**X-ray analyses**

### **Experimental**

Single-crystal X-ray diffraction data were collected at 183(1) K on a Rigaku OD Xcalibur / Ruby diffractometerusing a single wavelength X-ray source (Mo Ka radiation: l = 0.71073 Å) from a micro-focus sealed X-ray tube and an Oxford liquid-nitrogen Cryostream cooler. The selected suitable single crystals were mounted using polybutene oil on a flexible loop fixed on a goniometer head and immediately transferred to the diffractometer. Pre-experiment, data collection, data reduction and analytical absorption correction1 were performed with the program suite *CrysAlisPro*.2 Using *Olex2*,3 the structures were solved with the SHELXT4 small molecule structure solution program and refined with the *SHELXL2018/3* program package5 by full-matrix least-squares minimization on F2. *PLATON*6 was used to check the result of the X-ray analyses. CCDC 2115019 (**4**) and 2115020 (**3**) contain the supplementary crystallographic data for these compounds, and can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data\_request/cif.

**References**

1. Clark, R. C.; Reid, J. S. *Acta Cryst. A* **1995**, 51, 887.
2. *CrysAlisPro* (version 1.171.41.113a), Rigaku Oxford Diffraction Ltd, Yarnton, Oxfordshire, England, **2019**.
3. “*A complete structure solution, refinement and analysis program*” - Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H. *J. Appl. Cryst.* **2009**, 42, 339.
4. “*SHELXT - Integrated space-group and crystal-structure determination*” - Sheldrick, G. M. *Acta Cryst. A* **2015**, 71, 3.
5. “*Crystal structure refinement with SHELXL*” - Sheldrick, G. M. *Acta Cryst. C* **2015**, 71, 3.
6. “*Structure validation in chemical crystallography*” - Spek, A. L. *Acta Cryst. D* **2009**, *65*, 148.

|  |  |
| --- | --- |
| **Table S1. Crystal data and structure refinement for 3.** | |
| CCDC number | 2115020 |
| Empirical formula | C57H54Cl6N4O6P2Re2 |
| Formula weight | 1538.08 |
| Temperature/K | 183(1) |
| Crystal system | monoclinic |
| Space group | P21/c |
| a/Å | 11.0987(2) |
| b/Å | 9.01830(10) |
| c/Å | 30.4320(5) |
| α/° | 90 |
| β/° | 97.8700(10) |
| γ/° | 90 |
| Volume/Å3 | 3017.29(8) |
| Z | 2 |
| ρcalcg/cm3 | 1.693 |
| μ/mm‑1 | 4.378 |
| F(000) | 1508.0 |
| Crystal size/mm3 | 0.18 × 0.16 × 0.02 |
| Radiation | Mo Kα (λ = 0.71073) |
| 2Θ range for data collection/° | 5.264 to 56.564 |
| Index ranges | -14 ≤ h ≤ 14, -12 ≤ k ≤ 12, -40 ≤ l ≤ 40 |
| Reflections collected | 42433 |
| Independent reflections | 7462 [Rint = 0.0483, Rsigma = 0.0378] |
| Data/restraints/parameters | 7462/453/411 |
| Goodness-of-fit on F2 | 1.029 |
| Final R indexes [I>=2σ (I)] | R1 = 0.0311, wR2 = 0.0565 |
| Final R indexes [all data] | R1 = 0.0469, wR2 = 0.0616 |
| Largest diff. peak/hole / e Å-3 | 1.25/-0.66 |

|  |  |
| --- | --- |
| **Table S2. Crystal data and structure refinement for 4.** | |
| CCDC number | 2115019 |
| Empirical formula | C83H90Cl6N8O8P2Re2 |
| Formula weight | 1974.66 |
| Temperature/K | 183(1) |
| Crystal system | monoclinic |
| Space group | P21/c |
| a/Å | 14.0861(4) |
| b/Å | 12.5731(3) |
| c/Å | 26.9707(6) |
| α/° | 90 |
| β/° | 101.918(3) |
| γ/° | 90 |
| Volume/Å3 | 4673.7(2) |
| Z | 2 |
| ρcalcg/cm3 | 1.403 |
| μ/mm‑1 | 2.846 |
| F(000) | 1980.0 |
| Crystal size/mm3 | 0.37 × 0.26 × 0.03 |
| Radiation | Mo Kα (λ = 0.71073) |
| 2Θ range for data collection/° | 4.952 to 52.744 |
| Index ranges | -13 ≤ h ≤ 17, -15 ≤ k ≤ 15, -33 ≤ l ≤ 33 |
| Reflections collected | 36305 |
| Independent reflections | 9589 [Rint = 0.0471, Rsigma = 0.0482] |
| Data/restraints/parameters | 9589/106/550 |
| Goodness-of-fit on F2 | 1.122 |
| Final R indexes [I>=2σ (I)] | R1 = 0.0633, wR2 = 0.1541 |
| Final R indexes [all data] | R1 = 0.0807, wR2 = 0.1673 |
| Largest diff. peak/hole / e Å-3 | 2.68/-1.45 |

