

Supporting Information

Metal-mediated rearrangement of 1,2-diphenylhydrazine to *ortho*-semidine upon reaction with dichlorotris(triphenylphosphine)ruthenium(II)

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1. General considerations, materials, and methods

General Considerations and Materials

All reactions and manipulations were performed under anaerobic conditions employing either a nitrogen-filled glove box or standard Schlenk techniques. $\text{RuCl}_2(\text{PPh}_3)_3$ was prepared according to literature methods.¹ 2-aminodiphenylamine (*ortho*-semidine) was purchased from Sigma-Aldrich and used as received. 1,2-Diphenylhydrazine was purchased from TCI America and used as received. Solvents were obtained commercially, degassed, dried, and stored over molecular sieves or passed through a solvent purification system.

Physical Measurements

NMR data were obtained on a Bruker Avance III HD 400 MHz spectrometer. ^1H and $^{13}\text{C}\{^1\text{H}\}$ spectra were recorded in CDCl_3 and referenced internally to residual solvent. $^{31}\text{P}\{^1\text{H}\}$ spectra were referenced externally to 85% H_3PO_4 in D_2O . FTIR data were obtained on a Thermo Nicolet iS50 equipped with an ATR accessory with the following instrument parameters: 32 scans, 525-4000 cm^{-1} range, 4 cm^{-1} resolution. UV-vis data were collected on a Shimadzu 3101PC spectrophotometer using dichloromethane as solvent and a 1 cm cuvette at 25 °C under inert conditions. Melting points were obtained on a Stanford Research Systems MPA100 automated melting point system at a heating rate of 2 °C min^{-1} .

Computational Methods

The structures and gas-phase relative Gibbs free energies of reactants and products were calculated using density functional theory (DFT) methods. All calculations were performed using the PBE0 hybrid functional,² paired with the def2-TZVPPD basis set^{3,4} for all atoms and the Stuttgart quasi-relativistic pseudopotential⁵ for ruthenium.⁶⁻⁹ All molecular structures were fully optimized and confirmed as local minima or first-order transition states via diagonalization of the mass-weighted energy second derivatives with respect to nuclear coordinates (*i.e.* the Hessian matrix). Relative Gibbs free energies at 298.15 K were calculated at all stationary points, with thermal and entropic corrections obtained from standard rigid-rotor, harmonic oscillator approximations,¹⁰ using unscaled harmonic vibrational frequencies. All calculations were performed using the GAMESS quantum chemistry program.¹¹⁻¹³ The structures of **1** and **1b-1g** were reoptimized using the Solvation Model Density (SMD) method¹⁴ implemented within the Polarizable Continuum Model (PCM)^{15,16} to capture effects of solvation in chloroform, CHCl_3 . In addition, the structures of **1** and **1g** were optimized using SMD/PCM with toluene as the solvent. Relative free energies in solution were approximated by combining SMD/PCM relative electronic energies with the gas phase zero point, thermal, and entropic corrections.

Single-Crystal X-ray Diffraction

Crystals of α -**1** and β -**1** were grown as outlined below under inert atmosphere. Once obtained, the crystals were removed from the mother liquor, submersed in an inert oil, and examined microscopically. A suitable crystal was then placed in the 100 K nitrogen cold

stream provided by an Oxford Cryosystems Industries low-temperature apparatus on the goniometer head of a Bruker Apex II diffractometer equipped with a CCD detector and Mo K α radiation ($\lambda = 0.71073 \text{ \AA}$) from a fine-focus sealed tube. All data sets were reduced using Bruker SAINT, and a multi-scan absorption correction was applied using SADABS.¹⁷ Structure solution and refinement were conducted employing SHELXT-2015 and SHELXL-2018, respectively.^{18,19} CCDC 2201044 and 2201045 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif, or by emailing data_request@ccdc.cam.ac.uk, or by contacting The Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44 1223 336033.

Powder X-ray Diffraction

Powder samples were analyzed at room temperature using a Bruker D8 ADVANCE ECO equipped with a Cu-K α ($\lambda = 1.5418 \text{ \AA}$) and a LYNXEYE compound silicon strip detector, and Soller slits and a Nickel K β filter. Samples were prepared by grinding the material into a fine powder form. To run samples in an air-free environment sample was plated between double-sided Kapton® tape and Kapton® film on a poly(methyl methacrylate) (PMMA) sample holder. Data acquisition was conducted while rotating the sample at 30 rpm, and the pattern was acquired from 5–105° 2θ at 2.0° $2\theta \text{ min}^{-1}$, with an integration step size of 0.01° 2θ .

2. Synthesis

RuCl₂(PPh₃)₂(κ²-NH₂-1,2-C₆H₄-NHPPh) (1)

Method 1: A 50 mL flask equipped with a stir bar was charged with RuCl₂(PPh₃)₃ (200 mg, 0.209 mmol) and 1,2-diphenylhydrazine (46 mg, 0.25 mmol). Toluene (15 mL) was added, producing an orange solution. The solution was allowed to stir overnight. The solvent was removed *in vacuo* and the crude solid was suspended in Et₂O (10 mL), filtered, and washed with additional Et₂O (2 x 5 mL) to produce the orange solid product (141 mg, 76%). Single crystals (orange blocks) suitable for X-ray diffraction were obtained by vapor diffusion of pentane into a toluene solution. Mp: 89 °C (decomp.). ¹H NMR (400 MHz, CDCl₃): δ 7.43 (b, 12H, Ar CH), 7.28 (t, 6H, Ar CH, *J* = 7.2 Hz), 7.09 (t, 14H, Ar CH, *J* = 7.5 Hz), 6.93 (m, 6H, Ar CH and NH), 6.14 (b, 2H, Ar CH), 4.70 (b, 2H, NH₂). ¹³C{¹H} NMR (101 MHz, CDCl₃, 298 K): δ 147.17, 139.98, 135.42, 135.09, 135.05, 135.00, 129.24, 128.51, 127.61, 127.57, 127.52, 127.01, 126.84, 124.19 ppm. ³¹P{¹H} NMR (162 MHz, CDCl₃, 298 K): δ 44.3 ppm. ³¹P{¹H} NMR (162 MHz, CDCl₃, 218 K): δ 48.0 ppm (²*J*_{P,P} = 37 Hz), 38.2 ppm (²*J*_{P,P} = 37 Hz). FTIR (cm⁻¹): 3304w (v, N-H), 3247w (v, N-H), 3051w (v, C-H), 2227w, 1979w, 1617w, 1594w, 1572w, 1535w, 1493m, 1481m, 1469w, 1432m, 1366w, 1313w, 1269w, 1230w, 1191w, 1157w, 1114w, 1087m, 1050w, 1029w, 907m, 856w, 727s, 692s, 645w, 584w. UV/vis [chloroform; λ_{max}, nm (ε, M⁻¹ cm⁻¹): 492 (3470). Elemental analysis: element (theoretical, found) C (65.46, 65.11), H (4.81, 4.89), N (3.18, 3.39).

Method 2: A 50 mL flask equipped with a stir bar was charged with RuCl₂(PPh₃)₃ (200 mg, 0.209 mmol) and toluene (5 mL) producing a dark red solution. A separate 50 mL flask equipped with a stir bar was charged with *ortho*-semidine (46 mg, 0.25 mmol) and toluene (5 mL) forming a dark brown solution. The mixtures were combined forming a brown solution that turns orange over the course of hours. The solution was allowed to stir overnight. The solvent was removed *in vacuo* and the crude solid was suspended in Et₂O (10 mL), filtered, and washed with additional Et₂O (2 x 5 mL) to produce the orange solid product (131 mg, 71%).

3. NMR spectra

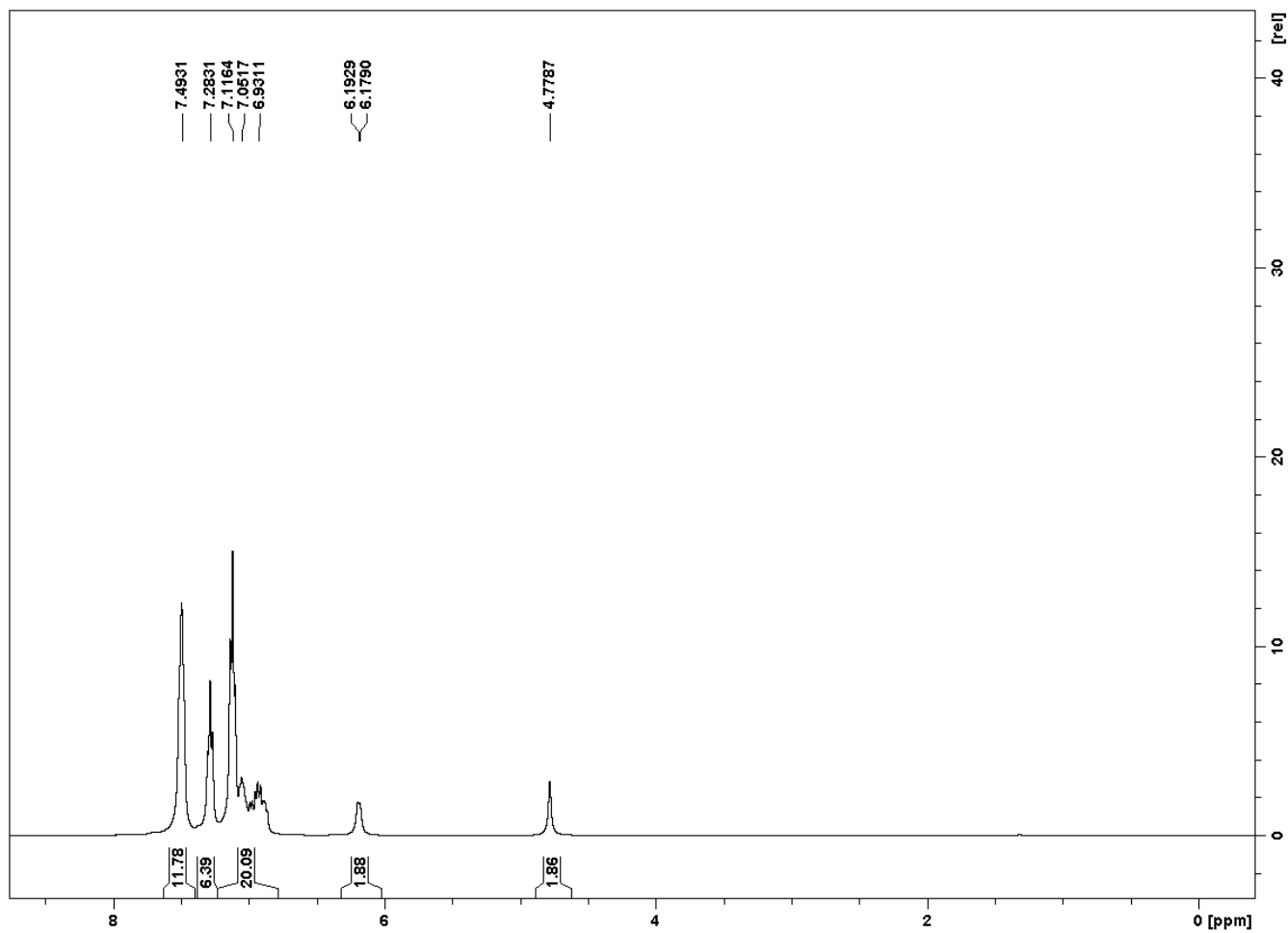


Figure S1. ^1H NMR spectrum of $\text{RuCl}_2(\text{PPh}_3)_2(\kappa^2\text{-NH}_2\text{-1,2-C}_6\text{H}_4\text{-NHPh})$ (1) in CDCl_3 normalized to 42 protons.

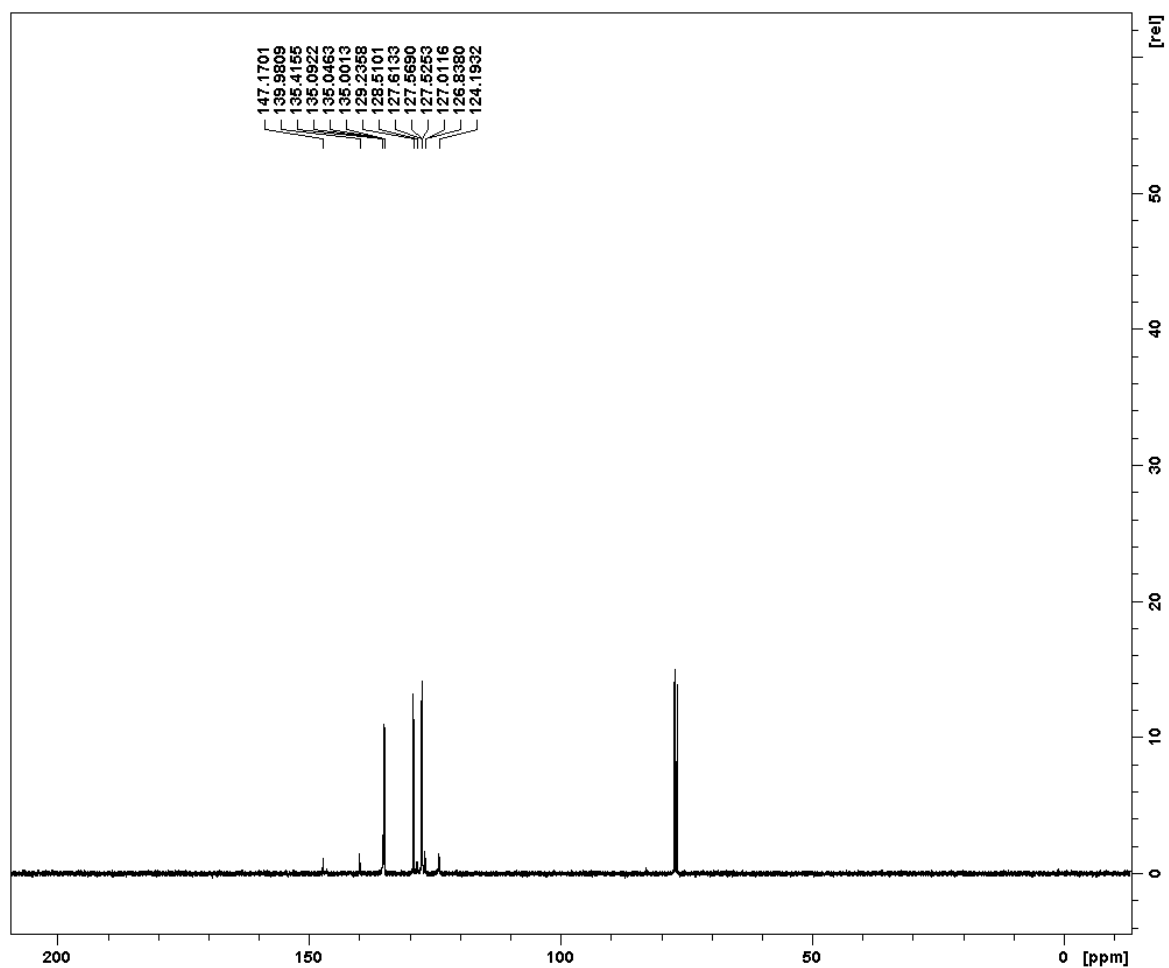


Figure S2. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of $\text{RuCl}_2(\text{PPh}_3)_2(\kappa^2\text{-NH}_2\text{-1,2-C}_6\text{H}_4\text{-NHPh})$ (**1**) in CDCl_3 .

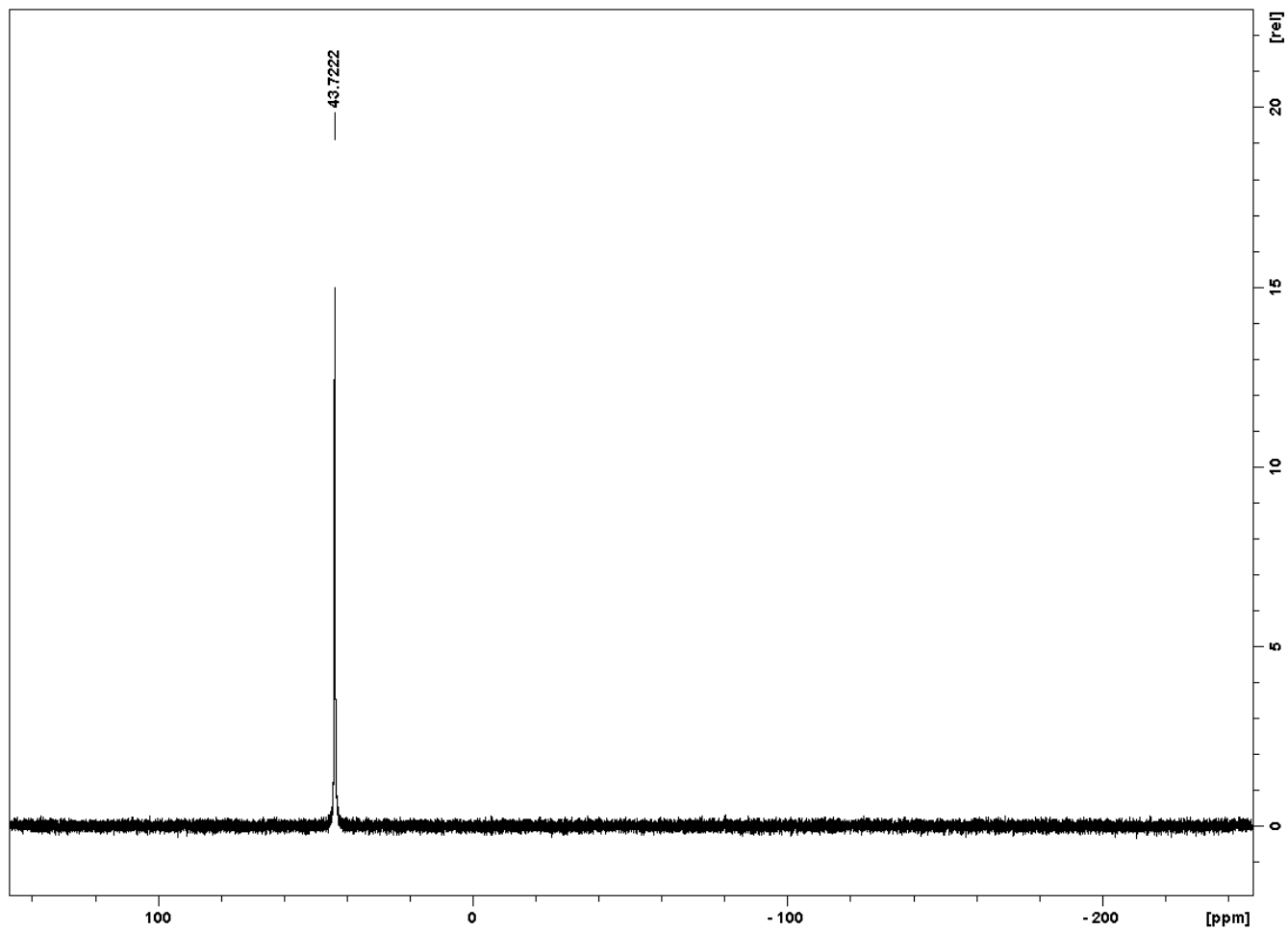


Figure S3. Room temperature $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of $\text{RuCl}_2(\text{PPh}_3)_2(\kappa^2\text{-NH}_2\text{-1,2-C}_6\text{H}_4\text{-NHPh})$ (**1**) in CDCl_3 .

