

Supporting Information for

14-Electron, 4-Coordinated Ruthenium(II) Chalcogenolate Complexes: Synthesis, Electronic Structure and Reactions with PhICl_2 and Organic Azides

Wai-Ming Ng, Xueying Guo, Wai-Man Cheung, Yat-Ming So, Man-Chun Chong, Herman H.-Y. Sung, Ian D. Williams*, Zhenyang Lin,* and Wa-Hung Leung*

*Department of Chemistry, The Hong Kong University of Science and Technology,
Clear Water Bay, Kowloon, Hong Kong, People's Republic of China*

*Corresponding authors, E-mail: chwill@ust.hk, chzlin@ust.hk, chleung@ust.hk

Table of Content

	Page no.
1. Computational comparison of complex 1 , 1_{Mes} and 2	3-35
2. NMR spectra	36-55
3. FT-IR spectrum of 4	56
4. Preliminary crystal structure of 3	57
5. Preliminary crystal structure of 5	58
6. Crystallographic data and experimental details for 2 , 4 , 6 , 8 , 9 , 10 and 11	59

Computational comparison of complex **1**, **1_{Mes}** and **2**.

Structural differences between **1** and **1_{Mes}** have been disclosed as shown below. Calculation results indicate that the structure did not change much with the replacement of R.

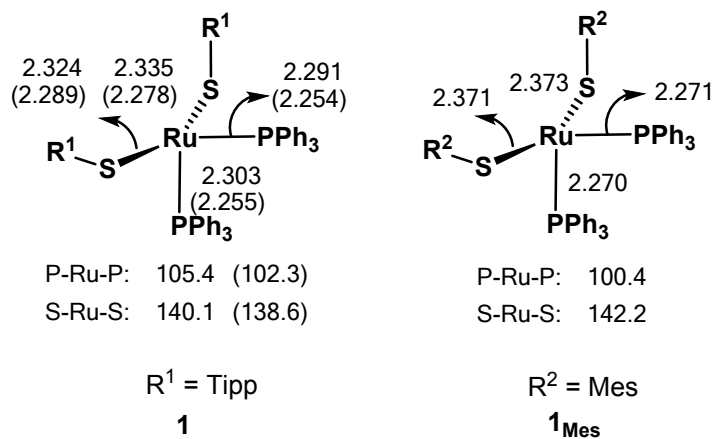
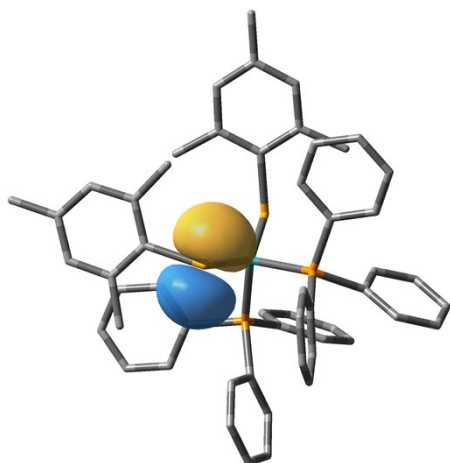


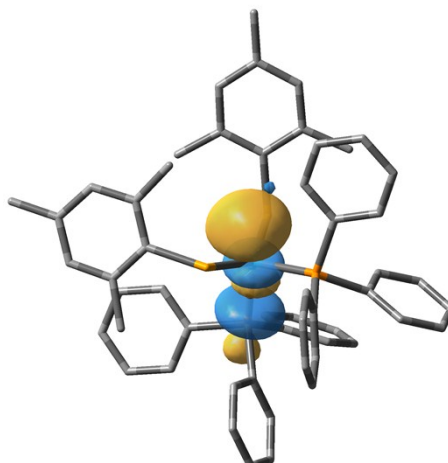
Fig. S1 Comparison of selected bond distances (Å) and angles (°) in calculated structures of **1** and **1_{Mes}**.

The orbital plots of the two donor-acceptor interactions in the selenolate complex **2** and simplified complex **1_{Mes}** are shown below. The second-order perturbation interaction energies of **2** are calculated to be 13.6 and 11.0 kcal/mol. The corresponding interaction energies for **1_{Mes}** are

12.8 and 10.4 kcal/mol.

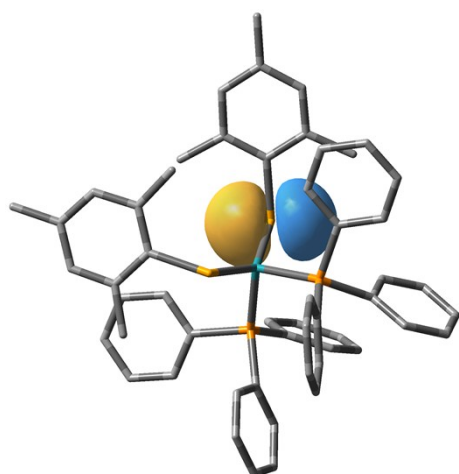


a **Se(p)**-lone-pair orbital
(donor orbital)

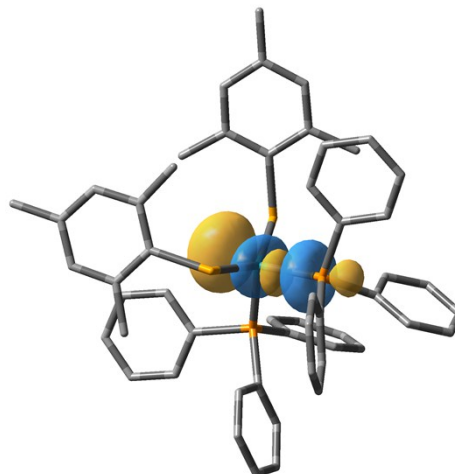


a **Ru-P** antibonding orbital
(acceptor orbital)

The first pair of $n \rightarrow \sigma^*$ (donor-acceptor) orbital interaction



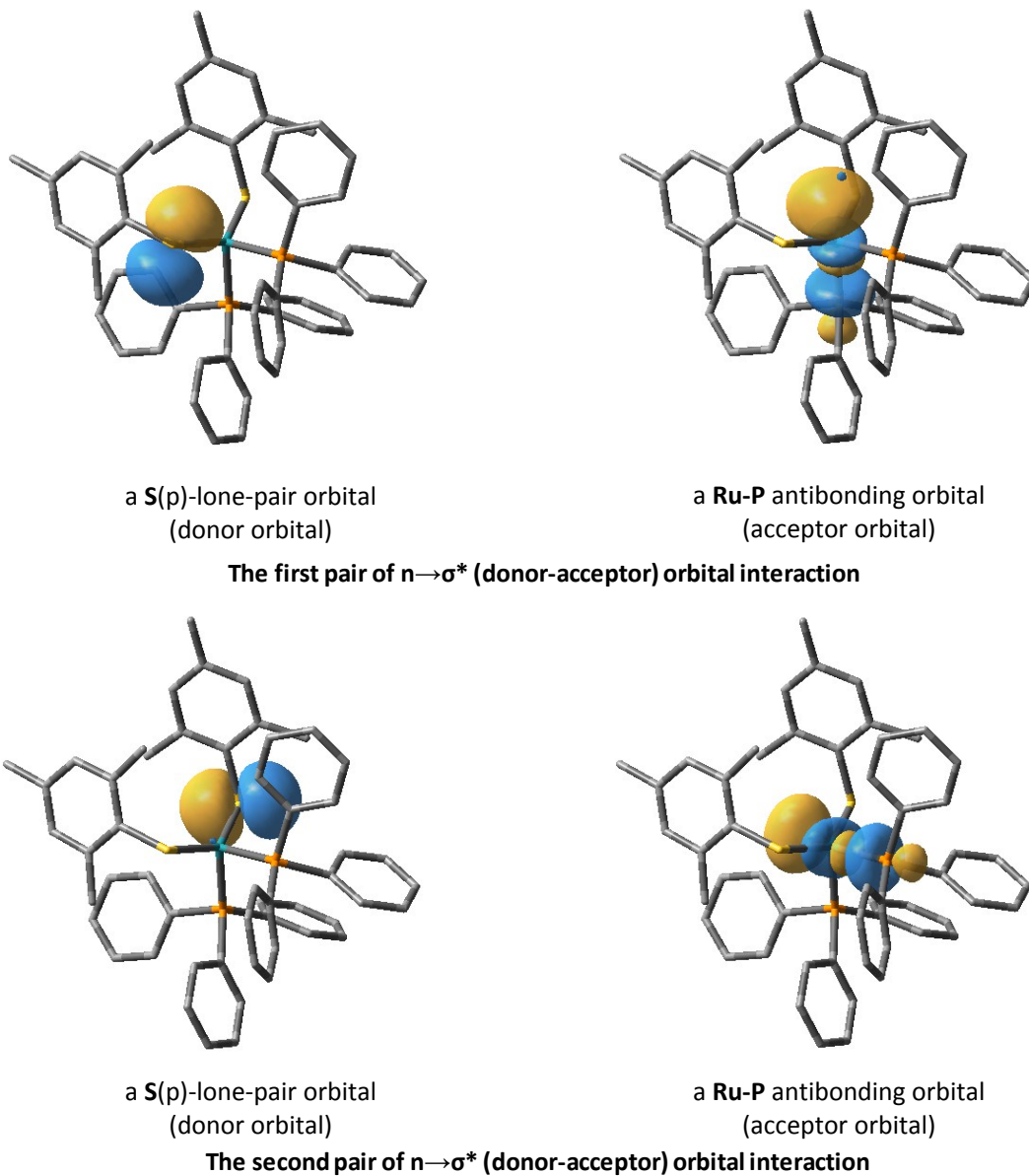
a **Se(p)**-lone-pair orbital
(donor orbital)



a **Ru-P** antibonding orbital
(acceptor orbital)

The first pair of $n \rightarrow \sigma^*$ (donor-acceptor) orbital interaction

(a)



(b)

Fig. S2 Plots of the orbitals with an isovalue of 0.045 1/bohr^{3/2} showing the $n \rightarrow \sigma^*$ (donor-acceptor) π -orbital interactions in **(a)** complex **2** **(b)** complex **1_{Mes}**. All hydrogen atoms are omitted for clarity.

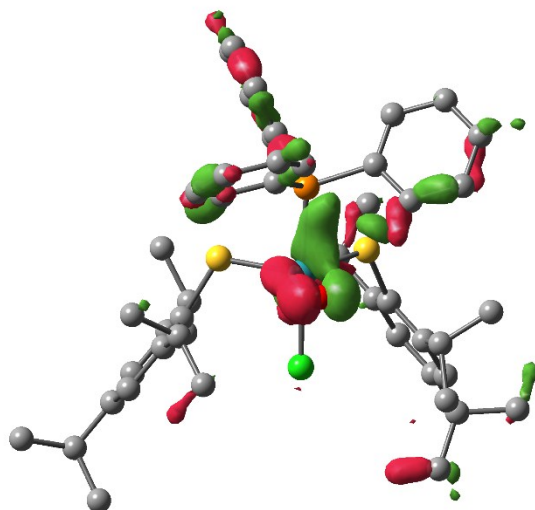


Fig. S3 Plot of the Ru-O π -bonding orbital in **4**. (isovalue=0.040 1/bohr^{3/2})

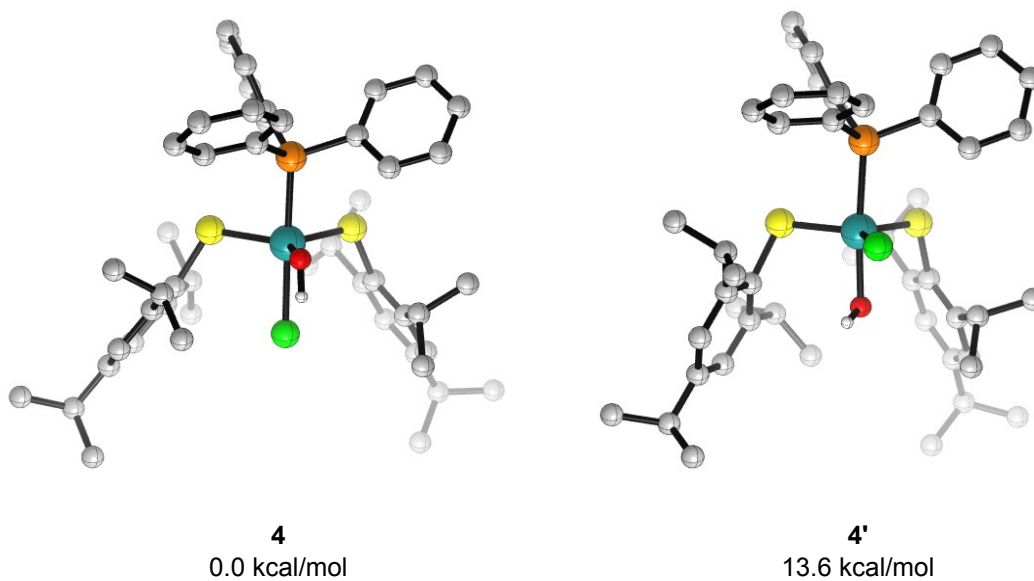


Fig. S4 Optimized structures of **4** and its geometric isomer **4'**. All the hydrogen atoms except for the one of hydroxide are omitted for clarity.

Cartesian Coordinates

complex **1**

44	0.448804000	0.048112000	-0.065381000
16	0.013463000	-0.892414000	-2.157469000
6	-1.464814000	-1.857845000	-1.808922000
6	-2.731788000	-1.236002000	-1.917405000
6	-3.864504000	-1.998350000	-1.631884000
6	-3.791586000	-3.331933000	-1.238374000
6	-2.534661000	-3.933368000	-1.187842000
6	-1.366886000	-3.231064000	-1.479682000
6	-2.877752000	0.196645000	-2.395640000
6	-4.209782000	0.853642000	-2.062894000

6	-2.644524000	0.280260000	-3.905965000
6	-0.026965000	-3.936704000	-1.479018000
6	0.044580000	-5.201107000	-0.633257000
6	0.409033000	-4.254431000	-2.910637000
16	-0.668164000	0.683997000	1.870894000
6	-2.067626000	1.740358000	1.460941000
6	-3.367113000	1.177096000	1.524770000
6	-4.460705000	2.015888000	1.311900000
6	-4.318459000	3.367957000	1.003101000
6	-3.031314000	3.892263000	0.946377000
6	-1.898047000	3.118411000	1.201502000
6	-3.588182000	-0.288056000	1.864871000
6	-4.957241000	-0.831364000	1.471371000
6	-3.387275000	-0.534175000	3.364033000
6	-0.538729000	3.779753000	1.302794000
6	-0.395821000	5.080550000	0.521727000
6	-0.194649000	4.029069000	2.773364000
15	1.720776000	-1.240017000	1.338896000
6	0.640120000	-2.282029000	2.435467000
6	-0.547859000	-2.767319000	1.878829000
6	-1.427920000	-3.529245000	2.635639000
6	-1.136629000	-3.812192000	3.967763000
6	0.045358000	-3.341340000	4.528693000
6	0.932231000	-2.582659000	3.767321000
6	2.792812000	-2.532016000	0.543621000
6	3.063639000	-2.512523000	-0.823007000
6	3.875478000	-3.489979000	-1.394878000
6	4.424594000	-4.491613000	-0.603073000
6	4.156276000	-4.519745000	0.764641000
6	3.342731000	-3.548954000	1.334578000
6	2.906136000	-0.437739000	2.514028000
6	2.428392000	0.285543000	3.615947000
6	3.311191000	0.975882000	4.438381000
6	4.677435000	0.970335000	4.163825000
6	5.156850000	0.269757000	3.062779000
6	4.277462000	-0.434287000	2.244389000
15	1.947215000	1.385270000	-1.191713000
6	1.031802000	2.401336000	-2.447955000
6	-0.276865000	2.777482000	-2.128023000
6	-1.032144000	3.546740000	-3.004270000
6	-0.490277000	3.944519000	-4.223697000
6	0.812068000	3.581328000	-4.549769000
6	1.572927000	2.819559000	-3.665994000
6	2.790255000	2.709074000	-0.200714000
6	2.713267000	2.711925000	1.188880000
6	3.353610000	3.702966000	1.929941000
6	4.065591000	4.705224000	1.282002000
6	4.139145000	4.714993000	-0.110532000
6	3.507678000	3.722290000	-0.848246000

6	3. 371685000	0. 661416000	-2. 120785000
6	3. 180864000	0. 024204000	-3. 353776000
6	4. 233511000	-0. 646949000	-3. 967153000
6	5. 482843000	-0. 703363000	-3. 354065000
6	5. 677437000	-0. 082520000	-2. 124063000
6	4. 629373000	0. 596365000	-1. 511349000
1	-4. 850180000	-1. 537476000	-1. 711163000
1	-2. 459702000	-4. 987643000	-0. 916255000
1	-2. 092451000	0. 788665000	-1. 899764000
1	-4. 161641000	1. 917832000	-2. 334875000
1	-5. 043854000	0. 414396000	-2. 631171000
1	-4. 447405000	0. 802550000	-0. 993155000
1	-2. 737243000	1. 320327000	-4. 250228000
1	-3. 395393000	-0. 323412000	-4. 437838000
1	-1. 647852000	-0. 079984000	-4. 188658000
1	0. 705831000	-3. 231149000	-1. 066145000
1	1. 091307000	-5. 529930000	-0. 569780000
1	-0. 530401000	-6. 028491000	-1. 075833000
1	-0. 317124000	-5. 043701000	0. 391926000
1	1. 415509000	-4. 698436000	-2. 910854000
1	0. 432797000	-3. 353507000	-3. 537173000
1	-0. 283934000	-4. 975100000	-3. 370284000
1	-5. 464587000	1. 592168000	1. 361589000
1	-2. 911424000	4. 955017000	0. 727870000
1	-2. 830321000	-0. 870885000	1. 310583000
1	-4. 963773000	-1. 923058000	1. 604114000
1	-5. 211860000	-0. 625496000	0. 423647000
1	-5. 757966000	-0. 424850000	2. 107031000
1	-3. 563014000	-1. 592488000	3. 605836000
1	-2. 373333000	-0. 279234000	3. 696703000
1	-4. 104601000	0. 069434000	3. 940507000
1	0. 204703000	3. 072498000	0. 907863000
1	0. 661477000	5. 381216000	0. 497628000
1	-0. 954425000	5. 904130000	0. 991066000
1	-0. 738359000	4. 986142000	-0. 517240000
1	0. 787880000	4. 515727000	2. 858985000
1	-0. 944019000	4. 691678000	3. 231513000
1	-0. 166826000	3. 093344000	3. 348766000
1	-0. 804661000	-2. 533832000	0. 844064000
1	-2. 354449000	-3. 883250000	2. 179594000
1	-1. 831259000	-4. 396815000	4. 569022000
1	0. 280900000	-3. 558521000	5. 569565000
1	1. 848914000	-2. 212514000	4. 225786000
1	2. 614312000	-1. 743105000	-1. 449270000
1	4. 077513000	-3. 451981000	-2. 464815000
1	5. 060865000	-5. 255060000	-1. 048451000
1	4. 577929000	-5. 305456000	1. 389583000
1	3. 132655000	-3. 583190000	2. 403861000
1	1. 357556000	0. 324437000	3. 820763000