**Cartesian coordinates and energies**

**B1**

Re 1.99299300 -0.05394000 0.22920800

Cl 2.04435100 2.16179600 1.17963000

Cl 1.47581700 0.87490300 -1.93775000

Cl 4.31784600 0.16107900 -0.27897800

O 1.85277900 -2.81195500 -0.90943800

N 1.89654300 -1.72866100 -0.48650000

P -1.53798800 0.01346800 0.05043200

C -2.67364800 -0.16085200 1.46622300

C -2.13871200 -0.30747100 2.75411800

C -4.06674600 -0.12594000 1.29067000

C -2.99164400 -0.42732100 3.85523300

H -1.06221200 -0.31501300 2.88818800

C -4.91378200 -0.24828500 2.39263500

H -4.49526500 0.00086400 0.30011500

C -4.37674300 -0.40008400 3.67612800

H -2.57087400 -0.53664000 4.85106500

H -5.99071100 -0.21985800 2.25053600

H -5.03830100 -0.49106800 4.53358500

C -1.97274700 1.53967500 -0.82695100

C -3.01882000 1.57532900 -1.76404100

C -1.28524500 2.71799900 -0.49605700

C -3.37777800 2.78533400 -2.36102400

H -3.54235400 0.66534500 -2.04459700

C -1.65044100 3.92296500 -1.09909700

H -0.45562000 2.68918700 0.20373800

C -2.69503700 3.95932400 -2.02718400

H -4.18202700 2.80810400 -3.09154500

H -1.10589700 4.82972900 -0.85141600

H -2.97132500 4.89923500 -2.49791800

C -1.81336100 -1.40001700 -1.06288300

C -2.37391100 -2.59246200 -0.57266500

C -1.38291300 -1.33413200 -2.40060200

C -2.50850100 -3.70067400 -1.41160900

H -2.70766500 -2.65740600 0.45863300

C -1.52068700 -2.44584100 -3.23317900

H -0.92379600 -0.42785700 -2.78258500

C -2.08400100 -3.62769300 -2.74152800

H -2.94396100 -4.61840900 -1.02577000

H -1.18151100 -2.38854500 -4.26374200

H -2.18877300 -4.49133100 -3.39300100

O -0.11980900 0.05196700 0.65661500

N 2.29081800 -0.72458500 1.89743400

O 2.45030500 -1.17394400 2.95815500

Zero-point correction= 0.300743 (Hartree/Particle)

Thermal correction to Energy= 0.329379

Thermal correction to Enthalpy= 0.330323

Thermal correction to Gibbs Free Energy= 0.236178

Sum of electronic and zero-point Energies= -2830.206665

Sum of electronic and thermal Energies= -2830.178030

Sum of electronic and thermal Enthalpies= -2830.177086

Sum of electronic and thermal Free Energies= -2830.271231

**B2**

Re 2.01375500 -0.12092100 0.04718900

Cl 2.15745100 0.75305300 2.28477900

Cl 1.53656800 2.15919200 -0.70363800

Cl 2.08718000 -2.35130600 1.02611600

O 1.90879600 -1.21705500 -2.73023000

N 1.91188700 -0.78950800 -1.64791500

P -1.53103500 -0.01621200 0.03724500

C -2.49104300 -1.29346200 0.90323800

C -1.80984300 -2.39426700 1.44566300

C -3.88502400 -1.18897100 1.04363100

C -2.52875800 -3.38933100 2.11498700

H -0.72931700 -2.46227200 1.35634100

C -4.59429000 -2.18797000 1.71109000

H -4.41819200 -0.32982200 0.64505200

C -3.91607800 -3.28970000 2.24561300

H -1.99801200 -4.23770600 2.53811600

H -5.67210500 -2.10306200 1.82057200

H -4.47003200 -4.06425800 2.76966400

C -2.03666500 1.61498400 0.64470500

C -3.15329200 2.27954700 0.11083000

C -1.32063300 2.18503400 1.70923400

C -3.55636000 3.50398400 0.64722800

H -3.69741100 1.85795000 -0.73021300

C -1.72944300 3.41129500 2.23685300

H -0.43816400 1.69019000 2.10348100

C -2.84568600 4.06854100 1.71125900

H -4.41662400 4.01911200 0.22821700

H -1.16504000 3.85628700 3.05142400

H -3.15667400 5.02510200 2.12320700

C -1.90795200 -0.10447100 -1.73977600

C -2.58139900 -1.20896600 -2.28710500

C -1.44739500 0.92161400 -2.58596900

C -2.79944200 -1.28197100 -3.66528800

H -2.93412700 -2.00929800 -1.64386900

C -1.66708600 0.83981900 -3.96137400

H -0.90383100 1.76728900 -2.17415000

C -2.34450000 -0.25887500 -4.50151200

H -3.32144900 -2.13862000 -4.08282300

H -1.30502400 1.63247500 -4.61029000

H -2.51374100 -0.31847400 -5.57349400

O -0.05132700 -0.30668700 0.33980500

N 3.80437700 0.05592400 -0.10195400

O 4.95112500 0.19442400 -0.19622900

Zero-point correction= 0.300928 (Hartree/Particle)

