SUPPORTING INFORMATION

Predicting the *Cis-Trans* Dichloro Configuration of Group 15-16 Chelated Ruthenium Olefin Metathesis Complexes: A DFT and Experimental Study

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Part I. DFT Calculations

BP86/LACVP*

Thermodynamic properties calculated assuming an ideal gas

In the tables below, the units for temperature
are kelvins, the units for U, H, and G are
kcal/mol and the units for Cv and S are cal/(mol K)

PhCH=CH$_2$

C1	-0.3735337579	-0.4474218383	0.0000000000
C2	1.0401223711	-0.3680593308	0.0000000000
C3	1.6902303249	0.8707777536	0.0000000000
C4	0.9475328287	2.0654232284	0.0000000000
C5	-0.4543176407	2.0064344618	0.0000000000
C6	-1.1038977093	0.7641901690	0.0000000000
H7	1.6359414605	-1.2875542161	0.0000000000
H8	2.7857545878	0.9075091856	0.0000000000
H9	1.4605410564	3.0337035426	0.0000000000
H10	-1.0446188137	2.9299610033	0.0000000000
H11	-2.2004063823	0.7234071385	0.0000000000
C12	-1.1127281970	-1.7226824556	0.0000000000
C13	-0.6033325129	-2.9729865825	0.0000000000
H14	-2.2071545108	-1.6123768655	0.0000000000
H15	-1.2615694985	-3.8474517775	0.0000000000
H16	0.4734058102	-3.1770715425	0.0000000000

SCFE: SCF energy: DFT(bp86) -309.62838568418 hartrees

NIMAG 0

HOMO energy: -0.19835
LUMO energy: -0.06303

The zero point energy (ZPE): 81.416 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	39.837	1.481	-10.396	17.54661
rot.	0.889	2.981	27.959	0.889	-7.447	12.56928

vib.	2.588	21.088	15.012	2.588	-1.888	3.18705
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	4.365	27.050	82.807	4.957	-19.732	33.30295

Total internal energy, Utot (SCFE + ZPE + U): -309.491684 hartrees
Total enthalpy, Htot (Utot + pV): -309.490740 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -309.530084 hartrees

H_2C=CH(C_6H_4)O*i*Pr

C1	0.0402779676	-0.0306001589	0.0483069218
C2	-0.0317229995	-0.1465784430	1.4527383650
C3	1.1140267644	-0.2614157194	2.2486680613
C4	2.3773081445	-0.2498815335	1.6398382645
C5	2.4930489168	-0.1239113699	0.2473116244
C6	1.3372803835	-0.0178276298	-0.5522434854
H7	-1.0184444071	-0.1250451301	1.9290215882
H8	1.0224624805	-0.3435929991	3.3370880552
H9	3.2863927048	-0.3303288579	2.2469609251
H10	3.4878934866	-0.1107184970	-0.2057027701
O11	1.3515659029	0.0760585271	-1.9227583112
C12	-1.1592456552	0.0912610162	-0.7984329758
C13	-2.4336218070	-0.1727200834	-0.4351382995
H14	-0.9672913396	0.4220906320	-1.8255164787
H15	-3.2588655128	-0.0296613907	-1.1401528714
H16	-2.7048351876	-0.5456080646	0.5593064419
C17	2.6115725365	0.1779396903	-2.6338341738
C18	2.2970214503	-0.2226789012	-4.0760350920
C19	3.1803941635	1.5984455734	-2.5247933419
H20	3.3218785258	-0.5563225399	-2.2036358158
H21	3.2143938230	-0.1929208800	-4.6895379239
H22	1.8802615582	-1.2429914791	-4.1150427804
H23	1.5603461436	0.4719843080	-4.5166243112
H24	4.1451388918	1.6686841989	-3.0584193131
H25	2.4788736394	2.3217838826	-2.9767886382
H26	3.3454842545	1.8904069323	-1.4740367469

SCFE: SCF energy: DFT(bp86) -502.77774671107 hartrees

NIMAG 0

HOMO energy: -0.17874
LUMO energy: -0.05536

The zero point energy (ZPE): 135.889 kcal/mol

is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	41.158	1.481	-10.790	18.21149
rot.	0.889	2.981	31.002	0.889	-8.355	14.10099
vib.	5.963	41.234	37.109	5.963	-5.101	8.60909
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	7.741	47.195	109.269	8.333	-24.245	40.92157

Total internal energy, Utot (SCFE + ZPE + U): -502.548859 hartrees
Total enthalpy, Htot (Utot + pV): -502.547914 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -502.599832 hartrees
H_2C=CH(C_6H_4)S*i*Pr

C1	0.0330843930	0.0764161477	0.0403758469
C2	0.0627871485	0.1776411964	1.4518432220
C3	1.2453811330	0.0230341624	2.1801540802
C4	2.4463025739	-0.2407376426	1.5009113642
C5	2.4491316074	-0.3533275887	0.1051938303
C6	1.2613967152	-0.1880072320	-0.6384607723
H7	-0.8687206847	0.4224082812	1.9741395450
H8	1.2349390288	0.1214243001	3.2713166002
H9	3.3830350683	-0.3648426648	2.0563313826
H10	3.3857806128	-0.5887411113	-0.4102806783
S11	1.2352638234	-0.4054242623	-2.4206915780
C12	-1.2302978250	0.2635402588	-0.6977094527
C13	-2.4691604015	0.0136686972	-0.2222935767
H14	-1.1241570563	0.6310929191	-1.7277690436
H15	-3.3576003149	0.2113400424	-0.8307790629
H16	-2.6427876048	-0.4089209894	0.7744157936
C17	2.8985303474	0.2146047453	-2.9861856798
C18	2.9446382728	-0.0437135453	-4.5010921885
C19	3.1178589387	1.6908097187	-2.6364169611
H20	3.6714222876	-0.4100138523	-2.5015228819
H21	3.9258921096	0.2705527594	-4.9004898825
H22	2.8023677621	-1.1123728179	-4.7378496585
H23	2.1631314492	0.5350464400	-5.0256139598
H24	4.1214094378	2.0138705946	-2.9734903380
H25	2.3634143467	2.3242760192	-3.1352820880
H26	3.0499640607	1.8657254495	-1.5493808208

SCFE: SCF energy: DFT(bp86) -825.77147092797 hartrees

NIMAG 0

HOMO energy: -0.18094
LUMO energy: -0.05935

The zero point energy (ZPE): 133.881 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	41.438	1.481	-10.874	18.35249
rot.	0.889	2.981	31.383	0.889	-8.468	14.29258
vib.	6.366	43.063	41.622	6.366	-6.044	10.20064
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	8.143	49.024	114.443	8.736	-25.385	42.84571

Total internal energy, Utot (SCFE + ZPE + U): -825.545142 hartrees
Total enthalpy, Htot (Utot + pV): -825.544197 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -825.598573 hartrees
H_2C=CH(C_6H_4)Se*i*Pr

C1	0.0512492318	0.2605039935	0.1078300924
C2	0.1162722911	0.4523228023	1.5112683899
C3	1.2847710228	0.2077247471	2.2372554386
C4	2.4369576659	-0.2462518069	1.5731290060
C5	2.4004339704	-0.4520734473	0.1876438307
C6	1.2304608304	-0.1885218666	-0.5496168792
H7	-0.7712270914	0.8369932779	2.0258225673
H8	1.3003013679	0.3763149576	3.3199621018
H9	3.3583188292	-0.4485241016	2.1310458128
H10	3.2871500482	-0.8400830387	-0.3254171387
Se11	1.2350258729	-0.5398059704	-2.4950750116
C12	-1.1964988729	0.5376664542	-0.6280908811
C13	-2.4452058693	0.4892202685	-0.1168904710
H14	-1.0661324554	0.7804024950	-1.6916223960
H15	-3.3159373620	0.7331080373	-0.7344171821
H16	-2.6490593683	0.1902393499	0.9182842824
C17	2.9136357266	0.5236458195	-3.0014809163
C18	3.1813034927	0.2306744594	-4.4808591779
C19	2.7386808193	2.0106417895	-2.6993229670
H20	3.7228141045	0.0966456844	-2.3841466425
H21	4.1015565664	0.7536460777	-4.8027236855
H22	3.3182667879	-0.8483589976	-4.6687432644
H23	2.3522337780	0.5916589677	-5.1164526129

H24	3.6716821107	2.5558955209	-2.9455646268
H25	1.9186917399	2.4422089258	-3.3003567782
H26	2.5152839064	2.1835497997	-1.6329805293

SCFE: SCF energy: DFT(bp86) -436.80899117002 hartrees

NIMAG 0

HOMO energy: -0.18040
LUMO energy: -0.06132

The zero point energy (ZPE): 132.940 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	42.149	1.481	-11.085	18.71010
rot.	0.889	2.981	31.757	0.889	-8.580	14.48082
vib.	6.717	44.108	45.029	6.717	-6.708	11.32158
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	8.495	50.069	118.935	9.087	-26.373	44.51250

Total internal energy, Utot (SCFE + ZPE + U): -436.583600 hartrees
Total enthalpy, Htot (Utot + pV): -436.582656 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -436.639166 hartrees

H_2C=CH(C_6H_4)NH*i*Pr

C1	0.0103798686	0.0060889763	0.0855252005
C2	-0.0559179069	-0.1764845368	1.4816558356
C3	1.0973125481	-0.2828842950	2.2695972944
C4	2.3537345871	-0.1926036472	1.6508196022
C5	2.4578322400	-0.0172982365	0.2645253302
C6	1.2983540374	0.0692996462	-0.5426233911
H7	-1.0451992449	-0.1939391848	1.9537729407
H8	1.0165253859	-0.4097365218	3.3545322670
H9	3.2693685997	-0.2585356567	2.2504913943
H10	3.4497032230	0.0362649605	-0.1936111832
N11	1.3632419823	0.2154061649	-1.9308430568
C12	-1.2138453271	0.1729374294	-0.7191671242
C13	-2.4062609284	-0.4210677897	-0.4909861002
H14	-1.1342301934	0.8690905078	-1.5690168746
H15	-3.2830439889	-0.1937243038	-1.1066891854
H16	-2.5462930690	-1.1497318944	0.3163039170
C17	2.6184354111	0.1420190990	-2.6929039811

C18	2.2933107448	-0.2820779876	-4.1331244906
C19	3.3574280364	1.4942521075	-2.6634852425
H20	3.2773030818	-0.6356679973	-2.2463592917
H21	3.2125559340	-0.3266111720	-4.7412128421
H22	1.8178934704	-1.2797636898	-4.1616559047
H23	1.6084124458	0.4462518523	-4.6066286241
H24	4.3370176009	1.4150647639	-3.1692191959
H25	2.7571077451	2.2667763463	-3.1765373033
H26	3.5303728580	1.8358352124	-1.6288962017
H27	0.5617751083	-0.1865161397	-2.4176120540

SCFE: SCF energy: DFT(bp86) -482.91070013756 hartrees

NIMAG 0

HOMO energy: -0.16385
LUMO energy: -0.05106

The zero point energy (ZPE): 143.633 kcal/mol
is not included in U, H, or G in the table below
T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	41.140	1.481	-10.785	18.20235
rot.	0.889	2.981	31.076	0.889	-8.377	14.13806
vib.	6.037	42.439	36.323	6.037	-4.792	8.08836
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	7.815	48.401	108.538	8.407	-23.953	40.42877

Total internal energy, Utot (SCFE + ZPE + U): -482.669353 hartrees
Total enthalpy, Htot (Utot + pV): -482.668409 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -482.719979 hartrees

H_2C=CH(C_6H_4)PH*i*Pr

C1	-0.0326942413	-0.0221534866	0.1301271031
C2	0.0024859171	-0.2192681787	1.5295769416
C3	1.2130000076	-0.3201298808	2.2236915599
C4	2.4236874952	-0.2156467205	1.5224448339
C5	2.4107990152	-0.0187236953	0.1332253187
C6	1.2012169394	0.0775628239	-0.5845342785
H7	-0.9458430137	-0.2611035232	2.0771453949
H8	1.2113152642	-0.4623559450	3.3102528311
H9	3.3800971944	-0.2841862692	2.0534117267
H10	3.3677755149	0.0517668528	-0.3934909047
P11	1.1472386521	0.3947712662	-2.4195979919

C12	-1.3252820012	0.0898381222	-0.5748135027
C13	-2.4835369671	-0.4994052851	-0.2089200193
H14	-1.3196882040	0.7123409704	-1.4829980050
H15	-3.4048078179	-0.3394241821	-0.7786189239
H16	-2.5520470058	-1.1686240004	0.6569891873
C17	2.9267767767	0.1263257462	-3.0067604210
C18	2.8834798884	-0.3272959830	-4.4797891117
C19	3.7378061740	1.4287484156	-2.8554149232
H20	3.3941718734	-0.6767750995	-2.4050887356
H21	3.9102307387	-0.4292915731	-4.8786804649
H22	2.3768901797	-1.3018171850	-4.5952779243
H23	2.3536694556	0.4094933666	-5.1122699781
H24	4.7781153211	1.2803184303	-3.2016340553
H25	3.2913982892	2.2384934220	-3.4613185115
H26	3.7778685969	1.7819314656	-1.8097913966
H27	0.6437182050	-0.8954483328	-2.8053047117

SCFE: SCF energy: DFT(bp86) -769.51821151576 hartrees

NIMAG 0

HOMO energy: -0.19184
LUMO energy: -0.06099

The zero point energy (ZPE): 139.051 kcal/mol
is not included in U, H, or G in the table below
T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	41.438	1.481	-10.874	18.35257
rot.	0.889	2.981	31.499	0.889	-8.503	14.35090
vib.	6.562	44.712	41.326	6.562	-5.760	9.72121
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	8.339	50.674	114.264	8.932	-25.136	42.42468

Total internal energy, Utot (SCFE + ZPE + U): -769.283330 hartrees
Total enthalpy, Htot (Utot + pV): -769.282386 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -769.336676 hartrees

(SIMes)$RuCl_2$=CHPh

C1	-0.6354000000	-4.0831000000	-1.0094000000
C2	-0.1535000000	-2.7448000000	-1.0216000000
C3	0.2769000000	-2.1954000000	-2.2623000000
C4	0.2022000000	-2.9471000000	-3.4379000000
C5	-0.2948000000	-4.2636000000	-3.4085000000

C6	-0.7093000000	-4.8300000000	-2.1900000000
C7	-0.1566000000	-1.9901000000	0.2243000000
Ru8	-0.0122000000	-0.1451000000	0.2220000000
Cl9	-2.2488000000	0.4202000000	-0.2702000000
C10	-0.0467000000	0.3302000000	2.1035000000
N11	0.1349000000	1.6359000000	2.5151000000
C12	-0.1977000000	1.8286000000	3.9428000000
C13	-0.1765000000	0.3876000000	4.4748000000
N14	-0.3076000000	-0.4104000000	3.2325000000
C15	0.4400000000	2.7829000000	1.6932000000
C16	-0.6007000000	3.5898000000	1.1692000000
C17	-0.2430000000	4.7080000000	0.3914000000
C18	1.0962000000	5.0646000000	0.1653000000
C19	2.1012000000	4.2951000000	0.7807000000
C20	1.8018000000	3.1634000000	1.5561000000
C21	-2.0579000000	3.3500000000	1.4977000000
C22	2.9089000000	2.4080000000	2.2574000000
C23	1.4545000000	6.2490000000	-0.7081000000
C24	-0.4691000000	-1.8318000000	3.3601000000
C25	-1.7802000000	-2.3646000000	3.3969000000
C26	-1.9262000000	-3.7524000000	3.5778000000
C27	-0.8160000000	-4.6044000000	3.7265000000
C28	0.4719000000	-4.0382000000	3.6801000000
C29	0.6732000000	-2.6579000000	3.4990000000
C30	-2.9897000000	-1.4764000000	3.1997000000
C31	-1.0031000000	-6.0915000000	3.9488000000
C32	2.0723000000	-2.0895000000	3.3903000000
Cl33	2.2943000000	0.0647000000	-0.2255000000
H34	0.7039000000	-1.1853000000	-2.2882000000
H35	-0.3388000000	-2.5745000000	1.1384000000
H36	-0.9623000000	-4.5181000000	-0.0573000000
H37	-1.0887000000	-5.8579000000	-2.1631000000
H38	-0.3503000000	-4.8490000000	-4.3334000000
H39	0.5409000000	-2.5098000000	-4.3838000000
H40	0.5463000000	2.4829000000	4.4280000000
H41	-1.1958000000	2.2994000000	4.0429000000
H42	0.7736000000	0.1407000000	4.9895000000
H43	-1.0098000000	0.1647000000	5.1626000000
H44	-1.0439000000	5.3259000000	-0.0353000000
H45	3.1523000000	4.5881000000	0.6610000000
H46	-2.7081000000	3.7282000000	0.6911000000
H47	-2.2902000000	2.2831000000	1.6317000000
H48	-2.3352000000	3.8934000000	2.4232000000
H49	2.7001000000	2.2839000000	3.3368000000
H50	3.0376000000	1.4012000000	1.8239000000
H51	3.8656000000	2.9487000000	2.1595000000

H52	2.3618000000	6.7625000000	-0.3429000000
H53	1.6596000000	5.9268000000	-1.7472000000
H54	0.6345000000	6.9871000000	-0.7494000000
H55	-2.9381000000	-4.1779000000	3.5968000000
H56	1.3496000000	-4.6908000000	3.7750000000
H57	2.2249000000	-1.5866000000	2.4172000000
H58	2.2822000000	-1.3420000000	4.1783000000
H59	2.8257000000	-2.8896000000	3.4834000000
H60	-3.9207000000	-2.0642000000	3.2678000000
H61	-3.0416000000	-0.6749000000	3.9606000000
H62	-2.9646000000	-0.9804000000	2.2113000000
H63	-0.1568000000	-6.6720000000	3.5414000000
H64	-1.0721000000	-6.3283000000	5.0281000000
H65	-1.9307000000	-6.4583000000	3.4753000000

SCFE: SCF energy: DFT(bp86) -2210.21892898923 hartrees

NIMAG 1 (-56.74 cm-1)

HOMO energy: -0.16370
LUMO energy: -0.09988

The zero point energy (ZPE): 324.880 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	44.896	1.481	-11.905	20.09257
rot.	0.889	2.981	37.100	0.889	-10.173	17.16920
vib.	20.923	126.315	149.488	20.923	-23.647	39.91139
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	22.700	132.277	231.483	23.293	-45.724	77.17315

Total internal energy, Utot (SCFE + ZPE + U): -2209.665025 hartrees
Total enthalpy, Htot (Utot + pV): -2209.664081 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2209.774066 hartrees

***cis*-(SIMes)RuCl$_2$=CH(C$_6$H$_4$)O*i*Pr**

C1	-0.8605144398	-3.0833569891	3.2666915812
C2	0.3869878845	-2.4171074117	3.1661514454
C3	1.6007506316	-3.1441541625	3.0783263919
C4	1.5304803073	-4.5499119136	3.0488646836
C5	0.3087028470	-5.2412928745	3.1209475161

C6	-0.8742482022	-4.4877906242	3.2355076350
N7	0.4373838183	-0.9881402234	3.3222162164
C8	0.1117851870	0.0008917167	2.4278788559
N9	0.1767968051	1.1916538781	3.1109413250
C10	0.7308290597	1.0421297882	4.4768502837
C11	0.6174241901	-0.4717603816	4.7029108774
Ru12	-0.0532786548	-0.0091094028	0.4073793165
Cl13	2.3185713908	0.0039725713	0.3968181201
C14	-0.2781946754	2.4839651910	2.6639345074
C15	-1.6403203198	2.8127913555	2.8862121243
C16	-2.0882173717	4.0967637042	2.5350029969
C17	-1.2199945477	5.0570485294	1.9837644909
C18	0.1339108222	4.7154764810	1.8252125150
C19	0.6384234192	3.4475174192	2.1733020286
C20	-2.5909465652	1.8148887621	3.5159767473
C21	-1.7334812056	6.4191736860	1.5649151396
C22	2.1187456750	3.1639726852	2.0633102331
C23	2.9415732535	-2.4460423481	3.0282269513
C24	0.2618533970	-6.7547858605	3.0597771648
C25	-2.1543305147	-2.3115933820	3.4057951487
C26	-0.0840173692	-1.8389588467	0.1874562717
C27	-1.3165500475	-2.5435278770	-0.1097431416
C28	-2.5265002955	-1.8028959559	-0.2242791717
C29	-3.7408403860	-2.4528134591	-0.4980021977
C30	-3.7501271416	-3.8479541283	-0.6709952704
C31	-2.5652265237	-4.5978627546	-0.5796793265
C32	-1.3600977676	-3.9462125650	-0.2996458366
O33	-2.3856142696	-0.4368303740	-0.0342706760
C34	-3.4402875870	0.4370342170	-0.6294490444
C35	-3.4504997500	0.3097329788	-2.1541358442
Cl36	0.0131345822	1.1326771234	-1.6972133459
C37	-3.1695193809	1.8566434534	-0.1580092231
H38	0.8524573053	-2.4251354198	0.1645330355
H39	-0.4232401505	-4.5091183961	-0.2184072246
H40	-2.5857891767	-5.6825871679	-0.7312415479
H41	-4.7011495293	-4.3478023113	-0.8884974522
H42	-4.6767230987	-1.8954612630	-0.5860660623
H43	-3.9655890455	2.5168859035	-0.5476908447
H44	-3.1761596437	1.9240928968	0.9393831254
H45	-2.1971573484	2.2115930649	-0.5377928404
H46	-4.2605153266	0.9422333010	-2.5609953674
H47	-2.4842629264	0.6543616772	-2.5580797213
H48	-3.6274439111	-0.7261414899	-2.4879312807
H49	-4.3949058130	0.0859806655	-0.1920411913
H50	-0.2562746438	-0.7481156080	5.3274373552
H51	1.5193906729	-0.9089749688	5.1621643204

H52	0.1450225811	1.6371343767	5.1978766305
H53	1.7803769747	1.3931902532	4.5022746189
H54	2.4659898709	-5.1190907145	2.9727366061
H55	-1.8388314647	-5.0067449322	3.3050815724
H56	3.7438466640	-3.1649492252	2.7891337314
H57	2.9467365126	-1.6430520876	2.2686428636
H58	3.1981075845	-1.9826165583	4.0017077593
H59	-2.1667798294	-1.6864307058	4.3186892687
H60	-2.3114644337	-1.6343059189	2.5479160294
H61	-3.0150207449	-2.9992776444	3.4588894386
H62	-0.5216429404	-7.1641650949	3.7223945351
H63	0.0350122945	-7.1078065388	2.0349874324
H64	1.2271108380	-7.2024446668	3.3534693374
H65	0.8315569730	5.4621352326	1.4246093055
H66	-3.1429050592	4.3545724869	2.6994821963
H67	-2.6368061625	0.8715631992	2.9430399304
H68	-2.2810912232	1.5474836029	4.5443111600
H69	-3.6113322416	2.2308144747	3.5764149390
H70	2.6250862706	3.9657598939	1.4999946057
H71	2.5905495145	3.1168934952	3.0650234175
H72	2.3198518214	2.2037793380	1.5553694267
H73	-2.6570879190	6.6887478589	2.1066967685
H74	-0.9844571579	7.2099156153	1.7476329321
H75	-1.9685690197	6.4383042321	0.4832075761

SCFE: SCF energy: DFT(bp86) -2403.36341625448 hartrees

NIMAG 1 (-42.51 cm-1)

HOMO energy: -0.15138
LUMO energy: -0.09455

The zero point energy (ZPE): 379.923 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	45.186	1.481	-11.991	20.23849
rot.	0.889	2.981	37.379	0.889	-10.256	17.31000
vib.	23.218	144.013	154.279	23.218	-22.780	38.44873
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	24.995	149.975	236.844	25.588	-45.027	75.99721

Total internal energy, Utot (SCFE + ZPE + U): -2402.718138 hartrees

Total enthalpy, Htot (Utot + pV): -2402.717194 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2402.829726 hartrees

***cis*-(SIMes)$RuCl_2$=$CH(C_6H_4)$S*i*Pr**

C1	-2.5977000000	-2.0454000000	0.1317000000
C2	-1.3031000000	-2.5850000000	-0.0796000000
C3	-1.1925000000	-3.9486000000	-0.4471000000
C4	-2.3394000000	-4.7372000000	-0.6006000000
C5	-3.6138000000	-4.1832000000	-0.3787000000
C6	-3.7473000000	-2.8341000000	-0.0026000000
C7	-0.1438000000	-1.7117000000	0.0724000000
Ru8	-0.2290000000	0.1089000000	0.4299000000
Cl9	-0.4482000000	1.4541000000	-1.5429000000
S10	-2.6037000000	-0.3124000000	0.6211000000
C11	-3.8661000000	0.4297000000	-0.5958000000
C12	-3.8665000000	1.9448000000	-0.3615000000
C13	0.0835000000	0.0578000000	2.4373000000
N14	0.1330000000	1.2296000000	3.1438000000
C15	0.5833000000	1.0492000000	4.5443000000
C16	0.5977000000	-0.4848000000	4.6950000000
N17	0.3699000000	-0.9583000000	3.3045000000
C18	-0.2154000000	2.5458000000	2.6618000000
C19	-1.5664000000	2.9682000000	2.7805000000
C20	-1.9001000000	4.2659000000	2.3570000000
C21	-0.9325000000	5.1514000000	1.8467000000
C22	0.4053000000	4.7234000000	1.8088000000
C23	0.7976000000	3.4365000000	2.2237000000
C24	-2.6246000000	2.0776000000	3.4017000000
C25	2.2610000000	3.0565000000	2.2300000000
C26	-1.3225000000	6.5290000000	1.3520000000
C27	0.3923000000	-2.3779000000	3.0686000000
C28	1.6207000000	-3.0070000000	2.7466000000
C29	1.6261000000	-4.4061000000	2.5940000000
C30	0.4694000000	-5.1849000000	2.7779000000
C31	-0.7238000000	-4.5304000000	3.1323000000
C32	-0.7858000000	-3.1351000000	3.2945000000
C33	2.8952000000	-2.2104000000	2.5808000000
C34	0.5167000000	-6.6932000000	2.6360000000
C35	-2.0860000000	-2.4799000000	3.7140000000
Cl36	2.1640000000	0.2529000000	0.1102000000
C37	-3.6384000000	0.0341000000	-2.0552000000
H38	0.8417000000	-2.1462000000	-0.1719000000
H39	-0.1957000000	-4.3728000000	-0.6152000000
H40	-2.2451000000	-5.7881000000	-0.8964000000

H41	-4.5102000000	-4.8025000000	-0.4980000000
H42	-4.7411000000	-2.4084000000	0.1766000000
H43	-4.6652000000	2.4015000000	-0.9748000000
H44	-4.0615000000	2.1985000000	0.6950000000
H45	-2.8995000000	2.3805000000	-0.6627000000
H46	-4.4533000000	0.4665000000	-2.6675000000
H47	-2.6749000000	0.4261000000	-2.4171000000
H48	-3.6568000000	-1.0598000000	-2.1940000000
H49	-4.8177000000	0.0010000000	-0.2256000000
H50	-0.2054000000	-0.8577000000	5.3589000000
H51	1.5594000000	-0.8706000000	5.0746000000
H52	-0.1156000000	1.5478000000	5.2387000000
H53	1.5843000000	1.4981000000	4.6835000000
H54	2.5706000000	-4.9004000000	2.3313000000
H55	-1.6358000000	-5.1210000000	3.2887000000
H56	3.7334000000	-2.8717000000	2.3040000000
H57	2.7918000000	-1.4290000000	1.8040000000
H58	3.1759000000	-1.6962000000	3.5205000000
H59	-2.0447000000	-2.1223000000	4.7616000000
H60	-2.3348000000	-1.6086000000	3.0842000000
H61	-2.9221000000	-3.1961000000	3.6468000000
H62	-0.4593000000	-7.1014000000	2.3203000000
H63	1.2754000000	-7.0079000000	1.8981000000
H64	0.7776000000	-7.1775000000	3.5969000000
H65	1.1791000000	5.4141000000	1.4508000000
H66	-2.9433000000	4.5979000000	2.4393000000
H67	-2.4099000000	1.8753000000	4.4694000000
H68	-3.6149000000	2.5626000000	3.3562000000
H69	-2.7020000000	1.0999000000	2.8959000000
H70	2.8729000000	3.8750000000	1.8154000000
H71	2.6250000000	2.8606000000	3.2575000000
H72	2.4473000000	2.1476000000	1.6286000000
H73	-2.2333000000	6.8995000000	1.8545000000
H74	-0.5150000000	7.2638000000	1.5170000000
H75	-1.5302000000	6.5124000000	0.2650000000

SCFE: SCF energy: DFT(bp86) -2726.38070611967 hartrees

NIMAG 2 (-42.04, -15.74 cm-1)

