

*Supporting Information*

**DFT Studies on the Distinct Mechanisms of C–H Activation and  
Oxidation Reactions Mediated by Mononuclear- and Binuclear-  
Palladium**

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**Table S1-1.** Some optimized Cartesian Coordinates of stationary points for the C-H activation, involved in the discussion on Pd(OAc)<sub>2</sub> as catalyst, computed at B2PLYP-IDSCRF/DGDZVP level in dichloromethane with bond lengths in Å.

..... s4

**Table S1-2.** Some optimized Cartesian Coordinates of stationary points for the oxidative process (Pd<sup>II</sup> to Pd<sup>III</sup>), involved in the discussion on PhI(OAc)<sub>2</sub> (**OX-a**), PhICl<sub>2</sub> (**OX-b**) and NCS (**OX-c**) as oxidant, computed at B2PLYP-IDSCRF/DGDZVP level in dichloromethane with bond lengths in Å.

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**Table S1-3.** Some optimized Cartesian Coordinates of stationary points for the oxidative process (Pd<sup>II</sup> to Pd<sup>IV</sup>), involved in the discussion on PhI(OAc)<sub>2</sub> (**OX-a**), PhICl<sub>2</sub> (**OX-b**) and NCS (**OX-c**) as oxidant, computed at B2PLYP-IDSCRF/DGDZVP level in dichloromethane with bond lengths in Å.

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**Table S1-4.** Some optimized Cartesian Coordinates of stationary points for the C-H activation, involved in the discussion on Pd(OAc)<sub>2</sub> as catalyst, computed at B3LYP-IDSCRF/DGDZVP level in dichloromethane with bond lengths in Å.

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**Table S1-5.** Some optimized Cartesian Coordinates of stationary points for the oxidative process (Pd<sup>II</sup> to Pd<sup>III</sup>), involved in the discussion on PhI(OAc)<sub>2</sub> (**OX-a**), PhICl<sub>2</sub> (**OX-b**) and NCS (**OX-c**) as oxidant, computed at B3LYP-IDSCRF/DGDZVP level in dichloromethane with bond lengths in Å.

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**Table S1-6.** Some optimized Cartesian Coordinates of stationary points for the oxidative process (Pd<sup>II</sup> to Pd<sup>IV</sup>), involved in the discussion on PhI(OAc)<sub>2</sub> (**OX-a**), PhICl<sub>2</sub> (**OX-b**) and NCS (**OX-c**) as oxidant, computed at B3LYP-IDSCRF/DGDZVP level in dichloromethane with bond lengths in Å.

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**Table S2-1.** Frequencies of some stationary points for the C-H activation, involved in the discussion on Pd(OAc)<sub>2</sub> as catalyst, computed at B3LYP-IDSCRF/DGDZVP level in dichloromethane.

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**Table S2-2.** Frequencies of some stationary points for the oxidative process ( $\text{Pd}^{\text{II}}$  to  $\text{Pd}^{\text{III}}$ ), involved in the discussion on  $\text{PhI}(\text{OAc})_2$  (**OX-a**),  $\text{PhICl}_2$  (**OX-b**) and  $\text{NCS}$  (**OX-c**) as oxidant, computed at B3LYP-IDSCRF/DGDZVP level in dichloromethane.

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**Table S2-3.** Frequencies of some stationary points for the oxidative process ( $\text{Pd}^{\text{II}}$  to  $\text{Pd}^{\text{IV}}$ ), involved in the discussion on  $\text{PhI}(\text{OAc})_2$  (**OX-a**),  $\text{PhICl}_2$  (**OX-b**) and  $\text{NCS}$  (**OX-c**) as oxidant, computed at B3LYP-IDSCRF/DGDZVP level in dichloromethane.

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**Table S3-1.** The total energies ( $E_{\text{tot}}/\text{a.u.} = E_{\text{elec}}/\text{a.u.} + \text{ZPE}/\text{a.u.}$ ), electronic energies ( $E_{\text{elec}}/\text{a.u.}$ ) and Gibbs free energies ( $G/\text{a.u.}$ ) for the C-H activation, involved in the discussion on  $\text{Pd}(\text{OAc})_2$  as catalyst, computed at B3LYP-IDSCRF/DGDZVP level in dichloromethane at 313K.

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**Table S3-2.** The total energies ( $E_{\text{tot}}/\text{a.u.} = E_{\text{elec}}/\text{a.u.} + \text{ZPE}/\text{a.u.}$ ), electronic energies ( $E_{\text{elec}}/\text{a.u.}$ ) and Gibbs free energies ( $G/\text{a.u.}$ ) for the oxidative process ( $\text{Pd}^{\text{II}}$  to  $\text{Pd}^{\text{III}}$ ), involved in the discussion on  $\text{PhI}(\text{OAc})_2$  (**OX-a**),  $\text{PhICl}_2$  (**OX-b**) and  $\text{NCS}$  (**OX-c**) as oxidant, computed at B3LYP-IDSCRF/DGDZVP level in dichloromethane at 238K(**OX-a**), 243K(**OX-b**), 195K(**OX-c**).

..... s130

**Table S3-3.** The total energies ( $E_{\text{tot}}/\text{a.u.} = E_{\text{elec}}/\text{a.u.} + \text{ZPE}/\text{a.u.}$ ), electronic energies ( $E_{\text{elec}}/\text{a.u.}$ ) and Gibbs free energies ( $G/\text{a.u.}$ ) for the oxidative process ( $\text{Pd}^{\text{II}}$  to  $\text{Pd}^{\text{IV}}$ ), involved in the discussion on  $\text{PhI}(\text{OAc})_2$  (**OX-a**),  $\text{PhICl}_2$  (**OX-b**) and  $\text{NCS}$  (**OX-c**) as oxidant, computed at B3LYP-IDSCRF/DGDZVP level in dichloromethane at 298K.

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**Table S3-4.** The electronic energies ( $E_{\text{elec}}/\text{a.u.}$ ) for the C-H activation, involved in the discussion on  $\text{Pd}(\text{OAc})_2$  as catalyst, computed at B2PLYP-IDSCRF/DGDZVP level in dichloromethane at 313K.

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**Table S3-5.** The electronic energies ( $E_{\text{elec}}/\text{a.u.}$ ) for the oxidative process ( $\text{Pd}^{\text{II}}$  to  $\text{Pd}^{\text{III}}$ ), involved in the discussion on  $\text{PhI}(\text{OAc})_2$  (**OX-a**),  $\text{PhICl}_2$  (**OX-b**) and  $\text{NCS}$  (**OX-c**) as oxidant, computed at B2PLYP-IDSCRF/DGDZVP level in dichloromethane at 238K(**OX-a**), 243K(**OX-b**), 195K(**OX-c**).

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**Table S3-6.** The electronic energies ( $E_{\text{elec}}/\text{a.u.}$ ) for the oxidative process ( $\text{Pd}^{\text{II}}$  to  $\text{Pd}^{\text{IV}}$ ), involved in the discussion on  $\text{PhI}(\text{OAc})_2$  (**OX-a**),  $\text{PhICl}_2$  (**OX-b**) and  $\text{NCS}$  (**OX-c**) as oxidant, computed at B2PLYP-IDSCRF/DGDZVP level in dichloromethane at 298K.

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**Table S4.** Calculated free energy barriers ( $\text{kcal mol}^{-1}$ ) with the oxidation of  $1\text{a} \rightarrow 2\text{a}$  for different calculation methods.

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**Table S5.** Calculated free energy barriers ( $\Delta G$ ,  $\text{kcal mol}^{-1}$ ) with the oxidation of B3LYP-IDSCRF+D3

s132

**Figure S1.** Gibbs free-energy profiles ( $\Delta G$ ,  $\text{kcal mol}^{-1}$ ) for the oxidative process ( $\text{Pd}^{\text{II}}$  to  $\text{Pd}^{\text{III}}$ ), involved in the discussion on  $\text{PhI}(\text{OAc})_2$  (**OX-a**) as oxidant, with the schematic representation of stationary points along the reaction coordinates in dichloromethane at 238K(**OX-a**).

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**Figure S2.** Gibbs free-energy profiles ( $\Delta G$ ,  $\text{kcal mol}^{-1}$ ) for the oxidative process ( $\text{Pd}^{\text{II}}$  to  $\text{Pd}^{\text{IV}}$ ), involved in the discussion on  $\text{NCS}$  (**OX-c**) as oxidant, with the schematic representation of stationary points along the reaction coordinates in dichloromethane at 298K.

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**Figure S3.** Gibbs free-energy profiles ( $\Delta G$ , kcal mol<sup>-1</sup>) for the oxidative process (Pd<sup>II</sup> to Pd<sup>IV</sup>), involved in the discussion on NFTPT (**OX-d**) as oxidant, computed at B3LYP-IDSCRF/DGDZVP level, with the schematic representation of stationary points along the reaction coordinates in DCE at 296K.

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**Figure S4.** Gibbs free-energy profiles ( $\Delta G$ , kcal mol<sup>-1</sup>) for the C-H activation process, involved in the mononuclear mechanism, computed at B3LYP-IDSCRF+D3/DGDZVP in dichloromethane at 298K.

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**Figure S5.** The bond length change (Å) and the change of  $\langle S^2 \rangle$  expectation value along the distance of O1-Pd (Å) under IRC of **TS1m-a**.

s134

**Table S1-1.** Some optimized Cartesian Coordinates of stationary points for the C-H activation, involved in the discussion on Pd(OAc)<sub>2</sub> as catalyst, computed at B3LYP-IDSCRF/DGDZVP level in dichloromethane with bond lengths in Å.

| Species                                  | Cartesian coordinates |              |              |              |
|------------------------------------------|-----------------------|--------------|--------------|--------------|
| <b>R</b>                                 | 6                     | -0.763498000 | 0.022345000  | -0.009396000 |
|                                          | 6                     | -1.499304000 | 1.178917000  | 0.310442000  |
|                                          | 6                     | -2.894807000 | 1.128294000  | 0.294848000  |
|                                          | 6                     | -3.524072000 | -0.077622000 | -0.030559000 |
|                                          | 6                     | -2.714765000 | -1.181946000 | -0.319074000 |
|                                          | 6                     | 0.724393000  | 0.019301000  | -0.010141000 |
|                                          | 6                     | 1.461407000  | 1.185494000  | -0.291213000 |
|                                          | 6                     | 2.860997000  | 1.164441000  | -0.282723000 |
|                                          | 6                     | 3.547424000  | -0.021468000 | 0.009472000  |
|                                          | 6                     | 2.821343000  | -1.188977000 | 0.285151000  |
|                                          | 6                     | 1.423106000  | -1.170567000 | 0.270063000  |
|                                          | 1                     | -0.990605000 | 2.095863000  | 0.589467000  |
|                                          | 1                     | -3.478273000 | 2.010821000  | 0.541820000  |
|                                          | 1                     | -4.605687000 | -0.166813000 | -0.054599000 |
|                                          | 1                     | -3.163714000 | -2.141397000 | -0.569551000 |
|                                          | 1                     | 0.948603000  | 2.109559000  | -0.543190000 |
|                                          | 1                     | 3.413758000  | 2.071907000  | -0.510842000 |
|                                          | 1                     | 4.633908000  | -0.036775000 | 0.018271000  |
|                                          | 1                     | 3.345756000  | -2.113518000 | 0.512545000  |
|                                          | 1                     | 0.858962000  | -2.073600000 | 0.480619000  |
|                                          | 7                     | -1.371808000 | -1.147459000 | -0.313434000 |
| <b>Pd<sub>2</sub>(μ-OAc)<sub>4</sub></b> | 46                    | 0.000228000  | 0.000285000  | 1.314242000  |
|                                          | 6                     | 1.876285000  | -1.860308000 | -0.000726000 |
|                                          | 8                     | 1.467122000  | -1.464076000 | 1.146834000  |
|                                          | 8                     | 1.467336000  | -1.463374000 | -1.148159000 |
|                                          | 6                     | 2.986445000  | -2.884892000 | -0.000971000 |
|                                          | 1                     | 2.933991000  | -3.501623000 | -0.898097000 |
|                                          | 1                     | 3.941502000  | -2.351000000 | -0.001098000 |
|                                          | 1                     | 2.934256000  | -3.501855000 | 0.896017000  |
|                                          | 6                     | -1.876474000 | 1.860629000  | 0.000343000  |
|                                          | 8                     | -1.466656000 | 1.464372000  | 1.147634000  |
|                                          | 8                     | -1.467568000 | 1.464321000  | -1.147353000 |
|                                          | 6                     | -2.987481000 | 2.884257000  | 0.000442000  |
|                                          | 1                     | -2.929363000 | 3.507702000  | -0.891719000 |
|                                          | 1                     | -3.942006000 | 2.349538000  | -0.010763000 |
|                                          | 1                     | -2.942057000 | 3.494569000  | 0.902298000  |
|                                          | 46                    | -0.000094000 | 0.000538000  | -1.314523000 |
|                                          | 6                     | 1.875989000  | 1.861275000  | 0.000090000  |
|                                          | 8                     | 1.466931000  | 1.464613000  | 1.147549000  |
|                                          | 8                     | 1.466455000  | 1.465231000  | -1.147449000 |

|                                                           |    |              |              |              |
|-----------------------------------------------------------|----|--------------|--------------|--------------|
|                                                           | 6  | 2.986752000  | 2.885176000  | 0.000260000  |
|                                                           | 1  | 3.941424000  | 2.350599000  | 0.001178000  |
|                                                           | 1  | 2.935437000  | 3.501607000  | -0.897130000 |
|                                                           | 1  | 2.934275000  | 3.502486000  | 0.896997000  |
|                                                           | 6  | -1.875680000 | -1.860633000 | 0.000005000  |
|                                                           | 8  | -1.466459000 | -1.464166000 | 1.147484000  |
|                                                           | 8  | -1.466633000 | -1.464078000 | -1.147497000 |
|                                                           | 6  | -2.986065000 | -2.884963000 | 0.000067000  |
|                                                           | 1  | -3.940957000 | -2.350776000 | 0.000962000  |
|                                                           | 1  | -2.934428000 | -3.501349000 | -0.897339000 |
|                                                           | 1  | -2.933427000 | -3.502285000 | 0.896786000  |
| <b>Pd<sub>2</sub>(OAc)<sub>2</sub>(μ-OAc)<sub>2</sub></b> | 46 | -1.501228000 | -0.130513000 | -0.002633000 |
|                                                           | 46 | 1.503769000  | -0.131907000 | 0.000528000  |
|                                                           | 6  | -0.001106000 | -1.941384000 | 1.873223000  |
|                                                           | 8  | 1.141037000  | -1.544614000 | 1.465061000  |
|                                                           | 8  | -1.141822000 | -1.547457000 | 1.458241000  |
|                                                           | 6  | -0.003141000 | -3.011931000 | 2.939990000  |
|                                                           | 1  | -0.000079000 | -3.986754000 | 2.443181000  |
|                                                           | 1  | 0.891658000  | -2.933931000 | 3.557132000  |
|                                                           | 1  | -0.902198000 | -2.936476000 | 3.551224000  |
|                                                           | 8  | -1.139906000 | -1.543732000 | -1.466451000 |
|                                                           | 6  | 0.001818000  | -1.942067000 | -1.874403000 |
|                                                           | 8  | 1.143029000  | -1.548930000 | -1.460176000 |
|                                                           | 6  | 0.002173000  | -3.013878000 | -2.939874000 |
|                                                           | 1  | 0.901071000  | -2.940303000 | -3.551575000 |
|                                                           | 1  | -0.001882000 | -3.988040000 | -2.441769000 |
|                                                           | 1  | -0.892798000 | -2.935587000 | -3.556717000 |
|                                                           | 8  | 2.112800000  | 1.539250000  | 1.097320000  |
|                                                           | 6  | 2.360766000  | 2.165734000  | -0.001673000 |
|                                                           | 8  | 2.113580000  | 1.537000000  | -1.099479000 |
|                                                           | 6  | 2.931753000  | 3.545766000  | -0.002930000 |
|                                                           | 1  | 4.022829000  | 3.471869000  | -0.004275000 |
|                                                           | 1  | 2.620118000  | 4.081775000  | 0.894490000  |
|                                                           | 1  | 2.617962000  | 4.080908000  | -0.900135000 |
|                                                           | 8  | -2.111497000 | 1.541727000  | -1.098413000 |
|                                                           | 6  | -2.359406000 | 2.166929000  | 0.001311000  |
|                                                           | 8  | -2.110672000 | 1.537601000  | 1.098561000  |
|                                                           | 6  | -2.932594000 | 3.546045000  | 0.004461000  |
|                                                           | 1  | -4.023526000 | 3.470294000  | 0.003045000  |
|                                                           | 1  | -2.619911000 | 4.084601000  | -0.891058000 |
|                                                           | 1  | -2.621808000 | 4.079681000  | 0.903589000  |
| <b>COM1<sup>bi</sup></b>                                  | 46 | -0.014266000 | 0.191792000  | -0.143597000 |
|                                                           | 6  | -0.637501000 | -2.202391000 | 1.501102000  |
|                                                           | 8  | 0.320003000  | -1.482741000 | 1.058634000  |

|  |    |              |              |              |
|--|----|--------------|--------------|--------------|
|  | 8  | -1.895176000 | -2.038457000 | 1.300076000  |
|  | 6  | -0.249863000 | -3.364596000 | 2.387699000  |
|  | 1  | -0.306053000 | -3.035675000 | 3.429720000  |
|  | 1  | -0.946214000 | -4.192821000 | 2.252292000  |
|  | 1  | 0.772808000  | -3.675754000 | 2.174070000  |
|  | 6  | -2.030921000 | 1.942577000  | -1.486105000 |
|  | 8  | -0.776680000 | 1.780513000  | -1.302591000 |
|  | 8  | -2.984222000 | 1.224251000  | -1.016006000 |
|  | 6  | -2.442793000 | 3.088367000  | -2.383262000 |
|  | 1  | -2.494446000 | 2.716602000  | -3.410959000 |
|  | 1  | -3.428957000 | 3.457777000  | -2.100335000 |
|  | 1  | -1.703556000 | 3.888489000  | -2.341516000 |
|  | 46 | -2.567179000 | -0.436348000 | 0.160480000  |
|  | 6  | -1.211548000 | -1.642642000 | -2.158057000 |
|  | 8  | -0.129870000 | -1.044301000 | -1.831510000 |
|  | 8  | -2.343667000 | -1.583542000 | -1.559048000 |
|  | 6  | -1.147288000 | -2.544365000 | -3.370246000 |
|  | 1  | -0.945595000 | -3.563892000 | -3.027728000 |
|  | 1  | -2.103353000 | -2.543088000 | -3.894426000 |
|  | 1  | -0.341581000 | -2.233104000 | -4.034684000 |
|  | 6  | -1.420180000 | 1.379450000  | 2.183107000  |
|  | 8  | -0.289510000 | 1.330829000  | 1.589305000  |
|  | 8  | -2.505171000 | 0.784086000  | 1.844476000  |
|  | 6  | -1.487327000 | 2.209229000  | 3.445340000  |
|  | 1  | -2.439389000 | 2.739726000  | 3.494700000  |
|  | 1  | -1.428369000 | 1.535095000  | 4.304863000  |
|  | 1  | -0.654799000 | 2.910987000  | 3.486176000  |
|  | 6  | 3.616401000  | 1.088806000  | -0.143872000 |
|  | 6  | 4.689352000  | 1.977718000  | 0.052508000  |
|  | 6  | 4.472679000  | 3.350955000  | -0.073822000 |
|  | 6  | 3.190351000  | 3.805059000  | -0.398943000 |
|  | 6  | 2.181874000  | 2.855323000  | -0.585469000 |
|  | 6  | 3.795292000  | -0.381322000 | -0.020593000 |
|  | 6  | 4.685277000  | -0.926655000 | 0.923754000  |
|  | 6  | 4.837042000  | -2.312862000 | 1.041134000  |
|  | 6  | 4.103169000  | -3.173877000 | 0.214262000  |
|  | 6  | 3.215587000  | -2.637431000 | -0.727985000 |
|  | 6  | 3.059913000  | -1.252905000 | -0.843544000 |
|  | 1  | 5.681323000  | 1.596941000  | 0.274716000  |
|  | 1  | 5.291405000  | 4.051132000  | 0.067123000  |
|  | 1  | 2.973964000  | 4.863631000  | -0.507579000 |
|  | 1  | 1.168721000  | 3.156155000  | -0.839225000 |
|  | 1  | 5.242208000  | -0.271793000 | 1.588711000  |
|  | 1  | 5.520989000  | -2.718649000 | 1.782369000  |

|                   |    |              |              |              |
|-------------------|----|--------------|--------------|--------------|
|                   | 1  | 4.219902000  | -4.250686000 | 0.306451000  |
|                   | 1  | 2.640403000  | -3.296643000 | -1.372649000 |
|                   | 1  | 2.376675000  | -0.846433000 | -1.581821000 |
|                   | 7  | 2.379219000  | 1.530077000  | -0.467017000 |
| TS1 <sup>bi</sup> | 46 | 0.012516000  | 0.121104000  | -0.304265000 |
|                   | 6  | -0.310607000 | -1.425323000 | 2.145627000  |
|                   | 8  | 0.568784000  | -0.921394000 | 1.362846000  |
|                   | 8  | -1.579104000 | -1.396040000 | 2.017750000  |
|                   | 6  | 0.228862000  | -2.114109000 | 3.381867000  |
|                   | 1  | 0.239371000  | -1.389270000 | 4.203352000  |
|                   | 1  | -0.422753000 | -2.942964000 | 3.665775000  |
|                   | 1  | 1.248628000  | -2.463785000 | 3.213112000  |
|                   | 6  | -2.047687000 | 1.206533000  | -2.059050000 |
|                   | 8  | -0.777450000 | 1.138177000  | -1.891785000 |
|                   | 8  | -2.957427000 | 0.709471000  | -1.319765000 |
|                   | 6  | -2.509925000 | 1.947735000  | -3.296277000 |
|                   | 1  | -2.732326000 | 1.212087000  | -4.076991000 |
|                   | 1  | -3.426808000 | 2.500475000  | -3.080521000 |
|                   | 1  | -1.730859000 | 2.619764000  | -3.659486000 |
|                   | 46 | -2.523433000 | -0.405308000 | 0.418455000  |
|                   | 6  | -1.439133000 | -2.463225000 | -1.353435000 |
|                   | 8  | -0.364840000 | -1.801978000 | -1.399256000 |
|                   | 8  | -2.490542000 | -2.141930000 | -0.693975000 |
|                   | 6  | -1.511057000 | -3.773749000 | -2.115640000 |
|                   | 1  | -1.136217000 | -4.572064000 | -1.465670000 |
|                   | 1  | -2.541513000 | -4.007669000 | -2.389177000 |
|                   | 1  | -0.877525000 | -3.729401000 | -3.003551000 |
|                   | 6  | -1.776841000 | 2.086485000  | 1.704062000  |
|                   | 8  | -0.658654000 | 1.973052000  | 1.153520000  |
|                   | 8  | -2.766556000 | 1.263343000  | 1.577039000  |
|                   | 6  | -2.047397000 | 3.255959000  | 2.637388000  |
|                   | 1  | -3.088566000 | 3.578492000  | 2.567333000  |
|                   | 1  | -1.863808000 | 2.929484000  | 3.666990000  |
|                   | 1  | -1.373478000 | 4.083774000  | 2.409640000  |
|                   | 6  | 3.332509000  | 1.128285000  | -0.262919000 |
|                   | 6  | 4.363196000  | 2.082934000  | -0.194924000 |
|                   | 6  | 4.066816000  | 3.436211000  | -0.345618000 |
|                   | 6  | 2.740352000  | 3.811975000  | -0.569577000 |
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|                   | 6  | 3.655409000  | -0.320515000 | -0.154831000 |
|                   | 6  | 4.585019000  | -0.773712000 | 0.798812000  |
|                   | 6  | 4.917724000  | -2.128868000 | 0.880121000  |
|                   | 6  | 4.335733000  | -3.049604000 | 0.000025000  |
|                   | 6  | 3.415062000  | -2.605246000 | -0.956356000 |

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|                          | 6  | 3.074550000  | -1.252038000 | -1.031525000 |
|                          | 1  | 5.390045000  | 1.755783000  | -0.057667000 |
|                          | 1  | 4.858856000  | 4.181230000  | -0.302814000 |
|                          | 1  | 2.455018000  | 4.852482000  | -0.701692000 |
|                          | 1  | 0.725220000  | 3.058660000  | -0.770308000 |
|                          | 1  | 5.032208000  | -0.069925000 | 1.497888000  |
|                          | 1  | 5.628393000  | -2.465484000 | 1.632257000  |
|                          | 1  | 4.597957000  | -4.104065000 | 0.059472000  |
|                          | 1  | 2.961564000  | -3.312064000 | -1.647965000 |
|                          | 1  | 2.368415000  | -0.916267000 | -1.786092000 |
|                          | 7  | 2.047879000  | 1.504136000  | -0.461079000 |
| <b>INT1<sup>bi</sup></b> | 46 | 0.422587000  | -0.657545000 | -0.419138000 |
|                          | 6  | -0.175005000 | -0.207497000 | 2.473181000  |
|                          | 8  | 0.770778000  | -0.383268000 | 1.629364000  |
|                          | 8  | -1.439680000 | -0.254983000 | 2.274009000  |
|                          | 6  | 0.252425000  | 0.095157000  | 3.891531000  |
|                          | 1  | 0.186505000  | 1.179147000  | 4.023859000  |
|                          | 1  | -0.423816000 | -0.382072000 | 4.602464000  |
|                          | 1  | 1.280796000  | -0.223246000 | 4.063235000  |
|                          | 6  | -1.605452000 | -0.609208000 | -2.606592000 |
|                          | 8  | -0.355126000 | -0.791542000 | -2.369056000 |
|                          | 8  | -2.524000000 | -0.313694000 | -1.771433000 |
|                          | 6  | -2.030136000 | -0.783131000 | -4.049850000 |
|                          | 1  | -2.264149000 | -1.839862000 | -4.212006000 |
|                          | 1  | -2.923986000 | -0.194131000 | -4.256796000 |
|                          | 1  | -1.219316000 | -0.504521000 | -4.723426000 |
|                          | 46 | -2.205024000 | -0.244164000 | 0.331054000  |
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|                          | 8  | -2.259153000 | -2.318082000 | 0.370762000  |
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|                          | 1  | -0.714374000 | -5.085902000 | -0.255457000 |
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|                          | 8  | -2.567062000 | 1.747696000  | 0.295528000  |
|                          | 6  | -2.534816000 | 4.013568000  | 0.947642000  |
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|                          | 1  | -3.335549000 | 4.007276000  | 1.693700000  |
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|                          | 6  | 2.468240000  | 1.489456000  | -0.547927000 |
|                          | 6  | 2.968233000  | 2.786850000  | -0.719481000 |
|                          | 6  | 2.137262000  | 3.792891000  | -1.214699000 |

