

## **Synthesis, Structural and Theoretical Studies of Dithiodiglycolamide Compounds of Palladium (II)**

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## Optimized Coordinates of Pd-nitrates in *cis* and *trans* isomers

### *cis*-[Pd(NO<sub>3</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>]

Pd	-0.0000525	-0.3423654	0.0000000
O	1.4208802	-1.9490511	-0.0000000
O	-1.4209345	-1.9493952	-0.0000000
O	1.2627420	1.2363678	-0.0000000
O	3.1686334	0.0314086	0.0000000
O	-1.2627653	1.2363698	-0.0000000
O	-3.1686483	0.0313844	0.0000000
O	-3.1932641	2.2268685	0.0000000
O	3.1932949	2.2268582	0.0000000
N	-2.6169700	1.1521919	0.0000000
N	2.6169566	1.1520836	0.0000000
H	-2.0091130	-1.7193393	0.7509854
H	-2.0091130	-1.7193393	-0.7509854
H	2.0091767	-1.7191769	-0.7509612
H	2.0091767	-1.7191769	0.7509612

### *trans*-[Pd(NO<sub>3</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>]

Pd	-0.0003645	-0.0004607	0.0004046
N	0.4526779	-0.1485355	2.9778434
O	-0.4244248	-0.2777228	1.9661330
O	1.6729514	0.0716106	2.7262129
O	-0.0022148	-0.2574605	4.1000019
N	-0.4525226	0.1482621	-2.9770943
O	0.4242555	0.2777202	-1.9651097
O	-1.6725067	-0.0726840	-2.7255323
O	0.0023856	0.2576627	-4.0989338
O	2.0413204	-0.2512796	0.2280343
H	2.5324479	0.4277819	-0.2715446
O	-2.0417686	0.2521080	-0.2285525
H	-2.5336582	-0.4278471	0.2691570
H	-2.1054672	0.0645910	-1.2346554
H	2.1068889	-0.0637463	1.2336355

## Optimized Coordinates of Pd-complexes with dithiodiglycolamide ligand

### [PdL<sub>1</sub>(Che)]<sup>2+</sup>

Pd	-0.0096070	-0.8782384	-0.0465071
C	-0.8043064	-0.1123116	2.9324235
C	0.5582550	0.4821879	2.5828183
H	-1.4799434	0.6554680	3.3332575
H	-0.7276294	-0.9139335	3.6803322
H	1.1188498	0.7121874	3.5006662
H	0.4719088	1.3826461	1.9637406

S	-1.6706871	-0.9895545	1.4979857
S	1.5485237	-0.7926608	1.5993915
C	-2.7335300	0.2676928	0.5895828
H	-2.2908971	1.2668176	0.7061389
H	-3.7298812	0.2422187	1.0420103
C	-2.6906755	-0.1447722	-0.8820506
O	-1.5880000	-0.5923463	-1.3740062
N	-3.7675221	-0.0246394	-1.6475380
C	2.8030494	0.2136257	0.6286198
H	3.7796757	0.0279816	1.0870937
H	2.5446913	1.2771215	0.7361769
C	2.7126265	-0.1975559	-0.8389905
O	1.5781315	-0.5525662	-1.3328559
N	3.7930827	-0.1574070	-1.6084128
C	-3.7306166	-0.4738392	-3.0551004
H	-4.6456006	-1.0447711	-3.2576460
H	-2.8523005	-1.1009756	-3.2236862
C	-5.0485884	0.5585421	-1.2013791
H	-4.9032812	1.2907734	-0.4013359
H	-5.7375877	-0.2334092	-0.8749491
C	3.7208654	-0.6019235	-3.0157416
H	2.7945363	-1.1555625	-3.1845964
H	4.5869768	-1.2450362	-3.2173044
C	5.1135854	0.3327442	-1.1669222
H	5.0273625	1.0401990	-0.3367457
H	5.5772944	0.8622910	-2.0074514
H	-3.6951691	0.4009096	-3.7188667
H	-5.4955000	1.0832915	-2.0536825
H	5.7584489	-0.5110735	-0.8829389
H	3.7564865	0.2725871	-3.6797984

