. BD*(1) C 15 - N 16	0.92	1.19	0.029
34. BD (1) C 24 - C 25	/638. BD*(1) N 16 - C 18	0.73	1.00	0.024
34. BD (1) C 24 - C 25	/639. BD*(1) N 16 - C 24	1.37	1.09	0.034
34. BD (1) C 24 - C 25	/649. BD*(1) C 24 - C 26	4.77	1.28	0.070
34. BD (1) C 24 - C 25	/650. BD*(1) C 25 - C 27	3.72	1.29	0.062
34. BD (1) C 24 - C 25	/651. BD*(1) C 25 - C 48	1.90	1.11	0.041
34. BD (1) C 24 - C 25	/654. BD*(1) C 26 - C 52	2.68	1.12	0.049
34. BD (1) C 24 - C 25	/657. BD*(1) C 27 - H 30	2.02	1.16	0.043
34. BD (1) C 24 - C 25	/681. BD*(1) C 48 - H 49	0.59	1.15	0.023
35. BD (2) C 24 - C 25	/362. RY*(3) C 27	0.92	0.97	0.029
35. BD (2) C 24 - C 25	/363. RY*(4) C 27	0.51	2.15	0.032
35. BD (2) C 24 - C 25	/631. BD*(2) C 7 -Ru 11	0.57	0.27	0.011
35. BD (2) C 24 - C 25	/636. BD*(1) C 15 - N 16	2.48	0.75	0.042
35. BD (2) C 24 - C 25	/638. BD*(1) N 16 - C 18	2.85	0.56	0.038
35. BD (2) C 24 - C 25	/653. BD*(2) C 26 - C 28	22.40	0.29	0.072
35. BD (2) C 24 - C 25	/656. BD*(2) C 27 - C 29	16.61	0.29	0.062
35. BD (2) C 24 - C 25	/682. BD*(1) C 48 - H 50	1.95	0.69	0.036
35. BD (2) C 24 - C 25	/683. BD*(1) C 48 - H 51	1.30	0.72	0.030

36. BD (1) C 24 - C 26	/281. RY*(1) N 16	1.00	1.73	0.037
36. BD (1) C 24 - C 26	/342. RY*(1) C 25	0.86	1.98	0.037
36. BD (1) C 24 - C 26	/343. RY*(2) C 25	1.01	1.70	0.037
36. BD (1) C 24 - C 26	/369. RY*(1) C 28	0.63	1.97	0.032
36. BD (1) C 24 - C 26	/370. RY*(2) C 28	0.78	1.50	0.031
36. BD (1) C 24 - C 26	/520. RY*(1) C 52	0.62	1.51	0.028
36. BD (1) C 24 - C 26	/636. BD*(1) C 15 - N 16	1.37	1.19	0.036
36. BD (1) C 24 - C 26	/638. BD*(1) N 16 - C 18	0.59	0.99	0.022
36. BD (1) C 24 - C 26	/639. BD*(1) N 16 - C 24	1.44	1.09	0.035
36. BD (1) C 24 - C 26	/647. BD*(1) C 24 - C 25	4.82	1.27	0.070
36. BD (1) C 24 - C 26	/651. BD*(1) C 25 - C 48	2.78	1.11	0.050
36. BD (1) C 24 - C 26	/652. BD*(1) C 26 - C 28	3.44	1.29	0.060
36. BD (1) C 24 - C 26	/654. BD*(1) C 26 - C 52	1.96	1.12	0.042
36. BD (1) C 24 - C 26	/659. BD*(1) C 28 - H 31	2.00	1.17	0.043
36. BD (1) C 24 - C 26	/686. BD*(1) C 52 - H 55	0.56	1.16	0.023
37. BD (1) C 25 - C 27	/333. RY*(1) C 24	0.77	2.01	0.035
37. BD (1) C 25 - C 27	/335. RY*(3) C 24	0.88	1.83	0.036
37. BD (1) C 25 - C 27	/378. RY*(1) C 29	1.03	2.00	0.041
37. BD (1) C 25 - C 27	/379. RY*(2) C 29	1.80	1.64	0.049
37. BD (1) C 25 - C 27	/499. RY*(1) C 48	0.63	1.52	0.028
37. BD (1) C 25 - C 27	/639. BD*(1) N 16 - C 24	4.19	1.08	0.060
37. BD (1) C 25 - C 27	/647. BD*(1) C 24 - C 25	4.10	1.27	0.064
37. BD (1) C 25 - C 27	/651. BD*(1) C 25 - C 48	1.88	1.10	0.041
37. BD (1) C 25 - C 27	/655. BD*(1) C 27 - C 29	3.70	1.28	0.062
37. BD (1) C 25 - C 27	/657. BD*(1) C 27 - H 30	1.39	1.16	0.036
37. BD (1) C 25 - C 27	/660. BD*(1) C 29 - C 56	3.03	1.11	0.052
37. BD (1) C 25 - C 27	/683. BD*(1) C 48 - H 51	0.51	1.15	0.022
38. BD (1) C 25 - C 48	/333. RY*(1) C 24	1.54	1.95	0.049
38. BD (1) C 25 - C 48	/360. RY*(1) C 27	1.01	1.90	0.039
38. BD (1) C 25 - C 48	/647. BD*(1) C 24 - C 25	2.36	1.20	0.048
38. BD (1) C 25 - C 48	/649. BD*(1) C 24 - C 26	2.83	1.21	0.052
38. BD (1) C 25 - C 48	/650. BD*(1) C 25 - C 27	2.34	1.22	0.048
38. BD (1) C 25 - C 48	/655. BD*(1) C 27 - C 29	2.35	1.22	0.048
38. BD (1) C 25 - C 48	/681. BD*(1) C 48 - H 49	0.65	1.08	0.024
38. BD (1) C 25 - C 48	/682. BD*(1) C 48 - H 50	0.67	1.06	0.024
38. BD (1) C 25 - C 48	/683. BD*(1) C 48 - H 51	0.81	1.09	0.027
39. BD (1) C 26 - C 28	/333. RY*(1) C 24	0.79	2.01	0.036
39. BD (1) C 26 - C 28	/335. RY*(3) C 24	0.88	1.82	0.036
39. BD (1) C 26 - C 28	/378. RY*(1) C 29	0.87	1.99	0.037
39. BD (1) C 26 - C 28	/379. RY*(2) C 29	1.95	1.64	0.051
39. BD (1) C 26 - C 28	/520. RY*(1) C 52	0.63	1.50	0.028
39. BD (1) C 26 - C 28	/639. BD*(1) N 16 - C 24	4.43	1.08	0.062
39. BD (1) C 26 - C 28	/649. BD*(1) C 24 - C 26	3.83	1.27	0.062
39. BD (1) C 26 - C 28	/654. BD*(1) C 26 - C 52	1.89	1.11	0.041
39. BD (1) C 26 - C 28	/658. BD*(1) C 28 - C 29	3.66	1.28	0.061
39. BD (1) C 26 - C 28	/659. BD*(1) C 28 - H 31	1.37	1.16	0.036
39. BD (1) C 26 - C 28	/660. BD*(1) C 29 - C 56	3.02	1.10	0.052
40. BD (2) C 26 - C 28	/648. BD*(2) C 24 - C 25	18.30	0.27	0.064

40. BD (2) C 26 - C 28	/656. BD*(2) C 27 - C 29	23.93	0.28	0.073
40. BD (2) C 26 - C 28	/684. BD*(1) C 52 - H 53	1.87	0.74	0.036
40. BD (2) C 26 - C 28	/685. BD*(1) C 52 - H 54	2.48	0.69	0.041
41. BD (1) C 26 - C 52	/333. RY*(1) C 24	1.52	1.93	0.049
41. BD (1) C 26 - C 52	/369. RY*(1) C 28	0.95	1.89	0.038
41. BD (1) C 26 - C 52	/647. BD*(1) C 24 - C 25	2.91	1.19	0.053
41. BD (1) C 26 - C 52	/649. BD*(1) C 24 - C 26	2.44	1.19	0.048
41. BD (1) C 26 - C 52	/652. BD*(1) C 26 - C 28	2.41	1.21	0.048
41. BD (1) C 26 - C 52	/658. BD*(1) C 28 - C 29	2.46	1.21	0.049
41. BD (1) C 26 - C 52	/684. BD*(1) C 52 - H 53	0.81	1.11	0.027
41. BD (1) C 26 - C 52	/685. BD*(1) C 52 - H 54	0.60	1.06	0.023
41. BD (1) C 26 - C 52	/686. BD*(1) C 52 - H 55	0.58	1.08	0.022
42. BD (1) C 27 - C 29	/342. RY*(1) C 25	0.89	1.98	0.038
42. BD (1) C 27 - C 29	/343. RY*(2) C 25	2.21	1.70	0.055
42. BD (1) C 27 - C 29	/369. RY*(1) C 28	0.59	1.97	0.031
42. BD (1) C 27 - C 29	/370. RY*(2) C 28	0.59	1.49	0.027
42. BD (1) C 27 - C 29	/541. RY*(1) C 56	0.75	1.47	0.030
42. BD (1) C 27 - C 29	/650. BD*(1) C 25 - C 27	3.62	1.28	0.061
42. BD (1) C 27 - C 29	/651. BD*(1) C 25 - C 48	3.00	1.10	0.051
42. BD (1) C 27 - C 29	/657. BD*(1) C 27 - H 30	1.47	1.16	0.037
42. BD (1) C 27 - C 29	/658. BD*(1) C 28 - C 29	3.76	1.29	0.062
42. BD (1) C 27 - C 29	/659. BD*(1) C 28 - H 31	2.28	1.16	0.046
42. BD (1) C 27 - C 29	/660. BD*(1) C 29 - C 56	1.81	1.11	0.040
42. BD (1) C 27 - C 29	/689. BD*(1) C 56 - H 59	0.60	1.14	0.023
43. BD (2) C 27 - C 29	/371. RY*(3) C 28	0.79	0.98	0.027
43. BD (2) C 27 - C 29	/648. BD*(2) C 24 - C 25	24.31	0.28	0.074
43. BD (2) C 27 - C 29	/653. BD*(2) C 26 - C 28	17.32	0.29	0.063
43. BD (2) C 27 - C 29	/687. BD*(1) C 56 - H 57	2.57	0.69	0.041
43. BD (2) C 27 - C 29	/689. BD*(1) C 56 - H 59	0.86	0.70	0.024
44. BD (1) C 27 - H 30	/342. RY*(1) C 25	1.35	1.81	0.044
44. BD (1) C 27 - H 30	/378. RY*(1) C 29	1.39	1.83	0.045
44. BD (1) C 27 - H 30	/647. BD*(1) C 24 - C 25	3.97	1.10	0.059
44. BD (1) C 27 - H 30	/650. BD*(1) C 25 - C 27	1.23	1.11	0.033
44. BD (1) C 27 - H 30	/655. BD*(1) C 27 - C 29	1.19	1.11	0.032
44. BD (1) C 27 - H 30	/658. BD*(1) C 28 - C 29	3.66	1.11	0.057
45. BD (1) C 28 - C 29	/351. RY*(1) C 26	0.82	1.98	0.036
45. BD (1) C 28 - C 29	/352. RY*(2) C 26	2.32	1.69	0.056
45. BD (1) C 28 - C 29	/360. RY*(1) C 27	0.54	1.96	0.029
45. BD (1) C 28 - C 29	/361. RY*(2) C 27	0.63	1.49	0.027
45. BD (1) C 28 - C 29	/541. RY*(1) C 56	0.75	1.47	0.030
45. BD (1) C 28 - C 29	/652. BD*(1) C 26 - C 28	3.50	1.28	0.060
45. BD (1) C 28 - C 29	/654. BD*(1) C 26 - C 52	2.81	1.12	0.050
45. BD (1) C 28 - C 29	/655. BD*(1) C 27 - C 29	3.79	1.28	0.062
45. BD (1) C 28 - C 29	/657. BD*(1) C 27 - H 30	2.36	1.16	0.047
45. BD (1) C 28 - C 29	/659. BD*(1) C 28 - H 31	1.44	1.16	0.037
45. BD (1) C 28 - C 29	/660. BD*(1) C 29 - C 56	1.83	1.11	0.040
45. BD (1) C 28 - C 29	/688. BD*(1) C 56 - H 58	0.62	1.14	0.024
46. BD (1) C 28 - H 31	/351. RY*(1) C 26	1.34	1.81	0.044

