Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Mechanistic study of the solvent-controlled Pd(II)-catalyzed chemoselective intermolecular 1,2-aminooxygenation and 1,2-oxyamination of conjugated dienes

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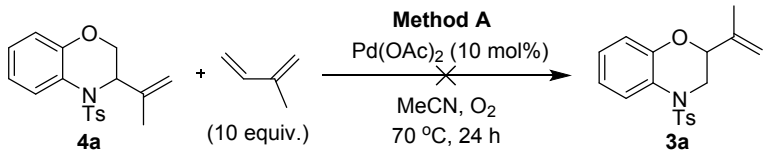
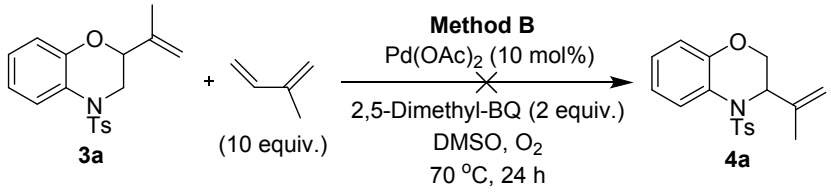
1. Experimental studies

1.1 The transformation between 3a and 4a

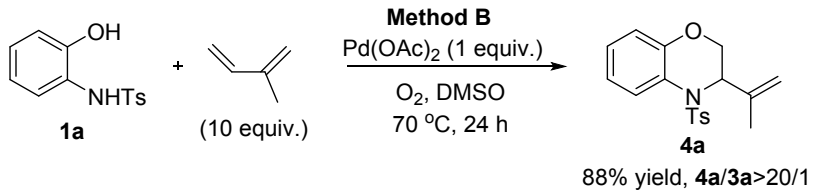


To a sealed tube (15 mL) were added **4a** (32.9 mg, 0.10 mmol, 1 equiv.), $Pd(OAc)_2$ (2.2 mg, 0.1 equiv.), followed by the solvent MeCN (1 mL). Afterwards, the system was degassed and recharged with O_2 balloon three times. Finally, the isoprene (1.0 mmol, 10 equiv.) was added and the tube was sealed and heated to 70 °C. After stirring for 24 h, the reaction mixture was cooled to room temperature, and the solvent was removed by rotary evaporation. The residue was purified by preparative TLC on silica gel (normal ratio: petroleum ether/EtOAc = 5/1) to give the substrate **4a**, and no product **3a** was detected.



To a sealed tube (15 mL) were added substrate **3a** (32.9 mg, 0.10 mmol, 1 equiv.), $Pd(OAc)_2$ (2.2 mg, 0.1 equiv.), 2,5-dimethyl-BQ (27.2 mg, 0.20 mmol, 2 equiv.), followed by the solvent DMSO (1 mL). Afterwards the system was degassed and recharged with O_2 balloon three times. Finally, the isoprene (1.0 mmol, 10 equiv.) was added and the tube was sealed and heated to 70 °C. After stirring for 24 h, the reaction mixture was cooled to room temperature, the mixture was purified by preparative TLC on silica gel (normal ratio: petroleum ether/EtOAc = 5/1) to give the substrate **3a**, and no product **4a** was detected.

1.2 The selectivity in the absence of quinone



To a sealed tube (15 mL) were added **1a** (52.7 mg, 0.20 mmol, 1 equiv.), $Pd(OAc)_2$ (45.0 mg, 1 equiv.), followed by the solvent DMSO (2 mL). Afterwards the system was degassed and recharged with O_2 (balloon) three times. Finally, the isoprene (2.0 mmol, 10 equiv.) was added and the tube was sealed and heated to 70 °C. After stirring for 24 h, the reaction mixture was cooled to room temperature, the mixture was purified by preparative TLC on silica gel (normal ratio: petroleum ether/EtOAc = 5/1) to give products **4a** and **3a** in 88% total yield (**4a**/**3a**>20/1).

2. DFT Calculation

Species	Zero-point Energy, a.u.	Free Energy (298 K), a.u.
2b in MeCN	**-155.854724**	**-155.880697**
2b in DMSO	**-155.852173**	**-155.878116**
Molecule MeCN	**-132.672753**	**-132.695694**
Molecule DMSO	**-553.057410**	**-553.085680**
5	**-1573.410357**	**-1573.470977**
Ts1-a	**-1596.558636**	**-1596.616150**
Ts1-b	**-1596.555862**	**-1596.613359**
Ts1-c	**-1463.862145**	**-1463.913815**
Ts1-d	**-1463.854251**	**-1463.905528**
6	**-1596.587907**	**-1596.646871**
Ts2	**-1596.573505**	**-1596.631331**
7	**-1596.594704**	**-1596.652483**
Ts3	**-1596.567801**	**-1596.627064**
8	**-1596.606763**	**-1596.665069**
9a	**-2414.195726**	**-2414.256705**
9b	**-2414.185190**	**-2414.244936**
9c	**-2414.194452**	**-2414.256530**
9d	**-2414.191797**	**-2414.251469**
9e	**-1861.086890**	**-1861.141050**
9f	**-1861.086908**	**-1861.140782**
Ts4-a	**-2016.946852**	**-2017.004274**
Ts4-b	**-2016.940911**	**-2016.999765**
Ts4-c	**-2016.941314**	**-2017.000935**
Ts4-d	**-2016.942286**	**-2017.001147**
Ts4-e	**-1463.848749**	**-1463.899688**

Ts4-f	**-1463.857146**	**-1463.908376**
10	**-2016.967280**	**-2017.026028**
Ts5	**-2016.956126**	**-2017.014741**
11	**-2016.979215**	**-2017.036087**
Ts6	**-2016.954090**	**-2017.012222**
12	**-2016.995547**	**-2017.054466**

The details include Cartesian coordinates, computed geometries of compounds, transition states, and computed total energies.

1,3-Butadiene **2b** in MeCN:
Sum of electronic and zero-point Energies= -155.854724
Sum of electronic and thermal Energies= -155.850088
Sum of electronic and thermal Enthalpies= -155.849144
Sum of electronic and thermal Free Energies= -155.880697
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.099085	0.729496	-0.556088
2	6	0	-0.099085	1.530120	0.494149
3	1	0	0.412111	1.167913	-1.502683
4	1	0	-0.460834	1.145569	1.445112
5	1	0	0.083075	2.598745	0.429209
6	6	0	-0.099085	-0.729496	-0.556088
7	6	0	0.099085	-1.530120	0.494149
8	1	0	-0.412111	-1.167913	-1.502683
9	1	0	0.460834	-1.145569	1.445112
10	1	0	-0.083075	-2.598745	0.429209

1,3-Butadiene **2b** in DMSO:
Sum of electronic and zero-point Energies= -155.852173
Sum of electronic and thermal Energies= -155.847557
Sum of electronic and thermal Enthalpies= -155.846612
Sum of electronic and thermal Free Energies= -155.878116

Standard orientation:

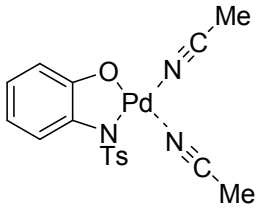
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.100670	0.729147	-0.555717
2	6	0	-0.100670	1.529698	0.493716
3	1	0	0.417950	1.166929	-1.501160
4	1	0	-0.467654	1.145870	1.442989
5	1	0	0.084165	2.597981	0.430179
6	6	0	-0.100670	-0.729147	-0.555717
7	6	0	0.100670	-1.529698	0.493716
8	1	0	-0.417950	-1.166929	-1.501160
9	1	0	0.467654	-1.145870	1.442989
10	1	0	-0.084165	-2.597981	0.430179

Molecule MeCN:
Sum of electronic and zero-point Energies= -132.672753
Sum of electronic and thermal Energies= -132.669195
Sum of electronic and thermal Enthalpies= -132.668250
Sum of electronic and thermal Free Energies= -132.695694
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.277042
2	7	0	0.000000	0.000000	1.435078
3	6	0	0.000000	0.000000	-1.178075
4	1	0	0.000000	1.028149	-1.546451
5	1	0	0.890403	-0.514074	-1.546451
6	1	0	-0.890403	-0.514074	-1.546451

Molecule DMSO:
Sum of electronic and zero-point Energies= -553.057410
Sum of electronic and thermal Energies= -553.051849
Sum of electronic and thermal Enthalpies= -553.050905
Sum of electronic and thermal Free Energies= -553.085680
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.000059	0.229282	-0.433025
2	8	0	0.000526	1.507578	0.374377
3	6	0	1.347187	-0.807999	0.180576
4	1	0	1.309299	-1.779310	-0.319309
5	1	0	2.288786	-0.310536	-0.060749
6	1	0	1.256929	-0.930647	1.263222
7	6	0	-1.347717	-0.807187	0.180593
8	1	0	-2.288999	-0.308801	-0.060085
9	1	0	-1.310856	-1.778246	-0.319850
10	1	0	-1.257130	-0.930470	1.263146



(5)

Sum of electronic and zero-point Energies= -1573.410357

Sum of electronic and thermal Energies= -1573.384290

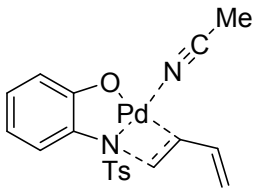
Sum of electronic and thermal Enthalpies= -1573.383345

Sum of electronic and thermal Free Energies= -1573.470977

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.982271	-2.913345	1.593300
2	6	0	-2.045230	-2.747627	0.572908
3	6	0	-1.081836	-1.746165	0.670441
4	6	0	-1.008197	-0.939509	1.820168
5	6	0	-1.956079	-1.105778	2.837382
6	6	0	-2.939034	-2.084991	2.714705
7	1	0	-3.736919	-3.689293	1.512807
8	1	0	-2.069222	-3.375965	-0.309905
9	1	0	-1.904986	-0.467187	3.714596
10	1	0	-3.669019	-2.209299	3.509761
11	8	0	-0.028985	-0.034660	1.921140

12	7	0	-0.096928	-1.469307	-0.345594
13	16	0	-0.738555	-0.923934	-1.778880
14	8	0	0.367635	-0.694178	-2.704806
15	46	0	1.300598	-0.259815	0.481400
16	8	0	-1.810488	-1.824725	-2.204712
17	6	0	-1.489386	0.653425	-1.417912
18	6	0	-2.753085	0.695571	-0.828652
19	6	0	-0.766030	1.821861	-1.638002
20	6	0	-3.284753	1.923614	-0.454838
21	1	0	-3.313454	-0.219052	-0.666692
22	6	0	-1.317784	3.044521	-1.268488
23	1	0	0.215398	1.772999	-2.098366
24	6	0	-2.577858	3.114008	-0.666125
25	1	0	-4.267533	1.960739	0.007047
26	1	0	-0.760335	3.958959	-1.451150
27	6	0	-3.174001	4.433296	-0.253972
28	1	0	-3.359635	4.456748	0.824924
29	1	0	-2.511813	5.266079	-0.503525
30	1	0	-4.135432	4.599362	-0.750852
31	6	0	3.329756	1.622864	2.098734
32	7	0	2.615046	0.950016	1.496740
33	6	0	4.225491	2.468261	2.862803
34	1	0	3.766202	3.450162	2.996609
35	1	0	4.404288	2.009770	3.837995
36	1	0	5.170693	2.572856	2.325882
37	6	0	3.505708	-0.797061	-1.741902
38	7	0	2.702655	-0.579234	-0.947422
39	6	0	4.503963	-1.075640	-2.755051
40	1	0	5.481217	-0.735891	-2.405537
41	1	0	4.534047	-2.151395	-2.942296
42	1	0	4.238891	-0.550821	-3.675652