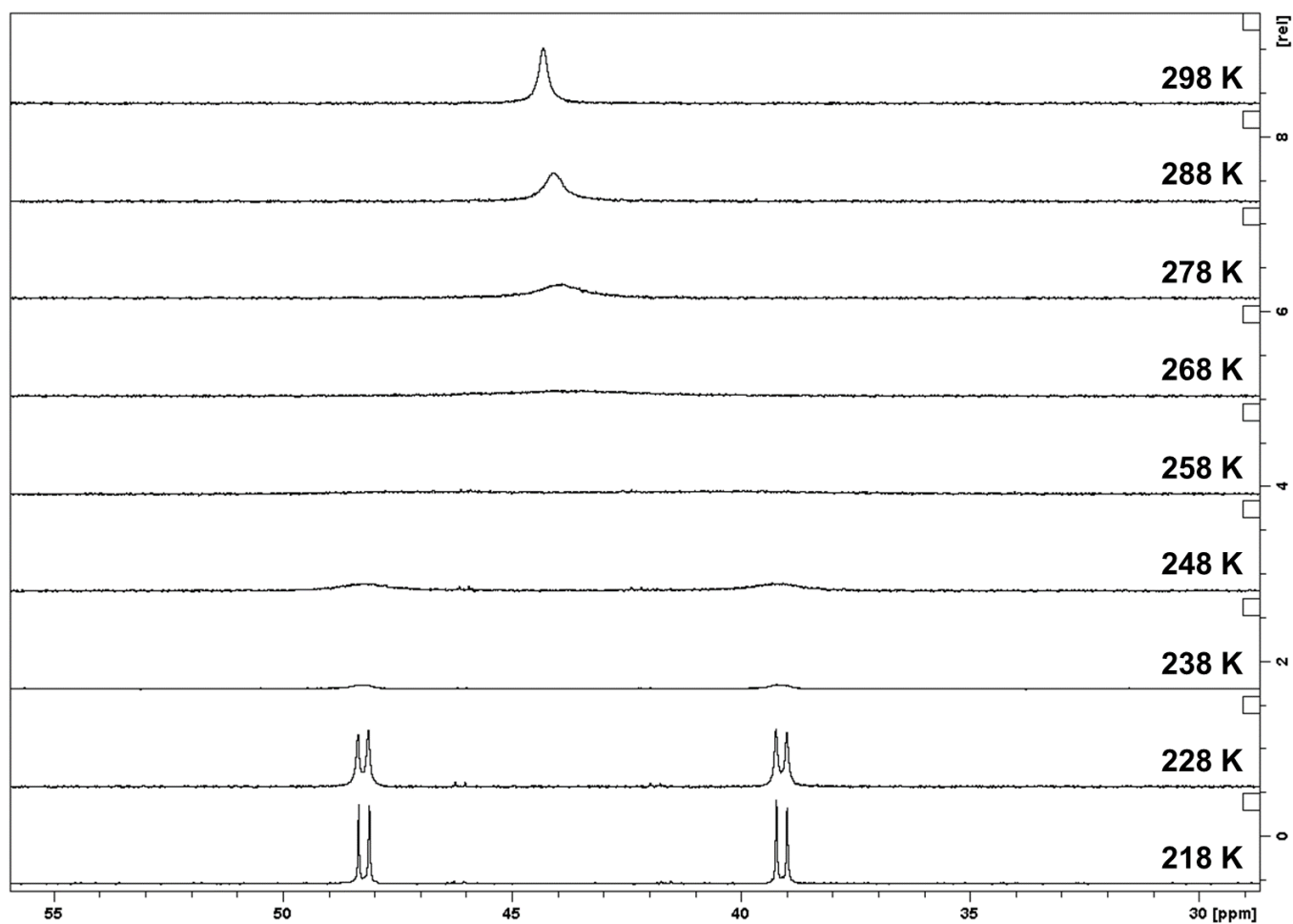


Figure S4. Variable temperature $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of $\text{RuCl}_2(\text{PPh}_3)_2(\kappa^2\text{-NH}_2\text{-1,2-C}_6\text{H}_4\text{-NHPh})$ (**1**) in CDCl_3 .

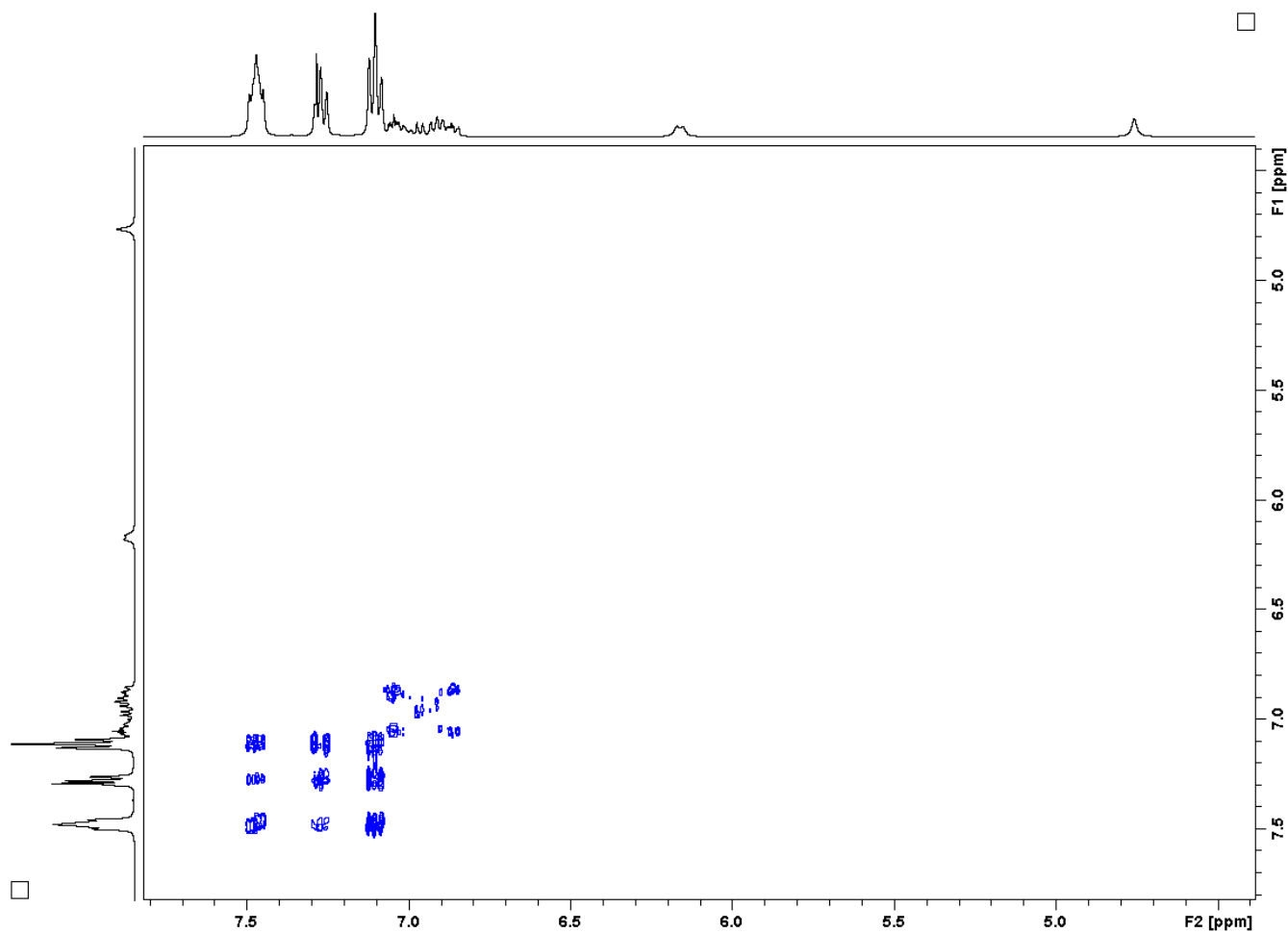


Figure S5. ¹H-¹H COSY NMR spectrum of RuCl₂(PPh₃)₂(κ²-NH₂-1,2-C₆H₄-NHPh) (**1**) in CDCl₃.

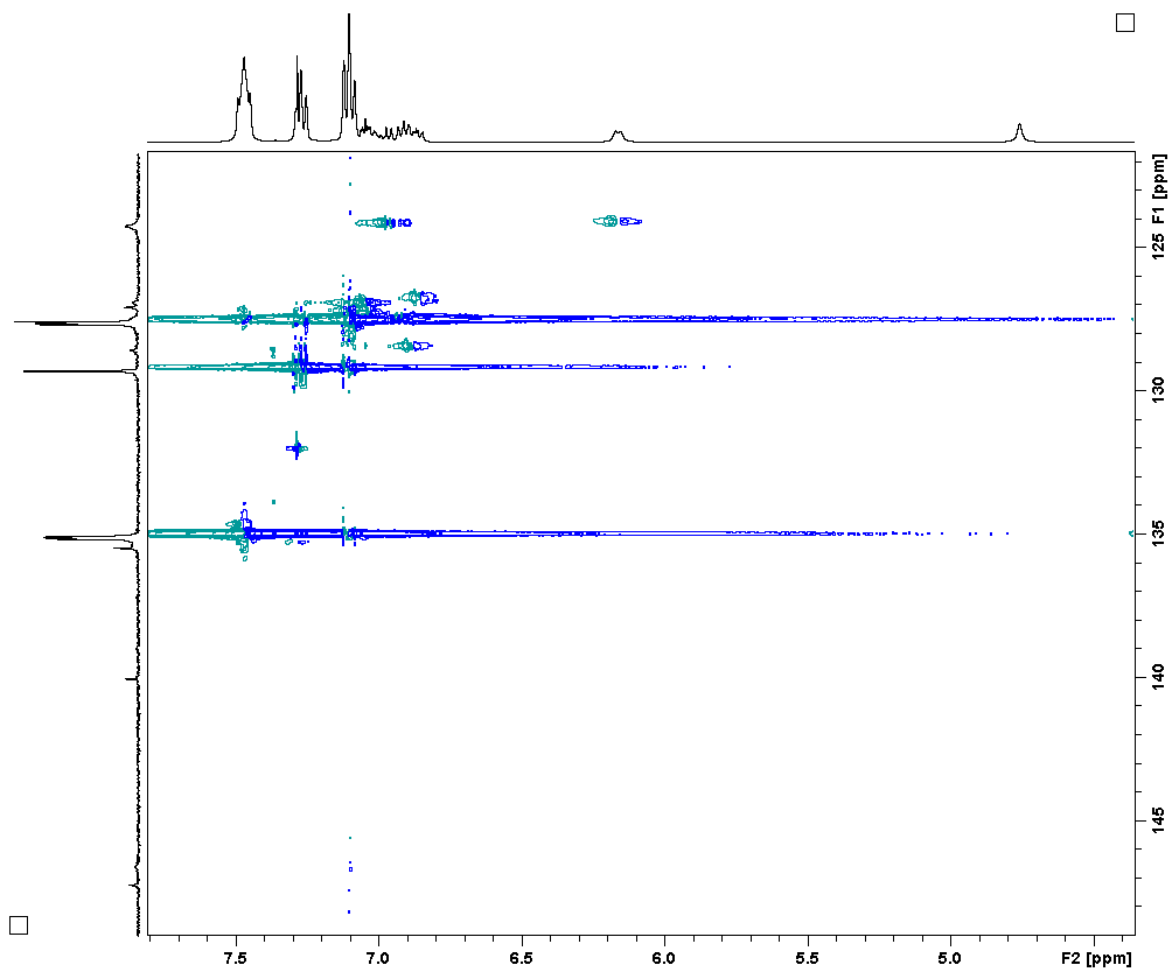


Figure S6. ^1H - ^{13}C HSQC NMR spectrum of $\text{RuCl}_2(\text{PPh}_3)_2(\kappa^2\text{-NH}_2\text{-1,2-C}_6\text{H}_4\text{-NHPh})$ (**1**) in CDCl_3 .

4. FTIR spectrum

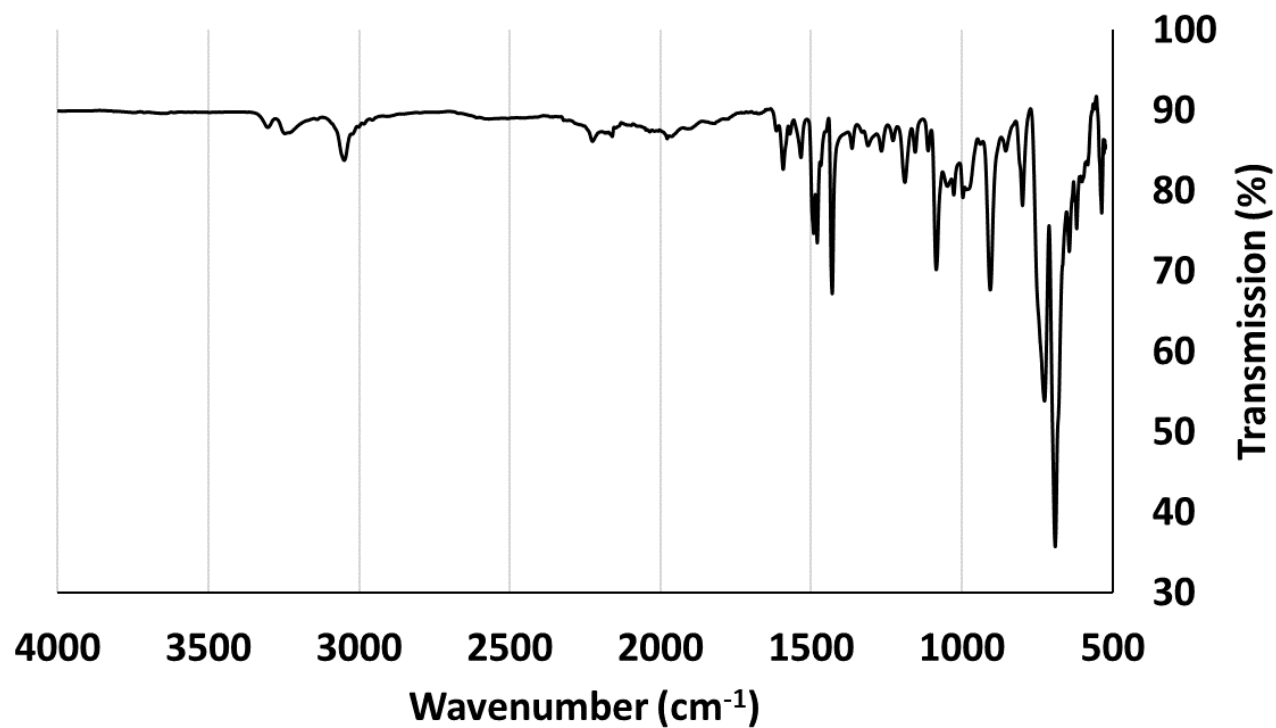


Figure S7. FTIR spectrum of $\text{RuCl}_2(\text{PPh}_3)_2(\kappa^2\text{-NH}_2\text{-1,2-C}_6\text{H}_4\text{-NHPh})$ (1).