HOMO energy: -0.15761
LUMO energy: -0.10121

The zero point energy (ZPE): 377.804 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	45.261	1.481	-12.013	20.27628
rot.	0.889	2.981	37.416	0.889	-10.267	17.32861
vib.	23.725	145.973	160.837	23.725	-24.228	40.89277
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	25.502	151.935	243.514	26.095	-46.509	78.49766

Total internal energy, Utot (SCFE + ZPE + U): -2725.737996 hartrees
Total enthalpy, Htot (Utot + pV): -2725.737052 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2725.852754 hartrees

***cis*-(SIMes)RuCl$_2$=CH(C$_6$H$_4$)Se*i*Pr**

C1	-1.5655077932	2.9091594579	2.9346859898
C2	-0.2327393726	2.4792282887	2.7004311680
C3	0.7328393142	3.3553302962	2.1418743074
C4	0.3027855350	4.6312027183	1.7319084637
C5	-1.0253701574	5.0630171666	1.8841116228
C6	-1.9397423756	4.1937130981	2.5057445592
N7	0.1539218175	1.1728137344	3.1783423672
C8	0.1214306458	-0.0015772071	2.4701313962
N9	0.4628695591	-1.0071891944	3.3335271412
C10	0.6353865718	-0.5244445286	4.7280707649
C11	0.6790078818	1.0028165884	4.5529355526
Ru12	-0.2212481267	0.0608500614	0.4720155311
Se13	-2.7726204920	-0.1513617343	0.7201047462
C14	-3.9519895937	0.6149455412	-0.8296717523
C15	-3.5673595267	0.0706794020	-2.1986832424
C16	0.4964775862	-2.4287600758	3.1099141765
C17	1.7430657490	-3.0501593979	2.8422572772
C18	1.7663117395	-4.4484502738	2.6936907445
C19	0.6079729285	-5.2351919041	2.8264234910
C20	-0.6028940625	-4.5895196003	3.1315499080
C21	-0.6813083848	-3.1943981665	3.2934586550
C22	3.0172157235	-2.2460345694	2.7271873348
C23	0.6740980409	-6.7422134886	2.6812271767
C24	-1.9957771660	-2.5548999021	3.6877029248
C25	2.1899175715	2.9753677236	2.0217838798
C26	-1.4591390750	6.4286216539	1.3939906528
C27	-2.5543136769	2.0522355971	3.6986912131
Cl28	2.1667198182	0.0208040914	0.0923711739
Cl29	-0.3880090202	1.4393495347	-1.4799725747

C30	-0.2798870951	-1.7590324226	0.1132712157
C31	-1.4767522471	-2.5832216495	-0.0563966833
C32	-1.3862318945	-3.9382792154	-0.4643414435
C33	-2.5413809547	-4.7082995524	-0.6465528098
C34	-3.8099965406	-4.1466988144	-0.4163030525
C35	-3.9248388122	-2.8060821805	-0.0009483644
C36	-2.7659206089	-2.0430380525	0.1647645022
C37	-3.8876552668	2.1369422314	-0.7121384266
H38	0.6785215285	-2.2530026785	-0.1304108760
H39	-0.3938973645	-4.3699691236	-0.6423654242
H40	-2.4561982224	-5.7510801832	-0.9731334964
H41	-4.7138886166	-4.7502358734	-0.5591184501
H42	-4.9132525379	-2.3700429901	0.1857063208
H43	-4.5961889505	2.5809870288	-1.4377853616
H44	-4.1718421631	2.4898457435	0.2953672399
H45	-2.8728709233	2.4992070366	-0.9468772054
H46	-4.2758339456	0.4775999514	-2.9479556535
H47	-2.5471226727	0.3844543896	-2.4721637064
H48	-3.6310644731	-1.0297991079	-2.2396092581
H49	-4.9464989360	0.2432477871	-0.5196738877
H50	-0.2180814383	-0.8580918841	5.3505497287
H51	1.5611865587	-0.9364052962	5.1636161047
H52	0.0443649150	1.5418016974	5.2770000102
H53	1.7070042674	1.4074899896	4.6218661990
H54	2.7241276503	-4.9361932789	2.4697415398
H55	-1.5171175369	-5.1860942691	3.2484295784
H56	3.8750323073	-2.9065368146	2.5152722404
H57	2.9435196784	-1.4916670820	1.9208216827
H58	3.2406116505	-1.7010853220	3.6649110121
H59	-2.0439272347	-2.3752139758	4.7803893132
H60	-2.1532926185	-1.5836354332	3.1892662705
H61	-2.8441938617	-3.2101448464	3.4279772226
H62	-0.2789491058	-7.1564332037	2.3080345351
H63	1.4762014649	-7.0466165661	1.9860113378
H64	0.8837580086	-7.2293826157	3.6531874167
H65	1.0395923083	5.3105951421	1.2847969903
H66	-2.9713455082	4.5291684896	2.6765779893
H67	-2.3474731253	2.0787936127	4.7873583206
H68	-3.5848106562	2.4211280529	3.5574729214
H69	-2.5269822004	0.9960335159	3.3855785337
H70	2.7682076518	3.8066834629	1.5849609347
H71	2.6315983356	2.7468695927	3.0108825397
H72	2.3323183387	2.0838048380	1.3828276575
H73	-2.3413213924	6.7977585499	1.9460641525
H74	-0.6505451956	7.1734023342	1.4995322719
H75	-1.7314073551	6.3943124695	0.3218392291

SCFE: SCF energy: DFT(bp86) -2337.41575486675 hartrees

NIMAG 2 (-41.58, -17.66 cm-1)

HOMO energy: -0.15535
LUMO energy: -0.10028

The zero point energy (ZPE): 376.762 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	45.476	1.481	-12.077	20.38430
rot.	0.889	2.981	37.559	0.889	-10.310	17.40059
vib.	24.176	147.101	164.687	24.176	-24.926	42.06987
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	25.953	153.063	247.722	26.545	-47.313	79.85476

Total internal energy, Utot (SCFE + ZPE + U): -2336.773988 hartrees
Total enthalpy, Htot (Utot + pV): -2336.773044 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2336.890745 hartrees

***cis*-(SIMes)RuCl$_2$=CH(C$_6$H$_4$)NH*i*Pr**

C1	0.6593000000	3.4552000000	2.1948000000
C2	-0.2819000000	2.4982000000	2.6539000000
C3	-1.6433000000	2.8514000000	2.8486000000
C4	-2.0652000000	4.1418000000	2.4894000000
C5	-1.1715000000	5.0905000000	1.9587000000
C6	0.1800000000	4.7305000000	1.8368000000
N7	0.1463000000	1.1938000000	3.0976000000
C8	0.0702000000	0.0033000000	2.4073000000
N9	0.3923000000	-0.9925000000	3.2979000000
C10	0.6172000000	-0.4819000000	4.6734000000
C11	0.7226000000	1.0341000000	4.4536000000
Ru12	-0.0961000000	0.0013000000	0.3891000000
Cl13	2.3166000000	0.1031000000	0.3783000000
C14	0.3410000000	-2.4200000000	3.1293000000
C15	-0.8904000000	-3.1025000000	3.2928000000
C16	-0.8944000000	-4.5073000000	3.2256000000
C17	0.2831000000	-5.2443000000	3.0156000000
C18	1.4944000000	-4.5391000000	2.8960000000

C19	1.5556000000	-3.1357000000	2.9627000000
C20	-2.1965000000	-2.3719000000	3.5272000000
C21	0.2480000000	-6.7558000000	2.9147000000
C22	2.8868000000	-2.4244000000	2.8796000000
C23	-2.6232000000	1.8877000000	3.4867000000
C24	-1.6555000000	6.4594000000	1.5278000000
C25	2.1401000000	3.1638000000	2.1327000000
C26	-0.0359000000	-1.8172000000	0.1147000000
C27	-1.2565000000	-2.5748000000	-0.1254000000
C28	-1.2732000000	-3.9629000000	-0.3985000000
C29	-2.4877000000	-4.6282000000	-0.6032000000
C30	-3.6980000000	-3.9182000000	-0.5269000000
C31	-3.6980000000	-2.5366000000	-0.2593000000
C32	-2.4815000000	-1.8682000000	-0.0700000000
N33	-2.3595000000	-0.4207000000	0.1793000000
C34	-3.3560000000	0.4068000000	-0.6285000000
C35	-3.2223000000	0.1552000000	-2.1345000000
Cl36	0.0075000000	1.2707000000	-1.6373000000
C37	-3.2126000000	1.8870000000	-0.2665000000
H38	0.9307000000	-2.3433000000	0.0141000000
H39	-0.3211000000	-4.5039000000	-0.4463000000
H40	-2.4961000000	-5.7016000000	-0.8240000000
H41	-4.6508000000	-4.4369000000	-0.6818000000
H42	-4.6493000000	-1.9958000000	-0.2151000000
H43	-3.9908000000	2.4662000000	-0.7959000000
H44	-3.3457000000	2.0594000000	0.8154000000
H45	-2.2222000000	2.2660000000	-0.5670000000
H46	-3.9877000000	0.7518000000	-2.6628000000
H47	-2.2250000000	0.4645000000	-2.4853000000
H48	-3.3832000000	-0.9050000000	-2.3923000000
H49	-4.3673000000	0.0786000000	-0.3050000000
H50	-0.2333000000	-0.7646000000	5.3270000000
H51	1.5354000000	-0.9194000000	5.0995000000
H52	0.1483000000	1.6229000000	5.1895000000
H53	1.7720000000	1.3859000000	4.4639000000
H54	2.4292000000	-5.0982000000	2.7575000000
H55	-1.8480000000	-5.0383000000	3.3457000000
H56	3.6881000000	-3.1329000000	2.6085000000
H57	2.8655000000	-1.6092000000	2.1321000000
H58	3.1655000000	-1.9719000000	3.8521000000
H59	-2.0475000000	-1.3790000000	3.9827000000
H60	-2.7372000000	-2.2256000000	2.5732000000
H61	-2.8618000000	-2.9573000000	4.1864000000
H62	-0.5328000000	-7.1884000000	3.5654000000
H63	0.0258000000	-7.0827000000	1.8802000000
H64	1.2167000000	-7.2037000000	3.1970000000

H65	0.8988000000	5.4683000000	1.4578000000
H66	-3.1182000000	4.4165000000	2.6366000000
H67	-2.6414000000	0.9069000000	2.9784000000
H68	-2.3655000000	1.6845000000	4.5443000000
H69	-3.6471000000	2.2990000000	3.4705000000
H70	2.6650000000	3.9505000000	1.5650000000
H71	2.5824000000	3.1415000000	3.1489000000
H72	2.3508000000	2.1920000000	1.6509000000
H73	-2.5613000000	6.7633000000	2.0817000000
H74	-0.8816000000	7.2316000000	1.6837000000
H75	-1.9109000000	6.4676000000	0.4506000000
H76	-2.6051000000	-0.2575000000	1.1674000000

SCFE: SCF energy: DFT(bp86) -2383.50391194208 hartrees

NIMAG 2 (-42.30, -17.43 cm-1)

HOMO energy: -0.14791
LUMO energy: -0.09589

The zero point energy (ZPE): 387.827 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	45.181	1.481	-11.990	20.23613
rot.	0.889	2.981	37.352	0.889	-10.248	17.29637
vib.	23.191	144.420	154.054	23.191	-22.740	38.38023
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	24.969	150.382	236.588	25.561	-44.977	75.91272

Total internal energy, Utot (SCFE + ZPE + U): -2382.846080 hartrees
Total enthalpy, Htot (Utot + pV): -2382.845136 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2382.957546 hartrees

***cis*-(SIMes)RuCl$_2$=CH(C$_6$H$_4$)PH*i*Pr**

C1	-0.7495000000	-3.1532000000	3.2930000000
C2	0.4226000000	-2.3809000000	3.0924000000
C3	1.6690000000	-2.9982000000	2.8154000000
C4	1.6965000000	-4.3986000000	2.6768000000
C5	0.5453000000	-5.1906000000	2.8317000000
C6	-0.6661000000	-4.5484000000	3.1451000000

N7	0.3837000000	-0.9600000000	3.3200000000
C8	0.0739000000	0.0510000000	2.4513000000
N9	0.1020000000	1.2227000000	3.1641000000
C10	0.6001000000	1.0433000000	4.5482000000
C11	0.5362000000	-0.4833000000	4.7190000000
Ru12	-0.2283000000	0.0961000000	0.4352000000
Cl13	2.2073000000	0.1686000000	0.1016000000
C14	-0.2538000000	2.5372000000	2.6831000000
C15	-1.5900000000	2.9813000000	2.8684000000
C16	-1.9367000000	4.2691000000	2.4260000000
C17	-0.9918000000	5.1295000000	1.8389000000
C18	0.3386000000	4.6878000000	1.7442000000
C19	0.7425000000	3.4095000000	2.1728000000
C20	-2.6133000000	2.1427000000	3.6072000000
C21	-1.3955000000	6.4942000000	1.3213000000
C22	2.2029000000	3.0256000000	2.1333000000
C23	2.9380000000	-2.1897000000	2.6854000000
C24	0.6090000000	-6.6980000000	2.6893000000
C25	-2.0669000000	-2.5206000000	3.6896000000
C26	-0.1849000000	-1.7365000000	0.1095000000
C27	-1.3543000000	-2.6005000000	-0.0713000000
C28	-2.6449000000	-2.0326000000	0.1056000000
C29	-3.7955000000	-2.8141000000	-0.0568000000
C30	-3.6710000000	-4.1736000000	-0.4042000000
C31	-2.3985000000	-4.7419000000	-0.5933000000
C32	-1.2440000000	-3.9648000000	-0.4278000000
P33	-2.5296000000	-0.2243000000	0.4695000000
C34	-3.8528000000	0.5793000000	-0.6180000000
C35	-3.7210000000	0.2073000000	-2.1051000000
Cl36	-0.4038000000	1.3641000000	-1.5948000000
C37	-3.8446000000	2.1031000000	-0.3927000000
H38	0.8032000000	-2.1875000000	-0.0913000000
H39	-0.2495000000	-4.4038000000	-0.5710000000
H40	-2.3103000000	-5.7979000000	-0.8741000000
H41	-4.5698000000	-4.7875000000	-0.5354000000
H42	-4.7921000000	-2.3753000000	0.0767000000
H43	-4.6708000000	2.5698000000	-0.9619000000
H44	-3.9767000000	2.3688000000	0.6720000000
H45	-2.8911000000	2.5351000000	-0.7409000000
H46	-4.5547000000	0.6649000000	-2.6711000000
H47	-2.7697000000	0.5816000000	-2.5170000000
H48	-3.7643000000	-0.8848000000	-2.2615000000
H49	-4.8039000000	0.1623000000	-0.2257000000
H50	-0.3329000000	-0.8096000000	5.3240000000
H51	1.4488000000	-0.9075000000	5.1701000000
H52	-0.0398000000	1.5893000000	5.2620000000

H53	1.6319000000	1.4343000000	4.6339000000
H54	2.6548000000	-4.8835000000	2.4497000000
H55	-1.5753000000	-5.1487000000	3.2817000000
H56	3.7968000000	-2.8474000000	2.4695000000
H57	2.8582000000	-1.4361000000	1.8775000000
H58	3.1657000000	-1.6401000000	3.6194000000
H59	-2.1703000000	-2.4693000000	4.7916000000
H60	-2.1654000000	-1.4946000000	3.3000000000
H61	-2.9173000000	-3.1124000000	3.3107000000
H62	-0.1607000000	-7.0708000000	1.9888000000
H63	1.5941000000	-7.0273000000	2.3174000000
H64	0.4321000000	-7.2018000000	3.6586000000
H65	1.0988000000	5.3615000000	1.3286000000
H66	-2.9715000000	4.6128000000	2.5553000000
H67	-2.5144000000	2.2732000000	4.7040000000
H68	-3.6410000000	2.4454000000	3.3416000000
H69	-2.5042000000	1.0668000000	3.3990000000
H70	2.7980000000	3.8251000000	1.6609000000
H71	2.6055000000	2.8743000000	3.1542000000
H72	2.3692000000	2.0928000000	1.5625000000
H73	-2.2938000000	6.8761000000	1.8374000000
H74	-0.5846000000	7.2329000000	1.4492000000
H75	-1.6291000000	6.4519000000	0.2401000000
H76	-3.2482000000	-0.1399000000	1.7086000000

SCFE: SCF energy: DFT(bp86) -2670.14573892683 hartrees

NIMAG 3 (-46.39, -29.54, -22.32 cm-1)

HOMO energy: -0.15913
LUMO energy: -0.10297

The zero point energy (ZPE): 383.343 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	45.261	1.481	-12.013	20.27630
rot.	0.889	2.981	37.449	0.889	-10.277	17.34514
vib.	23.310	145.062	155.641	23.310	-23.094	38.97828
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	25.088	151.024	238.352	25.680	-45.384	76.59973

Total internal energy, Utot (SCFE + ZPE + U): -2669.494862 hartrees

Total enthalpy, Htot (Utot + pV): -2669.493918 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2669.607167 hartrees

***trans*-(SIMes)RuCl$_2$=CH(C$_6$H$_4$)O*i*Pr**

C1	-0.5762000000	3.5757000000	1.1160000000
C2	0.4433000000	2.7730000000	1.6874000000
C3	1.8102000000	3.1511000000	1.5879000000
C4	2.1386000000	4.2551000000	0.7854000000
C5	1.1577000000	5.0058000000	0.1103000000
C6	-0.1903000000	4.6661000000	0.3100000000
N7	0.1059000000	1.6351000000	2.5091000000
C8	-0.0517000000	0.3245000000	2.0982000000
N9	-0.3402000000	-0.4017000000	3.2290000000
C10	-0.2603000000	0.4029000000	4.4710000000
C11	-0.2461000000	1.8410000000	3.9304000000
Ru12	0.0402000000	-0.1765000000	0.1922000000
Cl13	2.4145000000	-0.0117000000	-0.0002000000
C14	-0.5009000000	-1.8230000000	3.3624000000
C15	-1.8114000000	-2.3597000000	3.3712000000
C16	-1.9598000000	-3.7458000000	3.5590000000
C17	-0.8524000000	-4.5947000000	3.7407000000
C18	0.4349000000	-4.0262000000	3.7217000000
C19	0.6386000000	-2.6458000000	3.5363000000
C20	-3.0174000000	-1.4760000000	3.1377000000
C21	-1.0437000000	-6.0807000000	3.9694000000
C22	2.0391000000	-2.0766000000	3.4603000000
C23	2.8897000000	2.4258000000	2.3601000000
C24	1.5516000000	6.1559000000	-0.7939000000
C25	-2.0422000000	3.3673000000	1.4267000000
C26	-0.1509000000	-2.0199000000	0.2254000000
C27	-0.1912000000	-2.7542000000	-1.0218000000
C28	-0.0576000000	-2.0439000000	-2.2544000000
C29	-0.1022000000	-2.7200000000	-3.4827000000
C30	-0.2796000000	-4.1145000000	-3.4869000000
C31	-0.4130000000	-4.8378000000	-2.2887000000
C32	-0.3685000000	-4.1590000000	-1.0671000000
O33	0.1045000000	-0.6982000000	-2.0598000000
C34	0.3192000000	0.3115000000	-3.1153000000
C35	-0.9271000000	0.4797000000	-3.9887000000
Cl36	-2.2276000000	0.4370000000	-0.2367000000
C37	1.6411000000	0.0812000000	-3.8519000000
H38	-0.2470000000	-2.6172000000	1.1437000000
H39	-0.4718000000	-4.7007000000	-0.1193000000
H40	-0.5518000000	-5.9240000000	-2.3135000000

H41	-0.3152000000	-4.6388000000	-4.4490000000
H42	-0.0046000000	-2.1848000000	-4.4284000000
H43	1.8610000000	0.9700000000	-4.4706000000
H44	2.4557000000	-0.0452000000	-3.1199000000
H45	1.6195000000	-0.7962000000	-4.5191000000
H46	-0.8095000000	1.3906000000	-4.6031000000
H47	-1.0949000000	-0.3685000000	-4.6734000000
H48	-1.8159000000	0.6022000000	-3.3478000000
H49	0.4277000000	1.2143000000	-2.4908000000
H50	0.5003000000	2.4843000000	4.4272000000
H51	-1.2366000000	2.3313000000	4.0114000000
H52	0.6627000000	0.1514000000	5.0310000000
H53	-1.1253000000	0.1920000000	5.1230000000
H54	-0.9750000000	5.2771000000	-0.1554000000
H55	3.1943000000	4.5413000000	0.6915000000
H56	-2.6723000000	3.6989000000	0.5846000000
H57	-2.2851000000	2.3123000000	1.6201000000
H58	-2.3320000000	3.9700000000	2.3112000000
H59	2.6638000000	2.3932000000	3.4431000000
H60	2.9986000000	1.3868000000	2.0053000000
H61	3.8609000000	2.9351000000	2.2363000000
H62	2.4297000000	6.6989000000	-0.4004000000
H63	1.8225000000	5.7933000000	-1.8045000000
H64	0.7266000000	6.8794000000	-0.9151000000
H65	-2.9709000000	-4.1740000000	3.5546000000
H66	1.3113000000	-4.6761000000	3.8453000000
H67	2.2266000000	-1.6030000000	2.4781000000
H68	2.2167000000	-1.3027000000	4.2306000000
H69	2.7903000000	-2.8710000000	3.6078000000
H70	-3.9463000000	-2.0709000000	3.1588000000
H71	-3.1065000000	-0.6874000000	3.9089000000
H72	-2.9541000000	-0.9643000000	2.1591000000
H73	-0.1743000000	-6.6615000000	3.6144000000
H74	-1.1699000000	-6.3069000000	5.0459000000
H75	-1.9430000000	-6.4577000000	3.4509000000

SCFE: SCF energy: DFT(bp86) -2403.38117017747 hartrees

NIMAG 1 (-48.36 cm-1)

HOMO energy: -0.15194
LUMO energy: -0.09299

The zero point energy (ZPE): 379.748 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	45.186	1.481	-11.991	20.23849
rot.	0.889	2.981	37.520	0.889	-10.298	17.38083
vib.	24.076	146.190	167.550	24.076	-25.879	43.67932
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	25.853	152.151	250.256	26.446	-48.168	81.29863

Total internal energy, Utot (SCFE + ZPE + U): -2402.734803 hartrees
Total enthalpy, Htot (Utot + pV): -2402.733859 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2402.852764 hartrees

***trans*-(SIMes)RuCl$_2$=CH(C$_6$H$_4$)S*i*Pr**

C1	0.3535000000	-2.0326000000	-2.2509000000
C2	-0.0656000000	-2.6919000000	-1.0631000000
C3	-0.1318000000	-4.1089000000	-1.0649000000
C4	0.2342000000	-4.8381000000	-2.2020000000
C5	0.6803000000	-4.1690000000	-3.3556000000
C6	0.7485000000	-2.7641000000	-3.3784000000
C7	-0.3502000000	-1.9316000000	0.1473000000
Ru8	0.0097000000	-0.1243000000	0.3287000000
Cl9	-2.2446000000	0.6679000000	0.0200000000
S10	0.4469000000	-0.2379000000	-2.1683000000
C11	-1.0522000000	0.3494000000	-3.1486000000
C12	-0.9611000000	1.8815000000	-3.1206000000
C13	-0.1870000000	0.0924000000	2.3415000000
N14	-0.5062000000	-0.7828000000	3.3455000000
C15	-0.4935000000	-0.1631000000	4.6950000000
C16	-0.4028000000	1.3360000000	4.3704000000
N17	-0.0451000000	1.3267000000	2.9325000000
C18	-0.7102000000	-2.2039000000	3.2814000000
C19	-2.0359000000	-2.6954000000	3.1881000000
C20	-2.2294000000	-4.0886000000	3.1991000000
C21	-1.1521000000	-4.9879000000	3.3081000000
C22	0.1502000000	-4.4622000000	3.3969000000
C23	0.3995000000	-3.0769000000	3.3889000000
C24	-3.2076000000	-1.7504000000	3.0289000000
C25	1.8160000000	-2.5480000000	3.4450000000
C26	-1.3915000000	-6.4838000000	3.3529000000
C27	0.3749000000	2.5600000000	2.3102000000
C28	1.7609000000	2.8763000000	2.3002000000
C29	2.1630000000	4.0849000000	1.7072000000

C30	1.2371000000	4.9948000000	1.1655000000
C31	-0.1308000000	4.6988000000	1.2885000000
C32	-0.5900000000	3.5065000000	1.8805000000
C33	2.7851000000	1.9841000000	2.9658000000
C34	1.7064000000	6.2648000000	0.4861000000
C35	-2.0704000000	3.3183000000	2.1306000000
Cl36	2.4066000000	-0.2396000000	0.3841000000
C37	-1.0750000000	-0.2082000000	-4.5730000000
H38	-0.7773000000	-2.5185000000	0.9753000000
H39	-0.4547000000	-4.6227000000	-0.1510000000
H40	0.1871000000	-5.9330000000	-2.1886000000
H41	0.9855000000	-4.7405000000	-4.2397000000
H42	1.1180000000	-2.2426000000	-4.2674000000
H43	-1.8374000000	2.3057000000	-3.6449000000
H44	-0.9700000000	2.2633000000	-2.0863000000
H45	-0.0486000000	2.2388000000	-3.6326000000
H46	-1.9535000000	0.2044000000	-5.1047000000
H47	-0.1704000000	0.0845000000	-5.1377000000
H48	-1.1611000000	-1.3074000000	-4.5895000000
H49	-1.9334000000	0.0208000000	-2.5716000000
H50	0.3697000000	1.8620000000	4.9572000000
H51	-1.3667000000	1.8608000000	4.5164000000
H52	0.3781000000	-0.5312000000	5.2709000000
H53	-1.4087000000	-0.4337000000	5.2495000000
H54	-0.8728000000	5.4261000000	0.9332000000
H55	3.2335000000	4.3265000000	1.6818000000
H56	-2.6666000000	3.9318000000	1.4339000000
H57	-2.3836000000	2.2708000000	2.0034000000
H58	-2.3305000000	3.6459000000	3.1580000000
H59	2.5316000000	1.7984000000	4.0274000000
H60	2.8567000000	1.0067000000	2.4587000000
H61	3.7817000000	2.4571000000	2.9394000000
H62	2.6122000000	6.6725000000	0.9698000000
H63	1.9628000000	6.0765000000	-0.5744000000
H64	0.9270000000	7.0465000000	0.5018000000
H65	-3.2515000000	-4.4807000000	3.1144000000
H66	1.0031000000	-5.1498000000	3.4701000000
H67	2.0629000000	-1.9593000000	2.5412000000
H68	1.9766000000	-1.8846000000	4.3159000000
H69	2.5379000000	-3.3785000000	3.5227000000
H70	-4.1510000000	-2.3133000000	2.9276000000
H71	-3.3138000000	-1.0742000000	3.8986000000
H72	-3.0882000000	-1.1069000000	2.1368000000
H73	-0.5239000000	-7.0456000000	2.9647000000
H74	-1.5663000000	-6.8293000000	4.3902000000
H75	-2.2790000000	-6.7708000000	2.7616000000

SCFE: SCF energy: DFT(bp86) -2726.38421021158 hartrees

NIMAG 1 (-42.65 cm-1)

HOMO energy: -0.15286
LUMO energy: -0.10142

The zero point energy (ZPE): 377.925 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	45.261	1.481	-12.013	20.27628
rot.	0.889	2.981	37.652	0.889	-10.337	17.44705
vib.	24.291	147.851	166.368	24.291	-25.312	42.72208
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	26.068	153.813	249.281	26.660	-47.663	80.44542

Total internal energy, Utot (SCFE + ZPE + U): -2725.740407 hartrees
Total enthalpy, Htot (Utot + pV): -2725.739462 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2725.857904 hartrees

***trans*-(SIMes)RuCl$_2$=CH(C$_6$H$_4$)Se*i*Pr**

C1	0.5251000000	-2.0276000000	-2.2645000000
C2	0.1381000000	-2.6536000000	-1.0512000000
C3	0.1647000000	-4.0723000000	-0.9959000000
C4	0.5894000000	-4.8249000000	-2.0968000000
C5	0.9956000000	-4.1801000000	-3.2778000000
C6	0.9655000000	-2.7749000000	-3.3613000000
C7	-0.2236000000	-1.8889000000	0.1392000000
Ru8	0.0048000000	-0.0628000000	0.3525000000
Cl9	-2.2895000000	0.6059000000	0.0619000000
Se10	0.4491000000	-0.0617000000	-2.2892000000
C11	-1.3579000000	0.2084000000	-3.2544000000
C12	-1.5580000000	1.7242000000	-3.3248000000
C13	-0.2000000000	0.0931000000	2.3647000000
N14	-0.5690000000	-0.7928000000	3.3437000000
C15	-0.5755000000	-0.1945000000	4.7030000000
C16	-0.4789000000	1.3080000000	4.4015000000
N17	-0.0531000000	1.3149000000	2.9830000000
C18	-0.7575000000	-2.2150000000	3.2599000000