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|                   | 6  | 4.945177000  | -0.568756000 | 1.450678000  |
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|                   | 6  | 4.247852000  | -1.853515000 | -0.484803000 |
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|                   | 1  | 4.305178000  | -2.753003000 | -1.091483000 |
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| TS2 <sup>bi</sup> | 46 | -1.647582000 | -0.708015000 | -0.485841000 |
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|                   | 1  | -0.775527000 | 3.942714000  | -0.421217000 |
|                   | 1  | 0.363221000  | 3.753764000  | -1.768480000 |
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|                   | 8  | -1.496039000 | -2.693726000 | 0.145456000  |
|                   | 8  | 0.560223000  | -2.383467000 | 1.108743000  |
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|                   | 1  | -0.080779000 | -5.132552000 | 0.342592000  |
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| 6 | -4.029929000 | 0.598342000  | 3.523551000  |
| 6 | -2.810345000 | -0.078214000 | 3.607350000  |
| 6 | -2.181805000 | -0.471630000 | 2.429666000  |
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| 6 | 4.182293000  | 3.836771000  | -0.650425000 |
| 6 | 3.527539000  | 3.173431000  | 0.395137000  |
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| 6 | 6.036306000  | -2.422603000 | -0.220255000 |
| 6 | 3.802607000  | -2.400114000 | 0.654515000  |
| 7 | 3.678024000  | -1.074362000 | 0.466118000  |
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| <b>INT2<sup>bi</sup></b> | 46 | 1.565095000  | -0.315398000 | -0.479862000 |
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|                          | 8  | 1.830910000  | 0.623807000  | -2.281706000 |
|                          | 8  | 0.954544000  | 2.608274000  | -1.609034000 |
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|                          | 46 | -1.558371000 | -0.295037000 | 0.488627000  |
|                          | 6  | -0.602972000 | -2.014463000 | -1.796895000 |
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|                          | 8  | -1.592115000 | -1.425092000 | -1.250340000 |
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|                          | 6  | 4.754593000  | 1.678089000  | 1.657719000  |
|                          | 6  | 4.118080000  | 2.771489000  | 2.246001000  |
|                          | 6  | 2.766793000  | 2.992311000  | 1.971832000  |
|                          | 6  | 2.101010000  | 2.115646000  | 1.117679000  |
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|                   | 6  | -4.104935000 | 2.798801000  | -2.235684000 |
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|  | 8  | -1.829181000 | -0.657832000 | 2.350672000  |
|  | 6  | -1.151528000 | -0.273355000 | 4.582862000  |
|  | 1  | -2.193194000 | -0.054488000 | 4.833319000  |
|  | 1  | -0.960390000 | -1.316395000 | 4.857578000  |
|  | 1  | -0.483118000 | 0.373902000  | 5.153741000  |
|  | 6  | 3.178199000  | 0.817433000  | 1.351845000  |
|  | 6  | 3.975453000  | 1.069739000  | 2.472199000  |
|  | 6  | 4.379885000  | 0.006287000  | 3.277333000  |
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|  | 1  | 5.012536000  | 0.185841000  | 4.143755000  |
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|                    | 1  | -0.554719000 | 2.083964000  | 0.920476000  |
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|                    | 6  | 3.666722000  | 0.162913000  | 0.796298000  |
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| TS4 <sup>bi</sup> | 7 | 2.443645000  | 1.455639000  | 0.084050000  |
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| <b>1a</b> | 6 | 0.435052000  | -3.225386000 | 2.749290000  |
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|                            | 1  | -0.206261000 | -4.099482000 | -3.302052000 |
|                            | 1  | 0.015768000  | 0.212185000  | -3.164581000 |
|                            | 1  | 4.305901000  | -0.689198000 | -3.361854000 |
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|                            | 46 | -1.345363000 | 1.005511000  | -0.527355000 |
|                            | 6  | -0.854046000 | 2.890944000  | 1.743075000  |
|                            | 8  | -1.694089000 | 2.594438000  | 0.821031000  |
|                            | 8  | 0.266645000  | 2.329638000  | 1.949012000  |
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|                            | 6  | 0.864420000  | 2.938246000  | -1.653914000 |
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| <b>AcOH</b>                | 1  | 1.872642000  | 0.405667000  | 0.000743000  |
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|                            | 6  | -0.003350000 | 0.148535000  | -0.000891000 |
|                            | 6  | -1.040289000 | -0.940365000 | -0.000090000 |
|                            | 1  | -0.911228000 | -1.572517000 | 0.881485000  |
|                            | 1  | -2.035217000 | -0.498934000 | 0.000407000  |
|                            | 1  | -0.912249000 | -1.572736000 | -0.881647000 |
| <b>Pd(OAc)<sub>2</sub></b> | 46 | 0.000022000  | -0.000618000 | -0.000976000 |
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|                            | 6  | 3.951897000  | 0.000480000  | 0.015024000  |
|                            | 1  | 4.270672000  | 0.019527000  | 1.061459000  |
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|                          | 1  | 4.339848000  | 0.889328000  | -0.483720000 |
| <b>COM1<sup>mo</sup></b> | 6  | 2.082758000  | 0.863941000  | -0.678358000 |
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|                          | 6  | 0.744559000  | 2.743439000  | -0.868283000 |
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|                          | 1  | 3.751469000  | 0.713370000  | -2.055494000 |
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|                          | 8  | -0.954148000 | -0.696150000 | -1.586177000 |
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|                          | 6  | -0.247162000 | -2.985238000 | -2.003637000 |
|                          | 1  | -1.137813000 | -3.535596000 | -2.322913000 |
|                          | 1  | 0.257573000  | -2.595128000 | -2.888340000 |
|                          | 1  | 0.406342000  | -3.664350000 | -1.454969000 |
|                          | 6  | -2.573786000 | 2.850493000  | 2.812690000  |
|                          | 1  | -1.671753000 | 3.404868000  | 3.089343000  |
|                          | 1  | -3.263681000 | 3.537614000  | 2.320748000  |
|                          | 1  | -3.020845000 | 2.437531000  | 3.717560000  |
| <b>TS1<sup>mo</sup></b>  | 6  | -1.668881000 | -1.262706000 | -0.603555000 |
|                          | 6  | -2.450777000 | -2.067023000 | -1.452176000 |
|                          | 6  | -1.828128000 | -3.005234000 | -2.276735000 |
|                          | 6  | -0.435551000 | -3.129570000 | -2.229584000 |
|                          | 6  | 0.270952000  | -2.297408000 | -1.358512000 |
|                          | 6  | -2.292120000 | -0.269562000 | 0.306116000  |
|                          | 6  | -3.404335000 | 0.485479000  | -0.106481000 |

|                    |    |              |              |              |
|--------------------|----|--------------|--------------|--------------|
|                    | 6  | -3.989281000 | 1.417091000  | 0.757669000  |
|                    | 6  | -3.473342000 | 1.600291000  | 2.047153000  |
|                    | 6  | -2.365872000 | 0.849737000  | 2.463625000  |
|                    | 6  | -1.774765000 | -0.076771000 | 1.599356000  |
|                    | 1  | -3.532233000 | -1.973447000 | -1.441582000 |
|                    | 1  | -2.419664000 | -3.635502000 | -2.934939000 |
|                    | 1  | 0.093200000  | -3.847309000 | -2.849087000 |
|                    | 1  | 1.355182000  | -2.349247000 | -1.288407000 |
|                    | 1  | -3.797392000 | 0.370037000  | -1.113433000 |
|                    | 1  | -4.840498000 | 2.003994000  | 0.422337000  |
|                    | 1  | -3.929319000 | 2.321922000  | 2.719967000  |
|                    | 1  | -1.961644000 | 0.983475000  | 3.463556000  |
|                    | 1  | -0.917030000 | -0.655626000 | 1.928367000  |
|                    | 7  | -0.320856000 | -1.383380000 | -0.566097000 |
|                    | 46 | 1.321746000  | 0.466927000  | 0.110259000  |
|                    | 6  | 0.678093000  | 2.447947000  | -1.258378000 |
|                    | 8  | 0.022782000  | 2.022567000  | -0.225872000 |
|                    | 8  | 1.734407000  | 1.818321000  | -1.597759000 |
|                    | 6  | 2.464395000  | -1.233855000 | 1.630703000  |
|                    | 8  | 2.753151000  | -0.954406000 | 0.387972000  |
|                    | 8  | 1.537170000  | -0.596648000 | 2.202069000  |
|                    | 6  | 0.192374000  | 3.644654000  | -2.018576000 |
|                    | 1  | 0.972566000  | 4.409742000  | -2.024175000 |
|                    | 1  | -0.003469000 | 3.357831000  | -3.054751000 |
|                    | 1  | -0.716037000 | 4.041664000  | -1.564253000 |
|                    | 6  | 3.246660000  | -2.324652000 | 2.304519000  |
|                    | 1  | 3.082063000  | -2.294928000 | 3.381828000  |
|                    | 1  | 2.915086000  | -3.292187000 | 1.915588000  |
|                    | 1  | 4.309560000  | -2.217674000 | 2.078621000  |
| INT1 <sup>mo</sup> | 6  | -1.057134000 | 1.766388000  | -0.308045000 |
|                    | 6  | -1.481894000 | 3.068228000  | -0.614609000 |
|                    | 6  | -0.612332000 | 3.958353000  | -1.244251000 |
|                    | 6  | 0.685659000  | 3.536991000  | -1.549460000 |
|                    | 6  | 1.056765000  | 2.236302000  | -1.224216000 |
|                    | 6  | -1.954956000 | 0.810131000  | 0.382592000  |
|                    | 6  | -3.263287000 | 0.613326000  | -0.091477000 |
|                    | 6  | -4.117703000 | -0.285087000 | 0.555772000  |
|                    | 6  | -3.675652000 | -0.984144000 | 1.686694000  |
|                    | 6  | -2.376776000 | -0.778092000 | 2.169406000  |
|                    | 6  | -1.513448000 | 0.113332000  | 1.522872000  |
|                    | 1  | -2.482873000 | 3.374594000  | -0.330264000 |
|                    | 1  | -0.936470000 | 4.967481000  | -1.479456000 |
|                    | 1  | 1.401261000  | 4.194419000  | -2.031168000 |
|                    | 1  | 2.049649000  | 1.854217000  | -1.432540000 |

|                   |    |              |              |              |
|-------------------|----|--------------|--------------|--------------|
|                   | 1  | -3.603392000 | 1.139273000  | -0.980096000 |
|                   | 1  | -5.122720000 | -0.442696000 | 0.174206000  |
|                   | 1  | -4.340567000 | -1.681146000 | 2.189802000  |
|                   | 1  | -2.034228000 | -1.308624000 | 3.053987000  |
|                   | 1  | -0.511595000 | 0.280275000  | 1.911260000  |
|                   | 7  | 0.201993000  | 1.370694000  | -0.632759000 |
|                   | 46 | 0.821584000  | -0.598142000 | -0.419721000 |
|                   | 6  | 2.685447000  | 0.429789000  | 1.522927000  |
|                   | 8  | 2.615112000  | 0.091673000  | 0.254228000  |
|                   | 8  | 1.735198000  | 0.397613000  | 2.321865000  |
|                   | 6  | -0.061748000 | -2.831244000 | -1.007693000 |
|                   | 8  | -0.744912000 | -1.769322000 | -1.245507000 |
|                   | 8  | 1.097593000  | -2.694350000 | -0.462912000 |
|                   | 6  | 4.081256000  | 0.862193000  | 1.940610000  |
|                   | 1  | 4.462812000  | 1.624001000  | 1.256871000  |
|                   | 1  | 4.065638000  | 1.249487000  | 2.959850000  |
|                   | 1  | 4.756894000  | 0.003855000  | 1.889866000  |
|                   | 6  | -0.582755000 | -4.186457000 | -1.375317000 |
|                   | 1  | -0.214500000 | -4.443408000 | -2.373228000 |
|                   | 1  | -0.216187000 | -4.934532000 | -0.670983000 |
|                   | 1  | -1.672903000 | -4.178780000 | -1.395705000 |
| TS2 <sup>mo</sup> | 6  | -2.062311000 | 1.137395000  | -0.241278000 |
|                   | 6  | -3.030303000 | 2.138244000  | -0.367132000 |
|                   | 6  | -2.627375000 | 3.439392000  | -0.674816000 |
|                   | 6  | -1.267065000 | 3.708763000  | -0.855867000 |
|                   | 6  | -0.346375000 | 2.673145000  | -0.703931000 |
|                   | 6  | -2.364186000 | -0.279582000 | 0.059901000  |
|                   | 6  | -1.711850000 | -1.285685000 | -0.687922000 |
|                   | 6  | -1.897713000 | -2.636676000 | -0.362034000 |
|                   | 6  | -2.746544000 | -2.990194000 | 0.692161000  |
|                   | 6  | -3.414162000 | -1.993034000 | 1.418426000  |
|                   | 6  | -3.223036000 | -0.641993000 | 1.109327000  |
|                   | 1  | -4.079188000 | 1.887187000  | -0.245525000 |
|                   | 1  | -3.365053000 | 4.228823000  | -0.783569000 |
|                   | 1  | -0.915492000 | 4.703726000  | -1.107706000 |
|                   | 1  | 0.721872000  | 2.814550000  | -0.827998000 |
|                   | 1  | -1.150498000 | -1.033106000 | -1.588029000 |
|                   | 1  | -1.381832000 | -3.395193000 | -0.942190000 |
|                   | 1  | -2.892776000 | -4.036181000 | 0.946357000  |
|                   | 1  | -4.071598000 | -2.267444000 | 2.238905000  |
|                   | 1  | -3.710282000 | 0.126477000  | 1.703393000  |
|                   | 7  | -0.742986000 | 1.419997000  | -0.399965000 |
|                   | 46 | 0.557959000  | -0.149599000 | 0.036626000  |
|                   | 6  | 2.667766000  | 1.673397000  | 0.620986000  |

|                    |    |              |              |              |
|--------------------|----|--------------|--------------|--------------|
|                    | 8  | 1.716810000  | 1.039810000  | 1.268201000  |
|                    | 8  | 2.790869000  | 1.701194000  | -0.614937000 |
|                    | 6  | 1.818654000  | -2.473460000 | -0.550283000 |
|                    | 8  | 1.133312000  | -2.243569000 | -1.569935000 |
|                    | 8  | 1.781842000  | -1.698052000 | 0.506218000  |
|                    | 6  | 3.627539000  | 2.401409000  | 1.549222000  |
|                    | 1  | 3.073582000  | 3.001982000  | 2.274556000  |
|                    | 1  | 4.214105000  | 1.666317000  | 2.106975000  |
|                    | 1  | 4.297781000  | 3.036125000  | 0.968770000  |
|                    | 6  | 2.767796000  | -3.645524000 | -0.450989000 |
|                    | 1  | 3.786359000  | -3.287000000 | -0.628685000 |
|                    | 1  | 2.737429000  | -4.084482000 | 0.548292000  |
|                    | 1  | 2.519784000  | -4.393425000 | -1.204983000 |
| INT2 <sup>mo</sup> | 6  | -2.355777000 | -0.605951000 | 0.206065000  |
|                    | 6  | -3.572382000 | -1.284761000 | 0.301368000  |
|                    | 6  | -3.556811000 | -2.673264000 | 0.460346000  |
|                    | 6  | -2.331008000 | -3.345800000 | 0.519571000  |
|                    | 6  | -1.151231000 | -2.612234000 | 0.401564000  |
|                    | 6  | -2.194156000 | 0.855471000  | 0.035689000  |
|                    | 6  | -1.182346000 | 1.515664000  | 0.783976000  |
|                    | 6  | -0.918877000 | 2.879507000  | 0.554913000  |
|                    | 6  | -1.662478000 | 3.585354000  | -0.392589000 |
|                    | 6  | -2.680226000 | 2.935412000  | -1.108742000 |
|                    | 6  | -2.942978000 | 1.576553000  | -0.905198000 |
|                    | 1  | -4.504998000 | -0.731329000 | 0.266985000  |
|                    | 1  | -4.488995000 | -3.222934000 | 0.545995000  |
|                    | 1  | -2.282180000 | -4.420795000 | 0.653887000  |
|                    | 1  | -0.171164000 | -3.073326000 | 0.435146000  |
|                    | 1  | -0.741726000 | 1.040543000  | 1.664211000  |
|                    | 1  | -0.144802000 | 3.368046000  | 1.137184000  |
|                    | 1  | -1.464479000 | 4.638354000  | -0.568620000 |
|                    | 1  | -3.261374000 | 3.487010000  | -1.842292000 |
|                    | 1  | -3.702091000 | 1.073651000  | -1.497466000 |
|                    | 7  | -1.175292000 | -1.274733000 | 0.248552000  |
|                    | 46 | 0.440703000  | -0.031173000 | -0.120493000 |
|                    | 6  | 2.326680000  | -2.169033000 | -0.295690000 |
|                    | 8  | 1.527851000  | -1.497958000 | -1.092756000 |
|                    | 8  | 2.328604000  | -2.080727000 | 0.943817000  |
|                    | 6  | 2.426324000  | 1.896310000  | 0.468695000  |
|                    | 8  | 1.942107000  | 1.828102000  | 1.613523000  |
|                    | 8  | 1.973254000  | 1.230013000  | -0.567617000 |
|                    | 6  | 3.272835000  | -3.092692000 | -1.046412000 |
|                    | 1  | 2.719803000  | -3.703314000 | -1.763910000 |
|                    | 1  | 3.989602000  | -2.488546000 | -1.609992000 |

|                          |    |              |              |              |
|--------------------------|----|--------------|--------------|--------------|
|                          | 1  | 3.810599000  | -3.732793000 | -0.346575000 |
|                          | 6  | 3.626459000  | 2.769157000  | 0.150020000  |
|                          | 1  | 4.507161000  | 2.131628000  | 0.027525000  |
|                          | 1  | 3.473522000  | 3.309529000  | -0.786588000 |
|                          | 1  | 3.805552000  | 3.471828000  | 0.964658000  |
| <b>TS3<sup>mo</sup></b>  | 6  | 2.103668000  | -1.032471000 | -0.304354000 |
|                          | 6  | 3.135399000  | -1.908951000 | -0.666835000 |
|                          | 6  | 2.828556000  | -3.221158000 | -1.027447000 |
|                          | 6  | 1.493614000  | -3.640828000 | -1.021635000 |
|                          | 6  | 0.504765000  | -2.724856000 | -0.667094000 |
|                          | 6  | 2.281563000  | 0.350257000  | 0.169216000  |
|                          | 6  | 1.151909000  | 1.220388000  | 0.154283000  |
|                          | 6  | 1.248226000  | 2.444571000  | 0.846186000  |
|                          | 6  | 2.436175000  | 2.838803000  | 1.470646000  |
|                          | 6  | 3.556199000  | 1.999510000  | 1.423195000  |
|                          | 6  | 3.473340000  | 0.754651000  | 0.791043000  |
|                          | 1  | 4.163040000  | -1.561695000 | -0.673769000 |
|                          | 1  | 3.620627000  | -3.906824000 | -1.312710000 |
|                          | 1  | 1.215285000  | -4.652921000 | -1.295048000 |
|                          | 1  | -0.552823000 | -2.968962000 | -0.655086000 |
|                          | 1  | 0.364088000  | 1.542345000  | -0.903715000 |
|                          | 1  | 0.392339000  | 3.114202000  | 0.859719000  |
|                          | 1  | 2.489616000  | 3.792538000  | 1.988236000  |
|                          | 1  | 4.483461000  | 2.297489000  | 1.904618000  |
|                          | 1  | 4.327030000  | 0.083926000  | 0.831161000  |
|                          | 7  | 0.809950000  | -1.459159000 | -0.321735000 |
|                          | 46 | -0.610840000 | 0.006242000  | -0.034077000 |
|                          | 6  | -2.801216000 | -1.447044000 | 1.031639000  |
|                          | 8  | -2.168260000 | -1.364305000 | -0.118128000 |
|                          | 8  | -2.460455000 | -0.847352000 | 2.064118000  |
|                          | 6  | -1.559168000 | 2.412909000  | -1.154616000 |
|                          | 8  | -0.399892000 | 2.360976000  | -1.700363000 |
|                          | 8  | -1.946474000 | 1.618520000  | -0.229895000 |
|                          | 6  | -4.022015000 | -2.352036000 | 0.989214000  |
|                          | 1  | -4.786255000 | -1.897047000 | 0.352818000  |
|                          | 1  | -3.763983000 | -3.319951000 | 0.551856000  |
|                          | 1  | -4.422546000 | -2.490966000 | 1.994019000  |
|                          | 6  | -2.527104000 | 3.466462000  | -1.636541000 |
|                          | 1  | -2.898942000 | 3.166506000  | -2.620640000 |
|                          | 1  | -3.366741000 | 3.560818000  | -0.949381000 |
|                          | 1  | -2.010383000 | 4.420951000  | -1.750948000 |
| <b>INT3<sup>mo</sup></b> | 6  | 2.481860000  | 0.836134000  | 0.056118000  |
|                          | 6  | 3.565446000  | 1.719291000  | 0.130128000  |
|                          | 6  | 3.333052000  | 3.094346000  | 0.172240000  |

|          |    |              |              |              |
|----------|----|--------------|--------------|--------------|
|          | 6  | 2.017327000  | 3.565189000  | 0.135152000  |
|          | 6  | 0.972744000  | 2.643432000  | 0.061834000  |
|          | 6  | 2.558928000  | -0.623829000 | -0.003088000 |
|          | 6  | 1.317238000  | -1.299909000 | -0.068394000 |
|          | 6  | 1.282320000  | -2.695553000 | -0.135845000 |
|          | 6  | 2.484845000  | -3.421379000 | -0.136406000 |
|          | 6  | 3.717604000  | -2.756925000 | -0.069455000 |
|          | 6  | 3.756239000  | -1.361401000 | -0.003485000 |
|          | 1  | 4.578654000  | 1.333222000  | 0.153759000  |
|          | 1  | 4.167531000  | 3.786860000  | 0.229248000  |
|          | 1  | 1.793063000  | 4.626426000  | 0.158152000  |
|          | 1  | -0.067748000 | 2.947869000  | 0.002910000  |
|          | 1  | -3.115758000 | -0.161197000 | 0.301702000  |
|          | 1  | 0.331815000  | -3.215708000 | -0.185419000 |
|          | 1  | 2.456065000  | -4.507125000 | -0.188242000 |
|          | 1  | 4.644269000  | -3.323914000 | -0.069376000 |
|          | 1  | 4.717480000  | -0.856432000 | 0.046535000  |
|          | 7  | 1.200277000  | 1.314373000  | 0.027191000  |
|          | 46 | -0.300430000 | -0.138282000 | -0.031973000 |
|          | 6  | -2.725010000 | 2.164671000  | -0.183431000 |
|          | 8  | -2.043417000 | 3.130517000  | -0.562987000 |
|          | 8  | -2.233300000 | 0.982485000  | 0.113009000  |
|          | 6  | -2.789485000 | -2.061894000 | 0.120061000  |
|          | 8  | -3.622936000 | -1.081397000 | 0.365440000  |
|          | 8  | -1.563456000 | -1.907209000 | -0.086595000 |
|          | 6  | -4.232316000 | 2.284890000  | -0.017059000 |
|          | 1  | -4.567656000 | 3.283851000  | -0.297228000 |
|          | 1  | -4.741369000 | 1.542923000  | -0.638720000 |
|          | 1  | -4.506411000 | 2.088109000  | 1.023650000  |
|          | 6  | -3.411827000 | -3.429477000 | 0.089436000  |
|          | 1  | -4.088341000 | -3.491391000 | -0.767102000 |
|          | 1  | -2.643137000 | -4.195599000 | 0.007326000  |
|          | 1  | -4.006729000 | -3.581698000 | 0.992535000  |
| <b>B</b> | 6  | -3.356053000 | 0.522806000  | -0.619370000 |
|          | 6  | -4.497151000 | 0.868965000  | -1.361674000 |
|          | 6  | -4.414633000 | 1.835028000  | -2.362874000 |
|          | 6  | -3.186396000 | 2.459540000  | -2.599542000 |
|          | 6  | -2.089257000 | 2.075763000  | -1.834551000 |
|          | 6  | -3.437650000 | -0.484964000 | 0.464572000  |
|          | 6  | -4.119125000 | -1.694171000 | 0.241019000  |
|          | 6  | -4.216219000 | -2.649295000 | 1.258067000  |
|          | 6  | -3.644754000 | -2.398782000 | 2.512561000  |
|          | 6  | -2.976711000 | -1.188394000 | 2.742432000  |
|          | 6  | -2.867553000 | -0.233516000 | 1.725734000  |

|  |    |              |              |              |
|--|----|--------------|--------------|--------------|
|  | 1  | -5.443629000 | 0.393948000  | -1.126008000 |
|  | 1  | -5.295383000 | 2.107179000  | -2.936934000 |
|  | 1  | -3.072472000 | 3.224393000  | -3.360456000 |
|  | 1  | -1.112452000 | 2.523615000  | -1.975484000 |
|  | 1  | -4.547383000 | -1.902527000 | -0.736239000 |
|  | 1  | -4.731952000 | -3.587037000 | 1.069543000  |
|  | 1  | -3.721997000 | -3.139215000 | 3.304387000  |
|  | 1  | -2.543013000 | -0.983739000 | 3.718011000  |
|  | 1  | -2.353059000 | 0.703936000  | 1.922513000  |
|  | 7  | -2.168887000 | 1.126774000  | -0.877729000 |
|  | 46 | -0.345633000 | 0.566654000  | -0.024570000 |
|  | 6  | -0.260040000 | 3.026375000  | 1.525900000  |
|  | 8  | 0.037689000  | 2.564658000  | 0.341567000  |
|  | 8  | -0.745623000 | 2.351455000  | 2.457561000  |
|  | 6  | -0.809639000 | -1.739890000 | -1.714241000 |
|  | 8  | -0.593406000 | -1.425329000 | -0.459800000 |
|  | 8  | -0.920675000 | -0.935924000 | -2.654416000 |
|  | 6  | 0.034003000  | 4.509239000  | 1.690299000  |
|  | 1  | -0.605639000 | 5.084385000  | 1.014962000  |
|  | 1  | -0.148629000 | 4.823513000  | 2.718815000  |
|  | 1  | 1.071891000  | 4.717976000  | 1.418215000  |
|  | 6  | -0.924566000 | -3.243639000 | -1.924476000 |
|  | 1  | -1.720172000 | -3.646385000 | -1.291757000 |
|  | 1  | -1.133189000 | -3.466563000 | -2.972084000 |
|  | 1  | 0.009934000  | -3.729339000 | -1.628866000 |
|  | 6  | 2.498485000  | -0.494202000 | 0.175992000  |
|  | 6  | 3.569733000  | -1.115743000 | 0.835649000  |
|  | 6  | 3.560479000  | -1.226043000 | 2.226493000  |
|  | 6  | 2.484523000  | -0.691483000 | 2.942291000  |
|  | 6  | 1.444771000  | -0.092580000 | 2.234659000  |
|  | 6  | 2.498195000  | -0.311727000 | -1.293736000 |
|  | 6  | 2.816279000  | -1.382794000 | -2.145450000 |
|  | 6  | 2.839280000  | -1.197047000 | -3.531628000 |
|  | 6  | 2.558986000  | 0.062244000  | -4.076765000 |
|  | 6  | 2.249523000  | 1.134615000  | -3.229928000 |
|  | 6  | 2.211410000  | 0.951347000  | -1.844392000 |
|  | 1  | 4.408579000  | -1.482829000 | 0.253788000  |
|  | 1  | 4.386672000  | -1.705006000 | 2.743660000  |
|  | 1  | 2.441686000  | -0.737554000 | 4.025239000  |
|  | 1  | 0.582980000  | 0.343449000  | 2.728840000  |
|  | 1  | 3.021613000  | -2.365058000 | -1.727054000 |
|  | 1  | 3.069349000  | -2.035140000 | -4.183743000 |
|  | 1  | 2.582067000  | 0.206526000  | -5.153652000 |
|  | 1  | 2.042866000  | 2.116560000  | -3.647863000 |

|  |   |             |              |              |
|--|---|-------------|--------------|--------------|
|  | 1 | 1.988658000 | 1.789627000  | -1.189592000 |
|  | 7 | 1.447482000 | -0.011075000 | 0.885665000  |

**Table S1-2.** Some optimized Cartesian Coordinates of stationary points for the oxidative process (Pd<sup>II</sup> to Pd<sup>III</sup>), involved in the discussion on PhI(OAc)<sub>2</sub> (**OX-a**), PhICl<sub>2</sub> (**OX-b**) and NCS (**OX-c**) as oxidant, computed at B2PLYP-IDSCRF/DGDZVP level in dichloromethane with bond lengths in Å.