(Ts1-a)

Imaginary Freq.: -299.96 cm^{-1}

Sum of electronic and zero-point Energies= -1596.558636

Sum of electronic and thermal Energies= -1596.532621

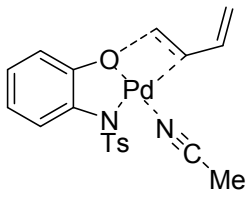
Sum of electronic and thermal Enthalpies= -1596.531677

Sum of electronic and thermal Free Energies= -1596.616150

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.550227	-3.036471	1.925616
2	6	0	-1.598606	-2.871471	0.923219
3	6	0	-0.868885	-1.688563	0.841093
4	6	0	-1.027190	-0.644415	1.797876
5	6	0	-2.037945	-0.813582	2.767494
6	6	0	-2.769481	-1.993406	2.830879
7	1	0	-3.117186	-3.958811	1.996240
8	1	0	-1.429713	-3.642637	0.178520
9	1	0	-2.205345	-0.016251	3.485964
10	1	0	-3.519069	-2.107112	3.609792
11	8	0	-0.252634	0.417247	1.778091
12	7	0	0.008423	-1.406857	-0.265716
13	16	0	-0.803270	-0.977191	-1.676167
14	8	0	0.209076	-0.727067	-2.698106
15	8	0	-1.822949	-1.987798	-1.942645
16	6	0	-1.638584	0.550309	-1.322721
17	6	0	-0.991185	1.756292	-1.583910
18	6	0	-2.896977	0.519462	-0.730717
19	6	0	-1.622259	2.945632	-1.247465
20	1	0	-0.008833	1.760480	-2.045049
21	6	0	-3.511105	1.721334	-0.391975
22	1	0	-3.388170	-0.427399	-0.533490
23	6	0	-2.887338	2.946657	-0.644111
24	1	0	-1.127134	3.890425	-1.453857
25	1	0	-4.490490	1.704435	0.077074
26	6	0	-3.569649	4.247134	-0.316297
27	1	0	-3.976960	4.702741	-1.226200
28	1	0	-4.397013	4.099912	0.382237
29	1	0	-2.868084	4.964525	0.119110
30	46	0	1.324892	-0.067515	0.478954
31	6	0	3.503245	-0.450492	-1.608768
32	6	0	3.321377	-0.583046	-2.924638
33	1	0	4.235453	0.272620	-1.252477
34	1	0	3.890046	0.026182	-3.621178
35	1	0	2.608247	-1.283228	-3.347356
36	6	0	2.833022	-1.199220	-0.519966
37	6	0	1.882421	-2.228360	-0.722732
38	1	0	3.448360	-1.334198	0.371997

39	1	0	1.760196	-2.989851	0.039889
40	1	0	1.559765	-2.500129	-1.720875
41	7	0	2.650453	1.265787	1.269012
42	6	0	3.386012	2.032131	1.715210
43	6	0	4.313752	2.996271	2.273219
44	1	0	4.084728	3.147566	3.330335
45	1	0	5.333125	2.618785	2.166965
46	1	0	4.212890	3.943919	1.739504



(Ts1-b)

Imaginary Freq.: -319.87 cm^{-1}

Sum of electronic and zero-point Energies= -1596.555862

Sum of electronic and thermal Energies= -1596.529974

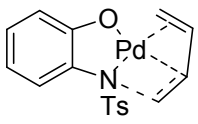
Sum of electronic and thermal Enthalpies= -1596.529030

Sum of electronic and thermal Free Energies= -1596.613359

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.177567	-1.873905	0.464412
2	6	0	-3.089885	-1.827218	-0.407361
3	6	0	-1.869848	-1.287828	0.005946
4	6	0	-1.778027	-0.764672	1.315315
5	6	0	-2.856388	-0.832671	2.193150
6	6	0	-4.060193	-1.388185	1.764855
7	1	0	-5.110762	-2.315840	0.129258
8	1	0	-3.171571	-2.226727	-1.411464
9	1	0	-2.742584	-0.432479	3.196366
10	1	0	-4.901295	-1.440961	2.449257
11	8	0	-0.644622	-0.095857	1.669462
12	7	0	-0.683090	-1.314929	-0.791050
13	16	0	-0.705489	-0.437554	-2.179926
14	8	0	0.502219	-0.787642	-2.928139
15	8	0	-1.996501	-0.554959	-2.865394
16	6	0	-0.544071	1.261578	-1.650675
17	6	0	0.726710	1.819086	-1.510850

18	6	0	-1.674675	1.957622	-1.235540
19	6	0	0.860561	3.077193	-0.939780
20	1	0	1.601288	1.267003	-1.839798
21	6	0	-1.524487	3.219376	-0.663202
22	1	0	-2.660822	1.520963	-1.354842
23	6	0	-0.260660	3.791097	-0.495636
24	1	0	1.850096	3.512543	-0.829802
25	1	0	-2.406785	3.763886	-0.338701
26	6	0	-0.089239	5.136787	0.157160
27	1	0	0.527059	5.797383	-0.460540
28	1	0	-1.052156	5.624115	0.328662
29	1	0	0.414812	5.033867	1.124617
30	46	0	0.860128	-0.835075	0.581311
31	6	0	1.884029	-0.428659	2.408322
32	6	0	0.646395	-0.491538	3.102104
33	1	0	2.481689	-1.338723	2.468962
34	1	0	0.263333	-1.459286	3.412178
35	1	0	0.268576	0.363731	3.650827
36	6	0	2.636976	0.842887	2.293283
37	6	0	2.123522	2.074570	2.379101
38	1	0	3.701207	0.726172	2.095565
39	1	0	2.754376	2.952566	2.280825
40	1	0	1.062806	2.249403	2.544819
41	6	0	3.372722	-1.877472	-1.030847
42	7	0	2.455057	-1.512948	-0.438493
43	6	0	4.525687	-2.332234	-1.782696
44	1	0	4.874239	-3.282738	-1.372647
45	1	0	4.244549	-2.464619	-2.829831
46	1	0	5.321948	-1.588033	-1.708200



(Ts1-c)

Imaginary Freq.: -323.60 cm^{-1}

Sum of electronic and zero-point Energies= -1463.862145

Sum of electronic and thermal Energies= -1463.841287

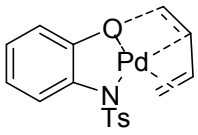
Sum of electronic and thermal Enthalpies= -1463.840343

Sum of electronic and thermal Free Energies= -1463.913815

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-0.489824	4.026700	0.155785
2	6	0	0.093544	2.949649	0.812041
3	6	0	0.306692	1.742419	0.141939
4	6	0	0.010277	1.612338	-1.246220
5	6	0	-0.614627	2.709330	-1.876717
6	6	0	-0.854129	3.889276	-1.187837
7	1	0	-0.659568	4.960423	0.681697
8	1	0	0.365750	3.020972	1.859332
9	1	0	-0.874842	2.613829	-2.927067
10	1	0	-1.316802	4.723434	-1.708548
11	8	0	0.321213	0.531137	-1.934713
12	7	0	0.780743	0.574816	0.828981
13	16	0	-0.252105	-0.096118	1.963693
14	8	0	0.440163	-1.249060	2.533202
15	8	0	-0.730555	0.940059	2.873776
16	6	0	-1.636668	-0.661891	1.004050
17	6	0	-1.625189	-1.960280	0.495519
18	6	0	-2.662933	0.224912	0.696818
19	6	0	-2.664985	-2.369552	-0.326888
20	1	0	-0.815446	-2.639107	0.743997
21	6	0	-3.694249	-0.201279	-0.135906
22	1	0	-2.659081	1.232278	1.099274
23	6	0	-3.710555	-1.496515	-0.659521
24	1	0	-2.667299	-3.381877	-0.721293
25	1	0	-4.496788	0.487731	-0.382101
26	6	0	-4.828556	-1.962955	-1.552364
27	1	0	-5.500798	-1.142756	-1.815162
28	1	0	-4.433877	-2.396406	-2.476566
29	1	0	-5.418877	-2.740846	-1.056071
30	46	0	1.464187	-0.661224	-0.706794
31	6	0	2.890252	-1.333379	0.685419
32	6	0	2.753481	0.020198	1.167701
33	1	0	2.638902	-2.114779	1.394723
34	1	0	2.627889	0.148379	2.234403
35	1	0	3.222887	0.852265	0.650626
36	6	0	3.340453	-1.779292	-0.608340
37	6	0	3.437379	-0.957418	-1.727785
38	1	0	3.378832	-2.857517	-0.738700
39	1	0	3.572708	-1.421017	-2.699772
40	1	0	3.703526	0.094820	-1.652502



(Ts1-d)

Imaginary Freq.: -344.76 cm^{-1}

Sum of electronic and zero-point Energies= -1463.854251

Sum of electronic and thermal Energies= -1463.833345

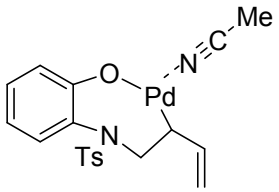
Sum of electronic and thermal Enthalpies= -1463.832401

Sum of electronic and thermal Free Energies= -1463.905528

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.514813	4.124136	-0.300757
2	6	0	0.450809	3.080466	0.618707
3	6	0	0.596957	1.749785	0.211315
4	6	0	0.803632	1.489812	-1.166247
5	6	0	0.895668	2.544521	-2.076599
6	6	0	0.743439	3.859426	-1.649531
7	1	0	0.408571	5.147495	0.045922
8	1	0	0.295019	3.284171	1.671451
9	1	0	1.068860	2.310097	-3.122664
10	1	0	0.809118	4.671131	-2.367382
11	8	0	0.844405	0.214741	-1.647239
12	7	0	0.620610	0.664268	1.143935
13	16	0	-0.731170	0.403787	2.030966
14	8	0	-0.429860	-0.688050	2.958944
15	8	0	-1.254222	1.652115	2.594037
16	6	0	-1.950681	-0.190633	0.867684
17	6	0	-2.069451	-1.559739	0.632258
18	6	0	-2.683556	0.726060	0.119036
19	6	0	-2.934774	-2.007681	-0.358094
20	1	0	-1.491055	-2.263455	1.222878
21	6	0	-3.542043	0.261990	-0.874022
22	1	0	-2.586273	1.789738	0.309546
23	6	0	-3.680114	-1.105691	-1.128339
24	1	0	-3.036565	-3.074627	-0.537368
25	1	0	-4.114809	0.975586	-1.459720
26	6	0	-4.626777	-1.607099	-2.185967
27	1	0	-4.895836	-0.815003	-2.889457
28	1	0	-4.185398	-2.435239	-2.748066