1	2. 927459000	1. 525071000	5. 297190000
1	5. 365948000	1. 516427000	4. 806800000
1	6. 222676000	0. 263332000	2. 839780000
1	4. 661851000	-0. 990535000	1. 389106000
1	-0. 720968000	2. 460114000	-1. 181574000
1	-2. 049366000	3. 828046000	-2. 727636000
1	-1. 082517000	4. 537719000	-4. 918568000
1	1. 243060000	3. 891280000	-5. 500633000
1	2. 590783000	2. 541720000	-3. 939670000
1	2. 131320000	1. 940473000	1. 690576000
1	3. 289224000	3. 682140000	3. 017805000
1	4. 563041000	5. 484201000	1. 857903000
1	4. 689786000	5. 501971000	-0. 623623000
1	3. 573034000	3. 735583000	-1. 936376000
1	2. 202430000	0. 045270000	-3. 832768000
1	4. 074829000	-1. 128532000	-4. 930996000
1	6. 304627000	-1. 230181000	-3. 836734000
1	6. 651139000	-0. 124445000	-1. 638285000
1	4. 787197000	1. 080265000	-0. 546077000
6	-4. 974915000	-4. 859226000	0. 394214000
6	-5. 052235000	-4. 107688000	-0. 931526000
1	-5. 872034000	-3. 373424000	-0. 851058000
1	-4. 745551000	-4. 181148000	1. 228256000
1	-5. 928781000	-5. 357688000	0. 613978000
1	-4. 197522000	-5. 636267000	0. 371508000
6	-5. 389598000	-5. 065453000	-2. 073460000
1	-5. 479652000	-4. 530789000	-3. 027838000
1	-4. 601806000	-5. 823793000	-2. 191169000
1	-6. 335370000	-5. 591474000	-1. 882449000
6	-6. 583923000	4. 160361000	1. 797250000
6	-5. 517287000	4. 240317000	0. 708913000
1	-5. 157908000	5. 282408000	0. 667361000
1	-6. 166381000	4. 386738000	2. 786567000
1	-7. 397219000	4. 870994000	1. 596304000
1	-7. 031958000	3. 157873000	1. 846238000
6	-6. 115039000	3. 901880000	-0. 656308000
1	-5. 365757000	3. 999331000	-1. 453710000
1	-6. 486043000	2. 866243000	-0. 674581000
1	-6. 959250000	4. 564090000	-0. 894423000
complex 2			
44	0. 093899000	0. 007752000	-0. 006984000
34	0. 896376000	0. 262509000	2. 329524000
34	0. 836017000	-0. 266483000	-2. 361522000
15	-1. 321734000	-1. 608267000	0. 710544000
15	-1. 338217000	1. 618230000	-0. 702214000
6	2. 516425000	1. 262036000	1. 929829000
6	3. 726630000	0. 564833000	1. 710626000
6	4. 877796000	1. 292197000	1. 418495000
1	5. 810664000	0. 750454000	1. 240645000
6	4. 874326000	2. 683291000	1. 325263000

6	3. 682122000	3. 350833000	1. 583283000
1	3. 661753000	4. 442708000	1. 543529000
6	2. 505129000	2. 670533000	1. 907344000
6	3. 820067000	-0. 930980000	1. 777771000
1	3. 367338000	-1. 329682000	2. 695800000
1	4. 868189000	-1. 256380000	1. 735069000
1	3. 301670000	-1. 399377000	0. 928028000
6	6. 127561000	3. 425643000	0. 970371000
1	5. 947490000	4. 504259000	0. 884630000
1	6. 541513000	3. 077818000	0. 012995000
1	6. 912119000	3. 278461000	1. 725965000
6	1. 281357000	3. 464316000	2. 246215000
1	0. 473171000	3. 298210000	1. 521973000
1	1. 501363000	4. 539292000	2. 252268000
1	0. 886439000	3. 183512000	3. 232861000
6	2. 454145000	-1. 274342000	-1. 977539000
6	2. 439139000	-2. 683462000	-1. 973254000
6	3. 611973000	-3. 369963000	-1. 648333000
1	3. 588446000	-4. 462211000	-1. 621089000
6	4. 803336000	-2. 708331000	-1. 371052000
6	4. 813749000	-1. 317198000	-1. 458099000
1	5. 748047000	-0. 780289000	-1. 273192000
6	3. 666369000	-0. 583393000	-1. 749700000
6	1. 217444000	-3. 472791000	-2. 332435000
1	0. 428274000	-3. 378990000	-1. 573563000
1	1. 456454000	-4. 539618000	-2. 427069000
1	0. 787724000	-3. 127671000	-3. 283128000
6	6. 041663000	-3. 456968000	-0. 980371000
1	6. 914101000	-3. 131603000	-1. 563113000
1	5. 923628000	-4. 537965000	-1. 124964000
1	6. 287764000	-3. 290235000	0. 079001000
6	3. 768120000	0. 912157000	-1. 809742000
1	3. 309785000	1. 317413000	-2. 722047000
1	4. 818560000	1. 230246000	-1. 776298000
1	3. 261187000	1. 380822000	-0. 953016000
6	-2. 227855000	1. 499596000	-2. 323219000
6	-3. 365244000	0. 695217000	-2. 460997000
1	-3. 776559000	0. 174644000	-1. 594807000
6	-3. 989234000	0. 559584000	-3. 695882000
1	-4. 880171000	-0. 061444000	-3. 780189000
6	-3. 471610000	1. 204012000	-4. 815548000
1	-3. 957004000	1. 092053000	-5. 783893000
6	-2. 329753000	1. 988374000	-4. 693513000
1	-1. 915279000	2. 491842000	-5. 565335000
6	-1. 713329000	2. 140052000	-3. 455779000
1	-0. 825479000	2. 765398000	-3. 370950000
6	-0. 434244000	3. 241503000	-0. 870074000
6	-1. 090592000	4. 457086000	-0. 640880000
1	-2. 151460000	4. 469429000	-0. 392857000

6	-0.389075000	5.655275000	-0.704623000
1	-0.909373000	6.593659000	-0.517999000
6	0.973687000	5.658728000	-0.994992000
1	1.521410000	6.599470000	-1.028413000
6	1.628308000	4.457644000	-1.242820000
1	2.694790000	4.440164000	-1.467176000
6	0.925383000	3.258115000	-1.186223000
1	1.435096000	2.318102000	-1.387960000
6	-2.665970000	2.125661000	0.496154000
6	-2.309320000	2.244377000	1.843593000
1	-1.319814000	1.916089000	2.169013000
6	-3.212587000	2.749376000	2.771228000
1	-2.916279000	2.832794000	3.815765000
6	-4.494889000	3.115818000	2.373297000
1	-5.206644000	3.500501000	3.102584000
6	-4.863042000	2.991587000	1.037554000
1	-5.861884000	3.281953000	0.715070000
6	-3.950439000	2.513451000	0.100141000
1	-4.241136000	2.461504000	-0.947609000
6	-2.186295000	-1.485094000	2.345652000
6	-1.646408000	-2.113436000	3.473350000
1	-0.753493000	-2.729796000	3.377343000
6	-2.243944000	-1.961475000	4.720283000
1	-1.809482000	-2.455737000	5.587647000
6	-3.392144000	-1.188926000	4.857036000
1	-3.863204000	-1.077277000	5.832478000
6	-3.934667000	-0.556063000	3.742686000
1	-4.830212000	0.056645000	3.838323000
6	-3.329239000	-0.691469000	2.498434000
1	-3.759981000	-0.178672000	1.637074000
6	-0.417984000	-3.230842000	0.877783000
6	0.954132000	-3.248200000	1.130498000
1	1.479869000	-2.305309000	1.265044000
6	1.648054000	-4.451926000	1.209175000
1	2.722988000	-4.436866000	1.389051000
6	0.972382000	-5.654630000	1.039812000
1	1.512102000	-6.599212000	1.090685000
6	-0.401502000	-5.649019000	0.806003000
1	-0.936674000	-6.588990000	0.679260000
6	-1.094892000	-4.447317000	0.726089000
1	-2.166509000	-4.456670000	0.528820000
6	-2.668096000	-2.124707000	-0.464754000
6	-3.949172000	-2.504193000	-0.049772000
1	-4.226226000	-2.445355000	1.001181000
6	-4.876733000	-2.983248000	-0.972043000
1	-5.872253000	-3.267225000	-0.633954000
6	-4.527953000	-3.116253000	-2.311906000
1	-5.251465000	-3.500708000	-3.029643000
6	-3.248828000	-2.759547000	-2.728729000

1	-2.966367000	-2.851522000	-3.776405000
6	-2.330273000	-2.255269000	-1.815861000
1	-1.342543000	-1.937606000	-2.156117000
complex I_{Mes}			
44	0.214752000	-0.013477000	0.000603000
15	-1.207298000	1.626534000	-0.662671000
15	-1.268416000	-1.607016000	0.646355000
6	2.501039000	-1.154604000	-1.925139000
6	3.734093000	-0.488406000	-1.726200000
6	4.878579000	-1.245725000	-1.492794000
1	5.826426000	-0.726942000	-1.326374000
6	4.852629000	-2.638926000	-1.442911000
6	3.640844000	-3.275916000	-1.687325000
1	3.601299000	-4.367794000	-1.686892000
6	2.468299000	-2.565106000	-1.951727000
6	3.852545000	1.006136000	-1.756977000
1	3.373583000	1.434056000	-2.648287000
1	4.908211000	1.308432000	-1.750078000
1	3.379453000	1.465087000	-0.875258000
6	6.099929000	-3.415637000	-1.145868000
1	5.896273000	-4.490589000	-1.066095000
1	6.557151000	-3.090690000	-0.200302000
1	6.859158000	-3.278693000	-1.928802000
6	1.221516000	-3.317738000	-2.293605000
1	0.439358000	-3.182360000	-1.535525000
1	1.421820000	-4.393643000	-2.373175000
1	0.800450000	-2.967956000	-3.247151000
6	2.462879000	1.105736000	1.954575000
6	2.459748000	2.517121000	2.020631000
6	3.644660000	3.209489000	1.774338000
1	3.629745000	4.301614000	1.809691000
6	4.842360000	2.553315000	1.501242000
6	4.839757000	1.160849000	1.512263000
1	5.775952000	0.626856000	1.331158000
6	3.679054000	0.420154000	1.730761000
6	1.229227000	3.285670000	2.385791000
1	0.442187000	3.181426000	1.627628000
1	1.451008000	4.355506000	2.487024000
1	0.804531000	2.924308000	3.333295000
6	6.090210000	3.321546000	1.186660000
1	6.991979000	2.751169000	1.443153000
1	6.126607000	4.276009000	1.727531000
1	6.151743000	3.558048000	0.113563000
6	3.768348000	-1.076636000	1.727755000
1	3.285191000	-1.513081000	2.612715000
1	4.817255000	-1.400964000	1.709532000
1	3.282243000	-1.507735000	0.838871000
6	-2.219340000	-1.479995000	2.232428000
6	-3.401604000	-0.735531000	2.315396000
1	-3.809552000	-0.250949000	1.426749000

6	-4.071377000	-0.605842000	3.527030000
1	-4.994190000	-0.028511000	3.568929000
6	-3.554687000	-1.192257000	4.678074000
1	-4.075844000	-1.084235000	5.628137000
6	-2.368064000	-1.914971000	4.610836000
1	-1.954659000	-2.373543000	5.507582000
6	-1.706895000	-2.062957000	3.396584000
1	-0.787406000	-2.645116000	3.354616000
6	-0.405179000	-3.248190000	0.851773000
6	-1.064611000	-4.455034000	0.590549000
1	-2.107847000	-4.456612000	0.276986000
6	-0.386510000	-5.662994000	0.706228000
1	-0.908996000	-6.594478000	0.492974000
6	0.953860000	-5.685454000	1.084997000
1	1.481950000	-6.634603000	1.164212000
6	1.610111000	-4.492048000	1.362956000
1	2.659478000	-4.489007000	1.657588000
6	0.933098000	-3.281970000	1.246518000
1	1.441566000	-2.346608000	1.470164000
6	-2.557122000	-2.076880000	-0.606661000
6	-2.183935000	-2.081510000	-1.954265000
1	-1.210094000	-1.683435000	-2.245080000
6	-3.053684000	-2.564118000	-2.925661000
1	-2.746815000	-2.553905000	-3.970463000
6	-4.317254000	-3.023101000	-2.569105000
1	-5.002982000	-3.390832000	-3.331324000
6	-4.704102000	-3.009716000	-1.231977000
1	-5.690288000	-3.369975000	-0.942719000
6	-3.825823000	-2.552286000	-0.253747000
1	-4.129125000	-2.581336000	0.791533000
6	-2.117377000	1.534136000	-2.274404000
6	-1.569467000	2.123000000	-3.419103000
1	-0.642670000	2.690767000	-3.348172000
6	-2.202658000	1.995204000	-4.650723000
1	-1.761924000	2.458265000	-5.532050000
6	-3.394940000	1.286546000	-4.755006000
1	-3.893053000	1.193438000	-5.718916000
6	-3.946384000	0.693861000	-3.623401000
1	-4.873891000	0.126961000	-3.694129000
6	-3.305812000	0.804547000	-2.394278000
1	-3.741827000	0.315116000	-1.521521000
6	-0.296012000	3.246598000	-0.823890000
6	1.053867000	3.250020000	-1.178788000
1	1.541718000	2.304679000	-1.405796000
6	1.767879000	4.442085000	-1.250818000
1	2.825722000	4.414988000	-1.512728000
6	1.135451000	5.648684000	-0.973982000
1	1.692282000	6.583552000	-1.018791000
6	-0.217076000	5.657702000	-0.639974000

1	-0.720661000	6.600160000	-0.429473000
6	-0.930745000	4.467321000	-0.564292000
1	-1.982527000	4.492593000	-0.281965000
6	-2.519101000	2.120777000	0.556463000
6	-3.766466000	2.625147000	0.169310000
1	-4.040730000	2.660748000	-0.883755000
6	-4.660279000	3.103619000	1.123175000
1	-5.629223000	3.486918000	0.806478000
6	-4.309968000	3.108880000	2.470283000
1	-5.007242000	3.492976000	3.213735000
6	-3.067416000	2.620824000	2.860873000
1	-2.788946000	2.604952000	3.913545000
6	-2.182951000	2.117548000	1.913636000
1	-1.225978000	1.699158000	2.230541000
16	0.955000000	0.172187000	2.245416000
16	1.011869000	-0.193547000	-2.227661000
complex 4			
44	-0.519346000	-0.160238000	-0.537564000
16	0.343210000	-2.033038000	0.302149000
6	2.113697000	-2.200597000	0.088351000
6	2.940997000	-2.047612000	1.218680000
6	4.295086000	-2.349695000	1.079651000
6	4.839874000	-2.776915000	-0.127307000
6	3.993982000	-2.899354000	-1.228449000
6	2.633733000	-2.616016000	-1.155285000
6	2.390979000	-1.623268000	2.566627000
6	3.422957000	-0.938881000	3.455028000
6	1.792988000	-2.820275000	3.309713000
6	1.760141000	-2.813708000	-2.377020000
6	2.434650000	-2.390673000	-3.677120000
6	1.289728000	-4.266366000	-2.452605000
16	-0.770740000	1.598902000	0.812096000
6	0.309747000	2.972116000	0.396210000
6	-0.029802000	3.793861000	-0.698263000
6	0.703854000	4.961276000	-0.893552000
6	1.755435000	5.325205000	-0.058984000
6	2.084664000	4.473263000	0.992550000
6	1.393973000	3.289020000	1.241828000
6	-1.142634000	3.478709000	-1.676871000
6	-0.630085000	3.424352000	-3.114417000
6	-2.297495000	4.466406000	-1.529337000
6	1.808134000	2.382965000	2.386133000
6	3.238307000	2.619388000	2.857229000
6	0.865352000	2.513854000	3.585389000
15	-2.656852000	-0.949717000	0.143635000
6	-2.900927000	-2.726127000	-0.264220000
6	-2.506971000	-3.164527000	-1.535289000
6	-2.669876000	-4.498006000	-1.888275000
6	-3.208612000	-5.403219000	-0.975930000
6	-3.591041000	-4.971837000	0.288941000

6	-3.440999000	-3.634319000	0.646536000
6	-3.078033000	-0.810484000	1.929538000
6	-2.057510000	-0.885553000	2.882871000
6	-2.361816000	-0.821980000	4.238124000
6	-3.683588000	-0.684431000	4.650848000
6	-4.704265000	-0.612560000	3.706875000
6	-4.404626000	-0.674158000	2.350292000
6	-4.042225000	-0.088870000	-0.712096000
6	-4.984640000	-0.778178000	-1.476906000
6	-6.017814000	-0.085385000	-2.102883000
6	-6.119909000	1.293928000	-1.965136000
6	-5.185719000	1.985446000	-1.197334000
6	-4.149782000	1.299852000	-0.576442000
1	4.958512000	-2.245864000	1.938823000
1	4.410566000	-3.224410000	-2.182892000
1	1.582074000	-0.895057000	2.381751000
1	2.925626000	-0.480369000	4.321344000
1	4.159375000	-1.653098000	3.850702000
1	3.967672000	-0.153883000	2.915006000
1	1.381445000	-2.507974000	4.280459000
1	2.572117000	-3.573197000	3.499434000
1	0.989484000	-3.304183000	2.739495000
1	0.871882000	-2.177356000	-2.263754000
1	1.705924000	-2.421003000	-4.498526000
1	3.259499000	-3.061206000	-3.958448000
1	2.823942000	-1.367425000	-3.601963000
1	0.648691000	-4.419644000	-3.332721000
1	0.717076000	-4.553422000	-1.559403000
1	2.148403000	-4.948867000	-2.538345000
1	0.445412000	5.603907000	-1.737656000
1	2.926196000	4.747221000	1.627982000
1	-1.537800000	2.479790000	-1.451225000
1	-1.426552000	3.071769000	-3.784242000
1	0.224080000	2.737862000	-3.193286000
1	-0.309018000	4.412276000	-3.474659000
1	-3.119348000	4.199666000	-2.209359000
1	-2.687443000	4.473183000	-0.500743000
1	-1.983439000	5.492439000	-1.769834000
1	1.748585000	1.346693000	2.007206000
1	3.503923000	1.880660000	3.623494000
1	3.353946000	3.608963000	3.322042000
1	3.961706000	2.537999000	2.035449000
1	1.167356000	1.821805000	4.385461000
1	0.907433000	3.535950000	3.990131000
1	-0.179378000	2.294299000	3.330675000
1	-2.073471000	-2.451571000	-2.240103000
1	-2.367016000	-4.834951000	-2.878281000
1	-3.326639000	-6.449570000	-1.253050000
1	-4.007596000	-5.677904000	1.005376000