Thermal correction to Energy= 0.329606

Thermal correction to Enthalpy= 0.330550

Thermal correction to Gibbs Free Energy= 0.236267

Sum of electronic and zero-point Energies= -2830.214464

Sum of electronic and thermal Energies= -2830.185787

Sum of electronic and thermal Enthalpies= -2830.184842

Sum of electronic and thermal Free Energies= -2830.279125

**D1**

Re 1.93044100 -0.04957700 0.02847200

Cl -0.03780100 -0.03240700 1.65244500

Cl 3.40455800 0.15532500 -1.81550200

Cl 1.82017500 2.32669800 0.16151700

O 3.98666100 -0.09519100 2.15939900

N 3.19162500 -0.08217900 1.32037900

N 1.87002800 -1.88732100 -0.05076100

O 1.81930600 -3.04069100 -0.04716500

Re -1.93045200 0.04959600 -0.02846900

N -3.19161300 0.08228000 -1.32039600

N -1.87004600 1.88734700 0.05066000

Cl -3.40457800 -0.15536700 1.81549300

Cl -1.82012100 -2.32666800 -0.16163500

O -3.98668100 0.09469900 -2.15939600

O -1.81924600 3.04071700 0.04750200

Cl 0.03779900 0.03250200 -1.65244400

Zero-point correction= 0.042501 (Hartree/Particle)

Thermal correction to Energy= 0.064203

Thermal correction to Enthalpy= 0.065147

Thermal correction to Gibbs Free Energy= -0.012643

Sum of electronic and zero-point Energies= -3437.799959

Sum of electronic and thermal Energies= -3437.778257

Sum of electronic and thermal Enthalpies= -3437.777313

Sum of electronic and thermal Free Energies= -3437.855103

**D2**

Re -1.95071000 0.03914600 -0.02684100

Cl 0.03689600 -0.05321000 -1.64209000

Cl -3.41905300 -0.07500900 1.82716100

Cl -1.93632600 -2.32262800 -0.12055700

O -3.99496200 0.10007800 -2.17029700

N -3.20867000 0.07986900 -1.32414100

N -1.84989500 1.87405000 0.01052900

O -1.77586600 3.03175600 -0.02590000

Re 1.95069500 0.03906200 0.02700600

N 3.20832000 0.07986800 1.32458200

N 1.84983400 1.87401500 -0.01057400

Cl 3.41923700 -0.07486900 -1.82709700

Cl 1.93664400 -2.32259400 0.11985000

O 3.99438400 0.10050400 2.17096600

O 1.77603500 3.03173800 0.02506600

Cl -0.03697100 -0.05361800 1.64192200

Zero-point correction= 0.042250 (Hartree/Particle)

Thermal correction to Energy= 0.064037

Thermal correction to Enthalpy= 0.064981

Thermal correction to Gibbs Free Energy= -0.013275

Sum of electronic and zero-point Energies= -3437.792640

Sum of electronic and thermal Energies= -3437.770853

Sum of electronic and thermal Enthalpies= -3437.769909

Sum of electronic and thermal Free Energies= -3437.848165

**D3**

Re -1.93874000 0.00045300 -0.00002400

Cl 0.00006400 -0.00082600 -1.65036700

Cl -1.73099800 -2.39343600 0.00046200

Cl -1.73091400 2.39390600 -0.00098600

O -3.97481000 -0.00165600 -2.15627500

N -3.19264400 -0.00072000 -1.30441000

N -3.19228100 0.00033100 1.30478400

O -3.97404100 -0.00079100 2.15701700

Re 1.93875600 -0.00039300 0.00000700

N 3.19262500 0.00062600 1.30443500

N 3.19228500 -0.00032600 -1.30480000

Cl 1.73084300 2.39339500 -0.00019200

Cl 1.73090300 -2.39384100 0.00075800

O 3.97498200 0.00133700 2.15612600

O 3.97414500 0.00041600 -2.15695100

Cl -0.00009100 0.00090300 1.65043200

Zero-point correction= 0.042405 (Hartree/Particle)

Thermal correction to Energy= 0.064152

Thermal correction to Enthalpy= 0.065096

Thermal correction to Gibbs Free Energy= -0.012348

Sum of electronic and zero-point Energies= -3437.780437

Sum of electronic and thermal Energies= -3437.758690

Sum of electronic and thermal Enthalpies= -3437.757746

Sum of electronic and thermal Free Energies= -3437.835190

**D4**

Re -1.84396500 -0.04281000 -0.00016100

Cl -3.67889800 0.14208500 1.39304400

Cl -2.71262000 0.08924900 -2.12736800

N -1.90149700 -1.85379800 0.03208400

O -1.92661800 -3.01010000 0.09222500

Re 1.84310000 0.04286700 -0.00057500

N 1.90049800 1.85383800 -0.03313900

Cl 2.71246700 -0.08942900 2.12647000

Cl 3.68421100 -0.14154400 -1.38627800

O 1.92617600 3.01008500 -0.09450500

N -0.07903500 -0.05194900 1.13858700

N 0.07841800 0.05180900 -1.13745600

O 0.29357500 0.08805400 -2.30492300

O -0.29250300 -0.08941200 2.30615600

Cl -1.61409200 2.34123400 0.11455000

Cl 1.61312000 -2.34115700 -0.11670900

Zero-point correction= 0.041610 (Hartree/Particle)