46. BD (1) C 28 - H 31	/378. RY*(1) C 29	1.37	1.82	0.045
46. BD (1) C 28 - H 31	/649. BD*(1) C 24 - C 26	3.96	1.10	0.059
46. BD (1) C 28 - H 31	/652. BD*(1) C 26 - C 28	1.23	1.11	0.033
46. BD (1) C 28 - H 31	/655. BD*(1) C 27 - C 29	3.77	1.11	0.058
46. BD (1) C 28 - H 31	/658. BD*(1) C 28 - C 29	1.17	1.11	0.032
47. BD (1) C 29 - C 56	/360. RY*(1) C 27	1.01	1.90	0.039
47. BD (1) C 29 - C 56	/369. RY*(1) C 28	1.05	1.90	0.040
47. BD (1) C 29 - C 56	/650. BD*(1) C 25 - C 27	2.36	1.22	0.048
47. BD (1) C 29 - C 56	/652. BD*(1) C 26 - C 28	2.37	1.22	0.048
47. BD (1) C 29 - C 56	/655. BD*(1) C 27 - C 29	2.22	1.22	0.046
47. BD (1) C 29 - C 56	/658. BD*(1) C 28 - C 29	2.24	1.22	0.047
47. BD (1) C 29 - C 56	/687. BD*(1) C 56 - H 57	0.67	1.07	0.024
47. BD (1) C 29 - C 56	/688. BD*(1) C 56 - H 58	0.61	1.07	0.023
47. BD (1) C 29 - C 56	/689. BD*(1) C 56 - H 59	0.62	1.07	0.023
48. BD (1) C 32 - C 33	/132. LP*(3)Ru 11	0.54	0.89	0.020
48. BD (1) C 32 - C 33	/316. RY*(1) N 21	0.94	1.72	0.036
48. BD (1) C 32 - C 33	/413. RY*(1) C 34	0.97	1.96	0.039
48. BD (1) C 32 - C 33	/414. RY*(2) C 34	0.82	1.70	0.033
48. BD (1) C 32 - C 33	/422. RY*(1) C 35	0.66	1.98	0.033
48. BD (1) C 32 - C 33	/423. RY*(2) C 35	0.73	1.51	0.030
48. BD (1) C 32 - C 33	/478. RY*(1) C 44	0.54	1.53	0.026
48. BD (1) C 32 - C 33	/637. BD*(1) C 15 - N 21	0.91	1.18	0.029
48. BD (1) C 32 - C 33	/642. BD*(1) C 17 - N 21	0.84	1.00	0.026
48. BD (1) C 32 - C 33	/646. BD*(1) N 21 - C 32	1.42	1.08	0.035
48. BD (1) C 32 - C 33	/663. BD*(1) C 32 - C 34	4.83	1.26	0.070
48. BD (1) C 32 - C 33	/664. BD*(1) C 33 - C 35	3.46	1.29	0.060
48. BD (1) C 32 - C 33	/665. BD*(1) C 33 - C 44	1.94	1.12	0.042
48. BD (1) C 32 - C 33	/668. BD*(1) C 34 - C 40	2.76	1.10	0.049
48. BD (1) C 32 - C 33	/671. BD*(1) C 35 - H 38	1.92	1.17	0.043
48. BD (1) C 32 - C 33	/679. BD*(1) C 44 - H 46	0.52	1.16	0.022
49. BD (2) C 32 - C 33	/132. LP*(3)Ru 11	2.32	0.45	0.030
49. BD (2) C 32 - C 33	/415. RY*(3) C 34	0.56	1.16	0.025
49. BD (2) C 32 - C 33	/424. RY*(3) C 35	0.86	1.00	0.029
49. BD (2) C 32 - C 33	/630. BD*(1) C 7 -Ru 11	0.66	0.60	0.019
49. BD (2) C 32 - C 33	/637. BD*(1) C 15 - N 21	2.72	0.74	0.044
49. BD (2) C 32 - C 33	/642. BD*(1) C 17 - N 21	3.12	0.56	0.040
49. BD (2) C 32 - C 33	/667. BD*(2) C 34 - C 36	23.07	0.29	0.073
49. BD (2) C 32 - C 33	/670. BD*(2) C 35 - C 37	15.65	0.30	0.061
49. BD (2) C 32 - C 33	/678. BD*(1) C 44 - H 45	2.14	0.76	0.039
49. BD (2) C 32 - C 33	/680. BD*(1) C 44 - H 47	0.73	0.72	0.022
50. BD (1) C 32 - C 34	/316. RY*(1) N 21	1.15	1.72	0.040
50. BD (1) C 32 - C 34	/404. RY*(1) C 33	0.94	1.98	0.039
50. BD (1) C 32 - C 34	/405. RY*(2) C 33	0.96	1.69	0.036
50. BD (1) C 32 - C 34	/431. RY*(1) C 36	0.70	1.97	0.033
50. BD (1) C 32 - C 34	/432. RY*(2) C 36	0.63	1.49	0.028
50. BD (1) C 32 - C 34	/457. RY*(1) C 40	0.62	1.51	0.028
50. BD (1) C 32 - C 34	/637. BD*(1) C 15 - N 21	1.03	1.18	0.031
50. BD (1) C 32 - C 34	/642. BD*(1) C 17 - N 21	0.69	1.00	0.023

50. BD (1) C 32 - C 34	/646. BD*(1) N 21 - C 32	1.29	1.08	0.033
50. BD (1) C 32 - C 34	/661. BD*(1) C 32 - C 33	4.70	1.27	0.069
50. BD (1) C 32 - C 34	/665. BD*(1) C 33 - C 44	2.70	1.12	0.049
50. BD (1) C 32 - C 34	/666. BD*(1) C 34 - C 36	3.70	1.29	0.062
50. BD (1) C 32 - C 34	/668. BD*(1) C 34 - C 40	1.86	1.10	0.041
50. BD (1) C 32 - C 34	/673. BD*(1) C 36 - H 39	2.03	1.16	0.044
50. BD (1) C 32 - C 34	/675. BD*(1) C 40 - H 41	0.56	1.14	0.023
51. BD (1) C 33 - C 35	/395. RY*(1) C 32	0.66	1.94	0.032
51. BD (1) C 33 - C 35	/397. RY*(3) C 32	0.89	1.81	0.036
51. BD (1) C 33 - C 35	/440. RY*(1) C 37	0.79	1.99	0.036
51. BD (1) C 33 - C 35	/441. RY*(2) C 37	2.05	1.65	0.052
51. BD (1) C 33 - C 35	/478. RY*(1) C 44	0.68	1.52	0.029
51. BD (1) C 33 - C 35	/646. BD*(1) N 21 - C 32	4.65	1.07	0.063
51. BD (1) C 33 - C 35	/661. BD*(1) C 32 - C 33	3.86	1.26	0.062
51. BD (1) C 33 - C 35	/665. BD*(1) C 33 - C 44	1.88	1.11	0.041
51. BD (1) C 33 - C 35	/669. BD*(1) C 35 - C 37	3.63	1.28	0.061
51. BD (1) C 33 - C 35	/671. BD*(1) C 35 - H 38	1.34	1.16	0.035
51. BD (1) C 33 - C 35	/674. BD*(1) C 37 - C 60	3.00	1.11	0.052
51. BD (1) C 33 - C 35	/680. BD*(1) C 44 - H 47	0.58	1.15	0.023
52. BD (1) C 33 - C 44	/395. RY*(1) C 32	1.52	1.87	0.048
52. BD (1) C 33 - C 44	/422. RY*(1) C 35	1.02	1.90	0.039
52. BD (1) C 33 - C 44	/661. BD*(1) C 32 - C 33	2.46	1.19	0.048
52. BD (1) C 33 - C 44	/663. BD*(1) C 32 - C 34	2.96	1.18	0.053
52. BD (1) C 33 - C 44	/664. BD*(1) C 33 - C 35	2.39	1.21	0.048
52. BD (1) C 33 - C 44	/669. BD*(1) C 35 - C 37	2.46	1.21	0.049
52. BD (1) C 33 - C 44	/678. BD*(1) C 44 - H 45	0.81	1.12	0.027
52. BD (1) C 33 - C 44	/679. BD*(1) C 44 - H 46	0.59	1.08	0.023
52. BD (1) C 33 - C 44	/680. BD*(1) C 44 - H 47	0.60	1.07	0.023
53. BD (1) C 34 - C 36	/395. RY*(1) C 32	0.75	1.95	0.034
53. BD (1) C 34 - C 36	/397. RY*(3) C 32	0.95	1.82	0.037
53. BD (1) C 34 - C 36	/440. RY*(1) C 37	1.15	2.00	0.043
53. BD (1) C 34 - C 36	/441. RY*(2) C 37	1.72	1.65	0.048
53. BD (1) C 34 - C 36	/457. RY*(1) C 40	0.68	1.51	0.029
53. BD (1) C 34 - C 36	/646. BD*(1) N 21 - C 32	4.12	1.08	0.060
53. BD (1) C 34 - C 36	/663. BD*(1) C 32 - C 34	4.08	1.26	0.064
53. BD (1) C 34 - C 36	/668. BD*(1) C 34 - C 40	1.85	1.10	0.040
53. BD (1) C 34 - C 36	/672. BD*(1) C 36 - C 37	3.64	1.29	0.061
53. BD (1) C 34 - C 36	/673. BD*(1) C 36 - H 39	1.39	1.16	0.036
53. BD (1) C 34 - C 36	/674. BD*(1) C 37 - C 60	2.95	1.12	0.051
53. BD (1) C 34 - C 36	/676. BD*(1) C 40 - H 42	0.69	1.14	0.025
54. BD (2) C 34 - C 36	/396. RY*(2) C 32	0.51	1.16	0.024
54. BD (2) C 34 - C 36	/662. BD*(2) C 32 - C 33	16.67	0.28	0.062
54. BD (2) C 34 - C 36	/670. BD*(2) C 35 - C 37	21.75	0.29	0.072
54. BD (2) C 34 - C 36	/676. BD*(1) C 40 - H 42	1.31	0.70	0.030
54. BD (2) C 34 - C 36	/677. BD*(1) C 40 - H 43	2.79	0.68	0.043
55. BD (1) C 34 - C 40	/395. RY*(1) C 32	1.56	1.89	0.049
55. BD (1) C 34 - C 40	/431. RY*(1) C 36	1.07	1.90	0.040
55. BD (1) C 34 - C 40	/661. BD*(1) C 32 - C 33	2.77	1.20	0.052

55. BD (1) C 34 - C 40	/663. BD*(1) C 32 - C 34	2.28	1.20	0.047
55. BD (1) C 34 - C 40	/666. BD*(1) C 34 - C 36	2.31	1.22	0.047
55. BD (1) C 34 - C 40	/672. BD*(1) C 36 - C 37	2.38	1.22	0.048
55. BD (1) C 34 - C 40	/675. BD*(1) C 40 - H 41	0.67	1.08	0.024
55. BD (1) C 34 - C 40	/676. BD*(1) C 40 - H 42	0.74	1.08	0.025
55. BD (1) C 34 - C 40	/677. BD*(1) C 40 - H 43	0.64	1.06	0.023
56. BD (1) C 35 - C 37	/404. RY*(1) C 33	0.75	1.98	0.035
56. BD (1) C 35 - C 37	/405. RY*(2) C 33	2.35	1.68	0.056
56. BD (1) C 35 - C 37	/432. RY*(2) C 36	0.69	1.49	0.029
56. BD (1) C 35 - C 37	/562. RY*(1) C 60	0.78	1.48	0.030
56. BD (1) C 35 - C 37	/664. BD*(1) C 33 - C 35	3.49	1.28	0.060
56. BD (1) C 35 - C 37	/665. BD*(1) C 33 - C 44	2.79	1.11	0.050
56. BD (1) C 35 - C 37	/671. BD*(1) C 35 - H 38	1.46	1.17	0.037
56. BD (1) C 35 - C 37	/672. BD*(1) C 36 - C 37	3.71	1.28	0.062
56. BD (1) C 35 - C 37	/673. BD*(1) C 36 - H 39	2.33	1.16	0.046
56. BD (1) C 35 - C 37	/674. BD*(1) C 37 - C 60	1.87	1.11	0.041
56. BD (1) C 35 - C 37	/692. BD*(1) C 60 - H 63	0.64	1.14	0.024
57. BD (2) C 35 - C 37	/434. RY*(4) C 36	0.73	2.04	0.038
57. BD (2) C 35 - C 37	/662. BD*(2) C 32 - C 33	25.12	0.27	0.074
57. BD (2) C 35 - C 37	/667. BD*(2) C 34 - C 36	18.43	0.28	0.064
57. BD (2) C 35 - C 37	/690. BD*(1) C 60 - H 61	0.50	0.70	0.018
57. BD (2) C 35 - C 37	/691. BD*(1) C 60 - H 62	2.45	0.70	0.041
57. BD (2) C 35 - C 37	/692. BD*(1) C 60 - H 63	0.69	0.70	0.022
58. BD (1) C 35 - H 38	/404. RY*(1) C 33	1.32	1.80	0.044
58. BD (1) C 35 - H 38	/440. RY*(1) C 37	1.38	1.82	0.045
58. BD (1) C 35 - H 38	/661. BD*(1) C 32 - C 33	4.02	1.09	0.059
58. BD (1) C 35 - H 38	/664. BD*(1) C 33 - C 35	1.21	1.10	0.033
58. BD (1) C 35 - H 38	/669. BD*(1) C 35 - C 37	1.21	1.11	0.033
58. BD (1) C 35 - H 38	/672. BD*(1) C 36 - C 37	3.84	1.10	0.058
59. BD (1) C 36 - C 37	/413. RY*(1) C 34	0.61	1.96	0.031
59. BD (1) C 36 - C 37	/414. RY*(2) C 34	2.43	1.69	0.058
59. BD (1) C 36 - C 37	/422. RY*(1) C 35	0.57	1.97	0.030
59. BD (1) C 36 - C 37	/423. RY*(2) C 35	0.62	1.50	0.027
59. BD (1) C 36 - C 37	/562. RY*(1) C 60	0.73	1.48	0.030
59. BD (1) C 36 - C 37	/666. BD*(1) C 34 - C 36	3.64	1.28	0.061
59. BD (1) C 36 - C 37	/668. BD*(1) C 34 - C 40	3.05	1.09	0.052
59. BD (1) C 36 - C 37	/669. BD*(1) C 35 - C 37	3.68	1.29	0.062
59. BD (1) C 36 - C 37	/671. BD*(1) C 35 - H 38	2.26	1.17	0.046
59. BD (1) C 36 - C 37	/673. BD*(1) C 36 - H 39	1.46	1.16	0.037
59. BD (1) C 36 - C 37	/674. BD*(1) C 37 - C 60	1.79	1.11	0.040
59. BD (1) C 36 - C 37	/690. BD*(1) C 60 - H 61	0.60	1.14	0.024
60. BD (1) C 36 - H 39	/413. RY*(1) C 34	1.31	1.79	0.043
60. BD (1) C 36 - H 39	/440. RY*(1) C 37	1.41	1.83	0.045
60. BD (1) C 36 - H 39	/663. BD*(1) C 32 - C 34	4.04	1.09	0.059
60. BD (1) C 36 - H 39	/666. BD*(1) C 34 - C 36	1.23	1.11	0.033
60. BD (1) C 36 - H 39	/669. BD*(1) C 35 - C 37	3.62	1.12	0.057
60. BD (1) C 36 - H 39	/672. BD*(1) C 36 - C 37	1.18	1.11	0.032
61. BD (1) C 37 - C 60	/422. RY*(1) C 35	1.04	1.90	0.040

