

Supporting Information to
Ru^{II}-hydride-*trop* complexes: X-ray single crystal determination and quantum
chemical calculations

Authors

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1. General Comments

All reactions and manipulations were routinely performed under dry nitrogen or argon atmosphere using standard Schlenk techniques. The argon was provided by PANGAS and further purified with an MBraun 100 HP gas purification system. Solvents were distilled under argon from sodium-benzophenone (THF, diethyl ether, n-hexane), sodium (toluene), potassium (DME) or calcium hydride (methylene chloride). Air sensitive compounds were stored and weighed in a glovebox (M Braun: 150-GI or lab master 130). Reactions in small quantities were performed within a glovebox. Substances are classified as: air sensitive: decompose rapidly on air (seconds to minutes); slightly air sensitive: decompose on air in solution in hours and as solid in hours to days, air stable: stable on air in solution and as solid (in the period observed, usually days).

Basic chemicals were ordered either at ABCR, Acros, Aldrich, Fluka, Lancaster or STREM and used as such.

Solution NMR spectra were recorded either on *Bruker Avance 700, 500, 400, 300, 250* or *200* spectrometers. The chemical shifts (δ) are measured according to IUPAC (Harris *et al.* 2002 & 2001) and expressed in parts per million (ppm) relative to TMS, CFCl₃, and H₃PO₄ for ¹H, ²H, ¹³C, and ³¹P respectively. Coupling constants J are given in Hertz (Hz) as absolute values, unless otherwise stated. The multiplicity of the signals is indicated as *s*, *d*, *t*, *q*, or *m* for singlets, doublets, triplets, quartets, or multiplets, respectively. The abbreviation br. is given for broadened signals. Quaternary carbon atoms are indicated as C^{quat}, aromatic units as CH^{ar} and CH^{ar} when not noted otherwise. The olefinic protons and ¹³C atoms of the coordinated C=C_{trop} unit in the central seven-membered ring are indicated as CH^{olef} and CH^{olef}. The benzylic protons and ¹³C atoms in the central seven-membered ring are indicated as CH^{benzyl} and CH^{benzyl}.

IR spectra were recorded on a *Perkin-Elmer-Spectrum 2000* FT-IR-Raman spectrometer with KBr beam splitter (range 500-4000 cm⁻¹). For solid compounds the ATR technique was

applied. The absorption bands are described as follows: strong (*s*), very strong (*vs*), middle (*m*), weak (*w*), or broad (*br*).

Melting points were determined with a Büchi melting-point apparatus and are not corrected. Samples were prepared in open glass capillaries.

Elemental analyses were performed by the microanalytical laboratory of the ETH Zürich.

X-ray diffraction was performed at 100 K either on a Bruker instrument equipped with an APEX II CCD area detector (Mo_{Kα} 0.70173 Å radiation) or Bruker-Venture equipped with a CMOS Photon-100 area detector (Mo_{Kα} 0.70173 Å radiation).

Most of the H atoms present were found in a difference Fourier map and were refined freely. Those H atoms which after the refinement did not refine properly were placed in idealized positions and refined using a riding model with appropriate displacement parameters $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{parent atom})$. Default effective X-H distances for T = 100 K were C-H = 1.00 (NCR₂), 0.99 (methylene), 0.98 (methyl), and 0.95 (aromatic).

Data Collection: *APEX2* (Bruker, v2012.4-3); cell refinement: *SAINT v7.68A* (Bruker, v2012.4-3); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL* and *DIAMOND v3.2i* (Brandenburg, 2012); software used to prepare material for publication: *SHELXTL*.

Quantum chemical calculations: The optimization of the molecules was performed using the (RI)-BP(86)/SV(P), BP(86)/TZVPP and PBE0/TZVPP functionals with the program TURBOMOLE Versions 6.4.0mpi (Eichkorn *et al.* 1995). Vibrational analyses and zero-point vibrational energy (ZPVE) corrections were calculated using the AOFORCE program implementation in TURBOMOLE. All calculated species are true minima on the energy hyper-surface as shown by the absence of imaginary frequencies.

2. Syntheses

Preparation of N-(pyridine-2-ylmethyl)tropimine = (*trop*NCH₂py); (py = pyridine, *trop* = 5H-dibenzo[*a,d*]cyclohepten-5-yl)

In a 50 mL round bottom flask, 1.00 g (9.34 mmol) of 2-pyridinecarboxaldehyde and 2.00 g (9.65 mmol) of *tropamine* were added to 30 mL of methanol. Two drops of acetic acid were added to the stirring solution. After several minutes a white precipitate began to form. The reaction was stirred at room temperature overnight. The precipitate was filtered on a glass frit, washed twice with methanol, and dried under reduced pressure to yield 1.65 g (59 %) of the

desired imine. ^1H NMR (250 MHz, CD_2Cl_2): δ [ppm] = 8.65 (d, J = 4.8 Hz, 1H, NCH , py), 8.42 (s, 1H, NCH), 7.86 (m, 1H, CH^{ar} , py), 7.72 (m, 2H, CH^{ar} , py), 7.42 (m, 6H, CH^{ar}), 7.35 (m, 2H, CH^{ar}), 7.19 (s, 2H, CH^{olef}), 5.22 (br, 1H, $\text{CH}^{\text{benzyl}}$). $^{13}\text{C}\{\text{H}\}$ NMR (63 MHz, CD_2Cl_2) δ [ppm] = 162.70 (s, 1C, C^{quart}), 154.74 (s, 1C, NCH), 149.42 (s, 1C, CH^{py}), 141.16 (br, 2C, C^{quart}), 136.47 (s, 1C, CH^{py}), 133.56 (br, 2C, C^{quart}), 131.10 (s, 2C, CH^{olef}), 128.53 (s, 2C, CH^{ar}), 128.53-128.24 (4, 2C, CH^{ar}), 126.33 (s, 1C, CH), 124.95 (s, 2C, CH^{ar}), 121.18 (s, 1C, CH^{py}), 50.30 (s, 1C, $\text{CH}^{\text{benzyl}}$). EA: Calcd. for $\text{C}_{21}\text{H}_{16}\text{N}_2$, C 85.11, H 5.44, N 9.45 ; found: C 84.93, H 5.59, N 9.39. Air stable.

Preparation of $[\text{Ru}^{\text{II}}(\text{H})_2(\text{N-(pyridine-2-ylmethyl)tropNH})(\text{PPh}_3)]$ (1)

This complex was prepared in two steps:

i) $[\text{Ru}(\text{Cl})_2(\text{PPh}_3)(\text{tropNCHpy})]$: Commercially available $[\text{Ru}(\text{Cl})_2(\text{PPh}_3)_4]$ (129 mg, 0.11 mmol) and *tropNCHpy* (33 mg, 0.11 mmol) were combined in a 25 mL Schlenk septum-capped. The air and moisture were purged with argon-vacuum cycles for 20 min. Dry and degassed THF (20 mL) was added with a syringe and the reaction mixture was stirred vigorously at room temperature overnight. 20 mL diethyl ether were added to the resulting deep purple suspension. The obtained purple precipitate was filtered, washed with ether (3 x 5 mL) and dried under reduced pressure. Yield: 74 mg, 96%. Two isomers are formed in a ratio 2.4:1. ^1H NMR (400 MHz, CD_2Cl_2): δ [ppm] = 8.64 (d, $^3J_{\text{HH}} = 8.1$ Hz, 1H, NCH), 8.16 (d, $^3J_{\text{HH}} = 5.4$ Hz, 1H, CH^{ar}), 8.04 (m, 6H, CH^{ar}), 7.75-7.67 (m, 2H, CH^{ar}), 7.49-7.41 (m, 9H, CH^{ar}), 7.30-7.28 (m, 3H, CH^{ar}), 7.18 (m, 6H, CH^{ar}), 5.82 (d, $^4J_{\text{PH}} = 6.3$ Hz, 1H, $\text{CH}^{\text{benzyl}}$), 5.35 (d, $^3J_{\text{HH}} = 2.3$ Hz, 2H, CH^{olef}); $^{13}\text{C}\{\text{H}\}$ NMR (101 MHz, CD_2Cl_2): δ [ppm] = 160.5 (s, NCH), 141.0 (s, CH^{ar}), 137.1 (s, CH^{ar}), 135.6 (s, CH^{ar}), 135.2 (d, $J_{\text{PC}} = 8.8$ Hz, CH^{ar}), 134.0 (s, CH^{ar}), 133.6 (s, CH^{ar}), 130.4 (s, CH^{ar}), 129.6 (d, $J_{\text{PC}} = 1.8$ Hz, CH^{ar}), 127.8 (d, $J_{\text{PC}} = 8.7$ Hz, CH^{ar}), 127.4 (s, CH^{ar}), 127.3 (s, CH^{ar}), 126.6 (s, CH^{ar}), 126.0 (s, CH^{ar}), 125.3 (s, CH^{ar}), 79.5 (s, $\text{CH}^{\text{benzyl}}$), 74.9 (s, CH^{olef}); $^{31}\text{P}\{\text{H}\}$ NMR (162 MHz, CD_2Cl_2): δ [ppm] = 27.5 (s), 26.1 (s). Air stable.

ii) $[\text{Ru}^{\text{II}}(\text{H})_2(\text{N-(pyridine-2-ylmethyl)tropNH})(\text{PPh}_3)]$ (1): $[\text{Ru}(\text{Cl})_2(\text{PPh}_3)(\text{tropNCHpy})]$ (74 mg, 0.10 mmol) and $\text{KO}^\text{t}\text{Bu}$ (22 mg, 0.20 mmol) were dissolved in dry THF and placed in a 100 mL stainless-steel reactor (*Parr 5500 Series Compact Reactor*) equipped with a small motor for mechanical stirring and a thermostat (*Parr 4836 controller*). The system was loaded with H_2 (8 bar) and stirred slowly at 65 °C overnight. Upon cooling to room temperature yellow crystals suitable for X-ray analysis were obtained. Yield: 41 mg, 62%. ^1H NMR (400 MHz, CD_2Cl_2): δ [ppm] = 8.35 (m, 1H, CH^{ar}), 7.89-7.83 (m, 3H, CH^{ar}), 7.79-7.73 (m, 2H, CH^{ar}), 7.42-7.34 (m, 8H, CH^{ar}), 7.21-6.97 (m, 7H, CH^{ar}), 6.84 (td, $J_{\text{HH}} = 7.4$ Hz, $J_{\text{HH}} = 3.2$ Hz,

1H, CH^{ar}), 6.76-6.59 (m, 4H, CH^{ar}), 6.84-6.44 (m, 1H), 5.36 (s, 1H, CH^{benzyl}), 5.19 (dd, ³J_{PH} = 15.0 Hz, ³J_{HH} = 7.7 Hz, 1H, CH^{olef}), 3.63 (dd, ³J_{PH} = 15.1 Hz, ³J_{HH} = 3.5 Hz, 1H, CH^{olef}), -3.37 (d, ²J_{PH} = 27.0 Hz, 1H, hydride), -11.47 (d, ²J_{PH} = 28.5 Hz, 1H, hydride); ¹³C{¹H} NMR (101 MHz, CD₂Cl₂): Carbon resonances are not well resolved due to low solubility of the compound in dichloromethane and common organic solvents. ³¹P{¹H} NMR (162 MHz, CD₂Cl₂): δ [ppm] = 64.8 (s). Air sensitive.

Preparation of [Ru^{II}(H)(Cl)(*tropdaetrop*)] (2)

We have recently published the detailed synthesis and chemistry of [K(DME)₂][Ru^{II}(H)(*tropN*-CH=CH-*Ntrop*)] (Rodríguez-Lugo *et al.* 2013). In this publication, the detailed synthesis and characterization of the ligand *N,N'*-bis(5*H*-dibenzo[*a,d*]cyclohepten-5-yl)-1,2-diaminoethane (*tropdaetrop*) is fully described.