29	1	0	-5.551663	-1.978343	-1.730452
30	46	0	1.289333	-0.978754	0.038084
31	6	0	2.817411	-2.511976	-0.084104
32	6	0	3.139195	-1.655792	0.979035
33	1	0	2.612927	-3.560066	0.117547
34	1	0	3.195184	-2.080320	1.976482
35	1	0	3.685469	-0.727238	0.823916
36	6	0	2.422394	-2.044396	-1.382617
37	6	0	2.584507	-0.715441	-1.936265
38	1	0	1.970611	-2.782749	-2.038750
39	1	0	2.417172	-0.602881	-2.999108
40	1	0	3.272633	-0.003041	-1.488540



(6)

Sum of electronic and zero-point Energies= -1596.587907

Sum of electronic and thermal Energies= -1596.561718

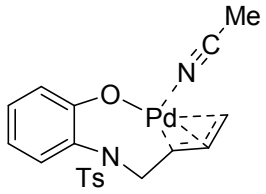
Sum of electronic and thermal Enthalpies= -1596.560774

Sum of electronic and thermal Free Energies= -1596.646871

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.914358	2.835290	1.441816
2	6	0	1.525303	1.520271	1.216775
3	6	0	0.404086	1.246151	0.438214
4	6	0	-0.419319	2.272395	-0.122014
5	6	0	0.042377	3.597478	0.089745
6	6	0	1.169940	3.863466	0.851667
7	1	0	2.783362	3.055277	2.052368
8	1	0	2.089651	0.694465	1.642277
9	1	0	-0.538343	4.409386	-0.339166
10	1	0	1.469126	4.897312	1.004929
11	8	0	-1.530567	2.025846	-0.755898
12	7	0	0.026863	-0.127054	0.126343
13	16	0	0.897670	-0.780289	-1.258260
14	8	0	0.425428	-2.147752	-1.415794

15	8	0	0.741616	0.184400	-2.332069
16	6	0	2.588266	-0.802683	-0.745577
17	6	0	3.079196	-1.902402	-0.042254
18	6	0	3.395507	0.298071	-1.030357
19	6	0	4.397414	-1.881450	0.395406
20	1	0	2.452685	-2.767794	0.144820
21	6	0	4.711529	0.294977	-0.589763
22	1	0	3.000787	1.141006	-1.585905
23	6	0	5.227657	-0.784657	0.136534
24	1	0	4.790769	-2.735164	0.938959
25	1	0	5.348273	1.146224	-0.811446
26	6	0	6.641906	-0.756379	0.646245
27	1	0	6.673554	-0.308953	1.646239
28	1	0	7.059472	-1.763620	0.722740
29	1	0	7.285466	-0.156364	-0.002252
30	46	0	-1.995612	-0.042111	-0.226232
31	6	0	-2.580986	-1.844705	1.990521
32	6	0	-2.505958	-1.362571	3.236952
33	1	0	-3.472938	-2.404603	1.710202
34	1	0	-3.311566	-1.533877	3.944864
35	1	0	-1.654944	-0.792088	3.600163
36	6	0	-1.594353	-1.695132	0.898632
37	6	0	-0.203514	-1.152905	1.226649
38	1	0	-1.556778	-2.570842	0.248755
39	1	0	0.591967	-1.901490	1.247081
40	1	0	-0.169511	-0.593288	2.160954
41	6	0	-5.155792	-0.235183	-0.553403
42	7	0	-4.011258	-0.186320	-0.424385
43	6	0	-6.595051	-0.301066	-0.717724
44	1	0	-6.829057	-0.879012	-1.614727
45	1	0	-7.037523	-0.784980	0.155698
46	1	0	-6.995478	0.709991	-0.819743



(Ts2)

Imaginary Freq.: -132.74 cm^{-1}

Sum of electronic and zero-point Energies= -1596.573505

Sum of electronic and thermal Energies= -1596.547920

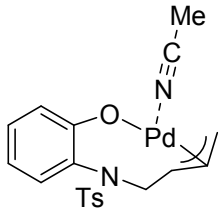
Sum of electronic and thermal Enthalpies= -1596.546976

Sum of electronic and thermal Free Energies= -1596.631331

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.108638	3.192593	0.131703
2	6	0	1.689731	1.912650	0.472819
3	6	0	0.471052	1.413043	0.014813
4	6	0	-0.425860	2.203054	-0.777562
5	6	0	0.064385	3.485226	-1.144325
6	6	0	1.286454	3.962729	-0.698435
7	1	0	3.053906	3.579223	0.497408
8	1	0	2.309794	1.282372	1.105198
9	1	0	-0.575570	4.105015	-1.766551
10	1	0	1.600825	4.962123	-0.989463
11	8	0	-1.620121	1.824031	-1.133602
12	7	0	0.084598	0.049226	0.331192
13	16	0	0.723139	-1.148345	-0.715168
14	8	0	0.161040	-2.415107	-0.262103
15	8	0	0.501848	-0.687680	-2.075992
16	6	0	2.468444	-1.166690	-0.410024
17	6	0	2.977188	-1.959362	0.616161
18	6	0	3.302160	-0.351380	-1.176034
19	6	0	4.341961	-1.922376	0.881485
20	1	0	2.324647	-2.610461	1.187515
21	6	0	4.661328	-0.331925	-0.898438
22	1	0	2.891769	0.254669	-1.975761
23	6	0	5.199969	-1.108978	0.135304
24	1	0	4.745580	-2.543221	1.675725
25	1	0	5.317535	0.296668	-1.493428
26	6	0	6.673794	-1.056046	0.432056
27	1	0	6.936949	-0.097142	0.891821
28	1	0	6.972990	-1.852360	1.117626
29	1	0	7.260711	-1.148199	-0.486647
30	46	0	-2.146496	0.176531	0.195561
31	6	0	-2.536207	0.100350	2.500258
32	6	0	-2.374236	1.455060	2.483835
33	1	0	-3.499239	-0.316743	2.784853
34	1	0	-3.197880	2.106467	2.757755
35	1	0	-1.413869	1.929774	2.300460
36	6	0	-1.580467	-0.800116	1.892283
37	6	0	-0.110581	-0.402759	1.755643

38	1	0	-1.784760	-1.865814	1.956913
39	1	0	0.556424	-1.231375	1.997352
40	1	0	0.157487	0.439680	2.394981
41	6	0	-4.728803	-1.622999	-0.962371
42	7	0	-3.835474	-1.013581	-0.555598
43	6	0	-5.851671	-2.388315	-1.474950
44	1	0	-5.971431	-2.187922	-2.541970
45	1	0	-5.665115	-3.453616	-1.322414
46	1	0	-6.761859	-2.098080	-0.945394



(7)

Sum of electronic and zero-point Energies= -1596.594704

Sum of electronic and thermal Energies= -1596.569062

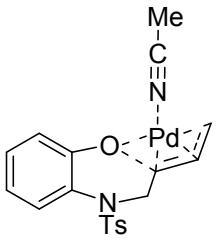
Sum of electronic and thermal Enthalpies= -1596.568117

Sum of electronic and thermal Free Energies= -1596.652483

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.421732	3.461726	-0.536867
2	6	0	1.241345	2.211975	0.042133
3	6	0	0.108806	1.435543	-0.217892
4	6	0	-0.950616	1.926328	-1.053600
5	6	0	-0.709365	3.193043	-1.653984
6	6	0	0.434192	3.934728	-1.406005
7	1	0	2.310368	4.046486	-0.323315
8	1	0	1.994353	1.810633	0.715879
9	1	0	-1.481655	3.579090	-2.314297
10	1	0	0.553552	4.902841	-1.886608
11	8	0	-2.079037	1.316624	-1.289340
12	7	0	0.033712	0.125187	0.383782
13	16	0	0.797208	-1.129928	-0.394061
14	8	0	0.396592	-2.349070	0.302419
15	8	0	0.559710	-0.985563	-1.823408
16	6	0	2.541174	-0.908346	-0.120222

17	6	0	3.121468	-1.418174	1.041686
18	6	0	3.291564	-0.166563	-1.028404
19	6	0	4.465671	-1.174040	1.289179
20	1	0	2.533526	-2.011631	1.733693
21	6	0	4.637399	0.067335	-0.764879
22	1	0	2.830276	0.223115	-1.929043
23	6	0	5.242026	-0.425916	0.394761
24	1	0	4.923649	-1.574836	2.189239
25	1	0	5.225626	0.644774	-1.472104
26	6	0	6.695511	-0.166902	0.686627
27	1	0	6.808260	0.412678	1.608886
28	1	0	7.236886	-1.107800	0.828356
29	1	0	7.174752	0.385081	-0.125468
30	46	0	-2.697007	0.085922	0.384838
31	6	0	-2.733085	0.261419	2.500988
32	6	0	-2.765837	1.544484	1.879800
33	1	0	-3.604292	-0.157139	2.996641
34	1	0	-3.685224	2.122189	1.944677
35	1	0	-1.859763	2.140049	1.779230
36	6	0	-1.656748	-0.571381	2.128003
37	6	0	-0.248720	-0.038563	1.823084
38	1	0	-1.723213	-1.628795	2.372336
39	1	0	0.481096	-0.712931	2.276944
40	1	0	-0.112538	0.940876	2.285699
41	6	0	-2.521920	-2.666688	-1.407939
42	7	0	-2.693931	-1.721398	-0.770278
43	6	0	-2.285380	-3.853782	-2.207578
44	1	0	-1.208976	-3.982226	-2.342397
45	1	0	-2.697679	-4.727667	-1.698715
46	1	0	-2.763916	-3.738161	-3.182421



(Ts3)

Imaginary Freq.: -285.05 cm^{-1}

Sum of electronic and zero-point Energies= -1596.567801

Sum of electronic and thermal Energies= -1596.542173

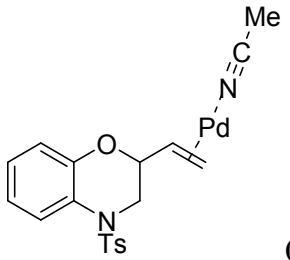
Sum of electronic and thermal Enthalpies= -1596.541229

Sum of electronic and thermal Free Energies= -1596.627064

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.800711	2.974114	-0.022220
2	6	0	-1.181261	1.697797	-0.421192
3	6	0	-0.500678	0.577371	0.054794
4	6	0	0.611357	0.701743	0.920600
5	6	0	1.001265	2.010925	1.284827
6	6	0	0.294641	3.117484	0.836400
7	1	0	-1.338234	3.844363	-0.383819
8	1	0	-2.013636	1.554151	-1.104210
9	1	0	1.860971	2.126946	1.939729
10	1	0	0.606717	4.110133	1.150620
11	8	0	1.252418	-0.358252	1.362526
12	7	0	-0.882936	-0.735346	-0.376558
13	16	0	-2.078246	-1.502578	0.525957
14	8	0	-2.202993	-2.842146	-0.044723
15	8	0	-1.853299	-1.372693	1.962951
16	6	0	-3.512971	-0.546581	0.112986
17	6	0	-4.079180	-0.689861	-1.153627
18	6	0	-4.032801	0.347475	1.040873
19	6	0	-5.184050	0.080059	-1.485207
20	1	0	-3.661302	-1.391139	-1.868591
21	6	0	-5.140219	1.114157	0.689701
22	1	0	-3.573620	0.449068	2.017845
23	6	0	-5.728858	0.993757	-0.571222
24	1	0	-5.634862	-0.026598	-2.467777
25	1	0	-5.548774	1.819167	1.407695
26	6	0	-6.932660	1.813571	-0.948637
27	1	0	-7.820510	1.177435	-1.033472
28	1	0	-7.140135	2.585637	-0.203848
29	1	0	-6.787043	2.297364	-1.919210
30	46	0	3.268573	-0.584781	-0.014132
31	6	0	2.482765	-2.534458	-0.160422
32	6	0	3.206804	-2.200279	-1.342640
33	1	0	2.937350	-3.212470	0.558352
34	1	0	4.125688	-2.748179	-1.537903
35	1	0	2.698443	-1.847335	-2.238631
36	6	0	1.182246	-2.050466	0.168376
37	6	0	0.206445	-1.577147	-0.868937
38	1	0	0.736770	-2.478836	1.058267
39	1	0	-0.225365	-2.476702	-1.320427