61. BD (1) C 37 - C 60	/431. RY*(1) C 36	0.94	1.89	0.038
61. BD (1) C 37 - C 60	/664. BD*(1) C 33 - C 35	2.41	1.21	0.048
61. BD (1) C 37 - C 60	/666. BD*(1) C 34 - C 36	2.36	1.21	0.048
61. BD (1) C 37 - C 60	/669. BD*(1) C 35 - C 37	2.29	1.22	0.047
61. BD (1) C 37 - C 60	/672. BD*(1) C 36 - C 37	2.20	1.21	0.046
61. BD (1) C 37 - C 60	/690. BD*(1) C 60 - H 61	0.61	1.08	0.023
61. BD (1) C 37 - C 60	/691. BD*(1) C 60 - H 62	0.67	1.08	0.024
61. BD (1) C 37 - C 60	/692. BD*(1) C 60 - H 63	0.59	1.07	0.023
62. BD (1) C 40 - H 41	/663. BD*(1) C 32 - C 34	3.78	1.08	0.057
62. BD (1) C 40 - H 41	/668. BD*(1) C 34 - C 40	0.62	0.92	0.021
63. BD (1) C 40 - H 42	/414. RY*(2) C 34	0.54	1.52	0.026
63. BD (1) C 40 - H 42	/666. BD*(1) C 34 - C 36	2.63	1.11	0.048
63. BD (1) C 40 - H 42	/667. BD*(2) C 34 - C 36	1.16	0.55	0.025
63. BD (1) C 40 - H 42	/668. BD*(1) C 34 - C 40	0.53	0.92	0.020
64. BD (1) C 40 - H 43	/415. RY*(3) C 34	0.83	1.42	0.031
64. BD (1) C 40 - H 43	/666. BD*(1) C 34 - C 36	0.56	1.10	0.022
64. BD (1) C 40 - H 43	/667. BD*(2) C 34 - C 36	4.26	0.54	0.047
64. BD (1) C 40 - H 43	/668. BD*(1) C 34 - C 40	0.59	0.92	0.021
65. BD (1) C 44 - H 45	/406. RY*(3) C 33	0.96	1.40	0.033
65. BD (1) C 44 - H 45	/662. BD*(2) C 32 - C 33	4.25	0.51	0.046
65. BD (1) C 44 - H 45	/664. BD*(1) C 33 - C 35	0.79	1.07	0.026
65. BD (1) C 44 - H 45	/665. BD*(1) C 33 - C 44	0.75	0.91	0.023
66. BD (1) C 44 - H 46	/661. BD*(1) C 32 - C 33	4.03	1.07	0.059
66. BD (1) C 44 - H 46	/662. BD*(2) C 32 - C 33	0.66	0.52	0.018
66. BD (1) C 44 - H 46	/665. BD*(1) C 33 - C 44	0.57	0.92	0.020
67. BD (1) C 44 - H 47	/662. BD*(2) C 32 - C 33	1.85	0.52	0.031
67. BD (1) C 44 - H 47	/664. BD*(1) C 33 - C 35	2.55	1.09	0.047
68. BD (1) C 48 - H 49	/647. BD*(1) C 24 - C 25	4.03	1.09	0.059
68. BD (1) C 48 - H 49	/651. BD*(1) C 25 - C 48	0.62	0.92	0.021
69. BD (1) C 48 - H 50	/344. RY*(3) C 25	0.87	1.40	0.031
69. BD (1) C 48 - H 50	/648. BD*(2) C 24 - C 25	3.65	0.54	0.044
69. BD (1) C 48 - H 50	/650. BD*(1) C 25 - C 27	1.17	1.10	0.032
69. BD (1) C 48 - H 50	/651. BD*(1) C 25 - C 48	0.53	0.92	0.020
70. BD (1) C 48 - H 51	/344. RY*(3) C 25	0.65	1.41	0.027
70. BD (1) C 48 - H 51	/648. BD*(2) C 24 - C 25	2.20	0.54	0.034
70. BD (1) C 48 - H 51	/650. BD*(1) C 25 - C 27	2.02	1.10	0.042
70. BD (1) C 48 - H 51	/651. BD*(1) C 25 - C 48	0.64	0.92	0.022
71. BD (1) C 52 - H 53	/353. RY*(3) C 26	0.70	1.44	0.028
71. BD (1) C 52 - H 53	/652. BD*(1) C 26 - C 28	2.02	1.08	0.042
71. BD (1) C 52 - H 53	/653. BD*(2) C 26 - C 28	2.90	0.52	0.038
71. BD (1) C 52 - H 53	/654. BD*(1) C 26 - C 52	0.76	0.91	0.023
72. BD (1) C 52 - H 54	/353. RY*(3) C 26	0.84	1.45	0.031
72. BD (1) C 52 - H 54	/652. BD*(1) C 26 - C 28	1.36	1.09	0.034
72. BD (1) C 52 - H 54	/653. BD*(2) C 26 - C 28	3.67	0.53	0.043
73. BD (1) C 52 - H 55	/649. BD*(1) C 24 - C 26	4.24	1.07	0.060
73. BD (1) C 52 - H 55	/654. BD*(1) C 26 - C 52	0.55	0.92	0.020
74. BD (1) C 56 - H 57	/380. RY*(3) C 29	1.10	1.38	0.035
74. BD (1) C 56 - H 57	/656. BD*(2) C 27 - C 29	4.15	0.54	0.046

74. BD (1) C 56 - H 57	/660. BD*(1) C 29 - C 56	0.55	0.92	0.020
75. BD (1) C 56 - H 58	/656. BD*(2) C 27 - C 29	0.80	0.54	0.020
75. BD (1) C 56 - H 58	/658. BD*(1) C 28 - C 29	3.19	1.10	0.053
76. BD (1) C 56 - H 59	/655. BD*(1) C 27 - C 29	3.19	1.10	0.053
76. BD (1) C 56 - H 59	/656. BD*(2) C 27 - C 29	0.99	0.54	0.023
76. BD (1) C 56 - H 59	/660. BD*(1) C 29 - C 56	0.50	0.92	0.019
77. BD (1) C 60 - H 61	/670. BD*(2) C 35 - C 37	1.01	0.54	0.023
77. BD (1) C 60 - H 61	/672. BD*(1) C 36 - C 37	3.08	1.09	0.052
78. BD (1) C 60 - H 62	/442. RY*(3) C 37	1.07	1.39	0.035
78. BD (1) C 60 - H 62	/670. BD*(2) C 35 - C 37	4.34	0.54	0.047
78. BD (1) C 60 - H 62	/672. BD*(1) C 36 - C 37	0.56	1.09	0.022
78. BD (1) C 60 - H 62	/674. BD*(1) C 37 - C 60	0.57	0.92	0.021
79. BD (1) C 60 - H 63	/441. RY*(2) C 37	0.54	1.46	0.025
79. BD (1) C 60 - H 63	/669. BD*(1) C 35 - C 37	3.34	1.10	0.054
79. BD (1) C 60 - H 63	/670. BD*(2) C 35 - C 37	0.71	0.54	0.019
80. BD (1) N 65 - O 66	/194. RY*(1) C 6	1.09	2.15	0.043
80. BD (1) N 65 - O 66	/195. RY*(2) C 6	0.90	2.26	0.040
80. BD (1) N 65 - O 66	/587. RY*(1) N 65	0.62	2.14	0.033
80. BD (1) N 65 - O 66	/616. BD*(1) C 1 - C 6	0.93	1.65	0.035
80. BD (1) N 65 - O 66	/628. BD*(1) C 6 - N 65	0.82	1.37	0.031
81. BD (2) N 65 - O 66	/148. LP (3) O 67	12.19	0.18	0.078
81. BD (2) N 65 - O 66	/606. RY*(2) O 67	1.57	1.45	0.043
81. BD (2) N 65 - O 66	/626. BD*(2) C 5 - C 6	3.02	0.46	0.037
81. BD (2) N 65 - O 66	/694. BD*(2) N 65 - O 66	7.49	0.32	0.053
82. BD (1) N 65 - O 67	/194. RY*(1) C 6	1.97	2.14	0.058
82. BD (1) N 65 - O 67	/587. RY*(1) N 65	0.80	2.13	0.037
82. BD (1) N 65 - O 67	/625. BD*(1) C 5 - C 6	0.73	1.64	0.031
82. BD (1) N 65 - O 67	/628. BD*(1) C 6 - N 65	0.78	1.37	0.030
83. CR (1) C 1	/158. RY*(1) C 2	0.60	11.56	0.075
83. CR (1) C 1	/159. RY*(2) C 2	1.75	11.34	0.126
83. CR (1) C 1	/194. RY*(1) C 6	0.89	11.17	0.089
83. CR (1) C 1	/195. RY*(2) C 6	1.61	11.28	0.120
83. CR (1) C 1	/614. BD*(1) C 1 - C 2	0.70	10.66	0.078
83. CR (1) C 1	/617. BD*(1) C 1 - I 12	2.26	10.18	0.138
83. CR (1) C 1	/618. BD*(1) C 2 - C 3	0.66	10.67	0.076
83. CR (1) C 1	/619. BD*(1) C 2 - C 7	0.82	10.59	0.084
83. CR (1) C 1	/625. BD*(1) C 5 - C 6	0.81	10.67	0.083
83. CR (1) C 1	/628. BD*(1) C 6 - N 65	1.06	10.40	0.096
84. CR (1) C 2	/132. LP*(3)Ru 11	1.14	10.28	0.101
84. CR (1) C 2	/149. RY*(1) C 1	2.05	11.21	0.135
84. CR (1) C 2	/168. RY*(2) C 3	1.58	10.84	0.117
84. CR (1) C 2	/204. RY*(2) C 7	0.70	12.31	0.083
84. CR (1) C 2	/206. RY*(4) C 7	0.59	11.49	0.074
84. CR (1) C 2	/616. BD*(1) C 1 - C 6	0.93	10.62	0.089
84. CR (1) C 2	/617. BD*(1) C 1 - I 12	0.87	10.13	0.085
84. CR (1) C 2	/620. BD*(1) C 3 - C 4	0.64	10.65	0.074
84. CR (1) C 2	/630. BD*(1) C 7 -Ru 11	1.13	10.43	0.100
85. CR (1) C 3	/158. RY*(1) C 2	0.60	11.51	0.074

85. CR (1) C 3	/159. RY*(2) C 2	1.67	11.29	0.123
85. CR (1) C 3	/177. RY*(2) C 4	1.73	10.75	0.122
85. CR (1) C 3	/180. RY*(5) C 4	0.51	11.13	0.067
85. CR (1) C 3	/212. RY*(1) H 8	0.67	10.66	0.075
85. CR (1) C 3	/614. BD*(1) C 1 - C 2	0.90	10.61	0.088
85. CR (1) C 3	/619. BD*(1) C 2 - C 7	0.78	10.54	0.082
85. CR (1) C 3	/623. BD*(1) C 4 - C 5	0.68	10.65	0.076
85. CR (1) C 3	/624. BD*(1) C 4 - H 64	0.59	10.54	0.071
86. CR (1) C 4	/168. RY*(2) C 3	1.51	10.84	0.114
86. CR (1) C 4	/171. RY*(5) C 3	0.70	11.13	0.079
86. CR (1) C 4	/185. RY*(1) C 5	0.96	11.25	0.093
86. CR (1) C 4	/186. RY*(2) C 5	0.95	10.85	0.091
86. CR (1) C 4	/189. RY*(5) C 5	0.58	11.20	0.072
86. CR (1) C 4	/583. RY*(1) H 64	0.65	10.64	0.074
86. CR (1) C 4	/618. BD*(1) C 2 - C 3	0.77	10.62	0.081
86. CR (1) C 4	/622. BD*(1) C 3 - H 8	0.61	10.54	0.072
86. CR (1) C 4	/625. BD*(1) C 5 - C 6	0.74	10.62	0.079
86. CR (1) C 4	/627. BD*(1) C 5 - H 9	0.63	10.55	0.073
87. CR (1) C 5	/177. RY*(2) C 4	1.72	10.76	0.121
87. CR (1) C 5	/180. RY*(5) C 4	0.60	11.14	0.073
87. CR (1) C 5	/194. RY*(1) C 6	2.23	11.13	0.141
87. CR (1) C 5	/196. RY*(3) C 6	0.51	11.08	0.067
87. CR (1) C 5	/216. RY*(1) H 9	0.83	10.69	0.084
87. CR (1) C 5	/616. BD*(1) C 1 - C 6	1.15	10.62	0.099
87. CR (1) C 5	/620. BD*(1) C 3 - C 4	0.67	10.65	0.076
87. CR (1) C 5	/624. BD*(1) C 4 - H 64	0.56	10.54	0.069
87. CR (1) C 5	/628. BD*(1) C 6 - N 65	0.58	10.35	0.071
88. CR (1) C 6	/150. RY*(2) C 1	2.56	11.41	0.153
88. CR (1) C 6	/186. RY*(2) C 5	1.76	10.90	0.124
88. CR (1) C 6	/588. RY*(2) N 65	0.74	11.37	0.082
88. CR (1) C 6	/614. BD*(1) C 1 - C 2	0.79	10.66	0.082
88. CR (1) C 6	/616. BD*(1) C 1 - C 6	0.94	10.67	0.090
88. CR (1) C 6	/617. BD*(1) C 1 - I 12	1.40	10.18	0.109
88. CR (1) C 6	/623. BD*(1) C 4 - C 5	0.56	10.70	0.069
88. CR (1) C 6	/625. BD*(1) C 5 - C 6	0.72	10.67	0.078
88. CR (1) C 6	/628. BD*(1) C 6 - N 65	0.90	10.40	0.089
89. CR (1) C 7	/132. LP*(3)Ru 11	8.81	10.27	0.280
89. CR (1) C 7	/158. RY*(1) C 2	1.21	11.50	0.106
89. CR (1) C 7	/220. RY*(1) H 10	0.51	10.95	0.066
89. CR (1) C 7	/230. RY*(7)Ru 11	0.55	10.85	0.069
89. CR (1) C 7	/232. RY*(9)Ru 11	0.71	11.16	0.080
89. CR (1) C 7	/614. BD*(1) C 1 - C 2	0.93	10.60	0.089
89. CR (1) C 7	/618. BD*(1) C 2 - C 3	0.54	10.62	0.068
90. CR (1)Ru 11	/132. LP*(3)Ru 11	0.74	3.11	0.045
90. CR (1)Ru 11	/204. RY*(2) C 7	2.78	5.15	0.107
90. CR (1)Ru 11	/241. RY*(18)Ru 11	0.57	6.62	0.055
90. CR (1)Ru 11	/243. RY*(20)Ru 11	1.33	36.09	0.196
90. CR (1)Ru 11	/272. RY*(1) C 15	1.48	4.46	0.073