Thermal correction to Energy= 0.063196

Thermal correction to Enthalpy= 0.064140

Thermal correction to Gibbs Free Energy= -0.012916

Sum of electronic and zero-point Energies= -3437.728081

Sum of electronic and thermal Energies= -3437.706495

Sum of electronic and thermal Enthalpies= -3437.705551

Sum of electronic and thermal Free Energies= -3437.782608

**D5**

Re -1.85281300 0.04096300 0.00302600

Cl -3.73398700 -0.08787600 -1.34521400

Cl -2.66732400 0.25512900 2.14808200

N -1.77413400 1.83684100 -0.25368100

O -1.72794300 2.97416900 -0.49505600

Re 1.85296300 0.04106000 -0.00315500

N 1.77377500 1.83693900 0.25348100

Cl 2.66734100 0.25559900 -2.14824000

Cl 3.73286400 -0.08748100 1.34684800

O 1.72710000 2.97417200 0.49514900

N -0.09362500 -0.11239000 -1.13486300

N 0.09375000 -0.11289700 1.13494500

O 0.31304800 -0.30192700 2.28536400

O -0.31334000 -0.30084800 -2.28532700

Cl -1.91028500 -2.31647900 0.12436300

Cl 1.91136200 -2.31628800 -0.12528200

Zero-point correction= 0.041371 (Hartree/Particle)

Thermal correction to Energy= 0.063041

Thermal correction to Enthalpy= 0.063985

Thermal correction to Gibbs Free Energy= -0.013663

Sum of electronic and zero-point Energies= -3437.720027

Sum of electronic and thermal Energies= -3437.698357

Sum of electronic and thermal Enthalpies= -3437.697413

Sum of electronic and thermal Free Energies= -3437.775061

**D6**

Re -1.95597400 -0.00004900 0.00001700

Cl -0.00003500 1.56934200 -0.00024200

Cl -3.23872000 -2.07730600 -0.00018900

Cl -3.23881400 2.07725600 0.00027100

O -3.04793600 0.00004200 2.77567800

N -2.47429000 0.00000300 1.77379900

N -2.47428900 0.00030800 -1.77378800

O -3.04808700 0.00054600 -2.77557300

Re 1.95590100 -0.00004600 0.00000200

N 2.47412400 0.00045900 1.77382300

N 2.47420000 -0.00021500 -1.77378800

Cl 3.23880700 -2.07723400 0.00051200

Cl 3.23914100 2.07701200 -0.00039200

O 3.04809000 0.00091900 2.77551200

O 3.04808200 -0.00025200 -2.77552700

Cl -0.00002400 -1.56947000 -0.00010300

Zero-point correction= 0.040330 (Hartree/Particle)

Thermal correction to Energy= 0.062954

Thermal correction to Enthalpy= 0.063898

Thermal correction to Gibbs Free Energy= -0.017125

Sum of electronic and zero-point Energies= -3437.701959

Sum of electronic and thermal Energies= -3437.679335

Sum of electronic and thermal Enthalpies= -3437.678391

Sum of electronic and thermal Free Energies= -3437.759414

**D7**

Re -1.83716200 -0.03501200 0.02319000

Cl -3.07706000 0.56662500 1.88112700

Cl -1.63412000 -2.34137400 0.18039900

N -3.17929300 -0.15180500 -1.14962300

O -4.03401100 -0.23830900 -1.93074500

Re 1.83718700 -0.03500400 -0.02322400

N 3.17935800 -0.15250000 1.14948600

Cl 1.63421400 -2.34127500 -0.18172700

Cl 3.07679100 0.56790500 -1.88091500

O 4.03389900 -0.23957900 1.93074200

N 0.04630800 -0.07013500 1.27495100

N -0.04626400 -0.06948000 -1.27493900

O -0.09108500 -0.20448300 -2.45677200

O 0.09109500 -0.20605600 2.45666900

Cl -1.50946300 2.22912100 -0.64325400

Cl 1.50952800 2.22876400 0.64462200

Zero-point correction= 0.040802 (Hartree/Particle)