40	1	0	0.702092	-1.016372	-1.663391
41	6	0	4.885641	2.162521	-0.537220
42	7	0	4.350843	1.148455	-0.394462
43	6	0	5.551345	3.439475	-0.717351
44	1	0	6.293462	3.575401	0.072467
45	1	0	6.047146	3.458979	-1.690478
46	1	0	4.813314	4.243171	-0.666648



(8)

Sum of electronic and zero-point Energies= -1596.606763

Sum of electronic and thermal Energies= -1596.581386

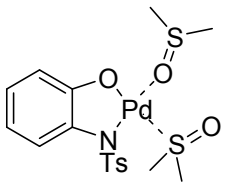
Sum of electronic and thermal Enthalpies= -1596.580442

Sum of electronic and thermal Free Energies= -1596.665069

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.634552	3.145906	-0.239440
2	6	0	-1.722884	1.776000	-0.448023
3	6	0	-0.753763	0.913923	0.071042
4	6	0	0.346072	1.444803	0.760765
5	6	0	0.443183	2.825844	0.949718
6	6	0	-0.547897	3.667402	0.464360
7	1	0	-2.398589	3.804215	-0.638881
8	1	0	-2.541676	1.360422	-1.024810
9	1	0	1.302010	3.220091	1.483349
10	1	0	-0.463059	4.737572	0.624683
11	8	0	1.366389	0.690515	1.233710
12	7	0	-0.809248	-0.498488	-0.164063
13	16	0	-1.910062	-1.368494	0.799840
14	8	0	-1.698826	-2.770848	0.454858
15	8	0	-1.815168	-0.969550	2.203047
16	6	0	-3.470672	-0.826431	0.170983
17	6	0	-3.836218	-1.176444	-1.129430

18	6	0	-4.292867	-0.043720	0.971866
19	6	0	-5.045418	-0.717536	-1.628698
20	1	0	-3.181741	-1.786090	-1.743653
21	6	0	-5.504490	0.404247	0.454185
22	1	0	-3.985684	0.219868	1.977723
23	6	0	-5.894687	0.080378	-0.847370
24	1	0	-5.337969	-0.977342	-2.642017
25	1	0	-6.150734	1.021024	1.071399
26	6	0	-7.202750	0.565955	-1.409682
27	1	0	-7.052699	1.061228	-2.374052
28	1	0	-7.884891	-0.273999	-1.579746
29	1	0	-7.692258	1.269192	-0.731862
30	46	0	3.852030	-0.679522	-0.716832
31	6	0	2.762062	-1.205184	1.061817
32	6	0	3.233316	-2.355948	0.434203
33	1	0	3.317480	-0.808847	1.911566
34	1	0	4.120272	-2.851197	0.824844
35	1	0	2.578163	-2.980480	-0.171936
36	6	0	1.329569	-0.734777	1.041684
37	6	0	0.536628	-1.088103	-0.211203
38	1	0	0.816735	-1.161332	1.914932
39	1	0	0.449915	-2.168252	-0.320131
40	1	0	1.031892	-0.686983	-1.101379
41	6	0	4.372079	1.462549	-0.632037
42	7	0	4.487203	1.132600	-1.764944
43	6	0	4.353812	2.298032	0.572907
44	1	0	3.417037	2.132247	1.107340
45	1	0	5.184850	2.011668	1.221540
46	1	0	4.450567	3.349802	0.292170



(9a)

Sum of electronic and zero-point Energies= -2414.195726

Sum of electronic and thermal Energies= -2414.166011

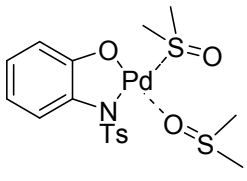
Sum of electronic and thermal Enthalpies= -2414.165067

Sum of electronic and thermal Free Energies= -2414.256705

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.687597	2.533985	-2.707221
2	6	0	-1.693448	2.692213	-1.740462
3	6	0	-0.953618	1.591349	-1.321503
4	6	0	-1.167276	0.320646	-1.891277
5	6	0	-2.172738	0.169154	-2.854319
6	6	0	-2.925094	1.272205	-3.251805
7	1	0	-3.266765	3.391856	-3.033679
8	1	0	-1.503612	3.660518	-1.290554
9	1	0	-2.345869	-0.812701	-3.285640
10	1	0	-3.697087	1.145217	-4.005790
11	8	0	-0.404023	-0.701497	-1.503446
12	7	0	0.038672	1.649683	-0.274464
13	16	0	-0.643330	1.851170	1.226675
14	8	0	0.429016	1.708404	2.218665
15	46	0	1.170549	-0.024898	-0.444004
16	16	0	3.091945	0.832934	0.488579
17	8	0	4.325611	0.519438	-0.292677
18	6	0	3.281495	0.237333	2.163828
19	1	0	2.390000	0.521579	2.725239
20	1	0	3.371857	-0.848833	2.108274
21	1	0	4.184360	0.677548	2.593345
22	6	0	3.030086	2.602085	0.737236
23	1	0	2.878172	3.064596	-0.239174
24	1	0	2.204727	2.836324	1.408281
25	1	0	3.991229	2.902214	1.160927
26	8	0	-1.419944	3.090222	1.244506
27	6	0	-1.788657	0.507841	1.474301
28	6	0	-3.066761	0.585348	0.921655
29	6	0	-1.368861	-0.637495	2.143156
30	6	0	-3.921813	-0.502838	1.040171
31	1	0	-3.389180	1.483106	0.405489
32	6	0	-2.242455	-1.713375	2.265007
33	1	0	-0.369546	-0.689407	2.562937
34	6	0	-3.525233	-1.665826	1.711733
35	1	0	-4.915658	-0.447743	0.604814
36	1	0	-1.916509	-2.607440	2.789236
37	6	0	-4.475329	-2.824514	1.850553
38	1	0	-4.989233	-3.026882	0.906154
39	1	0	-3.954578	-3.733074	2.163370
40	1	0	-5.244601	-2.603655	2.598867
41	16	0	1.679924	-3.236386	-0.634504

42	8	0	2.279852	-1.799327	-0.624413
43	6	0	0.220211	-3.201610	0.409136
44	1	0	-0.224882	-4.200301	0.401150
45	1	0	0.549959	-2.954338	1.419657
46	1	0	-0.479452	-2.455477	0.025949
47	6	0	0.892674	-3.450853	-2.232831
48	1	0	1.680169	-3.451778	-2.988536
49	1	0	0.385474	-4.419325	-2.228766
50	1	0	0.190832	-2.629805	-2.393347



(9b)

Sum of electronic and zero-point Energies= -2414.185190

Sum of electronic and thermal Energies= -2414.155650

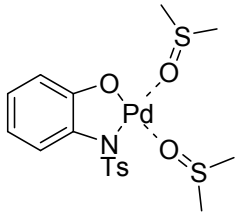
Sum of electronic and thermal Enthalpies= -2414.154705

Sum of electronic and thermal Free Energies= -2414.244936

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.072523	0.735206	-0.130038
2	6	0	-3.872801	0.968460	-0.802924
3	6	0	-2.710745	0.289618	-0.430945
4	6	0	-2.774828	-0.678616	0.591259
5	6	0	-3.981972	-0.911100	1.257237
6	6	0	-5.124979	-0.199521	0.901179
7	1	0	-5.965924	1.276287	-0.426564
8	1	0	-3.831558	1.686940	-1.611285
9	1	0	-4.006297	-1.657896	2.045691
10	1	0	-6.059179	-0.387930	1.422492
11	8	0	-1.676181	-1.375384	0.916826
12	7	0	-1.437100	0.406918	-1.076451
13	16	0	-0.805505	1.888466	-1.388826
14	8	0	0.093084	1.771789	-2.536122
15	46	0	-0.195570	-1.064834	-0.347900
16	16	0	2.598103	0.000891	-1.543363
17	8	0	1.356569	-0.933712	-1.715137

18	6	0	3.076081	-0.046403	0.191710
19	1	0	3.965174	0.580052	0.302724
20	1	0	2.257211	0.377651	0.777243
21	1	0	3.283337	-1.076519	0.487235
22	6	0	3.909670	-1.030486	-2.203125
23	1	0	3.722601	-1.161800	-3.270136
24	1	0	4.863967	-0.518623	-2.055350
25	1	0	3.890073	-1.991722	-1.685520
26	8	0	-1.861202	2.903138	-1.465081
27	6	0	0.225092	2.310882	0.015966
28	6	0	-0.167577	1.976273	1.311820
29	6	0	1.410876	3.004487	-0.205623
30	6	0	0.650200	2.317703	2.381598
31	1	0	-1.095122	1.441085	1.489259
32	6	0	2.216561	3.347035	0.877075
33	1	0	1.712358	3.254715	-1.216973
34	6	0	1.853933	3.005624	2.182308
35	1	0	0.351012	2.044165	3.389788
36	1	0	3.149265	3.875631	0.701079
37	6	0	2.719483	3.381768	3.354353
38	1	0	2.721086	2.594085	4.113040
39	1	0	3.751152	3.569758	3.046176
40	1	0	2.343367	4.293525	3.832150
41	16	0	0.885293	-2.828842	0.687340
42	8	0	2.247719	-3.250063	0.238642
43	6	0	-0.215717	-4.236893	0.663186
44	1	0	-1.188851	-3.911700	1.035910
45	1	0	-0.299085	-4.571947	-0.372220
46	1	0	0.210294	-5.022051	1.291826
47	6	0	0.920376	-2.455259	2.436812
48	1	0	1.580972	-1.596542	2.571990
49	1	0	-0.094895	-2.203814	2.749599
50	1	0	1.301989	-3.326446	2.973889



(9c)

Sum of electronic and zero-point Energies= -2414.194452

Sum of electronic and thermal Energies= -2414.164433

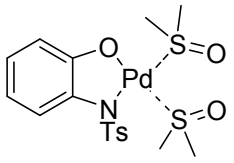
Sum of electronic and thermal Enthalpies= -2414.163489

