

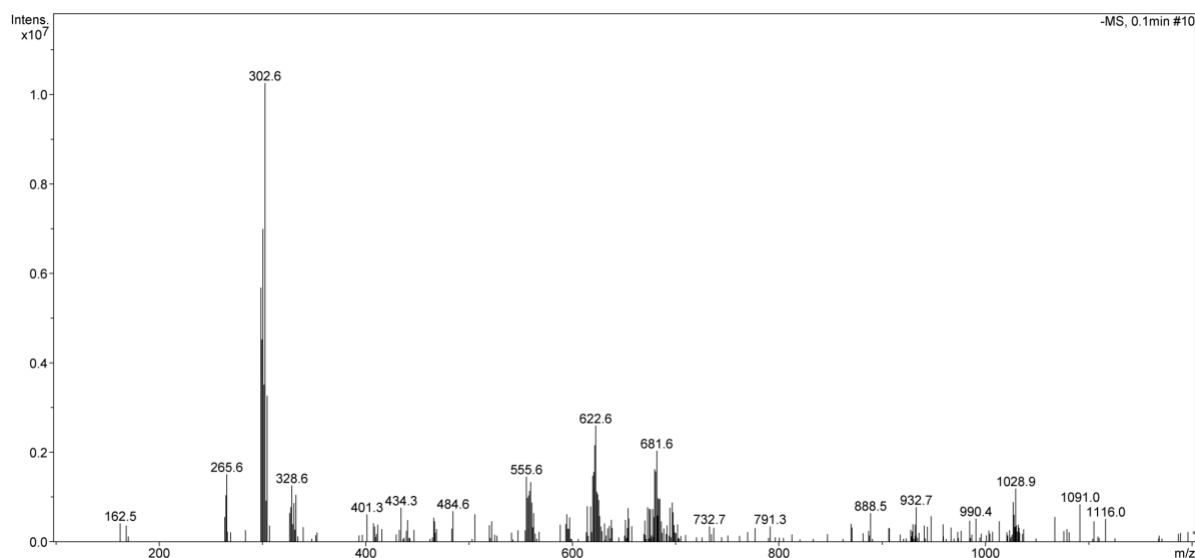
# Synthesis, crystal structure and anticancer activity of the complex [PtCl(C<sub>9</sub>H<sub>6</sub>NO)(C<sub>2</sub>H<sub>4</sub>)] by experimental and theoretical methods

Nguyen Thi Thanh Chi,<sup>a</sup> Ngo Tuan Cuong,<sup>a</sup> Tran Thu Trang,<sup>a</sup> Pham Van Thong,<sup>ab</sup> Nguyen Thi Bang Linh,<sup>a</sup> Nguyen Thi Khanh Ly<sup>a</sup> and Luc Van Meervelt<sup>c\*</sup>

<sup>a</sup>Department of Chemistry, Hanoi National University of Education, 136 Xuan Thuy, Cau Giay, Hanoi, Vietnam, <sup>b</sup>R&D Center, Vietnam Education and Technology Transfer JSC, Hanoi, Vietnam, and <sup>c</sup>Department of Chemistry, KU Leuven, Biomolecular Architecture, Celestijnenlaan 200F, Leuven (Heverlee), B-3001, Belgium

## Supporting Information

### I. Experimental ESI-MS, IR, <sup>1</sup>H-NMR and NOESY NMR spectrum of complex [PtCl(C<sub>9</sub>H<sub>6</sub>NO)(C<sub>2</sub>H<sub>4</sub>)].