90. CR (1)Ru 11	/273. RY*(2) C 15	0.57	3.97	0.042
90. CR (1)Ru 11	/619. BD*(1) C 2 - C 7	2.08	3.38	0.075
90. CR (1)Ru 11	/629. BD*(1) C 7 - H 10	0.90	3.38	0.049
90. CR (1)Ru 11	/630. BD*(1) C 7 -Ru 11	13.28	3.27	0.191
90. CR (1)Ru 11	/635. BD*(1)Ru 11 - C 15	2.63	3.29	0.087
90. CR (1)Ru 11	/636. BD*(1) C 15 - N 16	2.00	3.41	0.074
91. CR (2)Ru 11	/204. RY*(2) C 7	1.43	4.06	0.068
91. CR (2)Ru 11	/227. RY*(4)Ru 11	0.54	3.56	0.039
91. CR (2)Ru 11	/237. RY*(14)Ru 11	0.59	3.40	0.040
91. CR (2)Ru 11	/241. RY*(18)Ru 11	0.94	5.53	0.065
91. CR (2)Ru 11	/243. RY*(20)Ru 11	1.92	35.00	0.233
91. CR (2)Ru 11	/619. BD*(1) C 2 - C 7	0.77	2.29	0.037
91. CR (2)Ru 11	/630. BD*(1) C 7 -Ru 11	23.20	2.18	0.206
92. CR (3)Ru 11	/141. LP*(1) C 15	0.82	1.73	0.042
92. CR (3)Ru 11	/619. BD*(1) C 2 - C 7	0.50	2.30	0.031
92. CR (3)Ru 11	/629. BD*(1) C 7 - H 10	0.60	2.30	0.033
92. CR (3)Ru 11	/635. BD*(1)Ru 11 - C 15	1.59	2.21	0.056
93. CR (4)Ru 11	/631. BD*(2) C 7 -Ru 11	0.52	1.85	0.029
93. CR (4)Ru 11	/635. BD*(1)Ru 11 - C 15	3.16	2.21	0.078
93. CR (4)Ru 11	/636. BD*(1) C 15 - N 16	0.74	2.33	0.037
95. CR (2)Cl 13	/225. RY*(2)Ru 11	0.67	11.17	0.077
95. CR (2)Cl 13	/632. BD*(1)Ru 11 - I 12	2.61	10.96	0.157
95. CR (2)Cl 13	/633. BD*(1)Ru 11 -Cl 13	0.69	10.82	0.080
100. CR (2)Cl 14	/132. LP*(3)Ru 11	0.60	9.98	0.072
100. CR (2)Cl 14	/631. BD*(2) C 7 -Ru 11	0.98	9.79	0.092
100. CR (2)Cl 14	/635. BD*(1)Ru 11 - C 15	0.84	10.15	0.086
104. CR (1) C 15	/132. LP*(3)Ru 11	0.71	10.33	0.079
104. CR (1) C 15	/283. RY*(3) N 16	0.57	11.57	0.073
104. CR (1) C 15	/318. RY*(3) N 21	0.63	11.73	0.076
104. CR (1) C 15	/635. BD*(1)Ru 11 - C 15	0.67	10.51	0.079
104. CR (1) C 15	/638. BD*(1) N 16 - C 18	0.80	10.44	0.082
104. CR (1) C 15	/639. BD*(1) N 16 - C 24	1.39	10.53	0.109
104. CR (1) C 15	/642. BD*(1) C 17 - N 21	0.86	10.44	0.085
104. CR (1) C 15	/646. BD*(1) N 21 - C 32	1.28	10.52	0.104
105. CR (1) N 16	/273. RY*(2) C 15	3.08	15.26	0.194
105. CR (1) N 16	/301. RY*(3) C 18	1.32	14.99	0.126
105. CR (1) N 16	/333. RY*(1) C 24	1.64	15.53	0.142
105. CR (1) N 16	/635. BD*(1)Ru 11 - C 15	1.18	14.58	0.123
106. CR (1) C 17	/300. RY*(2) C 18	0.61	10.95	0.073
106. CR (1) C 17	/303. RY*(5) C 18	0.52	11.52	0.069
106. CR (1) C 17	/308. RY*(1) H 19	0.61	10.79	0.072
106. CR (1) C 17	/325. RY*(1) H 22	0.63	10.78	0.074
106. CR (1) C 17	/637. BD*(1) C 15 - N 21	0.60	10.61	0.072
106. CR (1) C 17	/646. BD*(1) N 21 - C 32	0.71	10.51	0.078
107. CR (1) C 18	/291. RY*(2) C 17	0.59	10.98	0.072
107. CR (1) C 18	/312. RY*(1) H 20	0.60	10.79	0.072
107. CR (1) C 18	/329. RY*(1) H 23	0.66	10.79	0.075
107. CR (1) C 18	/636. BD*(1) C 15 - N 16	0.61	10.62	0.072

107. CR (1) C 18	/639. BD*(1) N 16 - C 24	0.65	10.51	0.074
108. CR (1) N 21	/272. RY*(1) C 15	1.09	15.75	0.117
108. CR (1) N 21	/273. RY*(2) C 15	0.89	15.26	0.104
108. CR (1) N 21	/274. RY*(3) C 15	0.95	15.27	0.107
108. CR (1) N 21	/292. RY*(3) C 17	1.53	14.97	0.135
108. CR (1) N 21	/395. RY*(1) C 32	1.54	15.47	0.138
108. CR (1) N 21	/635. BD*(1)Ru 11 - C 15	1.09	14.58	0.119
109. CR (1) C 24	/343. RY*(2) C 25	1.80	11.09	0.126
109. CR (1) C 24	/352. RY*(2) C 26	1.88	11.08	0.129
109. CR (1) C 24	/636. BD*(1) C 15 - N 16	1.00	10.58	0.093
109. CR (1) C 24	/638. BD*(1) N 16 - C 18	0.64	10.38	0.073
109. CR (1) C 24	/647. BD*(1) C 24 - C 25	0.69	10.66	0.077
109. CR (1) C 24	/649. BD*(1) C 24 - C 26	0.67	10.66	0.076
109. CR (1) C 24	/650. BD*(1) C 25 - C 27	0.65	10.68	0.075
109. CR (1) C 24	/651. BD*(1) C 25 - C 48	0.82	10.50	0.083
109. CR (1) C 24	/652. BD*(1) C 26 - C 28	0.61	10.68	0.073
109. CR (1) C 24	/654. BD*(1) C 26 - C 52	0.80	10.51	0.082
110. CR (1) C 25	/335. RY*(3) C 24	1.55	11.19	0.118
110. CR (1) C 25	/337. RY*(5) C 24	0.60	12.06	0.076
110. CR (1) C 25	/361. RY*(2) C 27	1.43	10.85	0.111
110. CR (1) C 25	/500. RY*(2) C 48	1.22	10.81	0.102
110. CR (1) C 25	/639. BD*(1) N 16 - C 24	0.76	10.45	0.080
110. CR (1) C 25	/649. BD*(1) C 24 - C 26	0.88	10.64	0.087
110. CR (1) C 25	/650. BD*(1) C 25 - C 27	0.50	10.65	0.066
110. CR (1) C 25	/655. BD*(1) C 27 - C 29	0.76	10.65	0.081
110. CR (1) C 25	/657. BD*(1) C 27 - H 30	0.56	10.52	0.069
111. CR (1) C 26	/335. RY*(3) C 24	1.33	11.19	0.109
111. CR (1) C 26	/336. RY*(4) C 24	0.62	11.52	0.075
111. CR (1) C 26	/370. RY*(2) C 28	1.36	10.86	0.108
111. CR (1) C 26	/521. RY*(2) C 52	1.31	10.79	0.106
111. CR (1) C 26	/639. BD*(1) N 16 - C 24	0.81	10.45	0.083
111. CR (1) C 26	/647. BD*(1) C 24 - C 25	0.90	10.63	0.088
111. CR (1) C 26	/658. BD*(1) C 28 - C 29	0.78	10.65	0.082
111. CR (1) C 26	/659. BD*(1) C 28 - H 31	0.54	10.53	0.068
112. CR (1) C 27	/342. RY*(1) C 25	0.76	11.33	0.083
112. CR (1) C 27	/343. RY*(2) C 25	1.58	11.05	0.118
112. CR (1) C 27	/378. RY*(1) C 29	0.55	11.35	0.071
112. CR (1) C 27	/379. RY*(2) C 29	1.97	10.99	0.132
112. CR (1) C 27	/387. RY*(1) H 30	0.58	10.63	0.070
112. CR (1) C 27	/647. BD*(1) C 24 - C 25	0.86	10.62	0.086
112. CR (1) C 27	/651. BD*(1) C 25 - C 48	0.81	10.45	0.082
112. CR (1) C 27	/658. BD*(1) C 28 - C 29	0.75	10.63	0.080
112. CR (1) C 27	/660. BD*(1) C 29 - C 56	0.82	10.45	0.083
113. CR (1) C 28	/351. RY*(1) C 26	0.81	11.33	0.086
113. CR (1) C 28	/352. RY*(2) C 26	1.51	11.03	0.115
113. CR (1) C 28	/378. RY*(1) C 29	0.67	11.34	0.078
113. CR (1) C 28	/379. RY*(2) C 29	1.85	10.99	0.127
113. CR (1) C 28	/391. RY*(1) H 31	0.59	10.63	0.071

113. CR (1) C 28	/649. BD*(1) C 24 - C 26	0.83	10.62	0.085
113. CR (1) C 28	/654. BD*(1) C 26 - C 52	0.77	10.46	0.081
113. CR (1) C 28	/655. BD*(1) C 27 - C 29	0.77	10.63	0.081
113. CR (1) C 28	/660. BD*(1) C 29 - C 56	0.82	10.45	0.083
114. CR (1) C 29	/361. RY*(2) C 27	1.42	10.85	0.111
114. CR (1) C 29	/364. RY*(5) C 27	0.60	11.18	0.073
114. CR (1) C 29	/370. RY*(2) C 28	1.50	10.86	0.114
114. CR (1) C 29	/373. RY*(5) C 28	0.57	11.20	0.071
114. CR (1) C 29	/543. RY*(3) C 56	1.22	10.82	0.103
114. CR (1) C 29	/650. BD*(1) C 25 - C 27	0.74	10.65	0.080
114. CR (1) C 29	/652. BD*(1) C 26 - C 28	0.74	10.65	0.080
114. CR (1) C 29	/657. BD*(1) C 27 - H 30	0.61	10.52	0.072
114. CR (1) C 29	/659. BD*(1) C 28 - H 31	0.59	10.53	0.071
115. CR (1) C 32	/132. LP*(3)Ru 11	0.55	10.28	0.070
115. CR (1) C 32	/405. RY*(2) C 33	1.92	11.08	0.130
115. CR (1) C 32	/414. RY*(2) C 34	1.95	11.09	0.131
115. CR (1) C 32	/637. BD*(1) C 15 - N 21	0.91	10.57	0.088
115. CR (1) C 32	/642. BD*(1) C 17 - N 21	0.71	10.39	0.077
115. CR (1) C 32	/661. BD*(1) C 32 - C 33	0.66	10.66	0.075
115. CR (1) C 32	/663. BD*(1) C 32 - C 34	0.66	10.65	0.075
115. CR (1) C 32	/664. BD*(1) C 33 - C 35	0.60	10.68	0.072
115. CR (1) C 32	/665. BD*(1) C 33 - C 44	0.81	10.51	0.083
115. CR (1) C 32	/666. BD*(1) C 34 - C 36	0.63	10.68	0.074
115. CR (1) C 32	/668. BD*(1) C 34 - C 40	0.82	10.49	0.083
116. CR (1) C 33	/397. RY*(3) C 32	1.60	11.18	0.119
116. CR (1) C 33	/423. RY*(2) C 35	1.37	10.86	0.109
116. CR (1) C 33	/479. RY*(2) C 44	1.31	10.75	0.106
116. CR (1) C 33	/646. BD*(1) N 21 - C 32	0.86	10.44	0.085
116. CR (1) C 33	/663. BD*(1) C 32 - C 34	0.91	10.62	0.088
116. CR (1) C 33	/669. BD*(1) C 35 - C 37	0.77	10.65	0.081
116. CR (1) C 33	/671. BD*(1) C 35 - H 38	0.52	10.53	0.066
117. CR (1) C 34	/397. RY*(3) C 32	1.43	11.19	0.113
117. CR (1) C 34	/432. RY*(2) C 36	1.48	10.86	0.113
117. CR (1) C 34	/458. RY*(2) C 40	0.82	11.02	0.085
117. CR (1) C 34	/646. BD*(1) N 21 - C 32	0.75	10.45	0.080
117. CR (1) C 34	/661. BD*(1) C 32 - C 33	0.89	10.63	0.087
117. CR (1) C 34	/666. BD*(1) C 34 - C 36	0.53	10.65	0.068
117. CR (1) C 34	/672. BD*(1) C 36 - C 37	0.75	10.65	0.080
117. CR (1) C 34	/673. BD*(1) C 36 - H 39	0.56	10.53	0.069
118. CR (1) C 35	/404. RY*(1) C 33	0.85	11.32	0.088
118. CR (1) C 35	/405. RY*(2) C 33	1.49	11.02	0.114
118. CR (1) C 35	/440. RY*(1) C 37	0.76	11.34	0.083
118. CR (1) C 35	/441. RY*(2) C 37	1.79	11.00	0.125
118. CR (1) C 35	/449. RY*(1) H 38	0.60	10.63	0.071
118. CR (1) C 35	/661. BD*(1) C 32 - C 33	0.84	10.61	0.085
118. CR (1) C 35	/665. BD*(1) C 33 - C 44	0.77	10.46	0.080
118. CR (1) C 35	/672. BD*(1) C 36 - C 37	0.77	10.63	0.081
118. CR (1) C 35	/674. BD*(1) C 37 - C 60	0.82	10.46	0.083