Sum of electronic and thermal Free Energies= -2414.256530

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.247971	0.987246	-2.194201
2	6	0	-3.163434	1.651252	-1.620036
3	6	0	-1.978522	0.965078	-1.363579
4	6	0	-1.850690	-0.390376	-1.729428
5	6	0	-2.946384	-1.051253	-2.300116
6	6	0	-4.136251	-0.363441	-2.523082
7	1	0	-5.171384	1.524839	-2.385725
8	1	0	-3.237479	2.698070	-1.348251
9	1	0	-2.845313	-2.100097	-2.564601
10	1	0	-4.978392	-0.884335	-2.970249
11	8	0	-0.688736	-1.015629	-1.532995
12	7	0	-0.823556	1.558907	-0.736530
13	16	0	-1.075401	1.984418	0.844143
14	8	0	0.178892	2.525531	1.372385
15	46	0	0.723284	0.262396	-0.976026
16	16	0	2.916802	1.487706	0.795866
17	8	0	2.246506	1.611475	-0.607773
18	6	0	4.559004	0.858165	0.439050
19	1	0	5.134001	0.835321	1.368482
20	1	0	4.429731	-0.153814	0.051248
21	1	0	5.044954	1.494688	-0.303918
22	6	0	3.329619	3.181068	1.200799
23	1	0	2.385877	3.700747	1.365973
24	1	0	3.929609	3.185871	2.114371
25	1	0	3.882101	3.626527	0.370441
26	8	0	-2.270205	2.823413	0.952506
27	6	0	-1.415534	0.464931	1.720007
28	6	0	-2.684443	-0.103409	1.648534
29	6	0	-0.375115	-0.196311	2.370658
30	6	0	-2.902576	-1.351694	2.225998
31	1	0	-3.494002	0.417075	1.148117
32	6	0	-0.611565	-1.434634	2.951883
33	1	0	0.609550	0.257274	2.415208
34	6	0	-1.874673	-2.035264	2.880698
35	1	0	-3.889727	-1.800872	2.163899
36	1	0	0.198208	-1.948935	3.462696
37	6	0	-2.111973	-3.379135	3.515008

38	1	0	-1.304629	-4.076558	3.271735
39	1	0	-2.147978	-3.290423	4.606540
40	1	0	-3.056819	-3.816072	3.182188
41	16	0	1.811474	-2.668098	-1.318698
42	8	0	2.241927	-1.173359	-1.148213
43	6	0	3.361667	-3.525252	-1.050001
44	1	0	3.166972	-4.600638	-1.062771
45	1	0	4.032040	-3.263067	-1.870125
46	1	0	3.785467	-3.218169	-0.091422
47	6	0	0.967985	-3.112345	0.202673
48	1	0	0.013988	-2.583546	0.195759
49	1	0	0.798392	-4.192637	0.198202
50	1	0	1.580717	-2.817426	1.057659



(9d)

Sum of electronic and zero-point Energies= -2414.191797

Sum of electronic and thermal Energies= -2414.162517

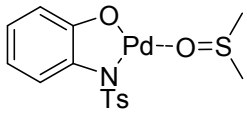
Sum of electronic and thermal Enthalpies= -2414.161573

Sum of electronic and thermal Free Energies= -2414.251469

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.424070	-2.518879	-2.112919
2	6	0	2.433284	-2.638115	-1.138645
3	6	0	1.486531	-1.629229	-0.979386
4	6	0	1.495528	-0.504235	-1.825465
5	6	0	2.498697	-0.387056	-2.795691
6	6	0	3.454921	-1.389528	-2.931143
7	1	0	4.163338	-3.304679	-2.231510
8	1	0	2.399777	-3.501669	-0.483618
9	1	0	2.509923	0.489846	-3.436712
10	1	0	4.224629	-1.292346	-3.691735
11	8	0	0.549364	0.429180	-1.696567
12	7	0	0.463638	-1.654915	0.038464
13	16	0	1.069681	-1.423544	1.566809

14	8	0	-0.070425	-1.460411	2.490665
15	46	0	-0.893271	-0.185803	-0.450592
16	16	0	-2.721388	-1.079882	0.629359
17	8	0	-3.957302	-0.949053	-0.206372
18	6	0	-2.999812	-0.339459	2.229243
19	1	0	-2.106137	-0.500560	2.833642
20	1	0	-3.167829	0.724122	2.048789
21	1	0	-3.880105	-0.805691	2.677713
22	6	0	-2.492435	-2.803291	1.035229
23	1	0	-2.320995	-3.336460	0.099024
24	1	0	-1.630534	-2.893078	1.696024
25	1	0	-3.410165	-3.149876	1.515928
26	8	0	2.174032	-2.347028	1.819817
27	6	0	1.731775	0.231405	1.589031
28	6	0	3.016147	0.452312	1.096281
29	6	0	0.913458	1.295960	1.959015
30	6	0	3.475530	1.757574	0.968301
31	1	0	3.646400	-0.384622	0.814631
32	6	0	1.390846	2.595993	1.830426
33	1	0	-0.086649	1.113652	2.340800
34	6	0	2.670916	2.846165	1.324725
35	1	0	4.475091	1.935046	0.581123
36	1	0	0.757209	3.427821	2.125117
37	6	0	3.183539	4.251360	1.160661
38	1	0	2.461473	4.985878	1.525567
39	1	0	4.122387	4.391354	1.706027
40	1	0	3.386965	4.467036	0.106404
41	16	0	-2.128179	1.704761	-0.996125
42	8	0	-2.957350	2.286802	0.103742
43	6	0	-3.139434	1.389285	-2.433301
44	1	0	-2.495606	1.010307	-3.230604
45	1	0	-3.866784	0.630822	-2.139075
46	1	0	-3.631688	2.318358	-2.729775
47	6	0	-1.005087	2.949212	-1.610727
48	1	0	-0.336814	3.218824	-0.790706
49	1	0	-0.430232	2.524088	-2.433691
50	1	0	-1.597848	3.809026	-1.930165



(9e)

Sum of electronic and zero-point Energies= -1861.086890

Sum of electronic and thermal Energies= -1861.063562

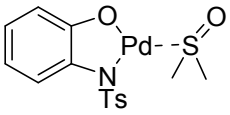
Sum of electronic and thermal Enthalpies= -1861.062618

Sum of electronic and thermal Free Energies= -1861.141050

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.191938	-3.672431	0.579554
2	6	0	1.135116	-2.881341	1.028646
3	6	0	0.618910	-1.891872	0.198289
4	6	0	1.102370	-1.717003	-1.109776
5	6	0	2.173815	-2.505405	-1.547342
6	6	0	2.710470	-3.471814	-0.700069
7	1	0	2.603709	-4.440775	1.225865
8	1	0	0.724324	-3.009949	2.023656
9	1	0	2.564405	-2.359616	-2.550121
10	1	0	3.534885	-4.085906	-1.051343
11	8	0	0.512157	-0.815351	-1.898266
12	7	0	-0.427802	-0.982748	0.615877
13	16	0	0.086313	0.126747	1.760816
14	8	0	-1.054537	0.999858	2.044843
15	46	0	-1.151972	-0.135929	-1.051661
16	16	0	-3.230436	0.428991	-0.253662
17	8	0	-4.196713	0.228829	-1.380621
18	6	0	-3.377238	2.106621	0.343564
19	1	0	-2.716016	2.228633	1.200712
20	1	0	-3.077536	2.767274	-0.472087
21	1	0	-4.422485	2.277921	0.611489
22	6	0	-3.733492	-0.524803	1.168319
23	1	0	-3.663440	-1.579325	0.897412
24	1	0	-3.054075	-0.293633	1.989434
25	1	0	-4.764415	-0.253818	1.407708
26	8	0	0.683392	-0.601742	2.875726
27	6	0	1.362054	1.098570	0.995750
28	6	0	2.666503	0.609381	0.977588
29	6	0	1.026399	2.280643	0.340270
30	6	0	3.642728	1.321050	0.290770
31	1	0	2.916605	-0.310320	1.495536
32	6	0	2.017312	2.982489	-0.335915
33	1	0	0.005465	2.649850	0.363630
34	6	0	3.334646	2.510920	-0.377943
35	1	0	4.661934	0.945672	0.275349

36	1	0	1.764591	3.911961	-0.838055
37	6	0	4.399258	3.252514	-1.139747
38	1	0	4.560610	2.789158	-2.119669
39	1	0	4.119592	4.295739	-1.307011
40	1	0	5.354014	3.229420	-0.606878



(9f)

Sum of electronic and zero-point Energies= -1861.086908

Sum of electronic and thermal Energies= -1861.063609

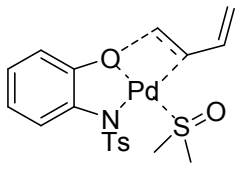
Sum of electronic and thermal Enthalpies= -1861.062665

Sum of electronic and thermal Free Energies= -1861.140782

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.177195	-3.690224	0.574646
2	6	0	1.123408	-2.895376	1.024109
3	6	0	0.614352	-1.900279	0.196115
4	6	0	1.101160	-1.723426	-1.110435
5	6	0	2.169708	-2.515628	-1.548300
6	6	0	2.699607	-3.487619	-0.703126
7	1	0	2.583650	-4.462914	1.219146
8	1	0	0.709640	-3.025190	2.017737
9	1	0	2.563302	-2.368469	-2.549696
10	1	0	3.521674	-4.104701	-1.054666
11	8	0	0.516663	-0.816395	-1.897020
12	7	0	-0.427880	-0.987110	0.615349
13	16	0	0.091037	0.118387	1.762139
14	8	0	-1.049522	0.988931	2.055131
15	46	0	-1.146445	-0.132954	-1.050967
16	16	0	-3.224425	0.435276	-0.254110
17	8	0	-4.190259	0.241239	-1.382456
18	6	0	-3.366721	2.111491	0.348203
19	1	0	-2.706347	2.228571	1.206788
20	1	0	-3.063833	2.773941	-0.464802
21	1	0	-4.411762	2.285297	0.615343
22	6	0	-3.730979	-0.521080	1.164862
23	1	0	-3.664362	-1.575012	0.890798

24	1	0	-3.050670	-0.294551	1.986600
25	1	0	-4.761036	-0.247385	1.404901
26	8	0	0.694792	-0.613777	2.870975
27	6	0	1.361586	1.095339	0.995153
28	6	0	2.662677	0.601010	0.954295
29	6	0	1.021236	2.284602	0.353173
30	6	0	3.633366	1.315333	0.259968
31	1	0	2.914744	-0.327126	1.456072
32	6	0	2.005155	2.988122	-0.328848
33	1	0	0.000978	2.654439	0.388949
34	6	0	3.322100	2.513982	-0.389077
35	1	0	4.648930	0.932082	0.221257
36	1	0	1.748677	3.919765	-0.825229
37	6	0	4.384800	3.298740	-1.109187
38	1	0	3.975619	3.808244	-1.985833
39	1	0	4.805116	4.066106	-0.449069
40	1	0	5.206263	2.654035	-1.432084



(Ts4-a)

Imaginary Freq.: -312.26 cm^{-1}

Sum of electronic and zero-point Energies= -2016.946852

Sum of electronic and thermal Energies= -2016.919461

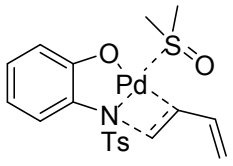
Sum of electronic and thermal Enthalpies= -2016.918517