5. UV-vis data

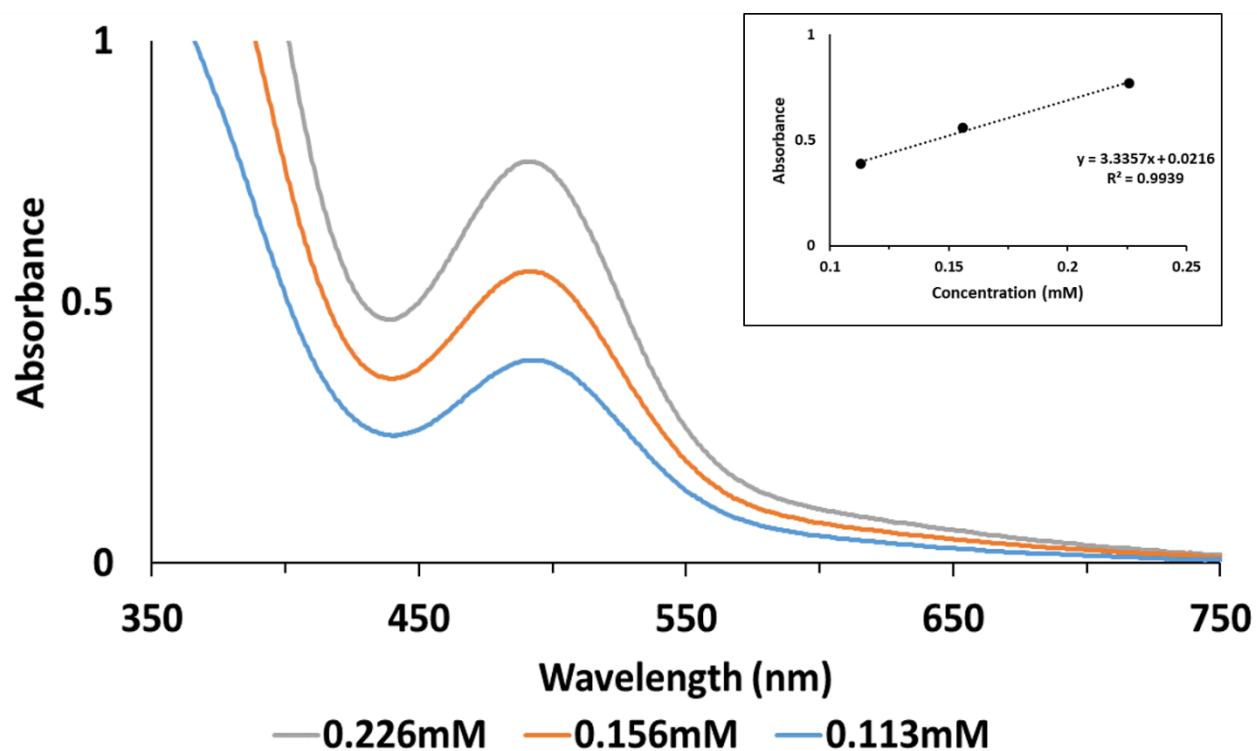


Figure S8. UV-vis spectra of $\text{RuCl}_2(\text{PPh}_3)_2(\kappa^2\text{-NH}_2\text{-1,2-C}_6\text{H}_4\text{-NHPh})$ (1) recorded under anaerobic conditions in dichloromethane. Beer-Lambert plot included for $\lambda_{\text{max}} = 492$ nm.

6. Single crystal X-ray diffraction data

Table S1. Crystallographic data for the polymorphs of compound **1**.

	α - 1	β - 1
chemical formula	C ₄₈ H ₄₂ Cl ₂ N ₂ P ₂ Ru	C ₄₈ H ₄₂ Cl ₂ N ₂ P ₂ Ru
formula weight	880.74	880.74
radiation source, λ (Å)	0.71073	0.71073
crystal system	monoclinic	orthorhombic
space group	<i>P2₁/n</i>	<i>P2₁2₁2₁</i>
<i>T</i> (K)	100(2)	100(2)
<i>a</i> (Å)	10.872(1)	12.798(3)
<i>b</i> (Å)	17.173(1)	12.949(3)
<i>c</i> (Å)	22.070(2)	24.832(5)
α (deg)	90	90
β (deg)	90.648(1)	90
γ (deg)	90	90
<i>V</i> (Å ³)	4120.2(6)	4115.4(2)
<i>Z</i>	4	4
<i>d</i> _{calc} (g cm ⁻³)	1.420	1.422
μ (mm ⁻¹)	0.625	0.625
<i>F</i> (000)	1808	1808
crystal size (mm)	0.37 x 0.18 x 0.17	0.10 x 0.05 x 0.02
reflections collected	88235	58890
data/parameters/restraints	10401 / 508 / 0	9119 / 508 / 0
<i>R</i> (int)	0.0295	0.0866
<i>R</i> ₁ [<i>I</i> > 2 σ (<i>I</i>)] ^a	0.0260	0.0358
w <i>R</i> ₂ (all data) ^a	0.0640	0.0781
Largest difference peak and hole (e ⁻ Å ⁻³)	0.421 and -0.273	0.673 and -0.597

$$^a R_1 = \frac{\sum ||F_o| - |F_c||}{\sum |F_o|}; wR_2 = \left\{ \frac{\sum [w(F_o^2 - F_c^2)^2]}{\sum [w(F_o^2)^2]} \right\}^{1/2}$$

Table S2. Relevant bond distances and angles of the first coordination sphere for the polymorphs and DFT-calculated structures in this study.

	Experimental ^a		DFT-calculated structures ^b							
	α -1	β -1	α -1	β -1	1b	1c	1d	1e	1f	1g
	Distances (Å)									
Ru – N1	2.160(1)	2.166(4)	2.145	2.147	2.117	2.144	2.117	2.140	2.125	2.214
Ru – N2	2.284(1)	2.306(4)	2.313	2.304	2.219	2.350	2.266	2.360	2.272	–
Ru – P1	2.3006(4)	2.295(1)	2.305	2.305	2.393	2.363	2.368	2.320	2.327	2.296
Ru – P2	2.3265(4)	2.324(1)	2.336	2.333	2.364	2.321	2.325	2.276	2.286	2.209
Ru – Cl1	2.4127(4)	2.389(1)	2.410	2.411	2.420	2.481	2.441	2.508	2.439	2.381
Ru – Cl2	2.4246(4)	2.424(1)	2.424	2.423	2.407	2.378	2.397	2.380	2.398	2.385
	Angles (°)									
N1-Ru1-N2	77.62(5)	76.26(1)	77.04	76.87	80.95	74.37	78.92	75.14	78.81	–
N1-Ru1-P1	90.96(4)	91.33(1)	91.11	91.13	90.04	166.60	165.80	98.84	96.44	159.35
N1-Ru1-P2	171.26(4)	169.45(1)	170.94	170.86	92.21	90.72	90.65	95.40	99.68	96.40
N1-Ru1-Cl1	81.50(4)	83.79(1)	81.16	80.99	172.59	78.91	78.58	80.48	79.47	81.60
N1-Ru1-Cl2	81.92(4)	81.82(1)	81.80	82.13	93.44	83.42	83.29	162.26	164.43	87.84
N2-Ru1-P1	168.57(3)	167.56(9)	168.14	167.99	102.30	103.97	102.73	158.78	167.57	–
N2-Ru1-P2	94.37(3)	93.30(9)	94.33	94.39	91.34	103.28	93.24	99.09	90.29	–
N2-Ru1-Cl1	90.70(4)	91.93(1)	90.90	90.76	91.77	75.89	87.06	74.07	83.13	–
N2-Ru1-Cl2	84.26(3)	81.62(1)	81.44	81.57	171.40	155.39	162.21	87.50	87.28	–
P1-Ru1-P2	97.05(1)	99.13(4)	97.53	97.62	166.35	102.53	103.27	101.75	101.88	103.96
P1-Ru1-Cl1	87.45(1)	85.85(4)	86.77	86.65	92.85	87.78	87.37	84.92	84.71	92.37
P2-Ru1-Cl1	102.30(1)	98.27(4)	101.97	102.05	86.58	169.47	168.97	172.68	173.40	97.17
P1-Ru1-Cl2	94.35(1)	97.58(4)	97.50	97.62	84.11	95.16	94.43	96.09	95.74	93.46
P2-Ru1-Cl2	93.92(1)	95.32(4)	94.31	94.06	82.32	87.22	87.26	90.87	87.24	95.67
Cl1-Ru1-Cl2	163.35(1)	165.28(4)	162.50	162.66	93.64	89.73	89.11	91.39	92.04	164.19

^a See crystallographic information file (CIF) for numbering scheme.

^b See Figure S8 for numbering scheme.

7. PXRD diffractograms

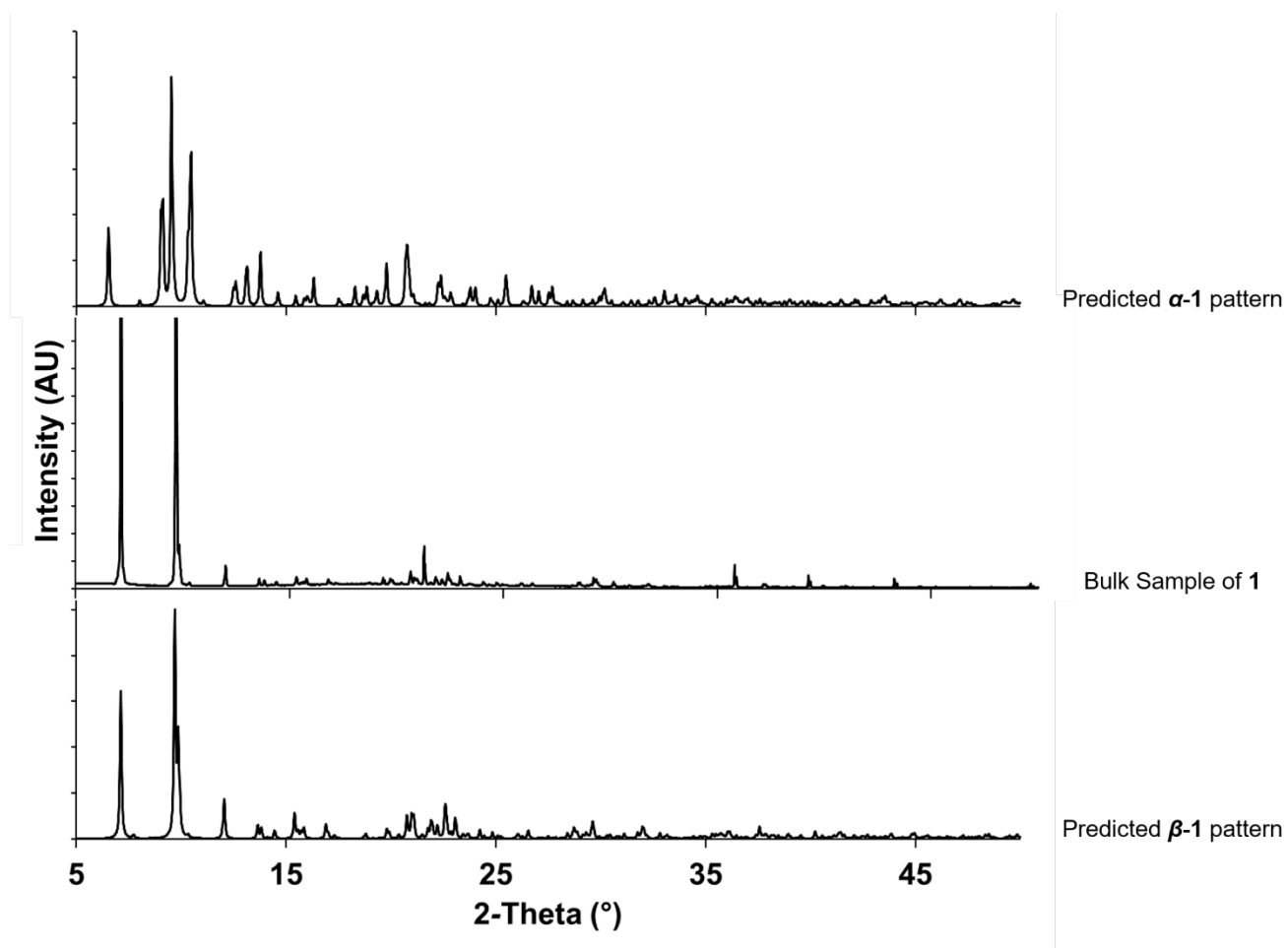


Figure S9. Powder X-ray diffraction pattern for the bulk sample of **1**, and the predicted powder patterns of the α and β polymorphs. Predicted powder patterns obtained from the single crystal diffraction data (CIF).

8. DFT numbering scheme, data, and coordinates

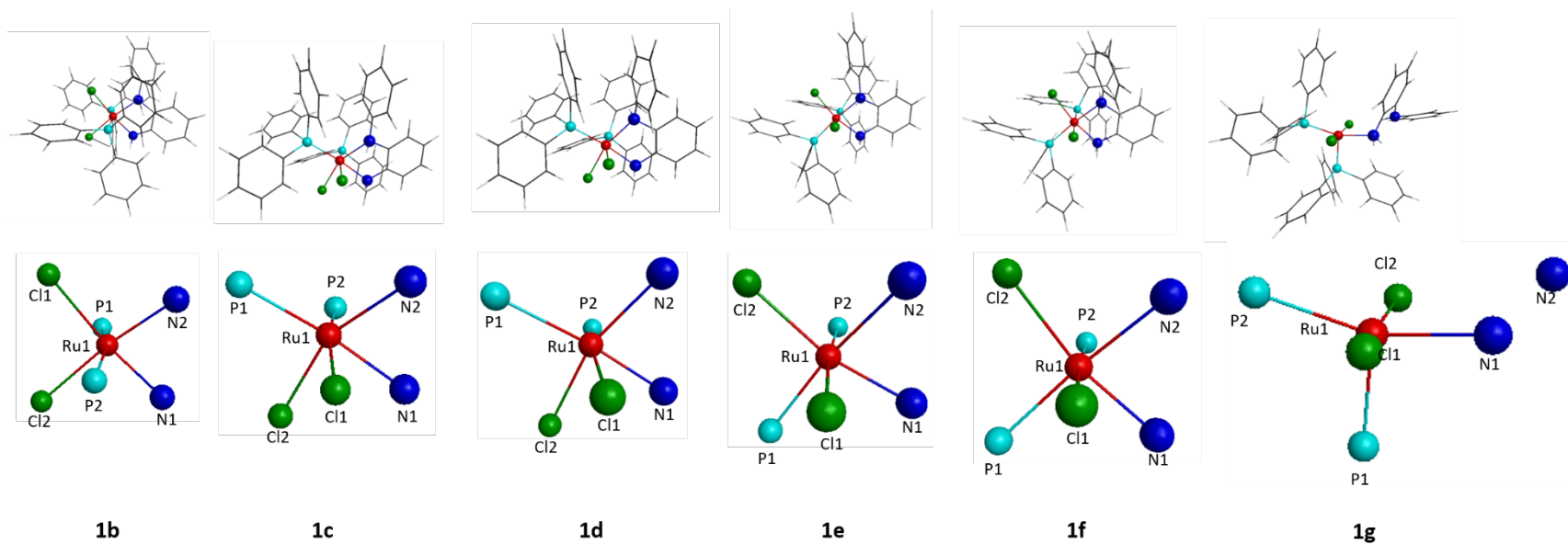


Figure S10. Numbering scheme for the $\text{RuCl}_2(\text{PPh}_3)_2(\kappa^2\text{-NH}_2\text{-1,2-C}_6\text{H}_4\text{-NHPh})$ predicted structures (**1b** – **1f**) and the monodentate structure $\text{RuCl}_2(\text{PPh}_3)_2(\text{NH}_2\text{-1,2-C}_6\text{H}_4\text{-NHPh})$ (**1g**).

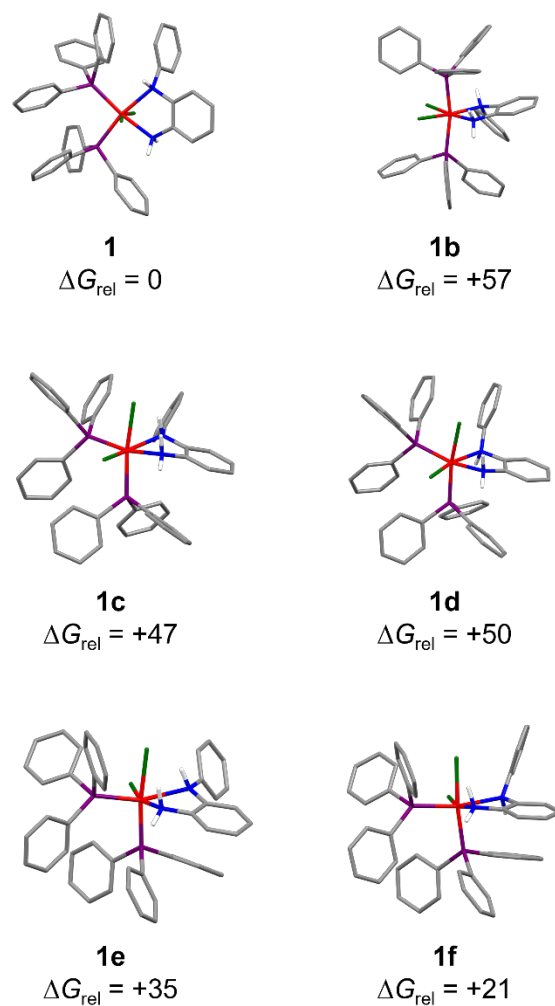


Figure S11. DFT-calculated structures and relative Gibbs free energies (kJ mol^{-1}) of compound **1** and its seven geometric isomers **1b** – **1f**. Color code: carbon (grey), hydrogen (white), nitrogen (blue), phosphorus (purple), chlorine (green), ruthenium (red). Phenyl hydrogen atoms are omitted for clarity.