Thermal correction to Energy= 0.062782

Thermal correction to Enthalpy= 0.063726

Thermal correction to Gibbs Free Energy= -0.014812

Sum of electronic and zero-point Energies= -3437.699478

Sum of electronic and thermal Energies= -3437.677498

Sum of electronic and thermal Enthalpies= -3437.676553

Sum of electronic and thermal Free Energies= -3437.755091

**D8**

Re -1.84211700 0.03839000 -0.00537700

Cl -3.18829800 -0.36439700 -1.83406200

Cl -1.58710900 2.33593000 -0.14558100

N -3.13837300 0.17576900 1.23202500

O -3.92670500 0.27965500 2.07849400

Re 1.84210800 -0.03825300 -0.00520800

N 3.13877800 -0.17535700 1.23175900

Cl 1.59080900 2.26483200 0.50585400

Cl 3.18825200 0.36287000 -1.83417000

O 3.92793600 -0.27963300 2.07742900

N -0.00009100 -0.00037300 -1.25416700

N -0.00006200 0.00054600 1.28458600

O -0.00049900 0.00121100 2.47202200

O -0.00003000 -0.00090500 -2.45304600

Cl -1.59086400 -2.26446900 0.50710600

Cl 1.58681600 -2.33576600 -0.14413400

Zero-point correction= 0.040736 (Hartree/Particle)

Thermal correction to Energy= 0.062717

Thermal correction to Enthalpy= 0.063661

Thermal correction to Gibbs Free Energy= -0.014938

Sum of electronic and zero-point Energies= -3437.695224

Sum of electronic and thermal Energies= -3437.673243

Sum of electronic and thermal Enthalpies= -3437.672299

Sum of electronic and thermal Free Energies= -3437.750898

**B1A**

Re -1.39288500 -0.81034200 -0.19826100

Cl -1.85187400 -0.57156000 2.26479800

Cl -0.28374700 -2.89248900 0.39158500

Cl -3.48504000 -1.94608700 -0.39815500

O -0.64683800 -1.05593300 -3.03056400

N -0.95302000 -0.95402900 -1.90063800

P 1.89732700 0.37993900 0.14908100

C 2.25205900 2.16637500 0.12262200

C 1.30264400 3.01755700 -0.46882600

C 3.43567500 2.69988100 0.65444100

C 1.55150900 4.39075600 -0.53445100

H 0.37513600 2.61102700 -0.86589000

C 3.67481200 4.07462800 0.58719800

H 4.16507800 2.05186300 1.13171400

C 2.73469800 4.92015100 -0.00961100

H 0.81650200 5.04636300 -0.99403000

H 4.59036600 4.48351800 1.00632200

H 2.92169800 5.98983800 -0.05989600

C 2.73717900 -0.38594700 1.56288000

C 4.10251800 -0.71459000 1.51901400

C 1.98935600 -0.63697100 2.72397000

C 4.72004200 -1.27320400 2.63953000

H 4.67863800 -0.55526100 0.61100100

C 2.61482600 -1.20060700 3.83865000

H 0.92535500 -0.42052700 2.74332700

C 3.97641100 -1.51364500 3.80003300

H 5.77507900 -1.53136000 2.60174500

H 2.03050600 -1.40800900 4.73075900

H 4.45672700 -1.95736400 4.66840300

C 2.58861700 -0.34747200 -1.36808000

C 3.09913800 0.45947900 -2.39855300

C 2.58140600 -1.74672500 -1.51677300

C 3.59884100 -0.12723000 -3.56359000

H 3.10605400 1.54014300 -2.29734800

C 3.07923200 -2.32405300 -2.68480700

H 2.16180100 -2.37847400 -0.73914900

C 3.58953800 -1.51713200 -3.70703400

H 3.98999900 0.50269400 -4.35800400

H 3.05810000 -3.40434200 -2.79821300

H 3.97398600 -1.97148900 -4.61659900

O 0.37272400 0.24480100 0.30164000

N -2.24720700 0.97379800 -0.57413500

O -1.89255000 1.74447100 -1.56797100

C -5.13339200 2.82764000 0.35472300

H -3.65353800 3.06141400 -1.23633000

C -5.16098800 1.85608400 1.31608100

H -3.70002100 0.27842300 1.69854500

H -5.80711500 3.64548800 0.15427500

H -5.85921100 1.67568600 2.11829300

C -3.36394900 1.50258400 0.05983800

N -4.06887900 1.04078800 1.10620700

N -4.00734200 2.59047300 -0.40912100

Zero-point correction= 0.375373 (Hartree/Particle)