C19	-2.0759000000	-2.7214000000	3.1539000000
C20	-2.2522000000	-4.1172000000	3.1533000000
C21	-1.1657000000	-5.0047000000	3.2647000000
C22	0.1302000000	-4.4644000000	3.3648000000
C23	0.3622000000	-3.0764000000	3.3663000000
C24	-3.2588000000	-1.7900000000	3.0007000000
C25	1.7724000000	-2.5302000000	3.4258000000
C26	-1.3891000000	-6.5033000000	3.2993000000
C27	0.4524000000	2.5364000000	2.4016000000
C28	1.8491000000	2.7889000000	2.4787000000
C29	2.3406000000	3.9812000000	1.9239000000
C30	1.4919000000	4.9327000000	1.3292000000
C31	0.1080000000	4.6963000000	1.3591000000
C32	-0.4408000000	3.5227000000	1.9120000000
C33	2.7887000000	1.8390000000	3.1886000000
C34	2.0606000000	6.1809000000	0.6866000000
C35	-1.9409000000	3.3965000000	2.0594000000
Cl36	2.4036000000	-0.0052000000	0.3560000000
C37	-1.3655000000	-0.4679000000	-4.6229000000
H38	-0.6335000000	-2.4992000000	0.9595000000
H39	-0.1357000000	-4.5669000000	-0.0637000000
H40	0.6128000000	-5.9189000000	-2.0346000000
H41	1.3384000000	-4.7678000000	-4.1373000000
H42	1.2900000000	-2.2698000000	-4.2776000000
H43	-2.5293000000	1.9398000000	-3.8098000000
H44	-1.5792000000	2.1708000000	-2.3167000000
H45	-0.7664000000	2.2117000000	-3.9241000000
H46	-2.3519000000	-0.3044000000	-5.1001000000
H47	-0.5943000000	-0.0427000000	-5.2919000000
H48	-1.2065000000	-1.5573000000	-4.5512000000
H49	-2.0927000000	-0.2398000000	-2.5658000000
H50	0.2603000000	1.8319000000	5.0310000000
H51	-1.4535000000	1.8231000000	4.5068000000
H52	0.2889000000	-0.5714000000	5.2850000000
H53	-1.4980000000	-0.4723000000	5.2408000000
H54	-0.5765000000	5.4554000000	0.9581000000
H55	3.4205000000	4.1741000000	1.9645000000
H56	-2.4614000000	4.0524000000	1.3407000000
H57	-2.2917000000	2.3669000000	1.8880000000
H58	-2.2546000000	3.7130000000	3.0746000000
H59	2.4881000000	1.6835000000	4.2429000000
H60	2.8133000000	0.8554000000	2.6899000000
H61	3.8153000000	2.2435000000	3.1919000000
H62	2.9507000000	6.5471000000	1.2291000000
H63	2.3765000000	5.9809000000	-0.3556000000
H64	1.3178000000	6.9970000000	0.6540000000

H65	-3.2689000000	-4.5207000000	3.0585000000
H66	0.9907000000	-5.1424000000	3.4392000000
H67	2.0180000000	-1.9482000000	2.5174000000
H68	1.9200000000	-1.8545000000	4.2892000000
H69	2.5039000000	-3.3510000000	3.5164000000
H70	-4.1916000000	-2.3640000000	2.8690000000
H71	-3.3895000000	-1.1405000000	3.8874000000
H72	-3.1336000000	-1.1211000000	2.1286000000
H73	-0.5106000000	-7.0541000000	2.9201000000
H74	-1.5740000000	-6.8557000000	4.3326000000
H75	-2.2656000000	-6.7968000000	2.6950000000

SCFE: SCF energy: DFT(bp86) -2337.42135286758 hartrees

NIMAG 1 (-40.91 cm-1)

HOMO energy: -0.15260
LUMO energy: -0.10059

The zero point energy (ZPE): 376.851 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	45.476	1.481	-12.077	20.38430
rot.	0.889	2.981	37.834	0.889	-10.392	17.53895
vib.	24.757	149.015	171.382	24.757	-26.340	44.45682
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	26.535	154.976	254.692	27.127	-48.809	82.38007

Total internal energy, Utot (SCFE + ZPE + U): -2336.778516 hartrees
Total enthalpy, Htot (Utot + pV): -2336.777572 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2336.898584 hartrees

***trans*-(SIMes)RuCl$_2$=CH(C$_6$H$_4$)NH*i*Pr**

C1	-0.3832000000	-4.2254000000	-0.9313000000
C2	-0.2577000000	-2.8150000000	-0.9812000000
C3	0.1391000000	-2.1926000000	-2.1933000000
C4	0.4969000000	-2.9776000000	-3.2972000000
C5	0.3823000000	-4.3787000000	-3.2282000000
C6	-0.0757000000	-5.0009000000	-2.0544000000
C7	-0.3981000000	-1.9837000000	0.2032000000

Ru8	0.0194000000	-0.1897000000	0.1015000000
Cl9	-2.2400000000	0.5884000000	-0.1894000000
N10	0.2345000000	-0.7335000000	-2.1385000000
C11	-0.6269000000	0.0854000000	-3.0771000000
C12	-0.1635000000	1.5445000000	-2.9558000000
C13	-0.0469000000	0.3580000000	2.0436000000
N14	0.1771000000	1.6590000000	2.4432000000
C15	-0.1476000000	1.8998000000	3.8679000000
C16	-0.2617000000	0.4716000000	4.4206000000
N17	-0.3671000000	-0.3391000000	3.1828000000
C18	0.6069000000	2.7743000000	1.6346000000
C19	-0.3407000000	3.6892000000	1.1100000000
C20	0.1363000000	4.7801000000	0.3566000000
C21	1.5074000000	5.0101000000	0.1570000000
C22	2.4222000000	4.1389000000	0.7768000000
C23	2.0017000000	3.0306000000	1.5308000000
C24	-1.8195000000	3.5841000000	1.4113000000
C25	3.0197000000	2.1831000000	2.2619000000
C26	1.9927000000	6.1706000000	-0.6874000000
C27	-0.5701000000	-1.7524000000	3.3415000000
C28	-1.8973000000	-2.2443000000	3.3956000000
C29	-2.0869000000	-3.6221000000	3.6074000000
C30	-1.0032000000	-4.5047000000	3.7731000000
C31	0.3008000000	-3.9792000000	3.7144000000
C32	0.5455000000	-2.6099000000	3.5019000000
C33	-3.0779000000	-1.3237000000	3.1724000000
C34	-1.2364000000	-5.9803000000	4.0291000000
C35	1.9621000000	-2.0889000000	3.3951000000
Cl36	2.4118000000	-0.2731000000	-0.0805000000
C37	-0.6277000000	-0.3563000000	-4.5505000000
H38	-0.7438000000	-2.4874000000	1.1185000000
H39	-0.6930000000	-4.6961000000	0.0093000000
H40	-0.1658000000	-6.0923000000	-2.0117000000
H41	0.6608000000	-4.9845000000	-4.0981000000
H42	0.8832000000	-2.5110000000	-4.2080000000
H43	-0.8207000000	2.1984000000	-3.5549000000
H44	-0.2016000000	1.8942000000	-1.9106000000
H45	0.8713000000	1.6652000000	-3.3318000000
H46	-1.2697000000	0.3360000000	-5.1250000000
H47	0.3853000000	-0.3131000000	-4.9955000000
H48	-1.0328000000	-1.3719000000	-4.6874000000
H49	-1.6506000000	0.0030000000	-2.6718000000
H50	0.6474000000	2.4925000000	4.3525000000
H51	-1.0986000000	2.4613000000	3.9507000000
H52	0.6312000000	0.1649000000	5.0010000000
H53	-1.1509000000	0.3211000000	5.0568000000

H54	-0.5943000000	5.4805000000	-0.0696000000
H55	3.4986000000	4.3347000000	0.6855000000
H56	-2.4136000000	4.0817000000	0.6263000000
H57	-2.1590000000	2.5388000000	1.4727000000
H58	-2.0546000000	4.0932000000	2.3676000000
H59	2.7897000000	2.1149000000	3.3424000000
H60	3.0488000000	1.1563000000	1.8589000000
H61	4.0279000000	2.6205000000	2.1610000000
H62	2.9240000000	6.6054000000	-0.2820000000
H63	2.2112000000	5.8462000000	-1.7233000000
H64	1.2371000000	6.9734000000	-0.7476000000
H65	-3.1114000000	-4.0162000000	3.6351000000
H66	1.1581000000	-4.6557000000	3.8287000000
H67	2.1610000000	-1.6728000000	2.3896000000
H68	2.1645000000	-1.2813000000	4.1234000000
H69	2.6891000000	-2.8973000000	3.5827000000
H70	-4.0239000000	-1.8912000000	3.1928000000
H71	-3.1425000000	-0.5387000000	3.9499000000
H72	-3.0029000000	-0.8045000000	2.1983000000
H73	-0.3970000000	-6.5941000000	3.6576000000
H74	-1.3381000000	-6.1875000000	5.1120000000
H75	-2.1623000000	-6.3348000000	3.5425000000
H76	1.2263000000	-0.4723000000	-2.2856000000

SCFE: SCF energy: DFT(bp86) -2383.52245131357 hartrees

NIMAG 1 (-43.61 cm-1)

HOMO energy: -0.15150
LUMO energy: -0.09628

The zero point energy (ZPE): 388.027 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	45.181	1.481	-11.990	20.23613
rot.	0.889	2.981	37.518	0.889	-10.297	17.37981
vib.	23.764	146.166	162.162	23.764	-24.584	41.49379
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	25.542	152.128	244.862	26.134	-46.871	79.10973

Total internal energy, Utot (SCFE + ZPE + U): -2382.863388 hartrees
Total enthalpy, Htot (Utot + pV): -2382.862443 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -2382.978785 hartrees

***trans*-(SIMes)RuCl$_2$=CH(C$_6$H$_4$)PH*i*Pr**

C1	0.2550370823	-2.1180803224	-2.2935185063
C2	-0.0748198093	-2.7732057890	-1.0717325132
C3	-0.1417474406	-4.1883260893	-1.0431048312
C4	0.1467426178	-4.9297888752	-2.1954016215
C5	0.5082291123	-4.2752734975	-3.3864024322
C6	0.5637392013	-2.8694279799	-3.4355281877
C7	-0.2777673039	-1.9782965125	0.1393766400
Ru8	0.0136534617	-0.1471231612	0.2964083036
Cl9	-2.2771424568	0.5791978992	0.0442260934
P10	0.2536798039	-0.2916148722	-2.0629558679
C11	-0.9862295435	0.4964155252	-3.2325951676
C12	-0.8206464557	2.0253581283	-3.1052367079
C13	-0.1628082132	0.0955405739	2.3862827705
N14	-0.4957795170	-0.7634784585	3.3941951367
C15	-0.4997516737	-0.1309952575	4.7401414379
C16	-0.3836596118	1.3632552630	4.4001280303
N17	-0.0199566676	1.3323235884	2.9611085433
C18	-0.6760876223	-2.1884619525	3.3330644715
C19	-1.9927696822	-2.7035201058	3.2446449046
C20	-2.1604887871	-4.1000847283	3.2523123372
C21	-1.0664486346	-4.9801114204	3.3506109766
C22	0.2270008289	-4.4313216364	3.4319562439
C23	0.4504840534	-3.0416040158	3.4270909870
C24	-3.1823743566	-1.7803862393	3.0926519850
C25	1.8576604073	-2.4861616901	3.4644479201
C26	-1.2795759799	-6.4803251489	3.3876749032
C27	0.3879106796	2.5608492254	2.3200201558
C28	1.7709592153	2.8887919060	2.3108945108
C29	2.1639569207	4.0938610694	1.7060709996
C30	1.2322469358	4.9871090579	1.1454307753
C31	-0.1331171862	4.6760925436	1.2552648313
C32	-0.5834008062	3.4860621175	1.8610631059
C33	2.8008349909	2.0044843991	2.9785947398
C34	1.6957947884	6.2545705240	0.4572099347
C35	-2.0647857581	3.2833404169	2.0912248487
Cl36	2.4216380407	-0.1624827775	0.3318235486
C37	-0.8814220687	0.0237344919	-4.6904855935
H38	-0.6125418370	-2.5497344538	1.0197078557
H39	-0.4000572431	-4.6913629629	-0.1030649589
H40	0.1030132479	-6.0247585403	-2.1668692340
H41	0.7496668468	-4.8604554595	-4.2815059035

H42	0.8571364188	-2.3707596394	-4.3660102315
H43	-1.5748256201	2.5383383839	-3.7308129682
H44	-0.9607530110	2.3569037213	-2.0624116851
H45	0.1786350374	2.3535352011	-3.4500428178
H46	-1.6277312248	0.5536305418	-5.3128451023
H47	0.1170514877	0.2411096035	-5.1160117997
H48	-1.0721948698	-1.0583168475	-4.7891603479
H49	-1.9705819846	0.2182902250	-2.8108876905
H50	0.3942952560	1.8841592583	4.9844209922
H51	-1.3391931792	1.9055575746	4.5343356753
H52	0.3571136260	-0.5054177414	5.3336709164
H53	-1.4273121444	-0.3846773876	5.2816269348
H54	-0.8799183569	5.3872063914	0.8783490837
H55	3.2322206663	4.3460637468	1.6831683663
H56	-2.6568815318	3.8102781380	1.3239330058
H57	-2.3507583066	2.2214661262	2.0563310918
H58	-2.3593497397	3.7022592684	3.0747043830
H59	2.5384470779	1.7972938919	4.0337706244
H60	2.8905417599	1.0364677646	2.4555403541
H61	3.7907914386	2.4921645275	2.9699917696
H62	2.5912593999	6.6772547049	0.9473471705
H63	1.9670932280	6.0578043587	-0.5980612063
H64	0.9081782732	7.0281694555	0.4552006878
H65	-3.1755817143	-4.5105436741	3.1705859879
H66	1.0928540336	-5.1036898872	3.4941701467
H67	2.0914874357	-1.9205803640	2.5423957921
H68	2.0083299226	-1.7928543435	4.3132471923
H69	2.5948039806	-3.3010227173	3.5642235112
H70	-4.1150677479	-2.3607589826	2.9914583914
H71	-3.2995951668	-1.1098084065	3.9653006078
H72	-3.0761154771	-1.1329076429	2.2017742187
H73	-0.3970550590	-7.0252702088	3.0091445877
H74	-1.4627979526	-6.8328378693	4.4211312021
H75	-2.1537668206	-6.7807304273	2.7831679215
H76	1.4818335704	0.1046847615	-2.6816210074

SCFE: SCF energy: DFT(bp86) -2670.14352463899 hartrees

NIMAG 1 (-44.87 cm-1)

HOMO energy: -0.15210
LUMO energy: -0.10021

The zero point energy (ZPE): 383.207 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	45.261	1.481	-12.013	20.27630
rot.	0.889	2.981	37.675	0.889	-10.344	17.45880
vib.	23.965	147.335	162.423	23.965	-24.462	41.28633
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	25.742	153.297	245.359	26.335	-46.819	79.02144

Total internal energy, Utot (SCFE + ZPE + U): -2669.491823 hartrees
Total enthalpy, Htot (Utot + pV): -2669.490878 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2669.607457 hartrees

***cis*-(SIMes)RuCl$_2$=CH(8-quinoline)**

C1	-4.2793000000	-3.2954000000	-0.4391000000
C2	-4.0006000000	-1.9191000000	-0.1787000000
C3	-2.6408000000	-1.5511000000	0.0378000000
C4	-1.5725000000	-2.4968000000	-0.0511000000
C5	-1.8916000000	-3.8338000000	-0.3265000000
C6	-3.2438000000	-4.2237000000	-0.5058000000
C7	-4.9722000000	-0.8772000000	-0.1480000000
C8	-4.5506000000	0.4295000000	0.0610000000
C9	-3.1781000000	0.7113000000	0.2694000000
N10	-2.2446000000	-0.2533000000	0.2929000000
Ru11	-0.1535000000	-0.0782000000	0.3699000000
Cl12	2.2467000000	-0.0388000000	0.1081000000
C13	-0.2490000000	-1.9118000000	0.1098000000
C14	0.1588000000	-0.0748000000	2.3791000000
N15	0.1613000000	1.1175000000	3.0534000000
C16	0.7647000000	1.0163000000	4.4023000000
C17	0.8155000000	-0.5068000000	4.6184000000
N18	0.5858000000	-1.0390000000	3.2497000000
C19	-0.3737000000	2.3664000000	2.5706000000
C20	-1.7465000000	2.6354000000	2.8134000000
C21	-2.2738000000	3.8648000000	2.3844000000
C22	-1.4733000000	4.8296000000	1.7430000000
C23	-0.1074000000	4.5512000000	1.5689000000
C24	0.4750000000	3.3376000000	1.9836000000
C25	-2.6221000000	1.6427000000	3.5510000000
C26	1.9615000000	3.1132000000	1.8294000000
C27	-2.0739000000	6.1284000000	1.2471000000
C28	0.6226000000	-2.4668000000	3.0703000000
C29	1.8685000000	-3.1070000000	2.8543000000

C30	1.8829000000	-4.5117000000	2.7658000000
C31	0.7161000000	-5.2846000000	2.9023000000
C32	-0.4965000000	-4.6174000000	3.1531000000
C33	-0.5667000000	-3.2165000000	3.2505000000
C34	3.1519000000	-2.3189000000	2.7267000000
C35	0.7623000000	-6.7936000000	2.7716000000
C36	-1.8872000000	-2.5408000000	3.5512000000
Cl37	-0.3887000000	1.1757000000	-1.6447000000
H38	0.6476000000	-2.5312000000	-0.0647000000
H39	-1.0895000000	-4.5759000000	-0.4076000000
H40	-3.4743000000	-5.2744000000	-0.7165000000
H41	-5.3177000000	-3.6070000000	-0.6028000000
H42	0.0233000000	-0.8694000000	5.3029000000
H43	1.7880000000	-0.8536000000	5.0056000000
H44	0.1404000000	1.5409000000	5.1459000000
H45	1.7714000000	1.4758000000	4.4045000000
H46	2.8424000000	-5.0151000000	2.5888000000
H47	-1.4167000000	-5.2023000000	3.2831000000
H48	3.9923000000	-2.9857000000	2.4697000000
H49	3.0647000000	-1.5410000000	1.9447000000
H50	3.4142000000	-1.8080000000	3.6741000000
H51	-1.8585000000	-1.9838000000	4.5070000000
H52	-2.1594000000	-1.8169000000	2.7636000000
H53	-2.6983000000	-3.2846000000	3.6249000000
H54	-0.0360000000	-7.2770000000	3.3619000000
H55	0.6264000000	-7.1087000000	1.7189000000
H56	1.7320000000	-7.2003000000	3.1082000000
H57	0.5360000000	5.3027000000	1.0940000000
H58	-3.3354000000	4.0798000000	2.5666000000
H59	-2.6159000000	0.6489000000	3.0712000000
H60	-2.2833000000	1.4983000000	4.5952000000
H61	-3.6663000000	1.9969000000	3.5902000000
H62	2.4163000000	3.9313000000	1.2462000000
H63	2.4670000000	3.0884000000	2.8149000000
H64	2.1845000000	2.1602000000	1.3141000000
H65	-2.9536000000	6.4244000000	1.8457000000
H66	-1.3413000000	6.9537000000	1.2801000000
H67	-2.4084000000	6.0321000000	0.1964000000
H68	-2.8170000000	1.7319000000	0.4226000000
H69	-5.2648000000	1.2591000000	0.0631000000
H70	-6.0306000000	-1.1126000000	-0.3101000000

SCFE: SCF energy: DFT(bp86) -2379.92836906358 hartrees

NIMAG 2 (-36.46, -18.48 cm-1)

HOMO energy: -0.14944
LUMO energy: -0.11319

The zero point energy (ZPE): 346.944 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	45.152	1.481	-11.981	20.22155
rot.	0.889	2.981	37.295	0.889	-10.231	17.26763
vib.	21.456	134.696	144.150	21.456	-21.522	36.32533
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	23.234	140.657	226.598	23.826	-43.734	73.81451

Total internal energy, Utot (SCFE + ZPE + U): -2379.338453 hartrees
Total enthalpy, Htot (Utot + pV): -2379.337509 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2379.445173 hartrees

***trans*-(SIMes)RuCl$_2$=CH(8-quinoline)**

C1	0.5478425732	-2.6849967531	3.5695711260
C2	-0.5947110638	-1.8744930850	3.3590968673
C3	-1.8965780706	-2.4279524166	3.3035875229
C4	-2.0328527164	-3.8193571562	3.4589255629
C5	-0.9225875737	-4.6568284058	3.6720368546
C6	0.3562335343	-4.0711126224	3.7211346577
N7	-0.4450354937	-0.4498024998	3.2528673335
C8	-0.0634477574	0.2788751218	2.1565529017
N9	0.0747493534	1.5789420661	2.5886890224
C10	-0.3631449990	1.7797893387	3.9905909463
C11	-0.4665784076	0.3381343642	4.5098896014
Ru12	0.0968597935	-0.2355274276	0.1837512565
Cl13	-2.1788730727	0.3830815910	-0.2072105882
C14	0.5229853519	2.7262944971	1.8347283313
C15	-0.4143476547	3.5978035840	1.2253717057
C16	0.0780030453	4.7143321142	0.5195413858
C17	1.4491794931	5.0105801667	0.4538821776
C18	2.3421289509	4.1804967826	1.1570480494
C19	1.9070843986	3.0477393500	1.8631016126
C20	-1.9079854063	3.4245787517	1.3931381583
C21	1.9594751055	6.1971426087	-0.3377873115
C22	2.8941414114	2.2298816785	2.6665844406
C23	-3.1039398549	-1.5550678820	3.0392494813

C24	-1.1027572574	-6.1495992049	3.8616895369
C25	1.9424670361	-2.0959358174	3.5627014222
N26	0.2041281467	-0.6506926213	-1.9402199437
C27	0.1145217539	-1.9934084591	-2.1923264192
C28	0.1579686734	-2.5418883142	-3.5077608533
C29	0.3040763767	-1.6213202876	-4.5854689364
C30	0.3950788346	-0.2629419624	-4.3116297809
C31	0.3410212071	0.1897616816	-2.9684745279
C32	-0.0250558724	-2.8107178222	-1.0271676683
C33	-0.1238124687	-4.1996836308	-1.2023603302
C34	-0.0843173289	-4.7598541881	-2.5054488262
C35	0.0533452136	-3.9600852005	-3.6379750878
C36	-0.0480640220	-2.0898948807	0.2331609591
Cl37	2.4659117538	0.0170750731	0.0773842797
H38	-0.1456936352	-2.6810736913	1.1550893653
H39	-0.2325490005	-4.8497125629	-0.3265916746
H40	-0.1637705906	-5.8467924322	-2.6217507877
H41	0.0829646009	-4.4097403046	-4.6374271662
H42	0.3718323247	2.3905724277	4.5425289629
H43	-1.3369132696	2.3065708343	4.0098856904
H44	0.3903278184	0.0516977644	5.1517684811
H45	-1.3955192242	0.1429917108	5.0725993338
H46	-0.6416898429	5.3814138694	0.0270678468
H47	3.4123649944	4.4253755436	1.1640071978
H48	-2.4532432962	3.9048838730	0.5628060955
H49	-2.2068539326	2.3654021218	1.4167854906
H50	-2.2478350879	3.9118494947	2.3292621313
H51	2.5736346265	2.1203630588	3.7201886076
H52	3.0043329610	1.2184780280	2.2386829920
H53	3.8861581235	2.7135746989	2.6667358618
H54	2.8106932765	6.6864830858	0.1691365872
H55	2.3159965013	5.8849805091	-1.3384673000
H56	1.1705311180	6.9540063279	-0.4907758359
H57	-3.0367835550	-4.2604733112	3.4029931853
H58	1.2353433960	-4.7115964955	3.8718075280
H59	2.1770561834	-1.6332963354	2.5852423786
H60	2.0660211915	-1.3072541955	4.3283522089
H61	2.6959680949	-2.8765732943	3.7630150189
H62	-4.0212198061	-2.1654237150	2.9833611040
H63	-3.2512336351	-0.8030172112	3.8378729791
H64	-2.9947979246	-0.9995192055	2.0890352477
H65	-0.2050739389	-6.7101633195	3.5468261278
H66	-1.2872922655	-6.3987756259	4.9245372636
H67	-1.9646311581	-6.5298959416	3.2851809200
H68	0.4112827146	1.2532407554	-2.7177957405
H69	0.5093654942	0.4696557818	-5.1169109408

H70	0.3439626273	-1.9915705850	-5.6165375871

SCFE: SCF energy: DFT(bp86) -2379.93249182542 hartrees

NIMAG 1 (-47.08 cm-1)
HOMO energy: -0.15034
LUMO energy: -0.10938

The zero point energy (ZPE): 346.948 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	45.152	1.481	-11.981	20.22155
rot.	0.889	2.981	37.527	0.889	-10.300	17.38406
vib.	22.093	136.729	152.636	22.093	-23.416	39.52140
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	23.870	142.691	235.315	24.463	-45.697	77.12701

Total internal energy, Utot (SCFE + ZPE + U): -2379.341555 hartrees
Total enthalpy, Htot (Utot + pV): -2379.340611 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2379.452417 hartrees

cis-(SIMes)RuCl$_2$=CH(C$_6$H$_4$)N=CMe$_2$

C1	-1.7932289225	2.7831876571	2.8089040688
C2	-0.4154239710	2.4919030903	2.6229323069
C3	0.4969746776	3.4953798242	2.2085964656
C4	-0.0185105734	4.7746417352	1.9212155020
C5	-1.3806094503	5.0877744228	2.0654309823
C6	-2.2502983253	4.0802127380	2.5233441609
N7	0.0595883637	1.1980077420	3.0413269020
C8	0.0394804702	0.0153012582	2.3410777253
N9	0.4012593564	-0.9710509506	3.2247629724
C10	0.5935635211	-0.4651466255	4.6076369518
C11	0.6209674908	1.0555556771	4.4056572109
Ru12	-0.1242088094	-0.0046198053	0.3051632337
Cl13	2.2847977059	0.1610412218	0.2924583350
C14	0.3917045750	-2.4022961589	3.0721409639
C15	1.6236132111	-3.0926105735	2.9390804540
C16	1.5983982870	-4.4999723523	2.9434658596
C17	0.4055694991	-5.2285373682	3.0985170871
C18	-0.7948155150	-4.5115155922	3.2520012819

C19	-0.8262633848	-3.1061924805	3.2484396180
C20	2.9358260133	-2.3521643170	2.8178174933
C21	0.4112155475	-6.7440600568	3.0903294126
C22	-2.1359593516	-2.3733053277	3.4404415692
C23	1.9829315542	3.2372365701	2.1113896670
C24	-1.9036447777	6.4679878814	1.7253441129
C25	-2.7558199830	1.7236002723	3.3026165065
C26	-0.0628941734	-1.8319342964	0.0845519864
C27	-1.3026762754	-2.5493645885	-0.1504141779
C28	-1.3978371804	-3.9523380151	-0.2785467419
C29	-2.6524148443	-4.5698165368	-0.3703596958
C30	-3.8197419425	-3.7896796739	-0.3090148571
C31	-3.7440342626	-2.3885174795	-0.2119771740
C32	-2.4871562809	-1.7577173818	-0.1846245583
N33	-2.2465992147	-0.3533406179	-0.0974304611
C34	-3.0317033853	0.5303652594	-0.6789989244
C35	-4.1513417253	0.2081231032	-1.6458711932
Cl36	-0.0765633755	0.9540039461	-1.9012175811
C37	-2.8136883108	1.9946854911	-0.4407150077
H38	0.8934496994	-2.3819414570	0.0419826992
H39	-0.4785144158	-4.5487995966	-0.2714600060
H40	-2.7249189989	-5.6596142156	-0.4601957808
H41	-4.8036639481	-4.2722420553	-0.3342937543
H42	-4.6647044391	-1.8042205551	-0.1309805952
H43	-3.7742182700	2.4699001942	-0.1553954737
H44	-2.0639483418	2.1792490333	0.3410453399
H45	-2.4617627548	2.4769346016	-1.3693366382
H46	-5.1443065949	0.2597035310	-1.1574215864
H47	-4.1511960587	0.9760276719	-2.4400314241
H48	-4.0438044789	-0.7837830389	-2.1102989732
H49	-0.2446898267	-0.7975714750	5.2525672852
H50	1.5303265250	-0.8615647185	5.0337888573
H51	0.0019379993	1.6054913798	5.1353508336
H52	1.6485509509	1.4649677397	4.4381986978
H53	2.5477031271	-5.0412334542	2.8363498435
H54	-1.7363915181	-5.0602671859	3.3854453943
H55	3.7533477995	-3.0505005691	2.5700074977
H56	2.8881595817	-1.5673199540	2.0395291784
H57	3.2093346943	-1.8522380180	3.7683384735
H58	-2.1358709763	-1.7598515894	4.3616662390
H59	-2.3408786477	-1.6908243179	2.5974552934
H60	-2.9743357625	-3.0860867586	3.5145917352
H61	-0.4168010736	-7.1557428881	3.6941278636
H62	0.2943632492	-7.1409563276	2.0633327865
H63	1.3588194309	-7.1482061165	3.4878987462
H64	0.6777094509	5.5532091245	1.5838428315