| Species                     | Cartesian coordinates |              |              |              |
|-----------------------------|-----------------------|--------------|--------------|--------------|
| <b>PhI(OAc)<sub>2</sub></b> | 6                     | 0.000002000  | -1.113402000 | -0.000014000 |
|                             | 6                     | 0.513868000  | -1.778954000 | -1.115380000 |
|                             | 6                     | -0.513860000 | -1.778939000 | 1.115362000  |
|                             | 6                     | 0.508412000  | -3.178752000 | -1.103139000 |
|                             | 6                     | -0.508398000 | -3.178737000 | 1.103141000  |
|                             | 6                     | 0.000009000  | -3.874671000 | 0.000006000  |
|                             | 1                     | 0.917109000  | -1.232762000 | -1.962396000 |
|                             | 1                     | -0.917104000 | -1.232736000 | 1.962368000  |
|                             | 1                     | 0.903995000  | -3.719739000 | -1.959791000 |
|                             | 1                     | -0.903977000 | -3.719714000 | 1.959801000  |
|                             | 1                     | 0.000011000  | -4.962474000 | 0.000015000  |
|                             | 53                    | -0.000003000 | 1.018347000  | -0.000029000 |
|                             | 8                     | -2.046005000 | 0.960178000  | -0.813945000 |
|                             | 6                     | -3.045159000 | 0.799232000  | 0.054153000  |
|                             | 8                     | -2.898312000 | 0.621792000  | 1.260442000  |
|                             | 6                     | -4.402901000 | 0.852177000  | -0.625644000 |
|                             | 1                     | -4.475735000 | 0.049366000  | -1.365669000 |
|                             | 1                     | -4.517345000 | 1.800696000  | -1.158428000 |
|                             | 1                     | -5.194211000 | 0.743387000  | 0.117198000  |
|                             | 8                     | 2.045976000  | 0.960192000  | 0.813958000  |
|                             | 6                     | 3.045159000  | 0.799253000  | -0.054105000 |
|                             | 8                     | 2.898362000  | 0.621814000  | -1.260402000 |
|                             | 6                     | 4.402874000  | 0.852184000  | 0.625747000  |
|                             | 1                     | 4.475738000  | 0.049232000  | 1.365617000  |
|                             | 1                     | 4.517235000  | 1.800606000  | 1.158719000  |
|                             | 1                     | 5.194215000  | 0.743580000  | -0.117089000 |
| <b>TS1a</b>                 | 6                     | -2.926043000 | 1.988561000  | 3.958548000  |
|                             | 6                     | 0.480194000  | -1.516920000 | 3.730841000  |
|                             | 6                     | -3.167632000 | -0.148623000 | 2.890980000  |
|                             | 6                     | -0.086323000 | -0.866138000 | 1.475797000  |
|                             | 6                     | -3.272030000 | 1.803495000  | 1.573939000  |
|                             | 6                     | 0.574323000  | 0.823119000  | 3.095916000  |
|                             | 1                     | 1.024643000  | 0.090323000  | 5.070668000  |
|                             | 1                     | -2.869197000 | 0.084107000  | 5.006802000  |
|                             | 1                     | -0.090492000 | -2.907864000 | 2.169357000  |
|                             | 6                     | 0.062603000  | 1.442376000  | 0.684924000  |
|                             | 6                     | -3.523789000 | 3.634458000  | -0.165404000 |

|  |    |              |              |              |
|--|----|--------------|--------------|--------------|
|  | 6  | -3.635355000 | 1.269847000  | -0.781883000 |
|  | 6  | 0.249839000  | 3.575152000  | -0.428942000 |
|  | 6  | -0.392216000 | 1.590882000  | -1.621483000 |
|  | 6  | -3.949010000 | 2.991984000  | -2.463481000 |
|  | 1  | -3.799388000 | 5.038449000  | -1.776841000 |
|  | 1  | -4.037363000 | 0.870833000  | -2.864929000 |
|  | 1  | -0.186475000 | 3.514991000  | -2.557235000 |
|  | 6  | 0.718741000  | -0.175760000 | 4.062717000  |
|  | 6  | -2.977793000 | 0.592675000  | 4.054938000  |
|  | 6  | 0.081894000  | -1.868848000 | 2.430779000  |
|  | 7  | -3.310292000 | 0.442721000  | 1.688690000  |
|  | 6  | 0.178022000  | 0.487712000  | 1.789248000  |
|  | 6  | -3.072208000 | 2.597180000  | 2.711917000  |
|  | 1  | -2.772955000 | 2.596506000  | 4.845390000  |
|  | 1  | 0.606172000  | -2.293426000 | 4.481604000  |
|  | 1  | -3.206947000 | -1.233128000 | 2.889628000  |
|  | 6  | -3.469918000 | 2.278321000  | 0.201832000  |
|  | 6  | 0.335266000  | 2.814777000  | 0.737045000  |
|  | 7  | -0.309022000 | 0.864339000  | -0.491441000 |
|  | 6  | -3.759010000 | 3.989319000  | -1.496470000 |
|  | 6  | -3.887051000 | 1.635063000  | -2.108273000 |
|  | 6  | -0.116530000 | 2.956427000  | -1.630016000 |
|  | 1  | 0.474686000  | 4.636891000  | -0.404703000 |
|  | 1  | -0.684634000 | 1.044975000  | -2.512080000 |
|  | 1  | -4.144284000 | 3.269633000  | -3.496886000 |
|  | 46 | -3.459219000 | -0.593637000 | -0.097481000 |
|  | 46 | -0.680107000 | -1.181803000 | -0.397686000 |
|  | 6  | -2.426626000 | -3.428408000 | 0.559848000  |
|  | 8  | -1.277535000 | -3.161817000 | 0.064043000  |
|  | 8  | -3.361718000 | -2.597415000 | 0.791492000  |
|  | 6  | -2.694035000 | -4.887684000 | 0.875653000  |
|  | 1  | -3.386964000 | -4.974506000 | 1.714255000  |
|  | 1  | -3.162459000 | -5.348077000 | -0.000211000 |
|  | 1  | -1.764670000 | -5.417577000 | 1.085823000  |
|  | 8  | -3.632189000 | -1.453842000 | -2.011705000 |
|  | 6  | -2.613149000 | -1.584047000 | -2.784291000 |
|  | 8  | -1.409221000 | -1.331944000 | -2.481685000 |
|  | 6  | -2.888944000 | -2.070977000 | -4.193690000 |
|  | 1  | -2.506679000 | -1.335928000 | -4.907249000 |
|  | 1  | -2.345254000 | -3.004097000 | -4.361902000 |
|  | 1  | -3.954922000 | -2.226571000 | -4.360893000 |
|  | 1  | -3.035813000 | 3.677481000  | 2.621589000  |
|  | 1  | -3.389551000 | 4.416338000  | 0.578059000  |
|  | 1  | 0.777794000  | 1.857355000  | 3.362024000  |

|              |    |              |              |              |
|--------------|----|--------------|--------------|--------------|
|              | 1  | 0.632140000  | 3.275782000  | 1.673061000  |
|              | 8  | 1.517545000  | -1.229377000 | -1.125980000 |
|              | 6  | 1.799998000  | -2.365438000 | -1.804129000 |
|              | 8  | 1.021046000  | -3.316713000 | -1.772210000 |
|              | 6  | 3.089559000  | -2.405402000 | -2.598392000 |
|              | 1  | 3.952100000  | -2.336068000 | -1.930274000 |
|              | 1  | 3.137781000  | -1.570318000 | -3.300576000 |
|              | 1  | 3.136257000  | -3.348247000 | -3.145395000 |
|              | 53 | 3.288417000  | 0.667800000  | -0.945040000 |
|              | 6  | 4.339775000  | -0.622098000 | 0.366906000  |
|              | 6  | 5.698677000  | -0.857736000 | 0.137059000  |
|              | 6  | 3.653934000  | -1.227021000 | 1.427905000  |
|              | 6  | 6.383343000  | -1.731071000 | 0.992668000  |
|              | 6  | 4.355284000  | -2.100999000 | 2.268051000  |
|              | 6  | 5.714934000  | -2.355020000 | 2.052922000  |
|              | 1  | 6.218089000  | -0.372910000 | -0.683372000 |
|              | 1  | 2.598733000  | -1.039644000 | 1.591550000  |
|              | 1  | 7.438995000  | -1.923698000 | 0.822878000  |
|              | 1  | 3.830096000  | -2.580692000 | 3.089646000  |
|              | 1  | 6.251488000  | -3.035841000 | 2.707803000  |
|              | 8  | 5.038320000  | 2.360434000  | -0.152177000 |
|              | 6  | 4.696854000  | 3.423389000  | -0.814319000 |
|              | 8  | 3.760212000  | 3.497916000  | -1.643845000 |
|              | 6  | 5.533459000  | 4.665703000  | -0.511186000 |
|              | 1  | 5.878192000  | 5.101012000  | -1.452476000 |
|              | 1  | 6.384754000  | 4.435446000  | 0.128958000  |
|              | 1  | 4.894656000  | 5.402868000  | -0.016211000 |
| <b>INT1a</b> | 6  | 3.564685000  | 3.002531000  | -0.618333000 |
|              | 6  | -1.034657000 | 4.137267000  | -0.950573000 |
|              | 6  | 1.920666000  | 1.814776000  | -1.902375000 |
|              | 6  | -0.919568000 | 1.903640000  | -0.049245000 |
|              | 6  | 2.956809000  | 0.725289000  | -0.086761000 |
|              | 6  | 0.245312000  | 3.719382000  | 1.066931000  |
|              | 1  | 0.072283000  | 5.650249000  | 0.127564000  |
|              | 1  | 2.512373000  | 3.835941000  | -2.328731000 |
|              | 1  | -2.053202000 | 2.427404000  | -1.807136000 |
|              | 6  | 0.251365000  | 1.370537000  | 2.034877000  |
|              | 6  | 3.903402000  | -0.820401000 | 1.690222000  |
|              | 6  | 2.126036000  | -1.557197000 | 0.184047000  |
|              | 6  | 1.251842000  | 0.553084000  | 4.075681000  |
|              | 6  | -0.046031000 | -0.884199000 | 2.656438000  |
|              | 6  | 3.063683000  | -3.091786000 | 1.810556000  |
|              | 1  | 4.613396000  | -2.295036000 | 3.092338000  |
|              | 1  | 1.508738000  | -3.614737000 | 0.404139000  |

|  |    |              |              |              |
|--|----|--------------|--------------|--------------|
|  | 1  | 0.859207000  | -1.544746000 | 4.491123000  |
|  | 6  | -0.208137000 | 4.601735000  | 0.082614000  |
|  | 6  | 2.656632000  | 2.977015000  | -1.682524000 |
|  | 6  | -1.400336000 | 2.782750000  | -1.016745000 |
|  | 7  | 2.069610000  | 0.724808000  | -1.125110000 |
|  | 6  | -0.115778000 | 2.360807000  | 1.019169000  |
|  | 6  | 3.715092000  | 1.871619000  | 0.184526000  |
|  | 1  | 4.150471000  | 3.894191000  | -0.415604000 |
|  | 1  | -1.402088000 | 4.828190000  | -1.705414000 |
|  | 1  | 1.194003000  | 1.727997000  | -2.703226000 |
|  | 6  | 3.014780000  | -0.548963000 | 0.634995000  |
|  | 6  | 1.020724000  | 1.600615000  | 3.183744000  |
|  | 7  | -0.250541000 | 0.127579000  | 1.796462000  |
|  | 6  | 3.923344000  | -2.088264000 | 2.278968000  |
|  | 6  | 2.164994000  | -2.828429000 | 0.763703000  |
|  | 6  | 0.705531000  | -0.709313000 | 3.816775000  |
|  | 1  | 1.849532000  | 0.720954000  | 4.966603000  |
|  | 1  | -0.495328000 | -1.833539000 | 2.385338000  |
|  | 1  | 3.091991000  | -4.082358000 | 2.258223000  |
|  | 46 | 0.935874000  | -0.995272000 | -1.320748000 |
|  | 46 | -1.326541000 | -0.056515000 | 0.010166000  |
|  | 6  | -1.480976000 | -0.128214000 | -2.994554000 |
|  | 8  | -2.186405000 | -0.018368000 | -1.933937000 |
|  | 8  | -0.223557000 | -0.320840000 | -3.045703000 |
|  | 6  | -2.240168000 | -0.032504000 | -4.303053000 |
|  | 1  | -1.555413000 | 0.126556000  | -5.136481000 |
|  | 1  | -2.779219000 | -0.971755000 | -4.460664000 |
|  | 1  | -2.978904000 | 0.769674000  | -4.256187000 |
|  | 8  | -0.080104000 | -2.824016000 | -1.368406000 |
|  | 6  | -1.083546000 | -3.061819000 | -0.596442000 |
|  | 8  | -1.613739000 | -2.239806000 | 0.204999000  |
|  | 6  | -1.674066000 | -4.454342000 | -0.684247000 |
|  | 1  | -2.074660000 | -4.753478000 | 0.285486000  |
|  | 1  | -2.502240000 | -4.431006000 | -1.399387000 |
|  | 1  | -0.933708000 | -5.175077000 | -1.033228000 |
|  | 8  | -3.043410000 | 0.559442000  | 1.297232000  |
|  | 6  | -4.214593000 | 0.059958000  | 1.009630000  |
|  | 8  | -4.495501000 | -0.638885000 | 0.022809000  |
|  | 6  | -5.268676000 | 0.404678000  | 2.064211000  |
|  | 1  | -5.210218000 | 1.459523000  | 2.341397000  |
|  | 1  | -5.079826000 | -0.188762000 | 2.964217000  |
|  | 1  | -6.266878000 | 0.171425000  | 1.688387000  |
|  | 1  | 1.428142000  | 2.586875000  | 3.377846000  |
|  | 1  | 0.871340000  | 4.095186000  | 1.872234000  |

|           |    |              |              |              |
|-----------|----|--------------|--------------|--------------|
|           | 1  | 4.586032000  | -0.055521000 | 2.051539000  |
|           | 1  | 4.417961000  | 1.874988000  | 1.010641000  |
| <b>2a</b> | 6  | -1.868935000 | 3.488567000  | 2.126863000  |
|           | 6  | 1.752495000  | 1.067408000  | 3.989029000  |
|           | 6  | -1.617333000 | 1.103226000  | 2.258745000  |
|           | 6  | 1.520345000  | 0.498637000  | 1.664568000  |
|           | 6  | -1.667050000 | 2.138967000  | 0.135588000  |
|           | 6  | 1.802449000  | 2.818239000  | 2.309464000  |
|           | 1  | 1.955923000  | 3.174065000  | 4.427319000  |
|           | 1  | -1.808469000 | 2.361593000  | 3.986224000  |
|           | 1  | 1.555973000  | -0.961099000 | 3.254991000  |
|           | 1  | -1.922913000 | 4.282086000  | 0.120368000  |
|           | 6  | 1.667588000  | 2.137644000  | -0.137615000 |
|           | 6  | -1.801992000 | 2.819546000  | -2.311483000 |
|           | 6  | -1.521060000 | 0.499750000  | -1.666443000 |
|           | 6  | 1.870755000  | 3.487270000  | -2.128790000 |
|           | 6  | 1.618344000  | 1.102042000  | -2.260764000 |
|           | 6  | -1.753463000 | 1.068705000  | -3.990995000 |
|           | 1  | 1.924145000  | 4.280638000  | -0.122187000 |
|           | 1  | -1.955949000 | 3.175444000  | -4.429323000 |
|           | 1  | -1.557400000 | -0.959805000 | -3.257000000 |
|           | 1  | 1.810810000  | 2.360328000  | -3.988165000 |
|           | 6  | 1.842763000  | 2.424723000  | 3.649285000  |
|           | 6  | -1.768318000 | 2.327618000  | 2.903081000  |
|           | 6  | 1.601341000  | 0.090092000  | 2.991566000  |
|           | 7  | -1.548672000 | 1.030036000  | 0.917449000  |
|           | 6  | 1.652085000  | 1.853660000  | 1.297006000  |
|           | 6  | -1.826329000 | 3.394745000  | 0.736561000  |
|           | 1  | -1.987637000 | 4.458295000  | 2.601189000  |
|           | 1  | 1.804244000  | 0.763208000  | 5.031692000  |
|           | 1  | -1.560037000 | 0.161126000  | 2.789263000  |
|           | 1  | 1.894418000  | 3.871544000  | 2.057856000  |
|           | 6  | -1.651999000 | 1.854900000  | -1.299026000 |
|           | 6  | 1.827448000  | 3.393408000  | -0.738533000 |
|           | 7  | 1.549151000  | 1.028711000  | -0.919466000 |
|           | 6  | -1.842904000 | 2.426078000  | -3.651298000 |
|           | 6  | -1.602478000 | 0.091371000  | -2.993515000 |
|           | 6  | 1.770112000  | 2.326335000  | -2.905051000 |
|           | 1  | -1.893418000 | 3.872923000  | -2.059887000 |
|           | 1  | 1.990021000  | 4.456946000  | -2.603075000 |
|           | 1  | 1.560617000  | 0.160153000  | -2.791742000 |
|           | 1  | -1.805758000 | 0.764564000  | -5.033656000 |
|           | 46 | -1.333553000 | -0.753848000 | -0.100045000 |
|           | 46 | 1.333029000  | -0.755029000 | 0.098306000  |

|                    |    |              |              |              |
|--------------------|----|--------------|--------------|--------------|
|                    | 6  | -0.097643000 | -2.708962000 | 1.837174000  |
|                    | 8  | 1.043232000  | -2.445964000 | 1.298648000  |
|                    | 8  | -1.165209000 | -2.053822000 | 1.660813000  |
|                    | 6  | -0.137286000 | -3.918157000 | 2.745895000  |
|                    | 1  | -0.828616000 | -3.736934000 | 3.570603000  |
|                    | 1  | -0.514377000 | -4.768985000 | 2.170305000  |
|                    | 1  | 0.856835000  | -4.160888000 | 3.122047000  |
|                    | 8  | -1.044804000 | -2.443869000 | -1.302421000 |
|                    | 6  | 0.095676000  | -2.707451000 | -1.841387000 |
|                    | 8  | 1.164231000  | -2.054073000 | -1.663775000 |
|                    | 6  | 0.133753000  | -3.915110000 | -2.752205000 |
|                    | 1  | 0.823964000  | -3.732616000 | -3.577578000 |
|                    | 1  | 0.511391000  | -4.766996000 | -2.178550000 |
|                    | 1  | -0.860921000 | -4.156876000 | -3.127522000 |
|                    | 6  | 4.283840000  | -0.961245000 | -0.544350000 |
|                    | 8  | 4.034565000  | -0.426682000 | -1.639476000 |
|                    | 6  | 5.686090000  | -1.466000000 | -0.209408000 |
|                    | 1  | 5.695609000  | -2.558095000 | -0.271504000 |
|                    | 1  | 6.409471000  | -1.061147000 | -0.919158000 |
|                    | 1  | 5.962863000  | -1.187827000 | 0.810056000  |
|                    | 8  | 3.433987000  | -1.178595000 | 0.423363000  |
|                    | 6  | -4.282364000 | -0.960956000 | 0.553332000  |
|                    | 8  | -4.030928000 | -0.426580000 | 1.647728000  |
|                    | 6  | -5.684030000 | -1.470693000 | 0.223074000  |
|                    | 1  | -5.689208000 | -2.562856000 | 0.284248000  |
|                    | 1  | -6.406246000 | -1.069095000 | 0.935871000  |
|                    | 1  | -5.965696000 | -1.192649000 | -0.795088000 |
|                    | 8  | -3.435675000 | -1.175384000 | -0.418353000 |
| <b>PhI</b>         | 53 | -1.562300000 | -0.000242000 | -0.002148000 |
|                    | 6  | 0.570226000  | 0.000186000  | 0.000479000  |
|                    | 6  | 1.259029000  | 1.219947000  | 0.000695000  |
|                    | 6  | 1.258750000  | -1.219686000 | 0.000693000  |
|                    | 6  | 2.660956000  | 1.210960000  | 0.000189000  |
|                    | 6  | 2.660635000  | -1.211078000 | 0.000187000  |
|                    | 6  | 3.364129000  | -0.000153000 | -0.000357000 |
|                    | 1  | 0.721260000  | 2.162642000  | 0.000877000  |
|                    | 1  | 0.720715000  | -2.162214000 | 0.000874000  |
|                    | 1  | 3.197898000  | 2.155516000  | -0.000091000 |
|                    | 1  | 3.197290000  | -2.155782000 | -0.000095000 |
|                    | 1  | 4.450251000  | -0.000315000 | -0.001230000 |
| <b>OAc-radical</b> | 8  | 0.819018000  | 1.044099000  | 0.000950000  |
|                    | 6  | 0.091727000  | 0.000476000  | -0.006740000 |
|                    | 8  | 0.818963000  | -1.044468000 | 0.000916000  |
|                    | 6  | -1.397312000 | 0.000026000  | -0.001774000 |

|           |    |              |              |              |
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|           | 1  | -1.741882000 | -0.003221000 | 1.035879000  |
|           | 1  | -1.772085000 | -0.894993000 | -0.500800000 |
|           | 1  | -1.771935000 | 0.898048000  | -0.495388000 |
| <b>1b</b> | 6  | -1.104799000 | -2.969300000 | -2.448051000 |
|           | 6  | 2.923495000  | -0.756684000 | -3.322833000 |
|           | 6  | -0.962141000 | -0.559438000 | -2.605455000 |
|           | 6  | 2.118036000  | 0.069199000  | -1.182951000 |
|           | 6  | -1.655300000 | -1.521664000 | -0.597228000 |
|           | 6  | 2.415108000  | -2.370340000 | -1.580234000 |
|           | 1  | 3.118747000  | -2.889569000 | -3.568723000 |
|           | 1  | -0.485055000 | -1.904357000 | -4.221911000 |
|           | 1  | 2.616273000  | 1.342021000  | -2.850334000 |
|           | 6  | 1.650891000  | -1.525091000 | 0.597637000  |
|           | 6  | -2.420184000 | -2.364442000 | 1.581409000  |
|           | 6  | -2.117513000 | 0.074224000  | 1.183130000  |
|           | 6  | 1.096443000  | -2.970829000 | 2.448824000  |
|           | 6  | 0.959389000  | -0.560601000 | 2.605316000  |
|           | 6  | -2.923355000 | -0.749000000 | 3.323901000  |
|           | 1  | -3.123672000 | -2.881303000 | 3.570601000  |
|           | 1  | -2.611535000 | 1.348819000  | 2.850470000  |
|           | 1  | 0.478924000  | -1.903833000 | 4.222208000  |
|           | 6  | 2.848516000  | -2.078644000 | -2.896541000 |
|           | 6  | -0.820547000 | -1.832088000 | -3.193033000 |
|           | 6  | 2.557411000  | 0.323370000  | -2.476463000 |
|           | 7  | -1.370767000 | -0.408543000 | -1.342151000 |
|           | 6  | 2.071071000  | -1.280024000 | -0.741039000 |
|           | 6  | -1.538901000 | -2.833787000 | -1.109942000 |
|           | 1  | -0.993255000 | -3.958332000 | -2.886065000 |
|           | 1  | 3.263234000  | -0.540366000 | -4.333292000 |
|           | 1  | -0.741761000 | 0.352068000  | -3.151344000 |
|           | 6  | -2.074148000 | -1.275216000 | 0.741591000  |
|           | 6  | 1.531254000  | -2.836753000 | 1.110794000  |
|           | 7  | 1.368567000  | -0.411079000 | 1.342031000  |
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|           | 6  | -2.555329000 | 0.329910000  | 2.476889000  |
|           | 6  | 0.814744000  | -1.832684000 | 3.193348000  |
|           | 1  | 0.982328000  | -3.959434000 | 2.887130000  |
|           | 1  | 0.740882000  | 0.351612000  | 3.150774000  |
|           | 1  | -3.261758000 | -0.531519000 | 4.334559000  |
|           | 46 | -1.431072000 | 1.345227000  | -0.195585000 |
|           | 46 | 1.433543000  | 1.342197000  | 0.194917000  |
|           | 6  | 0.425386000  | 3.242598000  | -1.867141000 |
|           | 8  | 1.461986000  | 2.947245000  | -1.171621000 |
|           | 8  | -0.714208000 | 2.687502000  | -1.795428000 |

|                          |    |              |              |              |
|--------------------------|----|--------------|--------------|--------------|
|                          | 6  | 0.586115000  | 4.386145000  | -2.850983000 |
|                          | 1  | 0.298794000  | 5.317013000  | -2.351280000 |
|                          | 1  | 1.622621000  | 4.477885000  | -3.177672000 |
|                          | 1  | -0.074633000 | 4.244512000  | -3.707468000 |
|                          | 8  | -1.455493000 | 2.951743000  | 1.169423000  |
|                          | 6  | -0.418363000 | 3.244957000  | 1.865092000  |
|                          | 8  | 0.720007000  | 2.687338000  | 1.793699000  |
|                          | 6  | -0.576743000 | 4.389019000  | 2.848747000  |
|                          | 1  | 0.081581000  | 4.244636000  | 3.706690000  |
|                          | 1  | -0.284495000 | 5.318827000  | 2.349942000  |
|                          | 1  | -1.613568000 | 4.484725000  | 3.173240000  |
|                          | 6  | 1.859408000  | -3.931614000 | 0.234809000  |
|                          | 1  | 1.763699000  | -4.947493000 | 0.611053000  |
|                          | 6  | 2.288892000  | -3.704794000 | -1.049173000 |
|                          | 1  | 2.536676000  | -4.546990000 | -1.691779000 |
|                          | 6  | -1.869212000 | -3.927587000 | -0.233446000 |
|                          | 1  | -1.776102000 | -4.943824000 | -0.609366000 |
|                          | 6  | -2.297464000 | -3.699359000 | 1.050698000  |
|                          | 1  | -2.546853000 | -4.540811000 | 1.693654000  |
| <b>PhICl<sub>2</sub></b> | 53 | -0.588859000 | -0.051699000 | -1.823236000 |
|                          | 6  | -0.551432000 | -0.021844000 | -3.950830000 |
|                          | 6  | 0.562822000  | -0.558398000 | -4.601866000 |
|                          | 6  | -1.641402000 | 0.532665000  | -4.627558000 |
|                          | 6  | 0.577281000  | -0.530295000 | -6.001831000 |
|                          | 6  | -1.604464000 | 0.541895000  | -6.027422000 |
|                          | 6  | -0.500949000 | 0.014905000  | -6.710734000 |
|                          | 1  | 1.395260000  | -0.981114000 | -4.049659000 |
|                          | 1  | -2.493672000 | 0.941383000  | -4.095369000 |
|                          | 1  | 1.431941000  | -0.939274000 | -6.532250000 |
|                          | 1  | -2.439325000 | 0.965246000  | -6.577732000 |
|                          | 1  | -0.481220000 | 0.028961000  | -7.796258000 |
|                          | 17 | 1.070600000  | 1.902395000  | -1.820035000 |
|                          | 17 | -2.243821000 | -2.005724000 | -1.932227000 |
| <b>TS1b</b>              | 6  | -4.739603000 | 0.547013000  | 2.468029000  |
|                          | 6  | -0.314062000 | 1.047370000  | 4.067440000  |
|                          | 6  | -2.992957000 | -1.121104000 | 2.323852000  |
|                          | 6  | -0.074494000 | 0.609713000  | 1.707855000  |
|                          | 6  | -3.862949000 | -0.217779000 | 0.355377000  |
|                          | 6  | -1.586158000 | 2.396670000  | 2.494124000  |
|                          | 1  | -1.672443000 | 2.612538000  | 4.653294000  |
|                          | 1  | -3.823041000 | -0.401905000 | 4.178528000  |
|                          | 1  | 0.994870000  | -0.479682000 | 3.230668000  |
|                          | 6  | -1.257157000 | 1.994898000  | 0.094428000  |
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|  | 6  | -2.874428000 | -1.104117000 | -1.685369000 |
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|  | 6  | -0.771437000 | 1.530277000  | -2.142325000 |
|  | 6  | -3.746527000 | -0.382421000 | -3.833060000 |
|  | 1  | -5.311100000 | 1.099595000  | -3.832343000 |
|  | 1  | -2.164610000 | -1.849817000 | -3.580753000 |
|  | 1  | -1.765107000 | 2.734252000  | -3.626868000 |
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|  | 6  | 0.277318000  | 0.304827000  | 3.009680000  |
|  | 7  | -2.995067000 | -1.066205000 | 0.988605000  |
|  | 6  | -0.985810000 | 1.657537000  | 1.446950000  |
|  | 6  | -4.760332000 | 0.617728000  | 1.056353000  |
|  | 1  | -5.409142000 | 1.172218000  | 3.053247000  |
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|  | 6  | -2.147606000 | 3.036179000  | -0.246015000 |
|  | 7  | -0.588206000 | 1.264929000  | -0.846587000 |
|  | 6  | -4.646269000 | 0.488180000  | -3.226979000 |
|  | 6  | -2.855310000 | -1.183859000 | -3.071541000 |
|  | 6  | -1.642865000 | 2.552123000  | -2.564421000 |
|  | 1  | -3.010958000 | 4.093102000  | -1.934579000 |
|  | 1  | -0.217259000 | 0.916274000  | -2.845257000 |
|  | 1  | -3.718462000 | -0.451640000 | -4.918280000 |
|  | 46 | -1.726766000 | -2.048572000 | -0.347361000 |
|  | 46 | 0.504022000  | -0.293484000 | 0.010521000  |
|  | 6  | 0.637198000  | -2.848062000 | 1.522736000  |
|  | 8  | 1.341825000  | -1.847002000 | 1.132639000  |
|  | 8  | -0.573985000 | -3.075196000 | 1.223106000  |
|  | 6  | 1.333001000  | -3.820119000 | 2.453589000  |
|  | 1  | 1.132748000  | -4.846050000 | 2.137283000  |
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|  | 1  | 0.918844000  | -3.694273000 | 3.459194000  |
|  | 8  | -0.579570000 | -2.924077000 | -1.868789000 |
|  | 6  | 0.478569000  | -2.367446000 | -2.332388000 |
|  | 8  | 1.000584000  | -1.287520000 | -1.916704000 |
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|  | 1  | 1.740602000  | -2.394783000 | -4.078934000 |
|  | 1  | 1.870023000  | -3.821344000 | -3.035655000 |
|  | 1  | 0.451561000  | -3.643101000 | -4.076427000 |
|  | 53 | 3.109211000  | 1.141631000  | -0.667878000 |
|  | 6  | 3.893175000  | -0.623232000 | 0.250234000  |
|  | 6  | 3.863226000  | -1.838705000 | -0.439680000 |

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|              | 6  | 4.486231000  | -0.479197000 | 1.508502000  |
|              | 6  | 4.483951000  | -2.942589000 | 0.152536000  |
|              | 6  | 5.079923000  | -1.605113000 | 2.093489000  |
|              | 6  | 5.085532000  | -2.829822000 | 1.414510000  |
|              | 1  | 3.376400000  | -1.918707000 | -1.404625000 |
|              | 1  | 4.501021000  | 0.478726000  | 2.019431000  |
|              | 1  | 4.488329000  | -3.895934000 | -0.369181000 |
|              | 1  | 5.548140000  | -1.515531000 | 3.069427000  |
|              | 1  | 5.559074000  | -3.696510000 | 1.867061000  |
|              | 17 | 1.684091000  | 3.331257000  | 0.540277000  |
|              | 17 | 5.045351000  | 0.861462000  | -2.501854000 |
|              | 6  | -2.779877000 | 3.753721000  | 0.829783000  |
|              | 1  | -3.478525000 | 4.550634000  | 0.585869000  |
|              | 6  | -2.504809000 | 3.449278000  | 2.139728000  |
|              | 1  | -2.985439000 | 4.012135000  | 2.937032000  |
|              | 6  | -5.630182000 | 1.463775000  | 0.281259000  |
|              | 1  | -6.319691000 | 2.121955000  | 0.804405000  |
|              | 6  | -5.602776000 | 1.437934000  | -1.091310000 |
|              | 1  | -6.276651000 | 2.078363000  | -1.656422000 |
| <b>INT1b</b> | 6  | -4.608818000 | 0.914658000  | 2.473851000  |
|              | 6  | -0.204710000 | 1.503999000  | 3.933258000  |
|              | 6  | -2.906975000 | -0.802654000 | 2.574702000  |
|              | 6  | -0.038626000 | 0.785034000  | 1.643929000  |
|              | 6  | -3.754097000 | -0.164024000 | 0.494059000  |
|              | 6  | -1.448910000 | 2.718227000  | 2.228292000  |
|              | 1  | -1.478496000 | 3.188476000  | 4.347253000  |
|              | 1  | -3.722097000 | 0.189295000  | 4.305203000  |
|              | 1  | 1.026811000  | -0.164351000 | 3.265013000  |
|              | 6  | -1.202301000 | 2.008504000  | -0.110161000 |
|              | 6  | -4.581498000 | 0.325868000  | -1.766710000 |
|              | 6  | -2.803892000 | -1.366899000 | -1.396984000 |
|              | 6  | -2.275321000 | 3.130781000  | -1.949455000 |
|              | 6  | -0.805604000 | 1.237188000  | -2.282824000 |
|              | 6  | -3.664449000 | -0.946660000 | -3.623556000 |
|              | 1  | -5.182647000 | 0.565837000  | -3.840135000 |
|              | 1  | -2.128872000 | -2.411381000 | -3.161863000 |
|              | 1  | -1.779841000 | 2.299637000  | -3.881157000 |
|              | 6  | -1.080438000 | 2.526196000  | 3.582530000  |
|              | 6  | -3.754132000 | 0.116282000  | 3.223444000  |
|              | 6  | 0.335872000  | 0.616785000  | 2.963556000  |
|              | 7  | -2.907214000 | -0.934659000 | 1.244464000  |
|              | 6  | -0.902852000 | 1.834436000  | 1.265820000  |
|              | 6  | -4.628552000 | 0.785668000  | 1.066304000  |
|              | 1  | -5.262296000 | 1.632454000  | 2.963097000  |