Thermal correction to Energy= 0.408148

Thermal correction to Enthalpy= 0.409092

Thermal correction to Gibbs Free Energy= 0.306239

Sum of electronic and zero-point Energies= -3056.367752

Sum of electronic and thermal Energies= -3056.334977

Sum of electronic and thermal Enthalpies= -3056.334033

Sum of electronic and thermal Free Energies= -3056.436886

**B2A**

Re 1.38312100 -0.35683800 0.12549000

Cl 1.67655600 1.92031900 1.20121600

Cl 1.36599900 -1.21972300 2.38442200

Cl 1.17009700 0.84433500 -1.98210700

O 0.69401300 -2.98397600 -0.98602700

N 0.99743100 -1.93388500 -0.56078400

P -2.14655000 0.16663200 0.03864000

C -3.15006600 -0.07995100 1.53740100

C -2.50465500 -0.54739900 2.69299100

C -4.52818000 0.18947400 1.56339700

C -3.24311500 -0.75380200 3.86218500

H -1.43450000 -0.73511000 2.67772900

C -5.25807300 -0.01975200 2.73438900

H -5.03335100 0.57024400 0.67970500

C -4.61568400 -0.49377900 3.88408400

H -2.73907400 -1.11336800 4.75513800

H -6.32382300 0.19269200 2.75131700

H -5.18532500 -0.65279100 4.79621300

C -2.56503400 1.77715700 -0.69196300

C -3.69184300 1.94776200 -1.51260400

C -1.74573800 2.87534600 -0.38713000

C -4.00636600 3.21339200 -2.01155800

H -4.31215000 1.09643700 -1.78112700

C -2.06607400 4.13748600 -0.89242800

H -0.85449000 2.73642400 0.21762600

C -3.19507700 4.30900900 -1.69862400

H -4.87606100 3.34065300 -2.65088600

H -1.42408300 4.98364200 -0.66328400

H -3.43774200 5.29276200 -2.09249800

C -2.59152900 -1.11650600 -1.17261600

C -3.37501900 -2.22549700 -0.81532800

C -2.07416100 -1.01984800 -2.47756700

C -3.64640700 -3.22229700 -1.75607900

H -3.76951500 -2.31564600 0.19211800

C -2.34639000 -2.02075000 -3.41010000

H -1.44155600 -0.18092500 -2.75459200

C -3.13420900 -3.12000200 -3.05203000

H -4.25171200 -4.07921800 -1.47287000

H -1.93491600 -1.94571800 -4.41288800

H -3.34178300 -3.89928600 -3.78084600

O -0.67843000 0.13648900 0.46822300

N 3.29829900 -0.75492200 -0.18174300

O 3.74246300 -1.88683500 -0.63659500

C 6.51213400 0.77945800 -0.09841600

H 5.79607800 -1.20635000 -0.67505900

C 5.75451000 1.82170400 0.36052300

H 3.58603200 1.89131400 0.71944900

H 7.57255800 0.69642000 -0.27628500

H 6.03266800 2.81980300 0.66107300

C 4.38678900 0.11995300 -0.02207900

N 4.44535000 1.39161000 0.39534600

N 5.63928700 -0.26349300 -0.32781200

Zero-point correction= 0.375308 (Hartree/Particle)