H65	-3.3148291026	4.3100126634	2.6645029308
H66	-2.8219242223	0.8783655871	2.5932650153
H67	-2.4400651193	1.2988429388	4.2739866283
H68	-3.7676673315	2.1443363435	3.4325738778
H69	2.4810563545	4.0503961382	1.5568366832
H70	2.4469531071	3.1952275413	3.1170839119
H71	2.2036063591	2.2829277160	1.5984702349
H72	-2.8027178278	6.7179891382	2.3159045826
H73	-1.1433164825	7.2470215376	1.9095240050
H74	-2.1845974022	6.5335659579	0.6566168046

SCFE: SCF energy: DFT(bp86) -2382.30686011300 hartrees

NIMAG 2 (-38.58, -12.36 cm-1)

HOMO energy: -0.14853
LUMO energy: -0.10286

The zero point energy (ZPE): 372.894 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	45.172	1.481	-11.987	20.23128
rot.	0.889	2.981	37.354	0.889	-10.248	17.29722
vib.	22.970	142.616	153.144	22.970	-22.690	38.29654
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	24.747	148.578	235.670	25.340	-44.925	75.82505

Total internal energy, Utot (SCFE + ZPE + U): -2381.673178 hartrees
Total enthalpy, Htot (Utot + pV): -2381.672234 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2381.784208 hartrees

***trans*-(SIMes)RuCl$_2$=CH(C$_6$H$_4$)N=CMe$_2$**

C1	1.8192000000	3.0438000000	1.7781000000
C2	0.4414000000	2.7045000000	1.8665000000
C3	-0.5553000000	3.5633000000	1.3379000000
C4	-0.1382000000	4.6808000000	0.5883000000
C5	1.2186000000	4.9898000000	0.3990000000
C6	2.1790000000	4.1755000000	1.0275000000
N7	0.0699000000	1.5484000000	2.6450000000
C8	-0.0977000000	0.2569000000	2.1902000000

N9	-0.4361000000	-0.4904000000	3.2906000000
C10	-0.3972000000	0.2774000000	4.5603000000
C11	-0.3069000000	1.7282000000	4.0648000000
Ru12	0.0774000000	-0.1943000000	0.2246000000
Cl13	2.4723000000	-0.2633000000	0.2053000000
C14	-0.6124000000	-1.9128000000	3.3955000000
C15	0.5111000000	-2.7485000000	3.6039000000
C16	0.2841000000	-4.1257000000	3.7896000000
C17	-1.0096000000	-4.6782000000	3.7766000000
C18	-2.1009000000	-3.8172000000	3.5540000000
C19	-1.9290000000	-2.4348000000	3.3648000000
C20	1.9201000000	-2.1969000000	3.5783000000
C21	-1.2283000000	-6.1585000000	4.0183000000
C22	-3.1148000000	-1.5353000000	3.0902000000
C23	-2.0267000000	3.3737000000	1.6348000000
C24	1.6428000000	6.1755000000	-0.4435000000
C25	2.8777000000	2.2520000000	2.5130000000
C26	-0.2863000000	-2.0063000000	0.2360000000
C27	-0.2151000000	-2.7347000000	-1.0148000000
C28	0.0769000000	-1.9896000000	-2.1990000000
C29	0.3533000000	-2.6752000000	-3.3972000000
C30	0.2498000000	-4.0763000000	-3.4411000000
C31	-0.1180000000	-4.8090000000	-2.2985000000
C32	-0.3392000000	-4.1413000000	-1.0883000000
N33	0.1762000000	-0.5976000000	-1.9695000000
C34	0.0266000000	0.3418000000	-2.8667000000
C35	-0.4798000000	0.1435000000	-4.2783000000
Cl36	-2.1492000000	0.5985000000	-0.2255000000
C37	0.3284000000	1.7634000000	-2.4715000000
H38	-0.5250000000	-2.5879000000	1.1391000000
H39	-0.5787000000	-4.6992000000	-0.1752000000
H40	-0.1998000000	-5.9007000000	-2.3491000000
H41	0.4699000000	-4.5998000000	-4.3787000000
H42	0.6890000000	-2.1350000000	-4.2860000000
H43	-0.6123000000	2.3145000000	-2.2875000000
H44	0.9454000000	1.8061000000	-1.5592000000
H45	0.8620000000	2.2780000000	-3.2939000000
H46	-1.0948000000	1.0163000000	-4.5622000000
H47	0.3548000000	0.0933000000	-5.0050000000
H48	-1.0866000000	-0.7699000000	-4.3818000000
H49	0.4545000000	2.3239000000	4.5977000000
H50	-1.2759000000	2.2603000000	4.1365000000
H51	0.4846000000	-0.0240000000	5.1597000000
H52	-1.3022000000	0.0772000000	5.1596000000
H53	-0.9052000000	5.3379000000	0.1571000000
H54	3.2426000000	4.4345000000	0.9442000000

H55	-2.6476000000	3.7916000000	0.8245000000
H56	-2.2966000000	2.3125000000	1.7392000000
H57	-2.3012000000	3.9091000000	2.5665000000
H58	2.6309000000	2.1417000000	3.5860000000
H59	2.9814000000	1.2389000000	2.0857000000
H60	3.8555000000	2.7588000000	2.4432000000
H61	2.5197000000	6.6885000000	-0.0092000000
H62	1.9287000000	5.8576000000	-1.4648000000
H63	0.8286000000	6.9140000000	-0.5447000000
H64	-3.1170000000	-4.2324000000	3.5235000000
H65	1.1481000000	-4.7853000000	3.9454000000
H66	2.1475000000	-1.7174000000	2.6074000000
H67	2.0812000000	-1.4314000000	4.3608000000
H68	2.6555000000	-3.0021000000	3.7457000000
H69	-4.0505000000	-2.1195000000	3.0683000000
H70	-3.2269000000	-0.7531000000	3.8652000000
H71	-3.0061000000	-1.0127000000	2.1213000000
H72	-0.3155000000	-6.7428000000	3.8091000000
H73	-1.5098000000	-6.3544000000	5.0713000000
H74	-2.0429000000	-6.5573000000	3.3875000000

SCFE: SCF energy: DFT(bp86) -2382.31811869208 hartrees

NIMAG 1 (-43.35 cm-1)

HOMO energy: -0.14747
LUMO energy: -0.09853

The zero point energy (ZPE): 372.758 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	45.172	1.481	-11.987	20.23128
rot.	0.889	2.981	37.482	0.889	-10.286	17.36142
vib.	23.721	144.796	162.850	23.721	-24.833	41.91243
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	25.499	150.758	245.503	26.091	-47.106	79.50513

Total internal energy, Utot (SCFE + ZPE + U): -2381.683457 hartrees
Total enthalpy, Htot (Utot + pV): -2381.682513 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2381.799159 hartrees

M06-L/LACVP*

PhCH=CH$_2$

C1	-0.3733664479	-0.4416789963	0.0000000000
C2	1.0279516401	-0.3670473443	0.0000000000
C3	1.6749254969	0.8593649163	0.0000000000
C4	0.9409963969	2.0448033387	0.0000000000
C5	-0.4487189602	1.9898735061	0.0000000000
C6	-1.0953015132	0.7602364869	0.0000000000
H7	1.6161410127	-1.2837772312	0.0000000000
H8	2.7631642998	0.8939308397	0.0000000000
H9	1.4526615744	3.0055205202	0.0000000000
H10	-1.0324779077	2.9088913335	0.0000000000
H11	-2.1850596871	0.7195973177	0.0000000000
C12	-1.1046450022	-1.7079991744	0.0000000000
C13	-0.5934176612	-2.9433285270	0.0000000000
H14	-2.1927376960	-1.6018506032	0.0000000000
H15	-1.2379396758	-3.8177128728	0.0000000000
H16	0.4778089864	-3.1371936504	0.0000000000

energy: -309.59627173278 hartrees

H$_2$C=CH(C$_6$H$_4$)O*i*Pr

C1	0.0557592582	-0.0599194342	0.0322161380
C2	-0.0084512384	-0.1566563743	1.4258016825
C3	1.1313258089	-0.2455670905	2.2116502986
C4	2.3806749104	-0.2278022360	1.6015890907
C5	2.4875455450	-0.1235223118	0.2189893394
C6	1.3370198992	-0.0474210334	-0.5696132843
H7	-0.9880896838	-0.1493682107	1.9015043710
H8	1.0465357303	-0.3177802305	3.2936793340
H9	3.2875777743	-0.2895289241	2.2006999870
H10	3.4729049458	-0.1077356693	-0.2373226847
O11	1.3482381597	0.0148481022	-1.9287655196
C12	-1.1395444247	0.0422349298	-0.8016791292
C13	-2.4068973786	-0.1271118570	-0.4066019940
H14	-0.9499319229	0.2788667765	-1.8473981545
H15	-3.2313403214	-0.0127741384	-1.1049979635
H16	-2.6799780661	-0.3901789097	0.6143275545
C17	2.5985725743	0.1585762273	-2.6156542153
C18	2.3146657856	-0.1977431621	-4.0571275829
C19	3.1309766138	1.5713101850	-2.4678574775
H20	3.3138355996	-0.5690387322	-2.1989804672

H21	3.2296614450	-0.1302204784	-4.6554953979
H22	1.9187936736	-1.2142500200	-4.1399524965
H23	1.5768772244	0.4924717783	-4.4824841011
H24	4.0964665757	1.6757188319	-2.9758733713
H25	2.4298198212	2.2837681761	-2.9180870351
H26	3.2670358816	1.8530168889	-1.4185438138

energy: -502.72633214088 hartrees

H_2C=CH(C_6H_4)S*i*Pr

C1	0.0503338915	0.0790914318	0.0189242035
C2	0.0134180822	0.1240982559	1.4200822880
C3	1.1541881293	-0.0368350202	2.1883606611
C4	2.3849799761	-0.2358473944	1.5654932645
C5	2.4564254352	-0.2934618076	0.1823039523
C6	1.3074629321	-0.1433520182	-0.5978813091
H7	-0.9420556605	0.3177223950	1.9056131017
H8	1.0869239664	0.0009400303	3.2734222246
H9	3.2882068361	-0.3674099895	2.1575589097
H10	3.4076945682	-0.4949558760	-0.3079408257
S11	1.3401795410	-0.4226211985	-2.3356478945
C12	-1.1730755304	0.2719181180	-0.7642873907
C13	-2.4260948486	0.0812520877	-0.3343656063
H14	-1.0237985690	0.6034130786	-1.7932172579
H15	-3.2791054644	0.2864012689	-0.9763658421
H16	-2.6573164935	-0.2961277945	0.6608077502
C17	2.9086670589	0.2205735050	-3.0098776844
C18	2.8083008760	-0.0818601620	-4.5002469197
C19	3.0744106964	1.7000861940	-2.7371216483
H20	3.7420917859	-0.3520401150	-2.5800977983
H21	3.7186460417	0.2376614992	-5.0193866566
H22	2.6605864367	-1.1502126554	-4.6939899190
H23	1.9616261297	0.4554844572	-4.9465448543
H24	4.0132073280	2.0681050150	-3.1705064844
H25	2.2466348948	2.2623031373	-3.1866043792
H26	3.0833505273	1.9144104939	-1.6629476165

energy: -825.68143510615 hartrees

H_2C=CH(C_6H_4)Se*i*Pr

C1	0.1165139060	0.2863422211	-0.0026339406
C2	0.2508349512	0.6944401951	1.3374713762

C3	1.4023396154	0.4561175801	2.0668265485
C4	2.4675130818	-0.2178245645	1.4741020255
C5	2.3602594768	-0.6391986057	0.1541765814
C6	1.2081514464	-0.3845268579	-0.5947195690
H7	-0.5657305626	1.2486233972	1.7981208246
H8	1.4758921622	0.8084089892	3.0947740121
H9	3.3817929993	-0.4057774689	2.0347846197
H10	3.1916083300	-1.1636206399	-0.3145090665
Se11	1.2797336636	-0.8493175144	-2.5213269962
C12	-1.1014712781	0.6050141025	-0.7491966635
C13	-2.2686495083	0.9992637869	-0.2279119243
H14	-1.0187706841	0.4930730885	-1.8310951057
H15	-3.1182124336	1.2301039394	-0.8645157856
H16	-2.4371656529	1.0970807503	0.8439361634
C17	2.6340758166	0.6552280168	-2.8443499026
C18	3.1052846418	0.6047491319	-4.2790799786
C19	2.0595915318	2.0050863815	-2.4726548137
H20	3.4587355704	0.4020525666	-2.1645119694
H21	3.8672717691	1.3784764718	-4.4443596681
H22	3.5480212739	-0.3626455773	-4.5383343479
H23	2.2824594513	0.8056102591	-4.9762424413
H24	2.8199982543	2.7860448093	-2.6195974034
H25	1.1963100837	2.2595110680	-3.1001783500
H26	1.7439983259	2.0514043020	-1.4244940101

energy: -436.72554285557 hartrees

H_2C=CH(C_6H_4)NH*i*Pr

C1	0.0095290614	0.0134452838	0.0753971507
C2	-0.0426936524	-0.2148832804	1.4530664746
C3	1.1067478501	-0.3114595219	2.2265560005
C4	2.3448743109	-0.1690019539	1.6091594840
C5	2.4335786819	0.0519100973	0.2403729656
C6	1.2783279182	0.1375967972	-0.5499638346
H7	-1.0231381486	-0.2842477311	1.9236034440
H8	1.0367802838	-0.4762036053	3.2993009570
H9	3.2605817918	-0.2310901011	2.1954369639
H10	3.4145074986	0.1437920634	-0.2181838794
N11	1.3382704048	0.3344822080	-1.9255734686
C12	-1.2179056991	0.1370921530	-0.7123018360
C13	-2.3687732787	-0.5031584696	-0.4749289027
H14	-1.1775924075	0.8319806298	-1.5565608439
H15	-3.2557402605	-0.3259047101	-1.0775446232
H16	-2.4645337713	-1.2306987758	0.3299501549

C17	2.5898071781	0.1435514945	-2.6549710910
C18	2.2713828908	-0.2892285715	-4.0749684162
C19	3.4221217510	1.4182991106	-2.6481259608
H20	3.1715008803	-0.6638786139	-2.1720190068
H21	3.1896531731	-0.4127427533	-4.6583772114
H22	1.7313509272	-1.2436879032	-4.0960520483
H23	1.6552130962	0.4655795188	-4.5811246484
H24	4.3990287819	1.2492283847	-3.1175224470
H25	2.9055907133	2.2101618886	-3.2038807364
H26	3.5928570354	1.7887766155	-1.6319313600
H27	0.5468813129	-0.0734129891	-2.4060733944

energy: -482.86056487123 hartrees

H_2C=CH(C_6H_4)PH*i*Pr

C1	0.2630057431	-0.0428168783	-0.0048118971
C2	0.2674231445	0.1997792648	1.3781083939
C3	1.3323840285	-0.1797072880	2.1777918297
C4	2.4278743612	-0.8254601038	1.6097784864
C5	2.4413428604	-1.0779174586	0.2447153160
C6	1.3764497298	-0.7003238569	-0.5839275581
H7	-0.6004457951	0.6781497838	1.8292330758
H8	1.3053325981	0.0181277988	3.2480099579
H9	3.2690494802	-1.1319870153	2.2290914324
H10	3.3057777120	-1.5738697452	-0.1976289830
P11	1.4727771697	-0.9869196040	-2.3985074266
C12	-0.8729604739	0.3898633007	-0.8252094417
C13	-1.7486839681	1.3524215897	-0.5152404244
H14	-0.9815303669	-0.1203846087	-1.7851461201
H15	-2.5706545749	1.6031431576	-1.1802754299
H16	-1.6759371250	1.9386358718	0.3997848788
C17	2.4954164470	0.5232051205	-2.8595986815
C18	3.0027653337	0.3933125231	-4.2883145805
C19	1.6842783451	1.7979134606	-2.6789600555
H20	3.3555770259	0.5571008980	-2.1732275395
H21	3.6213782867	1.2599471594	-4.5565782866
H22	3.6128183880	-0.5060973870	-4.4351008382
H23	2.1702400841	0.3523530548	-5.0025724229
H24	2.2799114605	2.6755377853	-2.9635418999
H25	0.7844247470	1.7927836418	-3.3088742547
H26	1.3600907467	1.9401243691	-1.6418217546
H27	2.5678309691	-1.8844760140	-2.3381912481

energy: -769.44111028459 hartrees

(SIMes)$RuCl_2$=CHPh

C1	-0.5022818509	3.6877050997	1.0450165835
C2	0.3752020499	2.7553245790	1.6192476458
C3	1.7709454003	2.9511565153	1.6091506047
C4	2.2771759536	4.0543264584	0.9257135282
C5	1.4364097524	4.9715315432	0.2831997998
C6	0.0568255031	4.7773221118	0.3655048634
N7	-0.1328557326	1.6641782988	2.3914091175
C8	-0.1826612529	0.3466772171	2.0369040132
N9	-0.3843934412	-0.3645026086	3.1775097651
C10	-0.3171951034	0.4744915188	4.3790666533
C11	-0.4744693325	1.8693734788	3.8026807212

Ru12	-0.2048280787	-0.1804091898	0.1641752047
Cl13	2.0459804252	0.2357363220	-0.5073135782
C14	-0.4179830232	-1.7765097200	3.3371864947
C15	-1.6642745011	-2.4090554827	3.4712491651
C16	-1.6777173582	-3.7953947506	3.6427178866
C17	-0.4961913525	-4.5439748280	3.6912183807
C18	0.7253848906	-3.8747726876	3.5581355484
C19	0.7902999125	-2.4899335750	3.3800505199
C20	-2.9331952847	-1.6177794475	3.3793075190
C21	-0.5425645703	-6.0294842863	3.8920928594
C22	2.0958260690	-1.7917447378	3.1488572716
C23	2.6755688987	2.0251694119	2.3620157309
C24	2.0135491233	6.1408547845	-0.4570418649
C25	-1.9856360783	3.5889844622	1.2246503017
C26	-0.1790360082	-2.0243512894	0.2074595174
C27	-0.1902867097	-2.7913097940	-1.0174735994
C28	0.0053354755	-2.2021556027	-2.2876329688
C29	-0.0436297783	-2.9747639894	-3.4391132956
C30	-0.2838636940	-4.3499904444	-3.3544999539
C31	-0.4720964092	-4.9510730281	-2.1077416864
C32	-0.4233884882	-4.1822448744	-0.9511072721
H33	0.2287192601	-1.1353394242	-2.3623820926
Cl34	-2.5494812409	0.2484187949	-0.0201782456
H35	-0.2136966477	-2.6156275693	1.1290313119
H36	-0.5711140302	-4.6425644946	0.0274170527
H37	-0.6539305096	-6.0228741278	-2.0402971525
H38	-0.3172411784	-4.9524348560	-4.2612090499
H39	0.1152845628	-2.5075457286	-4.4096912321
H40	0.1977528827	2.6096163107	4.2535219520
H41	-1.5073331668	2.2442774016	3.8872362857
H42	0.6496195430	0.3265583708	4.8904441041
H43	-1.1138554867	0.1981720772	5.0804847863
H44	-0.6136896104	5.5065977429	-0.0937081113
H45	3.3573575295	4.2120496189	0.9056340320
H46	-2.5169310834	4.1402237955	0.4410141612
H47	-2.3407611427	2.5523212388	1.2049844786
H48	-2.2895547273	4.0291357700	2.1866846125
H49	2.4125889356	1.9830341372	3.4301613945
H50	2.6141205442	1.0023460670	1.9687374845
H51	3.7198707479	2.3473832878	2.2891033627
H52	2.8380110219	6.6044396873	0.0995746306
H53	2.4231245595	5.8338185356	-1.4290070441
H54	1.2600577332	6.9132293994	-0.6493233260
H55	-2.6386173714	-4.3063777978	3.7315242512
H56	1.6545610787	-4.4478558984	3.5783287025
H57	2.1385572215	-1.3638604446	2.1335462689

H58	2.2521042187	-0.9560261780	3.8453536939
H59	2.9409392013	-2.4796343238	3.2593344159
H60	-3.8119429931	-2.2665195297	3.4589693763
H61	-3.0065118249	-0.8631691793	4.1758798521
H62	-2.9947770431	-1.0715785930	2.4266015433
H63	0.3717578536	-6.5162972294	3.5338472323
H64	-0.6499396010	-6.2863349105	4.9551009236
H65	-1.3947406273	-6.4822554557	3.3704406035

SCFE: SCF energy: DFT(m06-l) -2209.96887020770 hartrees

***cis*-(SIMes)RuCl$_2$=CH(C$_6$H$_4$)O*i*Pr**

C1	-1.6224000000	-3.7898000000	-0.1834000000
C2	-1.3633000000	-2.4096000000	-0.0906000000
C3	-2.4343000000	-1.5069000000	-0.2957000000
C4	-3.7211000000	-1.9701000000	-0.5595000000
C5	-3.9474000000	-3.3469000000	-0.6244000000
C6	-2.9048000000	-4.2605000000	-0.4443000000
C7	-0.0590000000	-1.8820000000	0.2294000000
Ru8	0.2268000000	-0.0698000000	0.3697000000
Cl9	0.5301000000	0.9021000000	-1.8492000000
O10	-2.0924000000	-0.1931000000	-0.1776000000
C11	-3.0122000000	0.8103000000	-0.7310000000
C12	-2.5349000000	2.1479000000	-0.2284000000
C13	0.1872000000	0.0347000000	2.3974000000
N14	0.4376000000	-0.9193000000	3.3334000000
C15	0.5131000000	-0.3593000000	4.6904000000
C16	0.7260000000	1.1146000000	4.4048000000
N17	0.1911000000	1.2398000000	3.0414000000
C18	0.3445000000	-2.3358000000	3.2015000000
C19	-0.9320000000	-2.9245000000	3.1129000000
C20	-1.0207000000	-4.3160000000	3.0599000000
C21	0.1165000000	-5.1292000000	3.1067000000
C22	1.3639000000	-4.5130000000	3.2358000000
C23	1.5058000000	-3.1212000000	3.3015000000
C24	-2.1739000000	-2.0861000000	3.1014000000
C25	2.8544000000	-2.5002000000	3.5010000000
C26	-0.0066000000	-6.6209000000	3.0079000000
C27	-0.4677000000	2.4491000000	2.6479000000
C28	-1.7298000000	2.7161000000	3.2287000000
C29	-2.3621000000	3.9246000000	2.9296000000
C30	-1.7873000000	4.8556000000	2.0578000000
C31	-0.5472000000	4.5541000000	1.4896000000
C32	0.1382000000	3.3644000000	1.7699000000

C33	-2.4250000000	1.6934000000	4.0773000000
C34	-2.5132000000	6.1220000000	1.7082000000
C35	1.4512000000	3.0768000000	1.1111000000
Cl36	2.6039000000	-0.2681000000	0.6380000000
C37	-3.0309000000	0.7267000000	-2.2422000000
H38	0.7780000000	-2.5943000000	0.3000000000
H39	-0.7924000000	-4.4810000000	-0.0302000000
H40	-3.0957000000	-5.3304000000	-0.5115000000
H41	-4.9569000000	-3.7043000000	-0.8258000000
H42	-4.5464000000	-1.2789000000	-0.7133000000
H43	-3.2138000000	2.9348000000	-0.5817000000
H44	-2.5159000000	2.1812000000	0.8652000000
H45	-1.5280000000	2.3586000000	-0.6136000000
H46	-3.7355000000	1.4684000000	-2.6386000000
H47	-2.0277000000	0.9460000000	-2.6293000000
H48	-3.3365000000	-0.2588000000	-2.6087000000
H49	-4.0002000000	0.5808000000	-0.2978000000
H50	-0.4270000000	-0.5599000000	5.2337000000
H51	1.3335000000	-0.8218000000	5.2500000000
H52	0.2017000000	1.7868000000	5.0922000000
H53	1.7932000000	1.3887000000	4.4018000000
H54	2.2612000000	-5.1326000000	3.2930000000
H55	-2.0079000000	-4.7771000000	2.9769000000
H56	3.6530000000	-3.2180000000	3.2843000000
H57	2.9923000000	-1.6268000000	2.8503000000
H58	2.9958000000	-2.1683000000	4.5408000000
H59	-2.3605000000	-1.6301000000	4.0855000000
H60	-2.1093000000	-1.2652000000	2.3736000000
H61	-3.0539000000	-2.6882000000	2.8464000000
H62	-0.8281000000	-7.0043000000	3.6266000000
H63	-0.2152000000	-6.9369000000	1.9758000000
H64	0.9144000000	-7.1260000000	3.3208000000
H65	-0.0873000000	5.2697000000	0.8054000000
H66	-3.3414000000	4.1324000000	3.3669000000
H67	-2.3852000000	0.7002000000	3.6098000000
H68	-1.9844000000	1.5883000000	5.0799000000
H69	-3.4800000000	1.9545000000	4.2189000000
H70	1.9943000000	4.0044000000	0.8940000000
H71	2.0930000000	2.4244000000	1.7127000000
H72	1.3184000000	2.5609000000	0.1450000000
H73	-3.2530000000	6.3897000000	2.4721000000
H74	-1.8265000000	6.9691000000	1.5908000000
H75	-3.0553000000	6.0202000000	0.7568000000

SCFE: SCF energy: DFT(m06-l) -2403.10793369686 hartrees

***cis*-(SIMes)RuCl$_2$=CH(C$_6$H$_4$)S*i*Pr**

C1	-2.7021000000	-1.6549000000	0.1196000000
C2	-1.5509000000	-2.4690000000	0.0520000000
C3	-1.7222000000	-3.8557000000	-0.1239000000
C4	-2.9966000000	-4.4023000000	-0.2317000000
C5	-4.1234000000	-3.5745000000	-0.1726000000
C6	-3.9796000000	-2.1975000000	0.0089000000
C7	-0.2426000000	-1.8531000000	0.1864000000
Ru8	0.0489000000	-0.0374000000	0.4074000000
Cl9	0.2043000000	1.3202000000	-1.6158000000
S10	-2.3780000000	0.0558000000	0.4680000000
C11	-3.4261000000	0.9386000000	-0.8036000000
C12	-3.1498000000	2.4217000000	-0.6330000000
C13	0.2191000000	-0.0351000000	2.4307000000
N14	0.1786000000	1.1540000000	3.0848000000
C15	0.7493000000	1.0613000000	4.4339000000
C16	0.7113000000	-0.4337000000	4.6887000000
N17	0.6011000000	-0.9776000000	3.3272000000
C18	-0.4469000000	2.3632000000	2.6478000000
C19	-1.7570000000	2.6173000000	3.1091000000
C20	-2.3534000000	3.8299000000	2.7681000000
C21	-1.6886000000	4.7816000000	1.9826000000
C22	-0.3930000000	4.4977000000	1.5519000000
C23	0.2601000000	3.3012000000	1.8801000000
C24	-2.4956000000	1.6091000000	3.9387000000
C25	1.6634000000	3.0586000000	1.4188000000
C26	-2.3722000000	6.0612000000	1.6034000000
C27	0.5747000000	-2.3937000000	3.1644000000
C28	1.7838000000	-3.1042000000	3.0848000000
C29	1.7160000000	-4.4943000000	2.9376000000
C30	0.5002000000	-5.1811000000	2.9107000000
C31	-0.6795000000	-4.4456000000	3.0636000000
C32	-0.6667000000	-3.0569000000	3.1989000000
C33	3.1058000000	-2.4102000000	3.1878000000
C34	0.4552000000	-6.6711000000	2.7450000000
C35	-1.9472000000	-2.3038000000	3.3991000000
Cl36	2.4849000000	-0.3152000000	0.3862000000
C37	-3.2036000000	0.4331000000	-2.2117000000
H38	0.6347000000	-2.5062000000	0.0557000000
H39	-0.8366000000	-4.4918000000	-0.1638000000
H40	-3.1186000000	-5.4767000000	-0.3636000000
H41	-5.1208000000	-4.0041000000	-0.2587000000
H42	-4.8591000000	-1.5569000000	0.0746000000
H43	-3.8082000000	2.9913000000	-1.3018000000