Cartesian coordinates for α -1:

Ru	-0.13928200	0.70863301	0.08619200
Cl	-0.09067400	1.10243106	2.47721410
Cl	-0.25338700	1.04712796	-2.29714394
P	-0.78567398	-1.52639306	0.28969499
P	2.11822295	0.34475499	-0.20476300
C	-1.19843996	-2.47849703	-1.23298395
C	-0.94381499	-3.84220505	-1.38180900
H	-0.43277001	-4.38843393	-0.60030800
C	-1.34829497	-4.51674986	-2.52465296
H	-1.13807595	-5.57538700	-2.62307811
C	-2.02479696	-3.84265304	-3.53091097
H	-2.34032202	-4.37039089	-4.42338705
C	-2.29582500	-2.49045396	-3.38608909
H	-2.82420301	-1.95184505	-4.16352701
C	-1.88496995	-1.81236899	-2.24804902
H	-2.08375406	-0.75329202	-2.15807295
C	-2.36377501	-1.78609502	1.23193204
C	-2.56639504	-1.12209702	2.44422889
H	-1.80429006	-0.44611299	2.81806493
C	-3.72684598	-1.31924701	3.18068409
H	-3.85713601	-0.79194200	4.11865711
C	-4.70840311	-2.18554306	2.72262311
H	-5.61550617	-2.33877802	3.29534411
C	-4.51432323	-2.85692000	1.52501905
H	-5.27076006	-3.53930998	1.15508294
C	-3.35477304	-2.66115594	0.78781998
H	-3.23398089	-3.19290400	-0.14586800
C	0.30474800	-2.71264005	1.18642604
C	1.46015799	-3.18537307	0.56291401
H	1.71250796	-2.85540700	-0.43705499
C	2.29428005	-4.09185886	1.19561303
H	3.18247104	-4.44529581	0.68606001

C	2.00036192	-4.53270388	2.47736692
H	2.65449905	-5.23827696	2.97564411
C	0.86608499	-4.05886984	3.11527896
H	0.62485999	-4.39208794	4.11792278
C	0.02296800	-3.16148305	2.47414303
H	-0.86479598	-2.82156205	2.98882794
C	2.71505499	-0.36557701	-1.79715705
C	1.93359101	-1.28927600	-2.48349094
H	0.93858898	-1.51767397	-2.13016009
C	2.39190006	-1.88780200	-3.64758992
H	1.75867403	-2.59945107	-4.16376591
C	3.63739896	-1.55736804	-4.15805197
H	3.99301291	-2.01673007	-5.07287216
C	4.41903687	-0.62077099	-3.49815106
H	5.38925219	-0.34346500	-3.89346290
C	3.96171308	-0.03088600	-2.32939601
H	4.58421707	0.70431602	-1.83514905
C	2.96041608	1.98645604	-0.23514500
C	2.91135597	2.76943803	-1.39148998
H	2.44477296	2.37263608	-2.28633404
C	3.44419503	4.04935598	-1.40067101
H	3.40483499	4.63880587	-2.30930591
C	4.02416420	4.57428312	-0.25318599
H	4.44204998	5.57398415	-0.26178399
C	4.06679010	3.80975699	0.90252602
H	4.51678324	4.20931721	1.80370700
C	3.53978705	2.52403092	0.91248298
H	3.58260894	1.93670404	1.82147598
C	3.18229389	-0.53545803	1.02436399
C	4.41544485	-1.08774304	0.67508101
H	4.74851799	-1.08074605	-0.35309801
C	5.22928476	-1.67022395	1.63398099
H	6.18216276	-2.09416389	1.33857501

C	4.82702398	-1.71364295	2.96073198
H	5.46435308	-2.16881800	3.70996094
C	3.59949994	-1.17878497	3.31594300
H	3.26511002	-1.21553504	4.34604979
C	2.78091407	-0.59821802	2.35716796
H	1.82139599	-0.18853900	2.64565110
N	-2.27494001	1.53142405	0.34156200
C	-2.18441200	2.94816995	0.64637101
C	-0.96845102	3.58929610	0.50898600
N	0.15484200	2.83331800	0.04030000
C	-3.29327989	3.65715003	1.09048104
C	-3.17874503	4.99731302	1.41427195
C	-1.95348895	5.63838816	1.28805900
C	-0.85225898	4.93492794	0.83378798
C	-3.35312891	1.25673103	-0.57732701
C	-3.36372304	1.85396695	-1.83307898
C	-4.40795708	1.60222197	-2.70665789
C	-5.44953680	0.76006299	-2.34032798
C	-5.44357395	0.17951301	-1.08273602
C	-4.40427303	0.43272999	-0.19835800
H	-2.45975900	1.04740596	1.21784699
H	0.98712701	3.09853411	0.55615997
H	0.32424399	3.01193905	-0.94955897
H	-4.24606991	3.14912200	1.18033302
H	-4.04494619	5.54136992	1.76994801
H	-1.85666800	6.68628120	1.54380703
H	0.11059000	5.42299795	0.73122698
H	-2.54557896	2.49482989	-2.12798309
H	-4.40283918	2.06680107	-3.68538904
H	-6.26269007	0.56498700	-3.02891493
H	-6.25419283	-0.47031900	-0.77564400
H	-4.41676998	-0.01210400	0.78881902

Cartesian coordinates for β -1:

Ru	0.00658885	0.03181645	-0.02261822
Cl	1.29621637	2.06493235	-0.14601861
Cl	-0.76976299	-2.23838139	-0.35878292
P	0.93032837	-0.26751047	2.06806302
P	-2.07795906	0.81854761	0.66973650
N	1.77338219	-0.74702460	-0.96142340
H	2.14626169	-1.53798163	-0.44751078
H	2.42816663	0.02999491	-0.86884713
N	-0.48864946	0.17330202	-2.26875663
H	-1.34631431	-0.37199751	-2.21349549
C	1.59537649	-1.09876680	-2.33839393
C	0.47794279	-0.62671465	-2.99948359
C	0.28313562	-0.93963522	-4.33858681
C	1.19352925	-1.73985159	-5.00571585
C	2.30939317	-2.22564793	-4.33717155
C	2.51004028	-1.90235424	-3.00699902
C	-0.77278554	1.41332257	-2.95015931
C	-2.06095028	1.69267058	-3.38673019
C	-2.32824254	2.88121748	-4.05154228
C	-1.31110024	3.78797722	-4.30030012
C	-0.01995280	3.49451113	-3.88203287
C	0.25363114	2.31442261	-3.21159005
C	2.58448195	-1.05757189	1.85525167
C	3.67633677	-0.28411633	1.45203435
C	4.90243387	-0.87587941	1.19027686
C	5.05704021	-2.25049734	1.31420362
C	3.97621465	-3.02795553	1.70064807
C	2.74819636	-2.43653131	1.97055686
C	0.21079786	-1.37810862	3.35843635
C	-0.62946957	-2.42069244	2.97324395
C	-1.11502159	-3.32111049	3.91117406
C	-0.77823025	-3.19189906	5.24871063

C	0.04478570	-2.14804697	5.64508009
C	0.53425610	-1.24965835	4.70999908
C	1.39502096	1.21247494	3.06320596
C	2.48003674	1.19781315	3.94177222
C	2.77670550	2.30275893	4.72554445
C	1.99324095	3.44445801	4.64600754
C	0.92134356	3.47643065	3.76794171
C	0.63340598	2.37313890	2.97867799
C	-2.87426758	0.09522954	2.16747236
C	-3.93266988	-0.80639380	2.09006238
C	-4.50917387	-1.32762527	3.24033308
C	-4.04560757	-0.94941801	4.48937988
C	-2.99045110	-0.05388796	4.58090878
C	-2.40707040	0.45440882	3.43239093
C	-2.29791689	2.62400913	0.96748072
C	-3.14581752	3.14651513	1.94462574
C	-3.32540059	4.51683998	2.06594276
C	-2.67089653	5.38601780	1.20519388
C	-1.83776855	4.87605333	0.22100480
C	-1.65064573	3.50684166	0.10309846
C	-3.44366336	0.56127292	-0.56128824
C	-4.36353540	1.56548178	-0.86188459
C	-5.39252853	1.34183443	-1.76579225
C	-5.52705240	0.10983428	-2.38768268
C	-4.62423611	-0.90071160	-2.09195304
C	-3.59390044	-0.67840856	-1.18799543
H	-0.58856595	-0.55206567	-4.85236406
H	1.02995813	-1.98920417	-6.04679585
H	3.02300954	-2.85625434	-4.85283709
H	3.37722826	-2.27463174	-2.47301674
H	-2.85950422	0.98240155	-3.21243763
H	-3.33919883	3.08809900	-4.38147497
H	-1.51932359	4.71381474	-4.82264328

H	0.78585631	4.19272375	-4.07411623
H	1.25628161	2.09876037	-2.87211108
H	3.55858231	0.78769410	1.33684433
H	5.74053431	-0.25900140	0.88749862
H	6.01628399	-2.71182799	1.11143339
H	4.08525085	-4.10150003	1.80000281
H	1.91341937	-3.05538106	2.27578402
H	-0.90445632	-2.52721286	1.93171644
H	-1.76706362	-4.12361193	3.58701491
H	-1.15971792	-3.89441371	5.98060513
H	0.30836734	-2.02740431	6.68955517
H	1.16273189	-0.43843415	5.04934549
H	3.10962915	0.31992334	4.01399088
H	3.62545729	2.26894784	5.39854431
H	2.22613502	4.30899382	5.25649357
H	0.31364223	4.36867046	3.67599916
H	-0.17083189	2.43439794	2.26035571
H	-4.32603168	-1.10525310	1.12854958
H	-5.33129597	-2.02830338	3.15279126
H	-4.50001335	-1.35158789	5.38702679
H	-2.60991740	0.24545178	5.54994583
H	-1.58425629	1.15136123	3.53107071
H	-3.67851663	2.48392677	2.61364698
H	-3.98571277	4.90346479	2.83347178
H	-2.81174541	6.45632792	1.30087578
H	-1.32170331	5.54322529	-0.45889577
H	-0.98192328	3.12403822	-0.65553874
H	-4.27951431	2.53831863	-0.39778426
H	-6.09131384	2.14095426	-1.98437047
H	-6.33041716	-0.06187624	-3.09440255
H	-4.71820784	-1.87271035	-2.56229162
H	-2.89838219	-1.47972238	-0.96059591

Cartesian coordinates for **1b**:

Ru	0.11230500	0.25995299	-0.03983400
N	0.09867700	-1.84810495	-0.73103398
C	0.32853499	-2.68743992	0.42791399
C	0.28913701	-2.13335490	1.69972396
N	0.11737700	-0.70788199	1.84281504
Cl	0.16187000	1.08413303	-2.31456304
Cl	0.40223601	2.44789195	0.92158902
P	-2.22074699	0.73085201	0.20648600
P	2.47434306	0.32731900	-0.11396500
C	-3.51148891	-0.55998701	-0.09490000
C	-2.79523206	2.16142392	-0.77296799
C	-2.80322194	1.18111503	1.91352904
C	3.20250511	0.30983299	1.57026398
C	3.37465811	1.73545897	-0.88114297
C	3.30682302	-1.05265403	-1.01142395
C	-3.60475898	-1.59690797	0.83639002
C	-2.82804799	2.07840490	-2.16602302
C	-1.92891002	1.51278102	2.94597006
C	3.26197195	-0.85641998	2.33727598
C	2.73311710	2.87304902	-1.35741794
C	2.90198207	-1.22406399	-2.33989692
C	-4.59736586	-2.55702209	0.74669403
C	-3.23441696	3.16435504	-2.92505002
C	-2.40766692	1.82525206	4.21406603
C	3.71336198	-0.82621700	3.65041494
C	3.47524405	3.90349889	-1.92074394
C	3.45845890	-2.21950889	-3.12894702
C	-5.51378107	-2.51298499	-0.29550400
C	-3.58770990	4.35548210	-2.30900502
C	-3.76826310	1.83074903	4.46711206
C	4.09986210	0.37425500	4.22584200
C	4.85428476	3.81179690	-2.01230502

C	4.43323612	-3.05865908	-2.60872602
C	-5.41987419	-1.50364602	-1.23884904
C	-3.52688193	4.45681715	-0.92799401
C	-4.65314388	1.52882802	3.43993592
C	4.02560806	1.54255402	3.48121905
C	5.50112915	2.67810893	-1.53834796
C	4.85486317	-2.88559699	-1.29932201
C	-4.43180895	-0.53191900	-1.13672197
C	-3.13315010	3.36800003	-0.16449900
C	-4.17579079	1.20403600	2.18195891
C	3.58077908	1.51323700	2.16877890
C	4.76484013	1.64750504	-0.97957599
C	4.29910803	-1.89069104	-0.50634199
C	0.61917299	-4.04181290	0.28432301
C	0.82958102	-4.83893108	1.39388704
C	0.74255502	-4.29147482	2.66807699
C	0.47929299	-2.94222212	2.81597400
C	-0.85426003	-2.38385892	-1.68431997
C	-1.86232996	-3.26030493	-1.30845702
C	-2.73267698	-3.76839304	-2.26155591
C	-2.60598302	-3.41216302	-3.59406209
C	-1.59973598	-2.53275299	-3.96559000
C	-0.72564101	-2.02171898	-3.02074409
H	0.98301899	-1.78665900	-1.23512900
H	0.89127499	-0.33873701	2.39535999
H	-0.72261399	-0.50488299	2.37890196
H	-2.91212201	-1.63990998	1.67028105
H	-2.50405312	1.17443395	-2.66294003
H	-0.86987603	1.59956300	2.73713589
H	2.95950699	-1.80547798	1.91196096
H	1.65886402	2.94879198	-1.28985298
H	2.16249490	-0.54297900	-2.75521111
H	-4.65996695	-3.33781409	1.49599898

H	-3.25418401	3.08215809	-4.00525999
H	-1.70551896	2.08359790	4.99825001
H	3.76450992	-1.74707603	4.21997213
H	2.96195102	4.78284979	-2.29115510
H	3.13299298	-2.33228898	-4.15634584
H	-6.29704094	-3.25835490	-0.36686400
H	-3.89670205	5.20630693	-2.90497899
H	-4.14144993	2.07963800	5.45362902
H	4.45424891	0.39991501	5.24942780
H	5.42687511	4.61910582	-2.45426893
H	4.86971188	-3.83627510	-3.22411704
H	-6.12923479	-1.45597398	-2.05667710
H	-3.78177500	5.38872099	-0.43731099
H	-5.72189999	1.54567099	3.61860609
H	4.31384897	2.48843694	3.92408490
H	6.57934523	2.59374189	-1.60705304
H	5.62935209	-3.52353311	-0.88947397
H	-4.40447283	0.26675799	-1.86515403
H	-3.07937288	3.46764588	0.91121298
H	-4.88280678	0.96678501	1.39700699
H	3.51597095	2.43354011	1.60393405
H	5.28114080	0.76495898	-0.62011200
H	4.66266108	-1.76070797	0.50414401
H	0.66615498	-4.46567583	-0.71116501
H	1.05862701	-5.88952398	1.26557899
H	0.89531702	-4.91215086	3.54232001
H	0.44204301	-2.49346399	3.80241799
H	-1.97471094	-3.55635810	-0.27585199
H	-3.51711988	-4.44679880	-1.94967103
H	-3.28567195	-3.81373596	-4.33565903
H	-1.48865700	-2.23646092	-5.00183582
H	0.03143500	-1.30570197	-3.30809498

Cartesian coordinates for 1c:

Ru	-0.27528700	0.51679999	-0.89691198
N	-1.66658998	1.91288602	0.38355699
C	-3.02964807	1.54435003	0.08877800
C	-3.27233195	0.88626701	-1.11694896
N	-2.14516306	0.58565402	-1.94356704
Cl	-0.11390500	2.72394204	-2.01760292
Cl	0.48763800	-0.53711498	-2.88788009
P	1.88518095	0.90628499	-0.02150800
P	-0.76779997	-1.60517204	-0.09669800
C	3.12388110	1.66666996	-1.16551101
C	2.88297510	-0.46753299	0.68527597
C	2.02023602	2.16251493	1.32931399
C	-2.28764296	-2.32403302	-0.89661801
C	-1.17064905	-1.83774400	1.68991005
C	0.31713101	-3.06066704	-0.42571399
C	2.98289609	1.63006699	-2.54798102
C	4.10162592	-0.86946797	0.14342000
C	1.59085000	3.45708489	1.03216696
C	-2.21759391	-2.57378793	-2.27169609
C	-2.22832298	-1.11659503	2.24526596
C	-0.16349199	-4.34110498	-0.13517299
C	3.95761895	2.18212104	-3.37002301
C	4.82084990	-1.91085303	0.71352100
C	1.76601899	4.48646688	1.94119799
C	-3.28569889	-3.14394212	-2.94632196
C	-2.57822394	-1.26541805	3.57847905
C	0.60463202	-5.46303892	-0.39164299
C	5.08191109	2.77899194	-2.82573891
C	4.34172916	-2.56034088	1.83992505
C	2.36936307	4.24478388	3.16753602
C	-4.44320202	-3.49044895	-2.26173902
C	-1.86189604	-2.12787890	4.39460421