Thermal correction to Energy= 0.408115

Thermal correction to Enthalpy= 0.409059

Thermal correction to Gibbs Free Energy= 0.304506

Sum of electronic and zero-point Energies= -3056.374537

Sum of electronic and thermal Energies= -3056.341731

Sum of electronic and thermal Enthalpies= -3056.340786

Sum of electronic and thermal Free Energies= -3056.445340

**B1B**

Re 1.35663300 -0.95041700 -0.12566300

Cl 0.80629300 -2.33221600 -2.04091100

Cl 0.10826100 -2.48618500 1.24065200

Cl 3.40789500 -2.16092900 0.05369600

O 2.06310400 0.62103400 2.27452500

N 1.77320500 0.02406600 1.29734100

P -1.93103300 0.39653600 -0.02409900

C -2.50409000 1.63588900 -1.22957400

C -1.56929000 2.18789500 -2.11875900

C -3.85122200 2.02687400 -1.29633400

C -1.98418100 3.13492300 -3.05989200

H -0.53283300 1.86735700 -2.07980000

C -4.25710500 2.97503100 -2.23652600

H -4.58659300 1.58841700 -0.62677200

C -3.32295200 3.53061500 -3.11827400

H -1.25869700 3.55435000 -3.75167700

H -5.30117500 3.27243600 -2.28678500

H -3.64228500 4.26377300 -3.85456200

C -3.06686700 -1.01627200 -0.07339900

C -4.24573100 -1.03847100 0.69016000

C -2.77187100 -2.07676700 -0.94533100

C -5.13047000 -2.11245300 0.57334900

H -4.46783300 -0.23447600 1.38688200

C -3.66145600 -3.14755400 -1.05265600

H -1.84360900 -2.08127900 -1.51003400

C -4.83913400 -3.16561300 -0.29961700

H -6.03856200 -2.13055900 1.17023400

H -3.42248600 -3.97373200 -1.71636800

H -5.52505600 -4.00472400 -0.38380000

C -2.01254500 1.13250900 1.63952900

C -2.20480900 2.51228400 1.81856100

C -1.80643500 0.30797900 2.76085000

C -2.20083500 3.05904700 3.10440000

H -2.35800100 3.15947000 0.96040500

C -1.80003900 0.86162900 4.04146800

H -1.63114100 -0.75624800 2.63171100

C -1.99981500 2.23520400 4.21515100

H -2.35292400 4.12712400 3.23566700

H -1.63260100 0.21967400 4.90188400

H -1.99452600 2.66253800 5.21460700

O -0.50738100 0.02057700 -0.45577500

N 2.35774100 1.61578800 -1.37393300

O 1.91403300 0.34106700 -1.46275000

C 5.19048500 2.95624400 0.23981100

H 3.46660300 3.88694000 -0.66490100

C 5.45793900 1.63485000 0.39347800

H 4.29729500 -0.09210100 -0.16477600

H 5.75373500 3.83021800 0.52530300

H 6.30042800 1.13376600 0.84339000

C 3.46518500 1.79205700 -0.65897400

N 4.40112200 0.92490900 -0.16653900

N 3.95936200 3.04553200 -0.40334500

Zero-point correction= 0.374429 (Hartree/Particle)

Thermal correction to Energy= 0.407570

Thermal correction to Enthalpy= 0.408514

Thermal correction to Gibbs Free Energy= 0.304478

Sum of electronic and zero-point Energies= -3056.350969

Sum of electronic and thermal Energies= -3056.317828

Sum of electronic and thermal Enthalpies= -3056.316883

Sum of electronic and thermal Free Energies= -3056.420920

**B2B**

Re -1.27289900 -0.78902700 0.07379300

Cl -2.03063500 0.83568200 -1.60345300

Cl -1.00679700 -2.31933500 -1.76322000

Cl -1.31908100 1.04089600 1.71905300

O -0.21790900 -2.79306500 1.96021000

N -0.65796800 -1.98407900 1.22636400

P 2.08944700 0.30839200 -0.11584400

C 3.15050400 -0.25514000 -1.48044300

C 2.60845500 -1.14405700 -2.42156500

C 4.47789500 0.18559200 -1.61167500

C 3.40069100 -1.59420800 -3.48224900

H 1.57642600 -1.47083800 -2.32874000

C 5.26145200 -0.26965800 -2.67251400

H 4.90131600 0.88661000 -0.89713000

C 4.72296600 -1.16143200 -3.60768800

H 2.97701600 -2.28047500 -4.21030300

H 6.28729200 0.07489600 -2.77255200

H 5.33403700 -1.51206700 -4.43549200

C 2.18424000 2.11787500 0.00262700

C 3.23664000 2.76512000 0.67020400

C 1.18785300 2.87131000 -0.63877700

C 3.29930700 4.15991300 0.68450700

H 3.99496300 2.18895100 1.19415200

C 1.25822300 4.26613800 -0.61784300

H 0.35684300 2.37063300 -1.12834200

C 2.31171100 4.91016400 0.03765000

H 4.11195000 4.65830100 1.20640200

H 0.48223400 4.84735400 -1.10840200

H 2.35986200 5.99605700 0.05298200

C 2.71721500 -0.39428800 1.43860900

C 3.62208100 -1.46839500 1.43848600

C 2.21892800 0.09686600 2.65927900

C 4.03131400 -2.03779300 2.64649200

H 4.00371200 -1.86261500 0.50166300

C 2.62991400 -0.47872400 3.86148900

H 1.49891800 0.91004800 2.66937300

C 3.53719100 -1.54350700 3.85650000

H 4.72993200 -2.86998500 2.63980100

H 2.23493100 -0.10083600 4.80042700

H 3.85295700 -1.99143600 4.79511800

O 0.65291700 -0.10845300 -0.45485100

N -4.30547900 -1.17494300 -0.02314300

O -3.07002900 -1.42034200 0.41295100

C -6.18009500 1.75111800 -0.56834400

H -6.35986600 -0.25255200 -1.34578200

C -5.20477800 2.26454100 0.22716400

H -3.42016500 1.34098400 0.99523000

H -7.05463400 2.20854500 -1.00242900

H -5.06457500 3.26183100 0.61305900

C -4.71103800 0.09577000 -0.11115300

N -4.32270400 1.23745500 0.52457500

N -5.87106800 0.41103300 -0.76169900

Zero-point correction= 0.374612 (Hartree/Particle)