Sum of electronic and thermal Free Energies= -2017.004274

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.643313	-3.624873	1.078277
2	6	0	-1.763501	-3.145909	0.107024
3	6	0	-1.039896	-1.974474	0.323197
4	6	0	-1.239372	-1.263454	1.528835
5	6	0	-2.101822	-1.755078	2.505696
6	6	0	-2.804663	-2.937141	2.278018
7	1	0	-3.181431	-4.551214	0.903010
8	1	0	-1.619977	-3.684825	-0.822587

9	1	0	-2.222046	-1.197099	3.429653
10	1	0	-3.477264	-3.317303	3.040883
11	8	0	-0.648852	-0.047263	1.672560
12	7	0	-0.057163	-1.483150	-0.600188
13	16	0	-0.662110	-0.897589	-2.012016
14	8	0	0.489201	-0.495405	-2.830122
15	8	0	-1.621429	-1.831261	-2.605177
16	6	0	-1.557933	0.582482	-1.578194
17	6	0	-0.883270	1.801349	-1.511939
18	6	0	-2.884531	0.480015	-1.174327
19	6	0	-1.550186	2.921889	-1.038046
20	1	0	0.154157	1.871581	-1.823794
21	6	0	-3.539165	1.613043	-0.696390
22	1	0	-3.401978	-0.471667	-1.231337
23	6	0	-2.883910	2.843741	-0.614126
24	1	0	-1.028100	3.873630	-0.987796
25	1	0	-4.575753	1.534552	-0.380969
26	6	0	-3.578901	4.067918	-0.081856
27	1	0	-3.558757	4.877896	-0.818111
28	1	0	-4.621975	3.859426	0.168284
29	1	0	-3.077665	4.436322	0.819545
30	46	0	1.057770	-0.130916	0.576055
31	6	0	1.775762	1.033150	2.218054
32	6	0	0.711171	0.542644	3.013676
33	1	0	2.730828	0.532835	2.377832
34	1	0	0.830883	-0.406179	3.527488
35	1	0	-0.042453	1.211015	3.414160
36	6	0	1.849446	2.454299	1.802453
37	6	0	0.825199	3.307283	1.697629
38	1	0	2.848632	2.797368	1.538996
39	1	0	0.987348	4.332863	1.380646
40	1	0	-0.199590	3.018656	1.920620
41	16	0	3.060078	-0.223301	-0.500946
42	8	0	4.274765	-0.121761	0.366130
43	6	0	3.125032	1.043811	-1.761724
44	1	0	2.294829	0.873659	-2.450058
45	1	0	3.024155	2.008623	-1.261299
46	1	0	4.087590	0.969510	-2.273649
47	6	0	3.168583	-1.707268	-1.491743
48	1	0	3.110909	-2.558699	-0.811717
49	1	0	2.328077	-1.713333	-2.188102
50	1	0	4.126952	-1.694244	-2.015728



(Ts4-b)

Imaginary Freq.: -273.49 cm^{-1}

Sum of electronic and zero-point Energies= -2016.940911

Sum of electronic and thermal Energies= -2016.913060

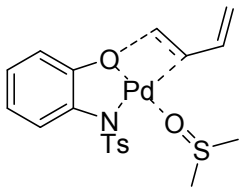
Sum of electronic and thermal Enthalpies= -2016.912116

Sum of electronic and thermal Free Energies= -2016.999765

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.295429	3.050250	-1.194604
2	6	0	1.916798	1.711050	-1.140550
3	6	0	0.748332	1.340962	-0.479552
4	6	0	-0.126347	2.312445	0.084713
5	6	0	0.311678	3.651535	0.075841
6	6	0	1.493791	4.005693	-0.565635
7	1	0	3.204887	3.341565	-1.709405
8	1	0	2.534786	0.939412	-1.590916
9	1	0	-0.318411	4.407280	0.535793
10	1	0	1.784909	5.052613	-0.591422
11	8	0	-1.305661	1.972079	0.561972
12	7	0	0.391413	-0.039374	-0.278669
13	16	0	1.115918	-0.746269	1.060070
14	8	0	0.958276	0.073789	2.259826
15	8	0	0.658874	-2.134089	1.104599
16	6	0	2.842576	-0.744457	0.633570
17	6	0	3.690264	0.211107	1.182064
18	6	0	3.311918	-1.678163	-0.289409
19	6	0	5.026753	0.231425	0.796034
20	1	0	3.309017	0.935427	1.893213
21	6	0	4.647343	-1.642887	-0.665042
22	1	0	2.646933	-2.426888	-0.707357
23	6	0	5.523379	-0.688217	-0.131332
24	1	0	5.692288	0.978469	1.218861
25	1	0	5.019021	-2.368320	-1.383235
26	6	0	6.972802	-0.678482	-0.533075
27	1	0	7.085675	-0.828293	-1.610757

28	1	0	7.456506	0.262504	-0.259788
29	1	0	7.513151	-1.490924	-0.034040
30	46	0	-1.655207	0.041687	-0.153366
31	6	0	-2.269177	-2.882641	-0.780944
32	6	0	-1.607645	-3.875652	-0.183013
33	1	0	-3.355529	-2.936221	-0.835995
34	1	0	-2.147990	-4.716741	0.241486
35	1	0	-0.527509	-3.877432	-0.079983
36	6	0	-1.707787	-1.673970	-1.430674
37	6	0	-0.330345	-1.464473	-1.669225
38	1	0	-2.365187	-1.234879	-2.183086
39	1	0	-0.028185	-0.823427	-2.490013
40	1	0	0.404265	-2.181060	-1.322789
41	16	0	-3.939658	0.172798	0.002072
42	8	0	-4.772031	-0.299924	-1.146704
43	6	0	-4.426568	1.835455	0.446095
44	1	0	-3.856671	2.147603	1.322864
45	1	0	-4.192373	2.485005	-0.398318
46	1	0	-5.500302	1.833300	0.647113
47	6	0	-4.412819	-0.717359	1.481740
48	1	0	-4.163165	-1.768408	1.324820
49	1	0	-3.847307	-0.319112	2.327613
50	1	0	-5.487255	-0.594479	1.637052



(Ts4-c)

Imaginary Freq.: -331.96 cm^{-1}

Sum of electronic and zero-point Energies= -2016.941314

Sum of electronic and thermal Energies= -2016.913184

Sum of electronic and thermal Enthalpies= -2016.912240

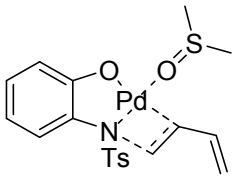
Sum of electronic and thermal Free Energies= -2017.000935

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.016207	-4.112732	0.692423
2	6	0	-1.109238	-3.411808	-0.102009

3	6	0	-0.716747	-2.116410	0.238418
4	6	0	-1.287596	-1.521495	1.387288
5	6	0	-2.175980	-2.229881	2.192150
6	6	0	-2.540505	-3.528733	1.843010
7	1	0	-2.290583	-5.127932	0.422562
8	1	0	-0.681991	-3.869894	-0.986662
9	1	0	-2.583524	-1.748067	3.076166
10	1	0	-3.231393	-4.081741	2.471958
11	8	0	-1.027990	-0.207428	1.633916
12	7	0	0.291559	-1.389084	-0.469988
13	16	0	-0.087406	-0.940788	-1.999316
14	8	0	1.113017	-0.325411	-2.574443
15	8	0	-0.713240	-2.036160	-2.745934
16	6	0	-1.314423	0.345267	-1.823633
17	6	0	-0.902266	1.671014	-1.688470
18	6	0	-2.652481	-0.001096	-1.672259
19	6	0	-1.840769	2.649855	-1.394405
20	1	0	0.145505	1.927392	-1.807456
21	6	0	-3.583801	0.992622	-1.377751
22	1	0	-2.966910	-1.033620	-1.782879
23	6	0	-3.194137	2.325579	-1.227388
24	1	0	-1.520126	3.682550	-1.285071
25	1	0	-4.630078	0.724541	-1.260419
26	6	0	-4.194587	3.401254	-0.900313
27	1	0	-4.222895	4.160005	-1.689312
28	1	0	-5.200452	2.989795	-0.785126
29	1	0	-3.925702	3.912491	0.030108
30	46	0	0.784547	0.181916	0.868740
31	6	0	0.830063	1.389032	2.628320
32	6	0	-0.191026	0.586665	3.203548
33	1	0	1.840654	1.146608	2.957461
34	1	0	0.087219	-0.326611	3.721235
35	1	0	-1.143152	1.019919	3.490487
36	6	0	0.582878	2.802379	2.264298
37	6	0	-0.602349	3.358020	1.987139
38	1	0	1.477554	3.419644	2.199782
39	1	0	-0.678863	4.410528	1.731848
40	1	0	-1.529622	2.789177	2.004107
41	16	0	3.522041	-0.224415	-0.642296
42	8	0	2.680789	0.747972	0.245720
43	6	0	3.992429	0.780244	-2.049229
44	1	0	4.686903	0.205071	-2.666896
45	1	0	3.077174	0.980809	-2.605533
46	1	0	4.457873	1.703743	-1.697920

47	6	0	5.101461	-0.280479	0.208020
48	1	0	4.944931	-0.790293	1.160561
49	1	0	5.800170	-0.856307	-0.404549
50	1	0	5.474147	0.733329	0.370206



(Ts4-d)

Imaginary Freq.: -292.03 cm^{-1}

Sum of electronic and zero-point Energies= -2016.942286

Sum of electronic and thermal Energies= -2016.914421

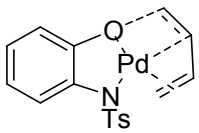
Sum of electronic and thermal Enthalpies= -2016.913477

Sum of electronic and thermal Free Energies= -2017.001147

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.493984	2.940859	-1.247831
2	6	0	2.051076	1.620947	-1.205164
3	6	0	0.811366	1.317277	-0.649413
4	6	0	-0.070494	2.336505	-0.183874
5	6	0	0.432357	3.655019	-0.173311
6	6	0	1.682661	3.942846	-0.708712
7	1	0	3.458852	3.180978	-1.681777
8	1	0	2.673092	0.813810	-1.582122
9	1	0	-0.200856	4.447572	0.215481
10	1	0	2.024637	4.974708	-0.722119
11	8	0	-1.299684	2.055675	0.178715
12	7	0	0.377350	-0.042023	-0.451870
13	16	0	0.926405	-0.724690	0.988011
14	8	0	0.443847	-2.103479	1.017927
15	46	0	-1.640271	0.097848	-0.525156
16	6	0	-2.239976	-2.808722	-1.153524
17	6	0	-1.668824	-3.850816	-0.545423
18	1	0	-3.324758	-2.789936	-1.245064
19	1	0	-2.279293	-4.656098	-0.146731
20	1	0	-0.595176	-3.932097	-0.409208
21	6	0	-1.577989	-1.634339	-1.765693