1	-3.740367000	-3.302169000	1.640009000
1	-1.019780000	-0.988671000	2.562336000
1	-1.560017000	-0.875335000	4.972900000
1	-3.919968000	-0.630182000	5.712307000
1	-5.739070000	-0.504003000	4.027252000
1	-5.204932000	-0.615523000	1.612036000
1	-4.915829000	-1.859407000	-1.587413000
1	-6.746359000	-0.631275000	-2.700049000
1	-6.928916000	1.832875000	-2.455581000
1	-5.261058000	3.065850000	-1.081686000
1	-3.417597000	1.844889000	0.022055000
6	7.012141000	-2.113301000	-1.190616000
6	6.314850000	-3.084097000	-0.239608000
1	6.753384000	-2.947468000	0.763081000
1	6.852528000	-1.071230000	-0.886482000
1	8.093743000	-2.304055000	-1.218611000
1	6.628492000	-2.221687000	-2.214920000
6	6.562680000	-4.529864000	-0.663731000
1	6.073062000	-5.238259000	0.016709000
1	6.176367000	-4.718119000	-1.675482000
1	7.638417000	-4.752101000	-0.675874000
6	1.650303000	7.832954000	-0.210607000
6	2.539786000	6.594686000	-0.294737000
1	3.292995000	6.666049000	0.507672000
1	1.119653000	7.882402000	0.748804000
1	2.246979000	8.748680000	-0.321311000
1	0.895241000	7.833131000	-1.009516000
6	3.282281000	6.550059000	-1.628726000
1	3.934117000	5.669937000	-1.694352000
1	2.577342000	6.503888000	-2.470873000
1	3.899761000	7.449015000	-1.761575000
8	-1.208669000	-0.186010000	-2.301174000
1	-0.449096000	0.106202000	-2.849265000
17	1.544696000	0.662412000	-1.558044000
geometric isomer 4'			
44	-0.498598000	-0.053301000	-0.461701000
16	0.173742000	-2.118106000	0.005873000
6	1.949089000	-2.310169000	-0.073506000
6	2.652646000	-2.503108000	1.135059000
6	4.012351000	-2.797812000	1.056090000
6	4.683864000	-2.878305000	-0.161008000
6	3.959045000	-2.670226000	-1.333353000
6	2.596472000	-2.386689000	-1.324155000
6	1.960784000	-2.444381000	2.484121000
6	2.885239000	-2.083985000	3.641846000
6	1.267138000	-3.774609000	2.790315000
6	1.859396000	-2.233032000	-2.636787000
6	2.602047000	-1.354807000	-3.635815000
6	1.540937000	-3.607476000	-3.223752000
16	-0.466832000	1.372939000	1.216229000

6	0.706153000	2.653393000	0.724141000
6	0.211721000	3.751594000	-0.016826000
6	1.094091000	4.786588000	-0.318309000
6	2.431544000	4.762184000	0.071672000
6	2.886403000	3.653161000	0.777651000
6	2.057543000	2.582409000	1.107901000
6	-1.237527000	3.884899000	-0.441239000
6	-1.413469000	4.410724000	-1.862060000
6	-1.991193000	4.759702000	0.559593000
6	2.650021000	1.415110000	1.866045000
6	3.847230000	0.817434000	1.130281000
6	3.003835000	1.841470000	3.290063000
15	-2.773831000	-0.706868000	0.106348000
6	-3.313810000	-2.306212000	-0.647085000
6	-2.719015000	-2.740055000	-1.836844000
6	-3.146664000	-3.916290000	-2.444496000
6	-4.165124000	-4.669825000	-1.869509000
6	-4.760879000	-4.243582000	-0.686088000
6	-4.338946000	-3.066805000	-0.077789000
6	-3.193826000	-0.914347000	1.893315000
6	-2.220426000	-1.443665000	2.746588000
6	-2.505626000	-1.661663000	4.089786000
6	-3.763511000	-1.349224000	4.595983000
6	-4.738239000	-0.822151000	3.754130000
6	-4.456841000	-0.606402000	2.408920000
6	-4.033405000	0.496812000	-0.499794000
6	-4.841837000	0.212515000	-1.601130000
6	-5.717962000	1.174477000	-2.095420000
6	-5.799117000	2.423787000	-1.491521000
6	-4.998054000	2.712938000	-0.389393000
6	-4.113298000	1.759110000	0.099755000
1	4.582320000	-2.952964000	1.973348000
1	4.473294000	-2.726080000	-2.294219000
1	1.189868000	-1.656304000	2.424424000
1	2.291081000	-1.886304000	4.543834000
1	3.574523000	-2.905312000	3.884978000
1	3.486167000	-1.190099000	3.429158000
1	0.755995000	-3.732416000	3.762907000
1	2.011142000	-4.583430000	2.835877000
1	0.525247000	-4.042794000	2.027012000
1	0.911623000	-1.724208000	-2.431593000
1	1.958508000	-1.154593000	-4.503218000
1	3.520658000	-1.827236000	-4.013731000
1	2.861197000	-0.395351000	-3.172231000
1	0.986810000	-3.504521000	-4.167528000
1	0.929370000	-4.205744000	-2.532875000
1	2.460551000	-4.173746000	-3.433834000
1	0.718697000	5.643585000	-0.880323000
1	3.936935000	3.617986000	1.073117000

1	-1.696656000	2.887373000	-0.428194000
1	-2.465842000	4.305124000	-2.160479000
1	-0.804297000	3.842880000	-2.576900000
1	-1.151569000	5.474901000	-1.951735000
1	-3.046314000	4.861173000	0.267537000
1	-1.951005000	4.340489000	1.574904000
1	-1.556167000	5.769155000	0.599050000
1	1.886023000	0.624899000	1.927108000
1	4.233129000	-0.056141000	1.675797000
1	4.673738000	1.537146000	1.037966000
1	3.539893000	0.486443000	0.128733000
1	3.393696000	0.993417000	3.870014000
1	3.775122000	2.625146000	3.291606000
1	2.125063000	2.238062000	3.817480000
1	-1.923220000	-2.151268000	-2.294349000
1	-2.676030000	-4.244816000	-3.369643000
1	-4.494549000	-5.593029000	-2.343707000
1	-5.557146000	-4.830949000	-0.231678000
1	-4.807844000	-2.742095000	0.850873000
1	-1.232590000	-1.688502000	2.353660000
1	-1.738103000	-2.072270000	4.744159000
1	-3.984520000	-1.514527000	5.649238000
1	-5.723918000	-0.575524000	4.145496000
1	-5.224025000	-0.192607000	1.754349000
1	-4.782450000	-0.762039000	-2.084323000
1	-6.339987000	0.942319000	-2.958251000
1	-6.487437000	3.173966000	-1.877341000
1	-5.063766000	3.686418000	0.095464000
1	-3.483044000	1.995903000	0.959543000
6	6.912047000	-1.825142000	-0.520154000
6	6.173970000	-3.123279000	-0.192776000
1	6.474922000	-3.435635000	0.821302000
1	6.654030000	-1.029470000	0.191249000
1	8.000461000	-1.973511000	-0.494248000
1	6.643408000	-1.470037000	-1.525374000
6	6.573368000	-4.232256000	-1.161150000
1	6.034648000	-5.165135000	-0.951757000
1	6.362795000	-3.950584000	-2.202353000
1	7.650549000	-4.434663000	-1.091166000
6	2.903689000	7.216069000	0.344028000
6	3.367376000	5.897516000	-0.271093000
1	4.350711000	5.650672000	0.162602000
1	2.780345000	7.131003000	1.431187000
1	3.629280000	8.015580000	0.141768000
1	1.938997000	7.532308000	-0.077497000
6	3.544819000	6.037130000	-1.781587000
1	3.895306000	5.099854000	-2.231956000
1	2.595933000	6.305482000	-2.267313000
1	4.272343000	6.825813000	-2.017106000

8	1.386788000	0.378684000	-1.051854000
1	1.303928000	1.142863000	-1.645139000
17	-1.249483000	0.584370000	-2.558985000
tosyl azide (TsN₃)			
16	-1.529521000	-0.722499000	0.307778000
8	-1.797733000	-2.102841000	-0.074626000
8	-2.062429000	-0.086588000	1.514685000
7	-2.130575000	0.196655000	-1.087431000
7	-2.244496000	1.400465000	-0.826344000
7	-2.370498000	2.517973000	-0.658693000
6	0.208920000	-0.384579000	0.191154000
6	0.744270000	0.668721000	0.925753000
1	0.108052000	1.249591000	1.590914000
6	2.099297000	0.944409000	0.798823000
1	2.536867000	1.764763000	1.367232000
6	2.914329000	0.183268000	-0.043141000
6	2.342224000	-0.868643000	-0.767397000
1	2.971965000	-1.466368000	-1.426289000
6	0.991638000	-1.162079000	-0.657938000
1	0.541233000	-1.981308000	-1.214636000
6	4.381262000	0.467794000	-0.151674000
1	4.614474000	1.502577000	0.125116000
1	4.750477000	0.294372000	-1.169854000
1	4.957914000	-0.187200000	0.516391000
complex 8			
44	-0.443419000	-0.625701000	-0.141075000
16	-2.642970000	-0.050104000	-0.133312000
6	-2.906415000	1.719232000	-0.310730000
6	-2.917918000	2.299975000	-1.596596000
6	-3.208453000	3.660590000	-1.696562000
6	-3.520468000	4.440441000	-0.589209000
6	-3.551894000	3.826606000	0.661785000
6	-3.243006000	2.479129000	0.835553000
6	-2.718289000	1.484480000	-2.856849000
6	-2.169580000	2.282949000	-4.031890000
6	-4.036236000	0.811561000	-3.248415000
6	-3.333802000	1.859252000	2.218671000
6	-3.302974000	2.874651000	3.356492000
6	-4.610604000	1.023200000	2.356533000
16	0.812882000	-0.572430000	1.755785000
6	2.128013000	0.631161000	1.499658000
6	1.891500000	2.018355000	1.593390000
6	2.987816000	2.876052000	1.534303000
6	4.298290000	2.415936000	1.411105000
6	4.495956000	1.044786000	1.286284000
6	3.437079000	0.136155000	1.302991000
6	0.522945000	2.604923000	1.862280000
6	0.185181000	3.799270000	0.976329000
6	0.438175000	2.955136000	3.348335000
6	3.728251000	-1.345149000	1.161992000

6	4.925502000	-1.663146000	0.272505000
6	3.926137000	-1.974776000	2.541903000
15	-1.056735000	-2.804018000	0.303227000
6	-1.570333000	-3.231494000	2.016457000
6	-2.198557000	-2.262861000	2.804164000
6	-2.650706000	-2.586532000	4.079125000
6	-2.481148000	-3.875270000	4.574520000
6	-1.860503000	-4.845771000	3.792756000
6	-1.405983000	-4.527185000	2.518056000
6	-2.467185000	-3.339491000	-0.758339000
6	-2.533927000	-2.887267000	-2.082968000
6	-3.586461000	-3.284951000	-2.898441000
6	-4.582583000	-4.121465000	-2.401225000
6	-4.522429000	-4.566839000	-1.085614000
6	-3.467886000	-4.178931000	-0.264328000
6	0.301225000	-3.984567000	-0.080103000
6	1.394622000	-4.075697000	0.788291000
6	2.452256000	-4.926346000	0.491654000
6	2.434503000	-5.682781000	-0.678052000
6	1.352797000	-5.589936000	-1.546180000
6	0.287368000	-4.745082000	-1.249654000
1	-3.201312000	4.134313000	-2.678561000
1	-3.812199000	4.427213000	1.533094000
1	-1.990259000	0.691969000	-2.642825000
1	-1.889299000	1.597067000	-4.839895000
1	-2.913487000	2.986326000	-4.434951000
1	-1.269714000	2.845667000	-3.752791000
1	-3.903174000	0.221438000	-4.166270000
1	-4.812543000	1.567184000	-3.441370000
1	-4.401935000	0.137505000	-2.461710000
1	-2.463280000	1.190140000	2.340820000
1	-3.155589000	2.358497000	4.314245000
1	-4.251778000	3.426212000	3.428805000
1	-2.498276000	3.611645000	3.240819000
1	-4.672400000	0.575321000	3.359103000
1	-4.665710000	0.214050000	1.617967000
1	-5.492465000	1.666440000	2.221052000
1	2.818493000	3.952555000	1.614627000
1	5.505864000	0.661645000	1.143682000
1	-0.230589000	1.831744000	1.652081000
1	-0.850890000	4.117206000	1.163965000
1	0.261458000	3.533600000	-0.087245000
1	0.834528000	4.665302000	1.171700000
1	-0.541397000	3.377877000	3.604711000
1	0.600145000	2.066142000	3.973881000
1	1.203380000	3.697930000	3.618569000
1	2.848405000	-1.812265000	0.691608000
1	4.962890000	-2.744615000	0.082193000
1	5.880436000	-1.388302000	0.744981000

1	4.860551000	-1.152931000	-0.697297000
1	4.116266000	-3.055293000	2.456444000
1	4.794548000	-1.522611000	3.044032000
1	3.050995000	-1.829449000	3.188781000
1	-2.333128000	-1.253439000	2.414089000
1	-3.134074000	-1.824677000	4.688379000
1	-2.832888000	-4.125391000	5.574130000
1	-1.727298000	-5.855628000	4.177058000
1	-0.921519000	-5.289426000	1.907859000
1	-1.758623000	-2.223439000	-2.470651000
1	-3.632183000	-2.928239000	-3.925979000
1	-5.410876000	-4.422200000	-3.040868000
1	-5.302000000	-5.216004000	-0.690363000
1	-3.434922000	-4.525786000	0.767671000
1	1.417091000	-3.477392000	1.700590000
1	3.295291000	-4.997315000	1.178525000
1	3.265689000	-6.346667000	-0.910413000
1	1.333033000	-6.179001000	-2.461486000
1	-0.556021000	-4.678629000	-1.935074000
6	-2.626546000	6.732077000	-0.161800000
6	-3.784396000	5.920102000	-0.741359000
1	-3.835111000	6.131483000	-1.822455000
1	-1.671291000	6.447464000	-0.622406000
1	-2.781028000	7.808222000	-0.321439000
1	-2.536320000	6.563437000	0.921496000
6	-5.110508000	6.347653000	-0.119333000
1	-5.949763000	5.764964000	-0.519930000
1	-5.101979000	6.214937000	0.971818000
1	-5.305197000	7.410557000	-0.316509000
6	6.775940000	2.866206000	0.982236000
6	5.435888000	3.414656000	1.452965000
1	5.156891000	4.252726000	0.789566000
1	6.719284000	2.418870000	-0.019912000
1	7.524538000	3.668312000	0.952436000
1	7.152738000	2.095906000	1.670696000
6	5.581963000	3.972865000	2.870694000
1	4.650968000	4.430091000	3.228536000
1	5.844227000	3.164206000	3.568195000
1	6.375461000	4.731390000	2.915672000
16	0.759372000	0.224800000	-2.411262000
8	0.291551000	1.244438000	-1.382319000
8	0.288827000	0.352218000	-3.801509000
7	0.341277000	-1.231833000	-1.725193000
6	2.540610000	0.335938000	-2.464484000
6	3.250485000	-0.598619000	-3.216042000
1	2.724359000	-1.415546000	-3.707871000
6	4.626862000	-0.464859000	-3.324756000
1	5.198845000	-1.197224000	-3.895152000
6	5.296700000	0.600762000	-2.711724000

6	4. 552089000	1. 537796000	-1. 995232000
1	5. 059286000	2. 384373000	-1. 529864000
6	3. 176123000	1. 407281000	-1. 851987000
1	2. 595337000	2. 125887000	-1. 274992000
6	6. 790878000	0. 701202000	-2. 767087000
1	7. 242284000	0. 214153000	-1. 888472000
1	7. 127857000	1. 745707000	-2. 765570000
1	7. 202165000	0. 210073000	-3. 657458000
complex 9			
44	0. 590837000	-0. 450887000	0. 086709000
16	-1. 795046000	2. 155539000	0. 032102000
16	2. 369254000	-0. 899564000	-2. 739703000
16	1. 633465000	0. 711880000	1. 699244000
16	-1. 011033000	-1. 967892000	0. 518928000
15	2. 054276000	-2. 304691000	0. 814440000
8	-1. 245827000	3. 517255000	-0. 038139000
8	-2. 168417000	1. 530408000	1. 310712000
8	1. 629543000	-1. 614939000	-3. 785854000
8	3. 294863000	-1. 587066000	-1. 829323000
7	-0. 647394000	1. 062275000	-0. 672177000
7	-0. 388739000	1. 440950000	-1. 922378000
7	0. 533235000	0. 824507000	-2. 506298000
7	1. 188229000	-0. 110534000	-1. 708395000
6	-3. 202234000	2. 133639000	-1. 070056000
6	-4. 342693000	1. 434751000	-0. 702768000
1	-4. 360489000	0. 865829000	0. 225014000
6	-5. 456688000	1. 482092000	-1. 532830000
1	-6. 364016000	0. 951158000	-1. 239893000
6	-5. 435511000	2. 198336000	-2. 729267000
6	-4. 274523000	2. 903827000	-3. 067874000
1	-4. 253029000	3. 483320000	-3. 991220000
6	-3. 161396000	2. 890253000	-2. 241847000
1	-2. 266777000	3. 455324000	-2. 490383000
6	-6. 622570000	2. 202484000	-3. 644526000
1	-6. 515807000	1. 440577000	-4. 430495000
1	-6. 741238000	3. 169601000	-4. 149044000
1	-7. 551536000	1. 983791000	-3. 103301000
6	3. 243200000	0. 477025000	-3. 463461000
6	4. 396398000	0. 938098000	-2. 837062000
1	4. 771756000	0. 438657000	-1. 944896000
6	5. 072010000	2. 018783000	-3. 389841000
1	5. 981029000	2. 386921000	-2. 912963000
6	4. 608285000	2. 639424000	-4. 552604000
6	3. 456424000	2. 139273000	-5. 168429000
1	3. 095253000	2. 607975000	-6. 083796000
6	2. 766533000	1. 061811000	-4. 632450000
1	1. 866603000	0. 672947000	-5. 102371000
6	5. 316453000	3. 833811000	-5. 115469000
1	5. 215263000	3. 887005000	-6. 206249000
1	6. 385425000	3. 823416000	-4. 870685000

1	4. 897889000	4. 763809000	-4. 705115000
6	1. 069345000	2. 395560000	1. 891047000
6	1. 595684000	3. 388584000	1. 039653000
6	1. 292748000	4. 714161000	1. 330505000
1	1. 678891000	5. 503841000	0. 683036000
6	0. 471244000	5. 072008000	2. 395087000
6	-0. 044918000	4. 063698000	3. 206901000
1	-0. 700659000	4. 333207000	4. 034879000
6	0. 235153000	2. 719189000	2. 981782000
6	2. 478916000	3. 059886000	-0. 147136000
1	2. 271735000	2. 021912000	-0. 447810000
6	3. 951528000	3. 133922000	0. 256194000
1	4. 599231000	2. 875263000	-0. 595649000
1	4. 176359000	2. 445031000	1. 083687000
1	4. 213767000	4. 151018000	0. 583537000
6	2. 196358000	3. 926682000	-1. 370044000
1	1. 124608000	3. 928134000	-1. 610439000
1	2. 744531000	3. 530071000	-2. 237808000
1	2. 521354000	4. 967483000	-1. 226632000
6	0. 070086000	6. 515986000	2. 577746000
1	0. 804442000	7. 129891000	2. 029220000
6	0. 068615000	6. 975716000	4. 031067000
1	-0. 715393000	6. 470721000	4. 612678000
1	-0. 131567000	8. 053899000	4. 091205000
1	1. 030547000	6. 777912000	4. 521512000
6	-1. 299809000	6. 738540000	1. 934466000
1	-1. 300208000	6. 421259000	0. 883961000
1	-1. 595101000	7. 795924000	1. 987262000
1	-2. 065392000	6. 143429000	2. 453176000
6	-0. 291640000	1. 656976000	3. 924202000
1	-0. 425696000	0. 731452000	3. 341284000
6	0. 735804000	1. 386751000	5. 025392000
1	0. 900005000	2. 294544000	5. 624892000
1	1. 708203000	1. 079699000	4. 615323000
1	0. 382474000	0. 595797000	5. 702729000
6	-1. 642251000	1. 995758000	4. 541103000
1	-1. 574086000	2. 828611000	5. 256159000
1	-2. 017705000	1. 127693000	5. 101057000
1	-2. 376695000	2. 252448000	3. 767926000
6	-2. 709529000	-1. 614467000	0. 071011000
6	-3. 653262000	-1. 521175000	1. 118276000
6	-5. 000209000	-1. 651138000	0. 788773000
1	-5. 748834000	-1. 603730000	1. 582876000
6	-5. 436236000	-1. 844326000	-0. 523629000
6	-4. 482132000	-1. 854680000	-1. 535453000
1	-4. 800189000	-1. 955932000	-2. 573304000
6	-3. 116745000	-1. 733383000	-1. 272301000
6	-3. 233957000	-1. 334891000	2. 562941000
1	-2. 252271000	-0. 835452000	2. 557619000