Commercially available [Ru(H)(Cl)(PPh₃)₃]•Toluene (88 mg, 0.09 mmol) and (*tropdaetrop*) (41 mg, 0.9 mmol) were combined in a 10 mL two-neck round-bottom flask which was connected to a reflux condenser with an argon inlet. The second neck was septum-capped. The air and moisture were purged with argon-vacuum cycles for 20 min. Dry and degassed THF (3 mL) was added with a syringe and the reaction mixture was stirred vigorously at 65 °C overnight. The pale yellow suspension was allowed to cool down to room temperature before 5 mL diethyl ether were added. The obtained pale yellow precipitate was filtered, washed with ether (3 x 5 mL) and dried under reduced pressure. Green rectangular platelet crystals suitable for X-ray analysis were obtained from DME/n-hexane. Yield: 35 mg, 70%. ¹H NMR (500 MHz, CD₂Cl₂): δ [ppm] = 7.60 (d, ³J_{HH} = 7.4 Hz, 2H, CH^{ar}), 7.52 (d, ³J_{HH} = 7.6 Hz, 2H, CH^{ar}), 7.32-7.30 (m, 4H, CH^{ar}), 7.20-7.13 (m, 8H, CH^{ar}), 4.58 (s, 2H, CH^{benzyl}), 4.29 (br, 2H, NH), 4.05 (d, ³J_{HH} = 9.2 Hz, 2H, CH^{olef}), 3.88 (d, ³J_{HH} = 9.2 Hz, 2H, CH^{olef}), 2.89 (br, 2H, CH₂), 2.43 (br, 2H, CH₂), -7.72 (s, 1H, hydride); ¹³C{¹H} NMR (126 MHz, CD₂Cl₂): δ [ppm] = 144.2 (s, C^{quat}), 142.9 (s, C^{quat}), 136.0 (s, C^{quat}), 135.3 (s, C^{quat}), 130.0 (s, CH^{ar}), 129.5 (s, CH^{ar}), 128.8 (s, CH^{ar}), 128.3 (s, CH^{ar}), 127.7 (s, CH^{ar}), 126.7 (s, CH^{ar}), 125.9 (s, CH^{ar}), 125.1 (s, CH^{ar}), 71.0 (s, CH^{olef}), 67.6 (s, CH^{benzyl}), 65.9 (s, CH^{olef}), 49.5 (s, 2 x CH₂).

Preparation of *N,N'*-bis(5*H*-dibenzo[*a,d*]cyclohepten-5-yl)-1,3-diaminopropane (*tropdaprop*)

i) Imine precursor: *N,N'*-bis(5*H*-dibenzo[*a,d*]cyclohepten-5-yl)diiminopropane (*trop₂dip*). 1,3-diaminopropane (270.0 mg, 3.60 mmol) and 1,4-diazabicyclo[2.2.2]octane (DABCO, 1.6 g, 14.40 mmol) were combined in a 50 mL two-neck round-bottom flask which was connected to a reflux condenser with an argon inlet. The second neck was septum-capped. Dry and

degassed toluene (4 mL) was added and the mixture was heated to 90 °C. TiCl₄ (0.44 mL, 3.96 mmol) in toluene (5 mL) was incorporated dropwise (10 min). Dibenzosuberone (1.5 g, 7.20 mmol) in toluene/chlorobenzene (4 mL) was added and the reddish suspension was refluxed for 24 h. After cooling to room temperature the mixture was filtered and the residue was washed with hot toluene. The filtrate was evaporated to dryness yielding a yellow oil, which was further purified by recrystallization in hot hexane. Yield: 1.2 g, 74% as colorless microcrystals. M.P: 144 °C. ¹H NMR (300.1 MHz, CDCl₃): δ [ppm] = 7.67-7.26 (m, 16H, CH^{ar}), 6.92-6.88 (m, 4H, CH^{olef}), 3.70-3.30 (m, 4H, CH₂), 2.20-1.99 (m, 2H, CH₂).

ii) Imine reduction: The imine *trop*₂dip (1.2 g, 2.66 mmol) dissolved in ethanol (30 mL) was treated slowly at 0°C with 3 equivalents of LiAlH₄ (125 mg, 3.3 mmol). The mixture was stirred overnight at room temperature. The reaction was quenched at 0°C with a mixture of (1:1) Celite and Na₂SO₄•10H₂O. The mixture was then stirred at room temperature during 3h, was filtered over a Celite pad filter and washed with ether. The filtrate was concentrated and a yellowish oily material was obtained. The oily material was recrystallized from hot hexane. Yield: 1.1 g, 91% as white solid. M.P: 137 °C. Three different conformers, namely the endo/endo, exo/exo, and endo/exo conformers with respect to the position of the NH group at the central seven-membered ring of the trop unit, were formed in a 1 : 1 : 1 ratio. The endo/endo, exo/exo conformers have mirror symmetry and show each one NH, one CH_{benzyl}, and two methylene CH₂ resonance. The endo/exo conformer has only rotational symmetry and shows two NH, two CH_{benzyl}, and three methylene CH₂ resonances. In total the conformer mixture therefore shows four NH, four CH_{benzyl}, and seven methylene CH₂ resonances. Only the four CH_{benzyl} resonances are really resolved ¹H NMR (300.1 MHz, CDCl₃): δ [ppm] = 7.60-6.54 (m, 60H), 4.90 (br, 1H, CH^{benzyl}), 4.77 (br, 2H, CH^{benzyl}), 4.66 (br, 1H, CH^{benzyl}), 4.63 (br, 1H, CH^{benzyl}), 3.90 (br, 2H, CH^{benzyl}), 2.79-1.28 (br, 24H); ¹³C{¹H} NMR (75.5 MHz, CDCl₃): δ [ppm] = 140.1 (br, C^{quat}), 133.8 (br, C^{quat}), 133.3 (br, C^{quat}), 131.2 (br, CH^{ar}), 130.5 (br, CH^{ar}), 130.0 (br, CH^{ar}), 129.6 (br, CH^{ar}), 128.6 (br, CH^{ar}), 127.7 (br, CH^{ar}), 127.0 (br, CH^{ar}), 125.5 (br, CH^{ar}), 122.5 (br, CH^{ar}), 69.9 (br, CH^{benzyl}), 69.5 (br, CH^{benzyl}), 61.2 (br, CH^{benzyl}), 61.2 (br, CH^{benzyl}), 51.5 (br, CH₂), 46.6 (br, CH₂), 45.8 (br, CH₂), 30.1 (br, CH₂). ATR IR (ν in cm⁻¹): 3287 w, 3214 w, 3013 w, 2898 w, 2831 w, 1483 m, 1431 s, 1100 m. Air stable.

Preparation of [Ru^{II}(H)(Cl)(*tropdaptrop*] (3)

Commercially available [Ru(H)(Cl)(PPh₃)₄]•Toluene (400.0 mg, 0.39 mmol) and *tropdaptrop* (180.0 mg, 0.39 mmol) were combined in a 25 mL two-neck round-bottom flask which was connected to a reflux condenser with an argon inlet. The second neck was septum-capped.

The air and moisture were purged with argon-vacuum cycles for 20 min. Dry and degassed toluene (5 mL) was added with a syringe and the reaction mixture was stirred vigorously at 80 °C overnight. The green brownish suspension was allowed to cool down to room temperature before 5 mL diethyl ether was added. The obtained green yellow precipitate was filtered, washed with ether (3 x 5 mL) and dried under reduced pressure. Crystals suitable for X-ray analysis were obtained from hot toluene. Yield: 190.0 mg, 83%. ¹H NMR (400.1 MHz, CD₂Cl₂): δ [ppm] = 7.60 (d, ³J_{HH} = 7.5 Hz, 2H, CH^{ar}), 7.55 (d, ³J_{HH} = 7.9 Hz, 3H, CH^{ar}), 7.49 (d, ³J_{HH} = 7.4 Hz, 1H, CH^{ar}), 7.35-7.17 (m, 10H, CH^{ar}), 5.13 (d, ³J_{HH} = 10.0 Hz, 1H, CH^{olef}), 5.03 (d, ³J_{HH} = 10.0 Hz, 1H, CH^{olef}), 4.59 (s, 1H, CH^{benzyl}), 4.57 (s, 1H, CH^{benzyl}), 4.26 (d, ³J_{HH} = 12.5 Hz, 1H, NH), 3.79 (d, ³J_{HH} = 12.1 Hz, 1H, NH), 3.68 (d, ³J_{HH} = 9.8 Hz, 1H, CH^{olef}), 3.63 (d, ³J_{HH} = 9.8 Hz, 1H, CH^{olef}), 3.44 (q, ³J_{HH} = 12.1 Hz, 1H, CH₂), 2.80 (d, ³J_{HH} = 11.9 Hz, 1H, CH₂), 2.48 (d, ³J_{HH} = 11.6 Hz, 1H, CH₂), 2.28 (q, ³J_{HH} = 12.2 Hz, 1H, CH₂), 1.77 (m, 1H, CH₂), 1.39 (m, 1H, CH₂), -7.03 (s, 1H, hydride); ¹³C{¹H} NMR (100.6 MHz, CD₂Cl₂): δ [ppm] = 141.9 (s, C^{quat}), 141.3 (s, C^{quat}), 139.7 (s, C^{quat}), 139.4 (s, C^{quat}), 136.0 (s, C^{quat}), 135.8 (s, C^{quat}), 134.2 (s, C^{quat}), 131.0 (s, C^{quat}), 130.0 (s, CH^{ar}), 129.4 (s, CH^{ar}), 128.3 (s, CH^{ar}), 128.2 (s, CH^{ar}), 127.7 (s, CH^{ar}), 127.6 (s, CH^{ar}), 127.4 (s, CH^{ar}), 127.3 (s, CH^{ar}), 127.2 (s, CH^{ar}), 127.1 (s, CH^{ar}), 126.9 (s, CH^{ar}), 126.5 (s, CH^{ar}), 126.2 (s, CH^{ar}), 125.6 (s, CH^{ar}), 124.8 (s, CH^{ar}), 86.7 (s, CH^{olef}), 84.8 (s, CH^{olef}), 72.2 (s, CH^{benzyl}), 71.4 (s, CH^{benzyl}), 69.6 (s, CH^{olef}), 65.8 (s, CH^{olef}), 55.1 (s, CH₂), 48.9 (s, CH₂), 28.7 (s, CH₂). EA Calcd. for C₃₃H₃₁ClN₂Ru, C 66.94, H 5.28, N 4.73; found: C 66.80, H 5.33, N 4.74. Air sensitive.

3. Inter- and intramolecular interactions for (1) and (2)

Figure 1 Experimental distances (Å) for the H^{δ-}-H^{δ+} interactions. Left: for **1** the shortest d_{intermol.}(H^{δ-}-H^{δ+}) = 1.83. Right: for **2** the shortest d_{intramol.}(H^{δ-}-H^{δ+}) = 2.08. All non relevant H atoms and solvent molecules have been omitted for clarity.

4. Quantum Chemical Calculations

Figure 2 Calculated species, showing two possible isomers for **2** and **3**. Complexes **2** and **3** are energetically favoured over **2a** and **3a** respectively.

Table 1 Total energies (Hartree) and zero-point vibrational energy (ZPVE) corrections (Hartree) using various functionals^a for all calculated species.

Complex (symmetr y)	RI-BP(86)/SV(P) ^a		BP(86)/TZVPP ^a		PBE0/TZVPP ^a	
	Total Energy	ZPVE	Total Energy	ZPVE	Total Energy	ZPVE
(1)-(C ₁)	- 2051.95649090	0.61513 01	- 2053.86983428	0.61342 43	- 2051.56372967	0.63560 95

	00		50		00	
(2)-(C _s)	-		-		-	
	1900.65714089	0.51865	1902.30431074	0.51662	1900.31020252	0.53597
	30	65	10	22	10	47
(2a)-(C _s)	-		-		-	
	1900.63566717	0.51892	1902.28363966	0.51667	1900.28977645	0.53626
	80	14	80	14	70	74
(3)-(C _s)	-		-		-	
	1939.94978461	0.54696	1941.64309348	0.54516	1939.60010248	0.56534
	70	76	80	73	00	63
(3a)-(C _s)	-		-		-	
	1939.93459117	0.54725			1939.58531047	0.56570
	50	41	Not calculated	---	40	18
Energy dif. (kJ mol ⁻¹)	(2)-(2a) RI-BP(86)/SV(P) -57	(2)-(2a) BP(86)/TZVPP -54	(2)-(2a) PBE0/TZVPP -54			
	(3)-(3a) RI-BP(86)/SV(P) -41	(3)-(3a) BP(86)/TZVPP Not calculated	(3)-(3a) PBE0/TZVPP -40			

^aAs implemented in the program TURBOMOLE (Eichkorn *et al.* 1995).

Table 2 Comparison of all calculated species with different functionals. Selected geometric parameters (Å, °) for (1-3). **3a** (RI-BP(86)/SV(P)) has not been included in the table.

