

Synthesis and Reactivity of the Unsaturated Trinuclear Phosphanido

Complex $[(\text{C}_6\text{F}_5)_2\text{Pt}(\mu\text{-PPh}_2)_2\text{Pt}(\mu\text{-PPh}_2)_2\text{Pt}(\text{PPh}_3)]$

Juan Forniés, Consuelo Fortuño,* Susana Ibáñez, and Antonio Martín

Departamento de Química Inorgánica Instituto de Síntesis Química y Catálisis

Homogénea, Universidad de Zaragoza - CSIC, 50009 Zaragoza, Spain.

Piero Mastrorilli,* and Vito Gallo

Dipartimento di Ingegneria Civile, Ambientale, del Territorio, Edile e di Chimica

(DICATECh), Politecnico di Bari, via Orabona 4, I-70125 Bari, Italy

Athanassios Tsipis*

Laboratory of Inorganic and General Chemistry, Department of Chemistry, University

of Ioannina, 451 10 Ioannina, Greece

Supporting Information

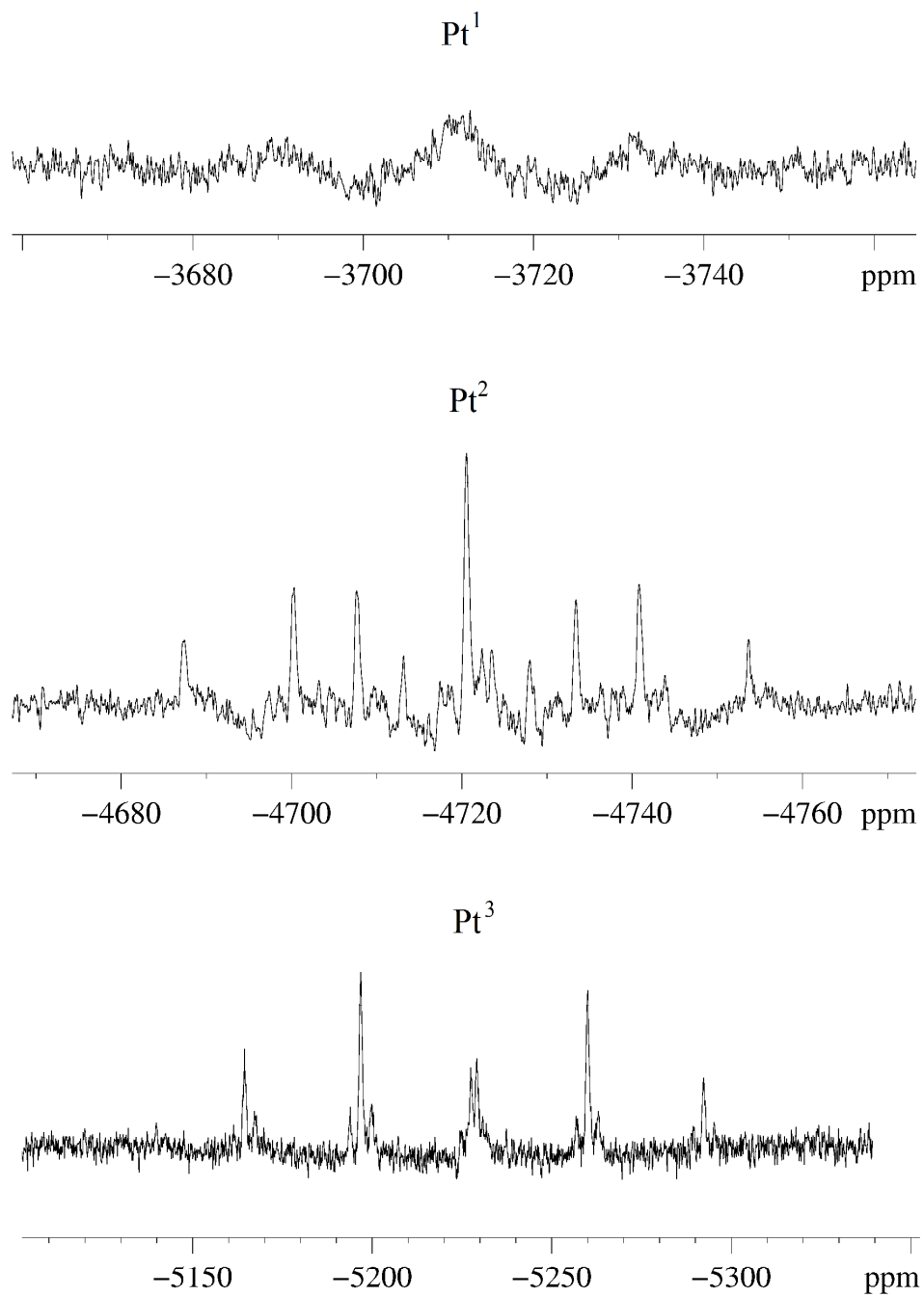


Figure S1. $^{195}\text{Pt}\{^1\text{H}\}$ spectrum of **1** (CDCl_3 , 298 K).

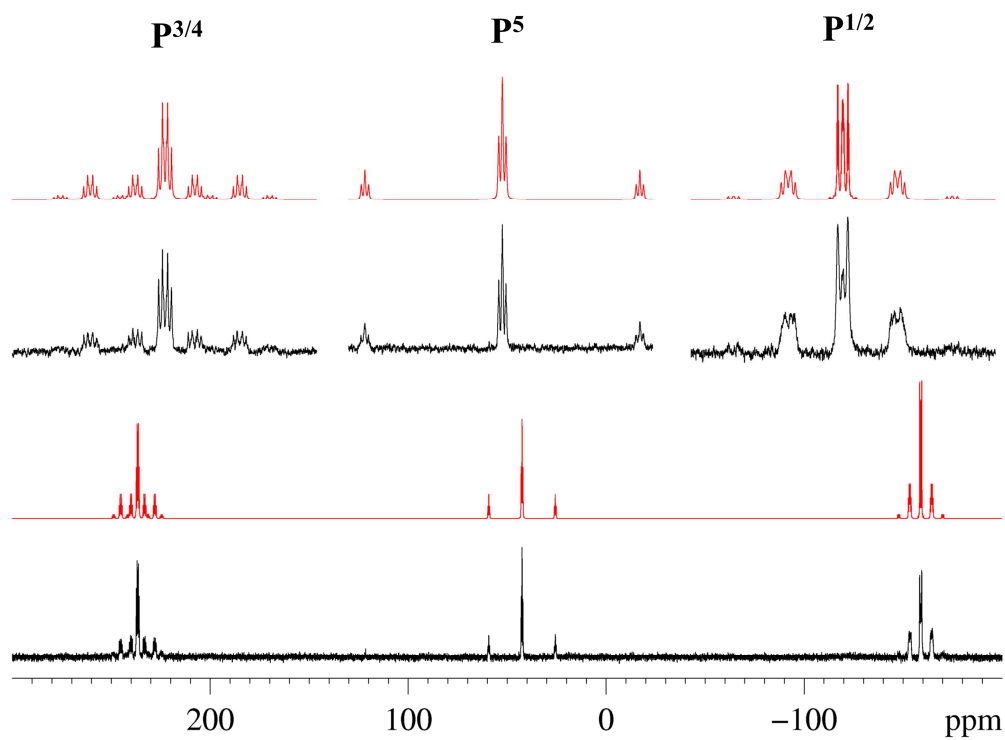


Figure S2. Experimental (black) and calculated (red) $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **1** (CDCl₃, 298 K)