6	-4.186233000	-0.439057000	3.347106000
1	-4.325042000	0.530152000	2.850120000
1	-3.775260000	-0.247407000	4.347273000
1	-5.172312000	-0.903522000	3.492321000
6	-3.079693000	-2.688731000	3.257034000
1	-4.035651000	-3.234090000	3.254692000
1	-2.769514000	-2.552043000	4.302731000
1	-2.325068000	-3.319451000	2.765583000
6	-6.911268000	-2.061453000	-0.784637000
1	-7.462986000	-1.366295000	-0.126902000
6	-7.341116000	-1.793284000	-2.220714000
1	-7.021888000	-0.801993000	-2.571924000
1	-8.433690000	-1.852137000	-2.308009000
1	-6.921305000	-2.541953000	-2.907882000
6	-7.300256000	-3.485939000	-0.383416000
1	-6.753976000	-4.213467000	-1.001119000
1	-8.375962000	-3.656841000	-0.527489000
1	-7.056785000	-3.692453000	0.666475000
6	-2.140510000	-1.775207000	-2.429070000
1	-1.156415000	-1.459396000	-2.057106000
6	-2.512846000	-0.804480000	-3.546927000
1	-3.447634000	-1.089926000	-4.051626000
1	-1.716159000	-0.791643000	-4.303040000
1	-2.629990000	0.219380000	-3.164934000
6	-1.987609000	-3.199608000	-2.961003000
1	-1.713980000	-3.899268000	-2.157443000
1	-1.204730000	-3.235654000	-3.732539000
1	-2.926294000	-3.558579000	-3.408376000
6	3.763030000	-1.874787000	1.372080000
6	4.432163000	-0.783152000	0.812069000
1	3.932390000	-0.179898000	0.057912000
6	5.718942000	-0.457881000	1.223205000
1	6.223040000	0.401017000	0.780513000
6	6.353185000	-1.218211000	2.201472000
1	7.360614000	-0.961458000	2.525156000
6	5.691830000	-2.299570000	2.773930000
1	6.177140000	-2.891816000	3.547884000
6	4.400714000	-2.622283000	2.367724000
1	3.881617000	-3.457034000	2.839069000
6	2.239300000	-3.754395000	-0.314944000
6	3.290131000	-4.658476000	-0.149475000
1	4.042460000	-4.491845000	0.620553000
6	3.393113000	-5.770921000	-0.977678000
1	4.218908000	-6.467642000	-0.842516000
6	2.451909000	-5.987182000	-1.979374000
1	2.538210000	-6.855219000	-2.630999000
6	1.407580000	-5.084903000	-2.152934000
1	0.674826000	-5.233023000	-2.944780000
6	1.300846000	-3.974019000	-1.324226000

1	0.489422000	-3.263328000	-1.478844000
6	1.338594000	-3.090376000	2.336633000
6	1.236791000	-2.335403000	3.512481000
1	1.634999000	-1.320636000	3.545999000
6	0.631106000	-2.868928000	4.642249000
1	0.563933000	-2.270689000	5.549934000
6	0.114497000	-4.162536000	4.615248000
1	-0.364488000	-4.578479000	5.500381000
6	0.210728000	-4.918356000	3.453134000
1	-0.191281000	-5.929796000	3.422347000
6	0.819372000	-4.386764000	2.318213000
1	0.877653000	-4.986060000	1.410541000
complex 10			
44	0.590837000	-0.450887000	0.086709000
16	-1.795046000	2.155539000	0.032102000
16	2.369254000	-0.899564000	-2.739703000
16	1.633465000	0.711880000	1.699244000
16	-1.011033000	-1.967892000	0.518928000
15	2.054276000	-2.304691000	0.814440000
8	-1.245827000	3.517255000	-0.038139000
8	-2.168417000	1.530408000	1.310712000
8	1.629543000	-1.614939000	-3.785854000
8	3.294863000	-1.587066000	-1.829323000
7	-0.647394000	1.062275000	-0.672177000
7	-0.388739000	1.440950000	-1.922378000
7	0.533235000	0.824507000	-2.506298000
7	1.188229000	-0.110534000	-1.708395000
6	-3.202234000	2.133639000	-1.070056000
6	-4.342693000	1.434751000	-0.702768000
1	-4.360489000	0.865829000	0.225014000
6	-5.456688000	1.482092000	-1.532830000
1	-6.364016000	0.951158000	-1.239893000
6	-5.435511000	2.198336000	-2.729267000
6	-4.274523000	2.903827000	-3.067874000
1	-4.253029000	3.483320000	-3.991220000
6	-3.161396000	2.890253000	-2.241847000
1	-2.266777000	3.455324000	-2.490383000
6	-6.622570000	2.202484000	-3.644526000
1	-6.515807000	1.440577000	-4.430495000
1	-6.741238000	3.169601000	-4.149044000
1	-7.551536000	1.983791000	-3.103301000
6	3.243200000	0.477025000	-3.463461000
6	4.396398000	0.938098000	-2.837062000
1	4.771756000	0.438657000	-1.944896000
6	5.072010000	2.018783000	-3.389841000
1	5.981029000	2.386921000	-2.912963000
6	4.608285000	2.639424000	-4.552604000
6	3.456424000	2.139273000	-5.168429000
1	3.095253000	2.607975000	-6.083796000
6	2.766533000	1.061811000	-4.632450000

1	1. 866603000	0. 672947000	-5. 102371000
6	5. 316453000	3. 833811000	-5. 115469000
1	5. 215263000	3. 887005000	-6. 206249000
1	6. 385425000	3. 823416000	-4. 870685000
1	4. 897889000	4. 763809000	-4. 705115000
6	1. 069345000	2. 395560000	1. 891047000
6	1. 595684000	3. 388584000	1. 039653000
6	1. 292748000	4. 714161000	1. 330505000
1	1. 678891000	5. 503841000	0. 683036000
6	0. 471244000	5. 072008000	2. 395087000
6	-0. 044918000	4. 063698000	3. 206901000
1	-0. 700659000	4. 333207000	4. 034879000
6	0. 235153000	2. 719189000	2. 981782000
6	2. 478916000	3. 059886000	-0. 147136000
1	2. 271735000	2. 021912000	-0. 447810000
6	3. 951528000	3. 133922000	0. 256194000
1	4. 599231000	2. 875263000	-0. 595649000
1	4. 176359000	2. 445031000	1. 083687000
1	4. 213767000	4. 151018000	0. 583537000
6	2. 196358000	3. 926682000	-1. 370044000
1	1. 124608000	3. 928134000	-1. 610439000
1	2. 744531000	3. 530071000	-2. 237808000
1	2. 521354000	4. 967483000	-1. 226632000
6	0. 070086000	6. 515986000	2. 577746000
1	0. 804442000	7. 129891000	2. 029220000
6	0. 068615000	6. 975716000	4. 031067000
1	-0. 715393000	6. 470721000	4. 612678000
1	-0. 131567000	8. 053899000	4. 091205000
1	1. 030547000	6. 777912000	4. 521512000
6	-1. 299809000	6. 738540000	1. 934466000
1	-1. 300208000	6. 421259000	0. 883961000
1	-1. 595101000	7. 795924000	1. 987262000
1	-2. 065392000	6. 143429000	2. 453176000
6	-0. 291640000	1. 656976000	3. 924202000
1	-0. 425696000	0. 731452000	3. 341284000
6	0. 735804000	1. 386751000	5. 025392000
1	0. 900005000	2. 294544000	5. 624892000
1	1. 708203000	1. 079699000	4. 615323000
1	0. 382474000	0. 595797000	5. 702729000
6	-1. 642251000	1. 995758000	4. 541103000
1	-1. 574086000	2. 828611000	5. 256159000
1	-2. 017705000	1. 127693000	5. 101057000
1	-2. 376695000	2. 252448000	3. 767926000
6	-2. 709529000	-1. 614467000	0. 071011000
6	-3. 653262000	-1. 521175000	1. 118276000
6	-5. 000209000	-1. 651138000	0. 788773000
1	-5. 748834000	-1. 603730000	1. 582876000
6	-5. 436236000	-1. 844326000	-0. 523629000
6	-4. 482132000	-1. 854680000	-1. 535453000

1	-4.800189000	-1.955932000	-2.573304000
6	-3.116745000	-1.733383000	-1.272301000
6	-3.233957000	-1.334891000	2.562941000
1	-2.252271000	-0.835452000	2.557619000
6	-4.186233000	-0.439057000	3.347106000
1	-4.325042000	0.530152000	2.850120000
1	-3.775260000	-0.247407000	4.347273000
1	-5.172312000	-0.903522000	3.492321000
6	-3.079693000	-2.688731000	3.257034000
1	-4.035651000	-3.234090000	3.254692000
1	-2.769514000	-2.552043000	4.302731000
1	-2.325068000	-3.319451000	2.765583000
6	-6.911268000	-2.061453000	-0.784637000
1	-7.462986000	-1.366295000	-0.126902000
6	-7.341116000	-1.793284000	-2.220714000
1	-7.021888000	-0.801993000	-2.571924000
1	-8.433690000	-1.852137000	-2.308009000
1	-6.921305000	-2.541953000	-2.907882000
6	-7.300256000	-3.485939000	-0.383416000
1	-6.753976000	-4.213467000	-1.001119000
1	-8.375962000	-3.656841000	-0.527489000
1	-7.056785000	-3.692453000	0.666475000
6	-2.140510000	-1.775207000	-2.429070000
1	-1.156415000	-1.459396000	-2.057106000
6	-2.512846000	-0.804480000	-3.546927000
1	-3.447634000	-1.089926000	-4.051626000
1	-1.716159000	-0.791643000	-4.303040000
1	-2.629990000	0.219380000	-3.164934000
6	-1.987609000	-3.199608000	-2.961003000
1	-1.713980000	-3.899268000	-2.157443000
1	-1.204730000	-3.235654000	-3.732539000
1	-2.926294000	-3.558579000	-3.408376000
6	3.763030000	-1.874787000	1.372080000
6	4.432163000	-0.783152000	0.812069000
1	3.932390000	-0.179898000	0.057912000
6	5.718942000	-0.457881000	1.223205000
1	6.223040000	0.401017000	0.780513000
6	6.353185000	-1.218211000	2.201472000
1	7.360614000	-0.961458000	2.525156000
6	5.691830000	-2.299570000	2.773930000
1	6.177140000	-2.891816000	3.547884000
6	4.400714000	-2.622283000	2.367724000
1	3.881617000	-3.457034000	2.839069000
6	2.239300000	-3.754395000	-0.314944000
6	3.290131000	-4.658476000	-0.149475000
1	4.042460000	-4.491845000	0.620553000
6	3.393113000	-5.770921000	-0.977678000
1	4.218908000	-6.467642000	-0.842516000
6	2.451909000	-5.987182000	-1.979374000

1	2.538210000	-6.855219000	-2.630999000
6	1.407580000	-5.084903000	-2.152934000
1	0.674826000	-5.233023000	-2.944780000
6	1.300846000	-3.974019000	-1.324226000
1	0.489422000	-3.263328000	-1.478844000
6	1.338594000	-3.090376000	2.336633000
6	1.236791000	-2.335403000	3.512481000
1	1.634999000	-1.320636000	3.545999000
6	0.631106000	-2.868928000	4.642249000
1	0.563933000	-2.270689000	5.549934000
6	0.114497000	-4.162536000	4.615248000
1	-0.364488000	-4.578479000	5.500381000
6	0.210728000	-4.918356000	3.453134000
1	-0.191281000	-5.929796000	3.422347000
6	0.819372000	-4.386764000	2.318213000
1	0.877653000	-4.986060000	1.410541000

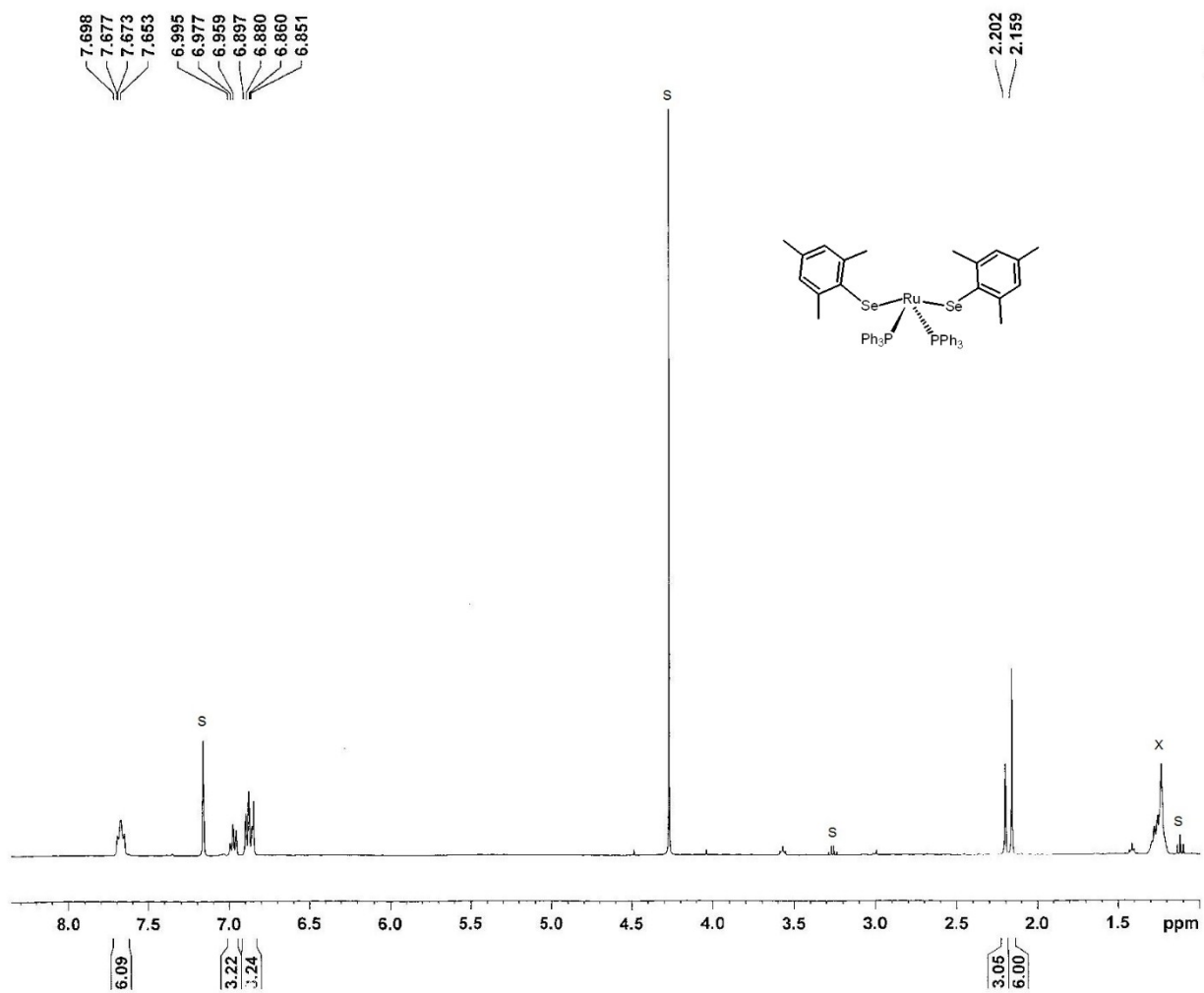


Figure S5. ^1H NMR (400 MHz, 298 K, C_6D_6) spectrum of **2** (X = impurity, S = residual solvent).

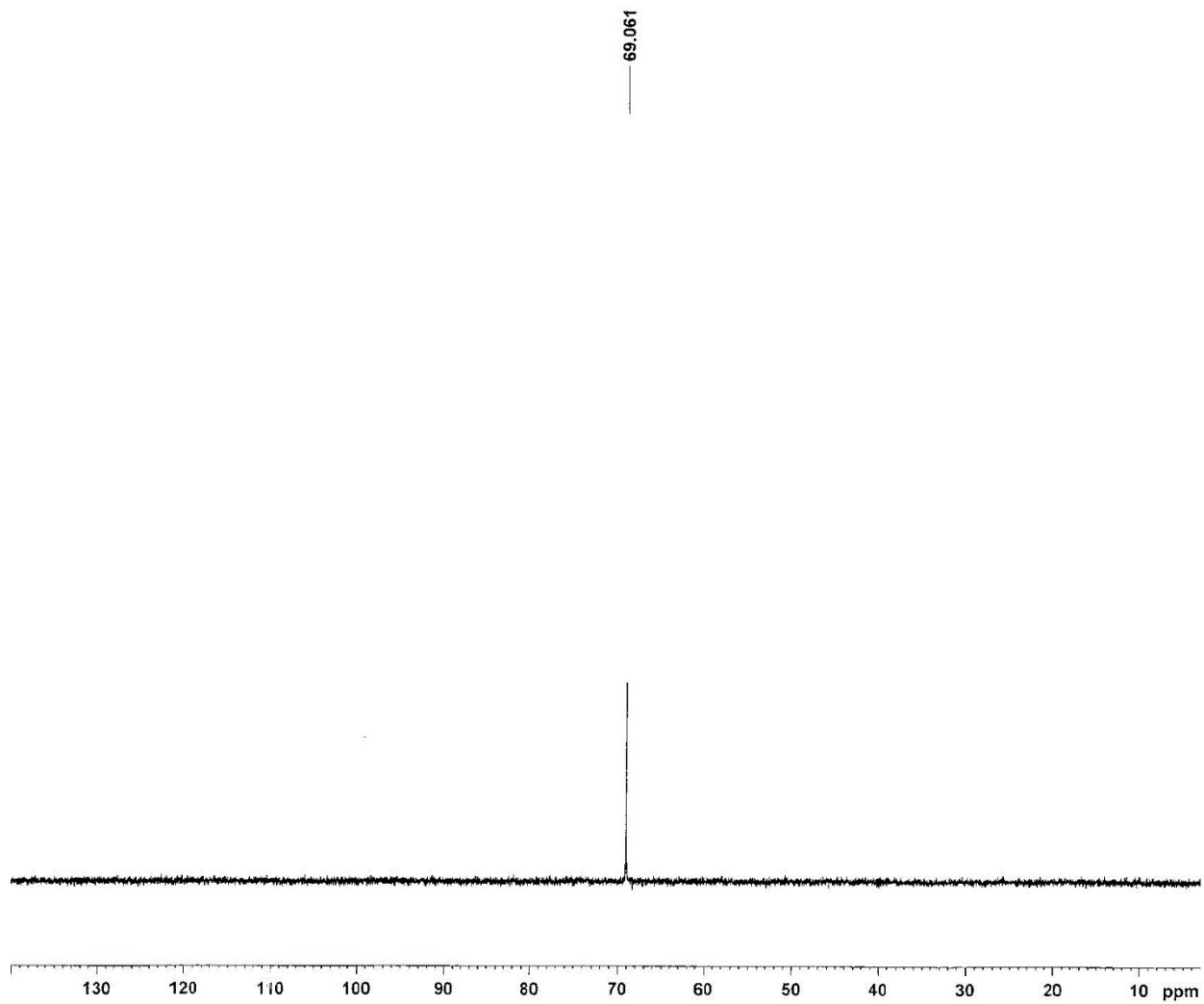


Figure S6. $^{31}\text{P}\{^1\text{H}\}$ NMR (162 MHz, 298 K, C_6D_6) spectrum of **2**.