119. CR (1) C 36	/413. RY*(1) C 34	0.98	11.31	0.094
119. CR (1) C 36	/414. RY*(2) C 34	1.32	11.04	0.108
119. CR (1) C 36	/441. RY*(2) C 37	2.05	11.00	0.134
119. CR (1) C 36	/453. RY*(1) H 39	0.59	10.62	0.071
119. CR (1) C 36	/663. BD*(1) C 32 - C 34	0.87	10.61	0.086
119. CR (1) C 36	/668. BD*(1) C 34 - C 40	0.81	10.44	0.082
119. CR (1) C 36	/669. BD*(1) C 35 - C 37	0.74	10.64	0.080
119. CR (1) C 36	/674. BD*(1) C 37 - C 60	0.80	10.46	0.082
120. CR (1) C 37	/423. RY*(2) C 35	1.44	10.86	0.112
120. CR (1) C 37	/426. RY*(5) C 35	0.56	11.13	0.070
120. CR (1) C 37	/432. RY*(2) C 36	1.27	10.85	0.105
120. CR (1) C 37	/435. RY*(5) C 36	0.66	11.13	0.077
120. CR (1) C 37	/564. RY*(3) C 60	1.37	10.72	0.108
120. CR (1) C 37	/664. BD*(1) C 33 - C 35	0.75	10.65	0.080
120. CR (1) C 37	/666. BD*(1) C 34 - C 36	0.74	10.64	0.080
120. CR (1) C 37	/671. BD*(1) C 35 - H 38	0.59	10.53	0.070
120. CR (1) C 37	/673. BD*(1) C 36 - H 39	0.61	10.52	0.072
121. CR (1) C 40	/413. RY*(1) C 34	1.08	11.33	0.099
121. CR (1) C 40	/466. RY*(1) H 41	0.62	10.75	0.073
121. CR (1) C 40	/470. RY*(1) H 42	0.71	10.87	0.078
121. CR (1) C 40	/474. RY*(1) H 43	0.59	10.77	0.071
121. CR (1) C 40	/663. BD*(1) C 32 - C 34	0.64	10.63	0.074
121. CR (1) C 40	/666. BD*(1) C 34 - C 36	0.54	10.65	0.068
122. CR (1) C 44	/404. RY*(1) C 33	1.11	11.33	0.100
122. CR (1) C 44	/487. RY*(1) H 45	0.94	10.92	0.090
122. CR (1) C 44	/491. RY*(1) H 46	0.59	10.74	0.071
122. CR (1) C 44	/495. RY*(1) H 47	0.60	10.80	0.072
122. CR (1) C 44	/661. BD*(1) C 32 - C 33	0.69	10.61	0.077
122. CR (1) C 44	/664. BD*(1) C 33 - C 35	0.57	10.63	0.070
123. CR (1) C 48	/342. RY*(1) C 25	1.12	11.35	0.101
123. CR (1) C 48	/508. RY*(1) H 49	0.61	10.75	0.072
123. CR (1) C 48	/512. RY*(1) H 50	0.60	10.79	0.072
123. CR (1) C 48	/516. RY*(1) H 51	0.75	11.02	0.081
123. CR (1) C 48	/647. BD*(1) C 24 - C 25	0.63	10.64	0.074
123. CR (1) C 48	/650. BD*(1) C 25 - C 27	0.56	10.65	0.070
124. CR (1) C 52	/351. RY*(1) C 26	1.11	11.33	0.100
124. CR (1) C 52	/529. RY*(1) H 53	1.05	10.93	0.096
124. CR (1) C 52	/533. RY*(1) H 54	0.58	10.79	0.071
124. CR (1) C 52	/537. RY*(1) H 55	0.60	10.75	0.072
124. CR (1) C 52	/649. BD*(1) C 24 - C 26	0.66	10.62	0.075
124. CR (1) C 52	/652. BD*(1) C 26 - C 28	0.59	10.63	0.071
125. CR (1) C 56	/378. RY*(1) C 29	1.09	11.37	0.100
125. CR (1) C 56	/550. RY*(1) H 57	0.61	10.74	0.072
125. CR (1) C 56	/554. RY*(1) H 58	0.60	10.74	0.072
125. CR (1) C 56	/558. RY*(1) H 59	0.61	10.74	0.072
125. CR (1) C 56	/655. BD*(1) C 27 - C 29	0.59	10.65	0.071
125. CR (1) C 56	/658. BD*(1) C 28 - C 29	0.59	10.65	0.071
126. CR (1) C 60	/440. RY*(1) C 37	1.09	11.36	0.099

126. CR (1) C 60	/571. RY*(1) H 61	0.61	10.74	0.072
126. CR (1) C 60	/575. RY*(1) H 62	0.63	10.75	0.074
126. CR (1) C 60	/579. RY*(1) H 63	0.60	10.74	0.072
126. CR (1) C 60	/669. BD*(1) C 35 - C 37	0.60	10.65	0.072
126. CR (1) C 60	/672. BD*(1) C 36 - C 37	0.60	10.64	0.072
127. CR (1) N 65	/195. RY*(2) C 6	1.55	15.60	0.139
127. CR (1) N 65	/588. RY*(2) N 65	0.51	15.69	0.080
128. CR (1) O 66	/587. RY*(1) N 65	2.62	20.01	0.205
128. CR (1) O 66	/588. RY*(2) N 65	1.62	20.22	0.162
128. CR (1) O 66	/628. BD*(1) C 6 - N 65	0.89	19.25	0.120
128. CR (1) O 66	/695. BD*(1) N 65 - O 67	0.69	19.39	0.105
129. CR (1) O 67	/587. RY*(1) N 65	3.17	20.02	0.226
129. CR (1) O 67	/588. RY*(2) N 65	1.07	20.23	0.131
129. CR (1) O 67	/628. BD*(1) C 6 - N 65	0.84	19.25	0.117
129. CR (1) O 67	/693. BD*(1) N 65 - O 66	0.69	19.40	0.105
130. LP (1)Ru 11	/141. LP*(1) C 15	2.12	0.12	0.018
130. LP (1)Ru 11	/203. RY*(1) C 7	2.78	1.41	0.057
130. LP (1)Ru 11	/617. BD*(1) C 1 - I 12	1.29	0.29	0.017
130. LP (1)Ru 11	/619. BD*(1) C 2 - C 7	3.31	0.70	0.043
130. LP (1)Ru 11	/629. BD*(1) C 7 - H 10	3.13	0.70	0.042
131. LP (2)Ru 11	/141. LP*(1) C 15	26.16	0.12	0.061
131. LP (2)Ru 11	/203. RY*(1) C 7	0.57	1.41	0.026
131. LP (2)Ru 11	/255. RY*(2)Cl 13	0.75	1.11	0.026
131. LP (2)Ru 11	/274. RY*(3) C 15	0.77	1.30	0.029
131. LP (2)Ru 11	/275. RY*(4) C 15	0.95	1.18	0.031
131. LP (2)Ru 11	/619. BD*(1) C 2 - C 7	0.61	0.70	0.019
131. LP (2)Ru 11	/629. BD*(1) C 7 - H 10	0.77	0.70	0.021
132. LP*(3)Ru 11	/149. RY*(1) C 1	0.67	0.93	0.078
132. LP*(3)Ru 11	/204. RY*(2) C 7	2.90	2.03	0.240
132. LP*(3)Ru 11	/227. RY*(4)Ru 11	1.96	1.53	0.173
132. LP*(3)Ru 11	/228. RY*(5)Ru 11	0.68	0.64	0.066
132. LP*(3)Ru 11	/229. RY*(6)Ru 11	1.41	0.84	0.109
132. LP*(3)Ru 11	/232. RY*(9)Ru 11	1.02	0.89	0.095
132. LP*(3)Ru 11	/233. RY*(10)Ru 11	0.68	0.76	0.072
132. LP*(3)Ru 11	/234. RY*(11)Ru 11	0.96	0.80	0.088
132. LP*(3)Ru 11	/235. RY*(12)Ru 11	0.64	0.51	0.058
132. LP*(3)Ru 11	/236. RY*(13)Ru 11	1.68	1.61	0.165
132. LP*(3)Ru 11	/237. RY*(14)Ru 11	2.57	1.38	0.189
132. LP*(3)Ru 11	/239. RY*(16)Ru 11	2.74	1.22	0.184
132. LP*(3)Ru 11	/240. RY*(17)Ru 11	0.74	0.73	0.074
132. LP*(3)Ru 11	/241. RY*(18)Ru 11	2.82	3.50	0.316
132. LP*(3)Ru 11	/243. RY*(20)Ru 11	3.67	32.98	1.106
132. LP*(3)Ru 11	/247. RY*(1) I 12	0.86	0.36	0.055
132. LP*(3)Ru 11	/254. RY*(1)Cl 13	0.53	0.62	0.058
132. LP*(3)Ru 11	/268. RY*(6)Cl 14	0.66	1.00	0.082
132. LP*(3)Ru 11	/272. RY*(1) C 15	2.04	1.35	0.163
132. LP*(3)Ru 11	/273. RY*(2) C 15	0.52	0.86	0.066
132. LP*(3)Ru 11	/630. BD*(1) C 7 -Ru 11	61.08	0.15	0.232

132. LP*(3)Ru 11	/632. BD*(1)Ru 11 - I 12	7.70	0.23	0.096
132. LP*(3)Ru 11	/633. BD*(1)Ru 11 -Cl 13	7.11	0.10	0.061
132. LP*(3)Ru 11	/635. BD*(1)Ru 11 - C 15	5.82	0.18	0.069
132. LP*(3)Ru 11	/636. BD*(1) C 15 - N 16	0.72	0.30	0.043
132. LP*(3)Ru 11	/637. BD*(1) C 15 - N 21	0.51	0.29	0.036
132. LP*(3)Ru 11	/678. BD*(1) C 44 - H 45	0.51	0.31	0.038
133. LP (1) I 12	/149. RY*(1) C 1	1.92	1.69	0.051
133. LP (1) I 12	/150. RY*(2) C 1	1.03	1.84	0.039
133. LP (1) I 12	/225. RY*(2)Ru 11	0.61	1.20	0.024
133. LP (1) I 12	/228. RY*(5)Ru 11	0.53	1.39	0.024
133. LP (1) I 12	/233. RY*(10)Ru 11	0.56	1.51	0.026
133. LP (1) I 12	/238. RY*(15)Ru 11	0.52	1.40	0.024
133. LP (1) I 12	/240. RY*(17)Ru 11	0.60	1.48	0.027
133. LP (1) I 12	/249. RY*(3) I 12	1.53	2.31	0.053
133. LP (1) I 12	/252. RY*(6) I 12	1.65	2.13	0.053
133. LP (1) I 12	/253. RY*(7) I 12	3.34	12.08	0.180
133. LP (1) I 12	/614. BD*(1) C 1 - C 2	0.80	1.08	0.026
133. LP (1) I 12	/632. BD*(1)Ru 11 - I 12	5.58	0.99	0.068
133. LP (1) I 12	/633. BD*(1)Ru 11 -Cl 13	3.37	0.85	0.049
134. LP (2) I 12	/615. BD*(2) C 1 - C 2	6.73	0.27	0.042
134. LP (2) I 12	/631. BD*(2) C 7 -Ru 11	1.00	0.30	0.016
134. LP (2) I 12	/634. BD*(1)Ru 11 -Cl 14	1.52	0.42	0.023
134. LP (2) I 12	/635. BD*(1)Ru 11 - C 15	0.68	0.66	0.019
134. LP (2) I 12	/683. BD*(1) C 48 - H 51	1.08	0.75	0.026
135. LP (1)Cl 13	/141. LP*(1) C 15	1.08	0.16	0.014
135. LP (1)Cl 13	/631. BD*(2) C 7 -Ru 11	0.96	0.29	0.015
135. LP (1)Cl 13	/632. BD*(1)Ru 11 - I 12	1.49	0.70	0.030
135. LP (1)Cl 13	/633. BD*(1)Ru 11 -Cl 13	1.61	0.57	0.028
135. LP (1)Cl 13	/634. BD*(1)Ru 11 -Cl 14	3.12	0.41	0.033
135. LP (1)Cl 13	/684. BD*(1) C 52 - H 53	2.93	0.77	0.043
136. LP (2)Cl 13	/149. RY*(1) C 1	0.53	1.98	0.029
136. LP (2)Cl 13	/150. RY*(2) C 1	0.67	2.13	0.034
136. LP (2)Cl 13	/225. RY*(2)Ru 11	2.81	1.49	0.058
136. LP (2)Cl 13	/232. RY*(9)Ru 11	0.61	1.93	0.031
136. LP (2)Cl 13	/238. RY*(15)Ru 11	1.35	1.68	0.043
136. LP (2)Cl 13	/240. RY*(17)Ru 11	1.07	1.77	0.039
136. LP (2)Cl 13	/248. RY*(2) I 12	0.57	1.26	0.024
136. LP (2)Cl 13	/249. RY*(3) I 12	1.36	2.60	0.054
136. LP (2)Cl 13	/252. RY*(6) I 12	2.00	2.42	0.063
136. LP (2)Cl 13	/253. RY*(7) I 12	4.01	12.36	0.201
136. LP (2)Cl 13	/632. BD*(1)Ru 11 - I 12	11.46	1.28	0.111
136. LP (2)Cl 13	/633. BD*(1)Ru 11 -Cl 13	8.51	1.14	0.090
136. LP (2)Cl 13	/635. BD*(1)Ru 11 - C 15	0.81	1.22	0.029
136. LP (2)Cl 13	/684. BD*(1) C 52 - H 53	1.73	1.34	0.043
137. LP (3)Cl 13	/132. LP*(3)Ru 11	5.45	0.46	0.046
137. LP (3)Cl 13	/632. BD*(1)Ru 11 - I 12	1.01	0.69	0.024
137. LP (3)Cl 13	/633. BD*(1)Ru 11 -Cl 13	0.82	0.56	0.019
137. LP (3)Cl 13	/678. BD*(1) C 44 - H 45	2.96	0.77	0.043

138. LP (1)Cl 14	/238. RY*(15)Ru 11	0.55	1.09	0.022
138. LP (1)Cl 14	/249. RY*(3) I 12	0.71	2.01	0.034
138. LP (1)Cl 14	/252. RY*(6) I 12	1.07	1.82	0.040
138. LP (1)Cl 14	/253. RY*(7) I 12	1.74	11.77	0.129
138. LP (1)Cl 14	/617. BD*(1) C 1 - I 12	0.54	0.30	0.011
138. LP (1)Cl 14	/632. BD*(1)Ru 11 - I 12	4.98	0.68	0.054
138. LP (1)Cl 14	/633. BD*(1)Ru 11 -Cl 13	3.70	0.54	0.041
139. LP (2)Cl 14	/132. LP*(3)Ru 11	1.01	1.07	0.030
139. LP (2)Cl 14	/226. RY*(3)Ru 11	1.06	1.53	0.036
139. LP (2)Cl 14	/228. RY*(5)Ru 11	0.54	1.71	0.028
139. LP (2)Cl 14	/231. RY*(8)Ru 11	0.61	1.60	0.028
139. LP (2)Cl 14	/631. BD*(2) C 7 -Ru 11	4.55	0.89	0.059
139. LP (2)Cl 14	/632. BD*(1)Ru 11 - I 12	0.55	1.30	0.025
139. LP (2)Cl 14	/634. BD*(1)Ru 11 -Cl 14	3.40	1.01	0.054
139. LP (2)Cl 14	/635. BD*(1)Ru 11 - C 15	2.81	1.25	0.055
140. LP (3)Cl 14	/132. LP*(3)Ru 11	12.94	0.44	0.068
140. LP (3)Cl 14	/630. BD*(1) C 7 -Ru 11	0.63	0.60	0.017
140. LP (3)Cl 14	/631. BD*(2) C 7 -Ru 11	0.92	0.26	0.014
140. LP (3)Cl 14	/635. BD*(1)Ru 11 - C 15	0.78	0.62	0.020
141. LP*(1) C 15	/274. RY*(3) C 15	0.54	1.17	0.038
141. LP*(1) C 15	/275. RY*(4) C 15	1.09	1.06	0.051
141. LP*(1) C 15	/277. RY*(6) C 15	0.97	1.98	0.066
141. LP*(1) C 15	/281. RY*(1) N 16	0.62	1.15	0.040
141. LP*(1) C 15	/287. RY*(7) N 16	0.76	2.10	0.060
141. LP*(1) C 15	/316. RY*(1) N 21	0.51	1.14	0.036
141. LP*(1) C 15	/322. RY*(7) N 21	0.53	2.21	0.051
141. LP*(1) C 15	/631. BD*(2) C 7 -Ru 11	0.60	0.13	0.012
141. LP*(1) C 15	/633. BD*(1)Ru 11 -Cl 13	0.64	0.41	0.022
142. LP (1) N 16	/141. LP*(1) C 15	131.12	0.15	0.139
142. LP (1) N 16	/275. RY*(4) C 15	0.74	1.21	0.029
142. LP (1) N 16	/276. RY*(5) C 15	1.30	2.25	0.053
142. LP (1) N 16	/277. RY*(6) C 15	0.76	2.13	0.040
142. LP (1) N 16	/299. RY*(1) C 18	0.54	1.30	0.026
142. LP (1) N 16	/302. RY*(4) C 18	0.70	2.29	0.039
142. LP (1) N 16	/335. RY*(3) C 24	0.89	1.40	0.034
142. LP (1) N 16	/644. BD*(1) C 18 - H 20	4.83	0.70	0.056
142. LP (1) N 16	/645. BD*(1) C 18 - H 23	3.70	0.71	0.050
142. LP (1) N 16	/647. BD*(1) C 24 - C 25	5.95	0.84	0.069
142. LP (1) N 16	/649. BD*(1) C 24 - C 26	5.26	0.84	0.065
143. LP (1) N 21	/141. LP*(1) C 15	129.36	0.15	0.138
143. LP (1) N 21	/276. RY*(5) C 15	1.31	2.25	0.053
143. LP (1) N 21	/277. RY*(6) C 15	0.92	2.13	0.043
143. LP (1) N 21	/290. RY*(1) C 17	0.54	1.28	0.026
143. LP (1) N 21	/293. RY*(4) C 17	0.67	2.26	0.038
143. LP (1) N 21	/397. RY*(3) C 32	0.90	1.39	0.035
143. LP (1) N 21	/399. RY*(5) C 32	0.51	2.50	0.035
143. LP (1) N 21	/641. BD*(1) C 17 - H 19	5.16	0.70	0.059
143. LP (1) N 21	/643. BD*(1) C 17 - H 22	3.45	0.70	0.048