C	1.86617100	-5.32614899	-0.95725298
C	5.23140001	2.82366204	-1.44597495
C	3.12712097	-2.17135906	2.38578606
C	2.79542994	2.96372890	3.47445607
C	-4.51703405	-3.26258707	-0.89810401
C	-0.79804403	-2.83960700	3.86201501
C	2.34399104	-4.06407022	-1.26466894
C	4.26097584	2.27456093	-0.62522399
C	2.40213490	-1.14300501	1.80571401
C	2.62624693	1.93099499	2.56102395
C	-3.44992590	-2.68435097	-0.22123501
C	-0.46003401	-2.70139909	2.52297306
C	1.57343400	-2.93843007	-1.00285804
C	-4.09789085	1.79989100	0.93959600
C	-5.38269901	1.40162003	0.59388101
C	-5.61814404	0.75663501	-0.60750800
C	-4.55614185	0.50410402	-1.46298099
C	-1.50954497	2.60410500	1.64141905
C	-1.03494000	1.95475495	2.76678801
C	-0.94236898	2.63837600	3.97078800
C	-1.31614101	3.97084093	4.05296087
C	-1.77056599	4.62763786	2.91846991
C	-1.86614501	3.94649291	1.71617198
H	-1.36027503	2.57076406	-0.35304800
H	-1.92070901	1.35719395	-2.57603598
H	-2.30314112	-0.24735101	-2.50125790
H	2.10904098	1.17099702	-2.98653197
H	4.49501991	-0.37009400	-0.73198402
H	1.13660204	3.66078806	0.06879800
H	-1.30960798	-2.32505393	-2.81195498
H	-2.79524302	-0.43049300	1.62946904
H	-1.15272498	-4.46511078	0.28933400
H	3.82439804	2.14737701	-4.44483519

H	5.76451778	-2.21056700	0.27286801
H	1.43211102	5.48525000	1.68638897
H	-3.20473504	-3.32991600	-4.01103592
H	-3.40948701	-0.69721800	3.97897005
H	0.21380500	-6.44650412	-0.15837300
H	5.83744621	3.21356893	-3.47010899
H	4.90793180	-3.36824203	2.28779793
H	2.50981498	5.05250311	3.87621403
H	-5.27514887	-3.94421697	-2.78726506
H	-2.13068891	-2.24387598	5.43779707
H	2.46675801	-6.20384121	-1.16601706
H	6.10360718	3.29205799	-1.00505996
H	2.73935390	-2.67213297	3.26539993
H	3.27701497	2.76144195	4.42427492
H	-5.40854979	-3.53843403	-0.34700400
H	-0.22827300	-3.51614404	4.48848486
H	3.31961799	-3.94513607	-1.72011006
H	4.39206314	2.32486510	0.44855300
H	1.45079398	-0.85698903	2.23762393
H	2.99789500	0.94759202	2.81337905
H	-3.53441405	-2.53333497	0.84586501
H	0.36553901	-3.27546000	2.12541199
H	1.93907297	-1.96368802	-1.28107703
H	-3.92623806	2.30339694	1.88087499
H	-6.20038080	1.60146499	1.27561796
H	-6.61822701	0.44220099	-0.87790698
H	-4.71505880	-0.01867300	-2.39927292
H	-0.72960800	0.92076200	2.69352698
H	-0.56322902	2.12531400	4.84617805
H	-1.23957396	4.50057411	4.99477100
H	-2.05068207	5.67309093	2.96754694
H	-2.22690010	4.45248890	0.82740599

Cartesian coordinates for **1d**:

Ru	-0.05709000	-0.31923601	0.96407998
N	-0.05012700	-2.18351507	-0.32358000
C	-1.09776998	-3.06714511	0.18105900
C	-1.77744699	-2.73666406	1.34306502
N	-1.36830902	-1.57289302	2.05615997
Cl	1.50238395	-1.48324597	2.43746209
Cl	-0.51568198	1.23006296	2.73483706
P	1.80034900	0.89420903	0.13576999
P	-1.85626602	0.61790299	-0.17138100
C	3.01454496	1.53534806	1.37761796
C	1.54920602	2.40662408	-0.88452399
C	3.03659296	-0.02660700	-0.89166999
C	-3.49955797	0.12959100	0.55252802
C	-2.08177400	0.14757900	-1.94754303
C	-2.19958901	2.42680192	-0.22307099
C	2.75691795	1.56720197	2.74225998
C	1.93892503	3.67537904	-0.45988300
C	3.74728990	-1.03979599	-0.24320300
C	-3.74518800	0.52924198	1.87067103
C	-2.30548096	-1.18704700	-2.30105591
C	-3.38401389	2.87887192	-0.81178701
C	3.70423198	2.07214499	3.62562203
C	1.73057902	4.78831005	-1.26198494
C	4.79580784	-1.68304300	-0.87684900
C	-4.95575809	0.24921501	2.48510098
C	-2.39502501	-1.57949495	-3.62940311
C	-3.69984889	4.22568321	-0.82198000
C	4.91790819	2.54759789	3.16104293
C	1.13834405	4.65475321	-2.50764894
C	5.14995813	-1.34039605	-2.17480612
C	-5.95321989	-0.42663801	1.79554605
C	-2.26529503	-0.64250201	-4.64230585

C	-2.84164691	5.14416122	-0.22942400
C	5.18843794	2.51516104	1.79881096
C	0.73650002	3.39909196	-2.93777108
C	4.43933821	-0.35252899	-2.83426809
C	-5.72864294	-0.80998302	0.48411801
C	-2.05793595	0.68760997	-4.31009102
C	-1.67490697	4.70326614	0.37034699
C	4.24742985	2.01083398	0.91859102
C	0.92937398	2.29133391	-2.12731910
C	3.39361000	0.30393299	-2.19552588
C	-4.51484394	-0.53242600	-0.13288900
C	-1.96929097	1.07757294	-2.98167205
C	-1.35495102	3.35119390	0.37525100
C	-1.45665801	-4.21742296	-0.51704800
C	-2.50118089	-5.00880003	-0.07445000
C	-3.19465089	-4.66254997	1.07846105
C	-2.82748699	-3.53352690	1.78589594
C	1.09052002	-2.95255899	-0.76756102
C	1.71229398	-3.85270596	0.08709500
C	2.72222590	-4.66736507	-0.39756700
C	3.11939597	-4.58921099	-1.72511494
C	2.50845098	-3.67496896	-2.56874704
C	1.49287200	-2.86015892	-2.09269094
H	-0.42152399	-1.73553503	-1.15831602
H	-0.69711697	-1.81236696	2.79408598
H	-2.15477300	-1.08484805	2.47336698
H	1.81735098	1.19394505	3.11963892
H	2.40808201	3.80066490	0.50666898
H	3.48465204	-1.30752695	0.77362400
H	-2.97716689	1.07250202	2.41270399
H	-2.45444989	-1.93707502	-1.53324795
H	-4.07207584	2.17097306	-1.25910199
H	3.48383904	2.08252311	4.68651390

H	2.03847098	5.76529598	-0.90812200
H	5.34173918	-2.45595598	-0.34948501
H	-5.12103605	0.57302201	3.50614691
H	-2.57740808	-2.62099504	-3.86725307
H	-4.62202406	4.55849791	-1.28372002
H	5.65543604	2.93628502	3.85385299
H	0.98434699	5.52316904	-3.13688207
H	5.97699594	-1.83964598	-2.66615701
H	-6.90143299	-0.64125699	2.27401209
H	-2.33609509	-0.94417799	-5.68032694
H	-3.09113002	6.19885302	-0.22897400
H	6.13722181	2.87716603	1.42020404
H	0.26811600	3.28035688	-3.90824604
H	4.70769405	-0.06891500	-3.84558702
H	-6.50300121	-1.32378304	-0.07362500
H	-1.96957600	1.43423796	-5.09088182
H	-1.00590897	5.40911484	0.84746897
H	4.47944593	1.98376203	-0.13922100
H	0.59618503	1.31991005	-2.47174692
H	2.88728690	1.10249102	-2.71966505
H	-4.38298607	-0.82503998	-1.16513801
H	-1.81510794	2.12169695	-2.74786592
H	-0.46473300	3.00915408	0.87920702
H	-0.90861201	-4.48588419	-1.41195202
H	-2.77595997	-5.89595509	-0.63145602
H	-4.01576090	-5.27615309	1.42779100
H	-3.35335708	-3.25362611	2.69134212
H	1.40643895	-3.90448594	1.12262595
H	3.20220494	-5.37050676	0.27257901
H	3.90663695	-5.23294401	-2.09815788
H	2.81609106	-3.59464192	-3.60396504
H	1.00395596	-2.15662909	-2.75857210

Cartesian coordinates for 1e:

Ru	-0.00482000	-0.73108000	-0.16978700
N	-1.93784297	-2.07663608	-0.32318801
C	-2.52489495	-2.14439201	0.97428203
C	-1.71189404	-1.81338894	2.06090498
N	-0.33705699	-1.44307601	1.82052600
Cl	0.81497300	-3.08686399	-0.42972001
Cl	-0.13637701	-0.45495200	-2.52967596
P	2.24252701	-0.18808500	0.01654800
P	-0.99874401	1.29023600	0.15697999
C	3.09074807	-1.49486804	1.00702405
C	3.05326700	1.26961601	0.83685702
C	3.14786410	-0.18660700	-1.58530700
C	-1.00192499	1.91818404	1.90425801
C	-2.79660892	1.35605896	-0.23782800
C	-0.45217100	2.79224992	-0.77698702
C	2.86178303	-1.52954900	2.38247395
C	4.33594894	1.13121605	1.37802696
C	2.94843411	-1.23679197	-2.48383403
C	0.07011400	1.59107804	2.73280191
C	-3.77080798	0.98421699	0.68918598
C	-0.91122502	4.06087685	-0.41789299
C	3.44998789	-2.49562192	3.18282700
C	5.00337601	2.21644306	1.92259300
C	3.62426996	-1.26460505	-3.69261599
C	0.14588501	2.04734802	4.04098701
C	-5.11944485	1.09825504	0.38331601
C	-0.51243198	5.18483019	-1.12256706
C	4.28986311	-3.44501996	2.61777401
C	4.40844202	3.47019601	1.93634403
C	4.48460293	-0.23352100	-4.04064989
C	-0.86213797	2.84688306	4.55525112
C	-5.51543903	1.56381595	-0.86264098

C	0.34864599	5.05936813	-2.20475292
C	4.53797102	-3.40933990	1.25512695
C	3.14384508	3.62539601	1.39473903
C	4.66803122	0.82672399	-3.16814494
C	-1.93479502	3.19032192	3.74597692
C	-4.55411911	1.89127004	-1.80730903
C	0.80574000	3.80447006	-2.57166100
C	3.94393897	-2.44285798	0.45536900
C	2.47807288	2.53520799	0.85091001
C	4.00818110	0.84874499	-1.94683397
C	-2.00286007	2.73371696	2.43833899
C	-3.20619392	1.78728497	-1.49882901
C	0.41179401	2.67727900	-1.86263704
C	-3.83398199	-2.54063392	1.21789002
C	-4.33884096	-2.55549908	2.50945902
C	-3.53988194	-2.19031692	3.58004904
C	-2.21963596	-1.83398795	3.34862900
C	-2.73765206	-2.27471089	-1.49334598
C	-2.28392792	-3.18932891	-2.43926597
C	-3.00113201	-3.40322804	-3.60366106
C	-4.18091917	-2.71281099	-3.83775997
C	-4.62782478	-1.79863906	-2.89679098
C	-3.91058302	-1.57339704	-1.73165500
H	-1.17751896	-2.77358603	-0.36982900
H	0.25464401	-2.27695608	1.82014298
H	-0.02856900	-0.84228599	2.57529402
H	2.24484897	-0.76890701	2.84924889
H	4.82754612	0.16783001	1.36902905
H	2.25142598	-2.02712393	-2.23955297
H	0.87978101	0.99761099	2.32936597
H	-3.48383093	0.61700797	1.66666603
H	-1.58131301	4.18420696	0.42233300
H	3.26155996	-2.50008297	4.25015688

H	5.99651194	2.07900500	2.33385801
H	3.45863700	-2.09025002	-4.37434101
H	1.00111794	1.78438401	4.65252495
H	-5.86037922	0.81930000	1.12323594
H	-0.87695599	6.16122580	-0.82541800
H	4.75195694	-4.20305204	3.23861909
H	4.93023586	4.31852913	2.36334896
H	5.00258923	-0.25265700	-4.99246502
H	-0.81120902	3.20401692	5.57685995
H	-6.56860018	1.66067898	-1.09872603
H	0.65979701	5.93829393	-2.75721502
H	5.19612694	-4.14220905	0.80376899
H	2.66341805	4.59646702	1.39007401
H	5.32929802	1.64384699	-3.43180799
H	-2.72833896	3.81897807	4.13271713
H	-4.85104322	2.23319697	-2.79149604
H	1.47599399	3.69104099	-3.41537404
H	4.14517784	-2.43446112	-0.60731602
H	1.50034499	2.69048595	0.42491299
H	4.17036819	1.68524301	-1.28089094
H	-2.85739589	3.01048207	1.83556998
H	-2.46621704	2.04679108	-2.24513412
H	0.75735998	1.69743598	-2.16660500
H	-4.46244907	-2.82764506	0.38637999
H	-5.36634922	-2.85643411	2.67411494
H	-3.93318105	-2.19015288	4.58871412
H	-1.57347000	-1.56010997	4.17571020
H	-1.35139406	-3.71335912	-2.26660991
H	-2.62985706	-4.11270189	-4.33334684
H	-4.74322510	-2.88111806	-4.74820423
H	-5.54187012	-1.24226499	-3.06835294
H	-4.26811409	-0.84971499	-1.01465094

Cartesian coordinates for 1f:

Ru	0.42393699	0.47431400	-0.08966000
N	2.65458798	0.11354600	-0.32927400
C	3.20280099	-0.12208300	0.98785299
C	2.40431404	0.07730200	2.10341406
N	1.08186698	0.60675299	1.92637098
Cl	1.10953701	2.81357193	0.00267500
Cl	0.28990301	0.51894200	-2.48308301
P	-1.71652400	1.31066203	0.27885199
P	0.03458600	-1.77479398	-0.22000200
C	-1.64734101	2.67021990	1.52908301
C	-3.20249701	0.46974400	1.01153803
C	-2.47732210	2.08758497	-1.20480597
C	-0.05790800	-2.71884489	1.36954296
C	1.38815796	-2.66497803	-1.10857904
C	-1.41213799	-2.45875812	-1.14590704
C	-1.52472901	2.31248999	2.87157512
C	-4.23735094	1.26570702	1.51817596
C	-1.72419703	2.98446989	-1.96558905
C	-0.64076400	-2.09417701	2.47177505
C	2.56149507	-3.06580305	-0.46478701
C	-1.79436100	-3.79303098	-1.00141001
C	-1.43759894	3.27508211	3.86523008
C	-5.38253498	0.69855702	2.04857206
C	-2.26708198	3.57543898	-3.09498501
C	-0.76776499	-2.74536705	3.68967795
C	3.60257006	-3.64755106	-1.17636299
C	-2.87263799	-4.30034685	-1.70881796
C	-1.48558295	4.62072086	3.53064203
C	-5.52397490	-0.68296403	2.09099102
C	-3.55341697	3.25792098	-3.50549197
C	-0.30171099	-4.04286003	3.83449602
C	3.49155092	-3.83246899	-2.54540300

C	-3.58348703	-3.48260593	-2.57658505
C	-1.62597203	4.98718119	2.20129108
C	-4.51266623	-1.48337698	1.59086299
C	-4.29559088	2.34194112	-2.77760196
C	0.27654701	-4.68325377	2.74893403
C	2.33698511	-3.42516804	-3.19895601
C	-3.20775390	-2.15774393	-2.72967100
C	-1.70291996	4.02141619	1.20790005
C	-3.36676788	-0.90770501	1.05400598
C	-3.76325107	1.76293802	-1.63379502
C	0.39300001	-4.03068686	1.53043699
C	1.29678500	-2.84427691	-2.49057603
C	-2.13135195	-1.64623106	-2.01812100
C	4.50127602	-0.59372401	1.14986205
C	4.98664904	-0.89499998	2.40944600
C	4.17638588	-0.71852601	3.52379990
C	2.89262605	-0.22773699	3.36908102
C	3.47870207	0.94926703	-1.16980803
C	4.13803911	2.05896401	-0.65968901
C	4.93364096	2.82834911	-1.49278104
C	5.07442904	2.50112391	-2.83344007
C	4.41307402	1.39183903	-3.33721995
C	3.61940289	0.61365300	-2.50938606
H	2.59745789	-0.78691101	-0.80003399
H	1.11120403	1.63186896	1.97741199
H	0.48379400	0.26946399	2.66958594
H	-1.53966200	1.26465702	3.15558195
H	-4.14752102	2.34430599	1.49490499
H	-0.70338202	3.20354509	-1.67909205
H	-1.03399098	-1.09171104	2.35819507
H	2.66885304	-2.92978001	0.60469002
H	-1.25906205	-4.44654799	-0.32504699
H	-1.34820199	2.97352791	4.90253401