	PBE0/TZVPP ^a					BP(86)/TZVPP ^a				RI-BP(86)/SV(P) ^a			
	(1) ^b	(2) ^c	(2a) ^c	(3) ^c	(3a) ^c	(1) ^b	(2) ^c	(2a) ^c	(3) ^c	(1) ^b	(2) ^c	(2a) ^c	(3) ^c
Ru-H0a	1.58	1.56	1.57	1.56	1.57	1.59	1.57	1.59	1.58	1.61	1.60	1.61	1.60
Ru-H0b	1.63	---	---	---	---	1.64	---	---	---	1.65	---	---	---
H0a-H0b	1.96	---	---	---	---	1.94	---	---	---	1.97	---	---	---
Ru-N1	2.172	2.105	2.121	2.179	2.195	2.189	2.122	2.138	2.196	2.190	2.129	2.150	2.201
Ru-N2	2.189	2.105	2.121	2.179	2.195	2.196	2.122	2.138	2.196	2.199	2.129	2.150	2.201
Ru-X	2.233	2.533	2.537	2.521	2.516	2.243	2.563	2.571	5.554	2.260	2.557	2.554	2.545
Ru-ct.1	2.061	2.034	2.033	2.034	2.034	2.101	2.053	2.049	2.053	2.100	2.054	2.052	2.057
Ru-ct.2	---	2.034	2.033	2.034	2.034	---	2.053	2.049	2.053	---	2.054	2.052	2.057
N1-Ru-H0a	90.5	84	82	85.1	84.5	89.7	83	81	84.5	89.2	84	81	84.6
N1-Ru-N2	78.0	79.4	77.0	90.7	87.8	78.0	79.4	77.2	90.8	78.2	79.3	77.1	91.0
N1-Ru-ct.1	88.2	90.4	91.1	87.6	88.2	87.9	90.4	91.1	87.5	88.2	90.5	91.2	87.5
N1-Ru-ct.2	---	168.5	166.5	175.6	171.7	---	168.5	166.6	175.9	---	168.9	166.7	176.4
N1-Ru-X	171.0	79.3	86.9	78.8	87.6	171.1	78.6	86.6	78.2	171.3	78.1	86.3	77.8
N1-Ru-H0b	86.9	---	---	---	---	86.7	---	---	---	86.5	---	---	---
N2-Ru-H0a	159.0	84	82	85	81.4	157.7	83	81	85	157.8	84	81	85
N2-Ru-ct.1	103.4	168.5	166.5	175.6	171.7	103.6	168.5	166.6	175.9	103.3	168.9	166.7	176.4
N2-Ru-X	104.9	79.3	86.9	78.8	87.6	104.7	78.6	86.6	78.2	104.4	78.1	86.3	77.8
N2-Ru-H0b	86.7	---	---	---	---	86.8	---	---	---	86.6	---	---	---
N2-Ru-ct.2	---	90.4	91.1	87.6	88.2	---	90.4	91.1	87.5	---	90.5	91.2	87.5
ct.1-Ru-ct.2	---	99.2	99.9	93.9	94.8	---	99.3	99.9	93.6	---	99.3	99.8	93.9
ct.1-Ru-X	99.2	104.2	99.0	104.7	99.5	99.4	104.6	99.1	105.1	99.1	104.3	99.1	105.0
ct.1-Ru-H0a	93.7	90	90	90.8	90.6	94.3	91	91	91.6	94.5	91	91	92
ct.1-Ru-H0b	167.6	---	---	---	---	167.1	---	---	---	167.7	---	---	---
ct.2-Ru-X	---	104.2	99.0	104.7	99.5	---	104.6	99.1	105.1	---	104.3	99.1	105.0
ct.2-Ru-H0a	---	90	90	90.8	90.6	---	91	91	91.6	---	91	91	92
H0a-Ru-X	83.9	158	166	157.0	164.6	84.9	156	165	155.1	85.6	156	164	155
H0a-Ru-H0b	75	---	---	---	---	73.9	---	---	---	74.3	---	---	---
H0b-Ru-X	84.8	---	---	---	---	85.0	---	---	---	85.4	---	---	---

^aAs implemented in the program TURBOMOLE (Eichkorn *et al.* 1995). ^bX = P, complex calculated with C_1 symmetry. ^cX = Cl, H0a = H0, complex calculated with C_s symmetry *ct.* = centroid of the coordinated C=C bond of the *trop* units.

4.1. Coordinates (xyz) and vibrational frequencies for all calculated species at the PBE0 functional with a valence triple-zeta (TZVPP) basis set:

(S)-[Ru^{II}(H)₂(N-(pyridine-2-ylmethyl)*trop*NH)(PPh₃)] (**1**)

10.52758762613911	10.70588814296669	4.16198297828105	ru
7.60837760855858	11.27136108960834	3.84318389209347	h
10.36704261665420	12.86675427596971	1.96579500154532	h
10.40848962046679	13.96273449232142	6.84148987245580	p
10.36147907465266	7.93961961594142	1.13548720902285	n
8.78417343134390	8.50041339063474	0.20950274806387	h
14.51668243176764	10.30980821554952	3.14288160779494	n
10.00467625871841	5.24623129653614	1.84248988238585	c
7.46982607236707	4.92969842492346	3.08290223399659	c
6.86843225547157	6.27966369533617	5.28298273351622	c
8.62668925734612	8.02369955730445	6.54096152175330	c
11.27095434519632	7.57277880119925	6.83477223349628	c
12.68598653246328	5.45417146464123	5.79229247216912	c
12.14149219552081	4.30690046585354	3.45637351192414	c
13.57708991860622	2.27151448502971	2.61778125059266	c
15.59077570381563	1.35023732408854	4.01041124743164	c
16.18535592689960	2.50392040036055	6.29071809356545	c
14.75772593690978	4.51465413635881	7.15034262803086	c
5.71085337996020	3.29699610386078	2.01512478322640	c
3.34037949087036	2.97039849923415	3.07674228731541	c
2.71959506087440	4.31090133494065	5.24201477247280	c
4.46334759198383	5.93622035000133	6.31640117230679	c
12.55598936281492	8.39266898432274	-0.48714058311863	c
14.88058558361849	9.00008470856134	1.00645985628517	c
17.27380964730988	8.35309324207840	0.15694326655706	c
19.36465009753148	9.08841903492504	1.53915248780837	c
18.98703145462718	10.44182799462095	3.74793490897186	c
16.54292245971752	10.99610298850830	4.47861122440919	c
13.18509904283195	16.10167617133544	6.87719635933875	c
14.14734425300695	16.81015510698571	4.52617538554742	c
16.16053928560060	18.47378331056913	4.34577701865666	c
17.26819827306248	19.44563675447978	6.51640310844512	c
16.33217744020401	18.75315741615100	8.86232826990147	c
14.29847422968428	17.10294619634979	9.04182566774777	c
7.94980918685146	16.42227045219644	6.42145320678886	c
7.88205656019870	18.51205184734540	8.02898753733105	c
6.08306538293073	20.38597544677110	7.71788231780435	c
4.32484946555013	20.21003345357095	5.77664413004059	c
4.38773560320748	18.15349057501216	4.15915146660168	c
6.19002976130225	16.27090452110831	4.47950967533793	c
9.98969552772841	13.16851859373373	10.21048908354017	c
11.98003572469670	12.08431749984797	11.56049107377461	c
11.64919017152876	11.25165034082919	14.02193307339127	c
9.30169686834511	11.45008380643777	15.17328682334739	c

7.29704043928133	12.48382960563671	13.84169230246349	c
7.63817990391560	13.33667309609899	11.38458710515852	c
9.99809435213103	4.11654687396577	0.10264067761483	h
7.75304103382369	8.95006328695806	8.14693740799614	h
12.06532069423768	8.26225209231504	8.59315472369254	h
13.10318581481157	1.40071918732635	0.82147330393430	h
16.68635398795836	-0.23612675298062	3.32323511528271	h
17.75938691021492	1.82199496961062	7.41032517123981	h
15.21345641070515	5.38472485361135	8.94956099692130	h
6.21300074663812	2.26759387277374	0.31337065892853	h
1.99045802387391	1.69576392895530	2.21500238493399	h
0.87214496861537	4.08843490774156	6.09758660073564	h
3.97393429328784	6.97582078401299	8.01336487994987	h
12.10857857803918	10.05519456034870	-1.63325348629589	h
12.91809364358371	6.80073563911669	-1.76208012265110	h
17.47433570605950	7.26639808788045	-1.56498470189445	h
21.25160668568554	8.59968484810428	0.91518266158879	h
20.55337016203399	11.05547628694668	4.90976055024738	h
16.17027368455505	12.04264423820051	6.19327250977229	h
13.29470612186183	16.02756448369636	2.83468548366515	h
16.87204450836532	19.00974128021672	2.50139790303680	h
18.84944000837706	20.73948234032413	6.37831454673605	h
17.17598938038481	19.50772245852342	10.56957896463182	h
13.57991259037781	16.60462712615714	10.89181876108912	h
9.25199959111533	18.68279557004220	9.54156822845887	h
2.91867043263499	21.67798944248678	5.52686489212427	h
3.03009889240389	18.00451218412422	2.63280517438955	h
13.82151160016443	11.89802863221664	10.68088502628951	h
6.25692701628296	14.66511549494814	3.21546344450203	h
13.22809447597190	10.43619046591846	15.04016154371002	h
9.03709658289463	10.79359906035185	17.09436947876745	h
5.45202072946133	12.63643572141512	14.71754393178666	h
6.05503792070968	14.14948132768635	10.37343462510126	h
6.05746207313728	21.99257585321291	8.98782431903313	h

vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules
#				IR	RAMAN
1			0.00	0.00000	- -
2			0.00	0.00000	- -
3			0.00	0.00000	- -
4			0.00	0.00000	- -
5			0.00	0.00000	- -
6			0.00	0.00000	- -
7	a		13.56	0.12696	YES YES
8	a		21.93	0.10148	YES YES
9	a		32.73	0.07182	YES YES
10	a		40.00	0.17114	YES YES
11	a		43.68	0.76537	YES YES
12	a		47.08	0.02912	YES YES
13	a		51.51	0.10911	YES YES
14	a		56.65	0.09417	YES YES
15	a		57.54	0.20754	YES YES
16	a		63.56	0.31998	YES YES
17	a		77.10	0.96159	YES YES
18	a		89.34	0.17946	YES YES
19	a		91.14	0.13966	YES YES
20	a		108.03	0.13903	YES YES
21	a		117.84	0.53981	YES YES
22	a		123.93	0.14636	YES YES
23	a		128.74	0.28990	YES YES
24	a		135.82	0.41510	YES YES

25	a	178.93	1.59044	YES	YES
26	a	185.53	0.37117	YES	YES
27	a	209.39	1.63882	YES	YES
28	a	214.86	0.19827	YES	YES
29	a	223.63	0.77805	YES	YES
30	a	232.32	3.84242	YES	YES
31	a	243.66	3.32648	YES	YES
32	a	248.17	2.37021	YES	YES
33	a	253.66	3.66500	YES	YES
34	a	259.46	5.34585	YES	YES
35	a	263.83	0.64485	YES	YES
36	a	277.46	0.77939	YES	YES
37	a	282.19	0.64023	YES	YES
38	a	322.19	0.68129	YES	YES
39	a	331.12	4.70410	YES	YES
40	a	332.75	1.50727	YES	YES
41	a	393.25	1.21674	YES	YES
42	a	400.32	20.03587	YES	YES
43	a	406.60	0.02665	YES	YES
44	a	411.48	0.61312	YES	YES
45	a	417.70	0.07138	YES	YES
46	a	427.89	5.81264	YES	YES
47	a	437.95	1.66635	YES	YES
48	a	438.96	11.22394	YES	YES
49	a	446.07	5.11696	YES	YES
50	a	447.47	19.29020	YES	YES
51	a	471.34	10.29368	YES	YES
52	a	480.40	6.26681	YES	YES
53	a	481.50	3.65175	YES	YES
54	a	502.21	4.19719	YES	YES
55	a	514.28	32.02385	YES	YES
56	a	527.11	11.81550	YES	YES
57	a	541.35	145.00050	YES	YES
58	a	547.38	133.71274	YES	YES
59	a	559.29	3.68302	YES	YES
60	a	572.04	1.15009	YES	YES
61	a	585.45	18.63868	YES	YES
62	a	596.99	6.56217	YES	YES
63	a	628.91	0.02674	YES	YES
64	a	630.12	0.89396	YES	YES
65	a	630.71	1.19764	YES	YES
66	a	631.50	3.08756	YES	YES
67	a	652.80	0.97199	YES	YES
68	a	664.00	27.41452	YES	YES
69	a	673.78	2.64004	YES	YES
70	a	678.11	2.24763	YES	YES
71	a	697.34	22.41008	YES	YES
72	a	705.70	11.28586	YES	YES
73	a	710.23	30.54420	YES	YES
74	a	713.48	20.10178	YES	YES
75	a	720.26	66.12893	YES	YES
76	a	724.43	12.64886	YES	YES
77	a	726.74	12.28420	YES	YES
78	a	741.59	27.45081	YES	YES
79	a	752.33	14.57006	YES	YES
80	a	760.78	26.31386	YES	YES
81	a	763.60	20.18588	YES	YES
82	a	765.14	8.81607	YES	YES
83	a	768.07	1.72083	YES	YES
84	a	770.80	91.51892	YES	YES
85	a	771.96	13.35852	YES	YES
86	a	775.21	1.18188	YES	YES