22	6	0	-0.179120	-1.468195	-1.873304
23	1	0	-2.148499	-1.174332	-2.575163
24	1	0	0.218811	-0.852202	-2.672461
25	1	0	0.500961	-2.201659	-1.456490
26	16	0	-4.629292	0.198354	0.560486
27	8	0	-3.734525	0.227811	-0.708511
28	6	0	-3.969121	-1.090478	1.623418
29	1	0	-4.540064	-1.089933	2.555936
30	1	0	-4.096311	-2.046647	1.113136
31	1	0	-2.909328	-0.897403	1.816465
32	6	0	-4.172770	1.624338	1.552434
33	1	0	-4.512960	2.516742	1.024430
34	1	0	-4.687151	1.543679	2.513680
35	1	0	-3.087569	1.653331	1.678486
36	8	0	0.646904	0.134601	2.137052
37	6	0	2.689339	-0.759929	0.760135
38	6	0	3.244422	-1.735578	-0.067250
39	6	0	3.484362	0.210356	1.358771
40	6	0	4.612482	-1.724549	-0.299076
41	1	0	2.619736	-2.498163	-0.520702
42	6	0	4.854733	0.205666	1.117752
43	1	0	3.037543	0.965777	1.995488
44	6	0	5.436819	-0.753449	0.285094
45	1	0	5.050787	-2.481063	-0.943931
46	1	0	5.479147	0.964972	1.579434
47	6	0	6.919120	-0.763920	0.028428
48	1	0	7.393357	-1.608726	0.540157
49	1	0	7.131060	-0.872943	-1.039535
50	1	0	7.392329	0.154269	0.384735



(Ts4-e)

Imaginary Freq.: -344.98 cm^{-1}

Sum of electronic and zero-point Energies= -1463.848749

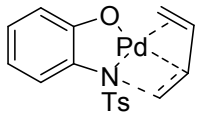
Sum of electronic and thermal Energies= -1463.827975

Sum of electronic and thermal Enthalpies= -1463.827031

Sum of electronic and thermal Free Energies= -1463.899688

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.327337	4.126158	-0.252771
2	6	0	0.315614	3.069422	0.653566
3	6	0	0.522854	1.752098	0.229317
4	6	0	0.737453	1.519502	-1.152343
5	6	0	0.777815	2.589167	-2.048886
6	6	0	0.564991	3.889798	-1.605025
7	1	0	0.174303	5.138955	0.107289
8	1	0	0.153680	3.253079	1.708947
9	1	0	0.959872	2.377375	-3.098273
10	1	0	0.590792	4.712848	-2.312408
11	8	0	0.836973	0.255068	-1.651014
12	7	0	0.599086	0.657162	1.147387
13	16	0	-0.734519	0.329821	2.041846
14	8	0	-0.390344	-0.776907	2.935775
15	8	0	-1.290453	1.545894	2.642064
16	6	0	-1.944849	-0.269099	0.870964
17	6	0	-2.023210	-1.633753	0.597213
18	6	0	-2.712962	0.644591	0.154734
19	6	0	-2.884275	-2.080832	-0.396978
20	1	0	-1.416897	-2.335402	1.161574
21	6	0	-3.566604	0.181939	-0.843043
22	1	0	-2.646889	1.705265	0.373266
23	6	0	-3.665266	-1.181570	-1.134121
24	1	0	-2.954891	-3.145066	-0.605307
25	1	0	-4.166644	0.893463	-1.403441
26	6	0	-4.608709	-1.684174	-2.193497
27	1	0	-4.896916	-0.886874	-2.883363
28	1	0	-4.156716	-2.496251	-2.770207
29	1	0	-5.524257	-2.078313	-1.738033
30	46	0	1.340031	-0.937696	0.020437
31	6	0	2.943036	-2.391200	-0.118133
32	6	0	3.217704	-1.532384	0.956171
33	1	0	2.791763	-3.450794	0.069948
34	1	0	3.293567	-1.966115	1.948413
35	1	0	3.717943	-0.576114	0.814283
36	6	0	2.527814	-1.928352	-1.411640
37	6	0	2.622456	-0.585864	-1.947296
38	1	0	2.116046	-2.680385	-2.078519
39	1	0	2.450700	-0.467854	-3.008840
40	1	0	3.275204	0.153803	-1.490666



(Ts4-f)

Imaginary Freq.: -327.71 cm^{-1}

Sum of electronic and zero-point Energies= -1463.857146

Sum of electronic and thermal Energies= -1463.836292

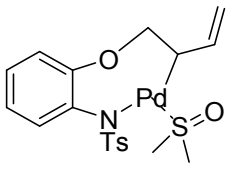
Sum of electronic and thermal Enthalpies= -1463.835348

Sum of electronic and thermal Free Energies= -1463.908376

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.415368	4.056883	0.107765
2	6	0	0.155224	2.978569	0.772557
3	6	0	0.334381	1.756712	0.119417
4	6	0	0.016833	1.610264	-1.262802
5	6	0	-0.596343	2.709985	-1.900833
6	6	0	-0.801966	3.905177	-1.227984
7	1	0	-0.559286	5.001796	0.621300
8	1	0	0.443145	3.059827	1.814921
9	1	0	-0.873640	2.604143	-2.945740
10	1	0	-1.256051	4.739888	-1.755396
11	8	0	0.299309	0.515015	-1.939128
12	7	0	0.792868	0.592245	0.820940
13	16	0	-0.241564	-0.040836	1.977624
14	8	0	0.445835	-1.178597	2.582206
15	8	0	-0.717813	1.024368	2.854112
16	6	0	-1.624769	-0.630173	1.029594
17	6	0	-1.626821	-1.949502	0.578171
18	6	0	-2.630859	0.258140	0.665292
19	6	0	-2.658676	-2.377861	-0.244260
20	1	0	-0.832933	-2.629898	0.869393
21	6	0	-3.654084	-0.187376	-0.167333
22	1	0	-2.618587	1.282253	1.022775
23	6	0	-3.682964	-1.503593	-0.634585
24	1	0	-2.671854	-3.407039	-0.592299
25	1	0	-4.440989	0.502968	-0.456525
26	6	0	-4.789035	-1.989533	-1.531423
27	1	0	-5.359956	-2.787068	-1.044092
28	1	0	-5.480642	-1.183783	-1.788571

29	1	0	-4.383206	-2.403945	-2.459860
30	46	0	1.425716	-0.684917	-0.704162
31	6	0	2.850608	-1.371704	0.683386
32	6	0	2.759141	-0.005684	1.139377
33	1	0	2.585263	-2.131113	1.411159
34	1	0	2.650903	0.147425	2.204565
35	1	0	3.243398	0.802914	0.598995
36	6	0	3.267048	-1.857557	-0.606878
37	6	0	3.371803	-1.063052	-1.745186
38	1	0	3.269092	-2.938920	-0.715219
39	1	0	3.479506	-1.551001	-2.708674
40	1	0	3.674298	-0.019076	-1.697027



(10)

Sum of electronic and zero-point Energies= -2016.967280

Sum of electronic and thermal Energies= -2016.939561

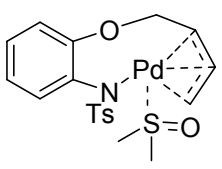
Sum of electronic and thermal Enthalpies= -2016.938617

Sum of electronic and thermal Free Energies= -2017.026028

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.900636	-3.567516	-0.751296
2	6	0	1.960001	-3.083560	0.154904
3	6	0	1.187685	-1.955048	-0.137814
4	6	0	1.415520	-1.329809	-1.383066
5	6	0	2.339379	-1.807750	-2.298421
6	6	0	3.085092	-2.941037	-1.980705
7	1	0	3.478257	-4.451467	-0.499446
8	1	0	1.802007	-3.581577	1.104709
9	1	0	2.475533	-1.292612	-3.244408
10	1	0	3.807485	-3.325556	-2.693245
11	8	0	0.722110	-0.148872	-1.631466
12	7	0	0.156726	-1.488000	0.730670
13	16	0	0.626631	-0.809233	2.130468
14	8	0	-0.600040	-0.514869	2.884842

15	8	0	1.669955	-1.585085	2.808268
16	6	0	1.358239	0.754318	1.664609
17	6	0	0.570673	1.904389	1.628302
18	6	0	2.667876	0.777637	1.194088
19	6	0	1.100386	3.078397	1.110790
20	1	0	-0.448455	1.878576	1.999091
21	6	0	3.184108	1.961610	0.672672
22	1	0	3.279431	-0.118149	1.229563
23	6	0	2.409615	3.123030	0.614931
24	1	0	0.487552	3.975468	1.083745
25	1	0	4.205034	1.979668	0.301490
26	6	0	2.952612	4.399631	0.031802
27	1	0	2.343979	4.725981	-0.818614
28	1	0	2.934207	5.205847	0.772411
29	1	0	3.981877	4.276259	-0.314094
30	46	0	-1.066117	-0.213071	-0.551481
31	6	0	-1.347043	0.694882	-2.358698
32	6	0	-0.047340	0.079482	-2.880395
33	1	0	-2.233438	0.299736	-2.855029
34	1	0	-0.212766	-0.885734	-3.363512
35	1	0	0.549986	0.727998	-3.526799
36	6	0	-1.379945	2.159897	-2.161195
37	6	0	-0.318764	2.975714	-2.108505
38	1	0	-2.373247	2.582627	-2.014268
39	1	0	-0.442830	4.040669	-1.937501
40	1	0	0.698938	2.613310	-2.231910
41	16	0	-3.160628	-0.224825	0.248365
42	8	0	-4.320247	-0.081196	-0.683320
43	6	0	-3.280567	1.005691	1.545327
44	1	0	-2.497770	0.795606	2.278670
45	1	0	-3.135090	1.986147	1.088739
46	1	0	-4.273202	0.932439	1.996764
47	6	0	-3.351654	-1.720877	1.214619
48	1	0	-3.278399	-2.567180	0.529737
49	1	0	-2.543263	-1.752318	1.949242
50	1	0	-4.330836	-1.697840	1.698489



(Ts5)

Imaginary Freq.: -73.39 cm^{-1}

Sum of electronic and zero-point Energies= -2016.956126

Sum of electronic and thermal Energies= -2016.928856

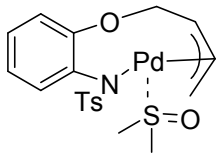
Sum of electronic and thermal Enthalpies= -2016.927912

Sum of electronic and thermal Free Energies= -2017.014741

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.138266	4.341219	-0.615046
2	6	0	-0.036463	3.343110	0.350127
3	6	0	-0.036383	1.986210	0.003420
4	6	0	-0.152275	1.673615	-1.372317
5	6	0	-0.242572	2.666315	-2.340117
6	6	0	-0.230502	4.006952	-1.963272
7	1	0	-0.128532	5.383417	-0.310871
8	1	0	0.055229	3.598703	1.399663
9	1	0	-0.334462	2.381871	-3.384202
10	1	0	-0.297903	4.780773	-2.721201
11	8	0	-0.244245	0.343153	-1.735682
12	7	0	0.161420	0.964081	0.971629
13	16	0	-1.000281	0.704019	2.061746
14	8	0	-0.477738	-0.264064	3.031686
15	8	0	-1.556341	1.958951	2.585866
16	6	0	-2.341244	-0.101864	1.192225
17	6	0	-2.546155	-1.468652	1.337083
18	6	0	-3.138079	0.644784	0.322107
19	6	0	-3.560150	-2.091949	0.612203
20	1	0	-1.920457	-2.038895	2.015343
21	6	0	-4.134177	0.007976	-0.405889
22	1	0	-2.985399	1.714285	0.218924
23	6	0	-4.362220	-1.368503	-0.272258
24	1	0	-3.724152	-3.158934	0.735441
25	1	0	-4.754419	0.589501	-1.082933
26	6	0	-5.449891	-2.038533	-1.069140
27	1	0	-6.418723	-1.560594	-0.890909
28	1	0	-5.247495	-1.964648	-2.143103
29	1	0	-5.539377	-3.097431	-0.813943
30	46	0	1.153005	-0.652269	-0.121728
31	6	0	1.365641	-1.414361	-1.984310
32	6	0	0.702265	-0.226766	-2.683219
33	1	0	2.367404	-1.630370	-2.352309
34	1	0	1.447948	0.525617	-2.951779