Cartessian Coordinates and energies of M1-M5

M1

```
Pt,0,1.5482607638,-0.0036076053,0.0004976998
Pt,0,-1.1216857058,0.0155501658,-0.0044181235
Cl,0,3.2562033797,1.6277517482,0.0082046551
Cl,0,3.2313739116,-1.6609947473,0.0036158219
P,0,0.169162304,1.8536139558,-0.0042884186
P,0,0.1436338493,-1.839391466,-0.0061258352
P,0,-3.359177711,0.0036057192,-0.0003978605
C,0,0.441110823,2.9483086257,-1.4407597274
H,0,-0.2689657736,3.7813155908,-1.409241476
H,0,1.4676054915,3.3270532522,-1.4046298531
H,0,0.2992034753,2.3834234853,-2.3641383819
H,0,-0.2750647036,3.7838348933,1.39571324
H,0,0.280293658,2.3846503148,2.356249744
H,0,1.4599522188,3.3241105641,1.4064362824
H,0,-0.333602246,-3.7630763089,1.3923020475
H,0,1.4097857547,-3.3358979049,1.3991914404
H,0,0.2508271334,-2.3759768703,2.3534459741
H,0,-0.3299744837,-3.7568359787,-1.4143807639
C,0,0.4320162522,2.9485525142,1.4338243511
H,0,0.2617537117,-2.3672428257,-2.366898419
H,0,1.4143074741,-3.3330133053,-1.4103846488
C,0,0.3891300966,-2.9412434503,1.4297542784
C,0,0.3945729474,-2.9362884235,-1.4447484152
C,0,-4.2107426326,1.5704786408,-0.4311043463
H,0,-5.2999556766,1.4560204183,-0.3993892869
H,0,-3.9050418523,2.3492053202,0.2724204236
H,0,-3.909585552,1.8818767091,-1.4349125767
H,0,-5.2400848334,-1.1336277535,-1.0858894904
H,0,-3.8297174405,-0.9836043908,-2.1675240746
H,0,-3.8224208691,-2.2044876573,-0.8851764842
H,0,-5.1886659808,-0.4018880287,1.5698114195
H,0,-3.7616342135,-1.4155512994,1.9256123976
H,0,-3.758491893,0.2982428265,2.3753189336
C,0,-4.147893966,-1.1936043516,-1.1428622958
C,0,-4.0948927116,-0.4198183768,1.6230717691
```

Sum of electronic and zero-point Energies=	-2461.475181
Sum of electronic and thermal Energies=	-2461.449791
Sum of electronic and thermal Enthalpies=	-2461.448847
Sum of electronic and thermal Free Energies=	-2461.531988

M2

Pt,0,0.1374515019,0.002065838,-0.005230835
 Pt,0,-2.5487345489,0.0048880305,-0.0071830641
 P,0,-1.2861758573,1.8612474848,0.1989153086
 P,0,-1.2903154354,-1.8538003606,-0.2203323337
 P,0,-4.7887349626,0.001358906,0.0059062355
 F,0,1.9600440653,1.2381770194,2.3791275381
 F,0,4.0586785519,2.9096783972,2.3639789712
 F,0,4.9243707971,4.012314982,0.0276877552
 F,0,3.6390444296,3.4253170464,-2.3013825038
 F,0,1.5326592388,1.7662461281,-2.3079584603
 F,0,1.5120772056,-1.7648996853,2.3074156577
 F,0,3.6117713724,-3.4320213987,2.315641647
 F,0,4.9096300026,-4.0262058033,-0.0046679803
 F,0,4.0631994273,-2.9222379549,-2.3473900877
 F,0,1.9713280886,-1.2424172341,-2.3773677789
 C,0,1.668461255,1.406477965,0.0329014564
 C,0,2.349392747,1.748012824,1.1963585672
 C,0,3.4385218974,2.6134058719,1.2179512198
 C,0,3.8831061086,3.1785086724,0.0294733644
 C,0,3.225768402,2.8747255973,-1.155964509
 C,0,2.1401976136,2.0052401966,-1.1309199722
 C,0,1.6638076294,-1.4078196926,-0.0330084955
 C,0,2.1260282149,-2.0071856517,1.13435206
 C,0,3.2080032454,-2.8808619233,1.1670949974
 C,0,3.8716549535,-3.1883507033,-0.0138586549
 C,0,3.436844908,-2.6225818398,-1.2056246392
 C,0,2.3509788412,-1.7529039972,-1.1917318324
 C,0,-1.1334901877,3.1699637633,-1.0723061486
 H,0,-1.9417171219,3.8969136813,-0.9406426386
 H,0,-0.1721655256,3.6845101762,-0.9773008097
 H,0,-1.2016285204,2.7293568689,-2.0683896739
 H,0,-1.8671507073,3.5199482735,1.8778817869
 H,0,-1.0954567869,2.0863184417,2.6088914847
 H,0,-0.1012028788,3.2972836588,1.7694631355
 H,0,-1.9473045652,-3.8942321818,0.910721989
 H,0,-0.1782744705,-3.6806842616,0.9521859477
 H,0,-1.2102865221,-2.730064262,2.0443330985
 H,0,-1.8711321762,-3.5021344372,-1.9090085722
 C,0,-1.0665665821,2.7812185728,1.7674793074
 H,0,-1.0883532432,-2.0697103411,-2.6300077938
 H,0,-0.1043119707,-3.2892394695,-1.790674929
 C,0,-1.1401027423,-3.1670062649,1.0467933274
 C,0,-1.0670383932,-2.7682923109,-1.7914618676
 C,0,-5.630898298,1.5728027299,-0.4261810335
 H,0,-6.7205726499,1.4667765025,-0.3843754608
 H,0,-5.3127271444,2.3524173116,0.2707649631
 H,0,-5.3376472129,1.8769278735,-1.4346508497
 H,0,-6.6930680983,-1.1233841439,-1.054691951
 H,0,-5.290603095,-0.9965785686,-2.1495771489
 H,0,-5.2851554214,-2.2073831482,-0.8578912812
 H,0,-6.6037667427,-0.3877481107,1.595609657
 H,0,-5.1775472394,-1.4031149966,1.9466843797
 H,0,-5.1642531268,0.3139261312,2.3833541099
 C,0,-5.602037803,-1.1949897909,-1.1205031107
 C,0,-5.5096464671,-0.4083994123,1.6394014507