H	-6.16821480	1.33942604	2.43111396
H	-1.66803706	4.27260923	-3.66858292
H	-1.23802805	-2.23856711	4.52428579
H	4.50021791	-3.95665503	-0.65378499
H	-3.15781498	-5.33800697	-1.58028400
H	-1.42164803	5.37776899	4.30304289
H	-6.41902208	-1.12786305	2.50967693
H	-3.97065806	3.71339512	-4.39605999
H	-0.39282200	-4.55406094	4.78538418
H	4.30195189	-4.28814316	-3.10169005
H	-4.42694807	-3.87922406	-3.12957692
H	-1.66972494	6.03503990	1.92892599
H	-4.60610723	-2.56267095	1.60924101
H	-5.29654598	2.07355499	-3.09506202
H	0.63845497	-5.70004988	2.84709907
H	2.24334598	-3.55660892	-4.27033615
H	-3.75205398	-1.50866497	-3.40538692
H	-1.80293798	4.32741308	0.17554800
H	-2.60571289	-1.55630505	0.65355200
H	-4.36141586	1.05023599	-1.08240700
H	0.84739703	-4.55343294	0.69879401
H	0.41004300	-2.51525807	-3.01565599
H	-1.82706594	-0.61698800	-2.15930200
H	5.12259007	-0.72568500	0.27238101
H	5.99534512	-1.27257895	2.52256393
H	4.54718494	-0.95713198	4.51293516
H	2.25659895	-0.07352100	4.23368502
H	4.01922607	2.33037901	0.37985700
H	5.43839502	3.69761610	-1.08870101
H	5.69442511	3.10876799	-3.48140502
H	4.51041412	1.12609005	-4.38290882
H	3.08707690	-0.24119499	-2.90736890

Cartesian coordinates for **1g**:

Ru	-0.08282200	0.10039600	0.54074103
Cl	0.73883897	0.44327399	2.74950790
Cl	-1.41511595	0.09869800	-1.43803096
P	-0.34421599	-2.15420794	0.88565600
P	1.85740805	0.25841099	-0.50260800
C	-0.36167499	-3.40670109	-0.45096099
C	0.58756399	-4.42608404	-0.49308899
H	1.32398295	-4.51272678	0.29602200
C	0.59465200	-5.34246778	-1.53552699
H	1.33945096	-6.12931919	-1.55070603
C	-0.35032299	-5.25815296	-2.54585600
H	-0.35007900	-5.97997522	-3.35410810
C	-1.29700601	-4.24325895	-2.51609707
H	-2.03781295	-4.16534090	-3.30320811
C	-1.30029202	-3.31984305	-1.48280501
H	-2.02484298	-2.51586509	-1.48517501
C	-2.07369089	-2.16289806	1.50952804
C	-2.42247105	-1.16834903	2.42618895
H	-1.67153597	-0.46857300	2.77928400
C	-3.71487904	-1.08514297	2.92199612
H	-3.96729207	-0.29735300	3.62133503
C	-4.67463589	-2.00219202	2.52368999
H	-5.68502903	-1.93699896	2.90944791
C	-4.33276081	-3.00733709	1.63115895
H	-5.07320404	-3.73618698	1.32302904
C	-3.04437995	-3.08650804	1.12447000
H	-2.79925990	-3.87744403	0.42825100
C	0.53688902	-3.05560398	2.21570492
C	1.84560502	-2.73163700	2.55277991
H	2.33460593	-1.90035796	2.06740093
C	2.51962399	-3.45353293	3.52844501
H	3.53822708	-3.18458605	3.78079200

C	1.88876104	-4.49912214	4.18279505
H	2.41264701	-5.05703497	4.95009613
C	0.57804602	-4.82343578	3.85891604
H	0.07461300	-5.63467979	4.37138605
C	-0.09308100	-4.10756111	2.88156509
H	-1.11713398	-4.36612701	2.64112806
C	2.14085293	-0.45267400	-2.17258692
C	1.29131305	-1.39007795	-2.73864007
H	0.40586099	-1.69522703	-2.20571494
C	1.55735600	-1.91364002	-3.99826908
H	0.87916398	-2.64345908	-4.42340422
C	2.67461109	-1.50052202	-4.70283985
H	2.88054609	-1.90572906	-5.68663788
C	3.52905989	-0.55549997	-4.14676523
H	4.40245724	-0.22078501	-4.69376421
C	3.26349592	-0.03412100	-2.89335895
H	3.93407297	0.70613497	-2.47299600
C	2.18284893	2.02294207	-0.92976499
C	1.33727598	2.58139801	-1.89439404
H	0.56173497	1.96792400	-2.34281707
C	1.47814095	3.90322399	-2.28216505
H	0.80794698	4.31754494	-3.02594495
C	2.47312188	4.69142008	-1.71744299
H	2.58554196	5.72569609	-2.01943707
C	3.32293606	4.14498520	-0.77029198
H	4.10925913	4.74870682	-0.33264399
C	3.18101311	2.81891298	-0.37727100
H	3.87025595	2.40908599	0.34822401
C	3.36698890	-0.29864699	0.37956199
C	4.11349201	-1.37809598	-0.09376200
H	3.82465410	-1.87803304	-1.00872004
C	5.22874594	-1.82685602	0.59888899
H	5.79219723	-2.66892910	0.21507999

C	5.62013102	-1.20158303	1.77222204
H	6.49501419	-1.54813600	2.30962491
C	4.87788486	-0.13565800	2.26020908
H	5.16271782	0.34906399	3.18631601
C	3.75505400	0.30509499	1.57801497
H	3.15470099	1.09628797	2.00427604
N	-2.39875102	3.11951995	-1.08152795
C	-2.71103811	3.13363791	0.27981400
C	-1.74170196	2.67805505	1.18557799
N	-0.45980501	2.27631903	0.69197899
C	-3.93904805	3.56225109	0.77979797
C	-4.19918919	3.54385400	2.13906288
C	-3.23656797	3.08472705	3.02643800
C	-2.01186800	2.65046096	2.54683089
C	-2.93200898	3.96183610	-2.04618907
C	-3.28758907	5.28576708	-1.77404296
C	-3.75443912	6.10594606	-2.78790689
C	-3.86837292	5.63933516	-4.08993816
C	-3.50539804	4.32828283	-4.36560917
C	-3.04816103	3.49534988	-3.35952592
H	-2.10212398	2.20351291	-1.41628897
H	0.26093799	2.52915502	1.36106598
H	-0.27828401	2.75027394	-0.18916699
H	-4.69524479	3.90315390	0.08438700
H	-5.16269207	3.87964606	2.50316691
H	-3.43261099	3.06994200	4.09145880
H	-1.24474800	2.29076600	3.22242093
H	-3.18432403	5.67423916	-0.76885998
H	-4.02387810	7.12967110	-2.55444694
H	-4.23315096	6.28723001	-4.87699318
H	-3.58686304	3.94289494	-5.37540579
H	-2.77676296	2.46865892	-3.58044195

SMD/PCM (CHCl₃) Cartesian coordinates for 1:

Ru	-0.15007775	0.70109522	0.08019862
Cl	-0.06929033	1.09733438	2.47864842
Cl	-0.30015132	1.00850046	-2.30841660
P	-0.78856707	-1.54790723	0.30012658
P	2.11915302	0.36132708	-0.22158490
C	-1.19547796	-2.51658964	-1.21594799
C	-0.91876143	-3.87630248	-1.36154008
H	-0.38769540	-4.41153574	-0.58579081
C	-1.33014286	-4.56704998	-2.49311447
H	-1.10253394	-5.62294865	-2.58703136
C	-2.03564191	-3.91309524	-3.49266171
H	-2.35796595	-4.45328903	-4.37573814
C	-2.32791924	-2.56409383	-3.35252714
H	-2.88110828	-2.04296851	-4.12568188
C	-1.90944147	-1.87120986	-2.22582889
H	-2.12970901	-0.81643212	-2.13558078
C	-2.37240553	-1.79913700	1.23573732
C	-2.60488510	-1.08700895	2.41463280
H	-1.85696757	-0.38774589	2.77289557
C	-3.77363610	-1.26797676	3.14283824
H	-3.92811227	-0.70023257	4.05368948
C	-4.73464870	-2.16897273	2.70868802
H	-5.65003490	-2.30835271	3.27237153
C	-4.51039839	-2.89236116	1.54636681
H	-5.25051355	-3.60324883	1.19621956
C	-3.34207869	-2.71141410	0.81856483
H	-3.20034790	-3.28456640	-0.08742836
C	0.30050015	-2.72523713	1.21100330
C	1.46536446	-3.19499612	0.60273927
H	1.73294497	-2.86130309	-0.39168629
C	2.28813243	-4.10843849	1.24108791
H	3.18155336	-4.46351004	0.74079394

C	1.97482717	-4.55612230	2.51640439
H	2.61931181	-5.26807642	3.01923823
C	0.83364272	-4.08108282	3.14268255
H	0.57805651	-4.41830254	4.14098740
C	0.00036072	-3.17979741	2.49300933
H	-0.89555717	-2.84281516	2.99652982
C	2.71084023	-0.36957037	-1.80845296
C	1.93933237	-1.32900023	-2.45700240
H	0.95281333	-1.56353688	-2.08349252
C	2.39779210	-1.96230745	-3.60302997
H	1.77538764	-2.70539093	-4.08839750
C	3.63542461	-1.63112247	-4.13451290
H	3.99348783	-2.12000704	-5.03347111
C	4.40561867	-0.65730679	-3.51534104
H	5.36883497	-0.37867421	-3.92784500
C	3.94629741	-0.03136153	-2.36501598
H	4.56116724	0.73227882	-1.90547121
C	2.94993544	2.00838256	-0.27163839
C	2.88575888	2.78741527	-1.42989981
H	2.40728402	2.39115906	-2.31830144
C	3.42314506	4.06561804	-1.45390916
H	3.37067771	4.65141010	-2.36473751
C	4.02278757	4.59379578	-0.31795898
H	4.44279194	5.59293842	-0.33714497
C	4.07928085	3.83507204	0.84158802
H	4.54332209	4.23779535	1.73483324
C	3.54793215	2.55104637	0.86475658
H	3.60476017	1.96994555	1.77713645
C	3.19996333	-0.49861002	1.00985646
C	4.47370911	-0.96224183	0.67611229
H	4.83273935	-0.90085471	-0.34164682
C	5.30292606	-1.51923227	1.63738573
H	6.28790379	-1.87279892	1.35308087

C	4.87554598	-1.62494981	2.95355773
H	5.52541971	-2.05852938	3.70552921
C	3.60779238	-1.18073487	3.29331589
H	3.25470281	-1.26798511	4.31471777
C	2.77552223	-0.62706840	2.32995582
H	1.78770447	-0.28458232	2.60606861
N	-2.29106092	1.51622438	0.33942032
C	-2.19038391	2.91343808	0.72333109
C	-0.98487842	3.56794095	0.55592853
N	0.12245560	2.82877374	0.02082252
C	-3.27961850	3.59054780	1.25626647
C	-3.15657210	4.91885710	1.62754476
C	-1.94409335	5.57621050	1.46033502
C	-0.86033422	4.90161943	0.92399794
C	-3.33861899	1.31025720	-0.63302773
C	-3.34221339	2.03519559	-1.81959260
C	-4.35456896	1.84184957	-2.74467254
C	-5.37062073	0.92645925	-2.50033188
C	-5.37411833	0.21788660	-1.30926764
C	-4.36796331	0.41514179	-0.37313038
H	-2.52453351	0.98343307	1.17381787
H	0.97571254	3.10324597	0.49620441
H	0.24984635	3.03246593	-0.97024715
H	-4.22349215	3.07183528	1.38032353
H	-4.00537491	5.44079304	2.05328035
H	-1.84361064	6.61513996	1.75075889
H	0.09134851	5.40547562	0.79263473
H	-2.55049276	2.74221873	-2.02232409
H	-4.34522104	2.40980077	-3.66794634
H	-6.15828276	0.77608442	-3.22941256
H	-6.16836166	-0.48782617	-1.09460473
H	-4.38990402	-0.12852591	0.56282330

SMD/PCM (CHCl₃) Cartesian coordinates for **1b**:

Ru	0.11395046	0.27527004	-0.03332962
N	0.09973326	-1.81686997	-0.75839573
C	0.32438898	-2.68335533	0.38515803
C	0.28496656	-2.15128899	1.66494977
N	0.10350619	-0.72747803	1.82903922
Cl	0.16712260	1.14293420	-2.30757022
Cl	0.39199725	2.47114825	0.95085943
P	-2.24013519	0.72207010	0.22104669
P	2.49114847	0.32113048	-0.08759052
C	-3.52809167	-0.57238793	-0.08047608
C	-2.83126235	2.15511703	-0.75239110
C	-2.82133794	1.16887641	1.92865813
C	3.22702980	0.34856337	1.59312952
C	3.40146041	1.70234561	-0.90050095
C	3.31160188	-1.08584368	-0.95164371
C	-3.60970473	-1.61462092	0.84646082
C	-2.88333225	2.07272816	-2.14491248
C	-1.95081627	1.47141826	2.97236729
C	3.23704982	-0.78785706	2.40590429
C	2.77230501	2.86316395	-1.33633780
C	2.93455315	-1.26131606	-2.28770351
C	-4.59856939	-2.57960868	0.75842363
C	-3.31261969	3.15300775	-2.90076971
C	-2.43373632	1.78212988	4.23974752
C	3.70238113	-0.72851419	3.71318316
C	3.50839520	3.87282014	-1.94495177
C	3.48120213	-2.27875090	-3.05539465
C	-5.52629519	-2.53128886	-0.27391320
C	-3.66598868	4.34400320	-2.28225946
C	-3.79661012	1.81458747	4.48005390
C	4.15455770	0.47321230	4.23664999
C	4.87659502	3.73751140	-2.12099838

C	4.41864538	-3.13959360	-2.50142574
C	-5.44846106	-1.51266515	-1.20941651
C	-3.58614731	4.44717550	-0.90142947
C	-4.67874050	1.53635836	3.44279337
C	4.13964987	1.61224699	3.44363928
C	5.51391554	2.58364916	-1.68316019
C	4.81393147	-2.96333146	-1.18377411
C	-4.46088505	-0.53964692	-1.11135566
C	-3.17210793	3.36116147	-0.14273085
C	-4.19589996	1.21224689	2.18646193
C	3.67953730	1.55204046	2.13691783
C	4.78086376	1.57497394	-1.07864177
C	4.26772785	-1.94479036	-0.41346040
C	0.61607677	-4.03443861	0.21625938
C	0.83077967	-4.84818029	1.31354940
C	0.74880683	-4.32084990	2.59695077
C	0.48250288	-2.97466278	2.76926374
C	-0.84064889	-2.33996677	-1.73242652
C	-1.86137891	-3.21132660	-1.37920725
C	-2.70694971	-3.72278547	-2.35318565
C	-2.54469705	-3.37271738	-3.68437552
C	-1.52699637	-2.49682474	-4.03396749
C	-0.67727023	-1.98477376	-3.06689477
H	0.98833257	-1.75235343	-1.25396395
H	0.85808527	-0.36752346	2.41135669
H	-0.75005615	-0.53897244	2.34496021
H	-2.91181469	-1.66235864	1.67552984
H	-2.56655574	1.16849709	-2.64551687
H	-0.88753510	1.52538681	2.78141403
H	2.88880062	-1.73839188	2.02119327
H	1.70694458	2.96877265	-1.20196950
H	2.22315764	-0.56789267	-2.72903848
H	-4.64739132	-3.36830592	1.50093091

H	-3.35594797	3.06655884	-3.98072386
H	-1.73318112	2.01167083	5.03487396
H	3.70983434	-1.62626827	4.32096004
H	3.00216889	4.76973963	-2.28392601
H	3.17629910	-2.39411139	-4.08931875
H	-6.30547285	-3.28163266	-0.34419420
H	-3.99448109	5.19048071	-2.87488556
H	-4.17392111	2.06111073	5.46603012
H	4.51724052	0.52278227	5.25688553
H	5.44685173	4.52611589	-2.59925008
H	4.84750938	-3.93675327	-3.09756303
H	-6.16787004	-1.46064544	-2.01889133
H	-3.84573627	5.37658167	-0.40706095
H	-5.74907494	1.56988204	3.61292171
H	4.48557663	2.55809379	3.84498763
H	6.58369017	2.46591473	-1.81443787
H	5.55900764	-3.61937475	-0.74782193
H	-4.44747114	0.26148647	-1.83746207
H	-3.11443210	3.46177721	0.93295920
H	-4.90200806	0.99157119	1.39556742
H	3.66760278	2.45066714	1.53475344
H	5.29363203	0.67910624	-0.74839705
H	4.61224365	-1.81752884	0.60412395
H	0.66631883	-4.44648647	-0.78457391
H	1.06215250	-5.89640856	1.16744888
H	0.90807819	-4.95457077	3.46104383
H	0.44508886	-2.54243588	3.76326704
H	-1.99725127	-3.50867629	-0.34985059
H	-3.49736261	-4.40343857	-2.06055713
H	-3.20419860	-3.77873373	-4.44248819
H	-1.38489640	-2.21009445	-5.06984472
H	0.09730310	-1.28274286	-3.34092402

SMD/PCM (CHCl₃) Cartesian coordinates for 1c:

Ru	-0.29476452	0.52077031	-0.90708303
N	-1.64857602	1.87994361	0.39497057
C	-3.02477431	1.53602195	0.10825334
C	-3.28753281	0.90162319	-1.10286009
N	-2.16906810	0.55888134	-1.93354428
Cl	-0.15653376	2.74387097	-2.03893852
Cl	0.48460144	-0.52204269	-2.92141199
P	1.88004363	0.91626239	-0.01743886
P	-0.78536105	-1.60977602	-0.09826621
C	3.13311791	1.64832175	-1.17281806
C	2.86384630	-0.44836035	0.72740316
C	2.03759646	2.20603323	1.30166936
C	-2.29009891	-2.34560323	-0.91382974
C	-1.20251131	-1.84472764	1.68290877
C	0.31846792	-3.05380583	-0.42136276
C	2.97140265	1.65020192	-2.55346298
C	4.08806038	-0.87110233	0.21421359
C	1.59756625	3.49262166	0.98806256
C	-2.20968866	-2.59055305	-2.28923965
C	-2.28461289	-1.14937413	2.22445321
C	-0.15177867	-4.34121704	-0.14291254
C	3.94247484	2.20356727	-3.38078332
C	4.80338430	-1.88796782	0.83230084
C	1.80535674	4.54658794	1.86211634
C	-3.26190066	-3.18065786	-2.97268653
C	-2.65417004	-1.31342328	3.55064631
C	0.62718129	-5.45466948	-0.40615043
C	5.09067202	2.76008892	-2.84169030
C	4.31159830	-2.49489641	1.97743332
C	2.45444131	4.33701468	3.07129836
C	-4.41550159	-3.55288839	-2.29484010
C	-1.93409085	-2.16756201	4.37309599