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|  | 1  | 0.080468000  | 1.375180000  | 4.974448000  |
|  | 1  | -2.218527000 | -1.437696000 | 3.122917000  |
|  | 6  | -3.713863000 | -0.395396000 | -0.908999000 |
|  | 6  | -2.062103000 | 3.032520000  | -0.557559000 |
|  | 7  | -0.609227000 | 1.127061000  | -0.966537000 |
|  | 6  | -4.534190000 | 0.030055000  | -3.151255000 |
|  | 6  | -2.792770000 | -1.655163000 | -2.753657000 |
|  | 6  | -1.641953000 | 2.239496000  | -2.806937000 |
|  | 1  | -2.926962000 | 3.905306000  | -2.346103000 |
|  | 1  | -0.296203000 | 0.515109000  | -2.912077000 |
|  | 1  | -3.643261000 | -1.174890000 | -4.686608000 |
|  | 46 | -1.681821000 | -2.141084000 | 0.071437000  |
|  | 46 | 0.432610000  | -0.359492000 | 0.041191000  |
|  | 6  | 0.754715000  | -2.681792000 | 1.852832000  |
|  | 8  | 1.401335000  | -1.743468000 | 1.249638000  |
|  | 8  | -0.483493000 | -2.918594000 | 1.742328000  |
|  | 6  | 1.578459000  | -3.538473000 | 2.789030000  |
|  | 1  | 1.327569000  | -4.590654000 | 2.640771000  |
|  | 1  | 2.643891000  | -3.372703000 | 2.631443000  |
|  | 1  | 1.320771000  | -3.274396000 | 3.819517000  |
|  | 8  | -0.530826000 | -3.246548000 | -1.277559000 |
|  | 6  | 0.435824000  | -2.708787000 | -1.928945000 |
|  | 8  | 0.864323000  | -1.523141000 | -1.772933000 |
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|  | 1  | 1.509728000  | -2.966283000 | -3.772217000 |
|  | 1  | 1.977833000  | -4.069832000 | -2.470325000 |
|  | 1  | 0.454172000  | -4.349463000 | -3.333626000 |
|  | 53 | 2.798833000  | 1.105601000  | -0.194335000 |
|  | 6  | 3.911631000  | -0.723509000 | -0.013776000 |
|  | 6  | 4.036342000  | -1.558429000 | -1.130195000 |
|  | 6  | 4.523417000  | -1.033840000 | 1.207081000  |
|  | 6  | 4.794520000  | -2.730726000 | -1.015475000 |
|  | 6  | 5.281507000  | -2.205932000 | 1.306206000  |
|  | 6  | 5.416726000  | -3.054112000 | 0.197832000  |
|  | 1  | 3.552382000  | -1.306520000 | -2.068050000 |
|  | 1  | 4.420829000  | -0.375571000 | 2.064809000  |
|  | 1  | 4.904316000  | -3.385610000 | -1.875917000 |
|  | 1  | 5.767650000  | -2.453796000 | 2.246036000  |
|  | 1  | 6.010724000  | -3.960264000 | 0.278373000  |
|  | 17 | 1.517491000  | 3.757155000  | -0.545711000 |
|  | 17 | 5.186208000  | 2.260691000  | -0.559554000 |
|  | 6  | -2.637794000 | 3.901615000  | 0.434257000  |
|  | 1  | -3.312554000 | 4.689479000  | 0.108231000  |
|  | 6  | -2.339207000 | 3.752969000  | 1.765732000  |

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|              | 1  | -2.779116000 | 4.426523000  | 2.497493000  |
|              | 6  | -5.477385000 | 1.534523000  | 0.176715000  |
|              | 1  | -6.147369000 | 2.279828000  | 0.598475000  |
|              | 6  | -5.455259000 | 1.309460000  | -1.177495000 |
|              | 1  | -6.112414000 | 1.879784000  | -1.830058000 |
| <b>INT2b</b> | 6  | -4.376900000 | 0.754649000  | 2.362308000  |
|              | 6  | -0.092514000 | 2.045247000  | 3.682935000  |
|              | 6  | -2.401692000 | -0.622294000 | 2.619568000  |
|              | 6  | 0.119865000  | 1.147423000  | 1.464317000  |
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|  | 17 | -2.606358000 | 0.158707000  | 0.613252000  |
|  | 1  | -3.737930000 | 3.715993000  | 1.652092000  |
|  | 1  | -4.672649000 | 4.135004000  | -1.146321000 |
|  | 6  | 0.663083000  | -4.686992000 | -2.818205000 |
|  | 6  | 1.725144000  | -3.752186000 | -2.246015000 |
|  | 7  | 1.126778000  | -2.849837000 | -1.362585000 |
|  | 6  | -0.192252000 | -3.130332000 | -1.211270000 |
|  | 6  | -0.614334000 | -4.316877000 | -2.054540000 |
|  | 1  | 0.583503000  | -4.515497000 | -3.894821000 |
|  | 1  | -0.961910000 | -5.110800000 | -1.387776000 |
|  | 8  | -0.975466000 | -2.495738000 | -0.461757000 |
|  | 8  | 2.925365000  | -3.771292000 | -2.504247000 |
|  | 1  | -1.453895000 | -4.033161000 | -2.693511000 |
|  | 1  | 0.980657000  | -5.721529000 | -2.671033000 |
|  | 6  | 0.161202000  | -3.565708000 | 3.572899000  |
|  | 6  | 0.521455000  | -2.750569000 | 2.348955000  |
|  | 7  | -0.232448000 | -1.627587000 | 2.246832000  |
|  | 6  | -1.045760000 | -1.475906000 | 3.389857000  |
|  | 6  | -0.855717000 | -2.685327000 | 4.302636000  |
|  | 1  | -0.254174000 | -4.520114000 | 3.237270000  |
|  | 1  | -0.499851000 | -2.332443000 | 5.273836000  |
|  | 8  | -1.747153000 | -0.505148000 | 3.625589000  |
|  | 8  | 1.434381000  | -3.090884000 | 1.552657000  |
|  | 1  | -1.823916000 | -3.166313000 | 4.457749000  |
|  | 1  | 1.062132000  | -3.783959000 | 4.150924000  |
|  | 6  | 1.422551000  | 4.301163000  | -0.547764000 |
|  | 1  | 1.883640000  | 5.261789000  | -0.330546000 |
|  | 6  | 1.028287000  | 4.006270000  | -1.828257000 |
|  | 1  | 1.171435000  | 4.728370000  | -2.627895000 |
|  | 6  | 4.865361000  | 2.777670000  | -0.607175000 |
|  | 1  | 5.279778000  | 3.628144000  | -1.143731000 |
|  | 6  | 5.041699000  | 2.676331000  | 0.750066000  |
|  | 1  | 5.593507000  | 3.440170000  | 1.292080000  |
|  | 1  | -5.692608000 | -0.155446000 | -0.358307000 |
|  | 8  | -6.162203000 | -1.019070000 | -0.630839000 |
|  | 8  | -7.576608000 | 0.386719000  | -1.706441000 |
|  | 6  | -7.219351000 | -0.751059000 | -1.399229000 |
|  | 6  | -7.964169000 | -1.993403000 | -1.830421000 |
|  | 1  | -7.304560000 | -2.859760000 | -1.886825000 |
|  | 1  | -8.743587000 | -2.200097000 | -1.090177000 |

|              |    |              |              |              |
|--------------|----|--------------|--------------|--------------|
|              | 1  | -8.450491000 | -1.815611000 | -2.789884000 |
| <b>INT1c</b> | 6  | 3.089347000  | -2.913754000 | 0.728241000  |
|              | 6  | 1.222321000  | -2.549995000 | -3.487781000 |
|              | 6  | 0.685136000  | -2.929866000 | 0.216597000  |
|              | 7  | 0.588849000  | -0.617019000 | -2.226217000 |
|              | 6  | 1.682971000  | -1.051479000 | 1.396577000  |
|              | 6  | 2.945761000  | -1.179141000 | -2.477254000 |
|              | 1  | 3.327979000  | -2.977915000 | -3.631890000 |
|              | 1  | 2.072890000  | -4.501867000 | -0.300412000 |
|              | 1  | -0.809008000 | -1.833923000 | -3.144491000 |
|              | 6  | 2.181279000  | 0.839249000  | -1.266434000 |
|              | 6  | 2.564404000  | 0.827597000  | 2.746089000  |
|              | 7  | 0.240014000  | 0.698947000  | 2.061306000  |
|              | 6  | 3.746954000  | 2.451542000  | -0.350362000 |
|              | 6  | 1.329565000  | 2.849295000  | -0.205756000 |
|              | 6  | 0.954730000  | 2.496413000  | 3.452013000  |
|              | 1  | 3.042504000  | 2.549510000  | 3.976865000  |
|              | 1  | -1.083763000 | 2.129119000  | 2.751503000  |
|              | 1  | 2.856101000  | 4.195870000  | 0.527446000  |
|              | 6  | 2.567724000  | -2.309067000 | -3.237885000 |
|              | 6  | 1.973090000  | -3.529313000 | 0.173891000  |
|              | 6  | 0.249384000  | -1.680166000 | -2.963464000 |
|              | 6  | 0.574638000  | -1.683707000 | 0.797450000  |
|              | 6  | 1.909089000  | -0.351895000 | -1.993015000 |
|              | 6  | 2.966095000  | -1.658656000 | 1.370487000  |
|              | 1  | 4.058427000  | -3.404219000 | 0.688601000  |
|              | 1  | 0.903894000  | -3.400586000 | -4.080807000 |
|              | 1  | -0.168835000 | -3.458099000 | -0.188677000 |
|              | 6  | 1.502078000  | 0.184503000  | 2.072076000  |
|              | 6  | 3.523194000  | 1.222680000  | -1.020508000 |
|              | 6  | 1.098486000  | 1.642293000  | -0.839768000 |
|              | 6  | 2.260016000  | 2.018375000  | 3.441761000  |
|              | 6  | -0.049360000 | 1.805363000  | 2.751295000  |
|              | 6  | 2.673251000  | 3.248021000  | 0.028396000  |
|              | 1  | 4.764614000  | 2.772756000  | -0.143527000 |
|              | 1  | 0.516942000  | 3.489696000  | 0.119667000  |
|              | 1  | 0.688664000  | 3.395138000  | 3.997816000  |
|              | 46 | -1.066502000 | -0.483419000 | 0.948974000  |
|              | 46 | -0.665868000 | 0.805974000  | -1.352755000 |
|              | 17 | -1.611350000 | -1.486467000 | 3.026551000  |
|              | 6  | -3.297892000 | 4.145264000  | -0.495509000 |
|              | 6  | -2.144573000 | 3.441168000  | -1.200170000 |
|              | 7  | -1.843429000 | 2.256683000  | -0.513299000 |
|              | 6  | -2.718811000 | 2.038638000  | 0.494757000  |

|    |   |              |              |              |
|----|---|--------------|--------------|--------------|
|    | 6 | -3.701407000 | 3.183069000  | 0.631977000  |
|    | 1 | -2.952337000 | 5.115930000  | -0.131909000 |
|    | 1 | -4.716345000 | 2.791075000  | 0.528218000  |
|    | 8 | -2.711289000 | 1.015923000  | 1.226868000  |
|    | 8 | -1.547170000 | 3.807388000  | -2.204910000 |
|    | 1 | -3.617861000 | 3.614995000  | 1.632384000  |
|    | 1 | -4.096243000 | 4.327336000  | -1.218060000 |
|    | 6 | -4.048764000 | -2.078025000 | -1.792399000 |
|    | 6 | -2.907968000 | -1.201873000 | -1.325902000 |
|    | 7 | -2.323662000 | -1.683633000 | -0.199951000 |
|    | 6 | -2.869971000 | -2.951576000 | 0.132761000  |
|    | 6 | -4.058832000 | -3.226915000 | -0.781313000 |
|    | 1 | -4.965789000 | -1.483660000 | -1.798873000 |
|    | 1 | -3.940463000 | -4.213332000 | -1.233514000 |
|    | 8 | -2.423691000 | -3.704344000 | 0.979108000  |
|    | 8 | -2.537566000 | -0.171688000 | -1.946240000 |
|    | 1 | -4.961136000 | -3.247842000 | -0.164878000 |
|    | 1 | -3.859137000 | -2.398575000 | -2.819848000 |
|    | 6 | 4.055057000  | -0.968024000 | 2.012830000  |
|    | 1 | 5.046009000  | -1.413426000 | 1.973292000  |
|    | 6 | 3.866044000  | 0.218734000  | 2.675376000  |
|    | 1 | 4.700561000  | 0.715335000  | 3.162876000  |
|    | 6 | 4.573892000  | 0.352394000  | -1.483386000 |
|    | 1 | 5.605703000  | 0.630796000  | -1.283013000 |
|    | 6 | 4.301086000  | -0.798812000 | -2.179794000 |
|    | 1 | 5.110521000  | -1.433284000 | -2.531013000 |
| 2c | 6 | 4.033527000  | -0.796287000 | -1.893384000 |
|    | 6 | 0.483619000  | 1.493448000  | -4.058714000 |
|    | 6 | 1.714635000  | -1.528268000 | -2.242199000 |
|    | 7 | -0.080947000 | 1.263467000  | -1.749169000 |
|    | 6 | 2.510595000  | -0.999490000 | -0.012956000 |
|    | 6 | 2.054418000  | 2.241966000  | -2.374099000 |
|    | 1 | 2.412749000  | 2.337163000  | -4.512403000 |
|    | 1 | 3.191987000  | -1.300015000 | -3.803145000 |
|    | 1 | -1.377542000 | 0.685790000  | -3.248695000 |
|    | 6 | 1.320202000  | 2.048804000  | -0.018668000 |
|    | 6 | 3.261254000  | -0.608879000 | 2.313831000  |
|    | 7 | 0.981482000  | -1.260185000 | 1.770044000  |
|    | 6 | 2.652668000  | 2.930185000  | 1.808230000  |
|    | 6 | 0.427352000  | 1.979461000  | 2.232981000  |
|    | 6 | 1.628441000  | -1.009294000 | 4.056169000  |
|    | 1 | 3.659281000  | -0.399367000 | 4.436585000  |
|    | 1 | -0.334288000 | -1.618583000 | 3.318788000  |
|    | 1 | 1.734678000  | 2.803025000  | 3.745055000  |

|    |              |              |              |
|----|--------------|--------------|--------------|
| 6  | 1.716054000  | 2.046483000  | -3.730475000 |
| 6  | 3.007919000  | -1.211664000 | -2.735212000 |
| 6  | -0.402615000 | 1.110495000  | -3.035523000 |
| 6  | 1.474899000  | -1.398497000 | -0.887153000 |
| 6  | 1.107759000  | 1.837944000  | -1.405925000 |
| 6  | 3.807356000  | -0.690854000 | -0.501002000 |
| 1  | 5.014052000  | -0.560039000 | -2.299139000 |
| 1  | 0.188947000  | 1.349549000  | -5.093083000 |
| 1  | 0.949781000  | -1.872100000 | -2.927036000 |
| 6  | 2.250639000  | -0.942410000 | 1.383051000  |
| 6  | 2.512851000  | 2.674447000  | 0.423330000  |
| 6  | 0.297141000  | 1.694687000  | 0.887828000  |
| 6  | 2.916438000  | -0.645604000 | 3.682449000  |
| 6  | 0.675532000  | -1.315283000 | 3.067798000  |
| 6  | 1.625683000  | 2.594849000  | 2.683251000  |
| 1  | 3.559541000  | 3.399395000  | 2.181679000  |
| 1  | -0.358265000 | 1.754892000  | 2.944497000  |
| 1  | 1.340181000  | -1.062427000 | 5.100881000  |
| 46 | -0.240776000 | -1.734852000 | 0.140608000  |
| 46 | -1.239224000 | 0.787332000  | -0.080712000 |
| 17 | 0.360353000  | -4.092356000 | 0.621942000  |
| 6  | -2.104354000 | 3.683367000  | -0.561746000 |
| 8  | -0.916601000 | 4.045242000  | -0.566745000 |
| 6  | -3.247004000 | 4.688787000  | -0.689406000 |
| 1  | -2.869252000 | 5.637798000  | -1.073924000 |
| 1  | -4.036385000 | 4.305315000  | -1.338781000 |
| 1  | -3.676130000 | 4.847560000  | 0.304775000  |
| 8  | -2.543742000 | 2.459790000  | -0.435656000 |
| 6  | -4.000865000 | 0.371732000  | 3.315213000  |
| 6  | -3.019245000 | 1.177766000  | 2.465305000  |
| 7  | -2.298752000 | 0.296742000  | 1.638446000  |
| 6  | -2.627665000 | -0.990341000 | 1.905884000  |
| 6  | -3.726236000 | -1.088833000 | 2.945214000  |
| 1  | -3.825028000 | 0.595906000  | 4.369787000  |
| 1  | -4.584417000 | -1.599841000 | 2.501430000  |
| 8  | -2.081606000 | -1.994165000 | 1.383628000  |
| 8  | -2.856617000 | 2.388393000  | 2.519130000  |
| 1  | -3.379043000 | -1.698362000 | 3.783343000  |
| 1  | -5.015990000 | 0.695294000  | 3.071427000  |
| 6  | -3.477010000 | -2.093540000 | -2.733224000 |
| 6  | -2.548751000 | -1.403866000 | -1.754949000 |
| 7  | -1.411094000 | -2.111351000 | -1.543799000 |
| 6  | -1.368550000 | -3.232794000 | -2.395629000 |
| 6  | -2.693964000 | -3.341297000 | -3.147820000 |

|                   |   |              |              |              |
|-------------------|---|--------------|--------------|--------------|
|                   | 1 | -4.419951000 | -2.313305000 | -2.225883000 |
|                   | 1 | -2.492588000 | -3.398357000 | -4.219481000 |
|                   | 8 | -0.409134000 | -3.975069000 | -2.540034000 |
|                   | 8 | -2.809252000 | -0.289946000 | -1.235166000 |
|                   | 1 | -3.180099000 | -4.274218000 | -2.849967000 |
|                   | 1 | -3.698540000 | -1.416406000 | -3.561998000 |
|                   | 6 | 4.818193000  | -0.307978000 | 0.452008000  |
|                   | 1 | 5.809462000  | -0.055215000 | 0.082542000  |
|                   | 6 | 4.562466000  | -0.272798000 | 1.799227000  |
|                   | 1 | 5.344913000  | 0.004389000  | 2.500968000  |
|                   | 6 | 3.496221000  | 3.036863000  | -0.566508000 |
|                   | 1 | 4.424139000  | 3.495269000  | -0.231785000 |
|                   | 6 | 3.279679000  | 2.834245000  | -1.905716000 |
|                   | 1 | 4.029776000  | 3.127259000  | -2.635848000 |
| Succinimide...OAc | 6 | -2.946700000 | -0.727268000 | 0.234754000  |
|                   | 6 | -1.513489000 | -1.152844000 | -0.066764000 |
|                   | 7 | -0.740764000 | -0.020610000 | -0.241604000 |
|                   | 6 | -1.458175000 | 1.152400000  | -0.100612000 |
|                   | 6 | -2.909315000 | 0.805710000  | 0.214892000  |
|                   | 1 | -3.607570000 | -1.156522000 | -0.521795000 |
|                   | 1 | -3.178574000 | 1.259666000  | 1.171689000  |
|                   | 8 | -0.995321000 | 2.286157000  | -0.218410000 |
|                   | 8 | -1.105839000 | -2.311044000 | -0.148389000 |
|                   | 1 | -3.550979000 | 1.247627000  | -0.550855000 |
|                   | 1 | -3.240304000 | -1.142702000 | 1.201892000  |
|                   | 1 | 0.311707000  | -0.045196000 | -0.443374000 |
|                   | 8 | 1.874527000  | -0.056692000 | -0.887655000 |
|                   | 8 | 2.326306000  | -0.028512000 | 1.334791000  |
|                   | 6 | 2.671558000  | -0.026447000 | 0.121964000  |
|                   | 6 | 4.164256000  | 0.021372000  | -0.223151000 |
|                   | 1 | 4.382753000  | 0.936276000  | -0.783586000 |
|                   | 1 | 4.780999000  | -0.004850000 | 0.677099000  |
|                   | 1 | 4.425178000  | -0.821882000 | -0.870085000 |
| succinimide       | 6 | 0.768606000  | -1.259028000 | -0.000145000 |
|                   | 6 | 1.169952000  | 0.208418000  | 0.000121000  |
|                   | 7 | 0.000001000  | 0.961928000  | 0.000011000  |
|                   | 6 | -1.169950000 | 0.208417000  | 0.000306000  |
|                   | 6 | -0.768605000 | -1.259028000 | 0.000220000  |
|                   | 1 | 1.201217000  | -1.738456000 | -0.880964000 |
|                   | 1 | -1.201230000 | -1.738641000 | 0.880928000  |
|                   | 8 | -2.301393000 | 0.675711000  | 0.000375000  |
|                   | 8 | 2.301393000  | 0.675717000  | -0.000524000 |
|                   | 1 | -1.201776000 | -1.738818000 | -0.880128000 |
|                   | 1 | 1.201789000  | -1.739004000 | 0.880093000  |

|  |   |             |             |              |
|--|---|-------------|-------------|--------------|
|  | 1 | 0.000001000 | 1.978641000 | -0.000162000 |
|--|---|-------------|-------------|--------------|

**Table S1-3.** Some optimized Cartesian Coordinates of stationary points for the oxidative process (Pd<sup>II</sup> to Pd<sup>IV</sup>), involved in the discussion on PhI(OAc)<sub>2</sub> (**OX-a**), PhICl<sub>2</sub> (**OX-b**) and NCS (**OX-c**) as oxidant, computed at B2PLYP-IDSCRF/DGDZVP level in dichloromethane with bond lengths in Å.

| Species   | Cartesian coordinates |              |              |              |
|-----------|-----------------------|--------------|--------------|--------------|
| <b>1m</b> | 6                     | -4.101208000 | -2.647569000 | -0.985212000 |
|           | 6                     | -2.879078000 | -3.326636000 | -1.043018000 |
|           | 6                     | -1.728165000 | -2.637374000 | -0.665810000 |
|           | 7                     | -1.739365000 | -1.359347000 | -0.239210000 |
|           | 6                     | -2.922008000 | -0.680369000 | -0.200068000 |
|           | 6                     | -4.119480000 | -1.317854000 | -0.566854000 |
|           | 1                     | -5.023904000 | -3.142194000 | -1.274717000 |
|           | 1                     | -2.811598000 | -4.357228000 | -1.374817000 |
|           | 1                     | -0.756870000 | -3.118590000 | -0.715450000 |
|           | 1                     | -5.056490000 | -0.772946000 | -0.545983000 |
|           | 6                     | -2.815999000 | 0.726864000  | 0.226445000  |
|           | 6                     | -3.956125000 | 1.481571000  | 0.568117000  |
|           | 6                     | -1.509491000 | 1.287290000  | 0.324419000  |
|           | 6                     | -3.824794000 | 2.789442000  | 1.040150000  |
|           | 6                     | -1.410103000 | 2.594548000  | 0.835840000  |
|           | 6                     | -2.545221000 | 3.341140000  | 1.186621000  |
|           | 1                     | -4.951230000 | 1.050911000  | 0.492081000  |
|           | 1                     | -4.708428000 | 3.362691000  | 1.307765000  |
|           | 1                     | -0.433434000 | 3.046415000  | 0.979640000  |
|           | 1                     | -2.428775000 | 4.347677000  | 1.582851000  |
|           | 46                    | 0.000044000  | -0.039424000 | 0.000615000  |
|           | 6                     | 4.101445000  | -2.648026000 | 0.984634000  |
|           | 6                     | 2.879249000  | -3.326885000 | 1.043446000  |
|           | 6                     | 1.728176000  | -2.637566000 | 0.666836000  |
|           | 7                     | 1.739289000  | -1.359596000 | 0.239961000  |
|           | 6                     | 2.922015000  | -0.680811000 | 0.199884000  |
|           | 6                     | 4.119642000  | -1.318419000 | 0.565950000  |
|           | 1                     | 5.024254000  | -3.142713000 | 1.273669000  |
|           | 1                     | 2.811831000  | -4.357357000 | 1.375630000  |
|           | 1                     | 0.756854000  | -3.118693000 | 0.717413000  |
|           | 1                     | 5.056723000  | -0.773666000 | 0.544303000  |
|           | 6                     | 2.815975000  | 0.726435000  | -0.226621000 |
|           | 6                     | 1.509532000  | 1.287196000  | -0.323552000 |
|           | 6                     | 3.955992000  | 1.480890000  | -0.569201000 |
|           | 6                     | 1.410044000  | 2.594626000  | -0.834509000 |
|           | 6                     | 3.824600000  | 2.788890000  | -1.040870000 |
|           | 6                     | 2.545059000  | 3.341010000  | -1.186033000 |
|           | 1                     | 4.951047000  | 1.049939000  | -0.494147000 |

|               |    |              |              |              |
|---------------|----|--------------|--------------|--------------|
|               | 1  | 0.433383000  | 3.046811000  | -0.977324000 |
|               | 1  | 4.708149000  | 3.361936000  | -1.309187000 |
|               | 1  | 2.428541000  | 4.347702000  | -1.581849000 |
| <b>TS1m-a</b> | 6  | 0.046715000  | -2.764437000 | 0.898450000  |
|               | 6  | -0.690958000 | -3.939512000 | 0.673015000  |
|               | 6  | -0.307998000 | -4.815171000 | -0.343160000 |
|               | 6  | 0.799682000  | -4.497344000 | -1.137462000 |
|               | 6  | 1.480051000  | -3.309854000 | -0.870464000 |
|               | 7  | 1.132308000  | -2.476911000 | 0.127733000  |
|               | 1  | -1.567473000 | -4.158040000 | 1.272602000  |
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|               | 6  | -0.718741000 | 0.151972000  | 3.925046000  |
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|               | 6  | -0.270230000 | -1.754688000 | 1.925212000  |
|               | 6  | 0.394115000  | -0.498491000 | 1.840411000  |
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|               | 1  | -0.868542000 | 0.888734000  | 4.712184000  |
|               | 1  | -1.673864000 | -2.984569000 | 3.040924000  |
|               | 46 | 1.827586000  | -0.412455000 | 0.378906000  |
|               | 6  | 2.208977000  | 1.585461000  | 0.427390000  |
|               | 6  | 1.263461000  | 2.600445000  | 0.643523000  |
|               | 6  | 3.517182000  | 1.961372000  | 0.018823000  |
|               | 6  | 1.612376000  | 3.954522000  | 0.536436000  |
|               | 1  | 0.238301000  | 2.342764000  | 0.890224000  |
|               | 6  | 3.864793000  | 3.324259000  | -0.077363000 |
|               | 6  | 2.920901000  | 4.318721000  | 0.189795000  |
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|               | 1  | 4.865246000  | 3.621779000  | -0.380023000 |
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|               | 6  | 6.062860000  | -1.281848000 | -1.006909000 |
|               | 6  | 6.628221000  | -0.002065000 | -0.969536000 |
|               | 6  | 5.823462000  | 1.085960000  | -0.633793000 |
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|               | 1  | 4.228533000  | -2.382445000 | -0.710547000 |
|               | 1  | 6.650685000  | -2.159363000 | -1.255039000 |
|               | 1  | 7.681378000  | 0.145001000  | -1.190527000 |
|               | 1  | 6.255124000  | 2.079435000  | -0.586467000 |
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|               | 1  | -2.084064000 | -1.292132000 | 4.787925000  |

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|         | 6  | -2.335272000 | 4.365457000  | 0.990382000  |
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|         | 1  | -2.565847000 | 3.431327000  | 2.927127000  |
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|         | 1  | -2.287185000 | 5.373636000  | 1.392719000  |
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|         | 1  | -7.151110000 | -0.621380000 | 0.764469000  |
|         | 1  | -7.180134000 | -2.272295000 | 0.064391000  |
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|         | 8  | -4.841066000 | -2.066033000 | -1.033258000 |
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|         | 53 | -2.562491000 | -0.174586000 | -0.807659000 |
| INT1m-a | 6  | 2.809699000  | -0.541672000 | -0.137639000 |
|         | 6  | 4.177178000  | -0.725466000 | 0.127016000  |
|         | 6  | 4.848498000  | 0.177348000  | 0.951732000  |
|         | 6  | 4.150702000  | 1.256788000  | 1.506859000  |
|         | 6  | 2.796080000  | 1.387632000  | 1.205742000  |
|         | 7  | 2.150721000  | 0.515449000  | 0.410293000  |
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|         | 1  | 4.638783000  | 1.978586000  | 2.153304000  |
|         | 1  | 2.191691000  | 2.200774000  | 1.598314000  |
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|         | 1  | 3.558369000  | -2.820942000 | -1.504829000 |