$[(\text{PdL}_1(\text{H}_2\text{O})_2)]^{2+}$

Pd	0.0521408	0.1207923	0.2300257
S	-2.0481866	0.7709417	0.9346639
S	-0.2894582	1.2479250	-1.7706977
O	-1.6848493	-0.8466922	3.3259467
C	-2.0424894	1.4392085	2.6801851
H	-1.0757829	1.9196811	2.8841854
H	-2.8422946	2.1886135	2.7086672
C	-2.2626429	2.3396584	-0.0501034
H	-3.3081208	2.6585710	0.0735200
H	-1.5956520	3.1152370	0.3462001
C	-2.2594318	0.2408945	3.6118829
N	2.9469451	3.2856333	-2.8435552
N	-3.0521195	0.3717163	4.6785737
C	0.7964660	2.7697012	-1.7473402
H	0.3005661	3.4844239	-2.4161538
H	0.8459460	3.1898154	-0.7334854

C	-1.9747926	2.0040012	-1.5014275
H	-2.0499769	2.8913681	-2.1445129
H	-2.6684698	1.2470992	-1.8942089
C	2.1944510	2.3609195	-2.2379447
C	2.5428798	4.6834256	-3.0645560
H	1.8312382	5.0263858	-2.3060672
C	-3.7293643	1.6138069	5.0873489
H	-3.1928898	2.5034509	4.7427569
C	4.2760821	2.9187933	-3.3685136
H	4.3348854	3.2191033	-4.4232573
C	-3.2984839	-0.7948631	5.5485907
H	-4.3812375	-0.8965579	5.7003568
O	2.5890069	1.1779988	-2.0665820
H	-2.9012591	-1.6957736	5.0760500
H	-2.8108924	-0.6384821	6.5206177
H	-3.7451198	1.6478811	6.1832936
H	-4.7676120	1.6298601	4.7246929
H	4.4188572	1.8395497	-3.2810338
H	5.0545657	3.4446147	-2.7989616
H	2.1155783	4.8134367	-4.0699863
H	3.4355975	5.3150395	-2.9835930
O	0.4540026	-0.7677758	2.0542856
O	1.8915961	-0.6116212	-0.4424765
H	2.2500689	0.0970170	-1.1166972
H	1.8265094	-1.4580444	-0.9275218
H	-0.4211114	-0.9148915	2.6183115
H	1.0067801	-1.5715804	2.0325293

[PdL<sub>1</sub>(NO<sub>3</sub>)]<sup>1+</sup>

Pd	-0.3979812	0.2452032	0.1005402
S	-2.6105146	0.7053270	0.5965979
S	-0.7311143	1.2149574	-1.9769969
O	-2.4744814	-0.9180738	2.6788550
C	-2.6951342	1.4219255	2.3007146
H	-1.8754992	2.1364337	2.4507748
H	-3.6574358	1.9503921	2.3744320
C	-2.8348663	2.2575503	-0.4210689
H	-3.8962117	2.5404496	-0.3642285
H	-2.2244596	3.0688326	-0.0042728
C	-2.6072483	0.1886786	3.2191998
N	1.2549928	4.3464038	-3.5075103
N	-2.6756491	0.3844901	4.5579663
C	0.3756259	2.7006989	-1.8721225
H	0.0923250	3.3235021	-1.0125263
H	1.3698627	2.2768543	-1.6811295
C	-2.4486194	1.9236745	-1.8468617
H	-2.4634827	2.7857242	-2.5252786
H	-3.0868112	1.1373013	-2.2739323

C	0.2632098	3.4717909	-3.2043993
C	2.4303455	4.6183062	-2.6804270
H	2.3279028	4.1911378	-1.6781776
C	-2.8489934	1.6802191	5.2101856
H	-2.9195710	2.4917690	4.4787564
C	1.1944735	5.0752180	-4.7796181
H	1.1408998	6.1573143	-4.5905229
C	-2.5792716	-0.7735160	5.4531267
H	-3.4987434	-0.8627279	6.0499056
O	-0.7260893	3.2708584	-3.9230275
H	-2.4437684	-1.6759668	4.8504625
H	-1.7228460	-0.6491654	6.1317976
H	-1.9970881	1.8867488	5.8758545
H	-3.7689901	1.6802464	5.8141757
H	0.3062294	4.7530604	-5.3300205
H	2.0954379	4.8606462	-5.3727182
H	2.5539050	5.7052863	-2.5694152
H	3.3402015	4.2122053	-3.1495078
O	0.4606254	-0.6941629	1.7904505
N	1.6130823	-0.8389650	1.1867876
O	1.6001528	-0.3513358	-0.0433193
O	2.5751976	-1.3522200	1.6802583