Sum of electronic and zero-point Energies=	-2995.462934
Sum of electronic and thermal Energies=	-2995.421034
Sum of electronic and thermal Enthalpies=	-2995.420090
Sum of electronic and thermal Free Energies=	-2995.540437

M3

Pt,0,17.3249341189,19.2489095578,7.8953038713
 Pt,0,14.4373788988,18.9008357825,5.6023195882
 Pt,0,12.3293593372,18.6491431211,3.913682978
 P,0,16.1900138439,17.6627778724,6.6700148614
 P,0,15.6552740149,20.4952507012,6.9131134978
 P,0,14.0041124526,17.1479326636,4.0606118218
 P,0,12.5972022348,20.378284133,5.3337742263
 P,0,10.5847414499,18.4407875728,2.5161358968
 F,0,20.0688936712,18.1295125555,6.5933787689
 F,0,21.970438267,16.4802903496,7.514854675
 F,0,21.7627842282,15.3843540752,10.0011838362
 F,0,19.6059768498,15.9709301715,11.5608065643
 F,0,17.6933878367,17.6249108769,10.6655217452
 F,0,19.8335497757,21.224678582,7.3883648656
 F,0,20.8753013799,23.2407530171,8.8185470953
 F,0,19.7657034994,23.9577501311,11.2023360847
 F,0,17.5794660641,22.6218973735,12.1315938673
 F,0,16.5138148524,20.6093512258,10.7173386245
 C,0,18.7975342964,17.9732711126,8.594666481
 C,0,19.9162985576,17.6341523672,7.8403425493
 C,0,20.9167422291,16.7770030347,8.287019297
 C,0,20.8157486912,16.2149290568,9.5528755336
 C,0,19.7146352373,16.5176695558,10.3432136373
 C,0,18.7410728519,17.3811530065,9.8521790891
 C,0,18.1364778551,20.8054786479,8.9925486156
 C,0,19.2467190751,21.5261383736,8.5645579386
 C,0,19.8080066458,22.5774690446,9.281644973
 C,0,19.24653012,22.9475591771,10.4968013586
 C,0,18.1330708394,22.2627485916,10.9657740404
 C,0,17.607847488,21.2184395626,10.21158029
 C,0,17.2581097432,16.5786334098,5.6368509897
 H,0,16.7118689048,15.7768652046,5.1328246132
 H,0,17.7946686037,17.1840596489,4.9023475993
 H,0,18.003103756,16.1331171147,6.3041320317
 H,0,15.5984487135,22.2838465714,5.1917914887
 H,0,17.0265727334,22.3736284773,6.2614979359
 H,0,16.9648259582,21.1580689378,4.9781574017
 H,0,14.7576218204,15.7159873011,7.2359336754
 H,0,16.1096770752,15.9562415425,8.3785794075
 H,0,14.6892325046,17.0067687132,8.4641095617
 H,0,13.9985898761,22.22931024,7.5749421386
 C,0,15.3436133736,16.4612680292,7.7801531773
 H,0,14.2148024811,20.9611075164,8.8201435223
 H,0,15.4551735389,22.1956911374,8.5964236905
 C,0,14.7207570311,21.5758895324,8.0718724276
 C,0,16.3616524941,21.6988137837,5.7114893941
 C,0,13.7923691636,15.4144307623,4.623644274
 H,0,13.4449269657,14.8134729437,3.776396147
 H,0,14.725532532,14.9830500692,4.9967000454
 H,0,13.0381713231,15.3766620623,5.4122721733
 H,0,14.8591509388,16.3996467172,1.9193608207
 H,0,15.4803239451,18.0118827212,2.3424211131
 H,0,16.1887655001,16.5637249312,3.0933838714
 H,0,11.8579358855,22.5619834956,4.6049563347
 H,0,13.3311171562,22.7191813115,5.58606277
 H,0,13.4373028489,22.149979305,3.9009877321
 H,0,10.5988030779,20.976541013,6.5668546593
 C,0,15.2619140213,17.0150670672,2.7306939054
 H,0,11.372112081,19.5246577162,7.2438490391
 H,0,12.0365257843,21.1340442168,7.6065232069