87	a	783.58	2.31186	YES	YES
88	a	794.96	3.28681	YES	YES
89	a	802.81	1.84741	YES	YES
90	a	828.37	9.12072	YES	YES
91	a	842.69	3.43985	YES	YES
92	a	865.39	11.26120	YES	YES
93	a	869.53	0.12136	YES	YES
94	a	873.66	5.41391	YES	YES
95	a	876.88	33.37587	YES	YES
96	a	879.76	2.81415	YES	YES
97	a	892.13	72.03572	YES	YES
98	a	896.57	4.11316	YES	YES
99	a	900.00	11.92699	YES	YES
100	a	903.60	20.54627	YES	YES
101	a	920.69	4.13753	YES	YES
102	a	946.63	8.96829	YES	YES
103	a	948.13	3.82621	YES	YES
104	a	953.19	0.06127	YES	YES
105	a	957.24	0.17669	YES	YES
106	a	961.59	0.99652	YES	YES
107	a	968.08	0.50106	YES	YES
108	a	979.88	59.69484	YES	YES
109	a	988.76	0.36996	YES	YES
110	a	990.35	6.70823	YES	YES
111	a	993.02	0.14767	YES	YES
112	a	1000.85	0.55127	YES	YES
113	a	1002.01	0.38476	YES	YES
114	a	1009.45	0.78284	YES	YES
115	a	1013.19	0.34961	YES	YES
116	a	1015.55	0.29282	YES	YES
117	a	1015.72	0.47996	YES	YES
118	a	1017.11	0.67572	YES	YES
119	a	1021.18	1.08857	YES	YES
120	a	1022.16	1.60073	YES	YES
121	a	1023.68	1.58102	YES	YES
122	a	1025.74	1.52570	YES	YES
123	a	1040.32	0.88620	YES	YES
124	a	1058.16	1.72212	YES	YES
125	a	1058.99	1.34138	YES	YES
126	a	1059.17	3.38375	YES	YES
127	a	1059.49	1.37737	YES	YES
128	a	1075.99	3.19299	YES	YES
129	a	1079.79	5.17096	YES	YES
130	a	1085.77	5.93060	YES	YES
131	a	1104.10	4.49811	YES	YES
132	a	1107.80	5.87038	YES	YES
133	a	1108.88	2.73977	YES	YES
134	a	1113.34	7.47088	YES	YES
135	a	1114.62	22.27819	YES	YES
136	a	1120.55	41.31748	YES	YES
137	a	1123.16	2.75154	YES	YES
138	a	1124.77	11.25615	YES	YES
139	a	1137.04	0.64128	YES	YES
140	a	1142.45	0.38429	YES	YES
141	a	1156.08	4.89222	YES	YES
142	a	1175.46	4.03583	YES	YES
143	a	1178.03	0.34503	YES	YES
144	a	1178.68	0.29335	YES	YES
145	a	1178.90	0.52018	YES	YES
146	a	1179.36	0.23868	YES	YES
147	a	1180.04	0.08955	YES	YES
148	a	1205.08	7.65513	YES	YES

149	a	1208.41	7.11987	YES	YES
150	a	1210.49	2.60977	YES	YES
151	a	1219.59	6.19387	YES	YES
152	a	1229.68	1.60529	YES	YES
153	a	1238.35	3.50691	YES	YES
154	a	1246.47	2.87765	YES	YES
155	a	1256.84	2.76619	YES	YES
156	a	1261.49	3.70338	YES	YES
157	a	1290.35	9.30011	YES	YES
158	a	1301.03	2.50871	YES	YES
159	a	1317.45	5.80938	YES	YES
160	a	1321.18	3.25155	YES	YES
161	a	1324.57	2.35465	YES	YES
162	a	1330.29	6.48124	YES	YES
163	a	1335.43	1.53041	YES	YES
164	a	1346.90	2.69059	YES	YES
165	a	1357.09	1.86098	YES	YES
166	a	1362.15	0.49629	YES	YES
167	a	1364.05	3.42281	YES	YES
168	a	1364.87	0.16384	YES	YES
169	a	1377.74	5.52794	YES	YES
170	a	1383.17	0.45343	YES	YES
171	a	1403.38	1.52479	YES	YES
172	a	1420.88	2.03598	YES	YES
173	a	1442.00	22.97415	YES	YES
174	a	1444.46	24.73086	YES	YES
175	a	1469.40	5.91081	YES	YES
176	a	1469.97	4.85093	YES	YES
177	a	1473.74	25.76979	YES	YES
178	a	1476.45	5.52529	YES	YES
179	a	1486.60	10.36632	YES	YES
180	a	1499.29	1.31824	YES	YES
181	a	1512.52	94.50393	YES	YES
182	a	1519.62	10.57182	YES	YES
183	a	1521.41	12.87787	YES	YES
184	a	1522.49	15.10170	YES	YES
185	a	1523.51	13.07173	YES	YES
186	a	1529.65	24.64798	YES	YES
187	a	1533.30	25.44225	YES	YES
188	a	1631.16	2.05992	YES	YES
189	a	1634.88	0.57466	YES	YES
190	a	1636.47	3.24460	YES	YES
191	a	1637.81	2.88488	YES	YES
192	a	1639.83	3.23296	YES	YES
193	a	1640.41	1.52785	YES	YES
194	a	1652.71	1.71891	YES	YES
195	a	1653.60	1.22496	YES	YES
196	a	1654.58	1.46468	YES	YES
197	a	1662.98	26.15660	YES	YES
198	a	1668.31	23.69048	YES	YES
199	a	1671.07	12.41204	YES	YES
200	a	1905.83	212.36965	YES	YES
201	a	2122.47	112.08573	YES	YES
202	a	3009.56	39.01804	YES	YES
203	a	3027.96	42.23404	YES	YES
204	a	3081.55	6.35316	YES	YES
205	a	3159.46	2.46182	YES	YES
206	a	3167.75	6.27339	YES	YES
207	a	3169.82	6.63930	YES	YES
208	a	3170.93	12.65178	YES	YES
209	a	3177.60	4.78196	YES	YES
210	a	3178.45	2.58567	YES	YES

211	a	3179.33	0.23073	YES	YES
212	a	3180.55	0.21861	YES	YES
213	a	3181.23	2.13038	YES	YES
214	a	3186.12	2.91728	YES	YES
215	a	3187.02	0.84319	YES	YES
216	a	3189.73	5.11092	YES	YES
217	a	3193.49	15.43198	YES	YES
218	a	3195.24	5.31037	YES	YES
219	a	3195.78	16.49318	YES	YES
220	a	3196.48	12.22617	YES	YES
221	a	3198.67	1.50483	YES	YES
222	a	3199.44	16.97592	YES	YES
223	a	3204.81	11.50547	YES	YES
224	a	3205.89	9.08918	YES	YES
225	a	3208.84	17.29180	YES	YES
226	a	3209.87	22.33231	YES	YES
227	a	3210.75	28.15851	YES	YES
228	a	3211.19	22.61467	YES	YES
229	a	3213.11	6.29876	YES	YES
230	a	3213.17	15.54094	YES	YES
231	a	3216.72	24.21889	YES	YES
232	a	3220.81	3.95296	YES	YES
233	a	3234.10	3.84522	YES	YES
234	a	3562.35	14.20721	YES	YES

(1S,2R)-[Ru^{II}(H)(Cl)(*tropdaetrop*)] (*C_s*) (**2**)

0.77371010778881	0.11046116270751	0.0000000000000000	ru
-2.07954859065377	0.87008170673178	0.0000000000000000	h
4.60563246975177	-2.75746412297697	0.0000000000000000	cl
-0.41333047423276	-2.71245663283353	-2.54083410510439	n
-0.41333047423276	-2.71245663283353	2.54083410510439	n
-0.63904715254230	-2.01994280475319	-5.24657732917666	c
-1.38019195672201	-3.65300027602309	-6.28472234409577	h
-2.41704404397147	0.15816209911037	-5.66275920139805	c
-1.96683488119837	2.50825870277586	-4.52060047443544	c
0.15664673341943	2.99186320993988	-2.78801240345499	c
0.00779167655403	4.83154045599755	-1.89552125124285	h
2.64474853310458	2.05393394825710	-3.06577612432679	c
4.14284049373011	3.24233101714850	-2.32374673999302	h
3.47366859795396	0.43593780628421	-5.16564269504089	c
1.95879701708342	-1.44418368662740	-6.26581284599836	c
-3.64588917973844	4.47714152514620	-5.02718203197682	c
-3.31789333433852	6.29923645478881	-4.14787378545613	h
-5.69561642151885	4.16102529718467	-6.62249269641964	c
-6.96016570961106	5.73108180342201	-6.98080286523484	h
-6.12226896412194	1.83669339756583	-7.75164583255796	c
-7.72366963501235	1.56117090916338	-8.99609684593763	h
-4.47866589279212	-0.14272327920226	-7.26009443978460	c
-4.79795405976089	-1.96940702397174	-8.13604862504311	h
5.89336152475344	0.80240794606348	-6.14752021947341	c
7.09420778609831	2.22101814114750	-5.28605724912781	h
6.78122773268397	-0.58747313155142	-8.17549418416442	c
5.25771948619751	-2.41254914609714	-9.27508946096849	c
5.93415860743351	-3.52081572213873	-10.85721948901617	h
2.86446520816939	-2.83146951848388	-8.30155325068103	c
1.67175622793358	-4.28045408676360	-9.12809245413592	h
-0.63904715254230	-2.01994280475319	5.24657732917666	c
1.95879701708342	-1.44418368662740	6.26581284599836	c
3.47366859795396	0.43593780628421	5.16564269504089	c
2.64474853310458	2.05393394825710	3.06577612432679	c

4.14284049373011	3.24233101714850	2.32374673999302	h
0.15664673341943	2.99186320993988	2.78801240345499	c
0.00779167655403	4.83154045599755	1.89552125124285	h
-1.96683488119837	2.50825870277586	4.52060047443544	c
-2.41704404397147	0.15816209911037	5.66275920139805	c
5.89336152475344	0.80240794606348	6.14752021947341	c
6.78122773268397	-0.58747313155142	8.17549418416442	c
8.66957640069931	-0.25092124463591	8.89179343955054	h
5.25771948619751	-2.41254914609714	9.27508946096849	c
2.86446520816939	-2.83146951848388	8.30155325068103	c
1.67175622793358	-4.28045408676360	9.12809245413592	h
-3.64588917973844	4.47714152514620	5.02718203197682	c
-3.31789333433852	6.29923645478881	4.14787378545613	h
-5.69561642151885	4.16102529718467	6.62249269641964	c
-6.96016570961106	5.73108180342201	6.98080286523484	h
-6.12226896412194	1.83669339756583	7.75164583255796	c
-4.47866589279212	-0.14272327920226	7.26009443978460	c
-4.79795405976089	-1.96940702397174	8.13604862504311	h
-2.65873120475051	-3.95029626125089	1.46154460632567	c
-4.29831018167861	-2.89832599827573	2.13121069626520	h
-2.81709821970642	-5.88251700209591	2.18751370011982	h
-2.65873120475051	-3.95029626125089	-1.46154460632567	c
-2.81709821970642	-5.88251700209591	-2.18751370011982	h
-4.29831018167861	-2.89832599827573	-2.13121069626520	h
1.13184829243867	-3.86680627252185	-2.38358252625074	h
1.13184829243867	-3.86680627252185	2.38358252625074	h
8.66957640069931	-0.25092124463591	-8.89179343955054	h
-1.38019195672201	-3.65300027602309	6.28472234409577	h
7.09420778609831	2.22101814114750	5.28605724912781	h
5.93415860743351	-3.52081572213873	10.85721948901617	h
-7.72366963501235	1.56117090916338	8.99609684593763	h

vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules
#				IR	RAMAN
1			0.00	0.00000	- -
2			0.00	0.00000	- -
3			0.00	0.00000	- -
4			0.00	0.00000	- -
5			0.00	0.00000	- -
6			0.00	0.00000	- -
7	a"		34.52	0.17260	YES YES
8	a'		35.87	0.10838	YES YES
9	a'		51.56	0.11087	YES YES
10	a"		58.62	0.14027	YES YES
11	a"		69.57	0.65868	YES YES
12	a"		90.10	0.02415	YES YES
13	a'		91.04	2.57001	YES YES
14	a'		108.78	1.25657	YES YES
15	a'		125.18	0.33799	YES YES
16	a"		128.76	0.11415	YES YES
17	a"		130.54	0.43371	YES YES
18	a'		134.33	0.29056	YES YES
19	a'		142.90	1.50451	YES YES
20	a"		148.26	3.04348	YES YES
21	a'		178.75	9.44979	YES YES
22	a'		205.59	0.04952	YES YES
23	a"		240.43	0.38012	YES YES
24	a'		240.47	16.89306	YES YES
25	a"		261.05	0.15133	YES YES
26	a"		277.55	10.03156	YES YES
27	a'		284.08	0.93855	YES YES