$[(\text{PdL}_1(\text{NO}_3)_2)]^0$

Pd	1.1124482	0.3317705	1.2171140
S	-1.1753943	0.5508098	1.5796924
S	0.7566644	0.7676512	-1.0405269
O	-3.3815927	3.1437308	2.0874240
C	-1.4617972	1.9223522	2.7997858
H	-1.0213444	1.5524286	3.7293350
H	-0.9209405	2.8079912	2.4518658
C	-1.7588400	1.3999693	0.0192437
H	-2.8502598	1.2868820	-0.0229574
H	-1.5431589	2.4721486	0.0981933
C	-2.9481851	2.2879968	2.8709329
N	2.1450322	3.2277880	-3.4259956
N	-3.7311484	1.6520301	3.7940620
C	1.1046971	2.5846044	-1.2539151
H	0.3364709	3.1528204	-0.7173451
H	2.0678684	2.7278247	-0.7572337
C	-1.0964812	0.7589686	-1.1792624
H	-1.3279446	1.3013484	-2.1077930
H	-1.3620227	-0.3010779	-1.2924899
C	1.0025577	2.9340021	-2.7366053
C	3.5149926	3.2076278	-2.9130844
H	3.5685078	2.8866003	-1.8698693
C	-3.2941338	0.6209539	4.7353733
H	-3.2573392	1.0219011	5.7616518

C	2.0286306	3.5905156	-4.8388278
H	2.4758458	4.5819779	-5.0078022
C	-5.1314499	2.0547019	3.9164282
H	-5.3318058	2.4111512	4.9389360
O	-0.1223245	2.9363132	-3.2619863
H	-5.3309480	2.8571647	3.2000838
H	-5.7927374	1.1992429	3.7084098
H	-2.3141921	0.2093458	4.4779959
H	-4.0169201	-0.2083291	4.7182355
H	0.9696768	3.6084386	-5.1119697
H	2.5588906	2.8548834	-5.4635029
H	3.9606367	4.2118183	-2.9918242
H	4.1232061	2.5138537	-3.5138953
O	1.7265271	-0.0431580	3.1532928
O	3.0711295	-0.1985465	0.8001395
N	0.9561360	-0.5289710	4.1406563
O	1.5301705	-0.7640181	5.1977926
O	-0.2668436	-0.7042469	3.9336262
N	3.9712852	0.7774403	0.5784938
O	5.1280535	0.4093147	0.4112552
O	3.5774047	1.9645893	0.5483746

[PdL<sub>1</sub>(NO<sub>3</sub>)(H<sub>2</sub>O)]<sup>1+</sup>

Pd	-0.1328188	0.6824802	0.5024127
S	-2.4174197	0.9794765	0.7467956
S	-0.3991359	1.5035705	-1.6821087
O	-2.9859169	-0.9514113	2.4509563
C	-2.7075152	1.4175043	2.5186987
H	-1.8267105	1.9317547	2.9215304
H	-3.5850370	2.0803826	2.5493030
C	-2.4484843	2.6582235	-0.0733793
H	-3.4811671	3.0362374	-0.0361155
H	-1.7836051	3.3544884	0.4513295
C	-2.9610736	0.0484028	3.1816121
N	2.9220842	3.0929639	-3.1578841
N	-3.1538015	0.0251579	4.5214819
C	0.7981886	2.9164300	-1.9003533
H	0.3304698	3.6018500	-2.6175148
H	0.9561326	3.4342035	-0.9444836
C	-2.0233431	2.4292957	-1.5168166
H	-1.9352795	3.3718872	-2.0717726
H	-2.7435423	1.7916225	-2.0473458
C	2.1093482	2.3090273	-2.4216346
C	2.6784498	4.5071860	-3.4576518
H	1.9977144	4.9623831	-2.7312505
C	-3.0517231	1.1891742	5.3979533
H	-3.0917493	2.1239343	4.8288913
C	4.1513601	2.5239615	-3.7285148