35	1	0	0.152107	-0.528748	-3.580614
36	6	0	0.562791	-2.579601	-1.615231
37	6	0	-0.774482	-2.565349	-1.420777
38	1	0	1.118621	-3.484334	-1.377370
39	1	0	-1.281826	-3.450947	-1.052030
40	1	0	-1.387874	-1.700525	-1.653714
41	16	0	3.317292	-0.866703	0.481748
42	8	0	3.939363	-2.227650	0.520031
43	6	0	3.519258	-0.087841	2.083926
44	1	0	3.129153	0.931041	2.029715
45	1	0	2.942079	-0.668580	2.805175
46	1	0	4.580364	-0.092584	2.343917
47	6	0	4.342435	0.208629	-0.522894
48	1	0	4.305956	-0.166932	-1.546885
49	1	0	3.930395	1.219671	-0.479704
50	1	0	5.365531	0.181911	-0.139381



(11)

Sum of electronic and zero-point Energies= -2016.979215

Sum of electronic and thermal Energies= -2016.951998

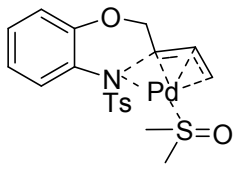
Sum of electronic and thermal Enthalpies= -2016.951054

Sum of electronic and thermal Free Energies= -2017.036087

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.522784	3.809326	0.455348
2	6	0	-1.032646	2.842195	-0.414907
3	6	0	-0.508256	1.622999	0.045502
4	6	0	-0.486655	1.418666	1.447081
5	6	0	-0.990278	2.386271	2.315335
6	6	0	-1.513792	3.578804	1.828642
7	1	0	-1.928209	4.734057	0.056152
8	1	0	-1.061796	3.005565	-1.486209
9	1	0	-0.954004	2.192903	3.383715
10	1	0	-1.901852	4.321377	2.518704
11	8	0	0.075985	0.283222	1.986182

12	7	0	-0.161322	0.600133	-0.869711
13	16	0	1.066951	0.790518	-1.886897
14	8	0	0.937123	-0.230894	-2.932679
15	8	0	1.216958	2.188480	-2.316450
16	6	0	2.554971	0.394799	-0.973506
17	6	0	3.315795	-0.713299	-1.322485
18	6	0	2.912017	1.179233	0.124904
19	6	0	4.433648	-1.047883	-0.560318
20	1	0	3.028167	-1.315887	-2.177072
21	6	0	4.023750	0.831668	0.879610
22	1	0	2.325996	2.052769	0.393309
23	6	0	4.800283	-0.288694	0.552002
24	1	0	5.025610	-1.916776	-0.835269
25	1	0	4.298534	1.439466	1.737958
26	6	0	6.003089	-0.649360	1.382500
27	1	0	5.725175	-0.812485	2.429004
28	1	0	6.483369	-1.558702	1.012610
29	1	0	6.745264	0.155933	1.368082
30	46	0	-0.864884	-1.312679	-0.099565
31	6	0	-1.041049	-1.937695	1.963162
32	6	0	-0.781664	-0.620089	2.684436
33	1	0	-1.944167	-2.436256	2.311904
34	1	0	-1.742810	-0.143325	2.898098
35	1	0	-0.304031	-0.851905	3.643898
36	6	0	-0.091752	-2.742631	1.301120
37	6	0	0.975533	-2.113482	0.610471
38	1	0	-0.345977	-3.779618	1.096028
39	1	0	1.555935	-2.715813	-0.083718
40	1	0	1.480110	-1.250309	1.030570
41	16	0	-3.131159	-0.816580	-0.533983
42	8	0	-4.045184	-1.996854	-0.692746
43	6	0	-3.251217	0.203739	-2.003188
44	1	0	-2.685060	1.122764	-1.840884
45	1	0	-2.815031	-0.358187	-2.830861
46	1	0	-4.305444	0.417425	-2.194136
47	6	0	-3.844227	0.309164	0.668176
48	1	0	-3.812914	-0.183620	1.641300
49	1	0	-3.255500	1.229532	0.691765
50	1	0	-4.877761	0.516368	0.379358



(Ts6)

Imaginary Freq.: -315.63 cm^{-1}

Sum of electronic and zero-point Energies= -2016.954090

Sum of electronic and thermal Energies= -2016.927195

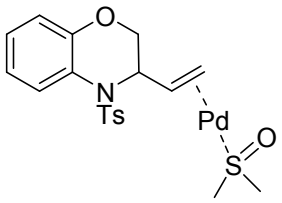
Sum of electronic and thermal Enthalpies= -2016.926250

Sum of electronic and thermal Free Energies= -2017.012222

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.103287	-0.165524	-0.197164
2	6	0	0.076248	-1.529514	1.376843
3	6	0	0.011215	2.271647	-0.602259
4	6	0	1.002188	1.404804	1.417586
5	6	0	1.321148	2.698581	1.820500
6	6	0	1.005157	3.776880	1.000293
7	1	0	0.079267	4.403804	-0.843150
8	1	0	-0.493245	2.092604	-1.545158
9	1	0	1.820234	2.841258	2.773577
10	1	0	1.261689	4.784243	1.312724
11	8	0	1.339698	0.363723	2.236446
12	6	0	0.341985	3.563924	-0.207769
13	16	0	0.934469	-0.743784	-1.486051
14	8	0	0.615845	-2.169334	-1.577486
15	8	0	0.718119	0.089400	-2.671398
16	6	0	2.649450	-0.585496	-1.029479
17	6	0	3.320350	-1.680539	-0.493141
18	6	0	3.280275	0.654642	-1.137307
19	6	0	4.630799	-1.527187	-0.051078
20	1	0	2.828489	-2.645553	-0.431593
21	6	0	4.586195	0.791869	-0.685323
22	1	0	2.760227	1.501896	-1.571301
23	6	0	5.278390	-0.291531	-0.130282
24	1	0	5.155921	-2.383442	0.362357
25	1	0	5.078885	1.756725	-0.766837
26	6	0	6.682313	-0.116474	0.381989
27	1	0	6.679451	0.426454	1.333818
28	1	0	7.170221	-1.080192	0.548436
29	1	0	7.290058	0.462470	-0.319840

30	46	0	-2.034758	-0.914929	0.206398
31	6	0	0.362050	1.173603	0.190787
32	6	0	0.274486	-0.539588	2.484942
33	1	0	1.003492	-1.949566	1.004564
34	1	0	-0.644320	0.009265	2.719377
35	1	0	0.560711	-1.118004	3.370181
36	6	0	-1.049892	-2.420473	1.328926
37	6	0	-2.321678	-2.180131	1.908063
38	1	0	-0.902546	-3.329713	0.752061
39	1	0	-2.447218	-1.489528	2.740073
40	1	0	-3.048564	-2.987298	1.874953
41	16	0	-3.778384	0.431202	-0.461905
42	8	0	-5.206590	-0.005188	-0.284030
43	6	0	-3.570661	0.927930	-2.177830
44	1	0	-2.576744	1.363301	-2.304934
45	1	0	-3.661973	0.031061	-2.793157
46	1	0	-4.348083	1.650820	-2.437239
47	6	0	-3.590834	2.044323	0.310715
48	1	0	-3.728313	1.908682	1.385027
49	1	0	-2.583356	2.420047	0.112169
50	1	0	-4.347457	2.724932	-0.088267



(12)

Sum of electronic and zero-point Energies= -2016.995547

Sum of electronic and thermal Energies= -2016.968398

Sum of electronic and thermal Enthalpies= -2016.967454

Sum of electronic and thermal Free Energies= -2017.054466

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.119919	-1.508210	0.729801
2	6	0	3.783376	-1.734705	1.031061
3	6	0	2.786934	-1.358197	0.131920
4	6	0	3.132615	-0.798995	-1.106839
5	6	0	4.478963	-0.584889	-1.411995
6	6	0	5.461120	-0.924807	-0.492085
7	1	0	5.890303	-1.792441	1.438392

8	1	0	3.490385	-2.186729	1.971312
9	1	0	4.731271	-0.144949	-2.371130
10	1	0	6.503625	-0.744829	-0.735562
11	8	0	2.224960	-0.450676	-2.045405
12	7	0	1.391883	-1.544983	0.427398
13	16	0	0.822915	-0.390585	1.536749
14	8	0	-0.621476	-0.572377	1.711022
15	8	0	1.664927	-0.528444	2.713778
16	6	0	1.114319	1.216818	0.840720
17	6	0	0.087313	1.879487	0.172145
18	6	0	2.386165	1.778294	0.941992
19	6	0	0.340295	3.115237	-0.404997
20	1	0	-0.896555	1.429189	0.094450
21	6	0	2.622833	3.014797	0.352656
22	1	0	3.178309	1.265171	1.476347
23	6	0	1.611444	3.697539	-0.330478
24	1	0	-0.462076	3.635357	-0.920647
25	1	0	3.611030	3.458004	0.430371
26	6	0	1.882546	5.019269	-0.993996
27	1	0	2.028780	4.879894	-2.070973
28	1	0	1.042832	5.707780	-0.864600
29	1	0	2.784084	5.489224	-0.593410
30	46	0	-2.158862	-0.928256	-0.150098
31	6	0	0.677332	-1.916962	-0.831366
32	6	0	0.853060	-0.827486	-1.879241
33	1	0	1.258525	-2.787026	-1.163510
34	1	0	0.520183	-1.185666	-2.855417
35	1	0	0.272325	0.064551	-1.627261
36	6	0	-0.738085	-2.408202	-0.631946
37	6	0	-1.712454	-2.418777	-1.637551
38	1	0	-0.805984	-3.160157	0.155276
39	1	0	-2.489049	-3.179760	-1.616500
40	1	0	-1.538354	-1.973461	-2.614611
41	16	0	-4.053384	0.420458	-0.063764
42	8	0	-5.147087	0.267240	-1.088676
43	6	0	-3.627171	2.170999	-0.003151
44	1	0	-2.942608	2.352033	0.829187
45	1	0	-3.142931	2.425724	-0.947790
46	1	0	-4.544308	2.752526	0.120495
47	6	0	-4.814606	0.293805	1.564264
48	1	0	-5.196806	-0.723216	1.670988
49	1	0	-4.055707	0.483184	2.327973
50	1	0	-5.631379	1.016258	1.640353