C	1.89097905	-5.30256796	-0.96477997
C	5.26430178	2.76431203	-1.46329796
C	3.08804512	-2.08988571	2.49195552
C	2.88898301	3.06298828	3.39703178
C	-4.50018597	-3.33127260	-0.93028796
C	-0.84657276	-2.85450339	3.85463786
C	2.36081648	-4.03324032	-1.25688624
C	4.29505444	2.21569133	-0.63980931
C	2.36915016	-1.08410060	1.86536050
C	2.68569756	2.00679588	2.51775599
C	-3.44891524	-2.73225379	-0.24618913
C	-0.48711190	-2.69790053	2.52270555
C	1.57849300	-2.91684175	-0.98682564
C	-4.08385468	1.81113315	0.96517724
C	-5.38115263	1.46599185	0.61006832
C	-5.63908005	0.86186481	-0.60938227
C	-4.58485794	0.58253455	-1.46567881
C	-1.47164130	2.53862476	1.67156124
C	-0.99581176	1.85708141	2.77616143
C	-0.88221329	2.51103830	3.99528384
C	-1.23922205	3.84586525	4.11182165
C	-1.70005858	4.53371811	2.99779201
C	-1.81423140	3.88257194	1.78030384
H	-1.36878538	2.56914210	-0.31896693
H	-1.99642229	1.27761030	-2.63713288
H	-2.34775829	-0.31372219	-2.42024612
H	2.07917452	1.22147787	-2.98500013
H	4.49384546	-0.40933168	-0.67609364
H	1.10480809	3.67170310	0.03914060
H	-1.30617654	-2.32043481	-2.82571268
H	-2.85687399	-0.47271103	1.60363007
H	-1.14051950	-4.47992945	0.27831244
H	3.79182839	2.19877076	-4.45474386

H	5.75247192	-2.20320439	0.41355172
H	1.45895302	5.53855658	1.59534502
H	-3.17410040	-3.35728550	-4.03885555
H	-3.50426507	-0.76568198	3.94130087
H	0.24459937	-6.44370556	-0.18023092
H	5.84556484	3.19358754	-3.48827195
H	4.87562370	-3.28219962	2.46432877
H	2.61990523	5.16318083	3.75348759
H	-5.23707485	-4.01875448	-2.82680631
H	-2.21938515	-2.29600120	5.41087818
H	2.50020742	-6.17396212	-1.17735803
H	6.15622044	3.19884562	-1.02576911
H	2.69286251	-2.55660534	3.38708878
H	3.40095878	2.88371897	4.33602428
H	-5.38903618	-3.62630105	-0.38390315
H	-0.27289996	-3.52271652	4.48707056
H	3.33983874	-3.90335274	-1.70324588
H	4.44712496	2.23700690	0.43226185
H	1.41517901	-0.78124017	2.27961493
H	3.06157947	1.02931941	2.78652096
H	-3.54388118	-2.58764458	0.82079870
H	0.35826012	-3.25171661	2.13853097
H	1.94010973	-1.93535364	-1.24605370
H	-3.89864612	2.28769803	1.91761601
H	-6.19246387	1.67866826	1.29631543
H	-6.65126371	0.59714562	-0.89005274
H	-4.76145649	0.09686406	-2.41888309
H	-0.71021855	0.81987965	2.67753530
H	-0.50294214	1.97249067	4.85581732
H	-1.14781523	4.35240841	5.06564522
H	-1.96937692	5.58090115	3.07432532
H	-2.18058753	4.41607618	0.90938002

SMD/PCM (CHCl₃) Cartesian coordinates for **1d**:

Ru	-0.06306731	-0.32900047	0.97505933
N	-0.07312745	-2.17599797	-0.32279897
C	-1.10555625	-3.07543063	0.19148372
C	-1.77520990	-2.75497794	1.36008692
N	-1.39283085	-1.56623435	2.05645084
Cl	1.49438155	-1.51588857	2.46308351
Cl	-0.48991135	1.22912455	2.76791525
P	1.79788697	0.89791483	0.12856676
P	-1.86253524	0.60655963	-0.17975207
C	3.01951146	1.53731668	1.37226319
C	1.54372871	2.41707778	-0.88085061
C	3.04868984	-0.00895203	-0.89600676
C	-3.51141739	0.14524694	0.54943603
C	-2.07881260	0.11187198	-1.94744408
C	-2.19941998	2.41782045	-0.25221947
C	2.79249740	1.51420426	2.74265838
C	1.90212142	3.68756652	-0.43316126
C	3.73866224	-1.04166865	-0.25669795
C	-3.74699354	0.54560035	1.86923492
C	-2.34644508	-1.21987092	-2.28049684
C	-3.36848831	2.86570311	-0.87515384
C	3.75235128	1.99290478	3.62840652
C	1.70491350	4.80587053	-1.23081982
C	4.80722046	-1.66862071	-0.87383246
C	-4.96953821	0.30998370	2.47946072
C	-2.44886374	-1.62908852	-3.60303760
C	-3.69400644	4.21080303	-0.88866621
C	4.95159340	2.50175452	3.15930009
C	1.15609431	4.67546463	-2.49699569
C	5.20053053	-1.29087090	-2.15115881
C	-5.98868704	-0.32504994	1.78241813
C	-2.28583169	-0.71117043	-4.62886810

C	-2.86081243	5.13267946	-0.26457664
C	5.19034386	2.53157330	1.79041457
C	0.78250158	3.41864991	-2.95027041
C	4.50760221	-0.28645793	-2.80527353
C	-5.77238750	-0.71435815	0.47063377
C	-2.02976513	0.61612940	-4.31738234
C	-1.70664573	4.69702959	0.36417800
C	4.23639631	2.05013847	0.90998703
C	0.96282786	2.30541086	-2.14313865
C	3.44452810	0.35499898	-2.17959642
C	-4.54723644	-0.47833660	-0.14184514
C	-1.93020332	1.02232683	-2.99436760
C	-1.37683427	3.34629083	0.37001914
C	-1.45646155	-4.23194456	-0.50170571
C	-2.47348523	-5.04507637	-0.03402949
C	-3.14637971	-4.71650934	1.13695085
C	-2.79378247	-3.57532787	1.83261275
C	1.07022345	-2.93295479	-0.78825104
C	1.69649255	-3.85405064	0.04082568
C	2.70953655	-4.65287638	-0.46478054
C	3.10528636	-4.53809881	-1.79066038
C	2.48373699	-3.60958552	-2.61139250
C	1.46676350	-2.80939317	-2.11247802
H	-0.46092236	-1.73517179	-1.15456378
H	-0.78999621	-1.79605246	2.85049963
H	-2.20763779	-1.07825136	2.41736555
H	1.86343157	1.11612391	3.12019587
H	2.33705950	3.81509876	0.54903501
H	3.44152093	-1.34110141	0.74147671
H	-2.96304655	1.06099987	2.41472483
H	-2.52029920	-1.95331717	-1.50236094
H	-4.03791952	2.15766263	-1.34961176
H	3.55460429	1.95953488	4.69418573

H	1.98726845	5.78362417	-0.85697860
H	5.33691502	-2.45771575	-0.35321930
H	-5.12654448	0.63279063	3.50268388
H	-2.66680884	-2.66745567	-3.82516885
H	-4.60333920	4.53950500	-1.37906456
H	5.69976711	2.87065744	3.85218358
H	1.01365089	5.54736948	-3.12503719
H	6.04018688	-1.77987170	-2.63220119
H	-6.94594765	-0.50757706	2.25719905
H	-2.36664772	-1.02496064	-5.66312742
H	-3.11808586	6.18598890	-0.26576799
H	6.12521744	2.92422485	1.40637481
H	0.35025254	3.30399251	-3.93806195
H	4.80215836	0.02070759	-3.80283689
H	-6.56294537	-1.19861698	-0.09137947
H	-1.91336572	1.34706271	-5.10981083
H	-1.05518126	5.40764523	0.85958266
H	4.44827127	2.07075405	-0.15225899
H	0.65598893	1.33370936	-2.51021981
H	2.95320153	1.16499913	-2.70026851
H	-4.42498064	-0.77105939	-1.17530096
H	-1.74268842	2.06422281	-2.77652788
H	-0.49383751	3.00883603	0.88979936
H	-0.93067956	-4.49112701	-1.41257298
H	-2.74353814	-5.93732929	-0.58633476
H	-3.94246578	-5.35116863	1.50763202
H	-3.30497193	-3.30812120	2.75114584
H	1.38669705	-3.94499707	1.07247829
H	3.19253540	-5.37251043	0.18640712
H	3.89544177	-5.16861820	-2.18124151
H	2.78405595	-3.50693154	-3.64726114
H	0.97115982	-2.09728408	-2.76397347

SMD/PCM (CHCl₃) Cartesian coordinates for 1e:

Ru	-0.00799294	-0.72048652	-0.19512500
N	-1.94999123	-2.05884910	-0.36373782
C	-2.53087902	-2.15826082	0.93936294
C	-1.72758591	-1.81718183	2.02708244
N	-0.36758259	-1.37900019	1.79441094
Cl	0.80720878	-3.09147310	-0.45177186
Cl	-0.09346277	-0.46465713	-2.57745409
P	2.25440717	-0.19622235	0.02708301
P	-0.99664789	1.31863713	0.14344381
C	3.09389806	-1.51384354	1.01211858
C	3.05308199	1.26049185	0.86026353
C	3.18644595	-0.19451836	-1.56241035
C	-0.96993786	1.95357394	1.88799846
C	-2.80582500	1.38188100	-0.20278126
C	-0.46830010	2.81349397	-0.81220806
C	2.79859281	-1.60619426	2.37249207
C	4.29136753	1.11586738	1.49431717
C	3.00865650	-1.24872971	-2.46062899
C	0.10529859	1.62757742	2.71342969
C	-3.73922467	0.95688814	0.74385732
C	-0.94714284	4.08091021	-0.47340363
C	3.39885974	-2.56490135	3.17370629
C	4.94267035	2.20695448	2.04967570
C	3.72156954	-1.29185188	-3.64803672
C	0.18550983	2.08465552	4.02160883
C	-5.10045671	1.06593311	0.49879563
C	-0.56819886	5.19970274	-1.19771194
C	4.32230663	-3.44561744	2.62658119
C	4.37779379	3.47232842	1.97722471
C	4.60324717	-0.27041140	-3.97525024
C	-0.81880659	2.88903761	4.53605509
C	-5.55253029	1.58535433	-0.70650947

C	0.29444087	5.07124805	-2.27891445
C	4.63768053	-3.35145569	1.28013515
C	3.15743685	3.63351631	1.34154940
C	4.76795912	0.79405349	-3.10326934
C	-1.89252675	3.23625159	3.72840405
C	-4.63379478	1.97557127	-1.67011619
C	0.77492017	3.81833959	-2.62391257
C	4.02718115	-2.39553833	0.47876927
C	2.50665474	2.53801513	0.79107457
C	4.06767082	0.82976758	-1.90400040
C	-1.96790516	2.77328038	2.42327452
C	-3.27241874	1.87382102	-1.42112005
C	0.39849067	2.69714570	-1.89515316
C	-3.82589650	-2.60175848	1.17876840
C	-4.32293034	-2.66338301	2.47182465
C	-3.52882433	-2.29869056	3.54732013
C	-2.22454524	-1.88706589	3.31841302
C	-2.77034307	-2.26922536	-1.51775098
C	-2.37523556	-3.24115968	-2.43295860
C	-3.12743902	-3.48125887	-3.57168555
C	-4.28690672	-2.75713515	-3.80945086
C	-4.67886877	-1.78776169	-2.89769483
C	-3.92503214	-1.53812814	-1.76022911
H	-1.19271660	-2.75599194	-0.41985846
H	0.26603991	-2.17029238	1.90942442
H	-0.13332458	-0.69808555	2.50739598
H	2.11924720	-0.89781284	2.83325911
H	4.76467752	0.14538257	1.55432796
H	2.30378652	-2.03510618	-2.22686601
H	0.91511917	1.03236842	2.31309319
H	-3.40986896	0.55641782	1.69422555
H	-1.61971498	4.20916080	0.36425221
H	3.15350747	-2.61419249	4.22852612

H	5.90098190	2.06424475	2.53636837
H	3.57739305	-2.12456560	-4.32724810
H	1.03680992	1.81299806	4.63511992
H	-5.80728292	0.74411041	1.25504005
H	-0.94887286	6.17519522	-0.91652250
H	4.79738855	-4.19428396	3.24989271
H	4.88744307	4.32499695	2.41122818
H	5.15424776	-0.30249965	-4.90861034
H	-0.76563656	3.24625182	5.55796576
H	-6.61564779	1.67841029	-0.89659470
H	0.59061056	5.94632578	-2.84621286
H	5.36468744	-4.02701902	0.84356946
H	2.70208454	4.61475372	1.27170169
H	5.44612885	1.60323358	-3.34991908
H	-2.68346953	3.86824322	4.11637163
H	-4.97485781	2.36625528	-2.62193942
H	1.45042145	3.70529246	-3.46443033
H	4.28904963	-2.34085846	-0.56948870
H	1.56256187	2.69588518	0.29491100
H	4.21886110	1.66805553	-1.23750222
H	-2.82683539	3.04858017	1.82639015
H	-2.57051635	2.19272661	-2.18130064
H	0.76667517	1.71919560	-2.17615652
H	-4.45280027	-2.89237785	0.34693426
H	-5.34020185	-3.00011230	2.63379669
H	-3.91661024	-2.33708572	4.55811691
H	-1.58359945	-1.60996020	4.14891768
H	-1.46914279	-3.80715132	-2.24937105
H	-2.80322099	-4.24088001	-4.27385187
H	-4.87970066	-2.94615602	-4.69683170
H	-5.58072758	-1.21194041	-3.07180977
H	-4.24393749	-0.77900356	-1.06143129

SMD/PCM (CHCl₃) Cartesian coordinates for **1f**:

Ru	0.42132780	0.48154718	-0.09857317
N	2.65577316	0.11001663	-0.31844753
C	3.20677352	-0.06884081	1.00969732
C	2.39431000	0.12363865	2.11449027
N	1.04131091	0.57594270	1.91936100
Cl	1.11384201	2.82983208	0.00245040
Cl	0.30441621	0.56341887	-2.50863743
P	-1.73297715	1.31315196	0.29707167
P	0.03770216	-1.77968919	-0.23374771
C	-1.65212035	2.67623782	1.54529369
C	-3.20411682	0.45621464	1.04102087
C	-2.52176833	2.10676432	-1.16617572
C	-0.09204923	-2.72379398	1.35124409
C	1.41153729	-2.66906905	-1.09297824
C	-1.38408566	-2.45993829	-1.20053184
C	-1.48915279	2.32301760	2.88513756
C	-4.21690559	1.23066950	1.62121832
C	-1.77814758	3.00725722	-1.93145788
C	-0.70069540	-2.10433221	2.44256473
C	2.57073593	-3.06970668	-0.42278305
C	-1.72254443	-3.81166649	-1.12053478
C	-1.39640641	3.28889656	3.87583590
C	-5.34603024	0.64174271	2.16477537
C	-2.34481621	3.63950944	-3.02707529
C	-0.85801953	-2.76029015	3.65480280
C	3.61704350	-3.67630506	-1.10636592
C	-2.77185607	-4.32456112	-1.86685836
C	-1.47986281	4.63364077	3.54234385
C	-5.49590635	-0.73955500	2.14069605
C	-3.65321040	3.36128545	-3.39874625
C	-0.39973751	-4.06049824	3.80269885
C	3.52692342	-3.88469458	-2.47385812

C	-3.49981880	-3.49319005	-2.70827627
C	-1.66250110	4.99607849	2.21628761
C	-4.50923777	-1.51834583	1.56185246
C	-4.38946629	2.44292879	-2.66630435
C	0.20301159	-4.69691849	2.72737122
C	2.38841176	-3.47517276	-3.15488887
C	-3.17133927	-2.14935565	-2.79399848
C	-1.74502933	4.02646494	1.22626126
C	-3.37912869	-0.92096198	1.01533747
C	-3.82935023	1.82241511	-1.55716610
C	0.35271505	-4.03776598	1.51579666
C	1.34331572	-2.87011600	-2.47352910
C	-2.12160730	-1.63497818	-2.04438424
C	4.52208567	-0.48593175	1.19108081
C	5.01124763	-0.72517765	2.46253753
C	4.18920183	-0.54498971	3.56835699
C	2.88499498	-0.11844053	3.39307094
C	3.49066901	0.88935912	-1.19969285
C	4.13508177	2.03879666	-0.76101547
C	4.95917797	2.73987961	-1.62789154
C	5.14793587	2.30386353	-2.93247366
C	4.50264263	1.15482414	-3.36604953
C	3.67447495	0.45084232	-2.50482702
H	2.59437203	-0.81362319	-0.74256289
H	1.00258029	1.58721197	2.06665349
H	0.45447367	0.14601673	2.62384439
H	-1.47590590	1.27739573	3.17548442
H	-4.12574673	2.30883932	1.64999211
H	-0.74696827	3.20105839	-1.66588485
H	-1.09546053	-1.10302138	2.32617068
H	2.66095114	-2.92510462	0.64723474
H	-1.17245877	-4.47790384	-0.46858335
H	-1.27235937	2.98938990	4.91047335