28	a'	292.52	5.58058	YES	YES
29	a"	325.94	1.39467	YES	YES
30	a"	329.12	4.25097	YES	YES
31	a'	329.26	0.89545	YES	YES
32	a'	332.95	0.71533	YES	YES
33	a"	339.71	11.00166	YES	YES
34	a'	358.68	1.66306	YES	YES
35	a"	399.32	0.01108	YES	YES
36	a'	402.73	0.37499	YES	YES
37	a"	422.17	24.62075	YES	YES
38	a"	439.41	27.73161	YES	YES
39	a'	446.77	2.75995	YES	YES
40	a'	458.10	0.60883	YES	YES
41	a"	458.21	0.28867	YES	YES
42	a"	478.83	0.05250	YES	YES
43	a'	480.32	7.17398	YES	YES
44	a'	482.17	1.25597	YES	YES
45	a"	515.53	46.05998	YES	YES
46	a"	558.40	2.53061	YES	YES
47	a'	560.23	15.48513	YES	YES
48	a"	568.56	13.74610	YES	YES
49	a'	572.90	7.65243	YES	YES
50	a"	574.54	0.64029	YES	YES
51	a'	586.24	9.91533	YES	YES
52	a'	603.64	6.37536	YES	YES
53	a"	614.16	1.67828	YES	YES
54	a'	629.34	3.65973	YES	YES
55	a"	642.18	12.61812	YES	YES
56	a'	643.99	9.74214	YES	YES
57	a"	649.41	13.74337	YES	YES
58	a'	686.35	0.38148	YES	YES
59	a"	713.43	1.58160	YES	YES
60	a"	720.30	0.92174	YES	YES
61	a'	724.29	1.01653	YES	YES
62	a"	745.76	4.75441	YES	YES
63	a'	747.90	2.17708	YES	YES
64	a"	763.86	0.00364	YES	YES
65	a'	764.79	29.12789	YES	YES
66	a"	770.21	92.54100	YES	YES
67	a'	772.59	33.11898	YES	YES
68	a'	782.85	9.57237	YES	YES
69	a"	783.28	3.87551	YES	YES
70	a'	798.23	2.04124	YES	YES
71	a"	805.15	0.90181	YES	YES
72	a'	830.93	10.70622	YES	YES
73	a"	834.84	0.30255	YES	YES
74	a'	857.03	1.48145	YES	YES
75	a"	859.68	36.94132	YES	YES
76	a'	873.34	4.85290	YES	YES
77	a"	878.95	2.51659	YES	YES
78	a'	887.82	0.81651	YES	YES
79	a'	897.84	33.17414	YES	YES
80	a"	898.00	0.91120	YES	YES
81	a'	902.07	4.33980	YES	YES
82	a"	906.77	9.43539	YES	YES
83	a'	912.22	0.63127	YES	YES
84	a"	916.31	1.11739	YES	YES
85	a'	929.39	5.55053	YES	YES
86	a"	936.96	62.32097	YES	YES
87	a'	963.64	2.22181	YES	YES
88	a"	964.24	0.31486	YES	YES
89	a"	968.98	1.53016	YES	YES

90	a'	969.06	1.94780	YES	YES
91	a'	975.79	12.65700	YES	YES
92	a"	994.38	0.02660	YES	YES
93	a'	994.89	0.04212	YES	YES
94	a"	997.79	0.07156	YES	YES
95	a'	998.32	0.00859	YES	YES
96	a"	999.87	26.65218	YES	YES
97	a"	1016.37	0.59290	YES	YES
98	a'	1036.90	15.88029	YES	YES
99	a'	1057.88	0.01128	YES	YES
100	a"	1060.49	54.04221	YES	YES
101	a'	1078.06	7.11736	YES	YES
102	a'	1080.93	5.29622	YES	YES
103	a"	1080.99	1.11496	YES	YES
104	a"	1083.13	9.41325	YES	YES
105	a'	1087.20	43.14857	YES	YES
106	a"	1092.21	0.45707	YES	YES
107	a"	1125.36	0.39398	YES	YES
108	a'	1127.78	2.78954	YES	YES
109	a"	1130.03	18.66434	YES	YES
110	a'	1133.51	6.46367	YES	YES
111	a'	1143.73	3.70476	YES	YES
112	a"	1161.01	27.30965	YES	YES
113	a"	1162.41	0.73585	YES	YES
114	a'	1166.09	4.23923	YES	YES
115	a"	1181.78	0.00324	YES	YES
116	a'	1181.89	0.09173	YES	YES
117	a"	1182.38	0.03585	YES	YES
118	a'	1182.43	0.09540	YES	YES
119	a"	1220.49	3.50637	YES	YES
120	a'	1220.63	8.50177	YES	YES
121	a"	1228.84	0.37844	YES	YES
122	a'	1230.02	4.18069	YES	YES
123	a'	1232.85	5.15555	YES	YES
124	a"	1233.16	0.49641	YES	YES
125	a"	1249.65	2.36993	YES	YES
126	a'	1254.69	2.02296	YES	YES
127	a'	1257.30	0.54217	YES	YES
128	a"	1265.26	1.69688	YES	YES
129	a'	1287.11	5.62307	YES	YES
130	a"	1289.30	13.46150	YES	YES
131	a"	1300.63	2.04363	YES	YES
132	a'	1305.54	9.29179	YES	YES
133	a'	1340.44	2.26397	YES	YES
134	a"	1345.47	0.28897	YES	YES
135	a"	1357.08	1.47014	YES	YES
136	a'	1361.52	0.04596	YES	YES
137	a'	1373.33	1.98808	YES	YES
138	a"	1373.40	0.65599	YES	YES
139	a"	1384.11	2.07954	YES	YES
140	a'	1386.39	2.67448	YES	YES
141	a"	1394.76	3.21470	YES	YES
142	a'	1398.89	4.75056	YES	YES
143	a"	1416.86	0.59833	YES	YES
144	a'	1419.24	3.72432	YES	YES
145	a"	1454.17	5.22781	YES	YES
146	a'	1456.51	5.55446	YES	YES
147	a"	1486.54	1.76495	YES	YES
148	a"	1492.05	1.66647	YES	YES
149	a'	1495.05	4.76111	YES	YES
150	a"	1502.83	1.35674	YES	YES
151	a'	1507.64	13.57051	YES	YES

152	a'	1516.89	4.28202	YES	YES
153	a''	1519.50	78.60131	YES	YES
154	a'	1522.24	2.17200	YES	YES
155	a''	1533.26	24.23195	YES	YES
156	a'	1534.03	22.28288	YES	YES
157	a''	1534.82	2.96125	YES	YES
158	a'	1535.93	11.24958	YES	YES
159	a''	1638.86	0.25787	YES	YES
160	a'	1639.20	0.41087	YES	YES
161	a''	1642.50	2.63467	YES	YES
162	a'	1643.39	0.28628	YES	YES
163	a''	1666.76	0.56042	YES	YES
164	a'	1666.95	9.47359	YES	YES
165	a''	1670.72	20.83809	YES	YES
166	a'	1671.39	4.06468	YES	YES
167	a'	2177.93	76.09359	YES	YES
168	a''	3027.41	19.84803	YES	YES
169	a'	3027.72	27.80095	YES	YES
170	a''	3032.29	19.77995	YES	YES
171	a'	3045.37	80.56637	YES	YES
172	a''	3109.48	0.01623	YES	YES
173	a'	3127.67	6.46975	YES	YES
174	a''	3147.57	0.11954	YES	YES
175	a'	3148.04	6.15785	YES	YES
176	a'	3162.79	30.71033	YES	YES
177	a''	3163.37	5.28713	YES	YES
178	a''	3174.37	0.46153	YES	YES
179	a'	3174.39	2.38886	YES	YES
180	a''	3175.23	6.79607	YES	YES
181	a'	3175.29	18.99329	YES	YES
182	a''	3181.60	2.03004	YES	YES
183	a'	3181.82	2.31914	YES	YES
184	a''	3185.92	2.49351	YES	YES
185	a'	3185.96	1.42787	YES	YES
186	a''	3197.73	2.83453	YES	YES
187	a'	3197.85	23.18912	YES	YES
188	a''	3199.41	4.59515	YES	YES
189	a'	3199.46	27.70101	YES	YES
190	a''	3212.97	7.58028	YES	YES
191	a'	3213.03	39.27349	YES	YES
192	a''	3213.37	26.80645	YES	YES
193	a'	3213.45	11.18391	YES	YES
194	a''	3367.00	15.80524	YES	YES
195	a'	3375.03	87.23855	YES	YES

(1S,2R)-[Ru^{II}(Cl)(H)(tropdaetrop)] (C_s) (2a)

0.13361748908083	0.39960981062757	0.00000000000000	ru
-4.58042627511774	1.27085354241698	0.00000000000000	cl
2.83575420132232	-0.84033758148908	0.00000000000000	h
-0.64444786684067	-2.63741957656770	-2.49530243553764	n
-0.64444786684067	-2.63741957656770	2.49530243553764	n
-0.67621333566535	-2.02172786341754	-5.23872484603299	c
-1.34085651951171	-3.68545795367584	-6.27837204994571	h
-2.34856559490734	0.16905678764412	-5.93558857118776	c
-1.97460051201516	2.58727832588578	-4.90991287460446	c
-0.06449597740193	3.17210983294137	-2.97901198497494	c
-0.27943006063272	5.04715958891564	-2.17751358660223	h
2.39140336427748	2.12438729884598	-2.90275409694954	c
3.84039946516598	3.30910761736340	-2.06261823300690	h
3.42537302512629	0.40868468367669	-4.84008105527353	c
2.02095961747652	-1.51709750277738	-6.01122711615101	c

-3.54233208029797	4.53585213227569	-5.73776386120782	c
-3.29608944078345	6.40035805975879	-4.92621327719948	h
-5.40196198310910	4.14159304930352	-7.53294816721105	c
-6.58883764792040	5.70002214186534	-8.12880815922867	h
-5.75563218386490	1.75157256163222	-8.54115250429711	c
-7.21816085116990	1.41088046773558	-9.93187462873294	h
-4.22475046599485	-0.21139299531889	-7.73028192157460	c
-4.49275960249218	-2.09171796445202	-8.50435425814469	h
5.93630209869618	0.73189418586469	-5.58244147165249	c
7.04214191691130	2.20479396001836	-4.68350561624668	h
7.02730576865453	-0.75288473368909	-7.43869219878217	c
5.61847329470739	-2.62934727813193	-8.60394067719665	c
6.44987052477125	-3.80509160941211	-10.05838821612090	h
3.13186045247971	-2.99937620541340	-7.87343357276207	c
2.01926928631772	-4.47301387334401	-8.76506255306059	h
-0.67621333566535	-2.02172786341754	5.23872484603299	c
2.02095961747652	-1.51709750277738	6.01122711615101	c
3.42537302512629	0.40868468367669	4.84008105527353	c
2.39140336427748	2.12438729884598	2.90275409694954	c
3.84039946516598	3.30910761736340	2.06261823300690	h
-0.06449597740193	3.17210983294137	2.97901198497494	c
-0.27943006063272	5.04715958891564	2.17751358660223	h
-1.97460051201516	2.58727832588578	4.90991287460446	c
-2.34856559490734	0.16905678764412	5.93558857118776	c
5.93630209869618	0.73189418586469	5.58244147165249	c
7.02730576865453	-0.75288473368909	7.43869219878217	c
8.97812714841768	-0.44160868885941	7.97704383438164	h
5.61847329470739	-2.62934727813193	8.60394067719665	c
3.13186045247971	-2.99937620541340	7.87343357276207	c
2.01926928631772	-4.47301387334401	8.76506255306059	h
-3.54233208029797	4.53585213227569	5.73776386120782	c
-3.29608944078345	6.40035805975879	4.92621327719948	h
-5.40196198310910	4.14159304930352	7.53294816721105	c
-6.58883764792040	5.70002214186534	-8.12880815922867	h
-5.75563218386490	1.75157256163222	-8.54115250429711	c
-4.22475046599485	-0.21139299531889	-7.73028192157460	c
-4.49275960249218	-2.09171796445202	-8.50435425814469	h
-2.82166944755812	-4.05013619530677	1.46596864255829	c
-4.52128629262353	-3.09047275888970	2.11081232011003	h
-2.80647211982051	-5.98430670200694	2.20444521814169	h
-2.82166944755812	-4.05013619530677	-1.46596864255829	c
-2.80647211982051	-5.98430670200694	-2.20444521814169	h
-4.52128629262353	-3.09047275888970	-2.11081232011003	h
0.92260331196495	-3.71876167824206	-2.27765508269770	h
0.92260331196495	-3.71876167824206	2.27765508269770	h
8.97812714841768	-0.44160868885941	-7.97704383438164	h
-1.34085651951171	-3.68545795367584	6.27837204994571	h
7.04214191691130	2.20479396001836	4.68350561624668	h
6.44987052477125	-3.80509160941211	10.05838821612090	h
-7.21816085116990	1.41088046773558	9.93187462873294	h

vibrational spectrum

#	mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules
#				IR	RAMAN
1			0.00	0.00000	- -
2			0.00	0.00000	- -
3			0.00	0.00000	- -
4			0.00	0.00000	- -
5			0.00	0.00000	- -
6			0.00	0.00000	- -
7	a'		36.03	0.10615	YES YES
8	a"		37.77	0.04357	YES YES