**Fig. S1.** Negative-mode ESI-MS spectrum of complex [PtCl(C<sub>9</sub>H<sub>6</sub>NO)(C<sub>2</sub>H<sub>4</sub>)].

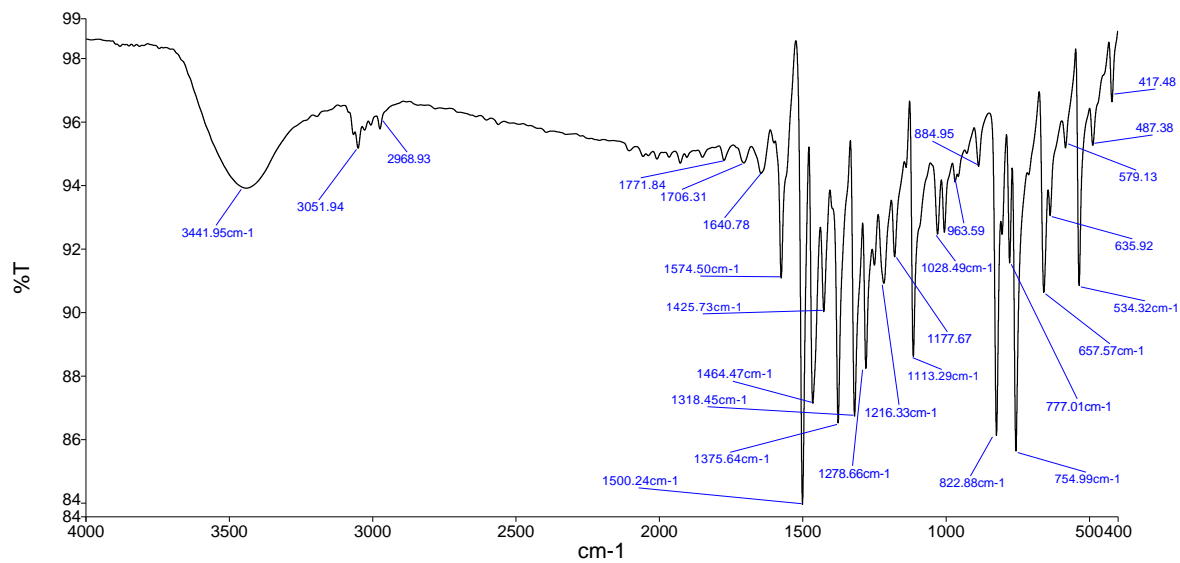


Fig. S2. IR spectrum of complex  $[\text{PtCl}(\text{C}_9\text{H}_6\text{NO})(\text{C}_2\text{H}_4)]$ .

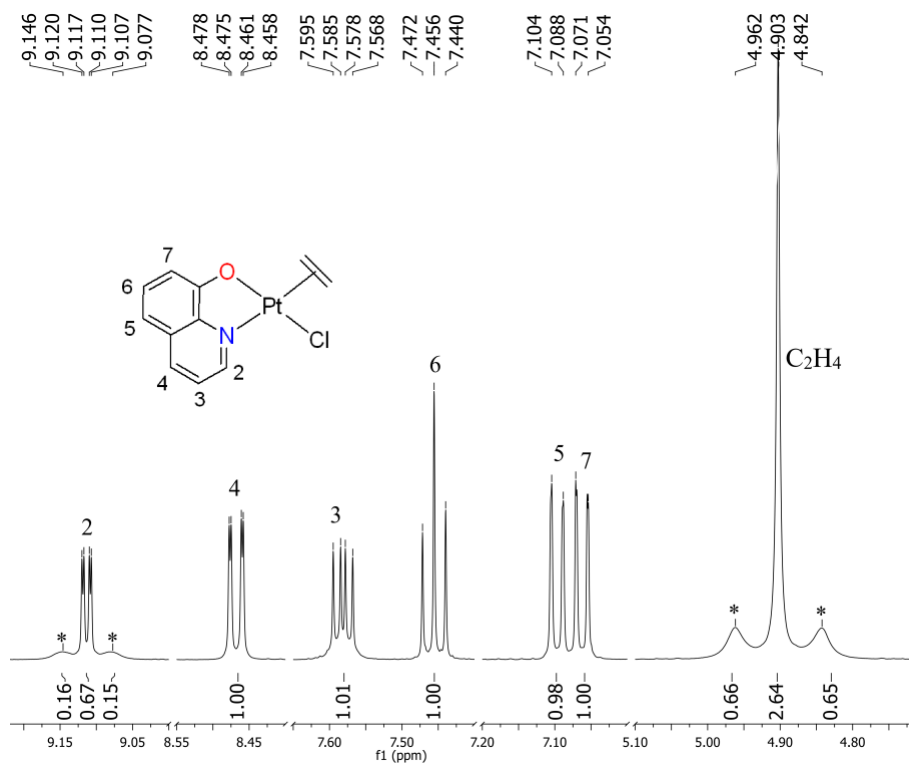


Fig. S3.  $^1\text{H}$  NMR spectrum of complex  $[\text{PtCl}(\text{C}_9\text{H}_6\text{NO})(\text{C}_2\text{H}_4)]$ .