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|             | 1  | 0.430159000  | 5.307965000  | -0.901920000 |
|             | 1  | 0.080395000  | 5.161455000  | 0.848240000  |
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| <b>2m-a</b> | 6  | -2.623333000 | 0.195697000  | -0.819248000 |
|             | 6  | -3.916654000 | 0.624652000  | -1.147957000 |
|             | 6  | -4.472921000 | 1.709755000  | -0.470148000 |
|             | 6  | -3.728784000 | 2.356129000  | 0.522714000  |
|             | 6  | -2.440105000 | 1.895400000  | 0.790183000  |
|             | 7  | -1.907885000 | 0.851839000  | 0.132072000  |
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|             | 6  | -0.616164000 | -3.249191000 | -2.393922000 |
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|                | 1  | -3.496563000 | -1.498742000 | -2.833605000 |
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|                | 6  | 2.276914000  | -1.836023000 | 1.511120000  |
|                | 6  | 2.791942000  | -0.441200000 | -0.430372000 |
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| <b>COM1m-b</b> | 6  | 0.127759000  | 3.733646000  | -3.037841000 |
|                | 6  | -0.252296000 | 2.523636000  | -3.628201000 |
|                | 6  | -0.841688000 | 1.554512000  | -2.818748000 |

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|  | 6  | 5.743971000  | 0.206146000  | -1.067414000 |

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|               | 17 | 2.119492000  | 1.048521000  | 2.432676000  |
| <b>TS1m-b</b> | 6  | -0.302982000 | 4.388450000  | -2.441111000 |
|               | 6  | -0.188597000 | 3.217201000  | -3.197952000 |
|               | 6  | -0.372862000 | 1.998652000  | -2.549518000 |
|               | 7  | -0.658381000 | 1.911312000  | -1.239683000 |
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|               | 1  | -0.685522000 | 5.203609000  | -0.490995000 |
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|         | 1  | -3.872546000 | -4.066838000 | 0.988953000  |
|         | 1  | 0.020179000  | -1.413220000 | 2.526049000  |
|         | 1  | -2.581005000 | -4.806856000 | 2.941363000  |
|         | 1  | -0.612398000 | -3.470076000 | 3.712280000  |
|         | 53 | 1.923679000  | -0.024480000 | 0.402843000  |
|         | 6  | 3.647543000  | -0.957540000 | -0.503942000 |
|         | 6  | 4.021251000  | -2.233303000 | -0.076743000 |
|         | 6  | 4.367304000  | -0.243501000 | -1.464091000 |
|         | 6  | 5.164779000  | -2.811578000 | -0.640164000 |
|         | 6  | 5.508145000  | -0.839014000 | -2.014897000 |
|         | 6  | 5.904902000  | -2.117818000 | -1.605266000 |
|         | 1  | 3.444639000  | -2.770620000 | 0.671077000  |
|         | 1  | 4.057855000  | 0.748795000  | -1.780399000 |
|         | 1  | 5.473462000  | -3.804384000 | -0.321116000 |
|         | 1  | 6.083811000  | -0.299426000 | -2.763382000 |
|         | 1  | 6.791992000  | -2.574056000 | -2.038349000 |
|         | 17 | 0.677405000  | -1.377580000 | -1.726610000 |
|         | 17 | 3.546111000  | 1.099948000  | 2.268603000  |
| INT1m-b | 6  | 2.509126000  | -4.612585000 | 0.025533000  |
|         | 6  | 1.784804000  | -4.300417000 | -1.131161000 |
|         | 6  | 1.244030000  | -3.021465000 | -1.249281000 |
|         | 7  | 1.404722000  | -2.092307000 | -0.288170000 |
|         | 6  | 2.103843000  | -2.374983000 | 0.844578000  |
|         | 6  | 2.670913000  | -3.646310000 | 1.019002000  |
|         | 1  | 2.944192000  | -5.599006000 | 0.152902000  |
|         | 1  | 1.639715000  | -5.026206000 | -1.924029000 |
|         | 1  | 0.676092000  | -2.701707000 | -2.118572000 |
|         | 1  | 3.228963000  | -3.882880000 | 1.917256000  |
|         | 6  | 2.189381000  | -1.268856000 | 1.816813000  |
|         | 6  | 2.901254000  | -1.371751000 | 3.029255000  |
|         | 6  | 1.525710000  | -0.052804000 | 1.536946000  |
|         | 6  | 2.941334000  | -0.302005000 | 3.925279000  |
|         | 6  | 1.551655000  | 1.018746000  | 2.428024000  |
|         | 6  | 2.265254000  | 0.888545000  | 3.630583000  |
|         | 1  | 3.428911000  | -2.287478000 | 3.278040000  |
|         | 1  | 3.496539000  | -0.399021000 | 4.853421000  |
|         | 1  | 1.025234000  | 1.942203000  | 2.211708000  |
|         | 1  | 2.286374000  | 1.719289000  | 4.331034000  |
|         | 46 | 0.598718000  | -0.039840000 | -0.319224000 |
|         | 6  | 4.465281000  | 2.094005000  | -2.305925000 |
|         | 6  | 4.475969000  | 0.702319000  | -2.148448000 |
|         | 6  | 3.378333000  | 0.091464000  | -1.551981000 |
|         | 7  | 2.322398000  | 0.812159000  | -1.125900000 |

|             |    |              |              |              |
|-------------|----|--------------|--------------|--------------|
|             | 6  | 2.278196000  | 2.165584000  | -1.273535000 |
|             | 6  | 3.364460000  | 2.825559000  | -1.868620000 |
|             | 1  | 5.306688000  | 2.601378000  | -2.767418000 |
|             | 1  | 5.310649000  | 0.095117000  | -2.480429000 |
|             | 1  | 3.326644000  | -0.980809000 | -1.411912000 |
|             | 1  | 3.340639000  | 3.902479000  | -1.988200000 |
|             | 6  | 1.059586000  | 2.792834000  | -0.776501000 |
|             | 6  | 0.065902000  | 1.950989000  | -0.228844000 |
|             | 6  | 0.833115000  | 4.182741000  | -0.798409000 |
|             | 6  | -1.109124000 | 2.466229000  | 0.304345000  |
|             | 6  | -0.347912000 | 4.711480000  | -0.275355000 |
|             | 6  | -1.308580000 | 3.857522000  | 0.280620000  |
|             | 1  | 1.579225000  | 4.852198000  | -1.216577000 |
|             | 1  | -1.881906000 | 1.870557000  | 0.777712000  |
|             | 1  | -0.511035000 | 5.785279000  | -0.291255000 |
|             | 1  | -2.227188000 | 4.236755000  | 0.721403000  |
|             | 53 | -1.553870000 | -1.042557000 | 1.029692000  |
|             | 6  | -3.130169000 | -1.053176000 | -0.407667000 |
|             | 6  | -4.122246000 | -0.074484000 | -0.303617000 |
|             | 6  | -3.139690000 | -2.056718000 | -1.382744000 |
|             | 6  | -5.171497000 | -0.118228000 | -1.233306000 |
|             | 6  | -4.200234000 | -2.075467000 | -2.294681000 |
|             | 6  | -5.212782000 | -1.108952000 | -2.221322000 |
|             | 1  | -4.099084000 | 0.697014000  | 0.468869000  |
|             | 1  | -2.349985000 | -2.797666000 | -1.440732000 |
|             | 1  | -5.957071000 | 0.630518000  | -1.174306000 |
|             | 1  | -4.228814000 | -2.842960000 | -3.063128000 |
|             | 1  | -6.032060000 | -1.129791000 | -2.934813000 |
|             | 17 | -0.358062000 | -0.246886000 | -2.566789000 |
|             | 17 | -4.054358000 | 2.384727000  | 2.214674000  |
| <b>2m-b</b> | 6  | -4.824057000 | -0.912913000 | -0.188309000 |
|             | 6  | -4.115043000 | -1.723603000 | -1.082531000 |
|             | 6  | -2.743676000 | -1.515214000 | -1.221704000 |
|             | 7  | -2.097011000 | -0.570529000 | -0.516357000 |
|             | 6  | -2.766353000 | 0.233773000  | 0.350795000  |
|             | 6  | -4.148300000 | 0.072635000  | 0.532007000  |
|             | 1  | -5.893740000 | -1.044415000 | -0.055062000 |
|             | 1  | -4.608609000 | -2.496183000 | -1.662514000 |
|             | 1  | -2.123964000 | -2.099053000 | -1.896390000 |
|             | 1  | -4.692188000 | 0.709705000  | 1.219914000  |
|             | 6  | -1.931262000 | 1.239751000  | 1.032404000  |
|             | 6  | -2.437608000 | 2.114290000  | 2.014764000  |
|             | 6  | -0.568674000 | 1.346999000  | 0.678370000  |
|             | 6  | -1.610387000 | 3.063988000  | 2.618069000  |

|        |    |              |              |              |
|--------|----|--------------|--------------|--------------|
|        | 6  | 0.262728000  | 2.297156000  | 1.268114000  |
|        | 6  | -0.263874000 | 3.158576000  | 2.244406000  |
|        | 1  | -3.479620000 | 2.056246000  | 2.315535000  |
|        | 1  | -2.015915000 | 3.729210000  | 3.375159000  |
|        | 1  | 1.304705000  | 2.386059000  | 0.979668000  |
|        | 1  | 0.381962000  | 3.900550000  | 2.707185000  |
|        | 46 | 0.018079000  | -0.052502000 | -0.711469000 |
|        | 6  | 1.750164000  | -2.768020000 | 2.919680000  |
|        | 6  | 0.395120000  | -2.886874000 | 2.587083000  |
|        | 6  | -0.105969000 | -2.104692000 | 1.551085000  |
|        | 7  | 0.678967000  | -1.244517000 | 0.875134000  |
|        | 6  | 2.001758000  | -1.113823000 | 1.172965000  |
|        | 6  | 2.555778000  | -1.881642000 | 2.208270000  |
|        | 1  | 2.173172000  | -3.362101000 | 3.724057000  |
|        | 1  | -0.264467000 | -3.567253000 | 3.114261000  |
|        | 1  | -1.144194000 | -2.155412000 | 1.245326000  |
|        | 1  | 3.607881000  | -1.785064000 | 2.450696000  |
|        | 6  | 2.720053000  | -0.154582000 | 0.334352000  |
|        | 6  | 1.983148000  | 0.496475000  | -0.679000000 |
|        | 6  | 4.088802000  | 0.142967000  | 0.481163000  |
|        | 6  | 2.590094000  | 1.406972000  | -1.540211000 |
|        | 6  | 4.701975000  | 1.063234000  | -0.370376000 |
|        | 6  | 3.956004000  | 1.690319000  | -1.378568000 |
|        | 1  | 4.678262000  | -0.340678000 | 1.255083000  |
|        | 1  | 2.014660000  | 1.897392000  | -2.317168000 |
|        | 1  | 5.757483000  | 1.289438000  | -0.250324000 |
|        | 1  | 4.434878000  | 2.404553000  | -2.044023000 |
|        | 17 | -0.614791000 | 1.499873000  | -2.386001000 |
|        | 17 | 0.544326000  | -1.899278000 | -2.290324000 |
| TS1m-c | 6  | 0.420043000  | 4.871865000  | -0.738644000 |
|        | 6  | 0.154222000  | 4.125999000  | -1.891481000 |
|        | 6  | -0.183618000 | 2.783541000  | -1.739526000 |
|        | 7  | -0.267602000 | 2.193352000  | -0.536963000 |
|        | 6  | -0.001996000 | 2.897996000  | 0.592173000  |
|        | 6  | 0.344725000  | 4.255572000  | 0.508832000  |
|        | 1  | 0.692368000  | 5.922624000  | -0.811483000 |
|        | 1  | 0.212960000  | 4.564648000  | -2.883718000 |
|        | 1  | -0.388732000 | 2.152721000  | -2.602577000 |
|        | 1  | 0.566131000  | 4.824026000  | 1.406634000  |
|        | 6  | -0.095167000 | 2.124486000  | 1.845067000  |
|        | 6  | 0.018140000  | 2.724414000  | 3.114657000  |
|        | 6  | -0.313836000 | 0.728636000  | 1.778622000  |
|        | 6  | -0.070615000 | 1.960935000  | 4.278630000  |
|        | 6  | -0.391838000 | -0.039589000 | 2.936876000  |

|      |    |              |              |              |
|------|----|--------------|--------------|--------------|
|      | 6  | -0.274395000 | 0.580294000  | 4.190607000  |
|      | 1  | 0.171854000  | 3.797590000  | 3.198912000  |
|      | 1  | 0.020464000  | 2.441903000  | 5.249880000  |
|      | 1  | -0.545645000 | -1.111303000 | 2.887899000  |
|      | 1  | -0.341591000 | -0.024110000 | 5.093414000  |
|      | 46 | -0.714821000 | 0.083454000  | -0.139713000 |
|      | 6  | -5.387387000 | -0.488983000 | -1.881915000 |
|      | 6  | -4.784339000 | 0.755404000  | -2.090898000 |
|      | 6  | -3.471526000 | 0.925719000  | -1.657939000 |
|      | 7  | -2.771319000 | -0.052842000 | -1.061704000 |
|      | 6  | -3.342495000 | -1.268007000 | -0.847375000 |
|      | 6  | -4.665137000 | -1.503444000 | -1.256421000 |
|      | 1  | -6.412885000 | -0.666441000 | -2.199161000 |
|      | 1  | -5.311707000 | 1.574478000  | -2.572139000 |
|      | 1  | -2.959816000 | 1.876084000  | -1.788653000 |
|      | 1  | -5.131912000 | -2.467775000 | -1.082837000 |
|      | 6  | -2.479227000 | -2.260465000 | -0.175359000 |
|      | 6  | -1.198850000 | -1.855381000 | 0.283217000  |
|      | 6  | -2.883891000 | -3.597658000 | 0.008772000  |
|      | 6  | -0.358350000 | -2.791230000 | 0.891864000  |
|      | 6  | -2.040177000 | -4.521170000 | 0.626227000  |
|      | 6  | -0.773841000 | -4.118678000 | 1.064965000  |
|      | 1  | -3.859435000 | -3.930133000 | -0.337664000 |
|      | 1  | 0.632768000  | -2.499737000 | 1.226987000  |
|      | 1  | -2.366858000 | -5.550407000 | 0.757783000  |
|      | 1  | -0.103978000 | -4.834646000 | 1.537989000  |
|      | 6  | 5.828670000  | -2.039686000 | -0.742852000 |
|      | 6  | 4.404961000  | -1.970908000 | -0.168086000 |
|      | 7  | 3.773838000  | -0.851859000 | -0.656532000 |
|      | 6  | 4.561121000  | -0.121710000 | -1.514023000 |
|      | 6  | 5.932990000  | -0.802429000 | -1.643848000 |
|      | 1  | 6.543966000  | -2.042145000 | 0.085283000  |
|      | 1  | 6.110816000  | -1.039197000 | -2.697342000 |
|      | 8  | 4.239075000  | 0.915261000  | -2.095638000 |
|      | 8  | 3.924757000  | -2.798604000 | 0.607859000  |
|      | 17 | 1.679621000  | -0.343080000 | -0.139681000 |
|      | 1  | 6.708272000  | -0.095705000 | -1.332475000 |
|      | 1  | 5.946989000  | -2.985960000 | -1.279585000 |
| 2m-c | 6  | 4.492687000  | 2.230077000  | 0.090288000  |
|      | 6  | 3.375165000  | 3.071793000  | 0.079119000  |
|      | 6  | 2.111136000  | 2.492126000  | -0.012061000 |
|      | 7  | 1.938114000  | 1.160010000  | -0.084000000 |
|      | 6  | 3.012903000  | 0.327144000  | -0.094831000 |
|      | 6  | 4.311761000  | 0.850351000  | 0.001035000  |

|  |    |              |              |              |
|--|----|--------------|--------------|--------------|
|  | 1  | 5.494760000  | 2.643370000  | 0.159366000  |
|  | 1  | 3.473728000  | 4.150643000  | 0.136258000  |
|  | 1  | 1.208588000  | 3.089713000  | -0.020451000 |
|  | 1  | 5.172437000  | 0.191623000  | -0.009528000 |
|  | 6  | 2.692958000  | -1.104760000 | -0.239453000 |
|  | 6  | 3.674932000  | -2.113326000 | -0.176890000 |
|  | 6  | 1.352891000  | -1.479858000 | -0.475400000 |
|  | 6  | 3.329812000  | -3.454580000 | -0.352340000 |
|  | 6  | 1.003406000  | -2.817012000 | -0.660648000 |
|  | 6  | 1.996830000  | -3.806471000 | -0.598733000 |
|  | 1  | 4.714030000  | -1.858504000 | 0.010714000  |
|  | 1  | 4.098085000  | -4.220793000 | -0.300304000 |
|  | 1  | -0.024192000 | -3.103757000 | -0.857967000 |
|  | 1  | 1.724431000  | -4.849318000 | -0.743180000 |
|  | 46 | 0.040654000  | 0.104882000  | -0.432676000 |
|  | 6  | -0.938769000 | -1.277926000 | 4.117834000  |
|  | 6  | 0.158619000  | -0.436795000 | 3.897105000  |
|  | 6  | 0.431341000  | -0.023916000 | 2.596675000  |
|  | 7  | -0.325067000 | -0.429337000 | 1.559697000  |
|  | 6  | -1.395651000 | -1.250685000 | 1.744508000  |
|  | 6  | -1.721859000 | -1.682529000 | 3.038544000  |
|  | 1  | -1.180535000 | -1.614766000 | 5.121444000  |
|  | 1  | 0.790706000  | -0.098079000 | 4.710599000  |
|  | 1  | 1.248617000  | 0.645921000  | 2.364145000  |
|  | 1  | -2.574935000 | -2.333008000 | 3.194431000  |
|  | 6  | -2.104291000 | -1.605978000 | 0.515408000  |
|  | 6  | -1.605570000 | -1.077317000 | -0.693374000 |
|  | 6  | -3.231424000 | -2.450812000 | 0.474995000  |
|  | 6  | -2.207886000 | -1.362835000 | -1.915064000 |
|  | 6  | -3.834836000 | -2.753621000 | -0.745965000 |
|  | 6  | -3.324467000 | -2.211753000 | -1.935096000 |
|  | 1  | -3.635557000 | -2.874572000 | 1.390216000  |
|  | 1  | -1.822067000 | -0.930130000 | -2.829840000 |
|  | 1  | -4.699489000 | -3.410748000 | -0.771683000 |
|  | 1  | -3.797648000 | -2.446534000 | -2.885638000 |
|  | 6  | -3.097377000 | 3.391757000  | -0.563461000 |
|  | 6  | -2.328670000 | 2.188732000  | -1.117686000 |
|  | 7  | -1.302755000 | 1.829339000  | -0.253779000 |
|  | 6  | -1.288262000 | 2.661325000  | 0.843057000  |
|  | 6  | -2.410959000 | 3.693806000  | 0.767213000  |
|  | 1  | -3.035347000 | 4.212390000  | -1.283279000 |
|  | 1  | -3.064343000 | 3.567964000  | 1.635099000  |
|  | 8  | -0.465473000 | 2.604570000  | 1.770421000  |
|  | 8  | -2.600410000 | 1.634840000  | -2.184213000 |

|  |    |              |             |              |
|--|----|--------------|-------------|--------------|
|  | 17 | 0.505394000  | 0.391296000 | -2.738003000 |
|  | 1  | -1.976595000 | 4.695670000 | 0.824726000  |
|  | 1  | -4.151533000 | 3.120205000 | -0.463745000 |

**Table S1-4.** Some optimized Cartesian Coordinates of stationary points for the C-H activation, involved in the discussion on Pd(OAc)<sub>2</sub> as catalyst, computed at B3LYP-IDSCRF/DGDZVP level in dichloromethane with bond lengths in Å.

| Species                                  | Cartesian coordinates |              |              |              |
|------------------------------------------|-----------------------|--------------|--------------|--------------|
| <b>R</b>                                 | 6                     | -0.765277000 | 0.022119000  | -0.003240000 |
|                                          | 6                     | -1.505819000 | 1.191623000  | 0.255622000  |
|                                          | 6                     | -2.899681000 | 1.138103000  | 0.243327000  |
|                                          | 6                     | -3.527879000 | -0.082204000 | -0.020296000 |
|                                          | 6                     | -2.715585000 | -1.196463000 | -0.252107000 |
|                                          | 6                     | 0.725735000  | 0.020182000  | -0.005524000 |
|                                          | 6                     | 1.467161000  | 1.194213000  | -0.238296000 |
|                                          | 6                     | 2.865281000  | 1.171504000  | -0.232541000 |
|                                          | 6                     | 3.550772000  | -0.024839000 | 0.009330000  |
|                                          | 6                     | 2.823719000  | -1.200203000 | 0.238089000  |
|                                          | 6                     | 1.426935000  | -1.178387000 | 0.226213000  |
|                                          | 1                     | -1.003192000 | 2.126759000  | 0.485243000  |
|                                          | 1                     | -3.484558000 | 2.033412000  | 0.445131000  |
|                                          | 1                     | -4.611012000 | -0.174755000 | -0.040392000 |
|                                          | 1                     | -3.164451000 | -2.169451000 | -0.455151000 |
|                                          | 1                     | 0.959552000  | 2.132149000  | -0.450121000 |
|                                          | 1                     | 3.418889000  | 2.088566000  | -0.424019000 |
|                                          | 1                     | 4.638777000  | -0.041834000 | 0.015704000  |
|                                          | 1                     | 3.346764000  | -2.135674000 | 0.427305000  |
|                                          | 1                     | 0.863650000  | -2.090513000 | 0.400509000  |
|                                          | 7                     | -1.376657000 | -1.157506000 | -0.246810000 |
| <b>Pd<sub>2</sub>(μ-OAc)<sub>4</sub></b> | 46                    | 0.000158000  | -0.000216000 | 1.317157000  |
|                                          | 6                     | 1.876544000  | -1.870074000 | -0.000178000 |
|                                          | 8                     | 1.471339000  | -1.472054000 | 1.144177000  |
|                                          | 8                     | 1.471277000  | -1.471667000 | -1.144360000 |
|                                          | 6                     | 2.978599000  | -2.908700000 | -0.000452000 |
|                                          | 1                     | 2.918853000  | -3.527139000 | -0.897740000 |
|                                          | 1                     | 3.942365000  | -2.387685000 | -0.003272000 |
|                                          | 1                     | 2.922254000  | -3.524227000 | 0.899033000  |
|                                          | 6                     | -1.876484000 | 1.870057000  | 0.000557000  |
|                                          | 8                     | -1.471060000 | 1.471748000  | 1.144716000  |
|                                          | 8                     | -1.471487000 | 1.471921000  | -1.143829000 |
|                                          | 6                     | -2.978465000 | 2.908775000  | 0.000316000  |
|                                          | 1                     | -2.911071000 | 3.534787000  | -0.891219000 |
|                                          | 1                     | -3.942195000 | 2.387937000  | -0.015806000 |
|                                          | 1                     | -2.929720000 | 3.516669000  | 0.905363000  |

|                                                         |    |              |              |              |
|---------------------------------------------------------|----|--------------|--------------|--------------|
|                                                         | 46 | -0.000115000 | 0.000140000  | -1.317110000 |
|                                                         | 6  | 1.875914000  | 1.870647000  | -0.000012000 |
|                                                         | 8  | 1.471076000  | 1.472044000  | 1.144253000  |
|                                                         | 8  | 1.470541000  | 1.472563000  | -1.144285000 |
|                                                         | 6  | 2.977828000  | 2.909424000  | -0.000090000 |
|                                                         | 1  | 3.941672000  | 2.388544000  | -0.001641000 |
|                                                         | 1  | 2.918781000  | 3.527256000  | -0.897836000 |
|                                                         | 1  | 2.920615000  | 3.525539000  | 0.898943000  |
|                                                         | 6  | -1.876054000 | -1.870535000 | -0.000185000 |
|                                                         | 8  | -1.470747000 | -1.472468000 | 1.144102000  |
|                                                         | 8  | -1.470874000 | -1.472216000 | -1.144443000 |
|                                                         | 6  | -2.978178000 | -2.909093000 | -0.000120000 |
|                                                         | 1  | -3.941898000 | -2.387998000 | 0.004163000  |
|                                                         | 1  | -2.922674000 | -3.523669000 | -0.900301000 |
|                                                         | 1  | -2.917714000 | -3.528491000 | 0.896465000  |
| Pd <sub>2</sub> (OAc) <sub>2</sub> (μ-OAc) <sub>2</sub> | 46 | -1.542230000 | -0.134318000 | 0.000020000  |
|                                                         | 46 | 1.542201000  | -0.134477000 | -0.000033000 |
|                                                         | 6  | -0.000096000 | -1.909378000 | 1.894091000  |
|                                                         | 8  | 1.138927000  | -1.526549000 | 1.475348000  |
|                                                         | 8  | -1.139090000 | -1.526377000 | 1.475447000  |
|                                                         | 6  | -0.000087000 | -2.953830000 | 2.992379000  |
|                                                         | 1  | 0.000881000  | -3.944379000 | 2.524373000  |
|                                                         | 1  | 0.897790000  | -2.861063000 | 3.605611000  |
|                                                         | 1  | -0.898770000 | -2.862236000 | 3.604592000  |
|                                                         | 8  | -1.139117000 | -1.526511000 | -1.475281000 |
|                                                         | 6  | -0.000138000 | -1.909391000 | -1.894086000 |
|                                                         | 8  | 1.138898000  | -1.526424000 | -1.475515000 |
|                                                         | 6  | -0.000201000 | -2.953865000 | -2.992352000 |
|                                                         | 1  | 0.897904000  | -2.861493000 | -3.605306000 |
|                                                         | 1  | 0.000157000  | -3.944404000 | -2.524329000 |
|                                                         | 1  | -0.898656000 | -2.861897000 | -3.604849000 |
|                                                         | 8  | 2.229529000  | 1.517505000  | 1.094674000  |
|                                                         | 6  | 2.501418000  | 2.131579000  | 0.000028000  |
|                                                         | 8  | 2.229499000  | 1.517561000  | -1.094652000 |
|                                                         | 6  | 3.132101000  | 3.488387000  | 0.000029000  |
|                                                         | 1  | 4.221563000  | 3.369943000  | -0.001626000 |
|                                                         | 1  | 2.846310000  | 4.038440000  | 0.899375000  |
|                                                         | 1  | 2.843832000  | 4.039545000  | -0.897860000 |
|                                                         | 8  | -2.229359000 | 1.517801000  | -1.094656000 |
|                                                         | 6  | -2.501168000 | 2.131868000  | 0.000015000  |
|                                                         | 8  | -2.229322000 | 1.517776000  | 1.094668000  |
|                                                         | 6  | -3.131678000 | 3.488758000  | 0.000001000  |
|                                                         | 1  | -4.221154000 | 3.370453000  | -0.002328000 |
|                                                         | 1  | -2.842841000 | 4.040081000  | -0.897608000 |

|                          |    |              |              |              |
|--------------------------|----|--------------|--------------|--------------|
|                          | 1  | -2.846317000 | 4.038572000  | 0.899626000  |
| <b>COM1<sup>bi</sup></b> | 46 | -0.194319000 | 0.169210000  | -0.055703000 |
|                          | 6  | -0.934854000 | -2.165298000 | 1.627119000  |
|                          | 8  | 0.058156000  | -1.488043000 | 1.200669000  |
|                          | 8  | -2.172195000 | -1.969913000 | 1.371759000  |
|                          | 6  | -0.618623000 | -3.314317000 | 2.562767000  |
|                          | 1  | -0.679398000 | -2.946367000 | 3.592911000  |
|                          | 1  | -1.350675000 | -4.115151000 | 2.442090000  |
|                          | 1  | 0.392747000  | -3.683616000 | 2.385554000  |
|                          | 6  | -2.088142000 | 1.940839000  | -1.523162000 |
|                          | 8  | -0.850848000 | 1.749451000  | -1.278038000 |
|                          | 8  | -3.077188000 | 1.259320000  | -1.086842000 |
|                          | 6  | -2.422514000 | 3.086098000  | -2.457216000 |
|                          | 1  | -2.398030000 | 2.709735000  | -3.485855000 |
|                          | 1  | -3.424585000 | 3.466920000  | -2.252563000 |
|                          | 1  | -1.680265000 | 3.881191000  | -2.365725000 |
|                          | 46 | -2.773466000 | -0.387297000 | 0.155695000  |
|                          | 6  | -1.337109000 | -1.690532000 | -2.072590000 |
|                          | 8  | -0.257404000 | -1.112072000 | -1.714761000 |
|                          | 8  | -2.488002000 | -1.587699000 | -1.526546000 |
|                          | 6  | -1.242954000 | -2.625381000 | -3.261257000 |
|                          | 1  | -1.055525000 | -3.638504000 | -2.888773000 |
|                          | 1  | -2.184351000 | -2.633294000 | -3.813886000 |
|                          | 1  | -0.415488000 | -2.335914000 | -3.911135000 |
|                          | 6  | -1.668016000 | 1.459324000  | 2.179137000  |
|                          | 8  | -0.519067000 | 1.369613000  | 1.631680000  |
|                          | 8  | -2.747867000 | 0.882383000  | 1.812007000  |
|                          | 6  | -1.759346000 | 2.324683000  | 3.419543000  |
|                          | 1  | -2.754122000 | 2.766294000  | 3.503390000  |
|                          | 1  | -1.590273000 | 1.689270000  | 4.295884000  |
|                          | 1  | -0.991626000 | 3.100045000  | 3.401652000  |
|                          | 6  | 3.808749000  | 1.055288000  | -0.126162000 |
|                          | 6  | 4.833776000  | 1.987035000  | 0.125661000  |
|                          | 6  | 4.548300000  | 3.351329000  | 0.082948000  |
|                          | 6  | 3.245885000  | 3.758421000  | -0.218093000 |
|                          | 6  | 2.290284000  | 2.768487000  | -0.462612000 |
|                          | 6  | 4.075609000  | -0.410361000 | -0.110236000 |
|                          | 6  | 5.091020000  | -0.962014000 | 0.693833000  |
|                          | 6  | 5.340310000  | -2.337652000 | 0.687882000  |
|                          | 6  | 4.582138000  | -3.187504000 | -0.126508000 |
|                          | 6  | 3.566466000  | -2.649220000 | -0.926595000 |
|                          | 6  | 3.312177000  | -1.275460000 | -0.915301000 |
|                          | 1  | 5.846855000  | 1.649782000  | 0.325812000  |
|                          | 1  | 5.332212000  | 4.082659000  | 0.270334000  |