H	4.1774131	2.7310999	-4.8074568
C	-3.3305354	-1.2668996	5.1919266
H	-4.2478145	-1.2466863	5.7974768
O	2.3747560	1.1143057	-2.1643222
H	-3.4053957	-2.0507932	4.4331621
H	-2.4701243	-1.4721085	5.8460522
H	-2.1129550	1.1641616	5.9736662
H	-3.8943637	1.1898172	6.1039424
H	4.1593558	1.4443790	-3.5585042
H	5.0325159	2.9789945	-3.2538591
H	2.2726954	4.6335113	-4.4733764
H	3.6324387	5.0469525	-3.3962892
O	-0.0180990	0.1584012	2.4721775
O	1.9406401	0.4536112	0.3208200
N	0.7238428	-0.9195518	2.8773317
O	0.6043814	-1.2031857	4.0542945
O	1.4445308	-1.5044598	2.0485382
H	2.0846227	-0.4316313	0.7496675
H	2.2218618	0.4766284	-0.6433226

[PdL<sub>2</sub>]<sup>2+</sup>

Pd	-0.1008409	-0.1621162	-0.1001387
S	-2.2558083	0.5639555	0.6148893
S	-0.4716898	1.0536206	-2.1339853
O	-2.4750268	-0.8576935	2.9514577
C	-2.2727365	1.4199264	2.2607004
H	-1.3249758	1.9511972	2.4186508
H	-3.0882164	2.1545546	2.1996626
C	-2.5231977	2.0498352	-0.4781752
H	-3.5816152	2.3303031	-0.3706209
H	-1.8974184	2.8822203	-0.1321736
C	-2.5263439	0.3316940	3.3166052
N	1.0351281	4.5898923	-3.3092461
N	-2.7870453	0.7271123	4.5796123
C	0.5257621	2.6022375	-1.9189417
H	0.2638817	3.0958700	-0.9737501
H	1.5581449	2.2358179	-1.8728350
C	-2.2136945	1.6512445	-1.9004019
H	-2.3272059	2.4792802	-2.6128202
H	-2.8388749	0.8142208	-2.2419632
C	0.2636397	3.4877992	-3.1559058
C	2.1068752	5.0054638	-2.4049651
H	2.2036459	4.3240242	-1.5542797
C	-2.8623701	2.1199093	5.0278448
H	-2.5135470	2.8126247	4.2556492
C	0.8163114	5.4612944	-4.4709005
H	0.5350732	6.4697454	-4.1344206

C	-3.0571746	-0.2817404	5.6126817
H	-4.0523961	-0.1083437	6.0460060
O	-0.6402827	3.1584285	-3.9401629
S	2.0523133	-0.8892772	-0.8212447
S	0.2722678	-1.3751043	1.9339952
O	2.2470977	0.4977143	-3.1803809
C	2.0493653	-1.7698741	-2.4542542
H	1.1027821	-2.3099469	-2.5879047
H	2.8712038	-2.4979218	-2.3961992
C	2.3362437	-2.3596461	0.2891582
H	3.3977711	-2.6286890	0.1842235
H	1.7204765	-3.2030640	-0.0480871
C	2.2801396	-0.6966821	-3.5307974
N	-1.2067003	-4.9274929	3.0988014
N	2.5019282	-1.1110963	-4.7952211
C	-0.7081163	-2.9338900	1.7136014
H	-0.4408360	-3.4222043	0.7671107
H	-1.7434543	-2.5761827	1.6672858
C	2.0222230	-1.9510527	1.7072345
H	2.1457821	-2.7709994	2.4273910
H	2.6356913	-1.1021061	2.0405399
C	-0.4389162	-3.8225814	2.9465729
C	-2.2809472	-5.3431963	2.1978385
H	-2.4112419	-4.6368726	1.3724106
C	2.5595676	-2.5106179	-5.2250797
H	2.2271133	-3.1907034	-4.4345421
C	-0.9726974	-5.8083229	4.2502559
H	-1.8902987	-5.8838148	4.8512037
C	2.7489349	-0.1184224	-5.8494986
H	1.9716710	-0.1967134	-6.6227226
O	0.4673107	-3.4944504	3.7285780
H	-3.0203598	-1.2754008	5.1596385
H	-2.3029522	-0.2093804	6.4089907
H	-2.2262727	2.2522680	5.9142067
H	-3.8963909	2.3807901	5.2993287
H	0.0155315	5.0416653	-5.0858813
H	1.7408547	5.5293326	-5.0621695
H	1.9019519	6.0151499	-2.0186384
H	3.0669713	5.0286342	-2.9420420
H	2.7313938	0.8817418	-5.4098036
H	3.7300713	-0.3047970	-6.3086372
H	3.5855392	-2.7805199	-5.5175391
H	1.9016420	-2.6525429	-6.0939703
H	-2.0580956	-6.3347207	1.7757967
H	-3.2301597	-5.4081822	2.7501398
H	-0.1661123	-5.3919081	4.8597655
H	-0.6927547	-6.8131024	3.9018600