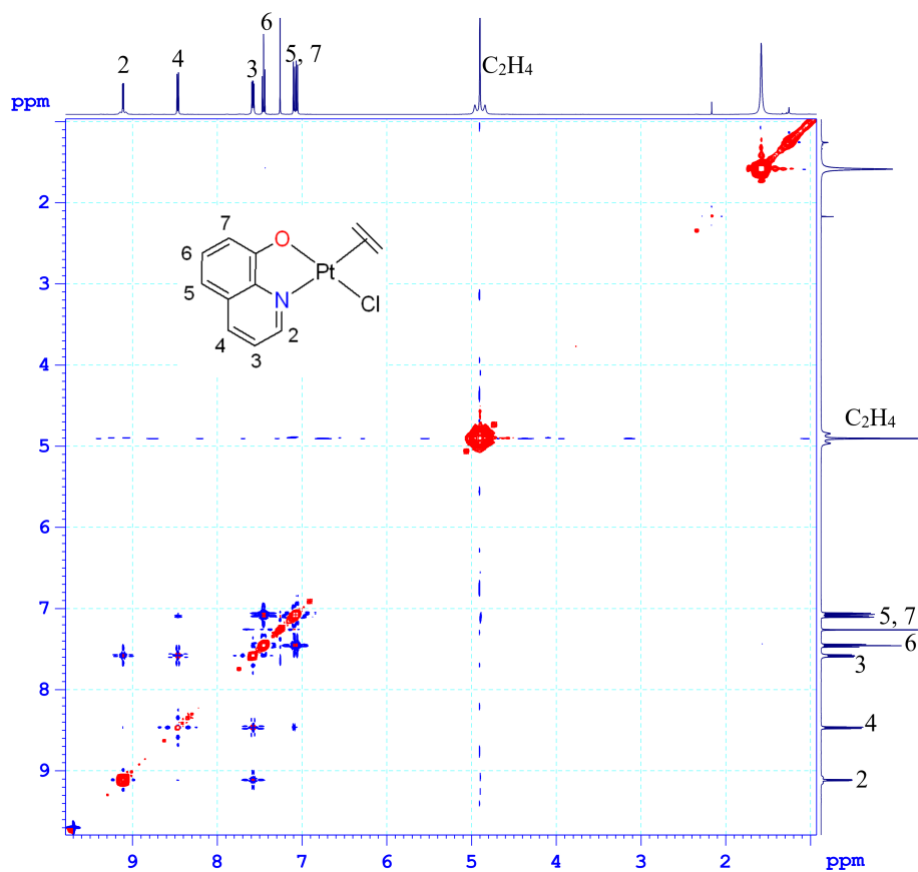


Fig. S4. NOESY NMR spectrum of complex  $[\text{PtCl}(\text{C}_9\text{H}_6\text{NO})(\text{C}_2\text{H}_4)]$ .

## II. DFT calculation results.

### II.1. The structure of complex (I)

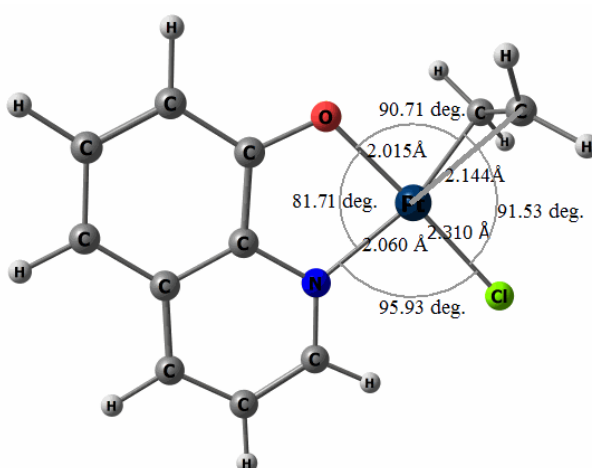


Fig. S5. The structure of complex (I) which is optimized using the CAM-B3LYP/6-311+G(d)/Aug-cc-pVDZ-PP combination of functional and basis set.

Table S1. Selected bond lengths (Å) and angles (°) for complex (I) determined by DFT and XRD (C<sub>g</sub> is the centroid of C=C olefin).