|                         |    |              |              |              |
|-------------------------|----|--------------|--------------|--------------|
|                         | 1  | 2.973717000  | 4.809943000  | -0.267652000 |
|                         | 1  | 1.263707000  | 3.039109000  | -0.703925000 |
|                         | 1  | 5.677580000  | -0.322969000 | 1.349944000  |
|                         | 1  | 6.122854000  | -2.745884000 | 1.324432000  |
|                         | 1  | 4.778081000  | -4.257927000 | -0.133802000 |
|                         | 1  | 2.970537000  | -3.301007000 | -1.562425000 |
|                         | 1  | 2.523108000  | -0.863978000 | -1.537300000 |
|                         | 7  | 2.551065000  | 1.453535000  | -0.417562000 |
| <b>TS1<sup>bi</sup></b> | 46 | 0.012516000  | 0.121104000  | -0.304265000 |
|                         | 6  | -0.310607000 | -1.425323000 | 2.145627000  |
|                         | 8  | 0.568784000  | -0.921394000 | 1.362846000  |
|                         | 8  | -1.579104000 | -1.396040000 | 2.017750000  |
|                         | 6  | 0.228862000  | -2.114109000 | 3.381867000  |
|                         | 1  | 0.239371000  | -1.389270000 | 4.203352000  |
|                         | 1  | -0.422753000 | -2.942964000 | 3.665775000  |
|                         | 1  | 1.248628000  | -2.463785000 | 3.213112000  |
|                         | 6  | -2.047687000 | 1.206533000  | -2.059050000 |
|                         | 8  | -0.777450000 | 1.138177000  | -1.891785000 |
|                         | 8  | -2.957427000 | 0.709471000  | -1.319765000 |
|                         | 6  | -2.509925000 | 1.947735000  | -3.296277000 |
|                         | 1  | -2.732326000 | 1.212087000  | -4.076991000 |
|                         | 1  | -3.426808000 | 2.500475000  | -3.080521000 |
|                         | 1  | -1.730859000 | 2.619764000  | -3.659486000 |
|                         | 46 | -2.523433000 | -0.405308000 | 0.418455000  |
|                         | 6  | -1.439133000 | -2.463225000 | -1.353435000 |
|                         | 8  | -0.364840000 | -1.801978000 | -1.399256000 |
|                         | 8  | -2.490542000 | -2.141930000 | -0.693975000 |
|                         | 6  | -1.511057000 | -3.773749000 | -2.115640000 |
|                         | 1  | -1.136217000 | -4.572064000 | -1.465670000 |
|                         | 1  | -2.541513000 | -4.007669000 | -2.389177000 |
|                         | 1  | -0.877525000 | -3.729401000 | -3.003551000 |
|                         | 6  | -1.776841000 | 2.086485000  | 1.704062000  |
|                         | 8  | -0.658654000 | 1.973052000  | 1.153520000  |
|                         | 8  | -2.766556000 | 1.263343000  | 1.577039000  |
|                         | 6  | -2.047397000 | 3.255959000  | 2.637388000  |
|                         | 1  | -3.088566000 | 3.578492000  | 2.567333000  |
|                         | 1  | -1.863808000 | 2.929484000  | 3.666990000  |
|                         | 1  | -1.373478000 | 4.083774000  | 2.409640000  |
|                         | 6  | 3.332509000  | 1.128285000  | -0.262919000 |
|                         | 6  | 4.363196000  | 2.082934000  | -0.194924000 |
|                         | 6  | 4.066816000  | 3.436211000  | -0.345618000 |
|                         | 6  | 2.740352000  | 3.811975000  | -0.569577000 |
|                         | 6  | 1.771007000  | 2.810863000  | -0.616099000 |
|                         | 6  | 3.655409000  | -0.320515000 | -0.154831000 |

|                    |    |              |              |              |
|--------------------|----|--------------|--------------|--------------|
|                    | 6  | 4.585019000  | -0.773712000 | 0.798812000  |
|                    | 6  | 4.917724000  | -2.128868000 | 0.880121000  |
|                    | 6  | 4.335733000  | -3.049604000 | 0.000025000  |
|                    | 6  | 3.415062000  | -2.605246000 | -0.956356000 |
|                    | 6  | 3.074550000  | -1.252038000 | -1.031525000 |
|                    | 1  | 5.390045000  | 1.755783000  | -0.057667000 |
|                    | 1  | 4.858856000  | 4.181230000  | -0.302814000 |
|                    | 1  | 2.455018000  | 4.852482000  | -0.701692000 |
|                    | 1  | 0.725220000  | 3.058660000  | -0.770308000 |
|                    | 1  | 5.032208000  | -0.069925000 | 1.497888000  |
|                    | 1  | 5.628393000  | -2.465484000 | 1.632257000  |
|                    | 1  | 4.597957000  | -4.104065000 | 0.059472000  |
|                    | 1  | 2.961564000  | -3.312064000 | -1.647965000 |
|                    | 1  | 2.368415000  | -0.916267000 | -1.786092000 |
|                    | 7  | 2.047879000  | 1.504136000  | -0.461079000 |
| INT1 <sup>bi</sup> | 46 | 0.421398000  | -0.623120000 | -0.351954000 |
|                    | 6  | -0.276399000 | -0.185568000 | 2.533859000  |
|                    | 8  | 0.698745000  | -0.323612000 | 1.718647000  |
|                    | 8  | -1.526326000 | -0.227312000 | 2.287512000  |
|                    | 6  | 0.102810000  | 0.067773000  | 3.980002000  |
|                    | 1  | 0.087985000  | 1.151439000  | 4.138573000  |
|                    | 1  | -0.629814000 | -0.386097000 | 4.650748000  |
|                    | 1  | 1.105223000  | -0.307711000 | 4.192107000  |
|                    | 6  | -1.567912000 | -0.590026000 | -2.598618000 |
|                    | 8  | -0.329977000 | -0.773650000 | -2.323422000 |
|                    | 8  | -2.510023000 | -0.294075000 | -1.796379000 |
|                    | 6  | -1.949902000 | -0.766470000 | -4.057433000 |
|                    | 1  | -2.195074000 | -1.821470000 | -4.223264000 |
|                    | 1  | -2.830617000 | -0.167589000 | -4.296332000 |
|                    | 1  | -1.114635000 | -0.503096000 | -4.709023000 |
|                    | 46 | -2.263196000 | -0.212188000 | 0.322785000  |
|                    | 6  | -1.272512000 | -3.014992000 | 0.257106000  |
|                    | 8  | -0.096943000 | -2.595253000 | 0.006298000  |
|                    | 8  | -2.306178000 | -2.287346000 | 0.373414000  |
|                    | 6  | -1.439710000 | -4.505628000 | 0.459424000  |
|                    | 1  | -1.207876000 | -4.739673000 | 1.504248000  |
|                    | 1  | -2.468976000 | -4.805739000 | 0.256291000  |
|                    | 1  | -0.743865000 | -5.056917000 | -0.175930000 |
|                    | 6  | -2.091976000 | 2.716289000  | 0.982048000  |
|                    | 8  | -1.035530000 | 2.609968000  | 1.610504000  |
|                    | 8  | -2.670551000 | 1.778001000  | 0.265856000  |
|                    | 6  | -2.887823000 | 4.020007000  | 0.961160000  |
|                    | 1  | -3.250141000 | 4.242156000  | -0.046223000 |
|                    | 1  | -3.764385000 | 3.912660000  | 1.609528000  |

|                         |    |              |              |              |
|-------------------------|----|--------------|--------------|--------------|
|                         | 1  | -2.270476000 | 4.841097000  | 1.331049000  |
|                         | 6  | 2.581056000  | 1.446634000  | -0.596785000 |
|                         | 6  | 3.119221000  | 2.722875000  | -0.811409000 |
|                         | 6  | 2.303230000  | 3.761766000  | -1.254923000 |
|                         | 6  | 0.949891000  | 3.506577000  | -1.482552000 |
|                         | 6  | 0.462833000  | 2.228611000  | -1.232917000 |
|                         | 6  | 3.457738000  | 0.317042000  | -0.188209000 |
|                         | 6  | 4.321069000  | 0.457456000  | 0.911430000  |
|                         | 6  | 5.168215000  | -0.590451000 | 1.282150000  |
|                         | 6  | 5.171522000  | -1.785084000 | 0.551623000  |
|                         | 6  | 4.325964000  | -1.925624000 | -0.554695000 |
|                         | 6  | 3.472344000  | -0.881794000 | -0.924407000 |
|                         | 1  | 4.183394000  | 2.876982000  | -0.657125000 |
|                         | 1  | 2.720714000  | 4.750702000  | -1.431764000 |
|                         | 1  | 0.271596000  | 4.278749000  | -1.834735000 |
|                         | 1  | -0.586161000 | 1.990895000  | -1.369484000 |
|                         | 1  | 4.311307000  | 1.376845000  | 1.493200000  |
|                         | 1  | 5.821379000  | -0.475580000 | 2.144545000  |
|                         | 1  | 5.832655000  | -2.599490000 | 0.840440000  |
|                         | 1  | 4.333906000  | -2.844398000 | -1.137130000 |
|                         | 1  | 2.851366000  | -0.985362000 | -1.811862000 |
|                         | 7  | 1.254502000  | 1.229375000  | -0.795241000 |
| <b>TS2<sup>bi</sup></b> | 46 | -1.706177000 | -0.591292000 | -0.510910000 |
|                         | 6  | -0.653342000 | 2.113575000  | -1.083677000 |
|                         | 8  | -1.729163000 | 1.420723000  | -1.042445000 |
|                         | 8  | 0.528787000  | 1.737103000  | -0.826812000 |
|                         | 6  | -0.827391000 | 3.567429000  | -1.487993000 |
|                         | 1  | -0.901284000 | 4.161161000  | -0.570428000 |
|                         | 1  | 0.044645000  | 3.911252000  | -2.048227000 |
|                         | 1  | -1.739517000 | 3.705818000  | -2.071201000 |
|                         | 6  | -0.469831000 | -2.966247000 | 0.658890000  |
|                         | 8  | -1.546389000 | -2.584744000 | 0.060737000  |
|                         | 8  | 0.523149000  | -2.247921000 | 0.949601000  |
|                         | 6  | -0.423479000 | -4.441200000 | 1.026402000  |
|                         | 1  | -1.424544000 | -4.874767000 | 1.057846000  |
|                         | 1  | 0.162389000  | -4.969032000 | 0.265599000  |
|                         | 1  | 0.079827000  | -4.570862000 | 1.987362000  |
|                         | 46 | 1.085627000  | -0.126686000 | 0.127991000  |
|                         | 6  | 0.411859000  | -1.163771000 | -2.570825000 |
|                         | 8  | -0.833341000 | -1.054668000 | -2.340674000 |
|                         | 8  | 1.350347000  | -0.934620000 | -1.744182000 |
|                         | 6  | 0.817001000  | -1.582154000 | -3.969149000 |
|                         | 1  | 1.820059000  | -2.011800000 | -3.966446000 |
|                         | 1  | 0.094112000  | -2.291534000 | -4.377228000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 1 | 0.820099000  | -0.692178000 | -4.608039000 |
| 6 | 0.466403000  | 1.599769000  | 2.499237000  |
| 8 | -0.484572000 | 2.168089000  | 1.958389000  |
| 8 | 1.165886000  | 0.602351000  | 2.005631000  |
| 6 | 0.972994000  | 2.013544000  | 3.880338000  |
| 1 | 1.203647000  | 1.138252000  | 4.493458000  |
| 1 | 1.898755000  | 2.588114000  | 3.765199000  |
| 1 | 0.227983000  | 2.638357000  | 4.377103000  |
| 6 | -4.104885000 | 0.240898000  | 1.148248000  |
| 6 | -4.793221000 | 0.554839000  | 2.329434000  |
| 6 | -4.184348000 | 0.364733000  | 3.567944000  |
| 6 | -2.885240000 | -0.144312000 | 3.608466000  |
| 6 | -2.240403000 | -0.415585000 | 2.407174000  |
| 6 | -4.782754000 | 0.371971000  | -0.168472000 |
| 6 | -5.451439000 | 1.562448000  | -0.500000000 |
| 6 | -6.120879000 | 1.681011000  | -1.721013000 |
| 6 | -6.141588000 | 0.606875000  | -2.619083000 |
| 6 | -5.491577000 | -0.587653000 | -2.287943000 |
| 6 | -4.814357000 | -0.706439000 | -1.070588000 |
| 1 | -5.816373000 | 0.913248000  | 2.262070000  |
| 1 | -4.721167000 | 0.596568000  | 4.485393000  |
| 1 | -2.366537000 | -0.319932000 | 4.546865000  |
| 1 | -1.222423000 | -0.788774000 | 2.388011000  |
| 1 | -5.425355000 | 2.406736000  | 0.185857000  |
| 1 | -6.621462000 | 2.613623000  | -1.972631000 |
| 1 | -6.664689000 | 0.699124000  | -3.568661000 |
| 1 | -5.515770000 | -1.432204000 | -2.973304000 |
| 1 | -4.345327000 | -1.651794000 | -0.807517000 |
| 7 | -2.829298000 | -0.220762000 | 1.210142000  |
| 6 | 4.859697000  | -3.155768000 | 0.636497000  |
| 6 | 4.869353000  | 0.998816000  | -0.262978000 |
| 6 | 5.675819000  | 1.537214000  | -1.283331000 |
| 6 | 5.689015000  | 2.912690000  | -1.532489000 |
| 6 | 4.902101000  | 3.775270000  | -0.759613000 |
| 6 | 4.094595000  | 3.248281000  | 0.255591000  |
| 6 | 4.072517000  | 1.872185000  | 0.498707000  |
| 1 | 6.279355000  | 0.879968000  | -1.905608000 |
| 1 | 6.309655000  | 3.309421000  | -2.333526000 |
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|                          | 6  | 2.015953000  | 2.644695000  | -3.748222000 |
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|                          | 1  | 1.799761000  | 1.974199000  | -4.585309000 |
|                          | 1  | 1.521120000  | 3.605139000  | -3.903655000 |
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|                          | 6  | 4.326857000  | 2.660077000  | 2.290367000  |
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|  | 1  | -1.835200000 | 3.197378000  | 0.572075000  |
|  | 6  | -1.461585000 | -0.508875000 | -2.169841000 |
|  | 46 | -1.374761000 | -0.180797000 | 0.722522000  |
|  | 7  | -1.572676000 | -1.250904000 | -1.035432000 |
|  | 6  | -1.750050000 | -2.580587000 | -1.100630000 |
|  | 6  | -1.829338000 | -3.246131000 | -2.321409000 |
|  | 6  | -5.119872000 | 0.517716000  | -0.794807000 |
|  | 8  | -4.323294000 | 0.932378000  | 0.133072000  |
|  | 1  | -2.819952000 | 1.077681000  | -0.302632000 |
|  | 8  | -4.781774000 | 0.196886000  | -1.957521000 |
|  | 6  | -6.594819000 | 0.434944000  | -0.380667000 |
|  | 1  | -6.954343000 | 1.429202000  | -0.093384000 |

|           |   |              |              |              |
|-----------|---|--------------|--------------|--------------|
|           | 1 | -7.210326000 | 0.048234000  | -1.196534000 |
|           | 1 | -6.700878000 | -0.211444000 | 0.497152000  |
|           | 6 | -1.519790000 | -1.125181000 | -3.423632000 |
|           | 1 | -1.437082000 | -0.525289000 | -4.325440000 |
|           | 6 | -1.708858000 | -2.504048000 | -3.500347000 |
|           | 1 | -1.769864000 | -2.994747000 | -4.469238000 |
|           | 1 | -1.833341000 | -3.100284000 | -0.150611000 |
|           | 1 | -1.989891000 | -4.320572000 | -2.338210000 |
|           | 6 | 4.061951000  | -1.229362000 | -2.224769000 |
|           | 1 | 4.621044000  | -0.673572000 | -2.974933000 |
|           | 6 | 4.030523000  | -2.623927000 | -2.290689000 |
|           | 1 | 4.559541000  | -3.141597000 | -3.087815000 |
|           | 1 | 3.302938000  | -4.439456000 | -1.371858000 |
|           | 1 | 2.101746000  | -3.264745000 | 0.453509000  |
| <b>1a</b> | 6 | 1.582262000  | -2.903545000 | 3.663155000  |
|           | 6 | -4.069096000 | -1.236408000 | 2.145467000  |
|           | 6 | 0.828079000  | -0.683976000 | 3.160216000  |
|           | 6 | -2.645394000 | -0.417208000 | 0.355915000  |
|           | 6 | 2.189029000  | -1.797350000 | 1.600530000  |
|           | 6 | -3.659382000 | -2.640335000 | 0.216691000  |
|           | 1 | -4.889264000 | -3.222574000 | 1.889524000  |
|           | 1 | 0.325190000  | -1.712795000 | 4.981388000  |
|           | 1 | -3.126395000 | 0.706982000  | 2.130994000  |
|           | 1 | 2.820001000  | -3.792783000 | 2.138853000  |
|           | 6 | -2.196782000 | -1.742587000 | -1.652759000 |
|           | 6 | 3.655986000  | -2.641728000 | -0.290320000 |
|           | 6 | 2.646803000  | -0.413338000 | -0.366016000 |
|           | 6 | -1.599367000 | -2.787958000 | -3.749579000 |
|           | 6 | -0.836478000 | -0.587055000 | -3.181976000 |
|           | 6 | 4.075350000  | -1.181095000 | -2.174410000 |
|           | 1 | -2.836226000 | -3.718610000 | -2.249502000 |
|           | 1 | 4.890740000  | -3.175753000 | -1.975621000 |
|           | 1 | 3.136592000  | 0.762991000  | -2.104522000 |
|           | 1 | -0.341776000 | -1.562048000 | -5.034694000 |
|           | 6 | -4.264453000 | -2.442687000 | 1.459634000  |
|           | 6 | 0.857926000  | -1.766581000 | 4.036050000  |
|           | 6 | -3.263090000 | -0.228296000 | 1.594857000  |
|           | 7 | 1.471184000  | -0.700813000 | 1.980800000  |
|           | 6 | -2.852158000 | -1.634033000 | -0.343675000 |
|           | 6 | 2.250925000  | -2.918337000 | 2.440258000  |
|           | 1 | 1.627108000  | -3.769659000 | 4.320064000  |
|           | 1 | -4.546939000 | -1.077741000 | 3.111045000  |
|           | 1 | 0.286233000  | 0.228844000  | 3.390229000  |
|           | 1 | -3.823525000 | -3.577532000 | -0.311525000 |

|                            |    |              |              |              |
|----------------------------|----|--------------|--------------|--------------|
|                            | 6  | 2.848703000  | -1.651142000 | 0.297271000  |
|                            | 6  | -2.264830000 | -2.837436000 | -2.525871000 |
|                            | 7  | -1.476380000 | -0.637339000 | -2.001724000 |
|                            | 6  | 4.265862000  | -2.407929000 | -1.524631000 |
|                            | 6  | 3.269354000  | -0.188388000 | -1.596449000 |
|                            | 6  | -0.872125000 | -1.642672000 | -4.089923000 |
|                            | 1  | 3.816538000  | -3.594702000 | 0.210031000  |
|                            | 1  | -1.648968000 | -3.633630000 | -4.432273000 |
|                            | 1  | -0.292475000 | 0.330634000  | -3.386105000 |
|                            | 1  | 4.557040000  | -0.994301000 | -3.133020000 |
|                            | 46 | 1.467357000  | 0.876275000  | 0.611188000  |
|                            | 46 | -1.465274000 | 0.898287000  | -0.585394000 |
|                            | 6  | -0.848207000 | 2.738766000  | 1.759017000  |
|                            | 8  | -1.722316000 | 2.387487000  | 0.897909000  |
|                            | 8  | 0.306045000  | 2.241252000  | 1.907639000  |
|                            | 6  | -1.238583000 | 3.880711000  | 2.686580000  |
|                            | 1  | -0.844157000 | 3.704645000  | 3.690420000  |
|                            | 1  | -0.786803000 | 4.805509000  | 2.310333000  |
|                            | 1  | -2.321713000 | 4.011553000  | 2.719500000  |
|                            | 8  | 1.729442000  | 2.406558000  | -0.828329000 |
|                            | 6  | 0.857178000  | 2.784710000  | -1.679907000 |
|                            | 8  | -0.299477000 | 2.297083000  | -1.841921000 |
|                            | 6  | 1.253698000  | 3.948795000  | -2.576774000 |
|                            | 1  | 0.861325000  | 3.799813000  | -3.585808000 |
|                            | 1  | 0.803880000  | 4.865171000  | -2.178237000 |
|                            | 1  | 2.337325000  | 4.076768000  | -2.603635000 |
| <b>AcOH</b>                | 1  | 1.886093000  | 0.406701000  | 0.000000000  |
|                            | 8  | 1.256449000  | -0.353101000 | 0.000000000  |
|                            | 8  | -0.227675000 | 1.350071000  | 0.000000000  |
|                            | 6  | 0.000000000  | 0.150906000  | 0.000000000  |
|                            | 6  | -1.041533000 | -0.939713000 | 0.000000000  |
|                            | 1  | -0.914236000 | -1.574995000 | 0.882024000  |
|                            | 1  | -2.038611000 | -0.499624000 | 0.000000000  |
|                            | 1  | -0.914236000 | -1.574995000 | -0.882024000 |
| <b>Pd(OAc)<sub>2</sub></b> | 46 | 0.000002000  | -0.000020000 | -0.000186000 |
|                            | 6  | -2.465399000 | -0.000668000 | 0.016485000  |
|                            | 8  | -1.791653000 | 1.091999000  | 0.018237000  |
|                            | 8  | -1.791021000 | -1.092824000 | 0.017801000  |
|                            | 6  | 2.465404000  | -0.000063000 | -0.016237000 |
|                            | 8  | 1.791295000  | -1.092432000 | -0.017999000 |
|                            | 8  | 1.791393000  | 1.092388000  | -0.018408000 |
|                            | 6  | -3.961385000 | 0.000002000  | -0.012971000 |
|                            | 1  | -4.292466000 | 0.061018000  | -1.055836000 |
|                            | 1  | -4.349619000 | -0.923574000 | 0.421580000  |

|                          |    |              |              |              |
|--------------------------|----|--------------|--------------|--------------|
|                          | 1  | -4.348797000 | 0.870732000  | 0.520993000  |
|                          | 6  | 3.961369000  | 0.000182000  | 0.013944000  |
|                          | 1  | 4.291723000  | 0.017988000  | 1.058687000  |
|                          | 1  | 4.349661000  | -0.905969000 | -0.456108000 |
|                          | 1  | 4.349383000  | 0.890946000  | -0.485109000 |
| <b>COM1<sup>mo</sup></b> | 6  | 2.375485000  | 0.910098000  | -0.548796000 |
|                          | 6  | 3.321777000  | 1.650768000  | -1.282939000 |
|                          | 6  | 2.898778000  | 2.734439000  | -2.052485000 |
|                          | 6  | 1.540544000  | 3.062895000  | -2.068921000 |
|                          | 6  | 0.671313000  | 2.283495000  | -1.299813000 |
|                          | 6  | 2.773520000  | -0.256604000 | 0.289945000  |
|                          | 6  | 3.950528000  | -0.984736000 | 0.030689000  |
|                          | 6  | 4.310706000  | -2.073252000 | 0.830908000  |
|                          | 6  | 3.502670000  | -2.454344000 | 1.908723000  |
|                          | 6  | 2.326784000  | -1.740596000 | 2.172912000  |
|                          | 6  | 1.963631000  | -0.656804000 | 1.369660000  |
|                          | 1  | 4.377534000  | 1.399553000  | -1.237385000 |
|                          | 1  | 3.619998000  | 3.317443000  | -2.622027000 |
|                          | 1  | 1.161938000  | 3.898934000  | -2.651911000 |
|                          | 1  | -0.394764000 | 2.508162000  | -1.275735000 |
|                          | 1  | 4.584031000  | -0.722908000 | -0.813376000 |
|                          | 1  | 5.219918000  | -2.627802000 | 0.607313000  |
|                          | 1  | 3.783806000  | -3.300470000 | 2.532547000  |
|                          | 1  | 1.690208000  | -2.028891000 | 3.007202000  |
|                          | 1  | 1.050423000  | -0.107483000 | 1.576576000  |
|                          | 7  | 1.065083000  | 1.237533000  | -0.560494000 |
|                          | 46 | -1.937902000 | -0.237549000 | 0.078833000  |
|                          | 6  | -1.893253000 | -2.053644000 | -1.589807000 |
|                          | 8  | -1.556158000 | -2.254284000 | -0.368212000 |
|                          | 8  | -2.253428000 | -0.861919000 | -1.901828000 |
|                          | 6  | -2.018953000 | 1.571969000  | 1.753432000  |
|                          | 8  | -2.363734000 | 1.769612000  | 0.533250000  |
|                          | 8  | -1.660225000 | 0.380814000  | 2.068323000  |
|                          | 6  | -1.891850000 | -3.162246000 | -2.595562000 |
|                          | 1  | -2.852631000 | -3.686687000 | -2.543222000 |
|                          | 1  | -1.769750000 | -2.759730000 | -3.603358000 |
|                          | 1  | -1.098185000 | -3.877322000 | -2.367166000 |
|                          | 6  | -2.007374000 | 2.684002000  | 2.755224000  |
|                          | 1  | -1.015728000 | 3.150423000  | 2.750205000  |
|                          | 1  | -2.747483000 | 3.441876000  | 2.489176000  |
|                          | 1  | -2.198869000 | 2.292995000  | 3.757020000  |
| <b>TS1<sup>mo</sup></b>  | 6  | -1.739114000 | -1.288062000 | -0.579616000 |
|                          | 6  | -2.514337000 | -2.140953000 | -1.387503000 |
|                          | 6  | -1.885586000 | -3.047556000 | -2.239377000 |

|                    |    |              |              |              |
|--------------------|----|--------------|--------------|--------------|
|                    | 6  | -0.489213000 | -3.093152000 | -2.262452000 |
|                    | 6  | 0.208947000  | -2.217189000 | -1.429975000 |
|                    | 6  | -2.388849000 | -0.336379000 | 0.362436000  |
|                    | 6  | -3.600368000 | 0.296581000  | 0.027726000  |
|                    | 6  | -4.217285000 | 1.174806000  | 0.923454000  |
|                    | 6  | -3.637795000 | 1.427908000  | 2.172696000  |
|                    | 6  | -2.433425000 | 0.800704000  | 2.514825000  |
|                    | 6  | -1.811100000 | -0.070723000 | 1.616849000  |
|                    | 1  | -3.598457000 | -2.111931000 | -1.323516000 |
|                    | 1  | -2.475817000 | -3.715174000 | -2.864002000 |
|                    | 1  | 0.050207000  | -3.785662000 | -2.903691000 |
|                    | 1  | 1.297428000  | -2.218175000 | -1.416827000 |
|                    | 1  | -4.053869000 | 0.126589000  | -0.946459000 |
|                    | 1  | -5.147100000 | 1.665528000  | 0.642885000  |
|                    | 1  | -4.119279000 | 2.109065000  | 2.871511000  |
|                    | 1  | -1.977004000 | 0.988464000  | 3.484732000  |
|                    | 1  | -0.879213000 | -0.555316000 | 1.892379000  |
|                    | 7  | -0.387567000 | -1.332179000 | -0.613103000 |
|                    | 46 | 1.397078000  | 0.540543000  | 0.014288000  |
|                    | 6  | 0.933120000  | 2.551266000  | -1.400979000 |
|                    | 8  | 0.207291000  | 2.170971000  | -0.403911000 |
|                    | 8  | 1.955010000  | 1.848944000  | -1.688368000 |
|                    | 6  | 2.460199000  | -1.168756000 | 1.602810000  |
|                    | 8  | 2.751618000  | -0.935693000 | 0.356143000  |
|                    | 8  | 1.565264000  | -0.475652000 | 2.153495000  |
|                    | 6  | 0.582114000  | 3.794592000  | -2.162587000 |
|                    | 1  | 1.163818000  | 4.631339000  | -1.759818000 |
|                    | 1  | 0.842633000  | 3.675427000  | -3.217027000 |
|                    | 1  | -0.480019000 | 4.023915000  | -2.053118000 |
|                    | 6  | 3.187578000  | -2.276263000 | 2.313449000  |
|                    | 1  | 3.247957000  | -2.059639000 | 3.382318000  |
|                    | 1  | 2.626676000  | -3.208453000 | 2.181791000  |
|                    | 1  | 4.186651000  | -2.415192000 | 1.893893000  |
| INT1 <sup>mo</sup> | 6  | -1.090627000 | 1.752533000  | -0.323651000 |
|                    | 6  | -1.514189000 | 3.045290000  | -0.673268000 |
|                    | 6  | -0.649701000 | 3.916025000  | -1.331226000 |
|                    | 6  | 0.647403000  | 3.486923000  | -1.624337000 |
|                    | 6  | 1.015611000  | 2.197645000  | -1.258694000 |
|                    | 6  | -2.001856000 | 0.838129000  | 0.412035000  |
|                    | 6  | -3.337893000 | 0.699040000  | -0.004694000 |
|                    | 6  | -4.214789000 | -0.131438000 | 0.697948000  |
|                    | 6  | -3.771076000 | -0.819970000 | 1.833776000  |
|                    | 6  | -2.445597000 | -0.674971000 | 2.259887000  |
|                    | 6  | -1.560454000 | 0.146175000  | 1.554594000  |