143. LP (1) N 21	/661. BD*(1) C 32 - C 33	5.69	0.84	0.067
143. LP (1) N 21	/663. BD*(1) C 32 - C 34	5.70	0.83	0.067
144. LP (1) O 66	/587. RY*(1) N 65	4.85	1.84	0.084
144. LP (1) O 66	/588. RY*(2) N 65	1.82	2.05	0.055
144. LP (1) O 66	/590. RY*(4) N 65	0.84	2.76	0.043
144. LP (1) O 66	/628. BD*(1) C 6 - N 65	3.64	1.08	0.057
144. LP (1) O 66	/695. BD*(1) N 65 - O 67	2.12	1.22	0.046
145. LP (2) O 66	/587. RY*(1) N 65	1.06	1.34	0.034
145. LP (2) O 66	/588. RY*(2) N 65	1.71	1.55	0.047
145. LP (2) O 66	/590. RY*(4) N 65	1.30	2.25	0.050
145. LP (2) O 66	/591. RY*(5) N 65	1.05	2.70	0.049
145. LP (2) O 66	/616. BD*(1) C 1 - C 6	0.56	0.85	0.020
145. LP (2) O 66	/623. BD*(1) C 4 - C 5	0.59	0.87	0.021
145. LP (2) O 66	/627. BD*(1) C 5 - H 9	0.73	0.77	0.022
145. LP (2) O 66	/628. BD*(1) C 6 - N 65	13.36	0.57	0.078
145. LP (2) O 66	/695. BD*(1) N 65 - O 67	18.77	0.71	0.105
146. LP (1) O 67	/587. RY*(1) N 65	5.45	1.84	0.089
146. LP (1) O 67	/588. RY*(2) N 65	1.14	2.05	0.043
146. LP (1) O 67	/590. RY*(4) N 65	0.54	2.76	0.035
146. LP (1) O 67	/628. BD*(1) C 6 - N 65	3.85	1.08	0.059
146. LP (1) O 67	/693. BD*(1) N 65 - O 66	1.86	1.23	0.043
147. LP (2) O 67	/587. RY*(1) N 65	0.75	1.34	0.029
147. LP (2) O 67	/588. RY*(2) N 65	1.66	1.55	0.047
147. LP (2) O 67	/590. RY*(4) N 65	2.02	2.26	0.062
147. LP (2) O 67	/591. RY*(5) N 65	0.54	2.71	0.035
147. LP (2) O 67	/625. BD*(1) C 5 - C 6	0.65	0.85	0.021
147. LP (2) O 67	/628. BD*(1) C 6 - N 65	11.87	0.58	0.074
147. LP (2) O 67	/632. BD*(1)Ru 11 - I 12	0.67	0.74	0.020
147. LP (2) O 67	/693. BD*(1) N 65 - O 66	18.92	0.73	0.106
148. LP (3) O 67	/589. RY*(3) N 65	3.72	2.27	0.096
148. LP (3) O 67	/592. RY*(6) N 65	0.59	1.93	0.035
148. LP (3) O 67	/594. RY*(8) N 65	0.95	1.22	0.036
148. LP (3) O 67	/606. RY*(2) O 67	0.78	1.27	0.033
148. LP (3) O 67	/694. BD*(2) N 65 - O 66	157.73	0.15	0.138
615. BD*(2) C 1 - C 2	/151. RY*(3) C 1	1.47	0.87	0.070
615. BD*(2) C 1 - C 2	/161. RY*(4) C 2	1.79	1.26	0.093
615. BD*(2) C 1 - C 2	/621. BD*(2) C 3 - C 4	172.24	0.02	0.082
615. BD*(2) C 1 - C 2	/631. BD*(2) C 7 -Ru 11	78.12	0.03	0.073
615. BD*(2) C 1 - C 2	/648. BD*(2) C 24 - C 25	0.62	0.04	0.007
621. BD*(2) C 3 - C 4	/170. RY*(4) C 3	1.57	0.70	0.078
621. BD*(2) C 3 - C 4	/179. RY*(4) C 4	2.18	0.70	0.091
626. BD*(2) C 5 - C 6	/187. RY*(3) C 5	2.40	1.04	0.101
626. BD*(2) C 5 - C 6	/198. RY*(5) C 6	0.62	1.66	0.065
626. BD*(2) C 5 - C 6	/200. RY*(7) C 6	0.51	1.78	0.061
626. BD*(2) C 5 - C 6	/621. BD*(2) C 3 - C 4	175.61	0.02	0.084
628. BD*(1) C 6 - N 65	/196. RY*(3) C 6	1.04	0.73	0.105
628. BD*(1) C 6 - N 65	/201. RY*(8) C 6	0.50	1.99	0.122
628. BD*(1) C 6 - N 65	/590. RY*(4) N 65	0.62	1.68	0.123

628. BD*(1) C 6 - N 65	/593. RY*(7) N 65	2.63	1.08	0.206
628. BD*(1) C 6 - N 65	/614. BD*(1) C 1 - C 2	1.36	0.26	0.064
628. BD*(1) C 6 - N 65	/623. BD*(1) C 4 - C 5	0.97	0.30	0.062
628. BD*(1) C 6 - N 65	/627. BD*(1) C 5 - H 9	0.97	0.20	0.051
630. BD*(1) C 7 -Ru 11	/149. RY*(1) C 1	0.67	0.78	0.081
630. BD*(1) C 7 -Ru 11	/158. RY*(1) C 2	0.57	1.07	0.087
630. BD*(1) C 7 -Ru 11	/159. RY*(2) C 2	1.48	0.86	0.127
630. BD*(1) C 7 -Ru 11	/160. RY*(3) C 2	0.60	0.74	0.076
630. BD*(1) C 7 -Ru 11	/204. RY*(2) C 7	9.96	1.88	0.485
630. BD*(1) C 7 -Ru 11	/206. RY*(4) C 7	0.97	1.06	0.116
630. BD*(1) C 7 -Ru 11	/220. RY*(1) H 10	2.06	0.53	0.118
630. BD*(1) C 7 -Ru 11	/226. RY*(3)Ru 11	3.59	0.31	0.118
630. BD*(1) C 7 -Ru 11	/227. RY*(4)Ru 11	12.36	1.38	0.467
630. BD*(1) C 7 -Ru 11	/228. RY*(5)Ru 11	4.71	0.48	0.171
630. BD*(1) C 7 -Ru 11	/229. RY*(6)Ru 11	6.94	0.69	0.249
630. BD*(1) C 7 -Ru 11	/230. RY*(7)Ru 11	3.05	0.43	0.130
630. BD*(1) C 7 -Ru 11	/231. RY*(8)Ru 11	0.86	0.38	0.065
630. BD*(1) C 7 -Ru 11	/232. RY*(9)Ru 11	7.03	0.73	0.259
630. BD*(1) C 7 -Ru 11	/233. RY*(10)Ru 11	4.87	0.60	0.196
630. BD*(1) C 7 -Ru 11	/234. RY*(11)Ru 11	2.87	0.65	0.156
630. BD*(1) C 7 -Ru 11	/235. RY*(12)Ru 11	6.41	0.36	0.173
630. BD*(1) C 7 -Ru 11	/236. RY*(13)Ru 11	11.70	1.46	0.472
630. BD*(1) C 7 -Ru 11	/237. RY*(14)Ru 11	14.09	1.22	0.475
630. BD*(1) C 7 -Ru 11	/239. RY*(16)Ru 11	12.35	1.07	0.415
630. BD*(1) C 7 -Ru 11	/240. RY*(17)Ru 11	5.39	0.57	0.201
630. BD*(1) C 7 -Ru 11	/241. RY*(18)Ru 11	15.07	3.35	0.813
630. BD*(1) C 7 -Ru 11	/242. RY*(19)Ru 11	2.15	1.40	0.198
630. BD*(1) C 7 -Ru 11	/243. RY*(20)Ru 11	18.87	32.82	2.851
630. BD*(1) C 7 -Ru 11	/247. RY*(1) I 12	7.64	0.20	0.141
630. BD*(1) C 7 -Ru 11	/254. RY*(1)Cl 13	2.29	0.47	0.118
630. BD*(1) C 7 -Ru 11	/256. RY*(3)Cl 13	1.80	0.48	0.106
630. BD*(1) C 7 -Ru 11	/263. RY*(1)Cl 14	0.69	0.49	0.067
630. BD*(1) C 7 -Ru 11	/265. RY*(3)Cl 14	0.99	0.50	0.080
630. BD*(1) C 7 -Ru 11	/266. RY*(4)Cl 14	1.45	0.58	0.105
630. BD*(1) C 7 -Ru 11	/268. RY*(6)Cl 14	2.41	0.85	0.164
630. BD*(1) C 7 -Ru 11	/270. RY*(8)Cl 14	1.58	0.76	0.125
630. BD*(1) C 7 -Ru 11	/272. RY*(1) C 15	12.01	1.19	0.420
630. BD*(1) C 7 -Ru 11	/273. RY*(2) C 15	5.43	0.70	0.218
630. BD*(1) C 7 -Ru 11	/282. RY*(2) N 16	1.17	1.35	0.143
630. BD*(1) C 7 -Ru 11	/317. RY*(2) N 21	0.55	1.33	0.097
630. BD*(1) C 7 -Ru 11	/500. RY*(2) C 48	0.53	0.40	0.052
630. BD*(1) C 7 -Ru 11	/516. RY*(1) H 51	1.60	0.61	0.112
630. BD*(1) C 7 -Ru 11	/629. BD*(1) C 7 - H 10	1.47	0.11	0.042
630. BD*(1) C 7 -Ru 11	/632. BD*(1)Ru 11 - I 12	99.64	0.08	0.214
630. BD*(1) C 7 -Ru 11	/635. BD*(1)Ru 11 - C 15	787.70	0.02	0.304
631. BD*(2) C 7 -Ru 11	/204. RY*(2) C 7	0.61	2.22	0.106
631. BD*(2) C 7 -Ru 11	/205. RY*(3) C 7	1.22	0.76	0.089
631. BD*(2) C 7 -Ru 11	/227. RY*(4)Ru 11	0.68	1.72	0.100