Complexes	Pt–N	Pt–Cl	Pt–O	Pt–C <sub>g</sub>	C=C <sub>olefinic</sub>	N–Pt–O	N–Pt–Cl	O–Pt–Cl
XRD	2.041(5)	2.2951(18)	2.004(4)	2.033(6)	1.379(10)	82.32(19)	95.90(15)	178.18(72)
DFT	2.060	2.310	2.015	2.029	1.386	81.71	95.93	177.64

## II.2. The DFT calculation results on energetics of the investigated reactions

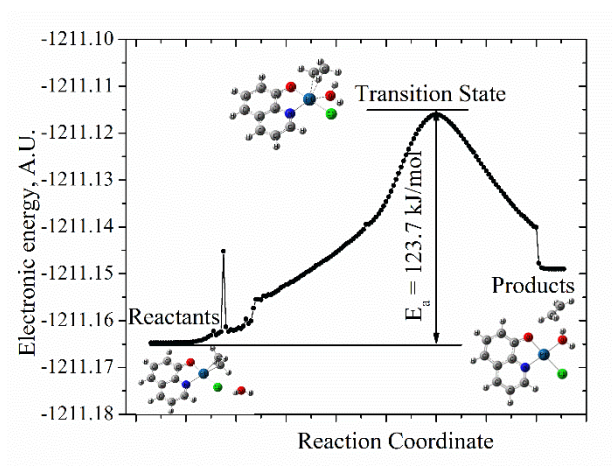


Figure S6. The reactants, transition state, products and activation energy  $E_a$  for the reaction step (2a).

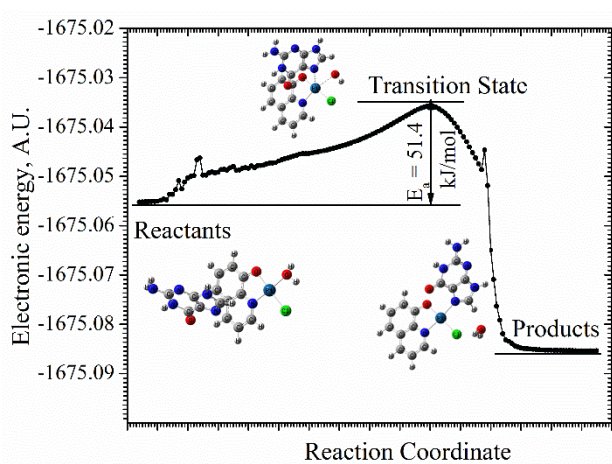
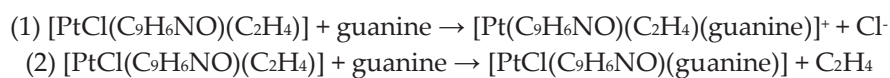


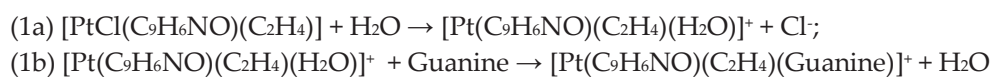
Figure S7. The reactants, transition state, products and activation energy  $E_a$  for the reaction step (2b).

Table S2. Calculated enthalpy change and free Gibbs energy for reaction pathways (1) and (2).

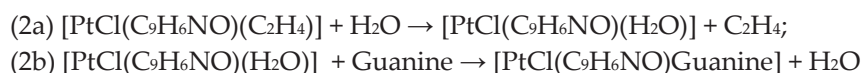


	Reaction (1)	Reaction (2)
$\Delta H^0_{298}$ , kJ/mol	377.6	-10.8
$\Delta G^0_{298}$ , kJ/mol	392.7	-8.9

Table S3. Calculated enthalpy change and free Gibbs energy for reaction steps (1a), (1b), (2a) and (2b).



and



Reaction steps	Step (1a)	Step (1b)	Step (2a)	Step (2b)
$\Delta H^0_{298}$ , kJ/mol	503.0	-125.4	40.7	-51.5
$\Delta G^0_{298}$ , kJ/mol	511.6	-118.9	36.2	-45.1