|                   |    |              |              |              |
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|                   | 1  | -2.514788000 | 3.363447000  | -0.395496000 |
|                   | 1  | -0.977453000 | 4.918858000  | -1.596775000 |
|                   | 1  | 1.365719000  | 4.129789000  | -2.125544000 |
|                   | 1  | 2.011624000  | 1.815160000  | -1.458661000 |
|                   | 1  | -3.687051000 | 1.219035000  | -0.894512000 |
|                   | 1  | -5.241690000 | -0.243133000 | 0.356435000  |
|                   | 1  | -4.455140000 | -1.463146000 | 2.383743000  |
|                   | 1  | -2.097198000 | -1.198222000 | 3.148018000  |
|                   | 1  | -0.537884000 | 0.264429000  | 1.906345000  |
|                   | 7  | 0.167109000  | 1.347798000  | -0.640094000 |
|                   | 46 | 0.842011000  | -0.621228000 | -0.433552000 |
|                   | 6  | 2.691083000  | 0.356668000  | 1.585638000  |
|                   | 8  | 2.606609000  | 0.100283000  | 0.302017000  |
|                   | 8  | 1.766027000  | 0.242417000  | 2.400157000  |
|                   | 6  | 0.061072000  | -2.878880000 | -1.105044000 |
|                   | 8  | -0.658200000 | -1.842295000 | -1.329170000 |
|                   | 8  | 1.190988000  | -2.709085000 | -0.520603000 |
|                   | 6  | 4.084395000  | 0.812166000  | 2.003958000  |
|                   | 1  | 4.426927000  | 1.631183000  | 1.364918000  |
|                   | 1  | 4.077679000  | 1.130560000  | 3.047892000  |
|                   | 1  | 4.790550000  | -0.015726000 | 1.881830000  |
|                   | 6  | -0.387375000 | -4.244807000 | -1.534882000 |
|                   | 1  | 0.035157000  | -4.460820000 | -2.522668000 |
|                   | 1  | -0.021855000 | -5.000519000 | -0.835693000 |
|                   | 1  | -1.476320000 | -4.282723000 | -1.607225000 |
| TS2 <sup>mo</sup> | 6  | -2.063647000 | 1.115703000  | -0.232184000 |
|                   | 6  | -3.023650000 | 2.124481000  | -0.365621000 |
|                   | 6  | -2.619354000 | 3.414706000  | -0.707956000 |
|                   | 6  | -1.260680000 | 3.671677000  | -0.912576000 |
|                   | 6  | -0.349321000 | 2.632164000  | -0.748346000 |
|                   | 6  | -2.393455000 | -0.290044000 | 0.098296000  |
|                   | 6  | -1.726710000 | -1.330755000 | -0.586161000 |
|                   | 6  | -1.962753000 | -2.667934000 | -0.240976000 |
|                   | 6  | -2.874430000 | -2.977600000 | 0.772291000  |
|                   | 6  | -3.554290000 | -1.947767000 | 1.437229000  |
|                   | 6  | -3.315674000 | -0.610589000 | 1.106049000  |
|                   | 1  | -4.074236000 | 1.886319000  | -0.223471000 |
|                   | 1  | -3.355873000 | 4.206765000  | -0.824701000 |
|                   | 1  | -0.903139000 | 4.658551000  | -1.193352000 |
|                   | 1  | 0.718238000  | 2.773136000  | -0.885941000 |
|                   | 1  | -1.122359000 | -1.116333000 | -1.470607000 |
|                   | 1  | -1.442231000 | -3.456278000 | -0.778814000 |
|                   | 1  | -3.061732000 | -4.014993000 | 1.040515000  |
|                   | 1  | -4.263543000 | -2.186356000 | 2.226891000  |

|                          |    |              |              |              |
|--------------------------|----|--------------|--------------|--------------|
|                          | 1  | -3.822663000 | 0.181501000  | 1.652915000  |
|                          | 7  | -0.745444000 | 1.388799000  | -0.412424000 |
|                          | 46 | 0.600095000  | -0.149224000 | -0.003050000 |
|                          | 6  | 2.724742000  | 1.699941000  | 0.649628000  |
|                          | 8  | 1.745871000  | 1.062063000  | 1.236631000  |
|                          | 8  | 2.928446000  | 1.731073000  | -0.572869000 |
|                          | 6  | 1.906272000  | -2.452082000 | -0.646938000 |
|                          | 8  | 1.200715000  | -2.228049000 | -1.650931000 |
|                          | 8  | 1.886522000  | -1.674143000 | 0.401864000  |
|                          | 6  | 3.640291000  | 2.422134000  | 1.633516000  |
|                          | 1  | 3.075393000  | 2.832936000  | 2.473573000  |
|                          | 1  | 4.359333000  | 1.699676000  | 2.035236000  |
|                          | 1  | 4.189470000  | 3.213632000  | 1.119703000  |
|                          | 6  | 2.857594000  | -3.627648000 | -0.562576000 |
|                          | 1  | 3.881777000  | -3.269472000 | -0.714146000 |
|                          | 1  | 2.812272000  | -4.091794000 | 0.426337000  |
|                          | 1  | 2.620986000  | -4.360464000 | -1.336490000 |
| <b>INT2<sup>mo</sup></b> | 6  | -2.360036000 | -0.601107000 | 0.174669000  |
|                          | 6  | -3.577126000 | -1.279489000 | 0.273137000  |
|                          | 6  | -3.568856000 | -2.669470000 | 0.400913000  |
|                          | 6  | -2.346343000 | -3.346973000 | 0.422483000  |
|                          | 6  | -1.167747000 | -2.613277000 | 0.304222000  |
|                          | 6  | -2.220204000 | 0.867549000  | 0.037335000  |
|                          | 6  | -1.173211000 | 1.522433000  | 0.738306000  |
|                          | 6  | -0.952161000 | 2.898486000  | 0.546370000  |
|                          | 6  | -1.768087000 | 3.623696000  | -0.321671000 |
|                          | 6  | -2.816041000 | 2.978205000  | -0.995337000 |
|                          | 6  | -3.039876000 | 1.608742000  | -0.824892000 |
|                          | 1  | -4.509579000 | -0.721391000 | 0.266562000  |
|                          | 1  | -4.504799000 | -3.216682000 | 0.489623000  |
|                          | 1  | -2.296873000 | -4.427077000 | 0.529917000  |
|                          | 1  | -0.192567000 | -3.087899000 | 0.307546000  |
|                          | 1  | -0.671826000 | 1.031247000  | 1.579349000  |
|                          | 1  | -0.151550000 | 3.383462000  | 1.097677000  |
|                          | 1  | -1.600994000 | 4.688130000  | -0.469366000 |
|                          | 1  | -3.454326000 | 3.543641000  | -1.671118000 |
|                          | 1  | -3.829510000 | 1.114390000  | -1.386287000 |
|                          | 7  | -1.182256000 | -1.274505000 | 0.184451000  |
|                          | 46 | 0.462197000  | -0.039518000 | -0.157268000 |
|                          | 6  | 2.377444000  | -2.198556000 | -0.202978000 |
|                          | 8  | 1.598320000  | -1.543075000 | -1.025462000 |
|                          | 8  | 2.378186000  | -2.078211000 | 1.029876000  |
|                          | 6  | 2.486993000  | 1.906997000  | 0.423472000  |
|                          | 8  | 2.042346000  | 1.870605000  | 1.580618000  |

|                   |    |              |              |              |
|-------------------|----|--------------|--------------|--------------|
|                   | 8  | 2.001078000  | 1.226417000  | -0.584145000 |
|                   | 6  | 3.331272000  | -3.152280000 | -0.916401000 |
|                   | 1  | 2.849564000  | -3.626865000 | -1.774786000 |
|                   | 1  | 4.185403000  | -2.576937000 | -1.290347000 |
|                   | 1  | 3.696411000  | -3.908370000 | -0.218512000 |
|                   | 6  | 3.687872000  | 2.763930000  | 0.045455000  |
|                   | 1  | 4.557330000  | 2.115255000  | -0.106664000 |
|                   | 1  | 3.505952000  | 3.295405000  | -0.892707000 |
|                   | 1  | 3.909287000  | 3.473860000  | 0.844710000  |
| TS3 <sup>mo</sup> | 6  | -2.099971000 | 1.046584000  | -0.288556000 |
|                   | 6  | -3.125900000 | 1.927374000  | -0.654736000 |
|                   | 6  | -2.815372000 | 3.240828000  | -1.003646000 |
|                   | 6  | -1.481583000 | 3.659408000  | -0.979221000 |
|                   | 6  | -0.500588000 | 2.738981000  | -0.618571000 |
|                   | 6  | -2.291422000 | -0.342124000 | 0.166942000  |
|                   | 6  | -1.162899000 | -1.215844000 | 0.172778000  |
|                   | 6  | -1.282892000 | -2.446339000 | 0.847130000  |
|                   | 6  | -2.489716000 | -2.848162000 | 1.427580000  |
|                   | 6  | -3.606191000 | -2.008774000 | 1.354114000  |
|                   | 6  | -3.501991000 | -0.756225000 | 0.741861000  |
|                   | 1  | -4.155802000 | 1.583179000  | -0.673731000 |
|                   | 1  | -3.605478000 | 3.929594000  | -1.294659000 |
|                   | 1  | -1.196912000 | 4.673958000  | -1.244078000 |
|                   | 1  | 0.555993000  | 2.990359000  | -0.594266000 |
|                   | 1  | -0.371560000 | -1.555640000 | -0.884691000 |
|                   | 1  | -0.429964000 | -3.120831000 | 0.881251000  |
|                   | 1  | -2.559180000 | -3.811393000 | 1.928580000  |
|                   | 1  | -4.550821000 | -2.313618000 | 1.799381000  |
|                   | 1  | -4.359020000 | -0.087143000 | 0.760587000  |
|                   | 7  | -0.806728000 | 1.472519000  | -0.287601000 |
|                   | 46 | 0.613948000  | -0.008005000 | 0.006476000  |
|                   | 6  | 2.876843000  | 1.460486000  | 1.049347000  |
|                   | 8  | 2.192151000  | 1.359340000  | -0.059722000 |
|                   | 8  | 2.609668000  | 0.862865000  | 2.104013000  |
|                   | 6  | 1.545403000  | -2.426810000 | -1.140383000 |
|                   | 8  | 0.388702000  | -2.357898000 | -1.683495000 |
|                   | 8  | 1.937295000  | -1.643491000 | -0.213958000 |
|                   | 6  | 4.079078000  | 2.392619000  | 0.941500000  |
|                   | 1  | 4.833604000  | 1.936317000  | 0.291661000  |
|                   | 1  | 3.788772000  | 3.343808000  | 0.485713000  |
|                   | 1  | 4.513999000  | 2.568270000  | 1.927239000  |
|                   | 6  | 2.490169000  | -3.506870000 | -1.617099000 |
|                   | 1  | 2.633848000  | -3.408094000 | -2.697041000 |
|                   | 1  | 3.450242000  | -3.439257000 | -1.105219000 |

|                          |    |              |              |              |
|--------------------------|----|--------------|--------------|--------------|
|                          | 1  | 2.037440000  | -4.486236000 | -1.434353000 |
| <b>INT3<sup>mo</sup></b> | 6  | 2.486846000  | 0.832268000  | 0.050279000  |
|                          | 6  | 3.572263000  | 1.714386000  | 0.113954000  |
|                          | 6  | 3.343682000  | 3.089296000  | 0.149848000  |
|                          | 6  | 2.029880000  | 3.562832000  | 0.116825000  |
|                          | 6  | 0.984963000  | 2.641351000  | 0.053265000  |
|                          | 6  | 2.566508000  | -0.629339000 | 0.000145000  |
|                          | 6  | 1.328052000  | -1.311209000 | -0.053118000 |
|                          | 6  | 1.301451000  | -2.704771000 | -0.112971000 |
|                          | 6  | 2.506053000  | -3.425830000 | -0.119081000 |
|                          | 6  | 3.735350000  | -2.756997000 | -0.063908000 |
|                          | 6  | 3.766438000  | -1.362245000 | -0.004548000 |
|                          | 1  | 4.586212000  | 1.326008000  | 0.135203000  |
|                          | 1  | 4.181725000  | 3.781356000  | 0.200174000  |
|                          | 1  | 1.805208000  | 4.625763000  | 0.136539000  |
|                          | 1  | -0.056669000 | 2.950739000  | 0.004984000  |
|                          | 1  | -3.111104000 | -0.134484000 | 0.204878000  |
|                          | 1  | 0.353058000  | -3.231546000 | -0.154325000 |
|                          | 1  | 2.480331000  | -4.513206000 | -0.166920000 |
|                          | 1  | 4.665714000  | -3.320559000 | -0.068254000 |
|                          | 1  | 4.726178000  | -0.851159000 | 0.036059000  |
|                          | 7  | 1.208454000  | 1.314598000  | 0.025173000  |
|                          | 46 | -0.296687000 | -0.147467000 | -0.024654000 |
|                          | 6  | -2.743447000 | 2.185665000  | -0.127934000 |
|                          | 8  | -2.062208000 | 3.187031000  | -0.380142000 |
|                          | 8  | -2.249251000 | 0.984974000  | 0.066089000  |
|                          | 6  | -2.800192000 | -2.053447000 | 0.100579000  |
|                          | 8  | -3.632215000 | -1.062440000 | 0.265775000  |
|                          | 8  | -1.565674000 | -1.918390000 | -0.054079000 |
|                          | 6  | -4.261239000 | 2.276690000  | -0.015231000 |
|                          | 1  | -4.592828000 | 3.303377000  | -0.177851000 |
|                          | 1  | -4.735100000 | 1.620905000  | -0.753413000 |
|                          | 1  | -4.586094000 | 1.941134000  | 0.975343000  |
|                          | 6  | -3.426963000 | -3.423466000 | 0.098549000  |
|                          | 1  | -4.099688000 | -3.508998000 | -0.760976000 |
|                          | 1  | -2.660342000 | -4.196116000 | 0.044157000  |
|                          | 1  | -4.031236000 | -3.552434000 | 1.001209000  |
| <b>B</b>                 | 6  | 2.826605000  | -1.132415000 | 0.227049000  |
|                          | 6  | 3.743406000  | -2.185547000 | 0.389840000  |
|                          | 6  | 3.340943000  | -3.389174000 | 0.961271000  |
|                          | 6  | 2.015394000  | -3.524246000 | 1.380604000  |
|                          | 6  | 1.152505000  | -2.451314000 | 1.192688000  |
|                          | 6  | 3.286201000  | 0.159859000  | -0.346570000 |
|                          | 6  | 4.112854000  | 0.161447000  | -1.484425000 |

|    |              |              |              |
|----|--------------|--------------|--------------|
| 6  | 4.594954000  | 1.363024000  | -2.010302000 |
| 6  | 4.269955000  | 2.578454000  | -1.395748000 |
| 6  | 3.456397000  | 2.581792000  | -0.256576000 |
| 6  | 2.961839000  | 1.382716000  | 0.265865000  |
| 1  | 4.776594000  | -2.034931000 | 0.091214000  |
| 1  | 4.052873000  | -4.201596000 | 1.091104000  |
| 1  | 1.648281000  | -4.437579000 | 1.840539000  |
| 1  | 0.113038000  | -2.510217000 | 1.497934000  |
| 1  | 4.360492000  | -0.776696000 | -1.977016000 |
| 1  | 5.221091000  | 1.349541000  | -2.900058000 |
| 1  | 4.649552000  | 3.514444000  | -1.800766000 |
| 1  | 3.207921000  | 3.521047000  | 0.233712000  |
| 1  | 2.339569000  | 1.407319000  | 1.156999000  |
| 7  | 1.538475000  | -1.291146000 | 0.622382000  |
| 46 | -0.045302000 | 0.064665000  | 0.298321000  |
| 6  | -0.003106000 | 0.964042000  | 3.096788000  |
| 8  | -0.441744000 | -0.001691000 | 2.336510000  |
| 8  | 0.657669000  | 1.941180000  | 2.706559000  |
| 6  | 0.214991000  | -0.924833000 | -2.465910000 |
| 8  | 0.293599000  | 0.155077000  | -1.734918000 |
| 8  | -0.072996000 | -2.060363000 | -2.059813000 |
| 6  | -0.381452000 | 0.795040000  | 4.565059000  |
| 1  | 0.012273000  | -0.152722000 | 4.945820000  |
| 1  | 0.014632000  | 1.621431000  | 5.158092000  |
| 1  | -1.470843000 | 0.759011000  | 4.667453000  |
| 6  | 0.528467000  | -0.661622000 | -3.937814000 |
| 1  | 1.546983000  | -0.272574000 | -4.035425000 |
| 1  | 0.429541000  | -1.581587000 | -4.517413000 |
| 1  | -0.149633000 | 0.099545000  | -4.336537000 |
| 6  | -2.885656000 | 1.129808000  | -0.382406000 |
| 6  | -3.785026000 | 2.147540000  | -0.741497000 |
| 6  | -3.387688000 | 3.481828000  | -0.707277000 |
| 6  | -2.087677000 | 3.786655000  | -0.297500000 |
| 6  | -1.239046000 | 2.738806000  | 0.042661000  |
| 6  | -3.332564000 | -0.288361000 | -0.388725000 |
| 6  | -4.052959000 | -0.788966000 | -1.487762000 |
| 6  | -4.519974000 | -2.106203000 | -1.489182000 |
| 6  | -4.287253000 | -2.934876000 | -0.385325000 |
| 6  | -3.581058000 | -2.438939000 | 0.716916000  |
| 6  | -3.101188000 | -1.126051000 | 0.717431000  |
| 1  | -4.800104000 | 1.880069000  | -1.020240000 |
| 1  | -4.085584000 | 4.270315000  | -0.981124000 |
| 1  | -1.728957000 | 4.810640000  | -0.239690000 |
| 1  | -0.222296000 | 2.922110000  | 0.374114000  |

|  |   |              |              |              |
|--|---|--------------|--------------|--------------|
|  | 1 | -4.228237000 | -0.156077000 | -2.355403000 |
|  | 1 | -5.061036000 | -2.485392000 | -2.353566000 |
|  | 1 | -4.654231000 | -3.959240000 | -0.384298000 |
|  | 1 | -3.406237000 | -3.074110000 | 1.583029000  |
|  | 1 | -2.565919000 | -0.746082000 | 1.582850000  |
|  | 7 | -1.619510000 | 1.444625000  | -0.008911000 |

**Table S1-5.** Some optimized Cartesian Coordinates of stationary points for the oxidative process ( $\text{Pd}^{\text{II}}$  to  $\text{Pd}^{\text{III}}$ ), involved in the discussion on  $\text{PhI}(\text{OAc})_2$  (**OX-a**),  $\text{PhICl}_2$  (**OX-b**) and  $\text{NCS}$  (**OX-c**) as oxidant, computed at B3LYP - IDSCRF/DGDZVP level in dichloromethane with bond lengths in Å.

| Species                     | Cartesian coordinates |              |              |              |
|-----------------------------|-----------------------|--------------|--------------|--------------|
| <b>PhI(OAc)<sub>2</sub></b> | 6                     | 0.000002000  | -1.113402000 | -0.000014000 |
|                             | 6                     | 0.513868000  | -1.778954000 | -1.115380000 |
|                             | 6                     | -0.513860000 | -1.778939000 | 1.115362000  |
|                             | 6                     | 0.508412000  | -3.178752000 | -1.103139000 |
|                             | 6                     | -0.508398000 | -3.178737000 | 1.103141000  |
|                             | 6                     | 0.000009000  | -3.874671000 | 0.000006000  |
|                             | 1                     | 0.917109000  | -1.232762000 | -1.962396000 |
|                             | 1                     | -0.917104000 | -1.232736000 | 1.962368000  |
|                             | 1                     | 0.903995000  | -3.719739000 | -1.959791000 |
|                             | 1                     | -0.903977000 | -3.719714000 | 1.959801000  |
|                             | 1                     | 0.000011000  | -4.962474000 | 0.000015000  |
|                             | 53                    | -0.000003000 | 1.018347000  | -0.000029000 |
|                             | 8                     | -2.046005000 | 0.960178000  | -0.813945000 |
|                             | 6                     | -3.045159000 | 0.799232000  | 0.054153000  |
|                             | 8                     | -2.898312000 | 0.621792000  | 1.260442000  |
|                             | 6                     | -4.402901000 | 0.852177000  | -0.625644000 |
|                             | 1                     | -4.475735000 | 0.049366000  | -1.365669000 |
|                             | 1                     | -4.517345000 | 1.800696000  | -1.158428000 |
|                             | 1                     | -5.194211000 | 0.743387000  | 0.117198000  |
|                             | 8                     | 2.045976000  | 0.960192000  | 0.813958000  |
|                             | 6                     | 3.045159000  | 0.799253000  | -0.054105000 |
|                             | 8                     | 2.898362000  | 0.621814000  | -1.260402000 |
|                             | 6                     | 4.402874000  | 0.852184000  | 0.625747000  |
|                             | 1                     | 4.475738000  | 0.049232000  | 1.365617000  |
|                             | 1                     | 4.517235000  | 1.800606000  | 1.158719000  |
|                             | 1                     | 5.194215000  | 0.743580000  | -0.117089000 |
| <b>TS1a</b>                 | 6                     | -4.254513000 | 1.259708000  | 4.135062000  |
|                             | 6                     | 0.484289000  | -1.141719000 | 3.708276000  |
|                             | 6                     | -3.749351000 | -0.624315000 | 2.741334000  |
|                             | 6                     | -0.020670000 | -0.589889000 | 1.409790000  |
|                             | 6                     | -4.108866000 | 1.467961000  | 1.730997000  |
|                             | 6                     | 0.609076000  | 1.163891000  | 2.975657000  |
|                             | 1                     | 1.013842000  | 0.516949000  | 4.991365000  |
|                             | 1                     | -3.900757000 | -0.752976000 | 4.882782000  |

|  |    |              |              |              |
|--|----|--------------|--------------|--------------|
|  | 1  | -0.058582000 | -2.594486000 | 2.199689000  |
|  | 6  | 0.141964000  | 1.693937000  | 0.535107000  |
|  | 6  | -4.487115000 | 3.517165000  | 0.281831000  |
|  | 6  | -3.940837000 | 1.350581000  | -0.709062000 |
|  | 6  | 0.284040000  | 3.811062000  | -0.618025000 |
|  | 6  | -0.261160000 | 1.785175000  | -1.778627000 |
|  | 6  | -4.345208000 | 3.280268000  | -2.122986000 |
|  | 1  | -4.807453000 | 5.134030000  | -1.107986000 |
|  | 1  | -3.875049000 | 1.307605000  | -2.863845000 |
|  | 1  | -0.103791000 | 3.694986000  | -2.755290000 |
|  | 6  | 0.725654000  | 0.209470000  | 3.988610000  |
|  | 6  | -3.963482000 | -0.102746000 | 4.014741000  |
|  | 6  | 0.114781000  | -1.544251000 | 2.415231000  |
|  | 7  | -3.818190000 | 0.138099000  | 1.637513000  |
|  | 6  | 0.240785000  | 0.774549000  | 1.675298000  |
|  | 6  | -4.327424000 | 2.048208000  | 2.987963000  |
|  | 1  | -4.426067000 | 1.703327000  | 5.113554000  |
|  | 1  | 0.587216000  | -1.887934000 | 4.494353000  |
|  | 1  | -3.521220000 | -1.673543000 | 2.579661000  |
|  | 6  | -4.178703000 | 2.153511000  | 0.434765000  |
|  | 6  | 0.373203000  | 3.075097000  | 0.562541000  |
|  | 7  | -0.179932000 | 1.082983000  | -0.638665000 |
|  | 6  | -4.566990000 | 4.079272000  | -0.993961000 |
|  | 6  | -4.033487000 | 1.919652000  | -1.980312000 |
|  | 6  | -0.032531000 | 3.158730000  | -1.813204000 |
|  | 1  | 0.467814000  | 4.883134000  | -0.606941000 |
|  | 1  | -0.514832000 | 1.218661000  | -2.669758000 |
|  | 1  | -4.416658000 | 3.714984000  | -3.118729000 |
|  | 46 | -3.537411000 | -0.573303000 | -0.306398000 |
|  | 46 | -0.576071000 | -0.977147000 | -0.479877000 |
|  | 6  | -2.250375000 | -3.389696000 | 0.250484000  |
|  | 8  | -1.069617000 | -2.986912000 | -0.017094000 |
|  | 8  | -3.295471000 | -2.675899000 | 0.299095000  |
|  | 6  | -2.406610000 | -4.877598000 | 0.521840000  |
|  | 1  | -3.157948000 | -5.043326000 | 1.297730000  |
|  | 1  | -2.760301000 | -5.362040000 | -0.395198000 |
|  | 1  | -1.454398000 | -5.328766000 | 0.805965000  |
|  | 8  | -3.473452000 | -1.122396000 | -2.340820000 |
|  | 6  | -2.405915000 | -1.327017000 | -3.014811000 |
|  | 8  | -1.220338000 | -1.211859000 | -2.592130000 |
|  | 6  | -2.595351000 | -1.760293000 | -4.460034000 |
|  | 1  | -1.864468000 | -1.259945000 | -5.100437000 |
|  | 1  | -2.409544000 | -2.837904000 | -4.527143000 |
|  | 1  | -3.609726000 | -1.555181000 | -4.806324000 |

|       |    |              |              |              |
|-------|----|--------------|--------------|--------------|
|       | 1  | -4.558538000 | 3.106478000  | 3.065452000  |
|       | 1  | -4.672204000 | 4.144116000  | 1.151794000  |
|       | 1  | 0.815912000  | 2.208066000  | 3.201091000  |
|       | 1  | 0.630551000  | 3.566400000  | 1.496185000  |
|       | 8  | 1.802094000  | -1.203714000 | -1.213959000 |
|       | 6  | 2.117179000  | -2.244389000 | -1.961883000 |
|       | 8  | 1.515298000  | -3.322396000 | -1.915721000 |
|       | 6  | 3.291975000  | -2.060325000 | -2.920865000 |
|       | 1  | 4.236034000  | -2.131219000 | -2.370421000 |
|       | 1  | 3.260398000  | -1.084491000 | -3.411768000 |
|       | 1  | 3.270161000  | -2.856285000 | -3.668405000 |
|       | 53 | 3.745765000  | 0.620236000  | -0.549712000 |
|       | 6  | 4.668962000  | -0.885983000 | 0.620898000  |
|       | 6  | 5.892616000  | -1.419108000 | 0.196959000  |
|       | 6  | 4.043063000  | -1.316188000 | 1.796280000  |
|       | 6  | 6.499959000  | -2.409012000 | 0.976925000  |
|       | 6  | 4.663755000  | -2.310399000 | 2.560182000  |
|       | 6  | 5.887951000  | -2.855179000 | 2.154614000  |
|       | 1  | 6.370699000  | -1.071549000 | -0.715026000 |
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|       | 1  | 6.630919000  | 4.320171000  | 1.075537000  |
|       | 1  | 5.868898000  | 5.357606000  | -0.175530000 |
| INT1a | 6  | 3.921503000  | 2.864731000  | -1.440200000 |
|       | 6  | -0.942938000 | 4.223280000  | -0.534868000 |
|       | 6  | 2.021674000  | 1.679580000  | -2.295736000 |
|       | 6  | -0.953525000 | 1.931332000  | 0.209184000  |
|       | 6  | 3.245962000  | 0.731349000  | -0.526259000 |
|       | 6  | 0.035063000  | 3.651086000  | 1.606002000  |
|       | 1  | -0.012379000 | 5.647933000  | 0.798217000  |
|       | 1  | 2.674947000  | 3.573275000  | -3.077041000 |
|       | 1  | -1.820802000 | 2.589427000  | -1.650753000 |
|       | 6  | -0.068105000 | 1.235883000  | 2.389091000  |
|       | 6  | 4.347139000  | -0.638790000 | 1.304970000  |
|       | 6  | 2.356477000  | -1.449057000 | 0.145330000  |
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|       | 6  | -0.369317000 | -1.060473000 | 2.787347000  |