Optimized coordinates of Pf complexed with thiodiglycolamide ligand

*cis*-[PdL<sub>2</sub>]<sup>2+</sup>

Pd	-0.1611405	-0.0720192	0.7573604
S	-0.8907654	1.4485718	-0.8053839
S	-0.8712486	-2.0745336	-0.1216415
C	-0.5388783	-2.3680476	-1.9188805
H	-0.3961475	-3.4511383	-2.0406462
H	0.3601682	-1.8115816	-2.2174644
C	0.5482226	-3.0722068	0.6009611
H	1.4563790	-2.8818417	0.0105951
H	0.2793358	-4.1316155	0.5349629
C	-1.4619259	2.6934677	0.4633665
H	-1.5400639	3.6742372	-0.0209706
H	-2.4756015	2.3671066	0.7408053
C	0.6326041	2.3605170	-1.3666372
H	1.2540251	2.6206391	-0.4988077
H	0.2616315	3.2789765	-1.8429363
C	1.3779869	1.4308767	-2.3346972
O	1.0528545	0.2276442	-2.3578591
N	2.3536683	1.9656620	-3.0994722
C	-1.7994004	-1.8007178	-2.5844059
O	-2.5212522	-1.0662991	-1.8825857
N	-2.0489998	-2.1192743	-3.8704718
C	0.7559911	-2.5662554	2.0115562
O	0.5757386	-1.3161042	2.2461591
N	1.1286245	-3.3786775	2.9969844
C	-0.5461627	2.6728517	1.6770676
O	0.2020670	1.6509091	1.8804919
N	-0.5252043	3.6978387	2.5274770
C	-3.2802699	-1.6364907	-4.5082736
C	-1.1986693	-2.9866123	-4.6890159
C	1.4713076	-4.8003909	2.8258207
C	1.2688382	-2.8614788	4.3710080
C	-1.3741519	4.8943582	2.4065293
C	0.3712508	3.6801033	3.6984793
C	2.7750142	3.3693393	-3.0824801
C	3.1037613	1.1041614	-4.0228718
H	2.3326611	-2.7314596	4.6140525
H	0.8283597	-3.5916711	5.0618229
H	0.7526669	-1.9028556	4.4602525
H	1.6736327	-5.0436320	1.7793347
H	0.6589805	-5.4351063	3.2077862
H	2.3819218	-5.0078463	3.4016881
H	-0.1931953	-3.0755302	-4.2640785
H	-1.0986113	-2.5483917	-5.6910607
H	-1.6412969	-3.9895111	-4.7921306
H	-3.8549741	-1.0568633	-3.7806908
H	-3.8784285	-2.4924406	-4.8522834

H	-3.0309214	-1.0058287	-5.3733621
H	2.7162456	3.7854662	-4.0983009
H	2.1449788	3.9744054	-2.4240904
H	3.8153980	3.4466871	-2.7338424
H	4.1802365	1.2044569	-3.8258051
H	2.7957405	0.0662426	-3.8758645
H	2.9029757	1.4045436	-5.0613407
H	-0.7824773	5.7492596	2.0483669
H	-1.7728189	5.1361936	3.3998741
H	-2.2211209	4.7230145	1.7364969
H	1.0489214	2.8260461	3.6328443
H	-0.2283864	3.6088762	4.6163231
H	0.9463941	4.6154018	3.7183024