9	a'	53.24	0.07302	YES	YES
10	a"	59.25	0.11005	YES	YES
11	a"	79.68	0.32572	YES	YES
12	a'	82.38	0.95326	YES	YES
13	a'	117.24	0.36310	YES	YES
14	a'	124.03	0.24325	YES	YES
15	a"	127.45	0.17004	YES	YES
16	a"	129.43	0.10942	YES	YES
17	a'	135.44	0.01912	YES	YES
18	a"	155.31	1.59525	YES	YES
19	a'	174.21	5.83142	YES	YES
20	a'	202.85	4.13286	YES	YES
21	a"	215.37	2.20988	YES	YES
22	a'	217.97	21.06769	YES	YES
23	a'	223.04	1.93854	YES	YES
24	a"	238.85	0.59864	YES	YES
25	a"	264.71	0.15971	YES	YES
26	a"	273.55	9.80542	YES	YES
27	a'	283.08	1.39940	YES	YES
28	a'	301.79	0.94549	YES	YES
29	a"	326.17	0.44044	YES	YES
30	a"	329.03	3.11945	YES	YES
31	a'	329.47	0.75805	YES	YES
32	a'	332.18	0.06974	YES	YES
33	a"	337.70	12.57667	YES	YES
34	a'	361.26	0.45300	YES	YES
35	a"	395.08	7.64310	YES	YES
36	a'	402.71	0.24259	YES	YES
37	a"	417.98	21.81144	YES	YES
38	a"	430.05	1.53269	YES	YES
39	a'	440.68	2.42633	YES	YES
40	a"	446.22	22.81786	YES	YES
41	a'	450.72	0.40818	YES	YES
42	a'	469.76	0.14158	YES	YES
43	a"	478.38	0.01639	YES	YES
44	a'	479.73	7.82962	YES	YES
45	a"	507.05	32.11034	YES	YES
46	a"	557.39	8.11594	YES	YES
47	a'	559.91	11.01777	YES	YES
48	a"	565.55	15.93377	YES	YES
49	a"	574.03	1.94464	YES	YES
50	a'	575.63	5.23158	YES	YES
51	a'	582.78	17.94691	YES	YES
52	a'	603.53	9.39606	YES	YES
53	a"	612.28	9.85611	YES	YES
54	a'	622.43	0.48969	YES	YES
55	a"	639.52	9.05211	YES	YES
56	a'	642.68	12.24129	YES	YES
57	a"	646.42	13.94725	YES	YES
58	a'	682.37	0.06275	YES	YES
59	a"	712.12	0.66464	YES	YES
60	a"	719.48	4.21048	YES	YES
61	a'	724.46	1.89026	YES	YES
62	a"	743.06	4.15712	YES	YES
63	a'	745.12	1.55966	YES	YES
64	a"	760.73	0.06773	YES	YES
65	a'	761.78	23.46703	YES	YES
66	a"	768.20	92.38604	YES	YES
67	a'	770.61	25.22825	YES	YES
68	a"	780.29	5.25529	YES	YES
69	a'	780.41	21.82033	YES	YES
70	a'	798.54	0.27615	YES	YES

71	a"	806.54	0.73945	YES	YES
72	a'	822.03	13.97461	YES	YES
73	a"	829.60	0.00007	YES	YES
74	a'	839.74	4.43874	YES	YES
75	a"	858.82	30.38400	YES	YES
76	a'	873.35	1.63334	YES	YES
77	a"	876.79	1.95612	YES	YES
78	a'	886.43	0.80818	YES	YES
79	a"	896.63	0.30800	YES	YES
80	a'	898.06	3.77352	YES	YES
81	a"	902.63	1.09196	YES	YES
82	a'	906.60	0.96142	YES	YES
83	a"	914.42	5.91050	YES	YES
84	a'	923.31	34.32898	YES	YES
85	a'	928.37	2.67023	YES	YES
86	a'	959.88	8.66430	YES	YES
87	a"	960.37	0.74848	YES	YES
88	a'	961.86	8.97356	YES	YES
89	a"	967.14	32.12219	YES	YES
90	a"	970.28	2.85822	YES	YES
91	a"	971.27	54.63228	YES	YES
92	a'	971.72	3.94797	YES	YES
93	a"	989.53	0.00114	YES	YES
94	a'	989.91	0.04285	YES	YES
95	a"	999.65	0.01366	YES	YES
96	a'	1000.15	0.04086	YES	YES
97	a"	1014.85	0.00085	YES	YES
98	a'	1020.03	12.73999	YES	YES
99	a'	1045.12	0.31351	YES	YES
100	a"	1055.30	66.84082	YES	YES
101	a'	1072.66	30.12619	YES	YES
102	a'	1078.51	5.61305	YES	YES
103	a"	1079.61	1.13131	YES	YES
104	a'	1083.13	3.44727	YES	YES
105	a"	1083.15	2.43292	YES	YES
106	a"	1088.57	0.41585	YES	YES
107	a'	1122.36	8.34437	YES	YES
108	a"	1124.67	0.00404	YES	YES
109	a'	1127.91	0.37733	YES	YES
110	a"	1129.70	8.88036	YES	YES
111	a'	1142.02	0.93543	YES	YES
112	a"	1162.00	13.55830	YES	YES
113	a"	1164.17	2.75889	YES	YES
114	a'	1166.09	5.18341	YES	YES
115	a"	1181.82	0.00053	YES	YES
116	a'	1181.89	0.09882	YES	YES
117	a"	1182.32	0.00000	YES	YES
118	a'	1182.34	0.10425	YES	YES
119	a'	1218.65	6.12718	YES	YES
120	a"	1218.72	2.04099	YES	YES
121	a"	1225.82	0.59982	YES	YES
122	a'	1226.24	11.36830	YES	YES
123	a'	1228.56	2.20294	YES	YES
124	a"	1228.93	1.20552	YES	YES
125	a"	1246.40	2.26111	YES	YES
126	a'	1252.70	0.04483	YES	YES
127	a'	1253.25	2.84062	YES	YES
128	a"	1261.90	4.84720	YES	YES
129	a'	1285.87	10.39634	YES	YES
130	a"	1287.26	8.80034	YES	YES
131	a"	1300.39	0.38450	YES	YES
132	a'	1308.66	9.83167	YES	YES

133	a'	1334.42	2.61708	YES	YES
134	a"	1339.97	0.19486	YES	YES
135	a"	1358.25	5.06610	YES	YES
136	a'	1363.03	2.26043	YES	YES
137	a"	1370.77	0.20999	YES	YES
138	a'	1371.03	1.11602	YES	YES
139	a"	1384.23	7.53013	YES	YES
140	a'	1386.76	4.54497	YES	YES
141	a"	1388.43	2.58335	YES	YES
142	a'	1395.39	3.89932	YES	YES
143	a"	1413.43	0.00041	YES	YES
144	a'	1415.63	4.83591	YES	YES
145	a"	1453.35	3.10764	YES	YES
146	a'	1455.80	5.90982	YES	YES
147	a"	1463.75	0.94097	YES	YES
148	a"	1479.92	17.07814	YES	YES
149	a'	1483.04	14.06071	YES	YES
150	a'	1492.70	4.62233	YES	YES
151	a"	1499.38	1.75928	YES	YES
152	a'	1511.33	9.22771	YES	YES
153	a"	1517.93	75.79436	YES	YES
154	a'	1520.29	7.86006	YES	YES
155	a"	1531.27	10.71617	YES	YES
156	a'	1532.24	26.12103	YES	YES
157	a"	1534.87	14.61961	YES	YES
158	a'	1535.77	5.49130	YES	YES
159	a"	1637.22	0.37931	YES	YES
160	a'	1637.63	0.47964	YES	YES
161	a"	1641.49	2.44137	YES	YES
162	a'	1642.21	0.28042	YES	YES
163	a"	1666.73	0.46666	YES	YES
164	a'	1666.92	8.74263	YES	YES
165	a"	1670.73	20.85232	YES	YES
166	a'	1671.39	4.59081	YES	YES
167	a'	2116.68	99.03851	YES	YES
168	a"	3028.38	8.03748	YES	YES
169	a'	3032.57	21.96657	YES	YES
170	a"	3032.67	35.01069	YES	YES
171	a'	3042.84	108.99059	YES	YES
172	a"	3143.97	0.00000	YES	YES
173	a'	3143.99	10.95639	YES	YES
174	a"	3145.96	0.47440	YES	YES
175	a'	3151.30	0.00093	YES	YES
176	a'	3162.84	27.99902	YES	YES
177	a"	3164.90	4.81864	YES	YES
178	a"	3172.22	2.64573	YES	YES
179	a'	3172.25	10.62150	YES	YES
180	a"	3176.58	4.43683	YES	YES
181	a'	3176.63	11.54311	YES	YES
182	a"	3182.64	1.79096	YES	YES
183	a'	3182.74	1.29119	YES	YES
184	a"	3185.99	2.38775	YES	YES
185	a'	3186.04	2.13084	YES	YES
186	a"	3198.25	2.57010	YES	YES
187	a'	3198.32	22.36651	YES	YES
188	a"	3199.21	5.38425	YES	YES
189	a'	3199.28	30.19561	YES	YES
190	a"	3212.89	13.48282	YES	YES
191	a'	3212.95	40.20184	YES	YES
192	a"	3213.27	21.06304	YES	YES
193	a'	3213.35	11.91754	YES	YES
194	a"	3520.89	0.49524	YES	YES

195	a'	3524.42	10.61336	YES	YES
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(1S,2R)-[Ru^{II}(H)(Cl)(*tropdaprop*)] (*C_s*) (3**)**

0.29691660004142	-0.45639552257960	0.0000000000000000	ru
-0.82936406251186	-5.08445164622870	0.0000000000000000	cl
-1.75462764010951	-0.30829084635176	-5.59653706684393	c
1.62481013291196	2.88774137761334	-4.66626473657688	c
2.77078483431097	1.24953633971451	-2.73934713328802	c
3.01554326390179	-1.41326735520216	-2.88006466271353	c
2.14154858725347	-2.98194449298685	-4.98791711435761	c
-0.07632340153617	-2.47611201054981	-6.33636429674890	c
2.72226658136797	5.23840751117589	-5.14359900509880	c
1.75680364562226	6.85586070130058	-6.95837531475315	c
-0.35563312288057	6.15321749476607	-8.34111205231511	c
-1.47730228194224	3.83331454505384	-7.87485513997024	c
3.58795089039171	-5.06625572579912	-5.70586093381329	c
2.90035655661162	-6.57724597912409	-7.72488487435487	c
0.71769553803085	-6.04297808534981	-9.07315515549011	c
-0.75902131989656	-4.00306333379054	-8.35927604452121	c
-1.75462764010951	-0.30829084635176	5.59653706684393	c
-0.07632340153617	-2.47611201054981	6.33636429674890	c
2.14154858725347	-2.98194449298685	4.98791711435761	c
3.01554326390179	-1.41326735520216	2.88006466271353	c
2.77078483431097	1.24953633971451	2.73934713328802	c
1.62481013291196	2.88774137761334	4.66626473657688	c
-0.51743627260863	2.20225906155066	6.05609887735642	c
3.58795089039171	-5.06625572579912	5.70586093381329	c
2.90035655661162	-6.57724597912409	7.72488487435487	c
0.71769553803085	-6.04297808534981	9.07315515549011	c
-0.75902131989656	-4.00306333379054	8.35927604452121	c
2.72226658136797	5.23840751117589	5.14359900509880	c
1.75680364562226	6.85586070130058	6.95837531475315	c
-0.35563312288057	6.15321749476607	8.34111205231511	c
-1.47730228194224	3.83331454505384	7.87485513997024	c
-2.59543873815530	-0.57316725770103	-2.92816376738645	n
-2.59543873815530	-0.57316725770103	2.92816376738645	n
-3.06355745413184	-2.43472758460473	-2.68454766128329	h
-3.06355745413184	-2.43472758460473	2.68454766128329	h
-0.51743627260863	2.20225906155066	-6.05609887735642	c
-4.82266372606657	1.00084550590612	-2.43905617784025	c
-6.16483692233806	0.32935241691241	0.0000000000000000	c
-4.82266372606657	1.00084550590612	2.43905617784025	c
-3.44480233574095	-0.40072484271553	-6.79214621247246	h
4.30554159236119	2.20532749892540	-1.77687659625723	h
4.67677366507569	-2.19223993074734	-1.96423687432023	h
4.37946635712056	5.78942364117816	-4.07055876179992	h
2.65443757775214	8.66539710126624	-7.29343104461878	h
-1.13210827010081	7.40548475897619	-9.76184928853486	h
-3.13755768487189	3.27207990066570	-8.93962148183001	h
5.28793828655093	-5.49532341260300	-4.64613937036545	h
4.06407231097621	-8.18109863157495	-8.24024229506830	h
0.15407576623217	-7.21969354174254	-10.65013895076133	h
-2.48760299777207	-3.59100735199264	-9.38283166014396	h
-3.44480233574095	-0.40072484271553	6.79214621247246	h
4.67677366507569	-2.19223993074734	1.96423687432023	h
4.30554159236119	2.20532749892540	1.77687659625723	h
5.28793828655093	-5.49532341260300	4.64613937036545	h
4.06407231097621	-8.18109863157495	8.24024229506830	h
0.15407576623217	-7.21969354174254	10.65013895076133	h
-2.48760299777207	-3.59100735199264	9.38283166014396	h