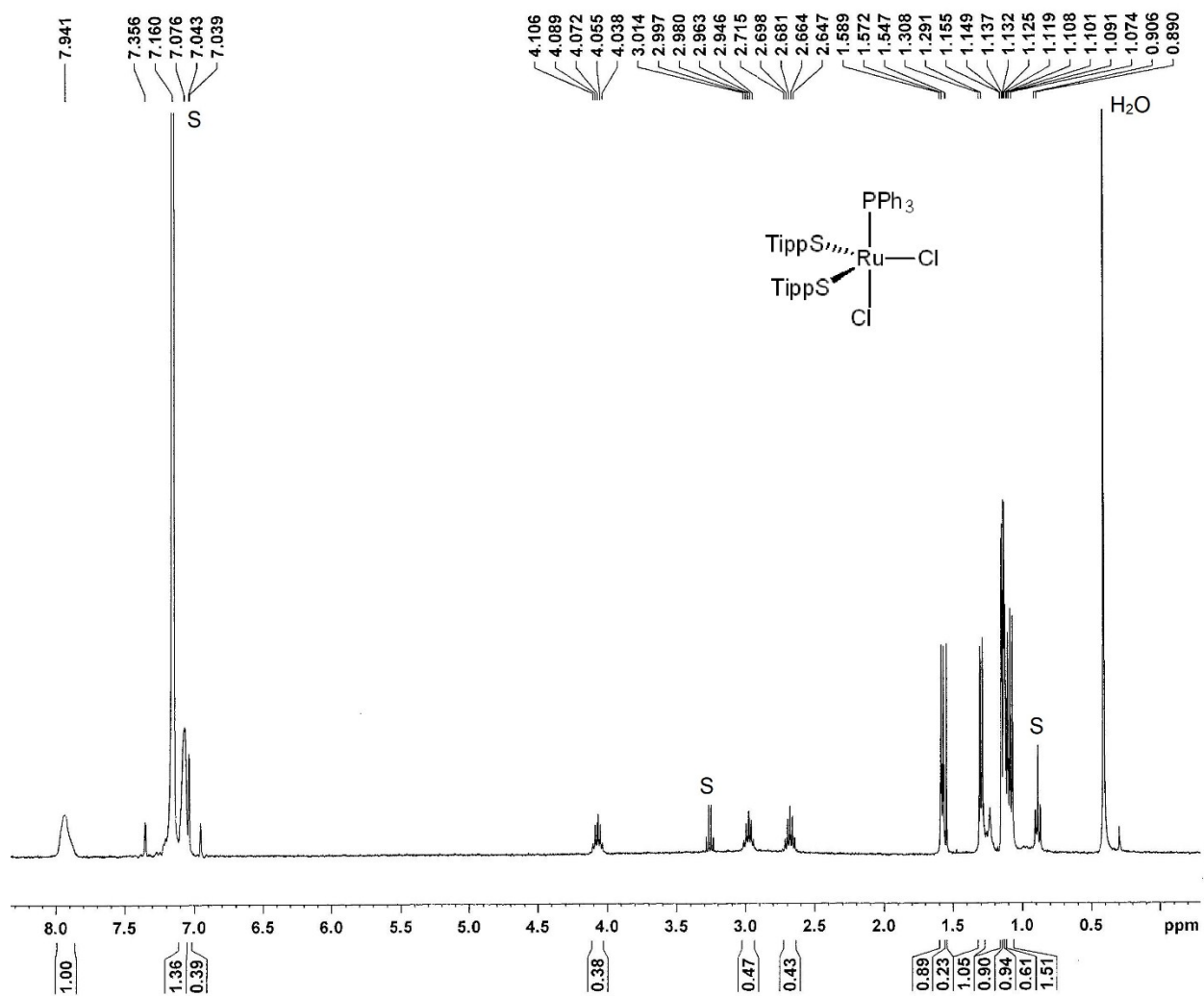


Figure S7. ^1H NMR (400 MHz, 298 K, C_6D_6) spectrum of **3** (X = impurity, S = residual solvent).

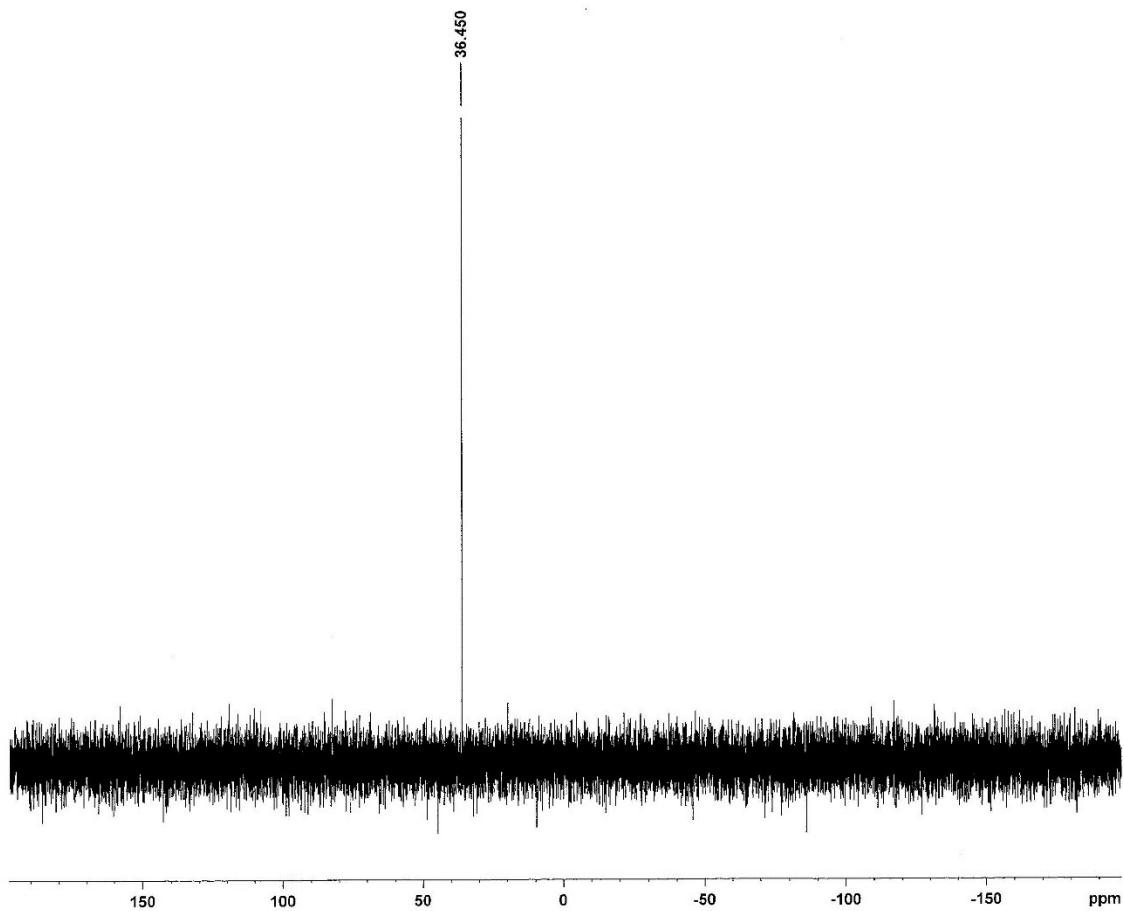


Figure S8. $^{31}\text{P}\{^1\text{H}\}$ NMR (162 MHz, 298 K, C_6D_6) spectrum of **3**.

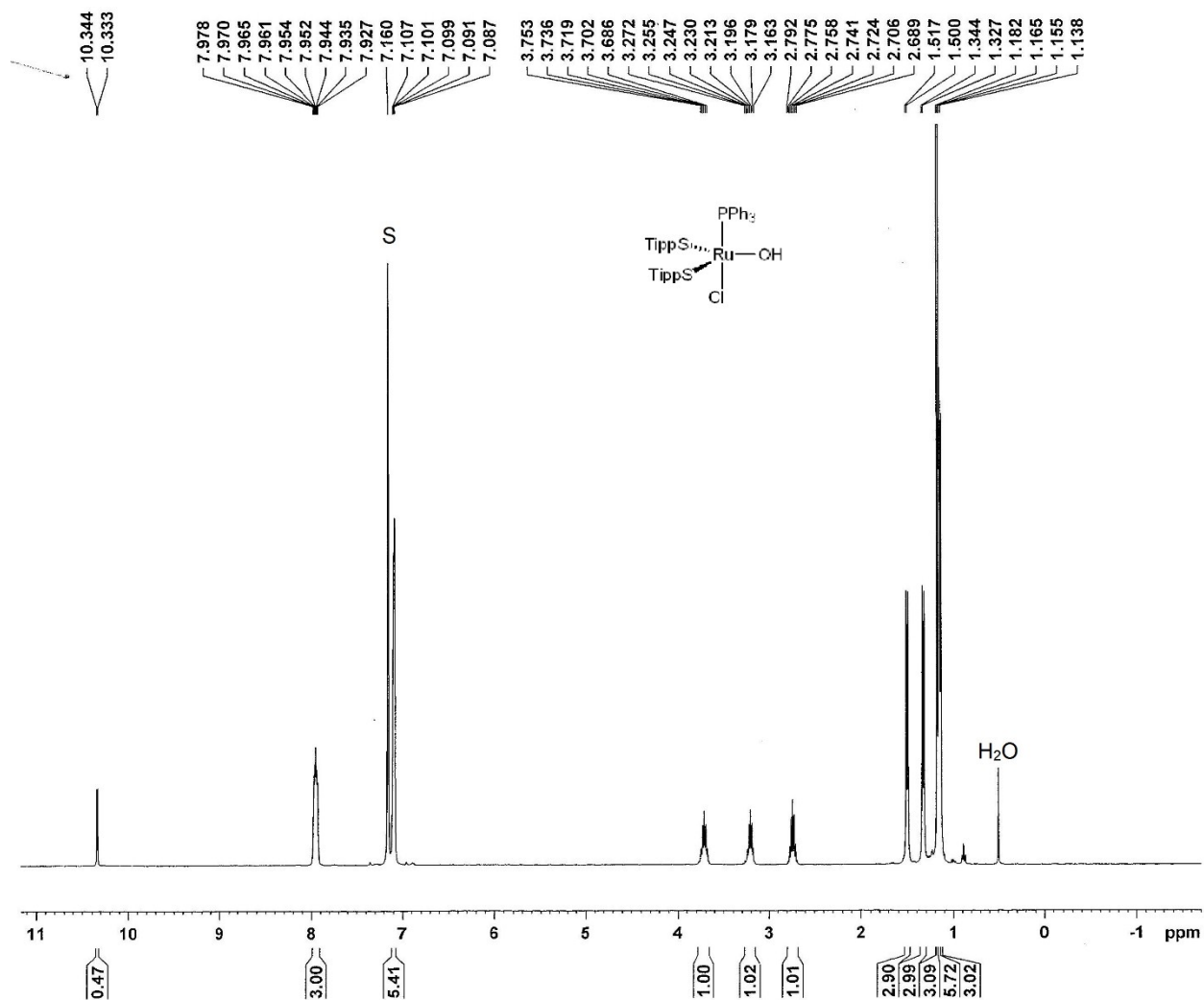


Figure S9. $^1\text{H NMR}$ (400 MHz, 298 K, C_6D_6) spectrum of **4** (X = impurity, S = residual solvent).

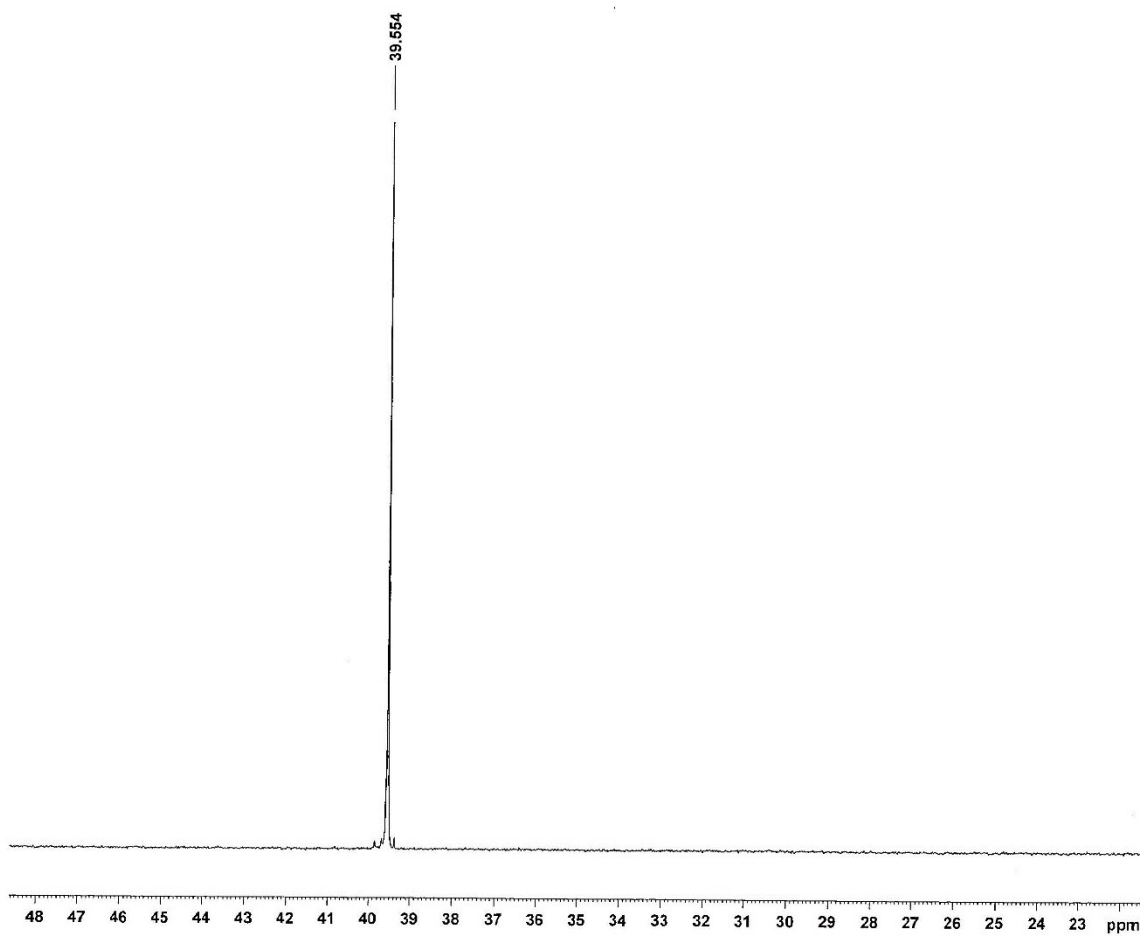


Figure S10. $^{31}\text{P}\{^1\text{H}\}$ NMR (162 MHz, 298 K, C_6D_6) spectrum of **4**. Figure

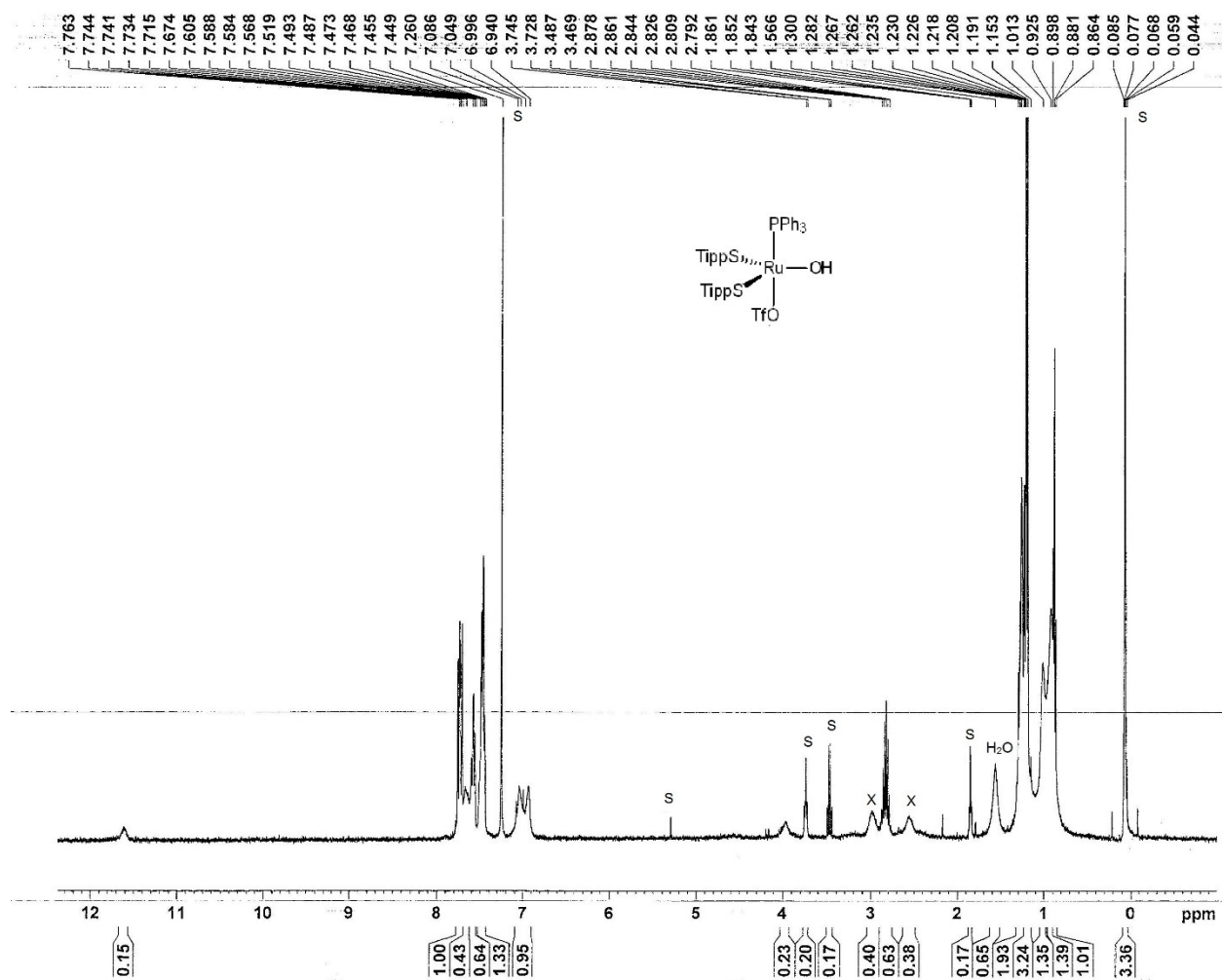


Figure S11. ^1H NMR (400 MHz, 298 K, CDCl_3) spectrum of **5** (X = impurity, S = residual solvent).