Thermal correction to Energy= 0.407768

Thermal correction to Enthalpy= 0.408713

Thermal correction to Gibbs Free Energy= 0.304596

Sum of electronic and zero-point Energies= -3056.354033

Sum of electronic and thermal Energies= -3056.320877

Sum of electronic and thermal Enthalpies= -3056.319932

Sum of electronic and thermal Free Energies= -3056.424049

**Dihapto 1**

Re -2.02152100 0.03820400 0.24965500

Cl -2.14241700 -2.27589400 0.92381800

Cl -1.37499200 -0.57406200 -1.94125300

Cl -4.28564700 -0.08878200 -0.43410400

O -1.92205200 2.94577000 -0.31697400

N -1.94493100 1.79218500 -0.11286800

P 1.54582300 -0.02545400 0.03623400

C 2.66807100 0.02318500 1.47430800

C 2.12400700 -0.03097500 2.76545100

C 4.06132700 0.08743600 1.30787100

C 2.96846900 -0.01466500 3.87974300

H 1.04813900 -0.09120800 2.89072100

C 4.89937400 0.10521900 2.42315500

H 4.49778700 0.12326100 0.31336900

C 4.35328100 0.05421900 3.71083800

H 2.54083600 -0.05929700 4.87770900

H 5.97638500 0.15532500 2.28756300

H 5.00781900 0.06498500 4.57842600

C 2.01517100 -1.45198100 -0.98342200

C 3.10438700 -1.40440800 -1.86915900

C 1.30142900 -2.64881500 -0.81271100

C 3.47912300 -2.54911700 -2.57535700

H 3.65119900 -0.47833800 -2.02547800

C 1.68308300 -3.78876600 -1.52305600

H 0.44189800 -2.68208200 -0.14977700

C 2.76989700 -3.74187600 -2.40084300

H 4.31744600 -2.50631100 -3.26559500

H 1.12020900 -4.70932700 -1.39674600

H 3.05984500 -4.63072100 -2.95516100

C 1.81505800 1.50198700 -0.91696500

C 2.25622900 2.66576700 -0.26266100

C 1.49772900 1.55601100 -2.28565700

C 2.38340100 3.86310800 -0.96917600

H 2.50256000 2.63906700 0.79474100

C 1.62890900 2.75570300 -2.98685800

H 1.13377200 0.67136900 -2.79703700

C 2.07174100 3.90850800 -2.33121400

H 2.72444400 4.75789800 -0.45565000

H 1.37746800 2.78962900 -4.04325600

H 2.17008500 4.84147300 -2.87996400

O 0.12567800 -0.16771300 0.61147300

N -1.69815500 0.43764500 2.23477700

O -2.88783800 0.42659800 2.31995100

Zero-point correction= 0.299546 (Hartree/Particle)

Thermal correction to Energy= 0.328341

Thermal correction to Enthalpy= 0.329285

Thermal correction to Gibbs Free Energy= 0.234756

Sum of electronic and zero-point Energies= -2830.170493

Sum of electronic and thermal Energies= -2830.141697

Sum of electronic and thermal Enthalpies= -2830.140753

Sum of electronic and thermal Free Energies= -2830.235282

**Dihapto 2**

Re -1.98266500 -0.08100800 -0.10956200

Cl -2.28930400 1.24137500 -2.10068300

Cl -1.87703900 -2.10322200 -1.50897600

Cl -1.46232500 1.98118600 1.07419900

O -1.86100100 -1.60825100 2.42867400

N -1.87157600 -1.01775200 1.41718800

P 1.46812900 0.00797100 -0.04457400

C 2.48513500 -1.04360000 -1.12167600

C 1.85073500 -1.94361200 -1.99129800

C 3.88752400 -0.95817400 -1.09515200

C 2.62417100 -2.75971800 -2.82282600

H 0.76639700 -1.99875300 -2.01937000

C 4.65020900 -1.77761700 -1.92719600

H 4.38746800 -0.25314100 -0.43642700

C 4.01826900 -2.67969900 -2.79135000

H 2.13011100 -3.45379700 -3.49707700

H 5.73441000 -1.70778700 -1.90611300

H 4.61457200 -3.31397600 -3.44214300

C 2.02205300 1.72588900 -0.20218400

C 3.12369400 2.21533200 0.51869700

C 1.35693400 2.55325500 -1.12140100

C 3.56316500 3.52446300 0.31257600

H 3.62879400 1.58997100 1.25010500

C 1.80293000 3.86123700 -1.31913200

H 0.48573200 2.18682100 -1.65617500

C 2.90416300 4.34615600 -0.60747300

H 4.41174800 3.90315600 0.87595600

H 1.27905000 4.50323600 -2.02156000

H 3.24409300 5.36685300 -0.76226900

C 1.69243100 -0.53584500 1.67321900

C 2.14811400 -1.83697700 1.94899900

C 1.33864400 0.31878300 2.73348300

C 2.25364100 -2.27460200 3.27047900

H 2.41892900 -2.50573700 1.13764600

C 1.44804700 -0.12630400 4.05128600

H 0.96087400 1.31565200 2.52973800

C 1.90579300 -1.42014700 4.32077700

H 2.60488200 -3.28167600 3.47746700

H 1.16834500 0.53597100 4.86581200

H 1.98736000 -1.76340700 5.34876900

O 0.01793600 -0.13303900 -0.56866800

N -3.95876400 -0.58439400 -0.26156300

O -4.04431200 0.47703700 0.28698300

Zero-point correction= 0.299821 (Hartree/Particle)

Thermal correction to Energy= 0.328452

Thermal correction to Enthalpy= 0.329396

Thermal correction to Gibbs Free Energy= 0.236600

Sum of electronic and zero-point Energies= -2830.170869

Sum of electronic and thermal Energies= -2830.142238

Sum of electronic and thermal Enthalpies= -2830.141294

Sum of electronic and thermal Free Energies= -2830.234090