4.37946635712056	5.78942364117816	4.07055876179992	h
2.65443757775214	8.66539710126624	7.29343104461878	h
-1.13210827010081	7.40548475897619	9.76184928853486	h
-3.13755768487189	3.27207990066570	8.93962148183001	h
-6.16564619368158	0.77412609588082	-4.00411887925412	h
-4.22737290011168	2.97649270419361	-2.42737969242701	h
-6.63670239981201	-1.68785314542385	0.0000000000000000	h
-7.96992585758113	1.33444306528585	0.0000000000000000	h
-6.16564619368158	0.77412609588082	4.00411887925412	h
-4.22737290011168	2.97649270419361	2.42737969242701	h
-0.18202985152861	2.46015712137109	0.0000000000000000	h

vibrational spectrum

#	mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules
#				IR	RAMAN
1			0.00	0.00000	- -
2			0.00	0.00000	- -
3			0.00	0.00000	- -
4			0.00	0.00000	- -
5			0.00	0.00000	- -
6			0.00	0.00000	- -
7	a"		27.48	0.15700	YES YES
8	a'		33.45	0.03148	YES YES
9	a'		51.71	0.13623	YES YES
10	a"		57.88	0.14229	YES YES
11	a"		71.07	0.38762	YES YES
12	a'		77.85	2.53105	YES YES
13	a'		100.64	1.32298	YES YES
14	a'		123.35	0.42124	YES YES
15	a'		128.04	0.49614	YES YES
16	a"		128.40	0.02551	YES YES
17	a"		129.84	0.31370	YES YES
18	a'		140.59	1.37241	YES YES
19	a"		149.41	1.89241	YES YES
20	a"		157.01	2.05491	YES YES
21	a'		174.46	6.42939	YES YES
22	a'		189.97	0.58621	YES YES
23	a"		232.92	0.65030	YES YES
24	a'		242.40	15.74649	YES YES
25	a"		258.67	0.14757	YES YES
26	a"		262.23	2.43103	YES YES
27	a'		274.89	4.16864	YES YES
28	a'		287.59	1.48025	YES YES
29	a'		294.93	2.34793	YES YES
30	a"		304.75	6.99741	YES YES
31	a"		324.94	1.01798	YES YES
32	a"		328.19	7.56078	YES YES
33	a'		328.31	1.20380	YES YES
34	a'		333.22	0.56157	YES YES
35	a'		351.69	0.68141	YES YES
36	a"		353.41	4.23291	YES YES
37	a"		403.30	0.02637	YES YES
38	a'		404.77	0.31424	YES YES
39	a'		422.32	0.00999	YES YES
40	a"		429.20	38.23669	YES YES
41	a'		451.39	1.07771	YES YES
42	a"		454.28	5.45404	YES YES
43	a'		455.55	3.08049	YES YES
44	a"		471.54	11.73012	YES YES
45	a'		479.83	6.47961	YES YES
46	a"		482.44	5.01396	YES YES
47	a'		502.54	10.47021	YES YES

48	a"	546.36	48.32716	YES	YES
49	a"	558.22	4.49791	YES	YES
50	a'	563.85	17.73246	YES	YES
51	a"	573.21	0.28238	YES	YES
52	a'	574.26	3.48600	YES	YES
53	a'	587.85	4.94743	YES	YES
54	a'	601.29	5.18499	YES	YES
55	a"	603.73	0.00009	YES	YES
56	a"	626.11	12.04676	YES	YES
57	a'	633.06	7.19046	YES	YES
58	a'	646.99	9.54515	YES	YES
59	a"	647.55	2.59592	YES	YES
60	a'	691.05	0.62001	YES	YES
61	a"	694.64	1.59297	YES	YES
62	a"	721.12	0.04610	YES	YES
63	a'	721.73	0.19630	YES	YES
64	a"	748.42	12.00245	YES	YES
65	a'	753.25	6.66677	YES	YES
66	a"	764.78	0.53765	YES	YES
67	a'	766.18	26.52688	YES	YES
68	a"	771.05	74.20821	YES	YES
69	a'	773.45	42.04559	YES	YES
70	a'	784.53	15.11229	YES	YES
71	a"	785.26	1.52196	YES	YES
72	a'	796.16	2.86535	YES	YES
73	a"	800.43	1.84615	YES	YES
74	a'	832.75	32.35835	YES	YES
75	a"	836.48	0.49040	YES	YES
76	a'	846.32	2.49953	YES	YES
77	a'	852.79	20.68457	YES	YES
78	a"	865.89	67.53176	YES	YES
79	a"	879.24	3.07601	YES	YES
80	a"	884.27	35.45693	YES	YES
81	a'	886.21	0.37744	YES	YES
82	a'	890.72	0.02313	YES	YES
83	a"	897.23	0.45688	YES	YES
84	a'	901.41	0.71135	YES	YES
85	a"	909.76	8.41577	YES	YES
86	a"	912.73	1.82322	YES	YES
87	a'	918.02	0.91833	YES	YES
88	a"	919.56	2.70015	YES	YES
89	a'	950.24	3.32311	YES	YES
90	a'	957.88	0.04503	YES	YES
91	a"	963.35	0.53806	YES	YES
92	a'	965.45	0.81000	YES	YES
93	a"	969.22	2.08299	YES	YES
94	a'	974.22	3.20865	YES	YES
95	a"	993.19	0.04628	YES	YES
96	a'	993.79	0.07559	YES	YES
97	a"	997.81	0.23891	YES	YES
98	a'	998.39	0.01717	YES	YES
99	a"	1017.82	43.27658	YES	YES
100	a"	1024.00	1.78829	YES	YES
101	a'	1043.82	40.81194	YES	YES
102	a"	1044.26	45.90926	YES	YES
103	a'	1069.99	6.39730	YES	YES
104	a"	1070.54	17.00508	YES	YES
105	a'	1079.32	6.21792	YES	YES
106	a"	1079.79	1.41658	YES	YES
107	a"	1080.07	1.87995	YES	YES
108	a'	1081.74	2.34294	YES	YES
109	a'	1087.80	7.96352	YES	YES

110	a'	1123.26	36.72509	YES	YES
111	a"	1126.19	1.15386	YES	YES
112	a'	1134.05	12.25002	YES	YES
113	a"	1140.28	0.13673	YES	YES
114	a'	1141.95	0.69409	YES	YES
115	a"	1146.38	0.32283	YES	YES
116	a"	1160.59	13.56943	YES	YES
117	a'	1166.98	2.43017	YES	YES
118	a'	1179.72	0.33896	YES	YES
119	a"	1181.30	0.00260	YES	YES
120	a'	1181.43	0.13389	YES	YES
121	a"	1181.71	0.00002	YES	YES
122	a'	1182.11	0.01794	YES	YES
123	a"	1222.08	9.18766	YES	YES
124	a"	1228.37	1.22140	YES	YES
125	a'	1228.67	11.82632	YES	YES
126	a"	1234.04	0.42438	YES	YES
127	a'	1234.49	3.56819	YES	YES
128	a"	1241.48	6.69369	YES	YES
129	a'	1246.98	1.69328	YES	YES
130	a"	1254.23	0.81256	YES	YES
131	a'	1267.50	0.96832	YES	YES
132	a'	1269.35	0.14041	YES	YES
133	a"	1276.04	8.26463	YES	YES
134	a"	1292.13	0.01314	YES	YES
135	a'	1298.15	7.17521	YES	YES
136	a"	1306.66	1.15068	YES	YES
137	a'	1312.68	11.48112	YES	YES
138	a'	1351.80	0.93946	YES	YES
139	a"	1353.82	0.07748	YES	YES
140	a"	1362.35	1.41663	YES	YES
141	a'	1366.01	1.34430	YES	YES
142	a"	1378.00	0.17309	YES	YES
143	a'	1380.38	3.47967	YES	YES
144	a"	1385.39	0.87962	YES	YES
145	a'	1386.76	6.04334	YES	YES
146	a"	1399.80	0.79364	YES	YES
147	a'	1415.40	1.03352	YES	YES
148	a"	1416.64	3.78786	YES	YES
149	a"	1420.89	0.01242	YES	YES
150	a'	1425.67	3.58523	YES	YES
151	a"	1454.08	4.47473	YES	YES
152	a'	1456.97	1.22041	YES	YES
153	a'	1463.38	17.32876	YES	YES
154	a"	1487.26	0.85649	YES	YES
155	a"	1494.11	4.03995	YES	YES
156	a'	1496.23	8.03128	YES	YES
157	a'	1501.56	10.19838	YES	YES
158	a"	1504.06	1.33836	YES	YES
159	a'	1511.13	20.43793	YES	YES
160	a"	1521.47	61.60468	YES	YES
161	a'	1525.56	1.06691	YES	YES
162	a"	1536.62	35.49646	YES	YES
163	a'	1537.70	13.88875	YES	YES
164	a"	1538.89	2.18855	YES	YES
165	a'	1539.72	19.36856	YES	YES
166	a"	1643.70	0.08827	YES	YES
167	a'	1644.36	0.84332	YES	YES
168	a"	1646.88	3.47830	YES	YES
169	a'	1648.24	0.09179	YES	YES
170	a"	1667.96	0.06052	YES	YES
171	a'	1668.15	7.80012	YES	YES

172	a"	1671.26	16.86811	YES	YES
173	a'	1672.09	4.25292	YES	YES
174	a'	2169.55	67.98330	YES	YES
175	a'	3009.13	36.78378	YES	YES
176	a"	3010.23	38.59223	YES	YES
177	a"	3023.16	41.17029	YES	YES
178	a'	3023.43	39.37749	YES	YES
179	a'	3038.51	17.87409	YES	YES
180	a'	3088.03	19.43334	YES	YES
181	a"	3099.36	0.39576	YES	YES
182	a'	3105.46	19.49146	YES	YES
183	a"	3148.82	0.50493	YES	YES
184	a'	3151.66	6.92438	YES	YES
185	a"	3164.75	7.15865	YES	YES
186	a'	3169.07	26.92857	YES	YES
187	a"	3174.55	1.54379	YES	YES
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189	a"	3175.69	8.79983	YES	YES
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192	a'	3181.74	2.26415	YES	YES
193	a"	3185.34	2.60629	YES	YES
194	a'	3185.42	1.58094	YES	YES
195	a"	3197.48	4.86019	YES	YES
196	a'	3197.59	22.06567	YES	YES
197	a"	3198.98	7.40203	YES	YES
198	a'	3199.06	25.59672	YES	YES
199	a"	3212.61	10.70147	YES	YES
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201	a"	3213.13	23.22621	YES	YES
202	a'	3213.21	16.36571	YES	YES
203	a"	3376.07	20.83319	YES	YES
204	a'	3381.77	67.83260	YES	YES