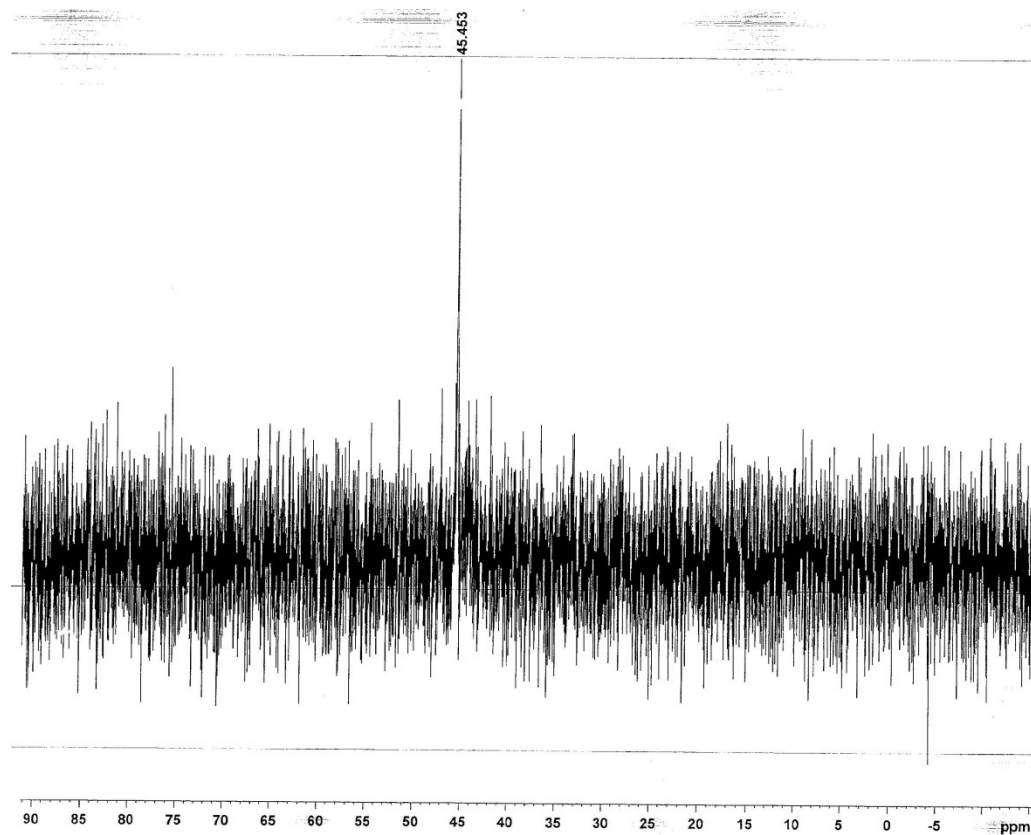


Figure S12. $^{31}\text{P}\{^1\text{H}\}$ NMR (162 MHz, 298 K, CDCl_3) spectrum of **5**.

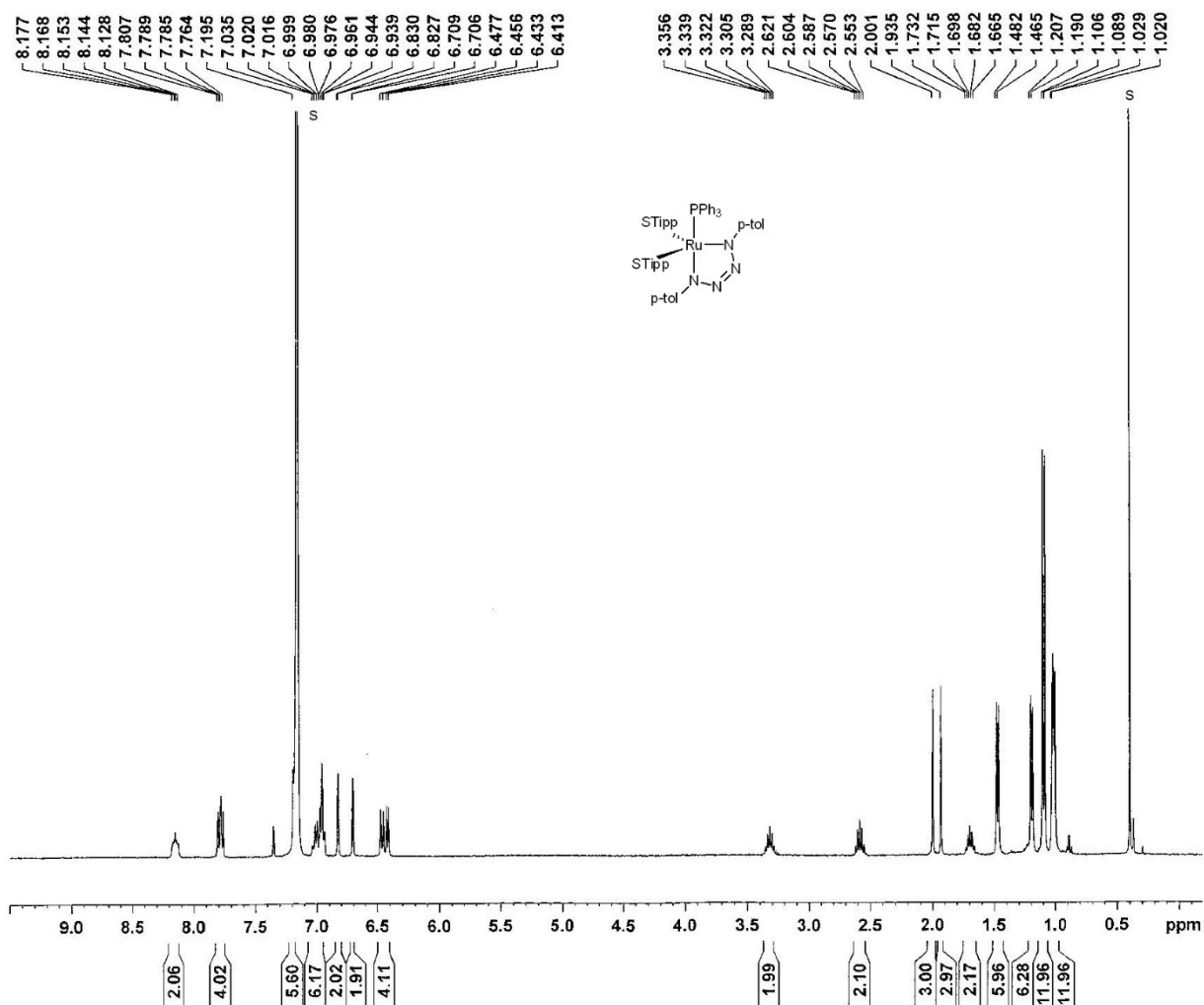


Figure S13. ^1H NMR (400 MHz, 298 K, C_6D_6) spectrum of 6 (X = impurity, S = residual solvent).

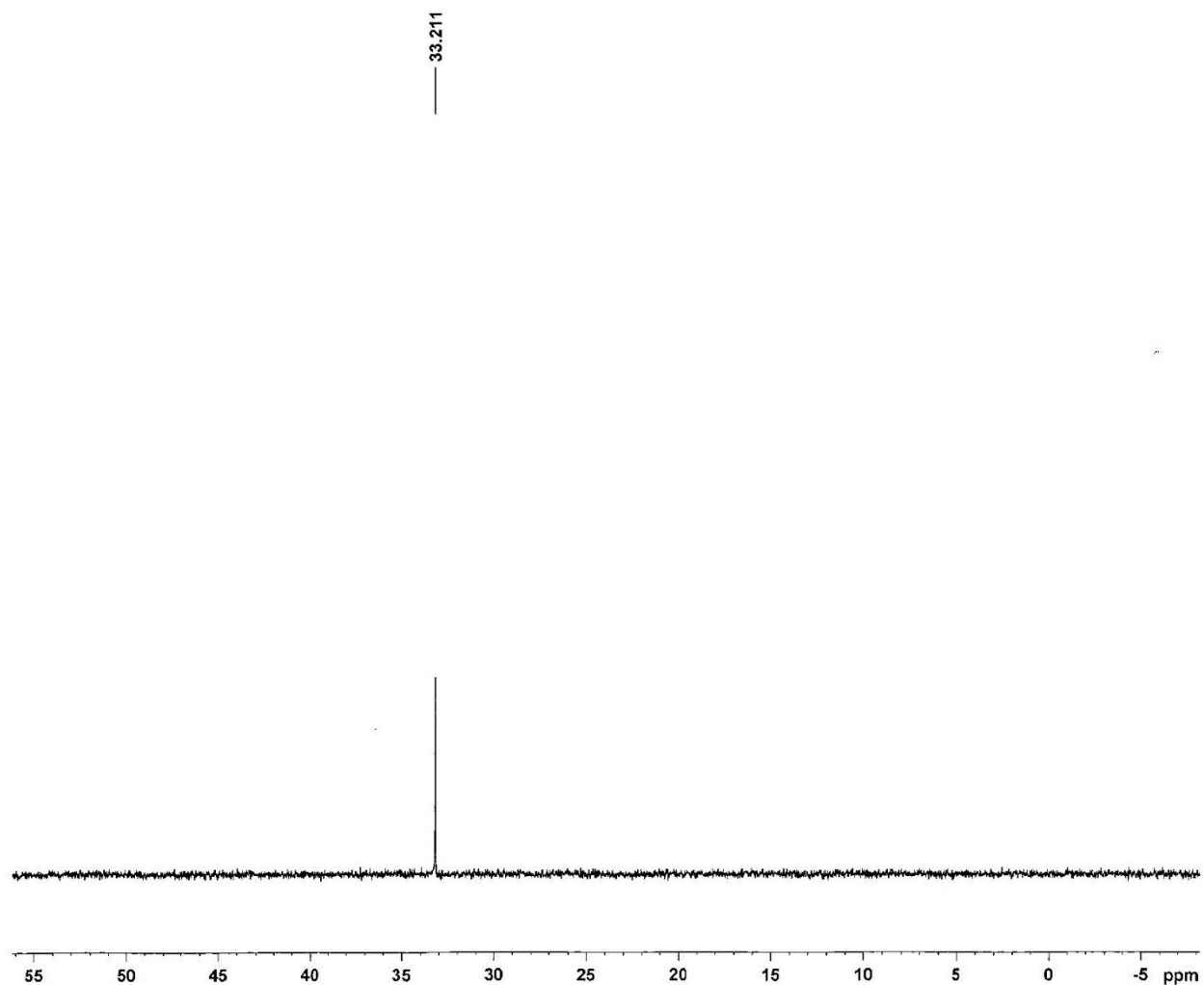


Figure S14. $^{31}\text{P}\{^1\text{H}\}$ NMR (162 MHz, 298 K, C_6D_6) spectrum of **6**.

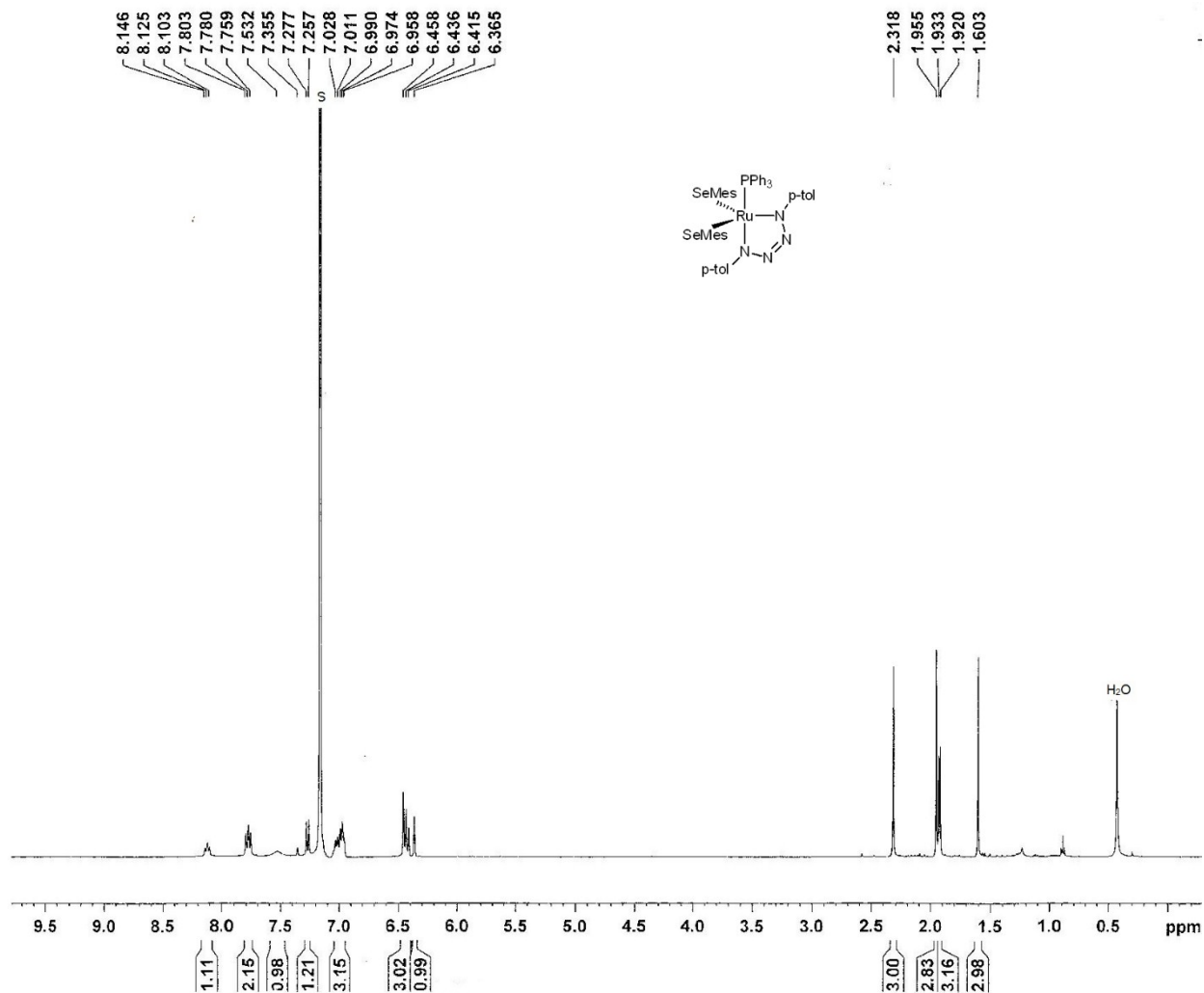


Figure S15. ^1H NMR (400 MHz, 298 K, C_6D_6) spectrum of 7 (X = impurity, S = residual solvent).

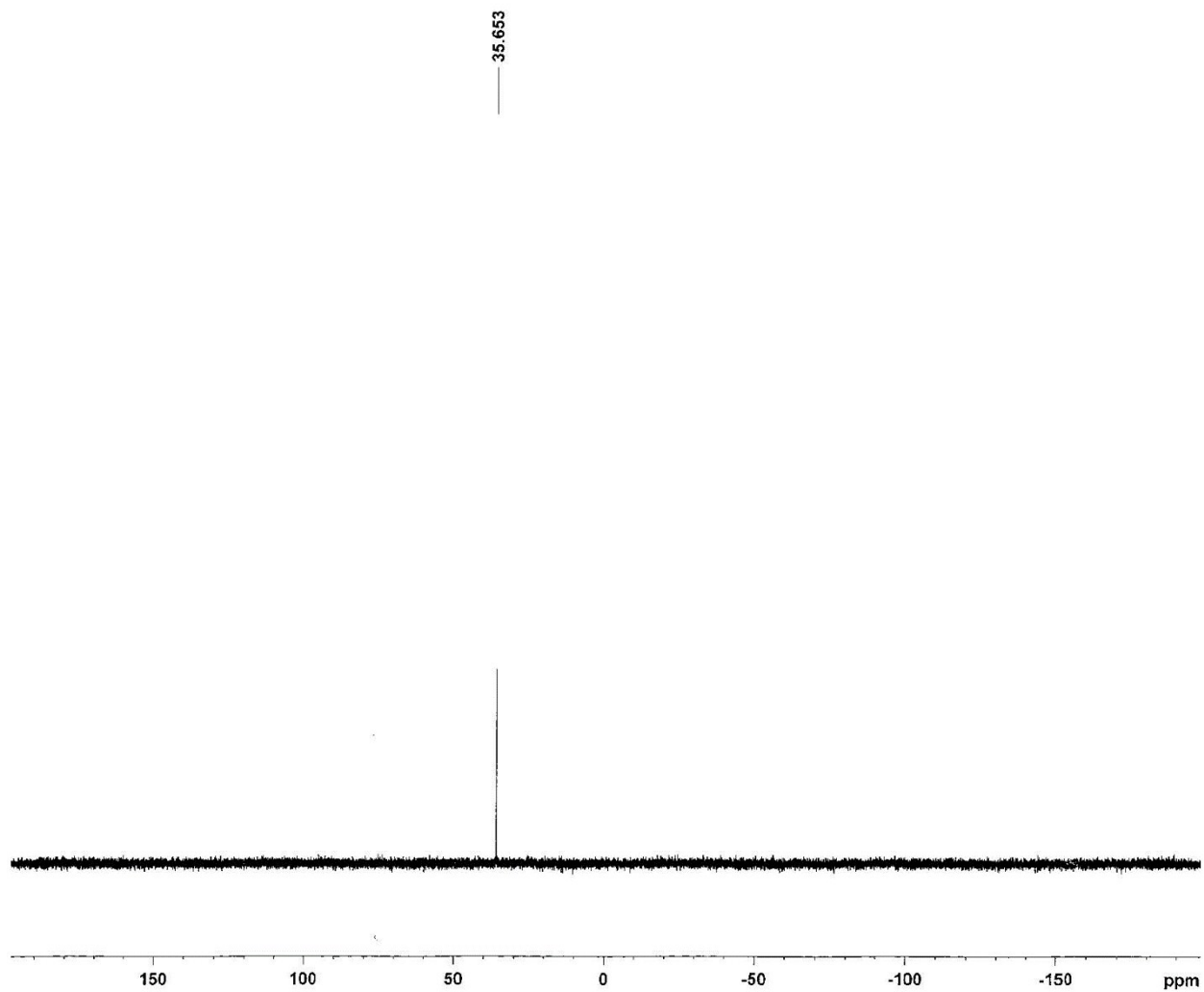


Figure S16. $^{31}\text{P}\{^1\text{H}\}$ NMR (162 MHz, 298 K, C_6D_6) spectrum of 7.