C,0,12.8385882862,22.121447458,4.8137809401
C,0,11.5570401483,20.5216497516,6.8390113514
C,0,10.1802464522,16.7509309997,1.9242215792
H,0,9.3163160637,16.7597734646,1.2503214536
H,0,11.0464065261,16.3390346511,1.3994430609
H,0,9.9608132449,16.1061378917,2.7795176283
H,0,8.1724195328,18.8676544912,2.4094778405
H,0,8.7146445539,18.4794160514,4.0635199648
H,0,9.0343169428,20.0869550886,3.3920071888
H,0,9.9134988338,19.238423869,0.3058970524
H,0,10.9151028356,20.4370766702,1.1701603592
H,0,11.6799361121,19.0202201612,0.4299359949
C,0,8.9654888621,19.0235960737,3.1487805644
C,0,10.7870951116,19.3739005917,0.9522832022

Sum of electronic and zero-point Energies=	-3956.676272
Sum of electronic and thermal Energies=	-3956.621206
Sum of electronic and thermal Enthalpies=	-3956.620262
Sum of electronic and thermal Free Energies=	-3956.770123

M4

Pt,0,0.8375772911,3.920335924,11.9151382511
 Pt,0,0.3373575643,6.0751074396,14.7634260813
 Pt,0,-0.3026414216,7.7778718496,17.8722450347
 P,0,-0.6812129475,5.4836960941,12.719123321
 P,0,2.0691134784,5.1324431793,13.4700308103
 P,0,-1.3946765475,6.9765529714,16.0646191583
 P,0,1.3346892689,6.6299910204,16.8161710981
 O,0,0.8855188603,8.4360238379,19.4829147882
 O,0,-1.9498194066,8.8049313649,18.6924417166
 F,0,-0.1715009498,4.6579077913,8.9194568753
 F,0,-1.894594306,3.4827342181,7.2408278135
 F,0,-3.1952403193,1.1979259965,7.9668246078
 F,0,-2.7339186332,0.1039506892,10.4216526697
 F,0,-1.0097626262,1.2544706539,12.1200254478
 F,0,1.9549708652,1.2396482756,13.3578722411
 F,0,3.8947885314,-0.4951791153,12.7220497411
 F,0,5.3842274528,-0.1395504583,10.4656929307
 F,0,4.8895338648,1.996047744,8.8432277817
 F,0,2.9457212701,3.740168422,9.4476811175
 C,0,-0.4832137044,3.0061924539,10.6029574471
 C,0,-0.7659997382,3.5201301065,9.3408002017
 C,0,-1.6597312899,2.9385046249,8.447498295
 C,0,-2.3256631194,1.7762493928,8.8105527091
 C,0,-2.0850839743,1.2246091014,10.0613722151
 C,0,-1.1808329914,1.8436714226,10.9180241687
 C,0,2.3379095666,2.5740206138,11.4270602974
 C,0,2.6407283503,1.4688592293,12.2173784193
 C,0,3.6447893941,0.5536361234,11.9191818886
 C,0,4.4072331977,0.7287272789,10.7726331931
 C,0,4.1497370441,1.8177452269,9.951439755
 C,0,3.1329282888,2.7035914212,10.2923592848
 C,0,-0.8967952548,6.9483932982,11.6129450305
 C,0,-2.4220269896,4.8898561786,12.8569410529
 C,0,3.3570497368,4.208354555,14.4126901813
 C,0,3.0981568114,6.4433776455,12.6706952286
 C,0,-2.4141135542,8.3058926084,15.293945678
 C,0,-2.6964765117,5.7904731925,16.6144421752
 C,0,1.8739370713,5.2139435284,17.8688764226
 C,0,2.8696331761,7.6508621301,16.7630258728
 C,0,0.4757625361,9.1588865693,20.4422932888
 C,0,-0.8232348202,9.6675178223,20.6199594537
 C,0,-1.9264723381,9.4766191066,19.7689420124
 C,0,1.5267312746,9.4825098847,21.4765757912
 C,0,-3.2417770728,10.1214218958,20.1339476112
 H,0,-1.5847250912,7.6754710921,12.0589622312
 H,0,-1.2804320993,6.6258921456,10.6394046123
 H,0,0.0696868721,7.4334221615,11.4537002067
 H,0,-3.0812816634,5.6765930777,13.2407530093
 H,0,-2.4555715123,4.0301804337,13.5313108112
 H,0,-2.7806773334,4.568856287,11.8729049557
 H,0,3.8718685706,4.8641665902,15.1235765148
 H,0,4.0912156349,3.7868178415,13.717372014
 H,0,2.887153351,3.3833990439,14.9536494582
 H,0,3.6064093654,7.0547344494,13.4244244314
 H,0,2.4586388728,7.0908642889,12.0656058594
 H,0,3.8404773997,5.981411018,12.0108715982
 H,0,-3.078492416,8.7509757801,16.0417101801
 H,0,-3.0085756318,7.8962981098,14.4698377364
 H,0,-1.7544309343,9.08193277,14.8976202404
 H,0,-3.3843417073,6.2811795658,17.3109783032