*trans*-[PdL<sub>2</sub>]<sup>2+</sup>

Pd	0.0754208	0.0494988	-0.0041058
S	-0.5141742	2.1409550	-0.9077887
S	0.6691815	-2.0418252	0.8941992
C	2.4480906	-1.9519415	0.3039688
H	2.5010113	-2.3168339	-0.7320395
H	3.0388312	-2.6158207	0.9452970
C	0.1461694	-3.4986802	-0.1301316
H	0.9184148	-4.2690220	0.0038020
H	0.0945398	-3.2108904	-1.1891737
C	-2.3014233	2.0491054	-0.3435022
H	-2.3721867	2.4319469	0.6851970
H	-2.8894861	2.6958705	-1.0049852
C	-0.0054950	3.5960553	0.1262357
H	0.0197659	3.3095293	1.1864598
H	-0.7701003	4.3706430	-0.0267836
C	1.3837464	3.9711930	-0.4115462
O	1.9659178	3.1294232	-1.1181322
N	1.8803311	5.1862638	-0.0932199
C	2.9116698	-0.5118991	0.3395650
O	2.0436521	0.4369515	0.3316090
N	4.2037490	-0.1979659	0.3366926
C	-1.2300443	-3.8773249	0.4373112
O	-1.8116033	-3.0242557	1.1307336
N	-1.7169893	-5.1058168	0.1580217
C	-2.7588317	0.6065659	-0.3624470
O	-1.8912357	-0.3411482	-0.3421426
N	-4.0534950	0.3009815	-0.3638663
C	-2.9863836	-5.5317957	0.7610901
C	-1.0456757	-6.1027923	-0.6808012
C	-4.4683773	-1.1152416	-0.3234399
C	-5.1296650	1.2965698	-0.5030253

C	1.2077081	6.1687921	0.7613108
C	3.1650630	5.6121808	-0.6626879
C	4.6053052	1.2219257	0.2729556
C	5.3093519	-1.1640826	0.4161167
H	-0.2626840	-5.6487193	-1.2971898
H	-1.7813835	-6.5539712	-1.3603722
H	-0.6061825	-6.9025912	-0.0650534
H	-2.8359850	-6.4805158	1.2951903
H	-3.3223434	-4.7656722	1.4652157
H	-3.7463078	-5.6810456	-0.0195239
H	-3.6621072	-1.7218636	0.1023147
H	-4.7066408	-1.4649889	-1.3384068
H	-5.3644123	-1.1919148	0.3031724
H	-4.8200142	2.2763659	-0.1272682
H	-5.9857108	0.9616445	0.0938061
H	-5.4441678	1.3833504	-1.5533740
H	0.8000721	6.9967246	0.1611533
H	0.3993374	5.7113725	1.3412939
H	1.9339629	6.5826493	1.4741901
H	3.9144916	5.7265555	0.1340231
H	3.0367281	6.5791250	-1.1691384
H	3.5018289	4.8635773	-1.3850274
H	5.5300542	1.2879799	-0.3117652
H	3.8141374	1.8098757	-0.2051543
H	4.7924352	1.6020930	1.2874853
H	5.9111086	-0.9565280	1.3115770
H	4.9474788	-2.1939200	0.4614755
H	5.9455437	-1.0548417	-0.4725998

*trans*-[PdL<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>]<sup>2+</sup>

Pd	-3.1485040	0.4384435	-0.1582079
S	-2.7290733	-1.9004705	-0.4320817
C	-4.2532646	-2.9348959	-0.1080261
C	-1.6275323	-2.4704907	0.9381392
C	-5.4832836	-2.3934505	-0.8358161
H	-3.9723938	-3.9566166	-0.3830408
H	-4.4549929	-2.8827426	0.9690692
H	-1.3772374	-3.5145451	0.7040888
H	-0.7117889	-1.8753370	0.8060477
C	-2.1905149	-2.3191094	2.3679635
N	-6.0550297	-3.1386856	-1.7989378
O	-5.9566657	-1.2872574	-0.4721910
N	-1.4957045	-2.9233981	3.3492529
O	-3.2455054	-1.6823048	2.5878716
C	-7.3440964	-2.7114040	-2.3691890
C	-5.5421820	-4.4284116	-2.2895005
C	-0.2547970	-3.6854835	3.1508892
C	-2.0058707	-2.8923169	4.7302939