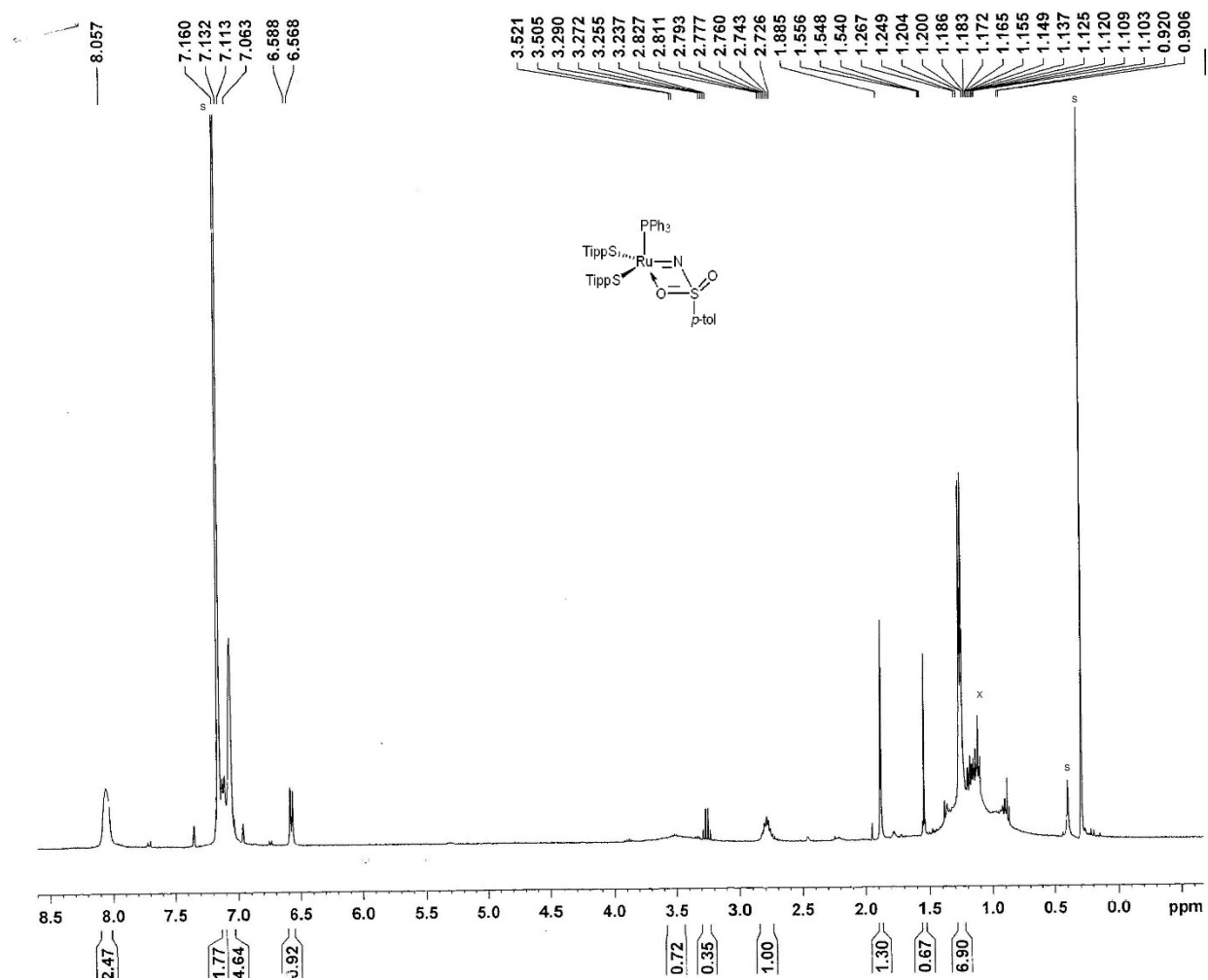


Figure S17. ^1H NMR (400 MHz, 298 K, C_6D_6) spectrum of **8** (X = impurity, S = residual solvent).

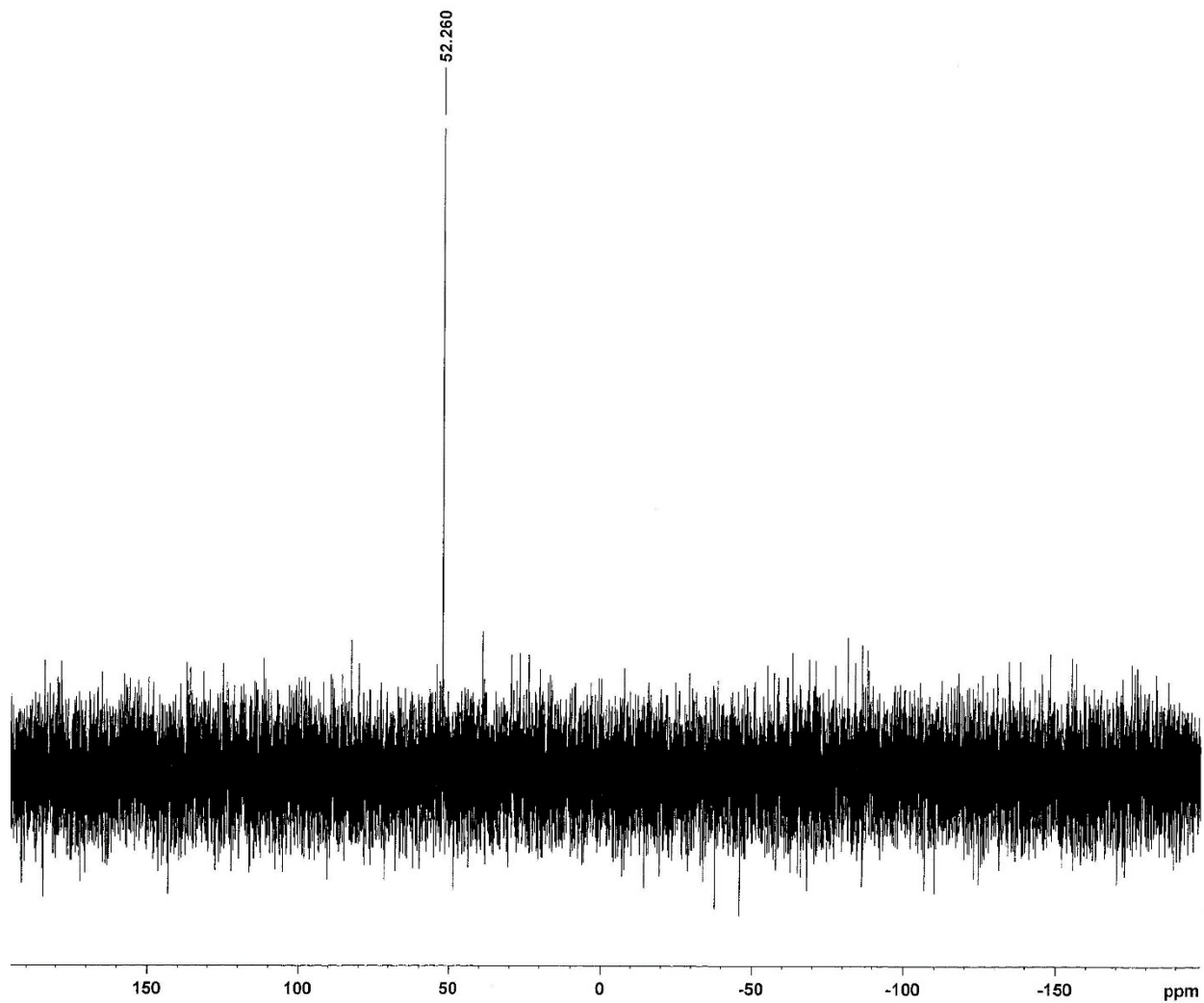


Figure S18. $^{31}\text{P}\{^1\text{H}\}$ NMR (162 MHz, 298 K, C_6D_6) spectrum of **8**.

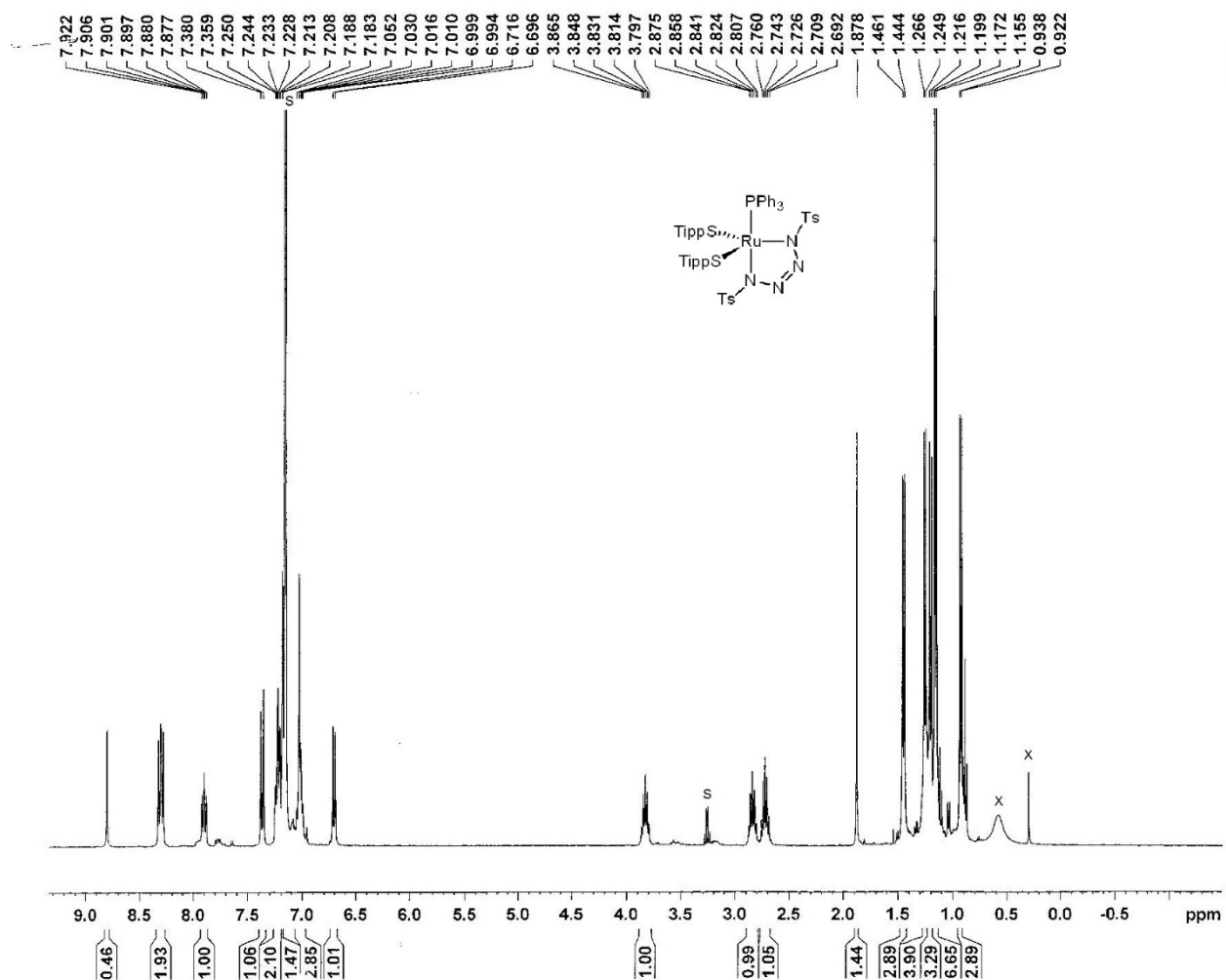


Figure S19. $^1\text{H NMR}$ (400 MHz, 298 K, C_6D_6) spectrum of **9** (X = impurity, S = residual solvent).

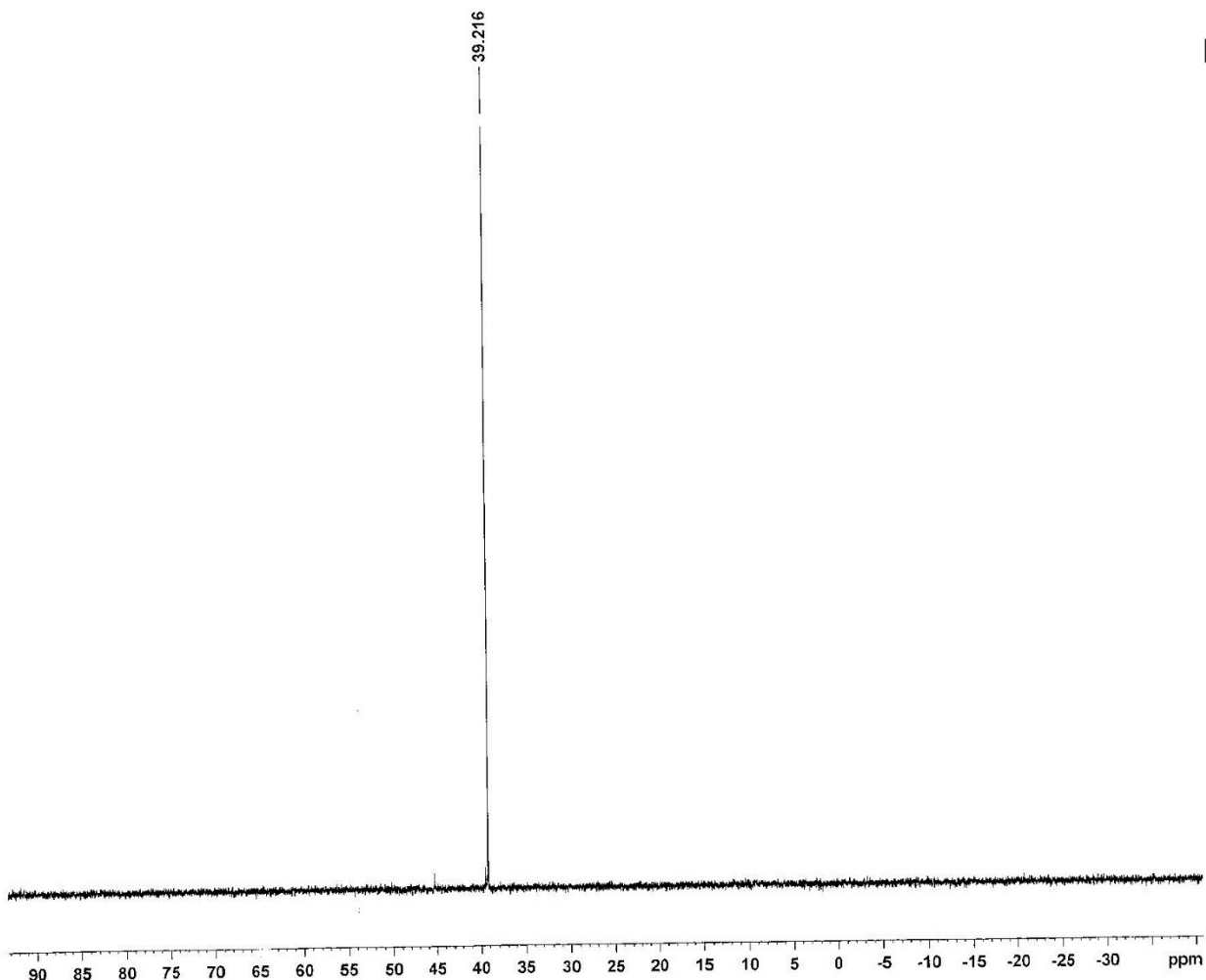


Figure S20. $^{31}\text{P}\{^1\text{H}\}$ NMR (162 MHz, 298 K, C_6D_6) spectrum of **9**.

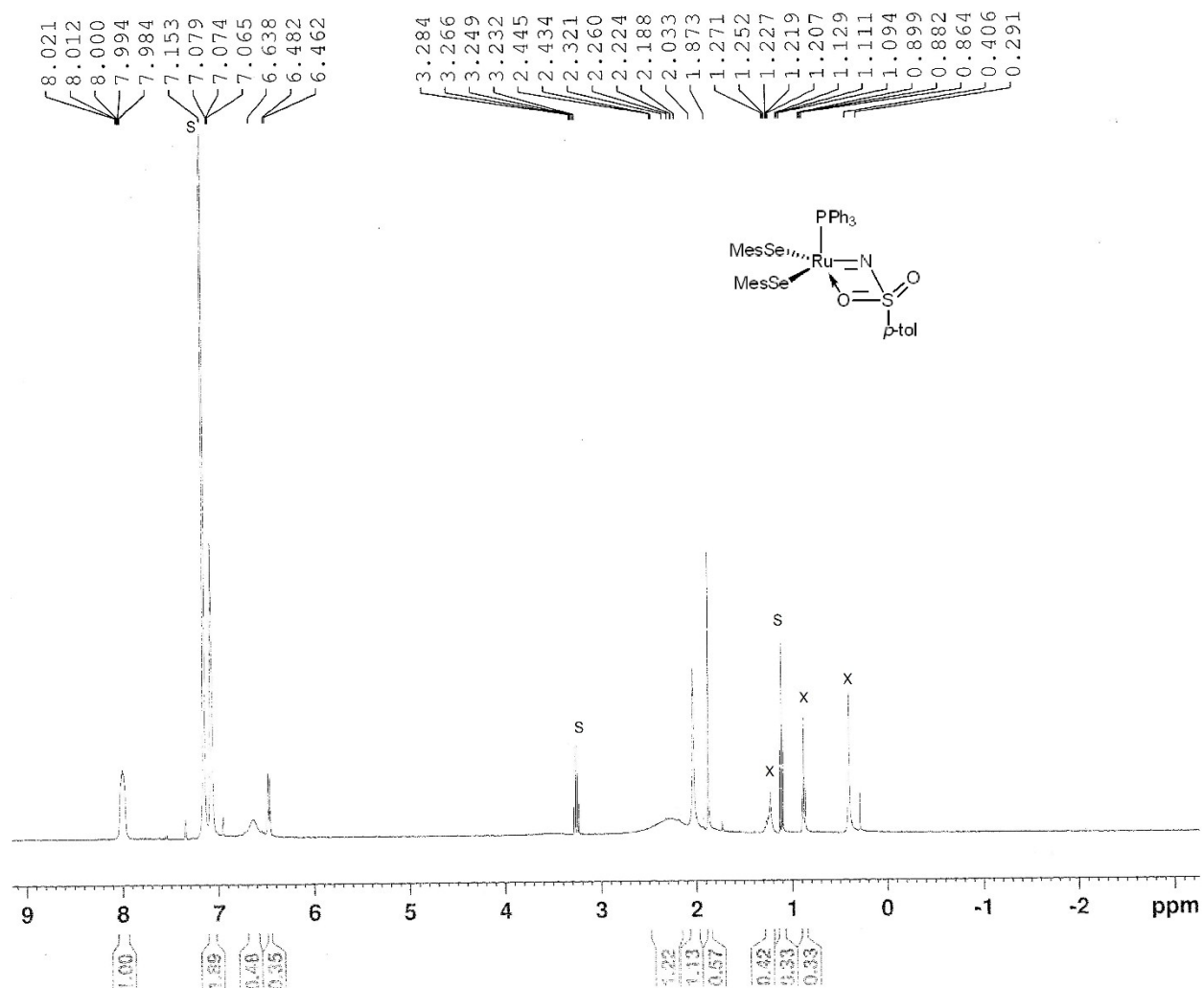


Figure S21. ^1H NMR (400 MHz, 298 K, C_6D_6) spectrum of **10** (X = impurity, S = residual solvent).