### II.3. Cartesian Coordinates of the complex compound in the reaction steps (2a,b)

#### Reactants $[\text{PtCl}(\text{C}_9\text{H}_6\text{NO})(\text{C}_2\text{H}_4)] + \text{H}_2\text{O}$ of step (2a)

Pt	0.800988000000	-0.239146000000	-0.192974000000
Cl	2.247858000000	1.561338000000	-0.449779000000
C	2.350837000000	-1.612843000000	0.426811000000
H	1.826630000000	-2.376074000000	0.991082000000
H	3.122632000000	-1.061386000000	0.953472000000
C	2.274011000000	-1.608252000000	-0.955258000000
H	2.986330000000	-1.042853000000	-1.544110000000
H	1.714631000000	-2.374803000000	-1.479703000000
C	-2.010569000000	0.108386000000	0.085658000000
C	-1.038618000000	2.217294000000	-0.096674000000
C	-1.769540000000	-1.293280000000	0.114676000000
C	-3.308897000000	0.646476000000	0.200280000000
C	-2.297754000000	2.829701000000	0.010866000000
H	-0.126733000000	2.788673000000	-0.214333000000
C	-2.862603000000	-2.126883000000	0.261372000000
C	-4.396684000000	-0.240129000000	0.348288000000
C	-3.416373000000	2.054919000000	0.157342000000

H	-2.360876000000	3.909736000000	-0.024021000000
C	-4.156808000000	-1.592130000000	0.375798000000
H	-2.702078000000	-3.197961000000	0.286956000000
H	-5.402345000000	0.153157000000	0.438414000000
H	-4.395864000000	2.513990000000	0.242106000000
H	-4.989720000000	-2.277394000000	0.489972000000
N	-0.907009000000	0.908058000000	-0.059893000000
O	-0.529746000000	-1.729657000000	0.001697000000
O	4.362676000000	0.536801000000	1.797744000000
H	5.272363000000	0.845718000000	1.789102000000
H	3.847982000000	1.116686000000	1.218079000000

**Transition state of the step (2a)**

Pt	-0.918900000000	-0.067516000000	-0.131295000000
Cl	-2.324151000000	1.792075000000	-0.092424000000
C	-2.646385000000	-1.552779000000	1.354306000000
H	-2.443450000000	-2.551254000000	0.982008000000
H	-3.608160000000	-1.109739000000	1.121443000000
C	-1.775923000000	-0.924608000000	2.154685000000
H	-2.008205000000	0.036455000000	2.597015000000
H	-0.851736000000	-1.398128000000	2.463362000000
C	1.894157000000	0.024455000000	-0.024456000000
C	1.051449000000	2.189342000000	0.139522000000
C	1.555803000000	-1.349677000000	-0.154015000000
C	3.229080000000	0.466743000000	0.060694000000
C	2.356544000000	2.705626000000	0.233250000000
H	0.176729000000	2.825287000000	0.160291000000
C	2.594210000000	-2.263678000000	-0.199473000000
C	4.257316000000	-0.497787000000	0.010213000000
C	3.430233000000	1.861096000000	0.193534000000
H	2.485429000000	3.775928000000	0.333420000000
C	3.925603000000	-1.825758000000	-0.117921000000
H	2.361469000000	-3.316863000000	-0.301082000000
H	5.292297000000	-0.182727000000	0.072404000000
H	4.441107000000	2.248638000000	0.262882000000
H	4.716031000000	-2.567649000000	-0.158136000000
N	0.834637000000	0.897037000000	0.015162000000
O	0.281995000000	-1.675645000000	-0.219000000000
O	-2.559592000000	-0.881521000000	-1.612673000000
H	-3.082258000000	-1.662063000000	-1.406059000000
H	-3.148702000000	-0.116727000000	-1.670149000000