H	-7.2243675	-2.5113562	-3.4431965
H	-8.0821868	-3.5142846	-2.2355346
H	-7.6839914	-1.8070027	-1.8594113
H	-4.4479831	-4.4370666	-2.3404882
H	-5.9171399	-4.5754787	-3.3086351
H	-5.8980843	-5.2634301	-1.6679648
H	0.2967137	-3.3453973	2.2683433
H	-0.4622231	-4.7628194	3.0624344
H	0.3904861	-3.5293254	4.0241918
H	-2.9843151	-2.4064823	4.7447099
H	-1.3073684	-2.3368534	5.3714267
H	-2.0943679	-3.9211873	5.1056519
O	-4.6200210	0.0902455	1.2238932
H	-5.2834548	-0.4612046	0.6511710
O	-1.6143680	0.8328893	-1.4740722
H	-1.5678548	0.2140246	-2.2259077
H	-4.1755794	-0.5657351	1.8522015
H	-1.6417714	1.8537570	-1.8706210
H	-2.1479534	3.0184957	1.7623356
C	-2.2967511	3.5550594	0.8155244
S	-3.7647783	2.7161161	0.0553083
C	-2.6612951	5.0415587	0.9982932
H	-1.4141231	3.4108059	0.1777337
C	-3.9192960	3.4368006	-1.6556968
N	-1.8878334	5.7839642	1.8203893
O	-3.6475805	5.4828054	0.3821184
H	-4.3518310	2.6231737	-2.2567680
H	-4.6559932	4.2340621	-1.5402509
C	-2.6290759	3.8957620	-2.3082014
C	-2.2410037	7.1891459	2.0646532
C	-0.6916679	5.3043417	2.5152167
N	-2.6083552	5.0852026	-2.9152944
O	-1.6092819	3.1350818	-2.3140030
H	-2.2798644	7.3697252	3.1478284
H	-1.4859703	7.8537471	1.6198561
H	-3.2189412	7.3951486	1.6214587
H	-0.3906882	4.3129038	2.1623964
H	-0.8662958	5.2620107	3.6010761
H	0.1416820	5.9955674	2.3249060
C	-3.7344739	6.0429480	-2.8905738
C	-1.4193180	5.4990573	-3.6801755
H	-4.0571121	6.2289265	-1.8585322
H	-4.5728578	5.6887738	-3.5060109
H	-3.3770205	6.9863085	-3.3148693
H	-1.7168093	5.7162233	-4.7149326
H	-0.6754204	4.6995729	-3.6664820
H	-0.9958886	6.4085447	-3.2321973

*trans*-[PdL<sub>2</sub>(NO<sub>3</sub>)<sub>2</sub>]<sup>0</sup>

Pd	-2.368339	0.236098	-0.528098
S	-1.727551	-2.054002	-0.815213
C	-3.241441	-3.040497	-1.131128
C	-1.037782	-2.715345	0.786942
C	-4.451226	-2.656216	-0.263162
H	-3.435597	-2.877056	-2.197457
H	-2.960345	-4.089252	-0.953253
H	-0.244410	-3.405640	0.475036
H	-0.590327	-1.841449	1.270171
C	-2.002459	-3.533175	1.642079
N	-5.647689	-3.175874	-0.666957
O	-4.329514	-1.939704	0.736891
N	-2.391286	-3.035660	2.851940
O	-2.319316	-4.665484	1.244536
C	-6.868762	-2.765295	0.024106
C	-5.835932	-3.933309	-1.903017
C	-2.338023	-1.631279	3.250847
C	-3.268126	-3.867490	3.673631
H	-7.486050	-2.135506	-0.635897
H	-7.448303	-3.652271	0.321296
H	-6.589939	-2.190736	0.912225
H	-4.967991	-4.566238	-2.119037
H	-6.025670	-3.263625	-2.758094
H	-6.701969	-4.596825	-1.776632
H	-1.662380	-1.049693	2.618992
H	-1.993551	-1.560944	4.293472
H	-3.341325	-1.184843	3.169340
H	-3.006768	-3.729288	4.732280
H	-3.141668	-4.915495	3.386305
H	-4.322458	-3.580745	3.525878
O	-3.772332	-0.214715	-1.963220
O	-0.864781	0.432686	0.849294
H	-1.093461	2.771444	1.163195
C	-1.461492	3.389136	0.331998
S	-2.975207	2.522679	-0.269498
C	-1.807819	4.802476	0.827332
H	-0.714889	3.391106	-0.470784
C	-3.004557	3.151733	-2.017727
N	-0.739479	5.589141	1.159853
O	-2.981754	5.171641	0.943314
H	-2.087135	2.816532	-2.511015
H	-3.872403	2.662404	-2.470822
C	-3.030510	4.681166	-2.106370
C	-0.980220	6.977661	1.544116
C	0.656350	5.220226	0.930222
N	-4.234399	5.315041	-1.992083
O	-1.965307	5.274930	-2.325008
H	-0.443484	7.207193	2.476738
H	-0.631952	7.663626	0.754681
H	-2.055219	7.115241	1.694444