H44	-3.3338000000	2.7576000000	0.3953000000
H45	-2.1083000000	2.6500000000	-0.8946000000
H46	-3.8734000000	0.9719000000	-2.8959000000
H47	-2.1682000000	0.6116000000	-2.5248000000
H48	-3.4226000000	-0.6371000000	-2.3039000000
H49	-4.4505000000	0.7106000000	-0.4682000000
H50	-0.1601000000	-0.7451000000	5.2896000000
H51	1.6152000000	-0.8136000000	5.1790000000
H52	0.1567000000	1.6479000000	5.1456000000
H53	1.7744000000	1.4634000000	4.4299000000
H54	2.6482000000	-5.0542000000	2.8416000000
H55	-1.6401000000	-4.9657000000	3.0656000000
H56	3.9231000000	-3.0718000000	2.8821000000
H57	3.1375000000	-1.5123000000	2.5573000000
H58	3.3113000000	-2.1017000000	4.2239000000
H59	-2.0470000000	-1.9416000000	4.4338000000
H60	-2.0178000000	-1.4218000000	2.7503000000
H61	-2.8163000000	-2.9383000000	3.1906000000
H62	-0.3669000000	-6.9788000000	2.0858000000
H63	1.3888000000	-7.0600000000	2.3231000000
H64	0.2964000000	-7.1792000000	3.7063000000
H65	0.1427000000	5.2340000000	0.9500000000
H66	-3.3651000000	4.0398000000	3.1231000000
H67	-1.9793000000	1.3730000000	4.8805000000
H68	-3.4969000000	1.9699000000	4.1986000000
H69	-2.6129000000	0.6594000000	3.3983000000
H70	2.2037000000	4.0061000000	1.3122000000
H71	2.2253000000	2.4077000000	2.0972000000
H72	1.6837000000	2.5621000000	0.4370000000
H73	-2.9749000000	6.4606000000	2.4288000000
H74	-1.6552000000	6.8333000000	1.3028000000
H75	-3.0562000000	5.9079000000	0.7565000000

SCFE: SCF energy: DFT(m06-l) -2726.08514212785 hartrees

cis-(SIMes)$RuCl_2$=CH(C_6H_4)Se_i_Pr

C1	-2.8787000000	-1.5713000000	0.3547000000
C2	-1.7447000000	-2.3603000000	0.0881000000
C3	-1.9434000000	-3.7050000000	-0.2846000000
C4	-3.2257000000	-4.2333000000	-0.3860000000
C5	-4.3357000000	-3.4311000000	-0.1083000000
C6	-4.1618000000	-2.0950000000	0.2666000000
C7	-0.4049000000	-1.8053000000	0.1916000000
Ru8	0.0301000000	-0.0319000000	0.4738000000

Cl9	0.1609000000	1.3714000000	-1.5197000000
Se10	-2.5222000000	0.3158000000	0.7945000000
C11	-3.5030000000	1.0238000000	-0.9093000000
C12	-3.3138000000	2.5204000000	-0.9546000000
C13	0.2270000000	-0.1067000000	2.4952000000
N14	0.1850000000	1.0626000000	3.1926000000
C15	0.5378000000	0.8921000000	4.6034000000
C16	0.5146000000	-0.6204000000	4.7661000000
N17	0.4876000000	-1.0980000000	3.3780000000
C18	-0.3947000000	2.2705000000	2.6956000000
C19	-1.7239000000	2.5513000000	3.0658000000
C20	-2.3426000000	3.6689000000	2.5029000000
C21	-1.6769000000	4.5053000000	1.6012000000
C22	-0.3434000000	4.2217000000	1.2987000000
C23	0.3277000000	3.1205000000	1.8399000000
C24	-2.4808000000	1.6694000000	4.0163000000
C25	1.7708000000	2.8831000000	1.5204000000
C26	-2.3888000000	5.6486000000	0.9438000000
C27	0.5526000000	-2.4997000000	3.1184000000
C28	1.8095000000	-3.1117000000	2.9838000000
C29	1.8427000000	-4.4742000000	2.6749000000
C30	0.6781000000	-5.2355000000	2.5348000000
C31	-0.5500000000	-4.6095000000	2.7605000000
C32	-0.6362000000	-3.2508000000	3.0744000000
C33	3.0733000000	-2.3326000000	3.1700000000
C34	0.7499000000	-6.6934000000	2.1886000000
C35	-1.9674000000	-2.6324000000	3.3749000000
Cl36	2.4097000000	-0.5515000000	0.1857000000
C37	-3.0624000000	0.3179000000	-2.1686000000
H38	0.4229000000	-2.4981000000	-0.0335000000
H39	-1.0686000000	-4.3237000000	-0.4927000000
H40	-3.3646000000	-5.2717000000	-0.6847000000
H41	-5.3409000000	-3.8433000000	-0.1895000000
H42	-5.0306000000	-1.4702000000	0.4756000000
H43	-3.8845000000	2.9338000000	-1.7987000000
H44	-3.6661000000	3.0060000000	-0.0372000000
H45	-2.2541000000	2.7674000000	-1.1042000000
H46	-3.6236000000	0.7378000000	-3.0164000000
H47	-1.9941000000	0.4801000000	-2.3593000000
H48	-3.2608000000	-0.7590000000	-2.1472000000
H49	-4.5438000000	0.7743000000	-0.6533000000
H50	-0.3786000000	-0.9844000000	5.3005000000
H51	1.3968000000	-1.0117000000	5.2866000000
H52	-0.1948000000	1.3984000000	5.2440000000
H53	1.5258000000	1.3342000000	4.8017000000
H54	2.8137000000	-4.9527000000	2.5335000000

H55	-1.4718000000	-5.1905000000	2.6788000000
H56	3.9517000000	-2.9756000000	3.0515000000
H57	3.1438000000	-1.5177000000	2.4365000000
H58	3.1280000000	-1.8808000000	4.1709000000
H59	-2.1404000000	-2.5619000000	4.4591000000
H60	-2.0522000000	-1.6145000000	2.9744000000
H61	-2.7871000000	-3.2247000000	2.9517000000
H62	-0.1353000000	-7.0219000000	1.6302000000
H63	1.6347000000	-6.9211000000	1.5825000000
H64	0.8103000000	-7.3200000000	3.0897000000
H65	0.1942000000	4.8649000000	0.6005000000
H66	-3.3838000000	3.8779000000	2.7607000000
H67	-2.2923000000	1.9353000000	5.0671000000
H68	-3.5609000000	1.7526000000	3.8520000000
H69	-2.2134000000	0.6097000000	3.8991000000
H70	2.1424000000	3.6509000000	0.8349000000
H71	2.3876000000	2.9095000000	2.4299000000
H72	1.9594000000	1.9139000000	1.0391000000
H73	-3.2351000000	6.0033000000	1.5437000000
H74	-1.7184000000	6.4967000000	0.7634000000
H75	-2.7893000000	5.3505000000	-0.0359000000

SCFE: SCF energy: DFT(m06-l) -2337.12509542207 hartrees

cis-(SIMes)$RuCl_2$=CH(C_6H_4)NH_i_Pr

C1	-2.3106000000	-1.7788000000	0.0610000000
C2	-1.1101000000	-2.5113000000	-0.0212000000
C3	-1.1686000000	-3.8992000000	-0.2409000000
C4	-2.3961000000	-4.5420000000	-0.3557000000
C5	-3.5786000000	-3.8076000000	-0.2488000000
C6	-3.5375000000	-2.4260000000	-0.0444000000
C7	0.1353000000	-1.7951000000	0.1576000000
Ru8	0.1602000000	0.0222000000	0.4106000000
Cl9	0.3076000000	1.3441000000	-1.6137000000
N10	-2.1666000000	-0.3442000000	0.2456000000
C11	-3.1278000000	0.4696000000	-0.5735000000
C12	-2.9316000000	1.9307000000	-0.2337000000
C13	0.2098000000	0.0243000000	2.4251000000
N14	0.2621000000	1.2173000000	3.0797000000
C15	0.8265000000	1.0779000000	4.4268000000
C16	0.6901000000	-0.4145000000	4.6835000000
N17	0.4863000000	-0.9499000000	3.3311000000
C18	-0.3435000000	2.4443000000	2.6592000000
C19	0.4179000000	3.4561000000	2.0522000000

C20	-0.2304000000	4.6504000000	1.7165000000
C21	-1.5764000000	4.8794000000	2.0058000000
C22	-2.2888000000	3.8735000000	2.6664000000
C23	-1.6962000000	2.6549000000	2.9948000000
C24	1.8860000000	3.3026000000	1.8158000000
C25	-2.4959000000	1.5928000000	3.6854000000
C26	-2.2459000000	6.1598000000	1.6073000000
C27	0.2919000000	-2.3543000000	3.1698000000
C28	-1.0045000000	-2.8813000000	3.3138000000
C29	-1.1861000000	-4.2593000000	3.1865000000
C30	-0.1165000000	-5.1190000000	2.9266000000
C31	1.1652000000	-4.5691000000	2.8391000000
C32	1.3991000000	-3.1963000000	2.9693000000
C33	-2.1874000000	-2.0008000000	3.5805000000
C34	-0.3440000000	-6.5860000000	2.7209000000
C35	2.7878000000	-2.6464000000	2.9018000000
Cl36	2.6028000000	0.0851000000	0.5252000000
C37	-2.9553000000	0.1829000000	-2.0512000000
H38	1.0765000000	-2.3581000000	0.0474000000
H39	-0.2353000000	-4.4599000000	-0.3061000000
H40	-2.4367000000	-5.6168000000	-0.5283000000
H41	-4.5420000000	-4.3086000000	-0.3325000000
H42	-4.4671000000	-1.8624000000	0.0229000000
H43	-3.6223000000	2.5478000000	-0.8200000000
H44	-3.1275000000	2.1288000000	0.8272000000
H45	-1.9043000000	2.2425000000	-0.4663000000
H46	-3.6630000000	0.7946000000	-2.6227000000
H47	-1.9383000000	0.4372000000	-2.3723000000
H48	-3.1504000000	-0.8681000000	-2.2938000000
H49	-4.1491000000	0.1768000000	-0.2672000000
H50	-0.1717000000	-0.6648000000	5.3265000000
H51	1.5835000000	-0.8585000000	5.1383000000
H52	0.2762000000	1.7012000000	5.1421000000
H53	1.8782000000	1.4025000000	4.4221000000
H54	2.0179000000	-5.2287000000	2.6658000000
H55	-2.1949000000	-4.6687000000	3.2774000000
H56	3.5079000000	-3.4293000000	2.6410000000
H57	2.8692000000	-1.8367000000	2.1624000000
H58	3.1002000000	-2.2235000000	3.8676000000
H59	-1.9580000000	-1.1784000000	4.2676000000
H60	-2.5689000000	-1.5466000000	2.6548000000
H61	-3.0161000000	-2.5762000000	4.0087000000
H62	-1.1416000000	-6.9716000000	3.3674000000
H63	-0.6481000000	-6.7953000000	1.6849000000
H64	0.5625000000	-7.1712000000	2.9129000000
H65	0.3493000000	5.4337000000	1.2249000000

H66	-3.3387000000	4.0363000000	2.9203000000
H67	-2.5709000000	0.6782000000	3.0800000000
H68	-2.0467000000	1.2806000000	4.6403000000
H69	-3.5156000000	1.9351000000	3.8948000000
H70	2.2567000000	4.0813000000	1.1417000000
H71	2.4447000000	3.3922000000	2.7591000000
H72	2.1469000000	2.3287000000	1.3824000000
H73	-3.0895000000	6.3993000000	2.2654000000
H74	-1.5496000000	7.0064000000	1.6251000000
H75	-2.6432000000	6.0959000000	0.5846000000
H76	-2.3719000000	-0.1267000000	1.2237000000

SCFE: SCF energy: DFT(m06-l) -2383.24814635021 hartrees

cis-(SIMes)RuCl$_2$=CH(C$_6$H$_4$)PH_i_Pr

C1	-0.7115000000	-3.0980000000	3.1545000000
C2	0.5142000000	-2.4076000000	3.1291000000
C3	1.7382000000	-3.0927000000	3.0279000000
C4	1.6974000000	-4.4769000000	2.8334000000
C5	0.4952000000	-5.1865000000	2.7828000000
C6	-0.6971000000	-4.4810000000	2.9679000000
N7	0.5107000000	-0.9941000000	3.3229000000
C8	0.1843000000	-0.0322000000	2.4274000000
N9	0.1146000000	1.1463000000	3.1028000000
C10	0.5881000000	1.0242000000	4.4853000000
C11	0.5721000000	-0.4795000000	4.6981000000
Ru12	0.0564000000	-0.0151000000	0.3967000000
Cl13	2.5271000000	-0.3942000000	0.2854000000
C14	-0.5021000000	2.3514000000	2.6435000000
C15	-1.8106000000	2.6342000000	3.0863000000
C16	-2.4069000000	3.8286000000	2.6738000000
C17	-1.7450000000	4.7271000000	1.8313000000
C18	-0.4405000000	4.4219000000	1.4326000000
C19	0.2109000000	3.2516000000	1.8350000000
C20	-2.5647000000	1.7075000000	3.9960000000
C21	-2.4335000000	5.9637000000	1.3387000000
C22	1.6321000000	2.9900000000	1.4359000000
C23	3.0459000000	-2.3745000000	3.1310000000
C24	0.4734000000	-6.6668000000	2.5426000000
C25	-2.0152000000	-2.3937000000	3.3826000000
C26	-0.2524000000	-1.8346000000	0.1681000000
C27	-1.5641000000	-2.4584000000	0.0533000000
C28	-2.7010000000	-1.6325000000	0.1989000000
C29	-3.9817000000	-2.1736000000	0.1278000000

C30	-4.1433000000	-3.5459000000	-0.0860000000
C31	-3.0240000000	-4.3704000000	-0.2384000000
C32	-1.7406000000	-3.8346000000	-0.1739000000
P33	-2.2401000000	0.1164000000	0.4179000000
C34	-3.3912000000	1.0015000000	-0.7419000000
C35	-3.2597000000	0.4954000000	-2.1714000000
Cl36	0.2186000000	1.2904000000	-1.6609000000
C37	-3.1955000000	2.5075000000	-0.6385000000
H38	0.6311000000	-2.4727000000	0.0108000000
H39	-0.8632000000	-4.4734000000	-0.2846000000
H40	-3.1588000000	-5.4379000000	-0.4110000000
H41	-5.1443000000	-3.9728000000	-0.1402000000
H42	-4.8592000000	-1.5334000000	0.2371000000
H43	-3.9135000000	3.0271000000	-1.2877000000
H44	-3.3438000000	2.8715000000	0.3864000000
H45	-2.1821000000	2.7879000000	-0.9561000000
H46	-3.9938000000	1.0016000000	-2.8128000000
H47	-2.2571000000	0.7035000000	-2.5648000000
H48	-3.4403000000	-0.5848000000	-2.2443000000
H49	-4.3958000000	0.7446000000	-0.3610000000
H50	-0.3074000000	-0.8267000000	5.2665000000
H51	1.4690000000	-0.8529000000	5.2058000000
H52	-0.0714000000	1.5701000000	5.1701000000
H53	1.5984000000	1.4517000000	4.5698000000
H54	2.6406000000	-5.0145000000	2.7191000000
H55	-1.6482000000	-5.0175000000	2.9463000000
H56	3.8851000000	-3.0707000000	3.0300000000
H57	3.1372000000	-1.6058000000	2.3508000000
H58	3.1548000000	-1.8664000000	4.1001000000
H59	-2.2212000000	-2.2642000000	4.4562000000
H60	-2.0346000000	-1.3958000000	2.9298000000
H61	-2.8513000000	-2.9635000000	2.9598000000
H62	-0.2627000000	-6.9367000000	1.7729000000
H63	1.4507000000	-7.0400000000	2.2163000000
H64	0.1961000000	-7.2209000000	3.4501000000
H65	0.0977000000	5.1191000000	0.7879000000
H66	-3.4219000000	4.0550000000	3.0089000000
H67	-2.4257000000	1.9751000000	5.0543000000
H68	-3.6429000000	1.7564000000	3.8011000000
H69	-2.2532000000	0.6615000000	3.8823000000
H70	2.0323000000	3.8300000000	0.8596000000
H71	2.2745000000	2.8412000000	2.3147000000
H72	1.7606000000	2.0926000000	0.8124000000
H73	-3.2197000000	6.2950000000	2.0276000000
H74	-1.7324000000	6.7946000000	1.1959000000
H75	-2.9133000000	5.7824000000	0.3658000000

H76	-2.8870000000	0.4493000000	1.6370000000

SCFE: SCF energy: DFT(m06-l) -2669.86007625593 hartrees

***trans*-(SIMes)RuCl$_2$=CH(C$_6$H$_4$)O*i*Pr**

C1	-0.6390000000	3.4600000000	1.1790000000
C2	0.4669000000	2.6937000000	1.5957000000
C3	1.7765000000	3.0130000000	1.1822000000
C4	1.9344000000	4.0124000000	0.2175000000
C5	0.8447000000	4.7181000000	-0.2997000000
C6	-0.4252000000	4.4516000000	0.2192000000
N7	0.2753000000	1.6151000000	2.5092000000
C8	0.1241000000	0.3111000000	2.1371000000
N9	0.0311000000	-0.4106000000	3.2818000000
C10	0.1910000000	0.4038000000	4.4919000000
C11	0.1634000000	1.8280000000	3.9500000000
Ru12	0.1213000000	-0.1548000000	0.2220000000
Cl13	2.5467000000	-0.2790000000	0.0371000000
C14	-0.2430000000	-1.7996000000	3.4087000000
C15	-1.5841000000	-2.2177000000	3.4508000000
C16	-1.8405000000	-3.5852000000	3.5750000000
C17	-0.8046000000	-4.5234000000	3.6595000000
C18	0.5163000000	-4.0662000000	3.6157000000
C19	0.8236000000	-2.7073000000	3.4929000000
C20	-2.6946000000	-1.2235000000	3.2937000000
C21	-1.1093000000	-5.9849000000	3.8072000000
C22	2.2399000000	-2.2311000000	3.3864000000
C23	2.9855000000	2.4034000000	1.8271000000
C24	1.0332000000	5.7349000000	-1.3856000000
C25	-1.9958000000	3.2938000000	1.7923000000
C26	-0.3099000000	-1.9530000000	0.2245000000
C27	-0.4947000000	-2.6419000000	-1.0253000000
C28	-0.2677000000	-1.9568000000	-2.2479000000
C29	-0.4643000000	-2.5863000000	-3.4734000000
C30	-0.8957000000	-3.9141000000	-3.4885000000
C31	-1.1234000000	-4.6159000000	-2.3015000000
C32	-0.9215000000	-3.9819000000	-1.0817000000
O33	0.1257000000	-0.6750000000	-2.0837000000
C34	0.5339000000	0.1555000000	-3.2071000000
C35	1.8827000000	-0.3051000000	-3.7203000000
Cl36	-2.1102000000	0.7107000000	-0.1711000000
C37	0.5582000000	1.5703000000	-2.6738000000
H38	-0.4722000000	-2.5554000000	1.1274000000
H39	-1.0966000000	-4.5073000000	-0.1410000000

H40	-1.4580000000	-5.6510000000	-2.3342000000
H41	-1.0549000000	-4.4056000000	-4.4476000000
H42	-0.2927000000	-2.0554000000	-4.4066000000
H43	0.7982000000	2.2694000000	-3.4841000000
H44	-0.4115000000	1.8460000000	-2.2420000000
H45	1.3299000000	1.6680000000	-1.8966000000
H46	2.2007000000	0.3285000000	-4.5571000000
H47	2.6232000000	-0.2255000000	-2.9152000000
H48	1.8667000000	-1.3445000000	-4.0673000000
H49	-0.2506000000	0.0528000000	-3.9742000000
H50	0.9964000000	2.4447000000	4.3134000000
H51	-0.7754000000	2.3560000000	4.1860000000
H52	1.1427000000	0.1560000000	4.9887000000
H53	-0.6190000000	0.1927000000	5.2027000000
H54	-1.2814000000	5.0289000000	-0.1357000000
H55	2.9422000000	4.2521000000	-0.1282000000
H56	-2.7876000000	3.4976000000	1.0641000000
H57	-2.1615000000	2.2811000000	2.1721000000
H58	-2.1237000000	4.0014000000	2.6259000000
H59	3.3887000000	3.0946000000	2.5831000000
H60	2.7668000000	1.4496000000	2.3171000000
H61	3.7778000000	2.2124000000	1.0965000000
H62	1.9765000000	6.2835000000	-1.2729000000
H63	1.0613000000	5.2553000000	-2.3747000000
H64	0.2152000000	6.4645000000	-1.4062000000
H65	-2.8770000000	-3.9288000000	3.5960000000
H66	1.3337000000	-4.7884000000	3.6674000000
H67	2.4148000000	-1.7100000000	2.4325000000
H68	2.4966000000	-1.5188000000	4.1837000000
H69	2.9453000000	-3.0666000000	3.4511000000
H70	-3.6744000000	-1.7016000000	3.4027000000
H71	-2.6337000000	-0.4134000000	4.0353000000
H72	-2.6599000000	-0.7405000000	2.3044000000
H73	-0.2576000000	-6.6086000000	3.5125000000
H74	-1.3518000000	-6.2400000000	4.8483000000
H75	-1.9732000000	-6.2832000000	3.2003000000

SCFE: SCF energy: DFT(m06-l) -2403.12721434024 hartrees

***trans*-(SIMes)$RuCl_2$=$CH(C_6H_4)$S*i*Pr**

C1	0.3837000000	-1.9279000000	-2.2585000000
C2	0.2247000000	-2.6136000000	-1.0340000000
C3	0.5656000000	-3.9786000000	-0.9763000000
C4	1.0879000000	-4.6226000000	-2.0896000000

C5	1.2683000000	-3.9232000000	-3.2845000000
C6	0.9206000000	-2.5742000000	-3.3688000000
C7	-0.1927000000	-1.9167000000	0.1638000000
Ru8	-0.2013000000	-0.0767000000	0.3338000000
Cl9	-2.6135000000	0.3986000000	0.2308000000
S10	-0.0002000000	-0.1935000000	-2.2579000000
C11	-1.6590000000	-0.0712000000	-3.0928000000
C12	-1.9609000000	1.4147000000	-3.1453000000
C13	-0.3097000000	0.1483000000	2.3396000000
N14	-0.6710000000	-0.7022000000	3.3336000000
C15	-0.6695000000	-0.0657000000	4.6553000000
C16	-0.6326000000	1.4071000000	4.2979000000
N17	-0.1793000000	1.3833000000	2.9038000000
C18	-0.7671000000	-2.1232000000	3.2703000000
C19	-2.0326000000	-2.7200000000	3.2046000000
C20	-2.0973000000	-4.1147000000	3.1378000000
C21	-0.9491000000	-4.9102000000	3.1516000000
C22	0.2967000000	-4.2788000000	3.2290000000
C23	0.4139000000	-2.8884000000	3.2900000000
C24	-3.2686000000	-1.8782000000	3.1433000000
C25	1.7607000000	-2.2348000000	3.2818000000
C26	-1.0460000000	-6.4046000000	3.0895000000
C27	0.5110000000	2.5189000000	2.3645000000
C28	1.8946000000	2.6144000000	2.6243000000
C29	2.5825000000	3.7332000000	2.1617000000
C30	1.9396000000	4.7512000000	1.4534000000
C31	0.5634000000	4.6465000000	1.2514000000
C32	-0.1793000000	3.5556000000	1.7182000000
C33	2.6121000000	1.5412000000	3.3823000000
C34	2.7154000000	5.9265000000	0.9411000000
C35	-1.6714000000	3.5768000000	1.6171000000
Cl36	2.1955000000	0.2802000000	0.2264000000
C37	-1.6344000000	-0.6979000000	-4.4708000000
H38	-0.4412000000	-2.5754000000	1.0048000000
H39	0.4442000000	-4.5104000000	-0.0305000000
H40	1.3712000000	-5.6723000000	-2.0269000000
H41	1.6923000000	-4.4268000000	-4.1518000000
H42	1.0835000000	-2.0169000000	-4.2903000000
H43	-2.9587000000	1.5730000000	-3.5731000000
H44	-1.9538000000	1.8576000000	-2.1430000000
H45	-1.2320000000	1.9411000000	-3.7760000000
H46	-2.6039000000	-0.5415000000	-4.9612000000
H47	-0.8621000000	-0.2377000000	-5.1028000000
H48	-1.4520000000	-1.7769000000	-4.4348000000
H49	-2.3771000000	-0.5764000000	-2.4335000000
H50	0.0572000000	1.9958000000	4.9141000000

H51	-1.6284000000	1.8732000000	4.3542000000
H52	0.2130000000	-0.3971000000	5.2287000000
H53	-1.5658000000	-0.3532000000	5.2175000000
H54	0.0351000000	5.4573000000	0.7463000000
H55	3.6543000000	3.8106000000	2.3554000000
H56	-2.0034000000	4.2288000000	0.8008000000
H57	-2.1034000000	2.5827000000	1.4536000000
H58	-2.1106000000	3.9778000000	2.5431000000
H59	2.1880000000	1.3833000000	4.3852000000
H60	2.5536000000	0.5874000000	2.8425000000
H61	3.6723000000	1.7891000000	3.5074000000
H62	3.4949000000	6.2351000000	1.6489000000
H63	3.2230000000	5.6881000000	-0.0037000000
H64	2.0679000000	6.7904000000	0.7532000000
H65	-3.0767000000	-4.5912000000	3.0616000000
H66	1.2052000000	-4.8846000000	3.2235000000
H67	1.9120000000	-1.6474000000	2.3605000000
H68	1.8960000000	-1.5401000000	4.1229000000
H69	2.5609000000	-2.9808000000	3.3376000000
H70	-4.1692000000	-2.5000000000	3.0987000000
H71	-3.3595000000	-1.2183000000	4.0173000000
H72	-3.2569000000	-1.2203000000	2.2618000000
H73	-0.1451000000	-6.8496000000	2.6501000000
H74	-1.1616000000	-6.8404000000	4.0916000000
H75	-1.9094000000	-6.7313000000	2.4979000000

SCFE: SCF energy: DFT(m06-l) -2726.08039266540 hartrees

***trans*-(SIMes)$RuCl_2$=$CH(C_6H_4)$Se*i*Pr**

C1	0.5489000000	-1.8723000000	-2.2086000000
C2	0.0116000000	-2.5360000000	-1.0814000000
C3	-0.2417000000	-3.9205000000	-1.1753000000
C4	0.0523000000	-4.6237000000	-2.3374000000
C5	0.6146000000	-3.9574000000	-3.4273000000
C6	0.8502000000	-2.5798000000	-3.3665000000
C7	-0.2478000000	-1.8513000000	0.1688000000
Ru8	0.1779000000	-0.0928000000	0.5320000000
Cl9	-2.0644000000	0.7767000000	0.0579000000
Se10	0.8897000000	0.0672000000	-2.0222000000
C11	-0.7783000000	0.6489000000	-3.0724000000
C12	-0.8260000000	2.1606000000	-3.0307000000
C13	-0.1404000000	-0.0272000000	2.5468000000
N14	-0.4829000000	-0.9070000000	3.5099000000
C15	-0.4671000000	-0.3100000000	4.8533000000
C16	-0.3474000000	1.1815000000	4.5618000000
N17	-0.0156000000	1.1920000000	3.1367000000
C18	-0.7806000000	-2.2925000000	3.3631000000
C19	-2.1345000000	-2.6593000000	3.2595000000
C20	-2.4457000000	-4.0185000000	3.1800000000
C21	-1.4510000000	-5.0022000000	3.2073000000
C22	-0.1153000000	-4.5966000000	3.2990000000
C23	0.2472000000	-3.2479000000	3.3831000000
C24	-3.2001000000	-1.6085000000	3.1743000000
C25	1.6821000000	-2.8259000000	3.4315000000
C26	-1.8151000000	-6.4566000000	3.1640000000
C27	0.2478000000	2.3629000000	2.3560000000
C28	1.5803000000	2.7351000000	2.0944000000
C29	1.8019000000	3.7562000000	1.1639000000
C30	0.7459000000	4.4436000000	0.5562000000
C31	-0.5578000000	4.1480000000	0.9664000000
C32	-0.8306000000	3.1411000000	1.8950000000
C33	2.7150000000	2.1202000000	2.8513000000
C34	0.9994000000	5.4553000000	-0.5198000000
C35	-2.2122000000	2.9550000000	2.4397000000
Cl36	2.6032000000	-0.4089000000	0.6748000000
C37	-0.7825000000	0.1085000000	-4.4865000000
H38	-0.7319000000	-2.4785000000	0.9331000000
H39	-0.6667000000	-4.4323000000	-0.3098000000
H40	-0.1455000000	-5.6931000000	-2.3927000000
H41	0.8569000000	-4.5064000000	-4.3361000000
H42	1.2899000000	-2.0671000000	-4.2210000000
H43	-1.7426000000	2.5073000000	-3.5265000000
H44	-0.8436000000	2.5362000000	-2.0011000000