631. BD*(2) C 7 -Ru 11	/241. RY*(18)Ru 11	0.69	3.69	0.148
631. BD*(2) C 7 -Ru 11	/243. RY*(20)Ru 11	0.91	33.16	0.508
631. BD*(2) C 7 -Ru 11	/630. BD*(1) C 7 -Ru 11	2.14	0.34	0.061
631. BD*(2) C 7 -Ru 11	/632. BD*(1)Ru 11 - I 12	0.88	0.42	0.042
631. BD*(2) C 7 -Ru 11	/634. BD*(1)Ru 11 -Cl 14	7.33	0.12	0.059
631. BD*(2) C 7 -Ru 11	/635. BD*(1)Ru 11 - C 15	6.91	0.36	0.102
632. BD*(1)Ru 11 - I 12	/149. RY*(1) C 1	9.74	0.70	0.264
632. BD*(1)Ru 11 - I 12	/150. RY*(2) C 1	10.04	0.85	0.297
632. BD*(1)Ru 11 - I 12	/153. RY*(5) C 1	0.74	0.84	0.081
632. BD*(1)Ru 11 - I 12	/156. RY*(8) C 1	0.96	1.64	0.129
632. BD*(1)Ru 11 - I 12	/158. RY*(1) C 2	5.71	1.00	0.241
632. BD*(1)Ru 11 - I 12	/168. RY*(2) C 3	1.65	0.33	0.075
632. BD*(1)Ru 11 - I 12	/171. RY*(5) C 3	0.70	0.62	0.068
632. BD*(1)Ru 11 - I 12	/189. RY*(5) C 5	0.79	0.69	0.076
632. BD*(1)Ru 11 - I 12	/194. RY*(1) C 6	2.16	0.61	0.115
632. BD*(1)Ru 11 - I 12	/195. RY*(2) C 6	2.73	0.72	0.141
632. BD*(1)Ru 11 - I 12	/196. RY*(3) C 6	2.94	0.57	0.132
632. BD*(1)Ru 11 - I 12	/203. RY*(1) C 7	4.50	0.74	0.185
632. BD*(1)Ru 11 - I 12	/204. RY*(2) C 7	6.85	1.80	0.356
632. BD*(1)Ru 11 - I 12	/206. RY*(4) C 7	3.10	0.99	0.179
632. BD*(1)Ru 11 - I 12	/220. RY*(1) H 10	1.04	0.45	0.070
632. BD*(1)Ru 11 - I 12	/224. RY*(1)Ru 11	8.31	0.31	0.162
632. BD*(1)Ru 11 - I 12	/225. RY*(2)Ru 11	1.27	0.21	0.053
632. BD*(1)Ru 11 - I 12	/226. RY*(3)Ru 11	7.55	0.23	0.134
632. BD*(1)Ru 11 - I 12	/227. RY*(4)Ru 11	1.25	1.30	0.130
632. BD*(1)Ru 11 - I 12	/228. RY*(5)Ru 11	10.05	0.40	0.206
632. BD*(1)Ru 11 - I 12	/229. RY*(6)Ru 11	9.21	0.61	0.243
632. BD*(1)Ru 11 - I 12	/230. RY*(7)Ru 11	1.21	0.35	0.067
632. BD*(1)Ru 11 - I 12	/231. RY*(8)Ru 11	1.75	0.30	0.074
632. BD*(1)Ru 11 - I 12	/234. RY*(11)Ru 11	3.40	0.57	0.143
632. BD*(1)Ru 11 - I 12	/235. RY*(12)Ru 11	4.23	0.28	0.112
632. BD*(1)Ru 11 - I 12	/236. RY*(13)Ru 11	8.36	1.38	0.349
632. BD*(1)Ru 11 - I 12	/237. RY*(14)Ru 11	5.38	1.14	0.255
632. BD*(1)Ru 11 - I 12	/238. RY*(15)Ru 11	9.48	0.41	0.203
632. BD*(1)Ru 11 - I 12	/239. RY*(16)Ru 11	3.31	0.99	0.186
632. BD*(1)Ru 11 - I 12	/240. RY*(17)Ru 11	1.48	0.49	0.088
632. BD*(1)Ru 11 - I 12	/241. RY*(18)Ru 11	3.09	3.27	0.327
632. BD*(1)Ru 11 - I 12	/243. RY*(20)Ru 11	6.59	32.74	1.514
632. BD*(1)Ru 11 - I 12	/247. RY*(1) I 12	10.49	0.12	0.117
632. BD*(1)Ru 11 - I 12	/249. RY*(3) I 12	11.36	1.33	0.398
632. BD*(1)Ru 11 - I 12	/250. RY*(4) I 12	6.90	0.27	0.141
632. BD*(1)Ru 11 - I 12	/251. RY*(5) I 12	0.60	0.29	0.043
632. BD*(1)Ru 11 - I 12	/252. RY*(6) I 12	16.69	1.15	0.450
632. BD*(1)Ru 11 - I 12	/253. RY*(7) I 12	20.74	11.09	1.562
632. BD*(1)Ru 11 - I 12	/261. RY*(8)Cl 13	0.55	0.68	0.063
632. BD*(1)Ru 11 - I 12	/264. RY*(2)Cl 14	0.80	0.39	0.057
632. BD*(1)Ru 11 - I 12	/268. RY*(6)Cl 14	1.22	0.77	0.100
632. BD*(1)Ru 11 - I 12	/272. RY*(1) C 15	5.10	1.11	0.239

632. BD*(1)Ru 11 - I 12	/273. RY*(2) C 15	4.88	0.62	0.176
632. BD*(1)Ru 11 - I 12	/274. RY*(3) C 15	0.72	0.63	0.069
632. BD*(1)Ru 11 - I 12	/275. RY*(4) C 15	2.22	0.51	0.109
632. BD*(1)Ru 11 - I 12	/282. RY*(2) N 16	0.64	1.27	0.092
632. BD*(1)Ru 11 - I 12	/487. RY*(1) H 45	0.58	0.46	0.053
632. BD*(1)Ru 11 - I 12	/516. RY*(1) H 51	4.52	0.53	0.159
632. BD*(1)Ru 11 - I 12	/593. RY*(7) N 65	0.74	0.92	0.085
632. BD*(1)Ru 11 - I 12	/605. RY*(1) O 67	0.67	0.71	0.071
632. BD*(1)Ru 11 - I 12	/614. BD*(1) C 1 - C 2	0.64	0.10	0.024
632. BD*(1)Ru 11 - I 12	/619. BD*(1) C 2 - C 7	4.93	0.03	0.038
632. BD*(1)Ru 11 - I 12	/676. BD*(1) C 40 - H 42	0.85	0.02	0.014
632. BD*(1)Ru 11 - I 12	/678. BD*(1) C 44 - H 45	2.40	0.07	0.041
632. BD*(1)Ru 11 - I 12	/679. BD*(1) C 44 - H 46	0.52	0.04	0.014
632. BD*(1)Ru 11 - I 12	/683. BD*(1) C 48 - H 51	2.11	0.03	0.026
632. BD*(1)Ru 11 - I 12	/684. BD*(1) C 52 - H 53	1.64	0.07	0.032
633. BD*(1)Ru 11 -Cl 13	/149. RY*(1) C 1	0.99	0.84	0.095
633. BD*(1)Ru 11 -Cl 13	/150. RY*(2) C 1	1.52	0.99	0.129
633. BD*(1)Ru 11 -Cl 13	/159. RY*(2) C 2	1.49	0.92	0.123
633. BD*(1)Ru 11 -Cl 13	/160. RY*(3) C 2	0.74	0.79	0.082
633. BD*(1)Ru 11 -Cl 13	/195. RY*(2) C 6	0.57	0.86	0.073
633. BD*(1)Ru 11 -Cl 13	/203. RY*(1) C 7	0.72	0.88	0.083
633. BD*(1)Ru 11 -Cl 13	/204. RY*(2) C 7	5.99	1.94	0.357
633. BD*(1)Ru 11 -Cl 13	/206. RY*(4) C 7	0.55	1.12	0.084
633. BD*(1)Ru 11 -Cl 13	/220. RY*(1) H 10	1.50	0.58	0.099
633. BD*(1)Ru 11 -Cl 13	/224. RY*(1)Ru 11	3.53	0.45	0.131
633. BD*(1)Ru 11 -Cl 13	/227. RY*(4)Ru 11	8.40	1.44	0.366
633. BD*(1)Ru 11 -Cl 13	/229. RY*(6)Ru 11	1.35	0.74	0.107
633. BD*(1)Ru 11 -Cl 13	/230. RY*(7)Ru 11	3.92	0.49	0.147
633. BD*(1)Ru 11 -Cl 13	/231. RY*(8)Ru 11	1.50	0.43	0.086
633. BD*(1)Ru 11 -Cl 13	/232. RY*(9)Ru 11	7.78	0.79	0.263
633. BD*(1)Ru 11 -Cl 13	/233. RY*(10)Ru 11	3.26	0.66	0.156
633. BD*(1)Ru 11 -Cl 13	/234. RY*(11)Ru 11	1.56	0.71	0.112
633. BD*(1)Ru 11 -Cl 13	/235. RY*(12)Ru 11	1.24	0.42	0.077
633. BD*(1)Ru 11 -Cl 13	/236. RY*(13)Ru 11	2.93	1.51	0.224
633. BD*(1)Ru 11 -Cl 13	/237. RY*(14)Ru 11	5.89	1.28	0.292
633. BD*(1)Ru 11 -Cl 13	/238. RY*(15)Ru 11	4.29	0.54	0.163
633. BD*(1)Ru 11 -Cl 13	/239. RY*(16)Ru 11	4.14	1.12	0.230
633. BD*(1)Ru 11 -Cl 13	/240. RY*(17)Ru 11	7.12	0.63	0.226
633. BD*(1)Ru 11 -Cl 13	/241. RY*(18)Ru 11	7.86	3.41	0.552
633. BD*(1)Ru 11 -Cl 13	/242. RY*(19)Ru 11	2.30	1.45	0.195
633. BD*(1)Ru 11 -Cl 13	/243. RY*(20)Ru 11	7.58	32.88	1.685
633. BD*(1)Ru 11 -Cl 13	/248. RY*(2) I 12	9.69	0.12	0.113
633. BD*(1)Ru 11 -Cl 13	/249. RY*(3) I 12	2.75	1.46	0.213
633. BD*(1)Ru 11 -Cl 13	/250. RY*(4) I 12	1.43	0.41	0.081
633. BD*(1)Ru 11 -Cl 13	/252. RY*(6) I 12	4.88	1.28	0.267
633. BD*(1)Ru 11 -Cl 13	/253. RY*(7) I 12	4.63	11.22	0.769
633. BD*(1)Ru 11 -Cl 13	/257. RY*(4)Cl 13	0.75	0.65	0.074
633. BD*(1)Ru 11 -Cl 13	/263. RY*(1)Cl 14	0.57	0.55	0.059

633. BD*(1)Ru 11 -Cl 13	/266. RY*(4)Cl 14	1.14	0.64	0.091
633. BD*(1)Ru 11 -Cl 13	/268. RY*(6)Cl 14	1.00	0.91	0.102
633. BD*(1)Ru 11 -Cl 13	/270. RY*(8)Cl 14	0.78	0.81	0.085
633. BD*(1)Ru 11 -Cl 13	/272. RY*(1) C 15	4.98	1.25	0.259
633. BD*(1)Ru 11 -Cl 13	/273. RY*(2) C 15	1.29	0.76	0.103
633. BD*(1)Ru 11 -Cl 13	/274. RY*(3) C 15	1.01	0.77	0.093
633. BD*(1)Ru 11 -Cl 13	/630. BD*(1) C 7 -Ru 11	95.15	0.06	0.181
633. BD*(1)Ru 11 -Cl 13	/632. BD*(1)Ru 11 - I 12	28.13	0.14	0.145
633. BD*(1)Ru 11 -Cl 13	/635. BD*(1)Ru 11 - C 15	107.93	0.08	0.203
633. BD*(1)Ru 11 -Cl 13	/678. BD*(1) C 44 - H 45	1.23	0.21	0.051
633. BD*(1)Ru 11 -Cl 13	/684. BD*(1) C 52 - H 53	0.67	0.20	0.036
634. BD*(1)Ru 11 -Cl 14	/132. LP*(3)Ru 11	1.16	0.06	0.018
634. BD*(1)Ru 11 -Cl 14	/204. RY*(2) C 7	1.67	2.10	0.163
634. BD*(1)Ru 11 -Cl 14	/227. RY*(4)Ru 11	0.53	1.60	0.080
634. BD*(1)Ru 11 -Cl 14	/228. RY*(5)Ru 11	0.52	0.70	0.053
634. BD*(1)Ru 11 -Cl 14	/232. RY*(9)Ru 11	0.66	0.95	0.070
634. BD*(1)Ru 11 -Cl 14	/235. RY*(12)Ru 11	0.73	0.58	0.057
634. BD*(1)Ru 11 -Cl 14	/236. RY*(13)Ru 11	0.71	1.68	0.096
634. BD*(1)Ru 11 -Cl 14	/237. RY*(14)Ru 11	2.27	1.44	0.160
634. BD*(1)Ru 11 -Cl 14	/239. RY*(16)Ru 11	1.10	1.28	0.105
634. BD*(1)Ru 11 -Cl 14	/240. RY*(17)Ru 11	1.23	0.79	0.087
634. BD*(1)Ru 11 -Cl 14	/241. RY*(18)Ru 11	1.57	3.57	0.209
634. BD*(1)Ru 11 -Cl 14	/243. RY*(20)Ru 11	1.72	33.04	0.666
634. BD*(1)Ru 11 -Cl 14	/264. RY*(2)Cl 14	0.68	0.69	0.060
634. BD*(1)Ru 11 -Cl 14	/272. RY*(1) C 15	0.75	1.41	0.089
634. BD*(1)Ru 11 -Cl 14	/273. RY*(2) C 15	0.50	0.92	0.059
634. BD*(1)Ru 11 -Cl 14	/630. BD*(1) C 7 -Ru 11	8.72	0.22	0.097
634. BD*(1)Ru 11 -Cl 14	/632. BD*(1)Ru 11 - I 12	4.06	0.30	0.074
634. BD*(1)Ru 11 -Cl 14	/633. BD*(1)Ru 11 -Cl 13	8.93	0.16	0.082
634. BD*(1)Ru 11 -Cl 14	/635. BD*(1)Ru 11 - C 15	0.85	0.24	0.029
635. BD*(1)Ru 11 - C 15	/149. RY*(1) C 1	0.55	0.76	0.058
635. BD*(1)Ru 11 - C 15	/158. RY*(1) C 2	1.63	1.05	0.118
635. BD*(1)Ru 11 - C 15	/159. RY*(2) C 2	1.28	0.84	0.093
635. BD*(1)Ru 11 - C 15	/160. RY*(3) C 2	2.00	0.71	0.108
635. BD*(1)Ru 11 - C 15	/204. RY*(2) C 7	22.01	1.86	0.574
635. BD*(1)Ru 11 - C 15	/206. RY*(4) C 7	4.50	1.04	0.197
635. BD*(1)Ru 11 - C 15	/220. RY*(1) H 10	5.25	0.50	0.147
635. BD*(1)Ru 11 - C 15	/226. RY*(3)Ru 11	6.22	0.28	0.120
635. BD*(1)Ru 11 - C 15	/227. RY*(4)Ru 11	20.79	1.36	0.479
635. BD*(1)Ru 11 - C 15	/228. RY*(5)Ru 11	6.64	0.46	0.158
635. BD*(1)Ru 11 - C 15	/229. RY*(6)Ru 11	13.02	0.66	0.267
635. BD*(1)Ru 11 - C 15	/230. RY*(7)Ru 11	7.01	0.41	0.153
635. BD*(1)Ru 11 - C 15	/231. RY*(8)Ru 11	2.22	0.35	0.080
635. BD*(1)Ru 11 - C 15	/232. RY*(9)Ru 11	10.93	0.71	0.253
635. BD*(1)Ru 11 - C 15	/233. RY*(10)Ru 11	6.87	0.58	0.182
635. BD*(1)Ru 11 - C 15	/234. RY*(11)Ru 11	4.27	0.63	0.149
635. BD*(1)Ru 11 - C 15	/235. RY*(12)Ru 11	6.59	0.34	0.135
635. BD*(1)Ru 11 - C 15	/236. RY*(13)Ru 11	15.97	1.43	0.435