H,0,-2.2245966628,4.9439829663,17.1194671991
H,0,-3.2532620272,5.413619717,15.7505960986
H,0,2.1945449312,5.5743756224,18.8519254074
H,0,2.6974115112,4.6759239154,17.3876739536
H,0,1.0379914859,4.5222179239,17.9992696745
H,0,3.1234850527,7.992718226,17.7716874599
H,0,2.7007525526,8.5217974619,16.1248636191
H,0,3.7016974693,7.0688041358,16.3521452104
H,0,-0.9905342806,10.274132084,21.5031644553
H,0,2.3637429854,9.9950697505,20.9912616202
H,0,1.9185775916,8.5494083672,21.8944539887
H,0,1.1432663841,10.1065751137,22.2867568126
H,0,-4.0102356676,9.3466074936,20.2230734168
H,0,-3.5505766582,10.7900112801,19.3236992827
H,0,-3.1902217236,10.6868029782,21.0669994787

Sum of electronic and zero-point Energies=	-3840.814267
Sum of electronic and thermal Energies=	-3840.757702
Sum of electronic and thermal Enthalpies=	-3840.756757
Sum of electronic and thermal Free Energies=	-3840.912417

M5

Pt,0,0.8772291294,3.9962592142,11.9223284096
 Pt,0,0.2517848542,6.0837761184,14.7529703269
 Pt,0,-0.5296551022,7.6908886787,17.9363134253
 P,0,-0.701316517,5.5206084521,12.6629320285
 P,0,2.0516836839,5.2664852561,13.4607832514
 P,0,-1.5573932365,6.7759678938,16.0710715006
 P,0,1.2205284425,6.5630047016,16.825240523
 C,0,-2.1470213107,9.290899615,20.6447658675
 P,0,-2.3658826505,8.8145622288,18.8841630279
 F,0,-0.2161130615,4.6628004178,8.9520406526
 F,0,-1.8938922731,3.3793433581,7.3039998348
 F,0,-3.0456752414,1.0266482801,8.0607467427
 F,0,-2.4828279782,-0.0251688293,10.5120804179
 F,0,-0.8009756467,1.2324071646,12.1760597583
 F,0,2.0683310085,1.4363239453,13.5157657271
 F,0,4.0347559414,-0.2913822761,12.953849606
 F,0,5.4826925037,-0.0411436244,10.6569931478
 F,0,4.9203948015,1.9835830209,8.919836618
 F,0,2.9469792504,3.7211768551,9.4526571596
 C,0,-0.4021944608,2.9975780421,10.6376558593
 C,0,-0.7346398499,3.4910319757,9.3800915548
 C,0,-1.6075626634,2.8539583267,8.504350038
 C,0,-2.1983246234,1.6563019775,8.8843946631
 C,0,-1.9060349382,1.1250114503,10.1334653169
 C,0,-1.0247656243,1.7992168,10.9721461457
 C,0,2.3977243575,2.6569590072,11.5013847686
 C,0,2.7331905633,1.6084923646,12.3516633744
 C,0,3.752138294,0.6981233849,12.0926426309
 C,0,4.4939348847,0.8210051517,10.9255910209
 C,0,4.2022719661,1.8541972786,10.044728239
 C,0,3.1719366675,2.7379233598,10.3481985396
 C,0,-0.931305132,7.0081070173,11.5942535129
 C,0,-2.4217614362,4.8618409222,12.7454672929
 C,0,3.3606880073,4.4069538984,14.43243766
 C,0,3.017506859,6.6483708902,12.7071991144
 C,0,-2.7506005522,7.9440426646,15.2887913996
 C,0,-2.6432848101,5.3830048913,16.5990116435
 C,0,1.7497946933,5.1117818794,17.834091206
 C,0,2.7459841567,7.6000206175,16.8194364242
 C,0,-3.9890264227,7.9651589942,18.9522648864
 N,0,0.7835327193,8.3781096145,19.500217171
 C,0,-2.7722585378,10.4273396247,18.1090408739
 H,0,-1.2659733631,9.9277976251,20.7595312696
 H,0,-2.0070842694,8.3971971624,21.2594110157
 H,0,-3.0256504188,9.8339352468,21.0078820587
 H,0,-1.6763685046,7.6916373098,12.0163868347