H45	0.0254000000	2.6048000000	-3.5632000000
H46	-1.6808000000	0.4705000000	-5.0060000000
H47	0.0894000000	0.4437000000	-5.0636000000
H48	-0.8161000000	-0.9862000000	-4.5146000000
H49	-1.6109000000	0.2301000000	-2.4937000000
H50	0.4344000000	1.6806000000	5.1474000000
H51	-1.2928000000	1.7159000000	4.7381000000
H52	0.3803000000	-0.7132000000	5.4292000000
H53	-1.3844000000	-0.5710000000	5.3960000000
H54	-1.3913000000	4.7253000000	0.5619000000
H55	2.8301000000	4.0292000000	0.9216000000
H56	-2.9425000000	3.5299000000	1.8614000000
H57	-2.5229000000	1.9050000000	2.4342000000
H58	-2.2697000000	3.3243000000	3.4741000000
H59	2.5712000000	2.2379000000	3.9344000000
H60	2.8133000000	1.0476000000	2.6515000000
H61	3.6640000000	2.5941000000	2.5826000000
H62	1.9240000000	6.0179000000	-0.3474000000
H63	1.1040000000	4.9660000000	-1.4985000000
H64	0.1747000000	6.1714000000	-0.6091000000
H65	-3.4918000000	-4.3174000000	3.0901000000
H66	0.6720000000	-5.3528000000	3.3022000000
H67	1.9513000000	-2.2174000000	2.5545000000
H68	1.9027000000	-2.2077000000	4.3126000000
H69	2.3495000000	-3.6935000000	3.4574000000
H70	-4.1916000000	-2.0572000000	3.0548000000
H71	-3.2319000000	-0.9744000000	4.0719000000
H72	-3.0279000000	-0.9326000000	2.3234000000
H73	-1.0197000000	-7.0648000000	2.7188000000
H74	-1.9917000000	-6.8529000000	4.1732000000
H75	-2.7343000000	-6.6294000000	2.5923000000

SCFE: SCF energy: DFT(m06-l) -2337.12069450286 hartrees

trans-(SIMes)$RuCl_2$=CH(C_6H_4)NH_i_Pr

C1	0.5863000000	-2.6429000000	3.5680000000
C2	-0.4922000000	-1.7547000000	3.4389000000
C3	-1.8250000000	-2.2012000000	3.4088000000
C4	-2.0606000000	-3.5747000000	3.5106000000
C5	-1.0117000000	-4.4933000000	3.6394000000
C6	0.2999000000	-4.0088000000	3.6651000000
N7	-0.2412000000	-0.3585000000	3.3317000000
C8	-0.0202000000	0.3433000000	2.1945000000
N9	0.1305000000	1.6462000000	2.5635000000

C10	-0.0280000000	1.8773000000	3.9984000000
C11	-0.1747000000	0.4605000000	4.5475000000
Ru12	0.1246000000	-0.1528000000	0.2486000000
Cl13	2.5567000000	-0.4478000000	0.1912000000
C14	0.4564000000	2.6922000000	1.6488000000
C15	-0.5620000000	3.5314000000	1.1584000000
C16	-0.2239000000	4.4679000000	0.1785000000
C17	1.0850000000	4.6061000000	-0.2947000000
C18	2.0892000000	3.8323000000	0.2937000000
C19	1.8050000000	2.8896000000	1.2868000000
C20	-1.9545000000	3.4891000000	1.7105000000
C21	1.3999000000	5.5569000000	-1.4110000000
C22	2.9267000000	2.2183000000	2.0203000000
C23	-2.9451000000	-1.2301000000	3.1837000000
C24	-1.2917000000	-5.9629000000	3.7553000000
C25	1.9980000000	-2.1420000000	3.5440000000
C26	-0.4438000000	-1.9024000000	0.2339000000
C27	-0.3422000000	-2.6727000000	-0.9865000000
C28	-0.6366000000	-4.0494000000	-1.0099000000
C29	-0.4119000000	-4.7988000000	-2.1586000000
C30	0.1296000000	-4.1847000000	-3.2893000000
C31	0.4215000000	-2.8175000000	-3.2851000000
C32	0.1576000000	-2.0492000000	-2.1536000000
N33	0.4598000000	-0.6428000000	-2.0267000000
C34	-0.1859000000	0.3454000000	-2.9417000000
C35	-0.0484000000	0.0555000000	-4.4304000000
Cl36	-2.0560000000	0.8634000000	-0.1817000000
C37	0.4035000000	1.7055000000	-2.6013000000
H38	-0.8709000000	-2.4264000000	1.1008000000
H39	-1.0190000000	-4.5183000000	-0.1012000000
H40	-0.6354000000	-5.8647000000	-2.1703000000
H41	0.3391000000	-4.7736000000	-4.1814000000
H42	0.8760000000	-2.3627000000	-4.1620000000
H43	-0.0731000000	2.4892000000	-3.2026000000
H44	0.2500000000	1.9643000000	-1.5448000000
H45	1.4851000000	1.7324000000	-2.8050000000
H46	-0.4704000000	0.8913000000	-5.0023000000
H47	1.0049000000	-0.0476000000	-4.7303000000
H48	-0.5873000000	-0.8478000000	-4.7343000000
H49	-1.2498000000	0.3443000000	-2.6642000000
H50	0.8461000000	2.4075000000	4.4021000000
H51	-0.9155000000	2.5015000000	4.1882000000
H52	0.6815000000	0.1484000000	5.1663000000
H53	-1.0829000000	0.3222000000	5.1508000000
H54	-1.0127000000	5.1005000000	-0.2343000000
H55	3.1269000000	3.9709000000	-0.0164000000

H56	-2.6951000000	3.7242000000	0.9388000000
H57	-2.2113000000	2.5044000000	2.1139000000
H58	-2.0679000000	4.2329000000	2.5143000000
H59	3.2960000000	2.8853000000	2.8146000000
H60	2.6276000000	1.2731000000	2.4829000000
H61	3.7668000000	1.9976000000	1.3548000000
H62	2.3914000000	6.0114000000	-1.2939000000
H63	1.3996000000	5.0398000000	-2.3816000000
H64	0.6609000000	6.3643000000	-1.4779000000
H65	-3.0895000000	-3.9392000000	3.4722000000
H66	1.1284000000	-4.7150000000	3.7511000000
H67	2.2360000000	-1.6687000000	2.5779000000
H68	2.1804000000	-1.3834000000	4.3188000000
H69	2.7107000000	-2.9584000000	3.7045000000
H70	-3.9190000000	-1.7303000000	3.2274000000
H71	-2.9510000000	-0.4204000000	3.9274000000
H72	-2.8561000000	-0.7417000000	2.2002000000
H73	-0.4238000000	-6.5648000000	3.4617000000
H74	-1.5447000000	-6.2440000000	4.7872000000
H75	-2.1404000000	-6.2657000000	3.1291000000
H76	1.4775000000	-0.5257000000	-2.0736000000

SCFE: SCF energy: DFT(m06-l) -2383.26352164448 hartrees

***trans*-(SIMes)RuCl$_2$=CH(C$_6$H$_4$)PH*i*Pr**

C1	-0.5339000000	3.3435000000	1.6589000000
C2	0.3507000000	2.4839000000	2.3299000000
C3	1.7407000000	2.7226000000	2.3450000000
C4	2.2385000000	3.7655000000	1.5677000000
C5	1.3973000000	4.5749000000	0.7964000000
C6	0.0199000000	4.3680000000	0.8804000000
N7	-0.1371000000	1.3465000000	3.0459000000
C8	-0.2261000000	0.1017000000	2.5193000000
N9	-0.5803000000	-0.7257000000	3.5238000000
C10	-0.6051000000	-0.0611000000	4.8361000000
C11	-0.5624000000	1.4110000000	4.4494000000
Ru12	-0.0062000000	-0.1323000000	0.4068000000
Cl13	2.4416000000	0.0162000000	0.4078000000
C14	-0.6814000000	-2.1420000000	3.4232000000
C15	-1.9547000000	-2.7164000000	3.2749000000
C16	-2.0350000000	-4.1041000000	3.1239000000
C17	-0.8925000000	-4.9125000000	3.1152000000
C18	0.3577000000	-4.3020000000	3.2648000000
C19	0.4898000000	-2.9169000000	3.4174000000

C20	-3.1749000000	-1.8507000000	3.1894000000
C21	-1.0092000000	-6.3996000000	2.9357000000
C22	1.8377000000	-2.2645000000	3.4597000000
C23	2.6532000000	1.8837000000	3.1861000000
C24	1.9696000000	5.6343000000	-0.0953000000
C25	-2.0192000000	3.2670000000	1.8403000000
C26	-0.1922000000	-1.9697000000	0.2012000000
C27	-0.0066000000	-2.7140000000	-1.0328000000
C28	0.2561000000	-2.0069000000	-2.2320000000
C29	0.5247000000	-2.7043000000	-3.4076000000
C30	0.4958000000	-4.1026000000	-3.4124000000
C31	0.2035000000	-4.8066000000	-2.2408000000
C32	-0.0431000000	-4.1214000000	-1.0553000000
P33	0.2266000000	-0.2139000000	-1.9395000000
C34	-1.0229000000	0.5756000000	-3.0507000000
C35	-0.8677000000	0.2181000000	-4.5202000000
Cl36	-2.3887000000	0.4501000000	0.1705000000
C37	-0.9411000000	2.0814000000	-2.8161000000
H38	-0.4629000000	-2.5855000000	1.0696000000
H39	-0.2529000000	-4.6625000000	-0.1303000000
H40	0.1798000000	-5.8957000000	-2.2556000000
H41	0.7035000000	-4.6446000000	-4.3345000000
H42	0.7665000000	-2.1668000000	-4.3244000000
H43	-1.7001000000	2.6021000000	-3.4150000000
H44	-1.1144000000	2.3297000000	-1.7627000000
H45	0.0402000000	2.4801000000	-3.1085000000
H46	-1.5918000000	0.7803000000	-5.1259000000
H47	0.1350000000	0.4690000000	-4.8946000000
H48	-1.0428000000	-0.8470000000	-4.7070000000
H49	-1.9956000000	0.2221000000	-2.6797000000
H50	0.1459000000	1.9995000000	5.0454000000
H51	-1.5495000000	1.8955000000	4.5165000000
H52	0.2717000000	-0.3735000000	5.4271000000
H53	-1.5053000000	-0.3421000000	5.3961000000
H54	-0.6555000000	5.0264000000	0.3310000000
H55	3.3161000000	3.9383000000	1.5471000000
H56	-2.5511000000	3.5135000000	0.9137000000
H57	-2.3574000000	2.2724000000	2.1451000000
H58	-2.3365000000	3.9949000000	2.6023000000
H59	2.3988000000	1.9528000000	4.2550000000
H60	2.5957000000	0.8267000000	2.8960000000
H61	3.6964000000	2.2007000000	3.0696000000
H62	2.8636000000	6.0961000000	0.3417000000
H63	2.2738000000	5.2122000000	-1.0617000000
H64	1.2435000000	6.4271000000	-0.3044000000
H65	-3.0158000000	-4.5639000000	2.9839000000

H66	1.2594000000	-4.9176000000	3.2355000000
H67	2.0293000000	-1.6981000000	2.5329000000
H68	1.9294000000	-1.5462000000	4.2860000000
H69	2.6354000000	-3.0070000000	3.5695000000
H70	-4.0830000000	-2.4558000000	3.0926000000
H71	-3.2929000000	-1.2085000000	4.0739000000
H72	-3.1175000000	-1.1767000000	2.3200000000
H73	-0.0935000000	-6.8297000000	2.5125000000
H74	-1.1919000000	-6.9100000000	3.8929000000
H75	-1.8432000000	-6.6631000000	2.2725000000
H76	1.4216000000	0.2272000000	-2.5508000000

SCFE: SCF energy: DFT(m06-l) -2669.84860530375 hartrees

***cis*-(SIMes)RuCl$_2$=CH(8-quinoline)**

C1	-4.5778000000	-2.7695000000	-0.1252000000
C2	-4.1058000000	-1.4357000000	-0.0234000000
C3	-2.7089000000	-1.2415000000	0.0836000000
C4	-1.7871000000	-2.3237000000	0.0318000000
C5	-2.2957000000	-3.6133000000	-0.0975000000
C6	-3.6874000000	-3.8269000000	-0.1581000000
C7	-4.9184000000	-0.2760000000	-0.0471000000
C8	-4.3201000000	0.9660000000	-0.0064000000
C9	-2.9210000000	1.0679000000	0.1077000000
N10	-2.1440000000	-0.0049000000	0.2003000000
Ru11	-0.0166000000	-0.1329000000	0.3196000000
Cl12	2.4058000000	-0.4070000000	0.2002000000
C13	-0.3953000000	-1.9339000000	0.1165000000
C14	0.1812000000	-0.1266000000	2.3376000000
N15	0.1171000000	1.0690000000	2.9748000000
C16	0.6508000000	1.0066000000	4.3381000000
C17	0.6906000000	-0.4912000000	4.5933000000
N18	0.5947000000	-1.0482000000	3.2375000000
C19	-0.5091000000	2.2549000000	2.4828000000
C20	-1.8728000000	2.4443000000	2.7833000000
C21	-2.4853000000	3.6271000000	2.3657000000
C22	-1.7817000000	4.6030000000	1.6530000000
C23	-0.4300000000	4.3805000000	1.3770000000
C24	0.2369000000	3.2243000000	1.7935000000
C25	-2.6575000000	1.3772000000	3.4835000000
C26	1.6976000000	3.0383000000	1.5236000000
C27	-2.4703000000	5.8436000000	1.1687000000
C28	0.6761000000	-2.4588000000	3.0505000000
C29	1.9364000000	-3.0703000000	2.9616000000

C30	1.9787000000	-4.4594000000	2.8096000000
C31	0.8205000000	-5.2386000000	2.7594000000
C32	-0.4143000000	-4.5981000000	2.8986000000
C33	-0.5101000000	-3.2131000000	3.0460000000
C34	3.1959000000	-2.2671000000	3.0509000000
C35	0.9008000000	-6.7210000000	2.5529000000
C36	-1.8437000000	-2.5569000000	3.2306000000
Cl37	0.0048000000	1.2827000000	-1.6329000000
H38	0.3919000000	-2.6876000000	-0.0348000000
H39	-1.6082000000	-4.4577000000	-0.1444000000
H40	-4.0659000000	-4.8439000000	-0.2481000000
H41	-5.6503000000	-2.9481000000	-0.1951000000
H42	-0.1562000000	-0.8448000000	5.2042000000
H43	1.6166000000	-0.8223000000	5.0760000000
H44	0.0002000000	1.5554000000	5.0294000000
H45	1.6503000000	1.4656000000	4.3697000000
H46	2.9522000000	-4.9455000000	2.7257000000
H47	-1.3305000000	-5.1927000000	2.8993000000
H48	4.0710000000	-2.8819000000	2.8166000000
H49	3.1731000000	-1.4227000000	2.3492000000
H50	3.3452000000	-1.8623000000	4.0621000000
H51	-1.9591000000	-2.1517000000	4.2465000000
H52	-1.9850000000	-1.7195000000	2.5353000000
H53	-2.6618000000	-3.2663000000	3.0644000000
H54	0.0543000000	-7.2433000000	3.0134000000
H55	0.8912000000	-6.9734000000	1.4839000000
H56	1.8244000000	-7.1398000000	2.9689000000
H57	0.1310000000	5.1341000000	0.8224000000
H58	-3.5438000000	3.7819000000	2.5861000000
H59	-2.6349000000	0.4391000000	2.9111000000
H60	-2.2603000000	1.1400000000	4.4814000000
H61	-3.7062000000	1.6708000000	3.6042000000
H62	2.0648000000	3.7995000000	0.8285000000
H63	2.2892000000	3.1177000000	2.4468000000
H64	1.9280000000	2.0570000000	1.0850000000
H65	-3.3177000000	6.1125000000	1.8094000000
H66	-1.7869000000	6.6994000000	1.1322000000
H67	-2.8648000000	5.7104000000	0.1518000000
H68	-2.4093000000	2.0285000000	0.1364000000
H69	-4.9115000000	1.8777000000	-0.0554000000
H70	-6.0009000000	-0.3766000000	-0.1216000000

Gas phase energy..... -2379.66719434718 hartrees

***trans*-(SIMes)$RuCl_2$=CH(8-quinoline)**

C1	0.1033000000	-4.1226000000	-3.5834000000
C2	0.1259000000	-2.7053000000	-3.5466000000
C3	0.0898000000	-2.0742000000	-2.2781000000
C4	0.0413000000	-2.8249000000	-1.0679000000
C5	0.0209000000	-4.2158000000	-1.1541000000
C6	0.0500000000	-4.8532000000	-2.4108000000
C7	0.1845000000	-1.8610000000	-4.6805000000
C8	0.2045000000	-0.4938000000	-4.5073000000
C9	0.1629000000	0.0391000000	-3.2033000000
N10	0.1053000000	-0.7279000000	-2.1288000000
Ru11	0.0457000000	-0.2208000000	0.0866000000
Cl12	2.3945000000	0.2781000000	-0.1668000000
C13	0.0253000000	-2.0715000000	0.1632000000
C14	-0.1264000000	0.2925000000	2.0522000000
N15	-0.4819000000	-0.4361000000	3.1428000000
C16	-0.5765000000	0.3697000000	4.3674000000
C17	-0.6210000000	1.7804000000	3.8156000000
N18	-0.1183000000	1.5956000000	2.4493000000
C19	-0.5214000000	-1.8500000000	3.2918000000
C20	0.6755000000	-2.5618000000	3.4705000000
C21	0.5929000000	-3.9409000000	3.6822000000
C22	-0.6351000000	-4.6086000000	3.7313000000
C23	-1.8057000000	-3.8650000000	3.5456000000
C24	-1.7741000000	-2.4851000000	3.3294000000
C25	1.9988000000	-1.8685000000	3.3674000000
C26	-3.0302000000	-1.7001000000	3.1038000000
C27	-0.7009000000	-6.0830000000	3.9995000000
C28	0.4973000000	2.7088000000	1.7963000000
C29	-0.2875000000	3.6826000000	1.1612000000
C30	0.3648000000	4.7987000000	0.6228000000
C31	1.7418000000	4.9828000000	0.7443000000
C32	2.4824000000	4.0252000000	1.4480000000
C33	1.8815000000	2.8946000000	1.9963000000
C34	-1.7822000000	3.6036000000	1.1424000000
C35	2.4183000000	6.1848000000	0.1559000000
C36	2.6667000000	1.9233000000	2.8225000000
Cl37	-2.3025000000	0.2903000000	-0.1869000000
H38	0.0055000000	-2.6570000000	1.0905000000
H39	-0.0177000000	-4.8057000000	-0.2371000000
H40	0.0334000000	-5.9411000000	-2.4567000000
H41	0.1298000000	-4.6287000000	-4.5483000000
H42	0.0143000000	2.4868000000	4.3634000000
H43	-1.6424000000	2.1922000000	3.7839000000
H44	0.3033000000	0.1820000000	5.0064000000
H45	-1.4700000000	0.0924000000	4.9404000000

H46	-0.2334000000	5.5617000000	0.1202000000
H47	3.5545000000	4.1757000000	1.5906000000
H48	-2.2010000000	4.1849000000	0.3133000000
H49	-2.1455000000	2.5743000000	1.0510000000
H50	-2.2005000000	4.0257000000	2.0692000000
H51	2.2531000000	1.8305000000	3.8393000000
H52	2.6608000000	0.9239000000	2.3693000000
H53	3.7106000000	2.2416000000	2.9180000000
H54	3.1706000000	6.6000000000	0.8384000000
H55	2.9434000000	5.9325000000	-0.7757000000
H56	1.7014000000	6.9800000000	-0.0791000000
H57	-2.7720000000	-4.3736000000	3.5650000000
H58	1.5158000000	-4.5101000000	3.8107000000
H59	2.1450000000	-1.4334000000	2.3655000000
H60	2.0870000000	-1.0366000000	4.0797000000
H61	2.8257000000	-2.5604000000	3.5596000000
H62	-3.9064000000	-2.3564000000	3.0676000000
H63	-3.2046000000	-0.9628000000	3.9011000000
H64	-2.9828000000	-1.1328000000	2.1638000000
H65	0.2382000000	-6.5859000000	3.7412000000
H66	-0.8923000000	-6.2857000000	5.0625000000
H67	-1.5100000000	-6.5639000000	3.4363000000
H68	0.1769000000	1.1142000000	-3.0248000000
H69	0.2510000000	0.1810000000	-5.3591000000
H70	0.2154000000	-2.2989000000	-5.6782000000

Gas phase energy..... -2379.66557709504 hartrees

***cis*-(SIMes)$RuCl_2$=CH(C_6H_4)N=CMe_2**

C1	-2.6218000000	-1.4563000000	-0.1925000000
C2	-1.5668000000	-2.4027000000	-0.1130000000
C3	-1.8658000000	-3.7737000000	-0.1181000000
C4	-3.1883000000	-4.2075000000	-0.1231000000
C5	-4.2221000000	-3.2692000000	-0.1087000000
C6	-3.9456000000	-1.9003000000	-0.1453000000
C7	-0.2338000000	-1.8907000000	0.1010000000
Ru8	0.0073000000	-0.0810000000	0.2909000000
Cl9	0.2737000000	0.9714000000	-1.8866000000
N10	-2.2024000000	-0.1102000000	-0.1817000000
C11	-2.8505000000	0.8474000000	-0.7811000000
C12	-2.4076000000	2.2576000000	-0.6232000000
C13	0.1017000000	-0.0705000000	2.3320000000
N14	0.0776000000	1.1223000000	2.9834000000
C15	0.6635000000	1.0446000000	4.3255000000

C16	0.6123000000	-0.4461000000	4.5954000000
N17	0.4784000000	-1.0054000000	3.2436000000
C18	-0.5349000000	2.3318000000	2.5442000000
C19	-1.9113000000	2.4965000000	2.8009000000
C20	-2.4993000000	3.7239000000	2.4987000000
C21	-1.7604000000	4.7725000000	1.9390000000
C22	-0.3980000000	4.5741000000	1.7002000000
C23	0.2451000000	3.3692000000	2.0095000000
C24	-2.7250000000	1.3668000000	3.3544000000
C25	1.7185000000	3.2013000000	1.8040000000
C26	-2.4279000000	6.0649000000	1.5758000000
C27	0.4927000000	-2.4234000000	3.1126000000
C28	1.7237000000	-3.1030000000	3.1474000000
C29	1.7037000000	-4.4995000000	3.0852000000
C30	0.5119000000	-5.2261000000	3.0219000000
C31	-0.6941000000	-4.5192000000	3.0481000000
C32	-0.7278000000	-3.1239000000	3.1080000000
C33	3.0202000000	-2.3670000000	3.2808000000
C34	0.5306000000	-6.7225000000	2.9253000000
C35	-2.0326000000	-2.3946000000	3.2086000000
Cl36	2.4440000000	-0.2550000000	0.4334000000
C37	-4.0356000000	0.6619000000	-1.6796000000
H38	0.6131000000	-2.5951000000	0.1178000000
H39	-1.0430000000	-4.4879000000	-0.0656000000
H40	-3.4155000000	-5.2725000000	-0.1046000000
H41	-5.2585000000	-3.6016000000	-0.0650000000
H42	-4.7645000000	-1.1869000000	-0.0960000000
H43	-3.2540000000	2.8714000000	-0.2766000000
H44	-1.5744000000	2.3562000000	0.0761000000
H45	-2.0814000000	2.6595000000	-1.5896000000
H46	-4.9786000000	0.8441000000	-1.1452000000
H47	-3.9878000000	1.4034000000	-2.4856000000
H48	-4.0846000000	-0.3378000000	-2.1200000000
H49	-0.2552000000	-0.7420000000	5.2106000000
H50	1.5158000000	-0.8303000000	5.0822000000
H51	0.0772000000	1.6402000000	5.0355000000
H52	1.6940000000	1.4341000000	4.3099000000
H53	2.6551000000	-5.0352000000	3.0951000000
H54	-1.6387000000	-5.0677000000	3.0312000000
H55	3.8665000000	-3.0120000000	3.0204000000
H56	3.0461000000	-1.4837000000	2.6292000000
H57	3.1856000000	-2.0271000000	4.3148000000
H58	-2.1382000000	-1.8886000000	4.1800000000
H59	-2.1216000000	-1.6141000000	2.4418000000
H60	-2.8814000000	-3.0783000000	3.0949000000
H61	-0.3640000000	-7.1710000000	3.3734000000

H62	0.5666000000	-7.0554000000	1.8783000000
H63	1.4093000000	-7.1500000000	3.4232000000
H64	0.1917000000	5.3850000000	1.2686000000
H65	-3.5649000000	3.8637000000	2.6950000000
H66	-2.7702000000	0.5303000000	2.6409000000
H67	-2.2966000000	0.9571000000	4.2807000000
H68	-3.7514000000	1.6837000000	3.5716000000
H69	2.1083000000	3.9569000000	1.1143000000
H70	2.2650000000	3.3144000000	2.7522000000
H71	1.9779000000	2.2110000000	1.4013000000
H72	-3.2939000000	6.2687000000	2.2171000000
H73	-1.7406000000	6.9154000000	1.6524000000
H74	-2.7940000000	6.0429000000	0.5394000000

Gas phase energy..... -2382.05189501824 hartrees

***trans*-(SIMes)$RuCl_2$=CH(C_6H_4)N=CMe_2**

C1	1.8736000000	2.8659000000	1.9809000000
C2	0.4846000000	2.6501000000	1.9103000000
C3	-0.3625000000	3.5444000000	1.2415000000
C4	0.2286000000	4.5989000000	0.5348000000
C5	1.6081000000	4.7952000000	0.5191000000
C6	2.4111000000	3.9343000000	1.2736000000
N7	-0.0408000000	1.5466000000	2.6435000000
C8	-0.1929000000	0.2692000000	2.1872000000
N9	-0.5575000000	-0.4697000000	3.2674000000
C10	-0.5315000000	0.2944000000	4.5201000000
C11	-0.4894000000	1.7230000000	4.0226000000
Ru12	-0.0638000000	-0.1383000000	0.2156000000
Cl13	2.3385000000	0.1537000000	0.0129000000
C14	-0.6659000000	-1.8820000000	3.3857000000
C15	0.5000000000	-2.6365000000	3.5793000000
C16	0.3643000000	-4.0071000000	3.8138000000
C17	-0.8879000000	-4.6261000000	3.8602000000
C18	-2.0240000000	-3.8448000000	3.6318000000
C19	-1.9382000000	-2.4710000000	3.3979000000
C20	1.8472000000	-1.9909000000	3.4822000000
C21	-1.0145000000	-6.0860000000	4.1753000000
C22	-3.1565000000	-1.6470000000	3.1273000000
C23	-1.8534000000	3.4609000000	1.3490000000
C24	2.2258000000	5.9058000000	-0.2721000000
C25	2.7400000000	1.9838000000	2.8214000000
C26	-0.1637000000	-1.9772000000	0.2010000000
C27	-0.0361000000	-2.6778000000	-1.0524000000

C28	0.0630000000	-1.9219000000	-2.2535000000
C29	0.3832000000	-2.5763000000	-3.4459000000
C30	0.5320000000	-3.9631000000	-3.4629000000
C31	0.3648000000	-4.7172000000	-2.3006000000
C32	0.0869000000	-4.0752000000	-1.1011000000
N33	-0.0438000000	-0.5447000000	-2.0577000000
C34	-0.3802000000	0.3470000000	-2.9285000000
C35	-0.8929000000	0.0719000000	-4.3063000000
Cl36	-2.4193000000	0.4270000000	-0.0836000000
C37	-0.2998000000	1.7797000000	-2.5216000000
H38	-0.2599000000	-2.6023000000	1.0992000000
H39	-0.0024000000	-4.6399000000	-0.1718000000
H40	0.4829000000	-5.7992000000	-2.3290000000
H41	0.7938000000	-4.4588000000	-4.3966000000
H42	0.5659000000	-2.0086000000	-4.3541000000
H43	-1.2933000000	2.1424000000	-2.2207000000
H44	0.3852000000	1.9177000000	-1.6759000000
H45	0.0410000000	2.3998000000	-3.3618000000
H46	-1.6167000000	0.8448000000	-4.5893000000
H47	-0.0815000000	0.1169000000	-5.0466000000
H48	-1.3702000000	-0.9094000000	-4.3860000000
H49	0.2063000000	2.3627000000	4.5794000000
H50	-1.4819000000	2.2028000000	4.0359000000
H51	0.3594000000	0.0182000000	5.1092000000
H52	-1.4175000000	0.0661000000	5.1254000000
H53	-0.4183000000	5.2963000000	-0.0014000000
H54	3.4888000000	4.1031000000	1.3135000000
H55	-2.3380000000	3.7546000000	0.4110000000
H56	-2.2042000000	2.4533000000	1.5902000000
H57	-2.2161000000	4.1461000000	2.1296000000
H58	2.4048000000	1.9608000000	3.8692000000
H59	2.7282000000	0.9531000000	2.4460000000
H60	3.7790000000	2.3302000000	2.8120000000
H61	3.0618000000	6.3693000000	0.2659000000
H62	2.6302000000	5.5358000000	-1.2244000000
H63	1.4985000000	6.6902000000	-0.5095000000
H64	-3.0081000000	-4.3174000000	3.6392000000
H65	1.2636000000	-4.6072000000	3.9672000000
H66	2.0078000000	-1.5496000000	2.4854000000
H67	1.9702000000	-1.1719000000	4.2055000000
H68	2.6469000000	-2.7170000000	3.6641000000
H69	-4.0653000000	-2.2568000000	3.1725000000
H70	-3.2674000000	-0.8250000000	3.8487000000
H71	-3.1037000000	-1.1777000000	2.1340000000
H72	-0.0772000000	-6.6242000000	3.9944000000
H73	-1.2774000000	-6.2434000000	5.2308000000