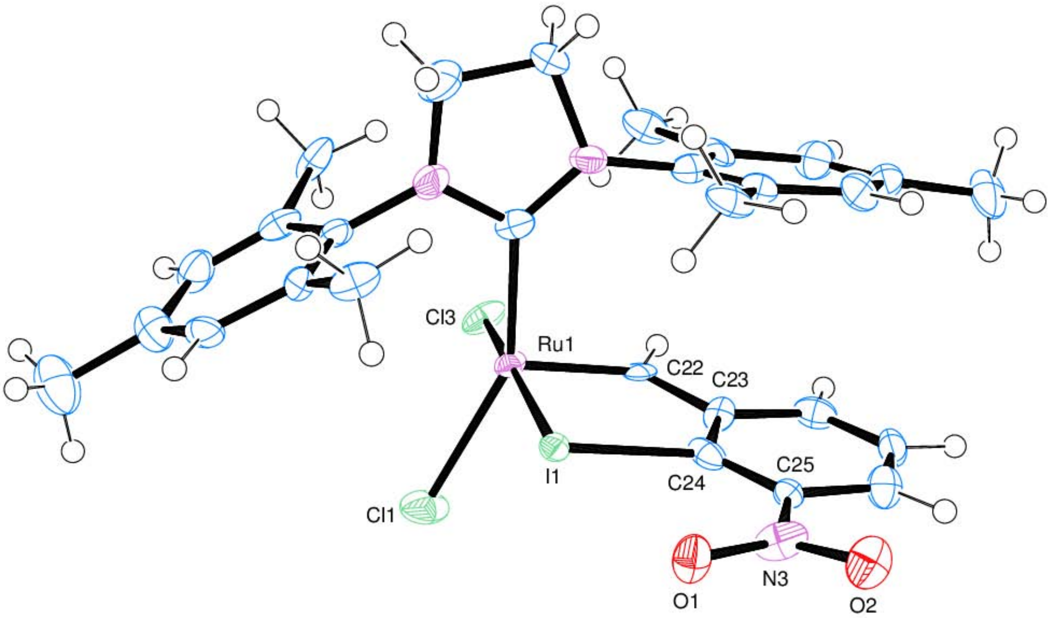
635. BD*(1)Ru 11 - C 15	/237. RY*(14)Ru 11	22.38	1.20	0.471
635. BD*(1)Ru 11 - C 15	/238. RY*(15)Ru 11	0.53	0.46	0.045
635. BD*(1)Ru 11 - C 15	/239. RY*(16)Ru 11	18.08	1.04	0.395
635. BD*(1)Ru 11 - C 15	/240. RY*(17)Ru 11	7.52	0.55	0.185
635. BD*(1)Ru 11 - C 15	/241. RY*(18)Ru 11	22.82	3.33	0.793
635. BD*(1)Ru 11 - C 15	/242. RY*(19)Ru 11	3.30	1.37	0.194
635. BD*(1)Ru 11 - C 15	/243. RY*(20)Ru 11	27.68	32.80	2.743
635. BD*(1)Ru 11 - C 15	/247. RY*(1) I 12	11.95	0.18	0.133
635. BD*(1)Ru 11 - C 15	/248. RY*(2) I 12	2.26	0.04	0.026
635. BD*(1)Ru 11 - C 15	/250. RY*(4) I 12	0.52	0.33	0.038
635. BD*(1)Ru 11 - C 15	/251. RY*(5) I 12	1.37	0.34	0.062
635. BD*(1)Ru 11 - C 15	/254. RY*(1)Cl 13	3.86	0.44	0.119
635. BD*(1)Ru 11 - C 15	/256. RY*(3)Cl 13	2.71	0.46	0.101
635. BD*(1)Ru 11 - C 15	/257. RY*(4)Cl 13	0.74	0.57	0.059
635. BD*(1)Ru 11 - C 15	/260. RY*(7)Cl 13	0.60	0.68	0.058
635. BD*(1)Ru 11 - C 15	/263. RY*(1)Cl 14	1.30	0.47	0.071
635. BD*(1)Ru 11 - C 15	/265. RY*(3)Cl 14	1.09	0.47	0.065
635. BD*(1)Ru 11 - C 15	/266. RY*(4)Cl 14	3.07	0.56	0.119
635. BD*(1)Ru 11 - C 15	/267. RY*(5)Cl 14	0.66	0.59	0.057
635. BD*(1)Ru 11 - C 15	/268. RY*(6)Cl 14	5.01	0.83	0.185
635. BD*(1)Ru 11 - C 15	/269. RY*(7)Cl 14	0.54	0.65	0.054
635. BD*(1)Ru 11 - C 15	/270. RY*(8)Cl 14	3.25	0.73	0.140
635. BD*(1)Ru 11 - C 15	/272. RY*(1) C 15	11.87	1.17	0.332
635. BD*(1)Ru 11 - C 15	/273. RY*(2) C 15	7.26	0.68	0.199
635. BD*(1)Ru 11 - C 15	/282. RY*(2) N 16	1.26	1.33	0.117
635. BD*(1)Ru 11 - C 15	/317. RY*(2) N 21	0.60	1.31	0.080
635. BD*(1)Ru 11 - C 15	/336. RY*(4) C 24	0.55	1.09	0.070
635. BD*(1)Ru 11 - C 15	/487. RY*(1) H 45	0.51	0.51	0.046
635. BD*(1)Ru 11 - C 15	/500. RY*(2) C 48	1.02	0.38	0.056
635. BD*(1)Ru 11 - C 15	/516. RY*(1) H 51	2.03	0.59	0.099
635. BD*(1)Ru 11 - C 15	/632. BD*(1)Ru 11 - I 12	126.97	0.06	0.181
635. BD*(1)Ru 11 - C 15	/637. BD*(1) C 15 - N 21	0.67	0.12	0.024
635. BD*(1)Ru 11 - C 15	/639. BD*(1) N 16 - C 24	3.19	0.02	0.020
635. BD*(1)Ru 11 - C 15	/646. BD*(1) N 21 - C 32	9.15	0.01	0.029
635. BD*(1)Ru 11 - C 15	/683. BD*(1) C 48 - H 51	0.80	0.09	0.023
648. BD*(2) C 24 - C 25	/334. RY*(2) C 24	0.70	0.87	0.050
648. BD*(2) C 24 - C 25	/344. RY*(3) C 25	0.75	0.87	0.052
648. BD*(2) C 24 - C 25	/636. BD*(1) C 15 - N 16	1.17	0.46	0.046
648. BD*(2) C 24 - C 25	/638. BD*(1) N 16 - C 18	1.68	0.27	0.041
648. BD*(2) C 24 - C 25	/653. BD*(2) C 26 - C 28	287.59	0.01	0.081
648. BD*(2) C 24 - C 25	/682. BD*(1) C 48 - H 50	1.63	0.41	0.052
648. BD*(2) C 24 - C 25	/683. BD*(1) C 48 - H 51	1.14	0.43	0.044
653. BD*(2) C 26 - C 28	/357. RY*(7) C 26	0.59	1.68	0.069
653. BD*(2) C 26 - C 28	/371. RY*(3) C 28	2.53	0.69	0.092
653. BD*(2) C 26 - C 28	/684. BD*(1) C 52 - H 53	0.71	0.46	0.038
653. BD*(2) C 26 - C 28	/685. BD*(1) C 52 - H 54	1.07	0.41	0.045
656. BD*(2) C 27 - C 29	/362. RY*(3) C 27	2.64	0.68	0.090
656. BD*(2) C 27 - C 29	/687. BD*(1) C 56 - H 57	1.49	0.41	0.052

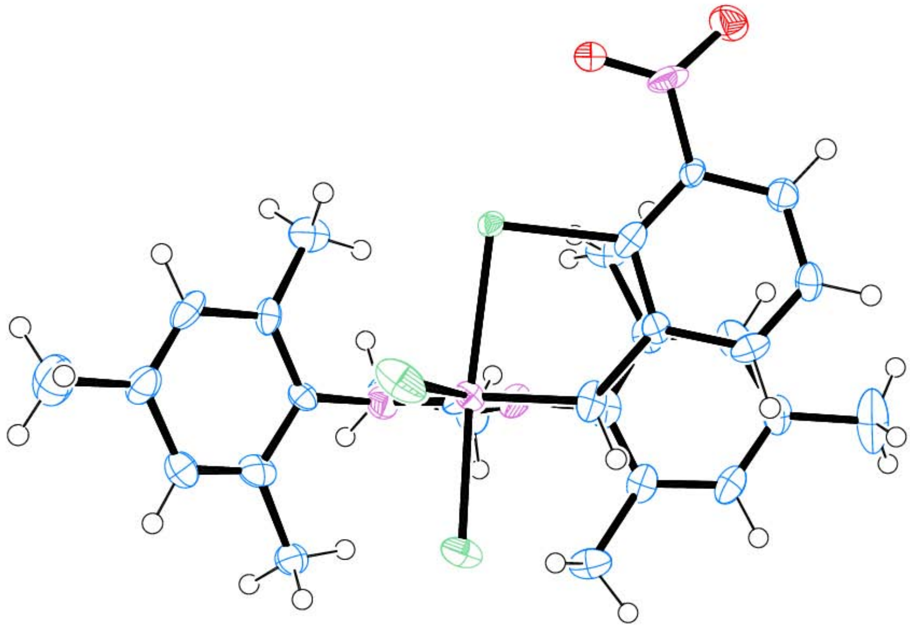
656. BD*(2) C 27 - C 29	/688. BD*(1) C 56 - H 58	0.51	0.41	0.031
662. BD*(2) C 32 - C 33	/406. RY*(3) C 33	0.78	0.89	0.054
662. BD*(2) C 32 - C 33	/637. BD*(1) C 15 - N 21	1.09	0.46	0.044
662. BD*(2) C 32 - C 33	/642. BD*(1) C 17 - N 21	1.65	0.28	0.042
662. BD*(2) C 32 - C 33	/670. BD*(2) C 35 - C 37	216.45	0.01	0.083
662. BD*(2) C 32 - C 33	/678. BD*(1) C 44 - H 45	1.49	0.47	0.053
662. BD*(2) C 32 - C 33	/680. BD*(1) C 44 - H 47	0.83	0.43	0.038
667. BD*(2) C 34 - C 36	/419. RY*(7) C 34	0.52	1.74	0.065
667. BD*(2) C 34 - C 36	/433. RY*(3) C 36	2.39	0.81	0.095
667. BD*(2) C 34 - C 36	/617. BD*(1) C 1 - I 12	0.55	0.02	0.006
667. BD*(2) C 34 - C 36	/670. BD*(2) C 35 - C 37	265.58	0.01	0.082
667. BD*(2) C 34 - C 36	/677. BD*(1) C 40 - H 43	1.39	0.40	0.050
670. BD*(2) C 35 - C 37	/424. RY*(3) C 35	1.65	0.71	0.076
670. BD*(2) C 35 - C 37	/446. RY*(7) C 37	0.53	1.68	0.066
670. BD*(2) C 35 - C 37	/690. BD*(1) C 60 - H 61	0.59	0.41	0.034
670. BD*(2) C 35 - C 37	/691. BD*(1) C 60 - H 62	1.34	0.41	0.051
694. BD*(2) N 65 - O 66	/589. RY*(3) N 65	3.77	2.12	0.142
694. BD*(2) N 65 - O 66	/594. RY*(8) N 65	1.20	1.08	0.057
694. BD*(2) N 65 - O 66	/597. RY*(2) O 66	3.09	1.14	0.094
694. BD*(2) N 65 - O 66	/603. RY*(8) O 66	0.71	2.13	0.062
694. BD*(2) N 65 - O 66	/606. RY*(2) O 67	1.13	1.13	0.057
694. BD*(2) N 65 - O 66	/626. BD*(2) C 5 - C 6	18.26	0.14	0.062

Citation of the program

Gaussian 03, Revision E.01,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

Crystallografic Information Data of complex 5





Experimental

The data were collected using the BRUKER KAPPA APEXII ULTRA controlled by APEXII software [i], equipped with MoKα rotating anode X-ray source (λ = 0.71073 Å, 50.0 kV, 22.0 mA) monochromatized by multi-layer optics and APEX-II CCD detector. The experiments were carried out at 100K using the Oxford Cryostream cooling device. The crystal was mounted on cactus needle with a droplet of Pantone-N oil and immediately cooled. Indexing, integration and initial scaling were performed with *SAINT* [ii] and *SADABS* [iii] software (Bruker, 2008). The data collection and processing statistics are reported in tables for according structures.

The crystal was positioned at 40 mm from the CCD camera. 1702 frames were measured at 0.5° intervals with a counting time of 20-30 sec.

The structures were solved by direct methods approach using the SHELXS-97 [iv] program and refined with the SHELXL-97 [v]. Multi-scan absorption correction have been applied in the scaling procedure.

The refinement was based on F^2 for all reflections except those with negative intensities. Weighted R factors wR and all goodness-of-fit S values were based on F^2, whereas conventional R factors were based on the amplitudes, with F set to zero for negative F^2. The $F_0^2 > 2\sigma(F_0^2)$ criterion was applied only for R factors calculation was not relevant to the choice of reflections for the refinement. The R factors based on F^2 are for all structures about twice as large as those based on F. The hydrogen atoms were located in idealized geometrical positions, except hydrogen in solvent molecule. Scattering factors were taken from Tables 4.2.6.8 and 6.1.1.4 from the International Crystallographic Tables Vol.C [vi].

Table 1. Crystal data and structure refinement for **5** · CH_2Cl_2.

Identification code	**5**
Empirical formula	$C_{29}H_{32}Cl_4IN_3O_2Ru$
Formula weight	824.35
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 8.2655(4) Å alpha = 90 °
	b = 14.6615(7) Å beta = 90.174(2) °
	c = 26.0185(12) Å gamma = 90 °
Volume	3153.0(3) A^3
Z, Calculated density	4, 1.737 Mg/m^3
Absorption coefficient	1.847 mm^{-1}
F(000)	1632
Crystal size	0.20 x 0.13 x 0.12 mm
Theta range for data collection	1.57 to 26.42 °.
Limiting indices	-10<=h<=10, -18<=k<=18, -32<=l<=32
Reflections collected / unique	49746 / 6464 [R(int) = 0.0324]
Completeness to theta = 26.00	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8088 and 0.7089
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6464 / 0 / 365
Goodness-of-fit on F^2	1.263
Final R indices [I>2sigma(I)]	R1 = 0.1175, wR2 = 0.3106

R indices (all data) R1 = 0.1184, wR2 = 0.3109
Largest diff. peak and hole 6.732 and -3.118 e.A^{-3}

i APEXII-2008v1.0 Bruker Nonius 2007
ii SAINT V7.34A Bruker Nonius 2007
iii SADABS-2008/1 Bruker Nonius area detector scaling and absorption correction, 2008
iv G. M. Sheldrick, Acta Crystallogr. **1990**, A46, 467-473.
v G. M. Sheldrick, SHELXL93. *Program for the Refinement of Crystal Structures.,* Univ. of Göttingen, Germany.
vi *International Tables for Crystallography*, Ed. A. J. C. Wilson, Kluwer:Dordrecht, **1992**, Vol.C.