**Products [PtCl(C<sub>9</sub>H<sub>6</sub>NO)(H<sub>2</sub>O)]<sup>0</sup> + C<sub>2</sub>H<sub>4</sub> of step (2a)**

Pt	0.810738000000	-0.433660000000	-0.162481000000
Cl	1.665442000000	-2.568180000000	0.120004000000
C	3.705596000000	3.083363000000	0.383478000000
H	3.470612000000	3.311825000000	-0.651411000000
H	4.747724000000	3.167460000000	0.674880000000
C	2.757817000000	2.747205000000	1.251279000000
H	2.992389000000	2.537433000000	2.290217000000
H	1.716627000000	2.668094000000	0.953823000000
C	-1.888030000000	0.302227000000	-0.000458000000
C	-1.672797000000	-1.992887000000	0.339952000000
C	-1.186696000000	1.510775000000	-0.261648000000
C	-3.288289000000	0.258684000000	0.144584000000
C	-3.064177000000	-2.115045000000	0.495504000000
H	-1.006577000000	-2.841856000000	0.408658000000
C	-1.933093000000	2.670545000000	-0.371181000000
C	-4.010869000000	1.464973000000	0.026573000000
C	-3.861604000000	-1.008549000000	0.400057000000
H	-3.481177000000	-3.094897000000	0.689821000000
C	-3.329706000000	2.631491000000	-0.225723000000
H	-1.424073000000	3.605288000000	-0.574000000000
H	-5.089115000000	1.457787000000	0.133873000000
H	-4.936811000000	-1.091585000000	0.518337000000
H	-3.883994000000	3.559325000000	-0.318253000000
N	-1.111312000000	-0.825468000000	0.101215000000
O	0.123170000000	1.455658000000	-0.380454000000
O	2.792321000000	0.098680000000	-0.496113000000
H	3.083682000000	0.893963000000	-0.015324000000
H	3.346960000000	-0.661398000000	-0.267648000000

**Reactants [PtCl(C<sub>9</sub>H<sub>6</sub>NO)(H<sub>2</sub>O)] + Guanine of step (2b)**

C	-1.507136000000	0.528875000000	-0.402798000000
C	-1.814430000000	-0.677081000000	1.567512000000
C	-1.430037000000	0.443888000000	-1.819070000000
C	-1.386572000000	1.746881000000	0.287779000000
C	-1.720540000000	0.502021000000	2.320983000000
H	-1.976038000000	-1.644073000000	2.023234000000
C	-1.223091000000	1.616453000000	-2.520237000000
C	-1.170425000000	2.922485000000	-0.464965000000
C	-1.503823000000	1.698327000000	1.696224000000
H	-1.799428000000	0.438812000000	3.398291000000
C	-1.094656000000	2.837642000000	-1.833530000000
H	-1.162738000000	1.578898000000	-3.601211000000
H	-1.063315000000	3.869780000000	0.049438000000

H	-1.389952000000	2.609313000000	2.268781000000
H	-0.933208000000	3.740294000000	-2.413808000000
N	-1.711137000000	-0.659030000000	0.254468000000
O	-1.560367000000	-0.745156000000	-2.376581000000
C	2.350190000000	1.498385000000	1.097614000000
C	2.324576000000	-0.553235000000	0.556897000000
C	3.478302000000	1.302672000000	0.321097000000
C	2.071872000000	2.818851000000	1.582922000000
H	2.064241000000	-1.594000000000	0.434391000000
H	4.130903000000	-0.487706000000	-0.597245000000
C	4.179459000000	3.398209000000	0.393879000000
H	3.006125000000	4.644214000000	1.548051000000
N	1.643205000000	0.322930000000	1.227974000000
N	3.455841000000	-0.016783000000	-0.016468000000
N	4.413094000000	2.205615000000	-0.061899000000
N	3.094190000000	3.713725000000	1.163212000000
N	5.072688000000	4.412651000000	0.151935000000
H	5.777426000000	4.167853000000	-0.526960000000
H	4.706356000000	5.345406000000	0.039318000000
O	1.156230000000	3.242209000000	2.256176000000
Pt	-1.859565000000	-2.178509000000	-0.999419000000
Cl	-2.234935000000	-3.910851000000	0.502642000000
H	-2.353143000000	-4.475598000000	-1.954973000000
H	-2.608758000000	-3.461428000000	-3.147911000000
O	-2.011604000000	-3.700868000000	-2.430050000000

#### Transition state of step (2b)

C	-2.305544000000	1.156592000000	-0.228255000000
C	-2.684930000000	0.001930000000	1.757002000000
C	-1.566745000000	1.168517000000	-1.442243000000
C	-3.216084000000	2.175131000000	0.110873000000
C	-3.603284000000	0.984683000000	2.167065000000
H	-2.451825000000	-0.859856000000	2.366519000000
C	-1.782163000000	2.224675000000	-2.312434000000
C	-3.404489000000	3.234337000000	-0.802920000000
C	-3.870656000000	2.053647000000	1.359150000000
H	-4.087719000000	0.871008000000	3.128767000000
C	-2.695564000000	3.237782000000	-1.981006000000
H	-1.233054000000	2.255157000000	-3.246065000000
H	-4.101172000000	4.029987000000	-0.565728000000
H	-4.579329000000	2.815851000000	1.665678000000
H	-2.841375000000	4.051579000000	-2.683943000000