H	-6.11352634	1.26585245	2.60860658
H	-1.75429034	4.34456968	-3.60138226
H	-1.34277546	-2.25357771	4.48160744
H	4.50112772	-3.98872566	-0.56247807
H	-3.02192235	-5.37657785	-1.78883052
H	-1.41281199	5.39258718	4.31347132
H	-6.37750673	-1.20102775	2.57097149
H	-4.09296942	3.85145354	-4.26014423
H	-0.51459438	-4.57694054	4.74871826
H	4.33976316	-4.36360598	-3.00765586
H	-4.32070589	-3.89434004	-3.29204202
H	-1.73985600	6.04291296	1.94466555
H	-4.60948277	-2.59724116	1.53002596
H	-5.40752411	2.20496130	-2.95354891
H	0.55932683	-5.71608353	2.82727194
H	2.31025195	-3.62604356	-4.22558498
H	-3.73328972	-1.49124229	-3.44711590
H	-1.88459098	4.33192492	0.19820249
H	-2.63567924	-1.55224347	0.55781156
H	-4.42509127	1.10968304	-1.00292659
H	0.82858449	-4.56003523	0.69603491
H	0.46662626	-2.54919219	-3.02040339
H	-1.85486686	-0.58972585	-2.12965608
H	5.15746641	-0.62795871	0.32522318
H	6.03368807	-1.06000245	2.59026670
H	4.56641865	-0.73546112	4.56607246
H	2.23611188	0.03306591	4.24922609
H	3.99449348	2.38591194	0.25291011
H	5.45735884	3.63652802	-1.27700889
H	5.79681540	2.85377097	-3.60422468
H	4.64146233	0.79938662	-4.38077450
H	3.16291809	-0.44010261	-2.84802246

SMD/PCM (CHCl₃) Cartesian coordinates for **1g**:

Ru	-0.09578462	0.09146255	0.55363518
Cl	0.73204684	0.45404440	2.76163888
Cl	-1.46329439	0.06873019	-1.40318394
P	-0.34019518	-2.17041469	0.89793754
P	1.84679747	0.25892782	-0.49965262
C	-0.34199297	-3.42689943	-0.43580997
C	0.62061304	-4.43453121	-0.47319046
H	1.36921453	-4.50171900	0.30643615
C	0.62709415	-5.36900425	-1.50008130
H	1.38175356	-6.14724064	-1.51023996
C	-0.32860178	-5.31204939	-2.50290561
H	-0.32805848	-6.04706383	-3.29974508
C	-1.28496909	-4.30587482	-2.48190737
H	-2.03332901	-4.24844599	-3.26428437
C	-1.28830886	-3.36672735	-1.46243978
H	-2.02622294	-2.57529402	-1.46977520
C	-2.06881475	-2.19690418	1.53140974
C	-2.40913415	-1.23134482	2.48258114
H	-1.65790737	-0.53403509	2.83960938
C	-3.69198656	-1.17290950	3.00753808
H	-3.93476462	-0.41623574	3.74435973
C	-4.65522718	-2.08171654	2.59607387
H	-5.65829563	-2.03655624	3.00440669
C	-4.32438803	-3.05401683	1.66319132
H	-5.06627321	-3.77759409	1.34456146
C	-3.04258871	-3.11284399	1.13503480
H	-2.80741978	-3.88718224	0.41724089
C	0.54479992	-3.06709838	2.23192143
C	1.84624195	-2.72919774	2.58513713
H	2.33075047	-1.88979876	2.10804629
C	2.52067471	-3.45225239	3.56095266
H	3.53413105	-3.17580438	3.82759094

C	1.89929926	-4.51549387	4.19731331
H	2.42523360	-5.07575321	4.96212196
C	0.59608948	-4.85494518	3.85637522
H	0.09978851	-5.68156481	4.35205889
C	-0.07541552	-4.13651037	2.88040733
H	-1.09159195	-4.41287136	2.62567830
C	2.11186576	-0.43285105	-2.18197036
C	1.25826812	-1.36421347	-2.75316811
H	0.38690409	-1.69168699	-2.20938206
C	1.50240803	-1.85615945	-4.03059006
H	0.82015061	-2.57770109	-4.46443892
C	2.60554814	-1.42223489	-4.74629164
H	2.79494548	-1.80409586	-5.74320412
C	3.46809697	-0.48892549	-4.18220091
H	4.33290577	-0.14103903	-4.73568869
C	3.22188234	0.00373148	-2.91254854
H	3.89970708	0.73607582	-2.48937368
C	2.16293526	2.02997398	-0.91015089
C	1.34151149	2.58338308	-1.89888740
H	0.59275889	1.96346319	-2.38192415
C	1.47577024	3.90932083	-2.27573729
H	0.82975858	4.31762409	-3.04430246
C	2.43767452	4.71007204	-1.67171240
H	2.54593897	5.74786139	-1.96485484
C	3.26256251	4.17021322	-0.69863421
H	4.02481079	4.78218079	-0.22995660
C	3.12838531	2.83904433	-0.31930190
H	3.80269551	2.43891239	0.42490765
C	3.36255217	-0.30981210	0.36407748
C	4.10603285	-1.38107824	-0.13321581
H	3.80281496	-1.87914085	-1.04453921
C	5.24112701	-1.82593608	0.52977830
H	5.80186224	-2.66142082	0.12640497

C	5.65696239	-1.20403111	1.69703615
H	6.54851961	-1.54629755	2.21009660
C	4.91665268	-0.14838316	2.21100354
H	5.22186947	0.33451387	3.13228345
C	3.77272868	0.28603402	1.55944729
H	3.17890382	1.07124388	2.00516987
N	-2.42124057	3.11629319	-1.12167668
C	-2.73052931	3.14044523	0.24114430
C	-1.76029789	2.69529819	1.15229189
N	-0.48129842	2.27549529	0.66643733
C	-3.96008730	3.57305074	0.73545659
C	-4.21796227	3.58157849	2.09596753
C	-3.25200176	3.14100718	2.98947001
C	-2.02936053	2.69543052	2.51427269
C	-2.90041924	3.98553753	-2.08831215
C	-3.26315355	5.30585289	-1.80367374
C	-3.67372513	6.15381479	-2.82041287
C	-3.72361875	5.71956444	-4.13840151
C	-3.35649300	4.41140604	-4.42605639
C	-2.95544553	3.55132675	-3.41796207
H	-2.11734700	2.20435596	-1.45653188
H	0.24590838	2.56811237	1.31190729
H	-0.30649897	2.71894503	-0.23184629
H	-4.72012568	3.90183449	0.03780562
H	-5.18184948	3.92252612	2.45573163
H	-3.44653630	3.14344716	4.05532169
H	-1.26369560	2.34754872	3.19742632
H	-3.20949411	5.67508268	-0.78734857
H	-3.94839811	7.17405748	-2.57523370
H	-4.04401159	6.38873863	-4.92791319
H	-3.38868403	4.04948282	-5.44787025
H	-2.67717505	2.52976179	-3.65517998

SMD/PCM (toluene) Cartesian coordinates for 1:

Ru	-0.14413518	0.70574862	0.08216618
Cl	-0.08009372	1.10409784	2.47880650
Cl	-0.27785513	1.02404821	-2.30547953
P	-0.78878319	-1.54038560	0.29441857
P	2.12285495	0.35792693	-0.21219254
C	-1.19942927	-2.49919796	-1.22664487
C	-0.93024558	-3.85991406	-1.37716663
H	-0.40628958	-4.40132332	-0.60091853
C	-1.33883369	-4.54199266	-2.51462173
H	-1.11706960	-5.59860945	-2.61270428
C	-2.03368545	-3.87829828	-3.51503038
H	-2.35320187	-4.41160059	-4.40312767
C	-2.31856847	-2.52861381	-3.36982822
H	-2.86241460	-1.99949527	-4.14380741
C	-1.90339959	-1.84392655	-2.23705792
H	-2.11628294	-0.78782529	-2.14414525
C	-2.36988568	-1.79363227	1.23368979
C	-2.58545732	-1.10481203	2.42953968
H	-1.83028042	-0.41676444	2.79401374
C	-3.74799776	-1.29415989	3.16514945
H	-3.88879228	-0.74568653	4.08971786
C	-4.71939373	-2.17924833	2.72169375
H	-5.62923813	-2.32595563	3.29224563
C	-4.51240253	-2.87763929	1.54141176
H	-5.26089907	-3.57548237	1.18341792
C	-3.35046959	-2.68872523	0.80585974
H	-3.22104144	-3.24253750	-0.11380012
C	0.29773563	-2.72819519	1.19582152
C	1.46395051	-3.18918562	0.58362633
H	1.73288691	-2.84210920	-0.40584081
C	2.28616166	-4.11029625	1.21125364
H	3.18112803	-4.45698452	0.70821559

C	1.97041976	-4.57600498	2.47926307
H	2.61447644	-5.29389048	2.97380066
C	0.82702357	-4.11154604	3.10864115
H	0.56891859	-4.46348572	4.10101604
C	-0.00515213	-3.20151615	2.47024488
H	-0.90235609	-2.87280536	2.97647166
C	2.71942163	-0.36475512	-1.80071521
C	1.94636095	-1.31212211	-2.46464515
H	0.95597661	-1.54484606	-2.10049248
C	2.40781522	-1.93346906	-3.61578584
H	1.78312373	-2.66608906	-4.11350965
C	3.64916158	-1.60185039	-4.13706017
H	4.00858593	-2.08038139	-5.04084539
C	4.42119169	-0.64017469	-3.50204659
H	5.38760185	-0.36123854	-3.90633965
C	3.95988321	-0.02709701	-2.34608769
H	4.57660627	0.72668082	-1.87306643
C	2.95917702	2.00309372	-0.25336346
C	2.90067816	2.78458095	-1.41033459
H	2.42515278	2.38982987	-2.30109215
C	3.43920517	4.06221342	-1.42906463
H	3.39147115	4.64978266	-2.33884358
C	4.03453970	4.58720875	-0.28957561
H	4.45596790	5.58566999	-0.30491024
C	4.08595133	3.82567430	0.86799288
H	4.54710674	4.22559834	1.76376450
C	3.55348253	2.54220915	0.88639498
H	3.60573435	1.95872927	1.79743266
C	3.19567442	-0.50979370	1.02032220
C	4.45632315	-1.00571370	0.68384856
H	4.80809402	-0.96653372	-0.33746767
C	5.27925682	-1.56852341	1.64694452
H	6.25393152	-1.94765425	1.36078095

C	4.85865688	-1.64834774	2.96676278
H	5.50370073	-2.08674240	3.71987343
C	3.60360861	-1.17193079	3.30925822
H	3.25542593	-1.23835576	4.33373928
C	2.77697849	-0.61219311	2.34477234
H	1.79812825	-0.24542837	2.62301970
N	-2.28452182	1.52684164	0.33878386
C	-2.18754649	2.93506026	0.68216175
C	-0.97627223	3.58157396	0.52624047
N	0.13866608	2.83076382	0.02646570
C	-3.28530598	3.63034582	1.17330718
C	-3.16438746	4.96533060	1.51830769
C	-1.94512296	5.61319828	1.36666894
C	-0.85378397	4.92208719	0.86974460
C	-3.35235023	1.28521132	-0.60279846
C	-3.36285114	1.94054532	-1.82923782
C	-4.39642191	1.71564889	-2.72318625
C	-5.42753983	0.84066653	-2.40672541
C	-5.42308474	0.20200330	-1.17724288
C	-4.39486885	0.42954549	-0.27283618
H	-2.49244475	1.01848519	1.19523776
H	0.98141086	3.10100174	0.52241677
H	0.29102072	3.02162576	-0.96346575
H	-4.23423433	3.11894679	1.28584421
H	-4.02070665	5.49996614	1.91150093
H	-1.84533024	6.65727472	1.63774586
H	0.10375765	5.41720200	0.74957663
H	-2.55688477	2.61241031	-2.08670712
H	-4.39163685	2.22728825	-3.67864180
H	-6.23192406	0.66581720	-3.11142635
H	-6.22740746	-0.47256243	-0.90788519
H	-4.40965462	-0.05928119	0.69315147

SMD/PCM (toluene) Cartesian coordinates for **1g**:

Ru	-0.09641241	0.08697950	0.55200797
Cl	0.73218256	0.44751087	2.75902009
Cl	-1.45737290	0.06891184	-1.40858150
P	-0.34055293	-2.17422390	0.89573729
P	1.84355474	0.26017064	-0.50151998
C	-0.34763685	-3.43145847	-0.43761703
C	0.60625845	-4.44726324	-0.47211730
H	1.35009754	-4.52137947	0.31130254
C	0.60962319	-5.37974548	-1.50050211
H	1.35777986	-6.16402197	-1.50862455
C	-0.34167469	-5.31391335	-2.50658560
H	-0.34398416	-6.04793882	-3.30413675
C	-1.29026604	-4.30059242	-2.48754787
H	-2.03535748	-4.23624039	-3.27226639
C	-1.28989816	-3.36228347	-1.46747315
H	-2.02008200	-2.56364679	-1.47711754
C	-2.06848478	-2.19708443	1.53013754
C	-2.40511894	-1.23215878	2.48297381
H	-1.65054083	-0.54022455	2.84324312
C	-3.68860054	-1.16821599	3.00495839
H	-3.92906094	-0.40994081	3.74065256
C	-4.65512753	-2.07166386	2.59076262
H	-5.65877676	-2.02183962	2.99672103
C	-4.32733107	-3.04442787	1.65770650
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C	-3.04568672	-3.10780120	1.13059223
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C	0.54521501	-3.06979656	2.22927713
C	1.84763050	-2.73240709	2.57859826
H	2.33207488	-1.89540434	2.09740305
C	2.52187634	-3.45093012	3.55739737
H	3.53549242	-3.17364311	3.82171392

C	1.89902484	-4.50857735	4.20079184
H	2.42430878	-5.06460524	4.96892548
C	0.59512198	-4.84766865	3.86351776
H	0.09771956	-5.66957617	4.36551905
C	-0.07646166	-4.13383627	2.88464856
H	-1.09410036	-4.40777779	2.63359594
C	2.11210799	-0.43173000	-2.18319917
C	1.26248860	-1.36765671	-2.75246525
H	0.39146113	-1.69579744	-2.20868421
C	1.50980425	-1.86234820	-4.02790022
H	0.83048999	-2.58769131	-4.45956182
C	2.61128592	-1.42584348	-4.74389362
H	2.80263019	-1.80936754	-5.73961020
C	3.46913433	-0.48704308	-4.18240309
H	4.33209705	-0.13627237	-4.73658848
C	3.22024989	0.00795807	-2.91448903
H	3.89395618	0.74472481	-2.49271655
C	2.15453553	2.03205347	-0.91361600
C	1.32356465	2.58542657	-1.89428389
H	0.57041544	1.96487188	-2.36965823
C	1.45233655	3.91213727	-2.26990962
H	0.79683203	4.32084417	-3.03002191
C	2.41898417	4.71289730	-1.67411685
H	2.52266955	5.75122786	-1.96636760
C	3.25358105	4.17293072	-0.70971072
H	4.01909399	4.78548241	-0.24747778
C	3.12434340	2.84141135	-0.33055735
H	3.80471492	2.44029927	0.40768424
C	3.36317205	-0.30083621	0.36177620
C	4.11430550	-1.36624837	-0.13623025
H	3.81534243	-1.86386168	-1.04913700
C	5.25102520	-1.80490088	0.52782762
H	5.81785488	-2.63568115	0.12379164

C	5.66049957	-1.18303359	1.69703233
H	6.55311298	-1.52062976	2.21103024
C	4.91238499	-0.13372646	2.21195459
H	5.21174526	0.34831554	3.13537359
C	3.76741242	0.29524437	1.55897808
H	3.16688895	1.07494462	2.00547075
N	-2.41233349	3.11436939	-1.11037612
C	-2.72719908	3.14182997	0.25066525
C	-1.76261914	2.68942046	1.16402829
N	-0.48397711	2.26808000	0.67925400
C	-3.95445013	3.58326316	0.74215013
C	-4.21672869	3.58797026	2.10158730
C	-3.25770640	3.13644505	2.99679065
C	-2.03604341	2.68504333	2.52496648
C	-2.88668990	3.98134351	-2.08132434
C	-3.24267483	5.30475426	-1.80351138
C	-3.65004778	6.14875698	-2.82437062
C	-3.70348620	5.70769835	-4.13951540
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C	-2.94432139	3.54044867	-3.40847683
H	-2.11528683	2.19858313	-1.44203806
H	0.24109252	2.54474115	1.33395040
H	-0.30308270	2.72146106	-0.21285917
H	-4.70936394	3.91923213	0.04260144
H	-5.17911291	3.93469357	2.45931816
H	-3.45615149	3.13653374	4.06176519
H	-1.27431667	2.33026958	3.20906591
H	-3.18667221	5.67812729	-0.78892821
H	-3.91997123	7.17136049	-2.58467412
H	-4.02186966	6.37389612	-4.93204165
H	-3.37758470	4.02950621	-5.44006968
H	-2.67222333	2.51582980	-3.63898039

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