H74	-1.8013000000	-6.5655000000	3.5805000000

Gas phase energy..... -2382.05879660977 hartrees

Single Point Energies

[hartree]	BP86/LACV3P**++// BP86/LACVP*	M06-L/LACV3P**++// M06-L/LACVP*
cis-(SIMes)RuCl$_2$=CH(C$_6$H$_4$)O*i*Pr	-2403.81130679733	-2403.52703782039
cis-(SIMes)RuCl$_2$=CH(C$_6$H$_4$)S*i*Pr	-2726.83739236758	-2726.51256814081
cis-(SIMes)RuCl$_2$=CH(C$_6$H$_4$)Se*i*Pr	-2337.84491740668	-2337.52654483699
cis-(SIMes)RuCl$_2$=CH(C$_6$H$_4$)NH*i*Pr	-2383.94696270786	-2383.66193085067
cis-(SIMes)RuCl$_2$=CH(C$_6$H$_4$)PH*i*Pr	-2670.60208972840	-2670.28627223548
(SIMes)RuCl$_2$=CHPh	-2210.61036224898	-2210.33177391813
trans-(SIMes)RuCl$_2$=CH(C$_6$H$_4$)O*i*Pr	-2403.82976718717	-2403.54662780807
trans-(SIMes)RuCl$_2$=CH(C$_6$H$_4$)S*i*Pr	-2726.84030279868	-2726.50682363163
trans-(SIMes)RuCl$_2$=CH(C$_6$H$_4$)Se*i*Pr	-2337.84968385204	-2337.52182258024
trans-(SIMes)RuCl$_2$=CH(C$_6$H$_4$)NH*i*Pr	-2383.96550517654	-2383.67717152704
trans-(SIMes)RuCl$_2$=CH(C$_6$H$_4$)PH*i*Pr	-2670.60015433103	-2670.27555058995
cis-(SIMes)RuCl$_2$=CH(8-quinoline)	-2380.36082860386	-2380.06803362130
trans-(SIMes)RuCl$_2$=CH(8-quinoline)	-2380.36546695852	-2380.06568682725
cis-(SIMes)RuCl$_2$=CH(C$_6$H$_4$)N=CMe$_2$	-2382.74491912127	-2382.46102797595
trans-(SIMes)RuCl$_2$=CH(C$_6$H$_4$)N=CMe$_2$	-2382.75695890323	-2382.46761703523
styrene	-309.71574463563	-309.67961012185
H$_2$C=CH(C$_6$H$_4$)OiPr	-502.92314826748	-502.86528099617
H$_2$C=CH(C$_6$H$_4$)SiPr	-825.92344509635	-825.82622316251
H$_2$C=CH(C$_6$H$_4$)SeiPr	-436.93260075774	-436.84547739255
H$_2$C=CH(C$_6$H$_4$)NHiPr	-483.05256872743	-482.99591665468
H$_2$C=CH(C$_6$H$_4$)PHiPr	-769.66992055779	-769.58514651235

Solution Phase Energies

Solvation energy will be computed using PBF
-solute cavity energy will not be included
-surface area terms will not be included
Solvent: dichloromethane
Internal dielectric constant: 1.00
Continuum dielectric constant: 8.93
Solvent probe molecule radius: 2.33

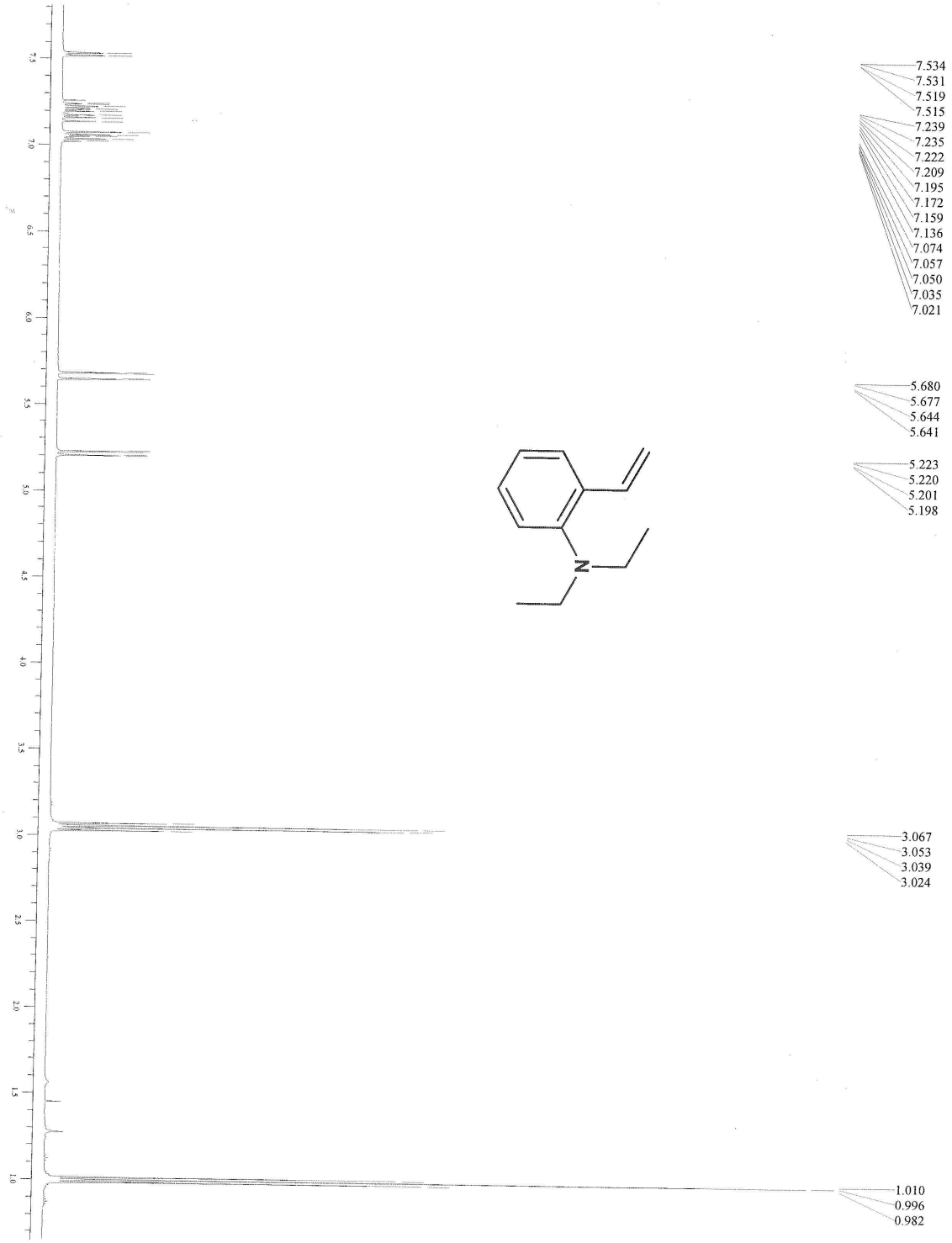
[hartree]	BP86/LACV3P**++// BP86/LACVP*	M06-L/LACV3P**++// M06-L/LACVP*
cis-(SIMes)$RuCl_2$=CH(C_6H_4)O*i*Pr	-2403.83953858992	-2403.55640153572
cis-(SIMes)$RuCl_2$=CH(C_6H_4)S*i*Pr	-2726.86680175987	-2726.54268102582
cis-(SIMes)$RuCl_2$=CH(C_6H_4)Se*i*Pr	-2337.87522258392	-2337.55746432696
cis-(SIMes)$RuCl_2$=CH(C_6H_4)NH*i*Pr	-2383.97732673790	-2383.69335018590
cis-(SIMes)$RuCl_2$=CH(C_6H_4)PH*i*Pr	-2670.63531922742	-2670.31922349679
trans-(SIMes)$RuCl_2$=CH(C_6H_4)O*i*Pr	-2403.84966818054	-2403.56691998239
trans-(SIMes)$RuCl_2$=CH(C_6H_4)S*i*Pr	-2726.86137560617	-2726.52747517518
trans-(SIMes)$RuCl_2$=CH(C_6H_4)Se*i*Pr	-2337.86900978212	-2337.54155466725
trans-(SIMes)$RuCl_2$=CH(C_6H_4)NH*i*Pr	-2383.98526329863	-2383.69676412108
trans-(SIMes)$RuCl_2$=CH(C_6H_4)PH*i*Pr	-2670.62065075559	-2670.29531539604
cis-(SIMes)$RuCl_2$=CH(8-quinoline)	-2380.39391348521	-2380.10237810973
trans-(SIMes)$RuCl_2$=CH(8-quinoline)	-2380.38876644599	-2380.08874713918
cis-(SIMes)$RuCl_2$=CH(C_6H_4)N=CMe_2	-2382.77730259727	-2382.49513483549
trans-(SIMes)$RuCl_2$=CH(C_6H_4)N=CMe_2	-2382.78013705015	-2382.48987058295

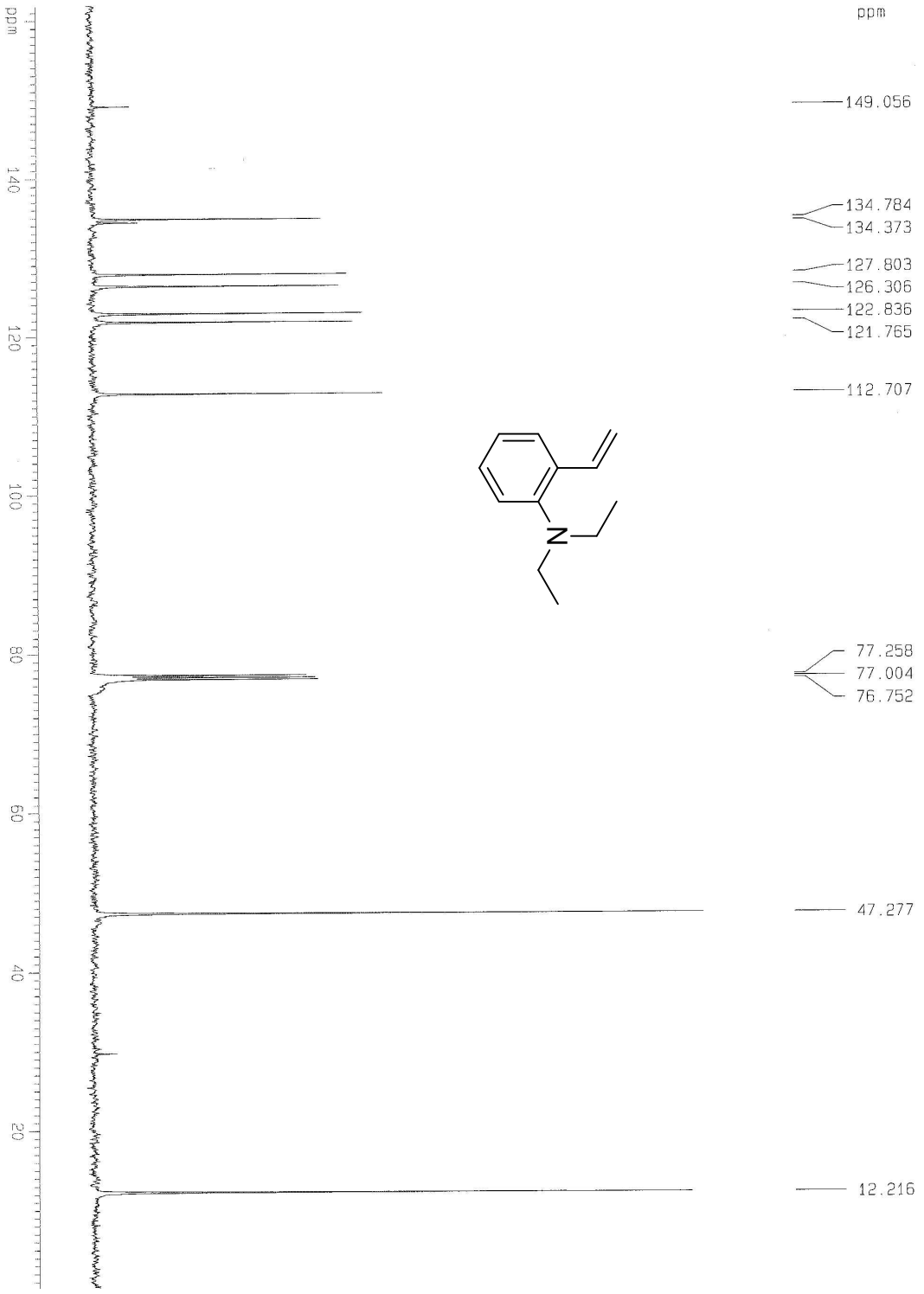
Solution Phase Energies

Solvation energy will be computed using PBF
-solute cavity energy will not be included
-surface area terms will not be included
Solvent: dichloromethane
Internal dielectric constant: 1.00
Continuum dielectric constant: 8.93
Solvent probe molecule radius: 2.33

[hartree]	BP86/LACVP*	M06-L/LACVP*
cis-(SIMes)$RuCl_2$=CH(C_6H_4)O*i*Pr	-2403.39166286943	-2403.13925893514
cis-(SIMes)$RuCl_2$=CH(C_6H_4)S*i*Pr	-2726.41019699187	-2726.11741246271
cis-(SIMes)$RuCl_2$=CH(C_6H_4)Se*i*Pr	-2337.44626822017	-2337.15810141947
cis-(SIMes)$RuCl_2$=CH(C_6H_4)NH*i*Pr	-2383.53446539027	-2383.28155662536
cis-(SIMes)$RuCl_2$=CH(C_6H_4)PH*i*Pr	-2670.17889780306	-2669.89522547148
trans-(SIMes)$RuCl_2$=CH(C_6H_4)O*i*Pr	-2403.40080925779	-2403.14900225916
trans-(SIMes)$RuCl_2$=CH(C_6H_4)S*i*Pr	-2726.40527475387	-2726.10289665314
trans-(SIMes)$RuCl_2$=CH(C_6H_4)Se*i*Pr	-2337.44073736004	-2337.14201287839
trans-(SIMes)$RuCl_2$=CH(C_6H_4)NH*i*Pr	-2383.54190932161	-2383.28460683939
trans-(SIMes)$RuCl_2$=CH(C_6H_4)PH*i*Pr	-2670.16380231438	-2669.86983848739
cis-(SIMes)$RuCl_2$=CH(8-quinoline)	-2379.96178731274	-2379.70402542959
trans-(SIMes)$RuCl_2$=CH(8-quinoline)	-2379.95540188057	-2379.69053060957
cis-(SIMes)$RuCl_2$=CH(C_6H_4)N=CMe_2	-2382.33922654385	-2382.08815941156
trans-(SIMes)$RuCl_2$=CH(C_6H_4)N=CMe_2	-2382.34097185359	-2382.08267111119

Part II. ^{1}H and ^{13}C NMR Spectra:

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7.097
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7.063
7.057
7.046
7.042
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6.815
6.812
6.799
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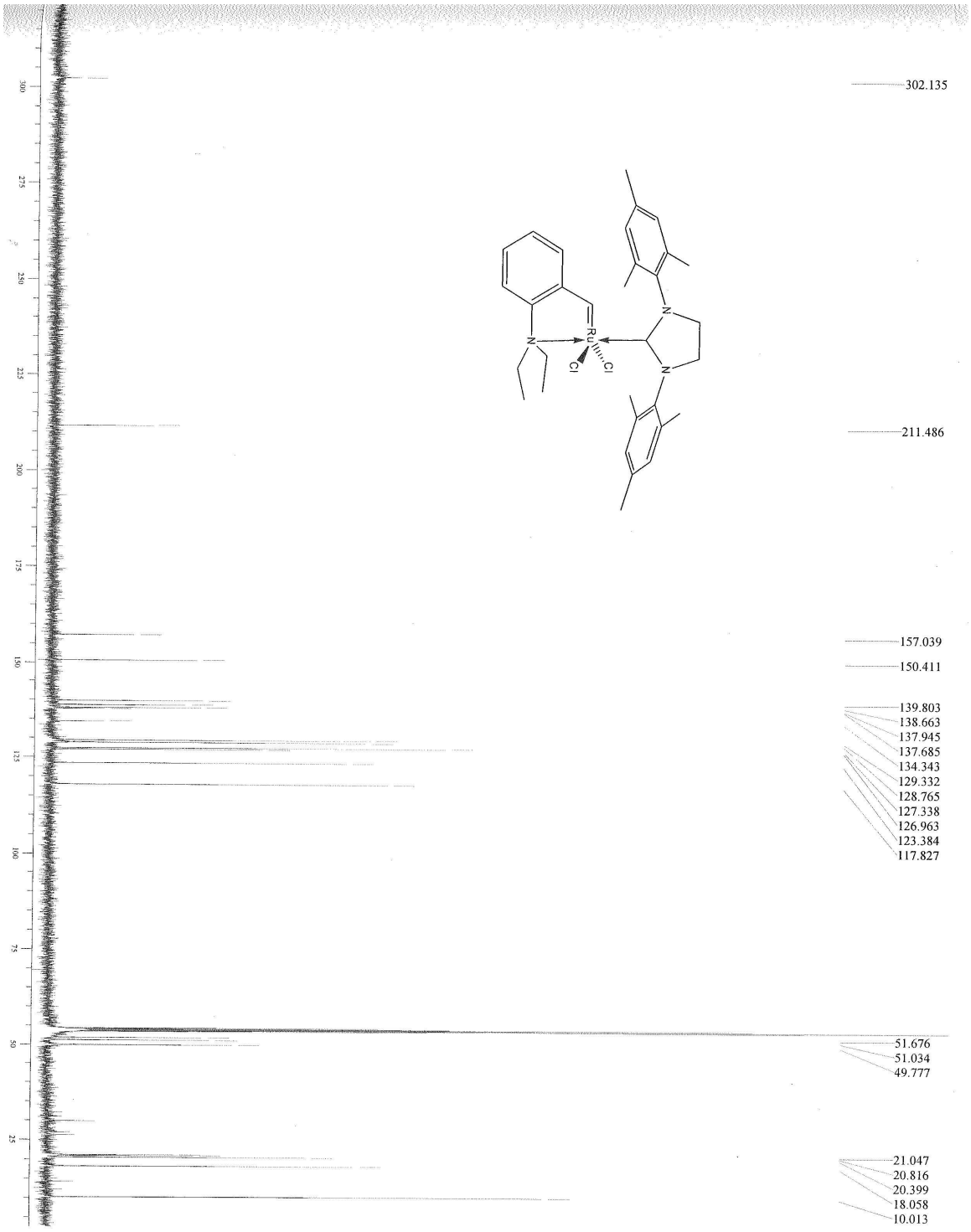
0.464
Ru
Cl
Cl
N
N
N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49.777
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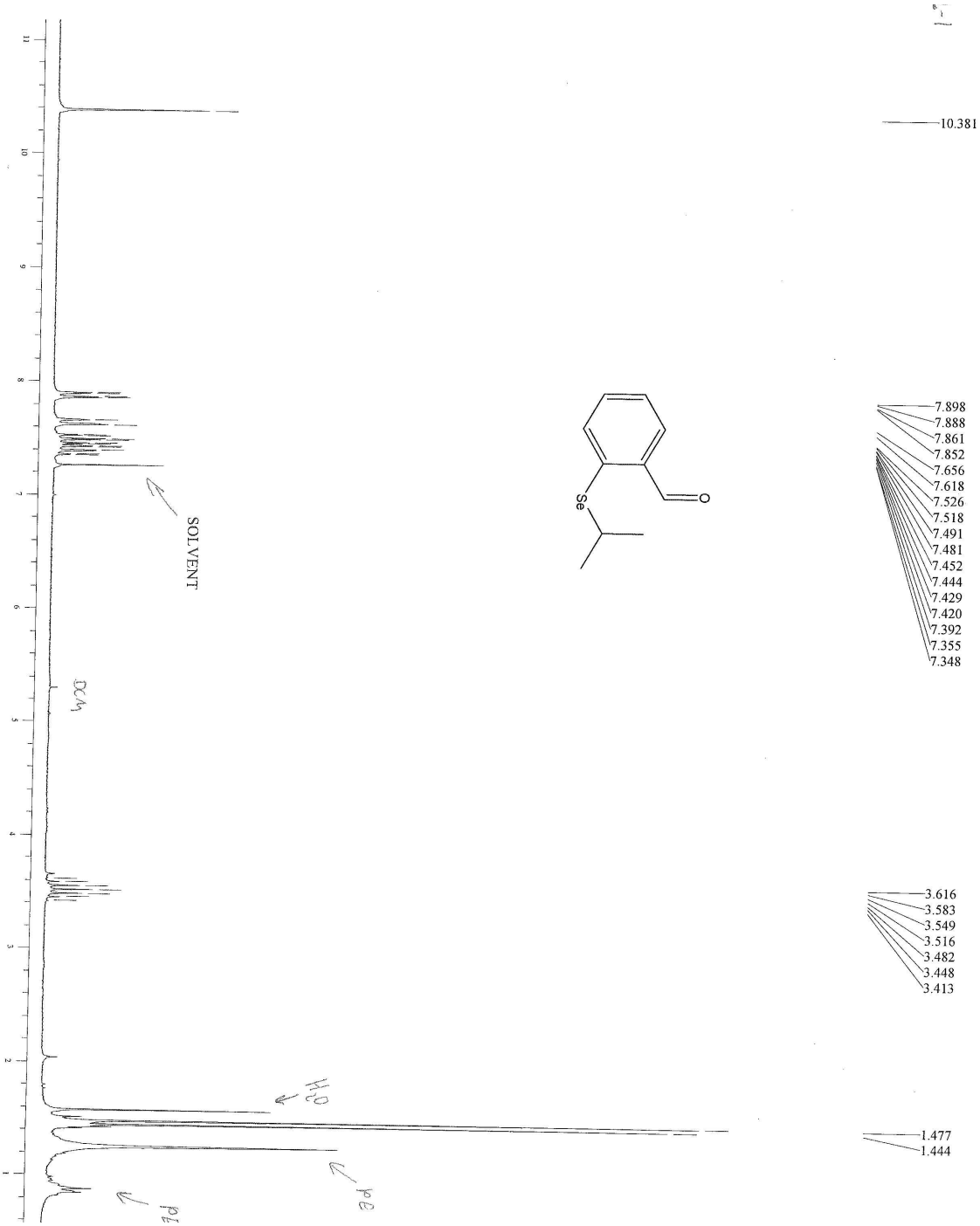
20.399
18.058
10.013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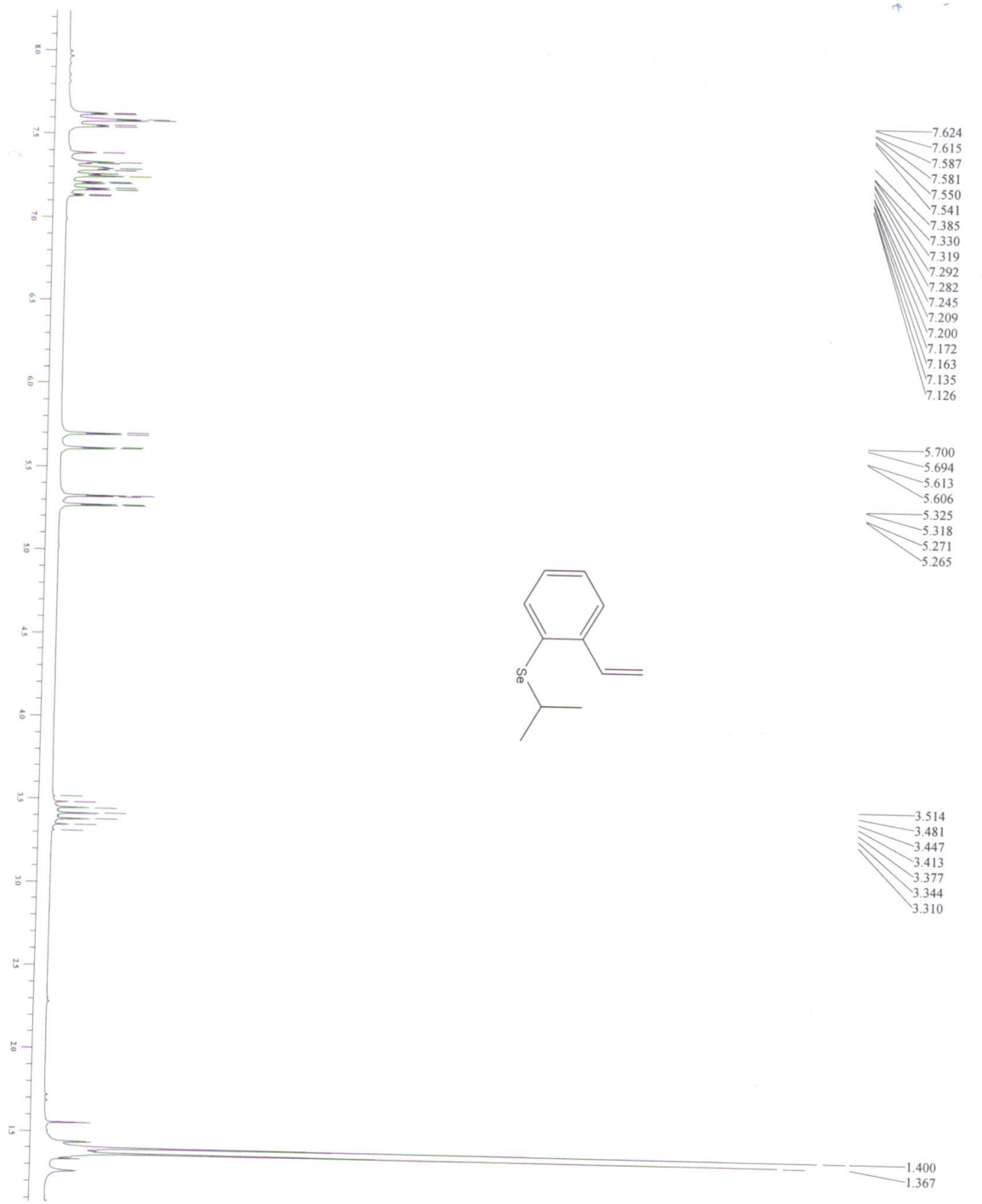
7.898
7.888
7.861
7.852
7.656
7.618
7.526
7.518
7.491
7.481
7.452
7.444
7.429
7.420
7.392
7.355
7.348
SOLVENT
3.616
3.583
3.549
3.516
3.482
3.448
3.413
1.477
1.444
O
Se