N	-2.065264000000	0.086667000000	0.598276000000
O	-0.727860000000	0.184114000000	-1.665252000000
C	2.519181000000	0.108283000000	0.087502000000
C	2.689558000000	-1.722750000000	-0.989178000000
C	3.839715000000	0.025897000000	-0.306372000000
C	2.090753000000	1.255906000000	0.836686000000
H	2.468522000000	-2.658736000000	-1.475366000000
H	4.774837000000	-1.511889000000	-1.419473000000
C	4.472993000000	1.946166000000	0.589329000000
H	2.977464000000	2.931758000000	1.618821000000
N	1.823231000000	-0.996929000000	-0.349817000000
N	3.937521000000	-1.149866000000	-0.992272000000
N	4.846405000000	0.906563000000	-0.096569000000
N	3.196444000000	2.134728000000	1.036980000000
N	5.392837000000	2.899569000000	0.933749000000
H	6.281670000000	2.800255000000	0.469305000000
H	5.083136000000	3.850345000000	1.054793000000
O	1.010917000000	1.551545000000	1.289925000000
Pt	-0.703415000000	-1.138089000000	-0.146785000000
Cl	-0.735988000000	-2.755886000000	1.539283000000
H	-0.129991000000	-3.644319000000	-0.638614000000
H	-0.571976000000	-3.158224000000	-2.054597000000
O	0.088728000000	-3.038388000000	-1.364963000000

**Products [PtCl(C<sub>9</sub>H<sub>6</sub>NO)Guanine]<sup>0</sup> + H<sub>2</sub>O of step (2b)**

C	2.791319000000	0.905233000000	0.155951000000
C	3.246685000000	-1.061780000000	-0.999854000000
C	1.781210000000	1.672269000000	0.805129000000
C	4.126439000000	1.347819000000	0.061203000000
C	4.595615000000	-0.690094000000	-1.136990000000
H	2.860573000000	-1.989649000000	-1.400346000000
C	2.159763000000	2.886802000000	1.354576000000
C	4.466516000000	2.591112000000	0.634831000000
C	5.030776000000	0.495681000000	-0.614046000000
H	5.269894000000	-1.355982000000	-1.660630000000
C	3.489058000000	3.326716000000	1.262316000000
H	1.409614000000	3.489519000000	1.852405000000
H	5.487010000000	2.950633000000	0.572975000000
H	6.069050000000	0.795005000000	-0.713232000000
H	3.747554000000	4.283899000000	1.703143000000
N	2.381933000000	-0.291550000000	-0.374708000000
O	0.561697000000	1.194345000000	0.853058000000
C	-2.536057000000	0.253516000000	-0.033347000000
C	-2.161466000000	-1.537491000000	1.120154000000

C	-3.734436000000	-0.097666000000	0.545674000000
C	-2.492994000000	1.379044000000	-0.926717000000
H	-1.685788000000	-2.402106000000	1.568340000000
H	-4.152644000000	-1.752249000000	1.803116000000
C	-4.907193000000	1.560784000000	-0.330371000000
H	-3.838735000000	2.750154000000	-1.638819000000
N	-1.569509000000	-0.662654000000	0.344941000000
N	-3.477673000000	-1.228605000000	1.268915000000
N	-4.932894000000	0.518561000000	0.449171000000
N	-3.783176000000	1.986554000000	-0.978556000000
N	-6.056532000000	2.257997000000	-0.565529000000
H	-6.831481000000	2.003799000000	0.025968000000
H	-6.001942000000	3.233001000000	-0.810475000000
O	-1.597805000000	1.824690000000	-1.597088000000
Pt	0.412261000000	-0.590413000000	-0.070592000000
Cl	0.308062000000	-2.684497000000	-1.098683000000
H	-0.175294000000	-3.879233000000	0.799179000000
H	0.162602000000	-4.289887000000	2.263164000000
O	-0.561427000000	-4.069289000000	1.671323000000