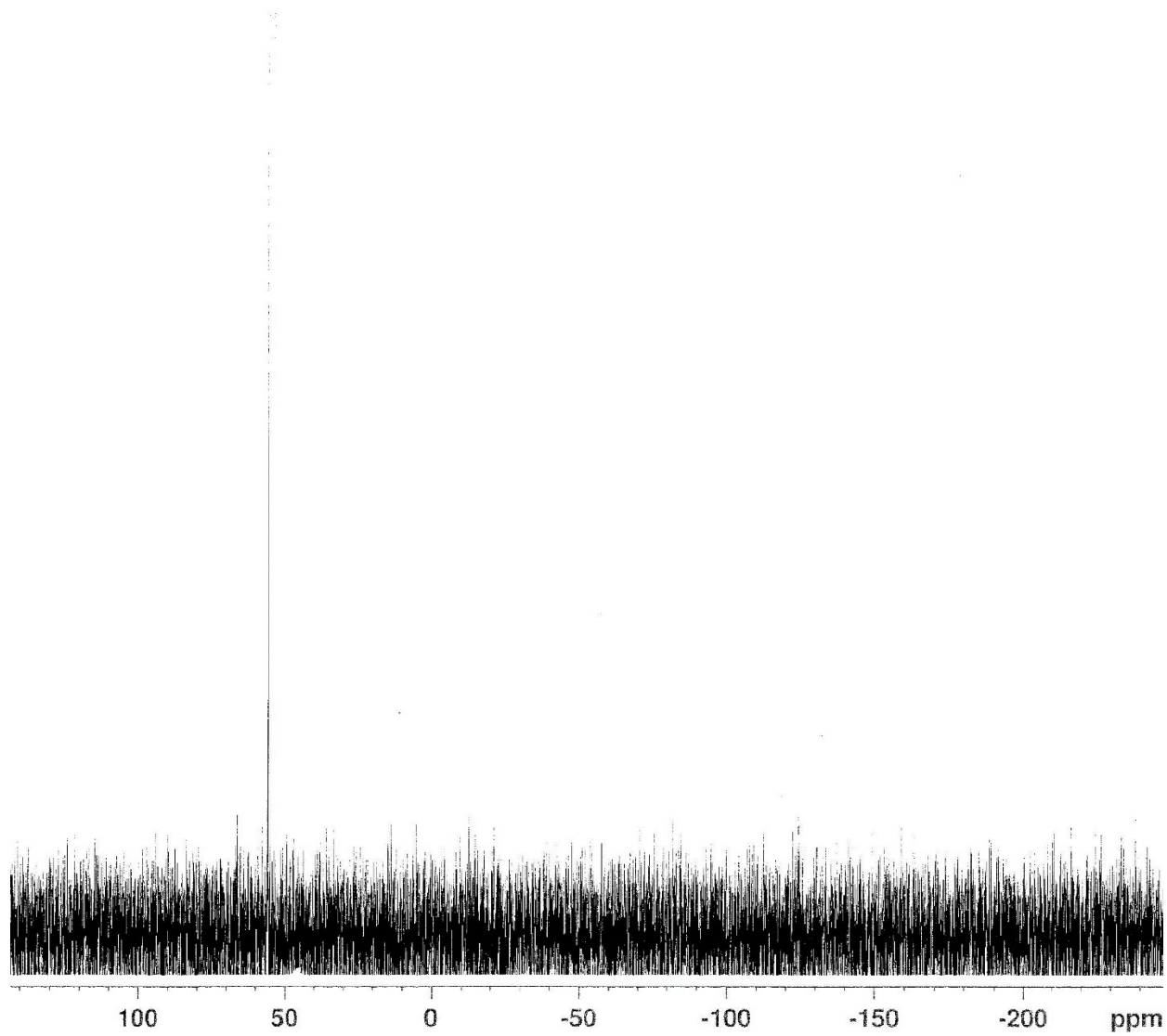


Figure S22. $^{31}\text{P}\{^1\text{H}\}$ NMR (162 MHz, 298 K, C_6D_6) spectrum of **10**.

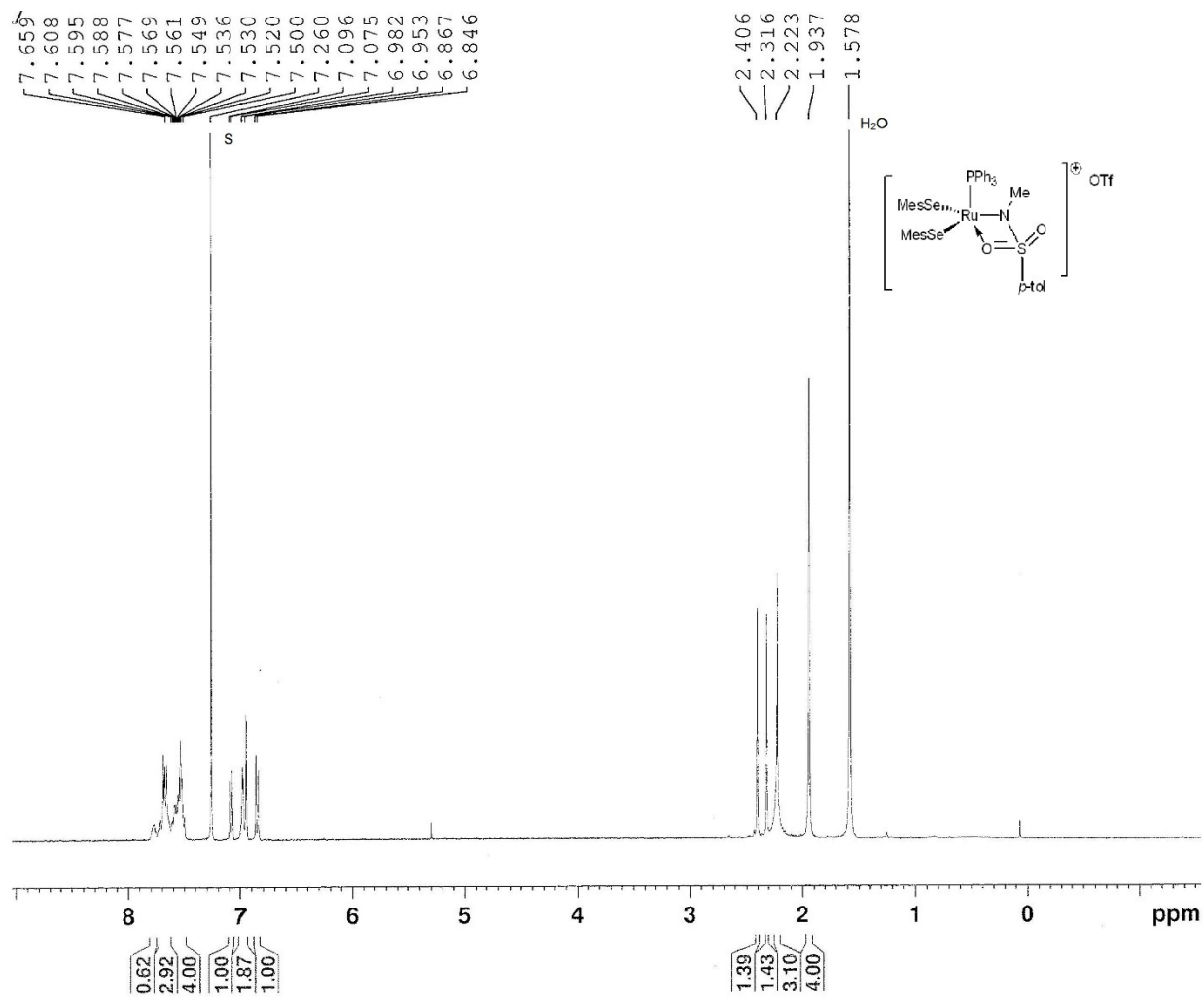


Figure S23. ^1H NMR (400 MHz, 298 K, CDCl_3) spectrum of **11** (X = impurity, S = residual solvent).

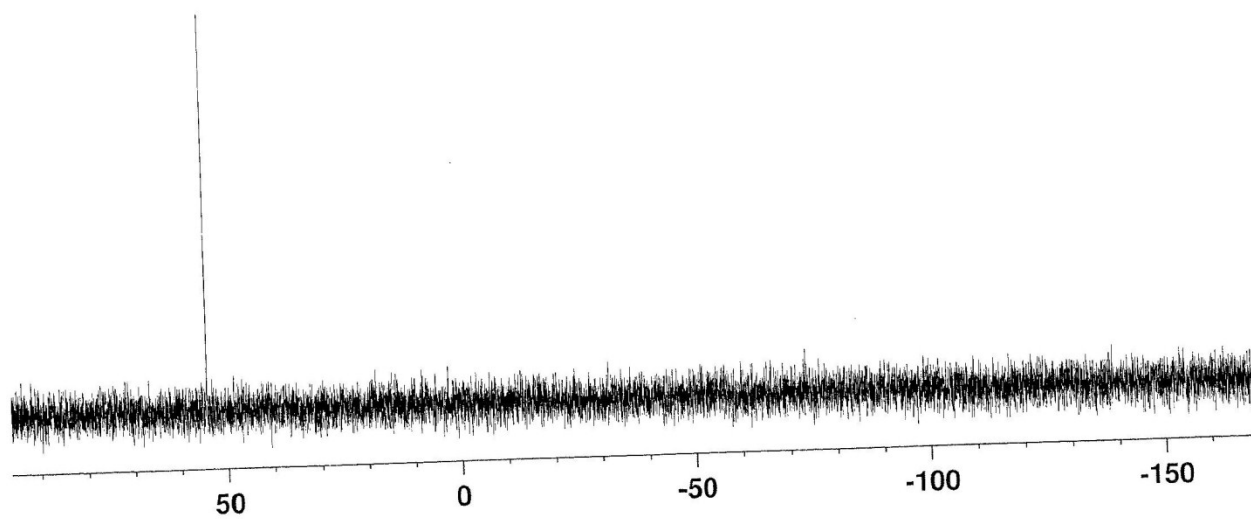


Figure S24. $^{31}\text{P}\{^1\text{H}\}$ NMR (162 MHz, 298 K, CDCl_3) spectrum of **11**.

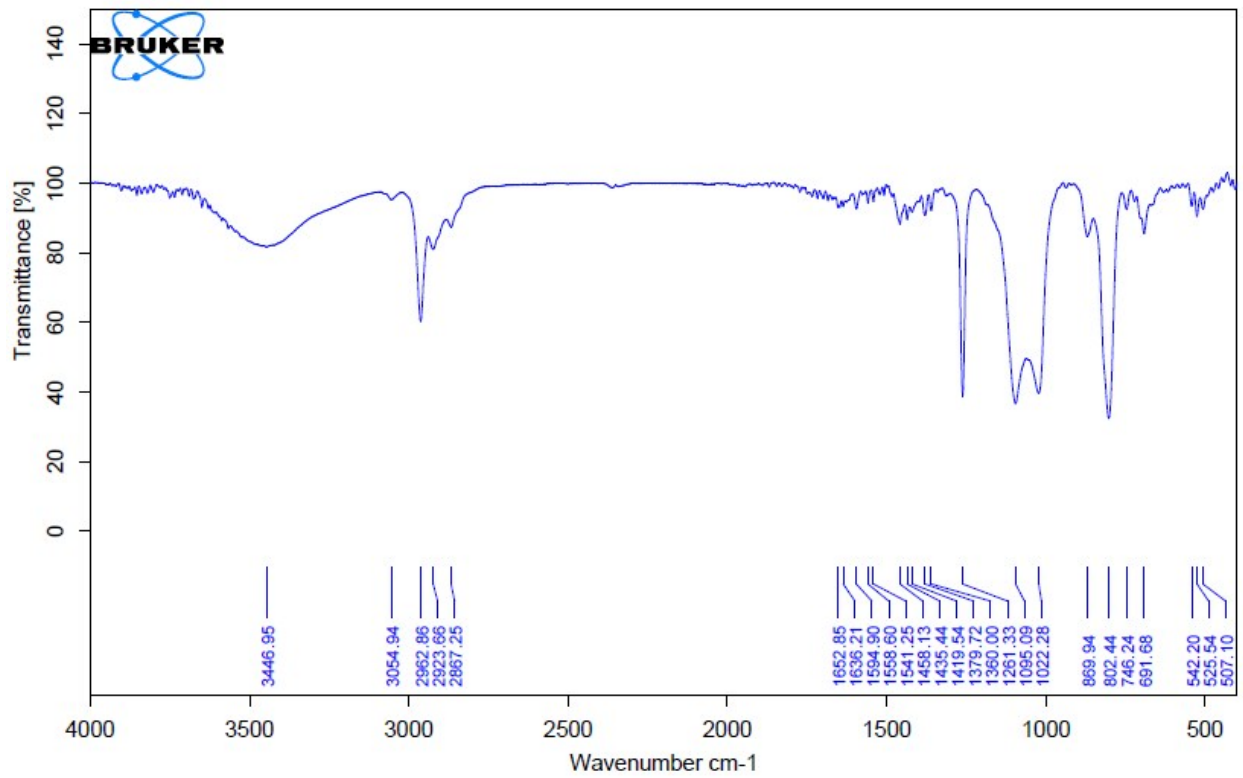


Figure S25. FT-IR spectrum of 4.

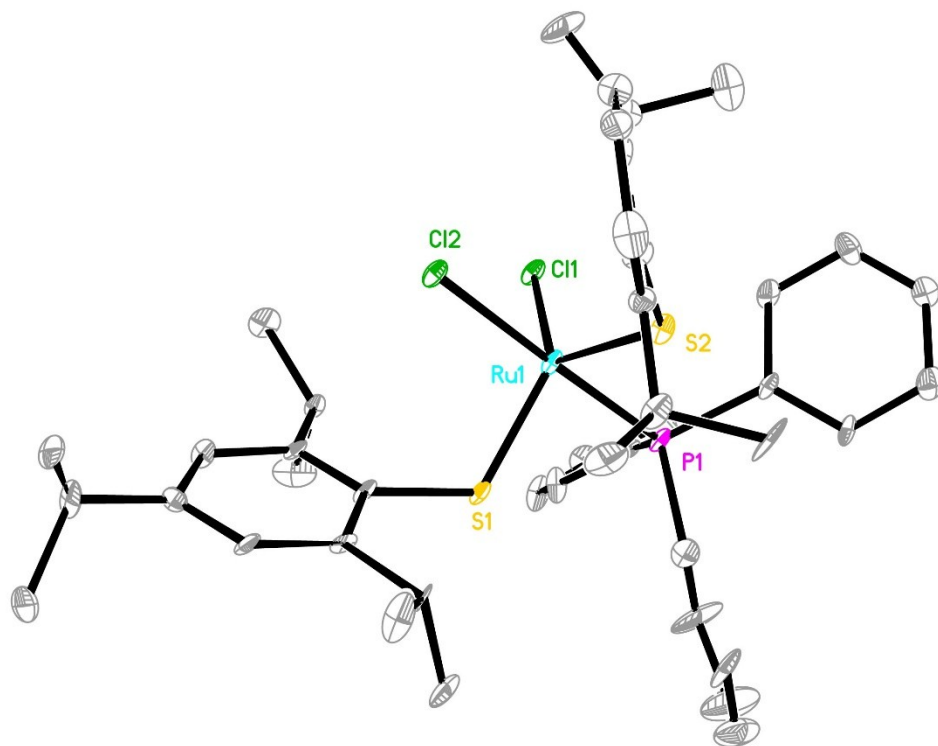


Figure S26. Preliminary crystal structure of [Ru^{IV}(STipp)₂Cl₂(PPh₃)] (**3**).

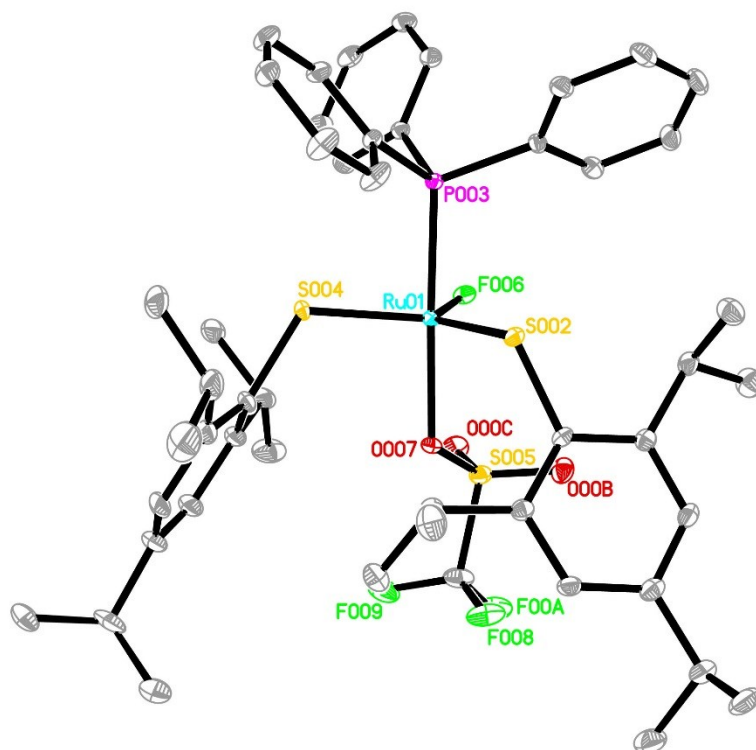


Figure S27. Preliminary crystal structure of [Ru^{IV}(STipp)₂(OH)(OTf)(PPh₃)] (5).

Table S1. Crystallographic data and experimental details for **2**, **4**, **6**, **8**, **9**, **10** and **11**.

	2	4	6	8	9 ·0.25C ₆ H ₁₄ ·0.5C ₄ H ₁₀ O	10 ·0.75C ₄ H ₈ O·0.25H ₂ O	11 ·1.5CH ₂ Cl ₂ ·0.25H ₂ O
Formula	C ₅₄ H ₅₂ P ₂ RuSe ₂	C ₄₈ H ₆₂ ClOPRuS ₂	C ₆₂ H ₇₅ N ₄ PRuS ₂	C ₅₅ H ₆₈ NO ₂ PRuS ₃	C _{65.5} H _{83.5} N ₄ O _{4.5} PRuS ₄	C ₄₆ H _{50.5} NO ₃ PRuS ₂ Se ₂	C ₄₅ H ₄₇ F ₃ NO ₅ PRuS ₂ Se ₂
Formula weight	1021.88	886.58	1072.42	1003.32	1259.17	987.39	1224.81
Crystal system	trigonal	triclinic	triclinic	monoclinic	monoclinic	triclinic	triclinic
Space group	P3 ₂	P-1	P-1	P2 ₁ /c	P2 ₁	P-1	P-1
<i>a</i> , Å	13.3542(4)	9.6919(3)	11.1803(5)	20.8430(4)	11.57442(18)	9.9055(3)	12.4019(5)
<i>b</i> , Å	13.3545(4)	14.1709(4)	14.8921(6)	13.9235(2)	42.0951(6)	14.8954(7)	20.0163(8)
<i>c</i> , Å	22.3819(6)	17.7259(6)	17.3032(7)	18.7630(4)	13.6150(3)	15.8159(7)	20.6971(8)
<i>α</i> , deg	90	78.473(3)	96.126(3)	90	90	70.854(4)	76.926(3)
<i>β</i> , deg	90	82.579(3)	93.546(3)	107.128(2)	98.1209(18)	82.761(3)	88.118(3)
<i>γ</i> , deg	120	72.678(3)	100.986(4)	90	90	72.261(3)	89.849(3)
<i>V</i> , Å ³	3456.7(2)	2270.91(13)	2801.9(2)	5203.64(18)	6567.0(2)	2098.80(16)	5001.9(3)
<i>Z</i>	3	2	2	4	4	2	4
<i>ρ</i> _{calc} , g cm ⁻³	1.473	1.297	1.271	1.281	1.274	1.562	1.626
<i>T</i> , K	100.00(10)	220.00(10)	100.01(10)	100.00(10)	99.9(2)	100.01(10)	100.01(10)
<i>μ</i> , mm ⁻¹	2.025	4.775	3.543	4.156	0.439	6.156	7.239
<i>F</i> (000)	1554.0	932.0	1132.0	2112.0	2654.0	1001.0	2462.0
Total reflections	21193	12355	15645	28996	39783	11466	28086
Independent reflections	8726	7932	9872	9259	23188	7294	17772
<i>R</i> _{int}	0.0830	0.0171	0.0808	0.0679	0.0417	0.0231	0.0458
GoF ^a	1.003	1.002	1.001	1.001	1.001	1.000	0.961
<i>R</i> ₁ , ^b <i>wR</i> ₂ ^c [<i>I</i> > 2σ(<i>I</i>)]	0.0670, 0.1105	0.0252, 0.0625	0.0446, 0.1067	0.0491, 0.1031	0.0472, 0.0974	0.0367, 0.0947	0.0449, 0.0952
<i>R</i> ₁ , <i>wR</i> ₂ (all data)	0.1245, 0.1284	0.0269, 0.0637	0.0552, 0.1133	0.0715, 0.1113	0.0557, 0.1023	0.0391, 0.0967	0.0750, 0.1070

$$^a \text{GoF} = [\sum w(|F_o| - |F_c|)^2 / (N_{\text{obs}} - N_{\text{param}})]^{1/2}. \quad ^b R_1 = \sum ||F_o| - |F_c|| / \sum |F_o|. \quad ^c wR_2 = [(\sum w|F_o| - |F_c|)^2 / \sum w^2 |F_o|]$$