193.385
136.341
136.048
133.766
133.492
132.065
126.704
SOLVENT
32.926
23.667
Se
O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7.550
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7.385
7.330
7.319
7.292
7.282
7.245
7.209
7.200
7.172
7.163
7.135
7.126
5.700
5.694
5.613
5.606
5.325
5.318
5.271
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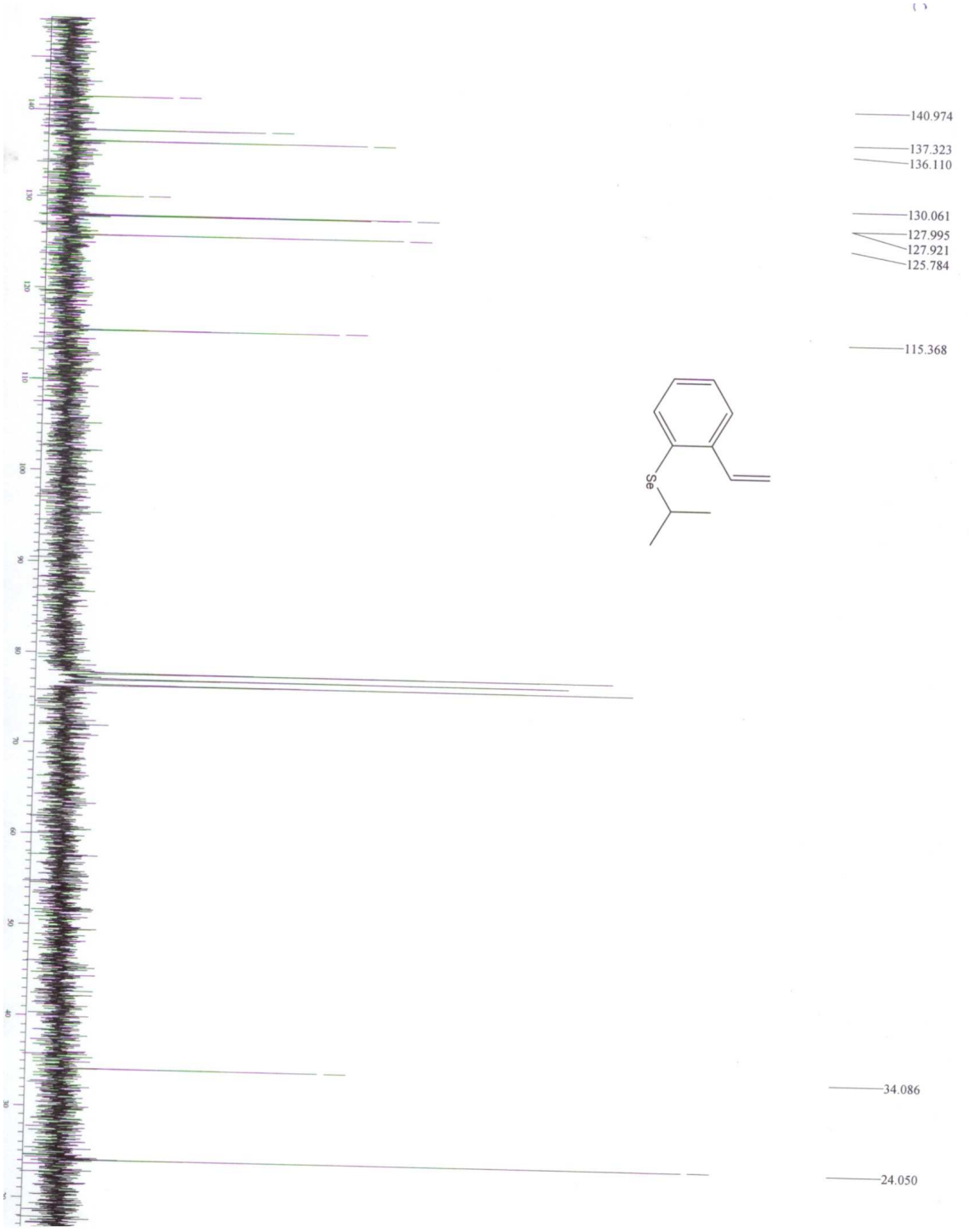
Se
3.514
3.481
3.447
3.413
3.377
3.344
3.310
1.400
1.367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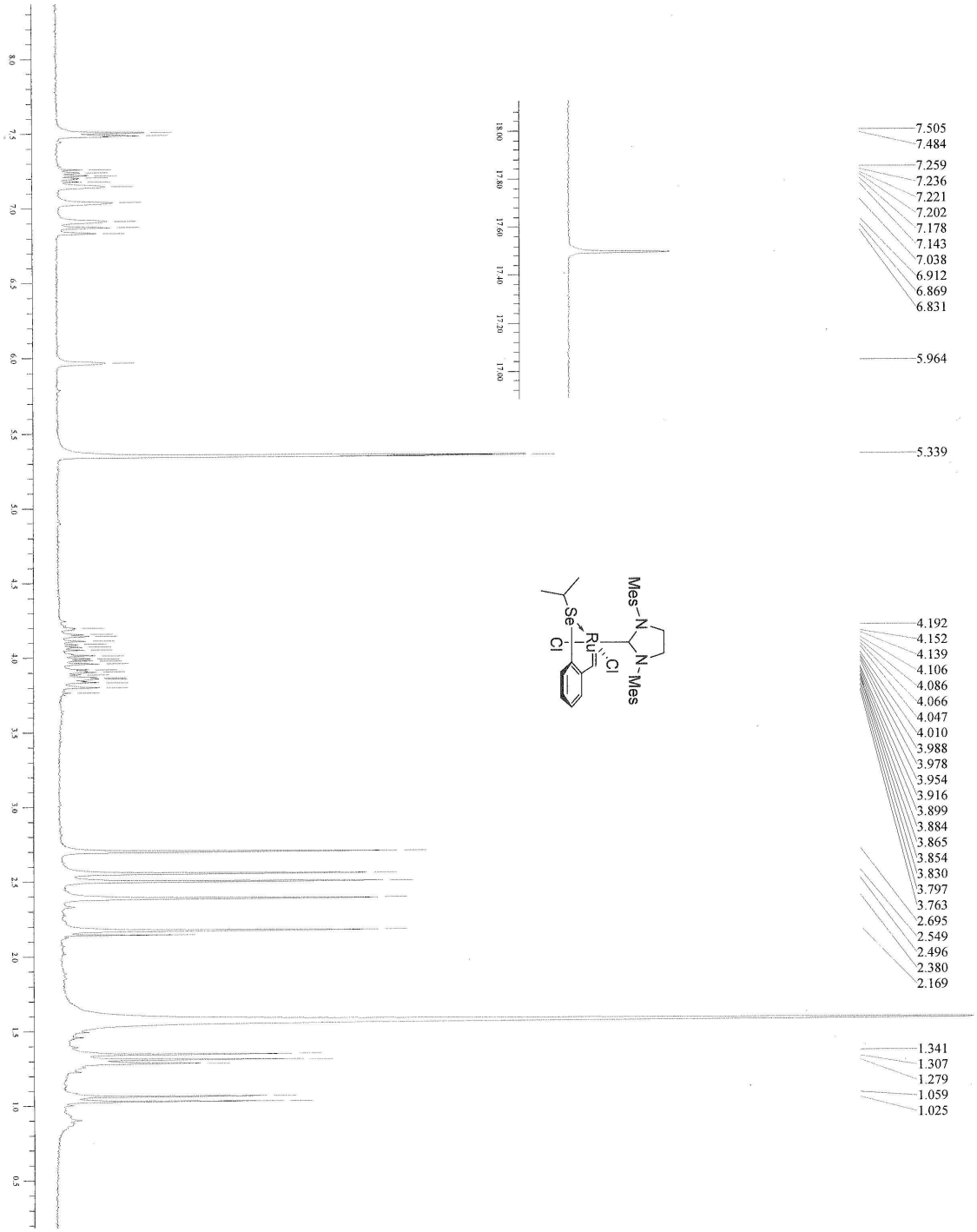
127.995
127.921
125.784
115.368
Se
34.086
24.050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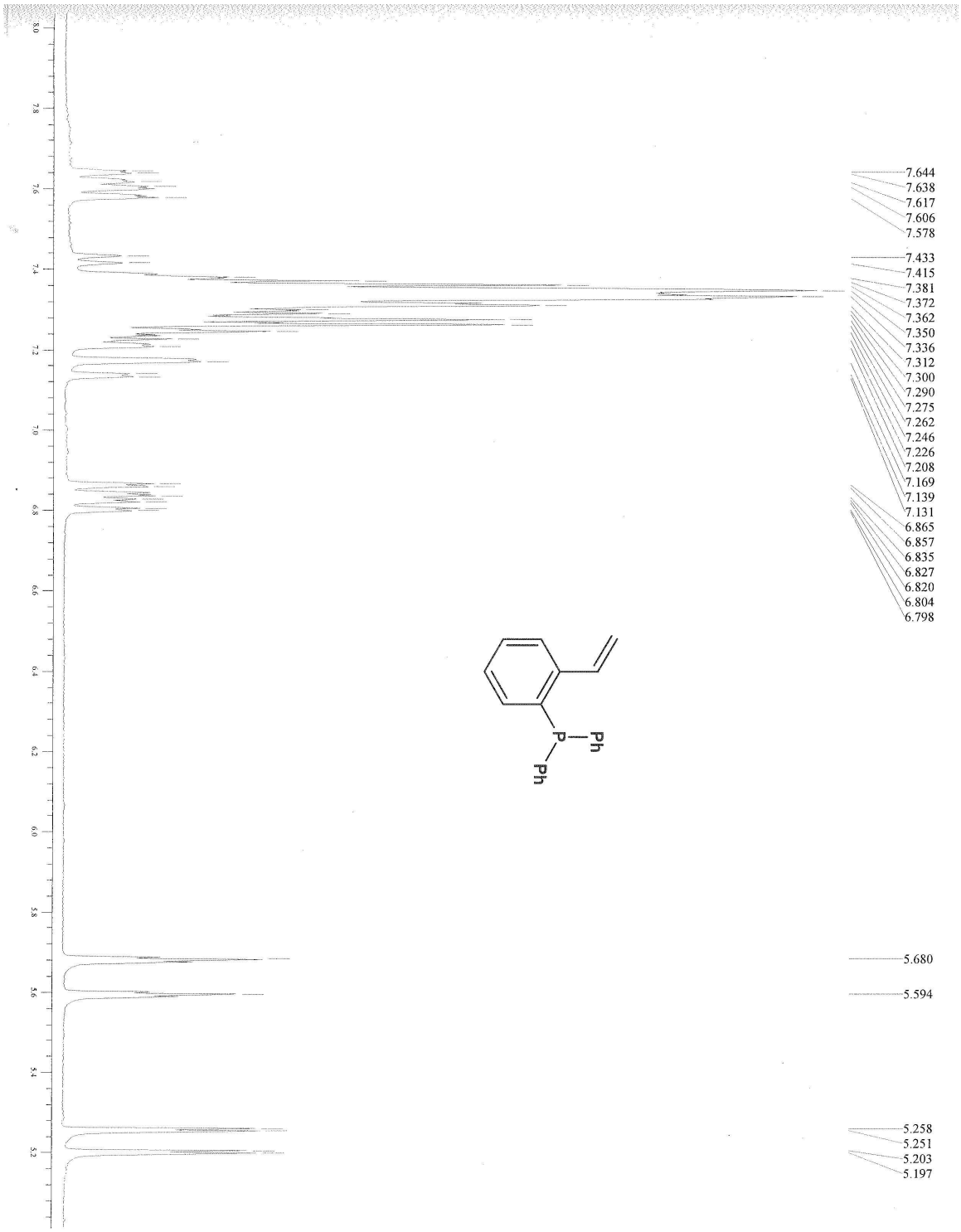
7.484
7.259
7.236
7.221
7.202
7.178
7.143
7.038
6.912
6.869
6.831
5.964
5.339
4.192
4.152
4.139
4.106
4.086
4.066
4.047
4.010
3.988
3.978
3.954
3.916
3.899
3.884
3.865
3.854
3.830
3.797
3.763
2.695
2.549
2.496
2.380
2.169
1.341
1.307
1.279
1.059
1.025
Mes
N
Se
Cl
Ru
Cl
N
Mes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7.381
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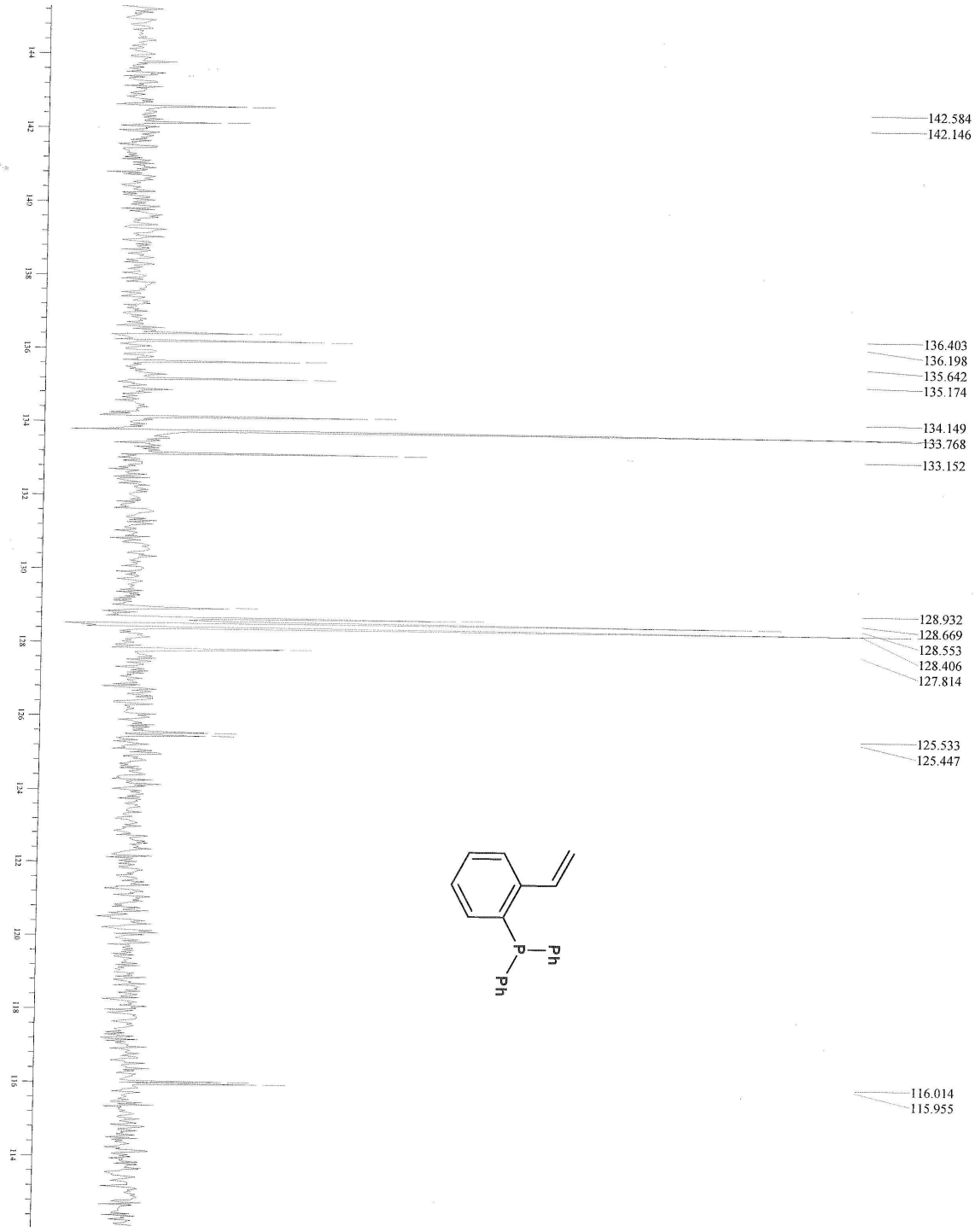
7.362
7.350
7.336
7.312
7.300
7.290
7.275
7.262
7.246
7.226
7.208
7.169
7.139
7.131
6.865
6.857
6.835
6.827
6.820
6.804
6.798
5.680
5.594
5.258
5.251
5.203
5.197
P
Ph
Ph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134.149
133.768
133.152
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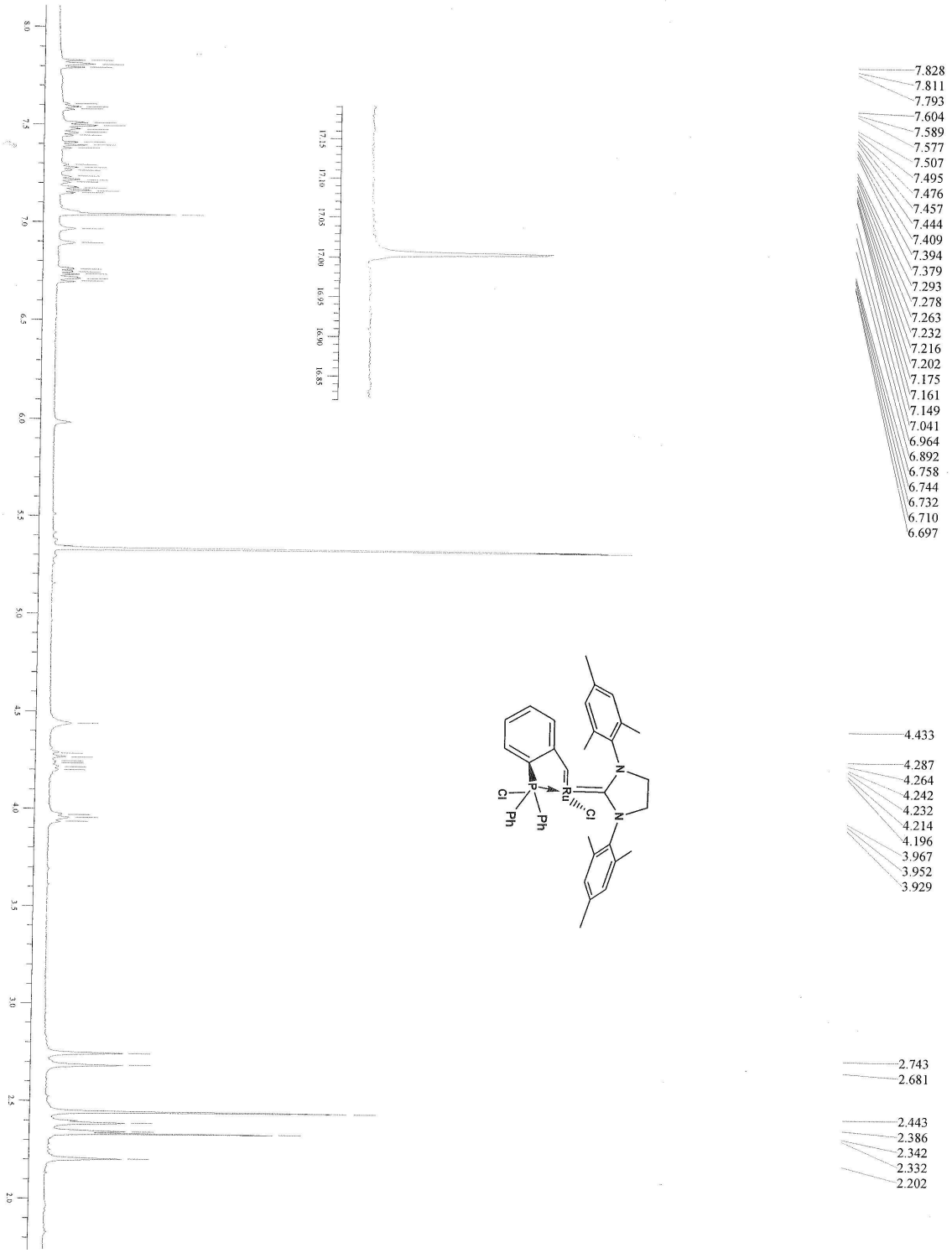
128.669
128.553
128.406
127.814
125.533
125.447
116.014
115.955
P
Ph
Ph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7.577
7.507
7.495
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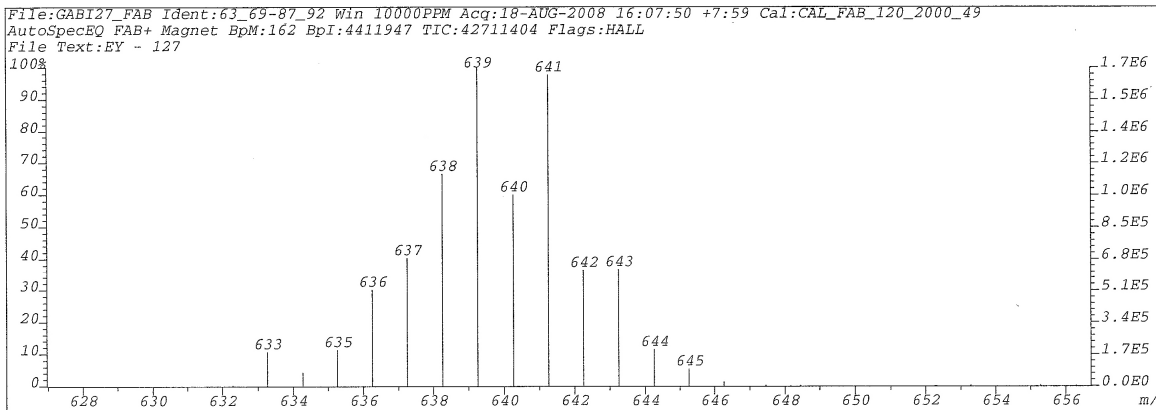
7.457
7.444
7.409
7.394
7.379
7.293
7.278
7.263
7.232
7.216
7.202
7.175
7.161
7.149
7.041
6.964
6.892
6.758
6.744
6.732
6.710
6.697
4.433
4.287
4.264
4.242
4.232
4.214
4.196
3.967
3.952
3.929
2.743
2.681
2.443
2.386
2.342
2.332
2.202
Cl
Ph
Ph
P
Ru
Cl
N
N

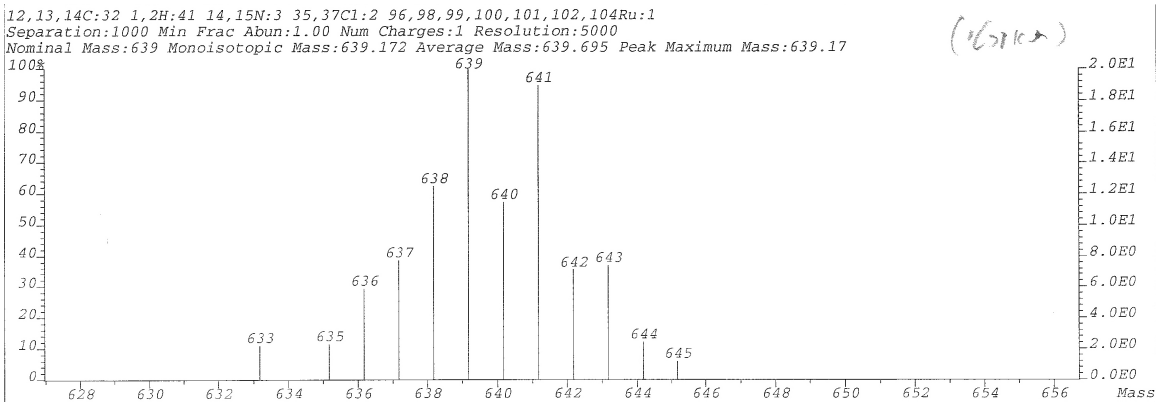
Part III. MS

Complex 14

Experimental MS (M^+)

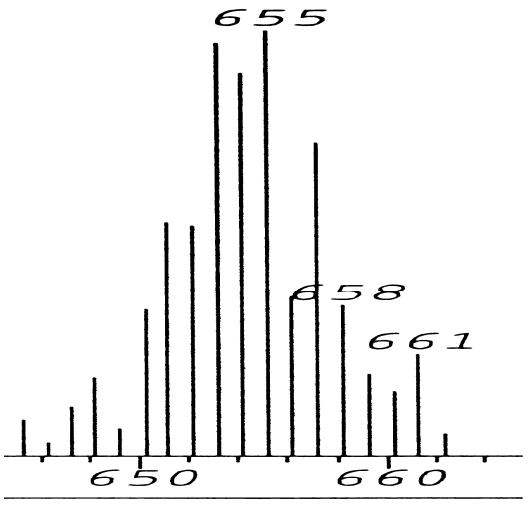


Theoretical isotopic distribution for (M^+)

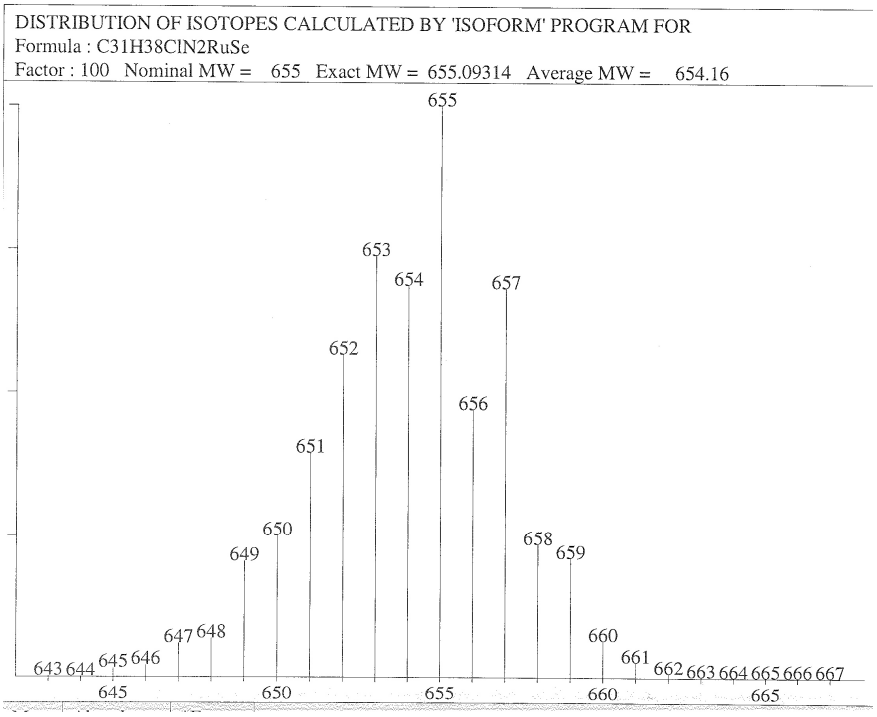


Complex 3-Se-*cis*

Experimental MS $(M\text{-}Cl)^+$

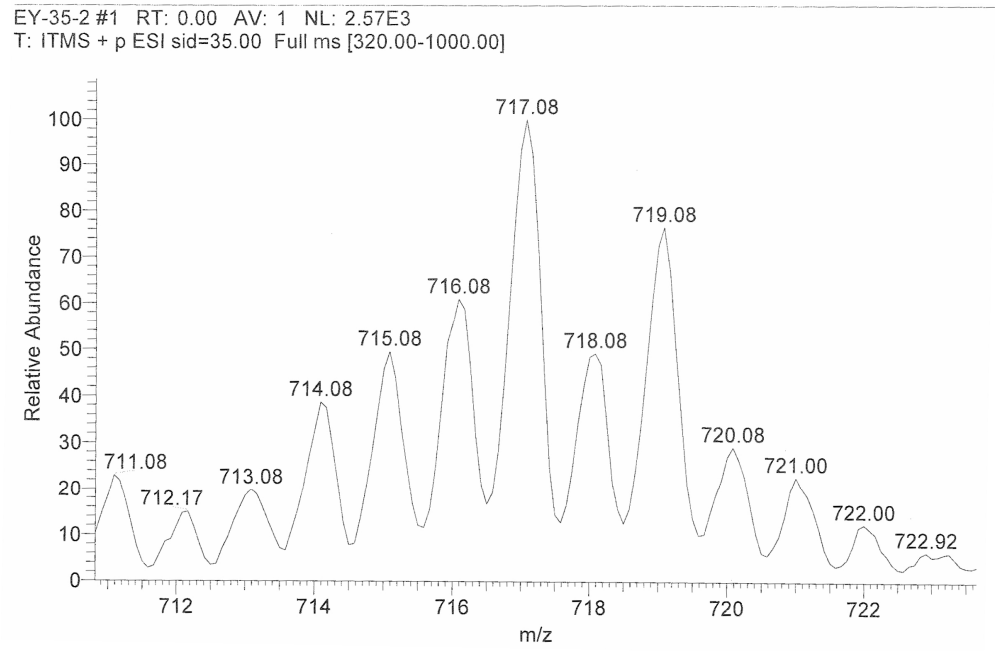


Theoretical isotopic distribution for $(M\text{-}Cl)^+$

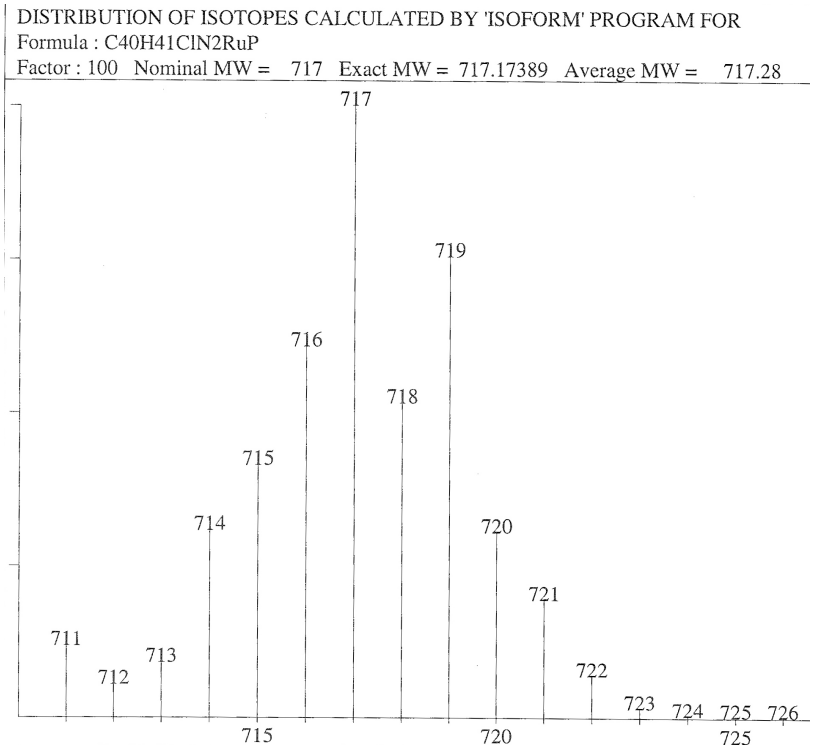


Complex 23

Experimental MS $(M-Cl)^+$



Theoretical isotopic distribution for $(M-Cl)^+$



Part IV. Crystal structure data

CIF files attached separately.