(1S,2R)-[Ru^{II}(Cl)(H)(tropdaprop)] (C_s) (3a**)**

0.33292563306162	0.14332594220779	0.000000000000000	ru
0.26902138402325	-2.82899134833107	0.000000000000000	h
-1.75658404765202	-0.31451450666038	-5.56091069119879	c
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2.86115012793848	1.47816378915300	-2.89607023394275	c
3.00907143210197	-1.18837280032868	-2.76372057011888	c
2.11212220938512	-2.94809443451118	-4.71613396048599	c
-0.10894306828325	-2.56212387320787	-6.10155492472818	c
2.81085900816299	5.19296537557352	-5.68921977287173	c
1.83431349132391	6.63160457219113	-7.64061161011206	c
-0.31331021509361	5.82787893790006	-8.90769443296091	c
-1.45480975968618	3.58483015671226	-8.18871628290755	c
3.54887355608360	-5.09825784924479	-5.23954328454581	c
2.84085758430214	-6.79996061942198	-7.09480499656950	c
0.64947845911450	-6.39170688558622	-8.47365758156016	c
-0.81103897105951	-4.28039949306815	-7.96000849300156	c
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1.69977199599101	2.91652782664867	4.96102941784397	c
-0.47881515453020	2.12672625572525	6.23668756215662	c
3.54887355608360	-5.09825784924479	5.23954328454581	c
2.84085758430214	-6.79996061942198	7.09480499656950	c

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-0.81103897105951	-4.28039949306815	7.96000849300156	c
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-1.45480975968618	3.58483015671226	8.18871628290755	c
-2.60353397221298	-0.41757487173311	-2.87561339563704	n
-2.60353397221298	-0.41757487173311	2.87561339563704	n
-3.04103347588393	-2.26307990713335	-2.58214310089313	h
-3.04103347588393	-2.26307990713335	2.58214310089313	h
-0.47881515453020	2.12672625572525	-6.23668756215662	c
-4.92628767164010	1.05390665060516	-2.45527900789148	c
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-4.92628767164010	1.05390665060516	2.45527900789148	c
-3.44541100173350	-0.4809711072448	-6.74931927898300	h
4.39131736193645	2.50073874465637	-1.99288972727053	h
4.66557760860021	-1.92005397141457	-1.80533129160681	h
4.47228900717583	5.84063402854756	-4.68150494078113	h
2.74115138240564	8.39201563197972	-8.16111048234425	h
-1.10638616750240	6.94653500298838	-10.42730625205327	h
-3.14801562090220	2.94991253690019	-9.15629864156481	h
5.26763889526423	-5.41876968493788	-4.16999300130387	h
4.00114004603047	-8.44581071753844	-7.46537795766491	h
0.07433489798639	-7.71218074816127	-9.92789126079918	h
-2.53472834364202	-3.95170435649619	-9.02095073342489	h
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0.07433489798639	-7.71218074816127	9.92789126079918	h
-2.53472834364202	-3.95170435649619	9.02095073342489	h
4.47228900717583	5.84063402854756	4.68150494078113	h
2.74115138240564	8.39201563197972	8.16111048234425	h
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-3.14801562090220	2.94991253690019	9.15629864156481	h
-6.23676803893891	0.69129657343736	-4.02113226587652	h
-4.41877870702698	3.04952876509605	-2.46447835900121	h
-6.65897004203260	-1.68663637512916	0.000000000000000	h
-8.07232520313059	1.29158485033028	0.000000000000000	h
-6.23676803893891	0.69129657343736	4.02113226587652	h
-4.41877870702698	3.04952876509605	2.46447835900121	h
-0.82719950304387	4.75326884151300	0.000000000000000	cl

vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules
#				IR	RAMAN
1			0.00	0.00000	- -
2			0.00	0.00000	- -
3			0.00	0.00000	- -
4			0.00	0.00000	- -
5			0.00	0.00000	- -
6			0.00	0.00000	- -
7	a"		27.61	0.07954	YES YES
8	a'		30.54	0.05289	YES YES
9	a'		52.69	0.09311	YES YES
10	a"		57.86	0.09852	YES YES
11	a'		72.54	1.33835	YES YES
12	a"		73.18	0.38401	YES YES
13	a'		114.73	0.21674	YES YES
14	a'		123.00	0.28752	YES YES
15	a"		124.44	0.19467	YES YES
16	a"		128.59	0.03736	YES YES

17	a'	131.45	0.04740	YES	YES
18	a"	151.38	1.34102	YES	YES
19	a'	169.09	1.62380	YES	YES
20	a'	176.67	6.63116	YES	YES
21	a'	190.72	1.77068	YES	YES
22	a"	209.84	1.34421	YES	YES
23	a'	227.00	18.85669	YES	YES
24	a"	230.29	1.41994	YES	YES
25	a"	260.16	1.37335	YES	YES
26	a"	273.06	1.73425	YES	YES
27	a'	274.84	2.90070	YES	YES
28	a'	291.78	1.91557	YES	YES
29	a"	300.55	8.67313	YES	YES
30	a'	308.81	0.65731	YES	YES
31	a"	324.78	0.05131	YES	YES
32	a'	327.05	1.00342	YES	YES
33	a"	327.24	8.03720	YES	YES
34	a'	331.91	0.16721	YES	YES
35	a'	349.84	0.05112	YES	YES
36	a"	358.52	3.47142	YES	YES
37	a"	399.21	6.16974	YES	YES
38	a'	408.51	0.18347	YES	YES
39	a'	419.83	0.01445	YES	YES
40	a"	423.02	16.93997	YES	YES
41	a'	443.74	1.80936	YES	YES
42	a"	444.14	23.19426	YES	YES
43	a'	452.63	2.04553	YES	YES
44	a"	469.74	11.20474	YES	YES
45	a'	480.04	7.56026	YES	YES
46	a"	480.06	2.20895	YES	YES
47	a'	503.13	6.31162	YES	YES
48	a"	546.85	46.65069	YES	YES
49	a"	556.62	8.69269	YES	YES
50	a'	564.65	15.17741	YES	YES
51	a"	573.72	0.65475	YES	YES
52	a'	575.72	6.18923	YES	YES
53	a'	583.07	9.50673	YES	YES
54	a'	600.69	8.68792	YES	YES
55	a"	604.30	6.18971	YES	YES
56	a"	623.68	0.95251	YES	YES
57	a'	628.71	2.81963	YES	YES
58	a'	645.20	12.01539	YES	YES
59	a"	645.26	3.49069	YES	YES
60	a'	685.27	0.05830	YES	YES
61	a"	690.51	2.64759	YES	YES
62	a"	721.02	0.97437	YES	YES
63	a'	723.88	1.08485	YES	YES
64	a"	746.30	11.02656	YES	YES
65	a'	751.72	4.97016	YES	YES
66	a"	763.74	1.37661	YES	YES
67	a'	764.98	27.70568	YES	YES
68	a"	770.63	76.95389	YES	YES
69	a'	772.95	35.92794	YES	YES
70	a"	782.42	1.69682	YES	YES
71	a'	783.23	15.47881	YES	YES
72	a'	795.66	1.09433	YES	YES
73	a"	800.71	1.37114	YES	YES
74	a"	832.67	0.00938	YES	YES
75	a'	834.19	9.98366	YES	YES
76	a'	848.76	1.55652	YES	YES
77	a"	872.27	25.67184	YES	YES
78	a"	877.68	1.25420	YES	YES

79	a'	881.82	2.27110	YES	YES
80	a'	888.15	0.71522	YES	YES
81	a"	895.00	24.61654	YES	YES
82	a"	897.97	6.04565	YES	YES
83	a'	899.67	19.30924	YES	YES
84	a'	905.32	24.84606	YES	YES
85	a"	906.52	1.54920	YES	YES
86	a"	915.12	17.90348	YES	YES
87	a'	915.69	1.43266	YES	YES
88	a"	930.11	28.45552	YES	YES
89	a'	941.44	7.23225	YES	YES
90	a'	953.71	0.90445	YES	YES
91	a"	962.45	1.47194	YES	YES
92	a'	964.91	1.15411	YES	YES
93	a"	968.76	3.06715	YES	YES
94	a'	972.40	2.78567	YES	YES
95	a"	991.55	0.30871	YES	YES
96	a'	992.11	0.07638	YES	YES
97	a"	998.76	0.38782	YES	YES
98	a'	999.33	0.01156	YES	YES
99	a"	1007.42	55.13930	YES	YES
100	a'	1021.50	37.75962	YES	YES
101	a"	1025.04	0.03353	YES	YES
102	a"	1042.93	24.89988	YES	YES
103	a"	1063.89	2.20039	YES	YES
104	a'	1066.51	9.43421	YES	YES
105	a"	1077.52	0.06250	YES	YES
106	a'	1077.75	0.40376	YES	YES
107	a'	1079.06	9.50701	YES	YES
108	a"	1081.17	0.39088	YES	YES
109	a'	1085.76	3.19285	YES	YES
110	a'	1114.27	33.07334	YES	YES
111	a"	1125.43	0.11486	YES	YES
112	a'	1132.00	1.90496	YES	YES
113	a"	1136.50	0.11169	YES	YES
114	a'	1139.97	2.01585	YES	YES
115	a"	1139.97	0.19191	YES	YES
116	a"	1161.56	11.72704	YES	YES
117	a'	1167.43	4.10194	YES	YES
118	a'	1181.18	3.50911	YES	YES
119	a"	1181.35	0.00840	YES	YES
120	a'	1181.49	0.06368	YES	YES
121	a"	1181.82	0.03132	YES	YES
122	a'	1183.17	3.62302	YES	YES
123	a"	1222.45	7.56013	YES	YES
124	a'	1228.26	10.29711	YES	YES
125	a"	1228.35	0.55561	YES	YES
126	a"	1233.22	0.30702	YES	YES
127	a'	1234.08	5.12868	YES	YES
128	a"	1241.45	1.50030	YES	YES
129	a'	1245.48	2.91479	YES	YES
130	a"	1252.26	1.22555	YES	YES
131	a'	1264.43	0.10380	YES	YES
132	a'	1268.62	0.83604	YES	YES
133	a"	1276.38	5.25387	YES	YES
134	a"	1291.16	0.32853	YES	YES
135	a'	1299.52	14.43709	YES	YES
136	a"	1303.77	0.48409	YES	YES
137	a'	1321.21	4.78151	YES	YES
138	a'	1347.87	0.96375	YES	YES
139	a"	1351.15	0.09350	YES	YES
140	a"	1363.82	4.87653	YES	YES

141	a'	1368.49	1.72178	YES	YES
142	a"	1375.99	0.10674	YES	YES
143	a'	1377.92	1.79236	YES	YES
144	a"	1386.13	3.06737	YES	YES
145	a'	1388.91	7.48332	YES	YES
146	a"	1395.60	1.68433	YES	YES
147	a'	1412.99	1.56349	YES	YES
148	a"	1415.17	1.21132	YES	YES
149	a"	1420.37	0.19102	YES	YES
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151	a"	1454.76	1.18220	YES	YES
152	a'	1456.49	0.06852	YES	YES
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156	a'	1488.19	27.76119	YES	YES
157	a'	1489.43	3.89739	YES	YES
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159	a'	1503.76	4.65349	YES	YES
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161	a'	1525.88	4.29963	YES	YES
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163	a'	1535.61	19.39602	YES	YES
164	a"	1537.91	12.24768	YES	YES
165	a'	1538.35	13.37545	YES	YES
166	a"	1642.13	0.11872	YES	YES
167	a'	1642.85	0.82816	YES	YES
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169	a'	1646.81	0.17116	YES	YES
170	a"	1666.52	1.17944	YES	YES
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172	a"	1670.76	16.18826	YES	YES
173	a'	1671.49	4.82109	YES	YES
174	a'	2116.87	97.53446	YES	YES
175	a'	2995.65	19.46204	YES	YES
176	a"	3013.76	44.93901	YES	YES
177	a'	3015.24	58.26689	YES	YES
178	a"	3027.60	41.94343	YES	YES
179	a'	3027.93	45.09042	YES	YES
180	a'	3088.74	17.92844	YES	YES
181	a"	3124.18	0.24182	YES	YES
182	a'	3127.62	3.95222	YES	YES
183	a"	3150.90	0.03657	YES	YES
184	a'	3153.68	5.99499	YES	YES
185	a"	3166.31	7.03540	YES	YES
186	a'	3168.48	28.87500	YES	YES
187	a"	3172.99	3.03457	YES	YES
188	a'	3173.02	8.46400	YES	YES
189	a"	3176.33	6.85846	YES	YES
190	a'	3176.41	12.75504	YES	YES
191	a"	3181.83	2.05208	YES	YES
192	a'	3182.06	1.77519	YES	YES
193	a"	3186.62	2.10927	YES	YES
194	a'	3186.68	2.41045	YES	YES
195	a"	3197.90	4.42912	YES	YES
196	a'	3198.00	21.93240	YES	YES
197	a"	3199.46	9.19490	YES	YES
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199	a"	3212.74	12.04251	YES	YES
200	a'	3212.79	42.54681	YES	YES
201	a"	3213.03	20.93747	YES	YES
202	a'	3213.12	11.01306	YES	YES

203	a"	3506.48	0.18438	YES	YES
204	a'	3507.31	6.85256	YES	YES

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