H	0.811173	4.141479	1.037038
H	1.279779	5.717907	1.685635
H	1.000066	5.535029	-0.069343
C	-5.456986	4.700996	-1.479586
C	-4.249066	6.774968	-2.037735
H	-5.436136	3.610987	-1.567068
H	-6.317284	5.076646	-2.053069
H	-5.593977	4.956537	-0.416655
H	-5.123017	7.112491	-2.613453
H	-3.328078	7.123816	-2.514248
H	-4.308544	7.190270	-1.018412
N	-5.065873	0.183135	-1.918225
O	-5.830230	-0.444570	-2.655829
O	-5.387068	1.130421	-1.186772
N	0.383133	0.742280	0.352708
O	0.508629	0.910053	-0.862592
O	1.265187	0.831575	1.205164

*trans*-[PdL<sub>2</sub>(H<sub>2</sub>O)(NO<sub>3</sub>)]<sup>1+</sup>

Pd	-2.7468072	0.4092480	-0.7556424
S	-2.2525454	-1.8928174	-1.2162460
C	-3.5834707	-3.0241613	-1.8437790
C	-1.6551671	-2.6645558	0.3554763
C	-4.9717821	-3.0032653	-1.2174568
H	-3.6902594	-2.7019973	-2.8916311
H	-3.1230197	-4.0168234	-1.8445803
H	-1.2871106	-3.6610821	0.0747304
H	-0.7974832	-2.0365716	0.6157418
C	-2.7204009	-2.8411262	1.4340707
N	-5.5968050	-4.1762437	-1.0297563
O	-5.5697149	-1.9105035	-1.0231041
N	-2.5356341	-2.2372189	2.6390057
O	-3.6961132	-3.5647680	1.1742006
C	-6.9813357	-4.1787286	-0.5401155
C	-4.9087204	-5.4762710	-1.0642139
C	-1.3850825	-1.4065910	3.0128098
C	-3.4812203	-2.5255478	3.7223414
H	-7.5580425	-4.9261744	-1.0997316
H	-7.0003691	-4.4296223	0.5307168
H	-7.4180913	-3.1878167	-0.6850309
H	-4.5576871	-5.7258630	-2.0749977
H	-5.6269857	-6.2454976	-0.7636899
H	-4.0774146	-5.4824810	-0.3465155
H	-0.9992148	-0.8360581	2.1616571
H	-0.5765295	-2.0132553	3.4505207
H	-1.7179529	-0.6855120	3.7702339
H	-2.9509210	-2.9854929	4.5695541

H	-4.2475968	-3.2114385	3.3515576
H	-3.9540730	-1.5934073	4.0650935
O	-4.7217990	0.3682796	-1.4365306
O	-0.8778764	0.4098117	0.0144026
H	-1.3022961	2.6615552	1.1634705
C	-1.5986800	3.4087848	0.4159999
S	-3.0855528	2.7222702	-0.4362184
C	-1.9950346	4.7624472	1.0347974
H	-0.8024230	3.5167920	-0.3310695
C	-2.8302016	3.3958698	-2.1492186
N	-1.0007845	5.4497363	1.6551378
O	-3.1674147	5.1553719	0.9586782
H	-1.8959152	2.9721887	-2.5320735
H	-3.6783507	3.0202498	-2.7327906
C	-2.6640545	4.9251376	-2.1231632
C	-1.2847553	6.7864711	2.1815526
C	0.4091474	5.0589990	1.6230065
N	-3.7748779	5.7052708	-2.2388363
O	-1.5142246	5.3711623	-2.0304921
H	-0.8926201	6.8700141	3.2047808
H	-0.8097874	7.5558273	1.5528962
H	-2.3674678	6.9406897	2.1873974
H	0.5237847	3.9717745	1.5578485
H	0.8880434	5.3875315	2.5546724
H	0.9354303	5.5249318	0.7745387
C	-5.1481125	5.2367203	-2.0690727
C	-3.6029665	7.1593279	-2.1841063
H	-5.2554493	4.1881045	-2.3642828
H	-5.8106316	5.8332176	-2.7106407
H	-5.4711953	5.3472147	-1.0214602
H	-4.2789651	7.6302685	-2.9105632
H	-2.5652209	7.4042212	-2.4263624
H	-3.8379655	7.5355248	-1.1758710
N	0.1529649	0.8125270	-0.8443722
O	-0.1544250	1.1855427	-1.9740086
O	1.2638867	0.7513090	-0.3441036
H	-5.0772005	-0.6321267	-1.2937667
H	-5.2874248	0.9311986	-0.8754936