 H,0,-1.248944444,6.6894811477,10.596326045
 H,0,0.0169936878,7.5417053502,11.4938490026
 H,0,-3.1331009129,5.5933367543,13.1442020135
 H,0,-2.4323893124,3.9619169867,13.3660894109
 H,0,-2.7377901942,4.5763677015,11.7365174451
 H,0,3.8433529044,5.0767940347,15.1525612788
 H,0,4.1209260481,4.0230175589,13.7437794745
 H,0,2.921311543,3.5537803782,14.9547706071
 H,0,3.4914227605,7.2688523997,13.4758532961
 H,0,2.3571134992,7.2756666426,12.1037858891
 H,0,3.7883096093,6.2337819961,12.0490870258
 H,0,-3.5801222575,8.215657734,15.9493601886
 H,0,-3.1647413619,7.4737728586,14.3918450308
 H,0,-2.2203022175,8.8489425352,14.9809192525

H,0,-3.4342791236,5.6984408511,17.2851878779
 H,0,-2.0323074687,4.619488807,17.0870865984
 H,0,-3.0966480239,4.9336688767,15.7102107104
 H,0,2.1023898894,5.4162494901,18.8257396698
 H,0,2.5585473333,4.5847378309,17.3182053661
 H,0,0.9127790388,4.4178831916,17.9468059243
 H,0,3.1017676763,7.811893753,17.833380598
 H,0,2.5443881584,8.5416240949,16.3016182364
 H,0,3.5372008885,7.0766564092,16.2734712564
 H,0,-3.8856904403,7.0185599903,19.489835245
 H,0,-4.3542041978,7.7491834264,17.9461067527
 H,0,-4.7245524851,8.5910920506,19.4681474935
 H,0,-3.0380843153,10.2840734054,17.0592966745
 H,0,-1.8991723075,11.0846186833,18.1510491851
 H,0,-3.6059644517,10.909928059,18.6296548344
 C,0,1.0341784212,7.6104643018,20.5727152316
 C,0,1.924007883,7.9879951896,21.5703741349
 C,0,2.5836496381,9.2085450828,21.4583629774
 C,0,2.3267692775,10.0042865341,20.3452461484
 C,0,1.4246787902,9.5529433778,19.3906554108
 H,0,0.5030942619,6.664487046,20.6154643095
 H,0,2.0937136041,7.3279317053,22.4145305344
 H,0,3.2872714955,9.5307236365,22.2199645693
 H,0,2.819842747,10.9607342991,20.2067057169
 H,0,1.2049901992,10.1327778809,18.4994060433

Sum of electronic and zero-point Energies=	-4204.609979
Sum of electronic and thermal Energies=	-4204.549016
Sum of electronic and thermal Enthalpies=	-4204.548072
Sum of electronic and thermal Free Energies=	-4204.712160

Full reference 59:

Gaussian 03, Revision B.03,
 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A.
 Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin,
 J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B.
 Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H.
 Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M.
 Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J.
 E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R.
 Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C.
 Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P.
 Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D.
 Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K.
 Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S.
 Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P.
 Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-
 Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B.
 Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian,
 Inc., Pittsburgh PA, 2003.