|    |              |              |              |
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| 1  | 5.166927000  | -1.958894000 | 2.799197000  |
| 1  | 1.672250000  | -3.408541000 | 0.730366000  |
| 1  | 0.246141000  | -1.843758000 | 4.693326000  |
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| 6  | 2.859074000  | 2.790940000  | -2.346141000 |
| 6  | -1.288996000 | 2.879747000  | -0.749905000 |
| 7  | 2.208535000  | 0.685530000  | -1.411468000 |
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| 6  | 4.115949000  | 1.829745000  | -0.527009000 |
| 1  | 4.594968000  | 3.719141000  | -1.447566000 |
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| 6  | 3.339607000  | -0.448083000 | 0.342688000  |
| 6  | 0.491911000  | 1.396954000  | 3.663261000  |
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| 6  | 4.384446000  | -1.814637000 | 2.057464000  |
| 6  | 2.408042000  | -2.625931000 | 0.892881000  |
| 6  | 0.173715000  | -0.959793000 | 4.065978000  |
| 1  | 1.045386000  | 0.408805000  | 5.496905000  |
| 1  | -0.736100000 | -2.001504000 | 2.388436000  |
| 1  | 3.454480000  | -3.730134000 | 2.426350000  |
| 46 | 1.019345000  | -1.026921000 | -1.291641000 |
| 46 | -1.374255000 | -0.031860000 | 0.068839000  |
| 6  | -1.464882000 | -0.112337000 | -2.956294000 |
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| 6  | -1.617059000 | -4.502122000 | -0.624953000 |
| 1  | -2.136164000 | -4.756081000 | 0.302159000  |
| 1  | -2.349538000 | -4.543409000 | -1.438851000 |
| 1  | -0.825471000 | -5.224282000 | -0.832598000 |
| 8  | -3.238967000 | 0.409251000  | 1.272533000  |
| 6  | -4.455249000 | 0.139679000  | 0.895406000  |
| 8  | -4.813945000 | -0.361496000 | -0.178517000 |
| 6  | -5.492230000 | 0.542120000  | 1.954838000  |
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| 1  | -5.147206000 | 0.292614000  | 2.961698000  |

|                    |   |              |              |              |
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|                    | 1 | 0.817878000  | 2.377979000  | 3.995876000  |
|                    | 1 | 0.538074000  | 3.963158000  | 2.518829000  |
|                    | 1 | 5.109401000  | 0.120696000  | 1.466780000  |
|                    | 1 | 4.941548000  | 1.869626000  | 0.177323000  |
| <b>OAc-radical</b> | 8 | 0.817900000  | 1.043402000  | 0.001491000  |
|                    | 6 | 0.096337000  | 0.000019000  | -0.007732000 |
|                    | 8 | 0.817760000  | -1.043473000 | 0.001489000  |
|                    | 6 | -1.395560000 | 0.000087000  | -0.003049000 |
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|                    | 1 | -1.773568000 | -0.896923000 | -0.500334000 |
|                    | 1 | -1.773576000 | 0.900066000  | -0.494908000 |
| <b>2a</b>          | 6 | -2.172978000 | 3.426609000  | 2.242685000  |
|                    | 6 | 1.833812000  | 1.202424000  | 3.934928000  |
|                    | 6 | -1.715541000 | 1.073510000  | 2.317656000  |
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|                    | 6 | -1.840029000 | 2.145715000  | 0.224765000  |
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|                    | 1 | 2.191151000  | 3.300495000  | 4.308768000  |
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|                    | 6 | -1.568448000 | 0.576958000  | -1.629558000 |
|                    | 6 | 2.173223000  | 3.426589000  | -2.242538000 |
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|                    | 6 | 2.021417000  | 2.536454000  | 3.553706000  |
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|                    | 7 | -1.632745000 | 1.032711000  | 0.979898000  |
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|            | 6  | 1.976021000  | 2.262691000  | -2.990936000 |
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|            | 6  | -0.089385000 | -3.914890000 | 2.738089000  |
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|            | 6  | 0.078499000  | -2.692381000 | -1.841773000 |
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|            | 8  | -3.456830000 | -1.188993000 | -0.387825000 |
| <b>Phi</b> | 53 | -1.564952000 | -0.000002000 | 0.000004000  |
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| <b>1b</b> | 6  | 2.517781000  | 2.539413000  | -3.219689000 |
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|           | 6  | -2.456232000 | 0.123403000  | -0.986901000 |
|           | 6  | 2.515160000  | 1.407190000  | -1.087053000 |
|           | 6  | -3.454006000 | 2.404013000  | -0.954868000 |
|           | 1  | -4.237231000 | 3.083944000  | -2.864060000 |
|           | 1  | 1.644412000  | 1.374275000  | -4.817097000 |
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|           | 6  | 2.456266000  | 0.123968000  | 0.986886000  |
|           | 6  | -2.518605000 | 2.538702000  | 3.219741000  |
|           | 6  | -1.612762000 | 0.317052000  | 2.936946000  |
|           | 6  | 3.404590000  | 1.101476000  | 3.001034000  |
|           | 1  | 4.236429000  | 3.084988000  | 2.864076000  |
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|           | 7  | 1.907140000  | 0.313159000  | -1.637260000 |
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|           | 6  | 2.763042000  | 0.024165000  | 2.335864000  |
|           | 6  | -1.905211000 | 1.419165000  | 3.763501000  |
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|           | 46 | 1.562375000  | -1.212062000 | -0.221130000 |
|           | 46 | -1.561996000 | -1.212405000 | 0.221107000  |

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|                          | 8  | -1.472838000 | -2.660927000 | -1.312891000 |
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|                          | 1  | 0.100229000  | -4.042246000 | -3.756541000 |
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|                          | 8  | -0.760824000 | -2.619024000 | 1.722906000  |
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|                          | 1  | -3.743267000 | 4.539480000  | 1.732616000  |
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|                          | 1  | -4.267430000 | 4.409305000  | -0.669301000 |
|                          | 6  | 3.486562000  | 3.649507000  | -1.162568000 |
|                          | 1  | 3.741868000  | 4.540520000  | -1.732538000 |
|                          | 6  | 3.776591000  | 3.573859000  | 0.173781000  |
|                          | 1  | 4.266150000  | 4.410430000  | 0.669359000  |
| <b>PhICl<sub>2</sub></b> | 53 | 1.142347000  | -0.000855000 | 0.000090000  |
|                          | 6  | -0.994284000 | 0.000932000  | 0.000157000  |
|                          | 6  | -1.656501000 | 0.002032000  | -1.228933000 |
|                          | 6  | -1.656788000 | 0.000560000  | 1.229117000  |
|                          | 6  | -3.055911000 | 0.002931000  | -1.215102000 |
|                          | 6  | -3.056199000 | 0.001363000  | 1.214937000  |
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|                          | 1  | -3.597298000 | 0.001083000  | 2.158008000  |
|                          | 1  | -4.838662000 | 0.003242000  | -0.000307000 |
|                          | 17 | 1.136185000  | -2.583649000 | -0.000516000 |
|                          | 17 | 1.142719000  | 2.582046000  | 0.000251000  |
| <b>TS1b</b>              | 6  | -5.332390000 | -0.498741000 | 2.731046000  |
|                          | 6  | -0.501623000 | 1.656967000  | 3.943382000  |
|                          | 6  | -3.190995000 | -1.571126000 | 2.414210000  |
|                          | 6  | -0.073626000 | 1.022401000  | 1.646057000  |
|                          | 6  | -4.323991000 | -0.750075000 | 0.552146000  |
|                          | 6  | -1.321842000 | 3.097422000  | 2.168528000  |
|                          | 1  | -1.602664000 | 3.474688000  | 4.289510000  |
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|  | 6  | -0.841339000 | 2.471068000  | -0.159238000 |
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|  | 6  | -3.191238000 | -1.106525000 | -1.578573000 |
|  | 6  | -1.503941000 | 3.824894000  | -2.043067000 |
|  | 6  | -0.268047000 | 1.766678000  | -2.303979000 |
|  | 6  | -4.269644000 | -0.368572000 | -3.625183000 |
|  | 1  | -6.182275000 | 0.609263000  | -3.458509000 |
|  | 1  | -2.352663000 | -1.383878000 | -3.542308000 |
|  | 1  | -0.875538000 | 3.021075000  | -3.948829000 |
|  | 6  | -1.182575000 | 2.799513000  | 3.546773000  |
|  | 6  | -4.226028000 | -1.141808000 | 3.266956000  |
|  | 6  | 0.059107000  | 0.758226000  | 2.997217000  |
|  | 7  | -3.238708000 | -1.378547000 | 1.096533000  |
|  | 6  | -0.756093000 | 2.193238000  | 1.235234000  |
|  | 6  | -5.406077000 | -0.287079000 | 1.335614000  |
|  | 1  | -6.141475000 | -0.160576000 | 3.375840000  |
|  | 1  | -0.388878000 | 1.440017000  | 5.004071000  |
|  | 1  | -2.312667000 | -2.081422000 | 2.798041000  |
|  | 6  | -4.308888000 | -0.599424000 | -0.865470000 |
|  | 6  | -1.489903000 | 3.628824000  | -0.644170000 |
|  | 7  | -0.250342000 | 1.562026000  | -0.988370000 |
|  | 6  | -5.359293000 | 0.135437000  | -2.927338000 |
|  | 6  | -3.182078000 | -0.992572000 | -2.959690000 |
|  | 6  | -0.888941000 | 2.896051000  | -2.869940000 |
|  | 1  | -1.989339000 | 4.703399000  | -2.464194000 |
|  | 1  | 0.223428000  | 1.018892000  | -2.919515000 |
|  | 1  | -4.244827000 | -0.287603000 | -4.710445000 |
|  | 46 | -1.826487000 | -1.948699000 | -0.363482000 |
|  | 46 | 0.534999000  | -0.079630000 | 0.071496000  |
|  | 6  | 0.603625000  | -2.676051000 | 1.560049000  |
|  | 8  | 1.249845000  | -1.595552000 | 1.331132000  |
|  | 8  | -0.527864000 | -2.987588000 | 1.090718000  |
|  | 6  | 1.261906000  | -3.652029000 | 2.521035000  |
|  | 1  | 1.048517000  | -4.679770000 | 2.219298000  |
|  | 1  | 2.338067000  | -3.483885000 | 2.573962000  |
|  | 1  | 0.835131000  | -3.499922000 | 3.518949000  |
|  | 8  | -0.654619000 | -2.575429000 | -2.001072000 |
|  | 6  | 0.490678000  | -2.120898000 | -2.332852000 |
|  | 8  | 1.121236000  | -1.179029000 | -1.766463000 |
|  | 6  | 1.157530000  | -2.805096000 | -3.516510000 |
|  | 1  | 1.871773000  | -2.134853000 | -3.998194000 |
|  | 1  | 1.700556000  | -3.684314000 | -3.151773000 |
|  | 1  | 0.411020000  | -3.149288000 | -4.235158000 |

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|--------------|----|--------------|--------------|--------------|
|              | 53 | 3.812489000  | 1.134253000  | -0.270558000 |
|              | 6  | 4.278313000  | -0.831638000 | 0.432337000  |
|              | 6  | 3.962836000  | -1.952474000 | -0.346025000 |
|              | 6  | 5.000563000  | -0.930894000 | 1.630162000  |
|              | 6  | 4.419125000  | -3.202440000 | 0.077362000  |
|              | 6  | 5.433710000  | -2.193016000 | 2.045403000  |
|              | 6  | 5.150395000  | -3.323228000 | 1.267404000  |
|              | 1  | 3.372309000  | -1.849959000 | -1.250004000 |
|              | 1  | 5.232286000  | -0.048432000 | 2.220838000  |
|              | 1  | 4.196994000  | -4.084439000 | -0.518884000 |
|              | 1  | 5.998970000  | -2.289728000 | 2.969252000  |
|              | 1  | 5.497054000  | -4.302032000 | 1.591186000  |
|              | 17 | 2.437538000  | 3.634433000  | 0.269810000  |
|              | 17 | 5.945230000  | 1.146065000  | -1.818561000 |
|              | 6  | -2.075879000 | 4.524857000  | 0.319135000  |
|              | 1  | -2.583171000 | 5.417390000  | -0.041329000 |
|              | 6  | -1.992668000 | 4.269185000  | 1.661860000  |
|              | 1  | -2.435340000 | 4.963174000  | 2.374131000  |
|              | 6  | -6.501916000 | 0.355246000  | 0.656003000  |
|              | 1  | -7.339506000 | 0.719535000  | 1.247262000  |
|              | 6  | -6.497760000 | 0.502527000  | -0.705525000 |
|              | 1  | -7.337848000 | 0.986871000  | -1.200132000 |
| <b>INT1b</b> | 6  | -5.120098000 | -0.053880000 | 2.882729000  |
|              | 6  | -0.187143000 | 1.986636000  | 3.733815000  |
|              | 6  | -3.032972000 | -1.246729000 | 2.644598000  |
|              | 6  | 0.084990000  | 1.107351000  | 1.500139000  |
|              | 6  | -4.194545000 | -0.616543000 | 0.725730000  |
|              | 6  | -1.104282000 | 3.243884000  | 1.866837000  |
|              | 1  | -1.245958000 | 3.847952000  | 3.948107000  |
|              | 1  | -3.908666000 | -0.721274000 | 4.543634000  |
|              | 1  | 0.855215000  | 0.137680000  | 3.263797000  |
|              | 6  | -0.780784000 | 2.362291000  | -0.404654000 |
|              | 6  | -5.311859000 | -0.061257000 | -1.392721000 |
|              | 6  | -3.149571000 | -1.286076000 | -1.374293000 |
|              | 6  | -1.556970000 | 3.507197000  | -2.379115000 |
|              | 6  | -0.362019000 | 1.411536000  | -2.492752000 |
|              | 6  | -4.265368000 | -0.766327000 | -3.466124000 |
|              | 1  | -6.130762000 | 0.306697000  | -3.371018000 |
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|              | 1  | -1.070887000 | 2.485115000  | -4.220799000 |
|              | 6  | -0.880728000 | 3.090611000  | 3.257582000  |
|              | 6  | -4.022403000 | -0.671433000 | 3.464579000  |
|              | 6  | 0.307064000  | 0.983379000  | 2.858606000  |
|              | 7  | -3.116785000 | -1.216994000 | 1.314801000  |

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|  | 6  | -0.606623000 | 2.236877000  | 1.002898000  |
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|  | 1  | -0.010171000 | 1.882937000  | 4.802569000  |
|  | 1  | -2.162489000 | -1.741327000 | 3.065382000  |
|  | 6  | -4.220945000 | -0.645677000 | -0.699221000 |
|  | 6  | -1.449731000 | 3.468771000  | -0.971025000 |
|  | 7  | -0.258391000 | 1.357623000  | -1.165922000 |
|  | 6  | -5.309828000 | -0.131713000 | -2.807326000 |
|  | 6  | -3.181765000 | -1.349062000 | -2.757817000 |
|  | 6  | -1.011231000 | 2.480920000  | -3.136353000 |
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|  | 1  | 0.080102000  | 0.591229000  | -3.050110000 |
|  | 1  | -4.273632000 | -0.823967000 | -4.553051000 |
|  | 46 | -1.782991000 | -2.031674000 | -0.098254000 |
|  | 46 | 0.568086000  | -0.175724000 | 0.010216000  |
|  | 6  | 0.719941000  | -2.590336000 | 1.759011000  |
|  | 8  | 1.363709000  | -1.553986000 | 1.361988000  |
|  | 8  | -0.450856000 | -2.916853000 | 1.422249000  |
|  | 6  | 1.452885000  | -3.467654000 | 2.758528000  |
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|  | 1  | 2.530611000  | -3.422292000 | 2.594621000  |
|  | 1  | 1.245154000  | -3.095166000 | 3.768012000  |
|  | 8  | -0.672901000 | -2.909312000 | -1.656030000 |
|  | 6  | 0.440959000  | -2.482215000 | -2.110357000 |
|  | 8  | 1.057085000  | -1.442127000 | -1.730529000 |
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|  | 1  | 1.579271000  | -2.671268000 | -3.932410000 |
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|  | 53 | 3.262798000  | 1.057283000  | -0.205760000 |
|  | 6  | 4.224932000  | -0.844632000 | 0.138475000  |
|  | 6  | 4.369249000  | -1.741807000 | -0.924831000 |
|  | 6  | 4.709771000  | -1.136344000 | 1.418369000  |
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|  | 6  | 5.509737000  | -3.267869000 | 0.579410000  |
|  | 1  | 3.982102000  | -1.504013000 | -1.911034000 |
|  | 1  | 4.590233000  | -0.430300000 | 2.235912000  |
|  | 1  | 5.135029000  | -3.668457000 | -1.512464000 |
|  | 1  | 5.741542000  | -2.595098000 | 2.622395000  |
|  | 1  | 6.015156000  | -4.215561000 | 0.751286000  |
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|  | 17 | 5.642722000  | 1.973089000  | -0.624677000 |

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|              | 6 | -1.796432000 | 4.363775000  | 1.278460000  |
|              | 1 | -2.186302000 | 5.137457000  | 1.937236000  |
|              | 6 | -6.323975000 | 0.583383000  | 0.750050000  |
|              | 1 | -7.127147000 | 1.053368000  | 1.313784000  |
|              | 6 | -6.359046000 | 0.559196000  | -0.618754000 |
|              | 1 | -7.195804000 | 1.012793000  | -1.146933000 |
| <b>INT2b</b> | 6 | -4.592944000 | 0.364041000  | 2.563395000  |
|              | 6 | -0.224500000 | 2.202178000  | 3.630356000  |
|              | 6 | -2.492026000 | -0.825798000 | 2.684411000  |
|              | 6 | 0.044208000  | 1.226276000  | 1.445722000  |
|              | 6 | -3.498582000 | -0.504181000 | 0.599284000  |
|              | 6 | -1.447030000 | 3.162901000  | 1.763251000  |
|              | 1 | -1.566417000 | 3.873467000  | 3.811014000  |
|              | 1 | -3.525249000 | -0.037346000 | 4.399706000  |
|              | 1 | 1.090419000  | 0.528643000  | 3.200298000  |
|              | 6 | -1.096953000 | 2.204505000  | -0.473879000 |
|              | 6 | -4.465000000 | -0.339155000 | -1.657008000 |
|              | 6 | -2.339706000 | -1.522718000 | -1.288870000 |
|              | 6 | -2.109980000 | 3.112878000  | -2.461785000 |
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|              | 1 | -5.149789000 | -0.361777000 | -3.716774000 |
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|              | 6 | -3.548788000 | -0.148660000 | 3.319751000  |
|              | 6 | 0.376733000  | 1.232478000  | 2.784047000  |
|              | 7 | -2.472868000 | -0.978972000 | 1.361862000  |
|              | 6 | -0.844365000 | 2.190790000  | 0.925786000  |
|              | 6 | -4.592823000 | 0.189632000  | 1.161229000  |
|              | 1 | -5.414477000 | 0.891151000  | 3.044683000  |
|              | 1 | 0.034941000  | 2.203307000  | 4.687093000  |
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|              | 6 | -1.951722000 | 3.162343000  | -1.060409000 |
|              | 7 | -0.452247000 | 1.255525000  | -1.211002000 |
|              | 6 | -4.370932000 | -0.681278000 | -3.027878000 |
|              | 6 | -2.274528000 | -1.888224000 | -2.614428000 |
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|              | 1 | -3.247726000 | -1.713574000 | -4.537636000 |

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|           | 8  | 0.224935000  | -3.055623000 | -1.036475000 |
|           | 6  | 1.142116000  | -2.483261000 | -1.733376000 |
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|           | 6  | 4.580220000  | 0.086607000  | -0.149605000 |
|           | 6  | 4.889004000  | -0.757743000 | -1.224583000 |
|           | 6  | 5.193027000  | -0.092587000 | 1.098023000  |
|           | 6  | 5.814831000  | -1.791875000 | -1.043175000 |
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|           | 17 | 1.682402000  | 4.374288000  | -0.962995000 |
|           | 17 | -2.394682000 | -4.050615000 | 0.507920000  |
|           | 6  | -2.580391000 | 4.121898000  | -0.190469000 |
|           | 1  | -3.246536000 | 4.861974000  | -0.628786000 |
|           | 6  | -2.336493000 | 4.121672000  | 1.156419000  |
|           | 1  | -2.810957000 | 4.864918000  | 1.794302000  |
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|           | 1  | -6.465114000 | 1.199730000  | 0.684693000  |
|           | 6  | -5.559034000 | 0.399207000  | -1.077059000 |
|           | 1  | -6.353217000 | 0.749850000  | -1.733229000 |
| <b>2b</b> | 6  | -3.031448000 | -0.883336000 | 3.083277000  |
|           | 6  | -1.021441000 | 3.460436000  | 2.467771000  |
|           | 6  | -0.671703000 | -0.374972000 | 2.957204000  |
|           | 6  | -0.188399000 | 2.152804000  | 0.628231000  |
|           | 6  | -1.688528000 | -1.492240000 | 1.175797000  |
|           | 6  | -2.574224000 | 2.765084000  | 0.733941000  |

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|  | 1  | -3.122292000 | 3.926696000  | 2.484533000  |
|  | 1  | -1.920292000 | 0.129315000  | 4.636999000  |
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|  | 6  | -3.031270000 | 0.883578000  | -3.083361000 |
|  | 6  | -0.671565000 | 0.375031000  | -2.957227000 |
|  | 6  | -1.021653000 | -3.460414000 | -2.467759000 |
|  | 1  | -3.122538000 | -3.926522000 | -2.484571000 |
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|  | 6  | 0.063890000  | 2.832796000  | 1.799826000  |
|  | 7  | -0.587541000 | -0.925575000 | 1.747719000  |
|  | 6  | -1.488383000 | 2.126041000  | 0.081921000  |
|  | 6  | -2.951095000 | -1.489549000 | 1.809786000  |
|  | 1  | -3.981975000 | -0.856920000 | 3.613364000  |
|  | 1  | -0.823572000 | 3.987325000  | 3.399395000  |
|  | 1  | 0.242390000  | 0.038191000  | 3.372639000  |
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|  | 6  | -2.950910000 | 1.489773000  | -1.809861000 |
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|  | 6  | -2.311884000 | -3.427724000 | -1.957220000 |
|  | 6  | 0.063704000  | -2.832839000 | -1.799795000 |
|  | 6  | -1.891969000 | 0.335786000  | -3.655637000 |
|  | 1  | -3.981783000 | 0.857243000  | -3.613477000 |
|  | 1  | 0.242513000  | -0.038187000 | -3.372642000 |
|  | 1  | -0.823797000 | -3.987338000 | -3.399367000 |
|  | 46 | 1.130938000  | -1.207532000 | 0.594069000  |
|  | 46 | 1.131074000  | 1.207451000  | -0.594054000 |
|  | 6  | 3.068575000  | 0.891052000  | 1.658349000  |
|  | 8  | 2.754669000  | 1.613675000  | 0.642807000  |
|  | 8  | 2.477000000  | -0.162544000 | 2.015538000  |
|  | 6  | 4.262681000  | 1.364645000  | 2.463108000  |
|  | 1  | 5.138154000  | 0.782760000  | 2.154681000  |
|  | 1  | 4.464453000  | 2.422309000  | 2.287514000  |
|  | 1  | 4.092364000  | 1.174750000  | 3.525426000  |
|  | 8  | 2.754514000  | -1.613885000 | -0.642771000 |
|  | 6  | 3.068555000  | -0.891270000 | -1.658270000 |
|  | 8  | 2.477059000  | 0.162358000  | -2.015516000 |
|  | 6  | 4.262610000  | -1.364904000 | -2.463085000 |
|  | 1  | 4.090576000  | -1.178273000 | -3.525725000 |

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|           | 6  | -3.866368000 | 2.722921000  | 0.095164000  |
|           | 1  | -4.707527000 | 3.200531000  | 0.594589000  |
|           | 6  | -4.048588000 | -2.117751000 | 1.119700000  |
|           | 1  | -5.029755000 | -2.111348000 | 1.590288000  |
|           | 6  | -3.866593000 | -2.722652000 | -0.095248000 |
|           | 1  | -4.707774000 | -3.200208000 | -0.594689000 |
|           | 17 | 1.461962000  | 3.406455000  | -1.750417000 |
|           | 17 | 1.461661000  | -3.406548000 | 1.750543000  |
| <b>1c</b> | 6  | 2.678170000  | -4.075287000 | -1.377017000 |
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|           | 6  | 0.394370000  | -3.204545000 | -1.542227000 |
|           | 7  | 0.784018000  | 1.317749000  | -2.064900000 |
|           | 6  | 1.741751000  | -2.683906000 | 0.383395000  |
|           | 6  | 3.065616000  | 2.103370000  | -2.404495000 |
|           | 1  | 3.985092000  | 1.458937000  | -4.263720000 |
|           | 1  | 1.359545000  | -4.451514000 | -3.026768000 |
|           | 1  | -0.066629000 | 0.144001000  | -3.529516000 |
|           | 6  | 1.744668000  | 2.682156000  | -0.383157000 |
|           | 6  | 3.062675000  | -2.106684000 | 2.405203000  |
|           | 7  | 0.781921000  | -1.318852000 | 2.065074000  |
|           | 6  | 2.681850000  | 4.073021000  | 1.377254000  |
|           | 6  | 0.397220000  | 3.204343000  | 1.542013000  |
|           | 6  | 1.969399000  | -0.720369000 | 4.059747000  |
|           | 1  | 3.982197000  | -1.463484000 | 4.264831000  |
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|           | 6  | 1.478485000  | -3.956014000 | -2.064394000 |
|           | 6  | 0.828881000  | 0.685916000  | -3.237233000 |
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|           | 6  | 2.838834000  | 3.431309000  | 0.125024000  |
|           | 6  | 0.511444000  | 2.562727000  | 0.316534000  |
|           | 6  | 3.088321000  | -1.427367000 | 3.644149000  |
|           | 6  | 0.827043000  | -0.687249000 | 3.237524000  |

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|     | 6  | 1.481871000  | 3.954948000  | 2.064323000  |
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|     | 1  | -0.521840000 | 3.147359000  | 2.118555000  |
|     | 1  | 1.956355000  | -0.189351000 | 5.007691000  |
|     | 46 | -0.822467000 | -1.429634000 | 0.687041000  |
|     | 46 | -0.820631000 | 1.430279000  | -0.687320000 |
|     | 6  | -4.194954000 | 2.760325000  | 1.850523000  |
|     | 6  | -3.171702000 | 2.844305000  | 0.716955000  |
|     | 7  | -2.349268000 | 1.720748000  | 0.728393000  |
|     | 6  | -2.712933000 | 0.876796000  | 1.723563000  |
|     | 6  | -3.869039000 | 1.433360000  | 2.544159000  |
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|     | 6  | -2.713386000 | -0.874180000 | -1.724352000 |
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|     | 1  | 4.881665000  | -4.081244000 | 0.268115000  |
|     | 6  | 4.156763000  | -2.873983000 | 1.868448000  |
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|     | 1  | 4.885818000  | 4.076664000  | -0.267269000 |
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| NCS | 6  | -1.892957000 | -0.770159000 | 0.000127000  |
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|             | 6  | 0.602087000  | 1.631599000  | 2.516755000  |
|             | 7  | 3.296909000  | -0.522406000 | 1.375974000  |
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|             | 6  | 4.973243000  | 1.241849000  | 1.450632000  |
|             | 1  | 5.745617000  | 1.678032000  | 3.433020000  |
|             | 1  | 1.344638000  | 3.082731000  | 3.935176000  |
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|             | 6  | 1.230975000  | 3.606634000  | 0.560130000  |
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|  | 8  | 2.972254000  | -3.992107000 | -2.163330000 |
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| <b>INT1c</b> | 6  | 2.962333000  | -3.148805000 | 1.001273000  |
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|              | 6  | 1.630431000  | -1.203435000 | 1.581768000  |
|              | 6  | 3.055239000  | -0.964769000 | -2.723783000 |
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|    | 6 | 2.413322000  | -1.558134000 | 0.131921000  |
|    | 6 | 2.399262000  | 1.931551000  | -2.508746000 |
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|    | 1 | 3.009596000  | -2.252414000 | -3.586400000 |
|    | 1 | -1.186331000 | 0.637965000  | -3.460143000 |
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|  | 1  | 4.982042000  | -1.939118000 | -2.074324000 |
|  | 1  | 0.515147000  | 1.030756000  | -5.211092000 |
|  | 1  | 0.701009000  | -2.105984000 | -2.636801000 |
|  | 6  | 2.092720000  | -1.362442000 | 1.503128000  |
|  | 6  | 2.936579000  | 2.520391000  | 0.246597000  |
|  | 7  | 0.694342000  | 1.722951000  | 0.735714000  |
|  | 6  | 2.761807000  | -1.080032000 | 3.818745000  |
|  | 6  | 0.390508000  | -1.256843000 | 3.215776000  |
|  | 6  | 2.045697000  | 2.602361000  | 2.493464000  |
|  | 1  | 4.027164000  | 3.265416000  | 1.970136000  |
|  | 1  | 0.005518000  | 1.855490000  | 2.676898000  |
|  | 1  | 1.144527000  | -1.008520000 | 5.228163000  |
|  | 46 | -0.478168000 | -1.643025000 | 0.266073000  |
|  | 46 | -1.022506000 | 0.987529000  | -0.186778000 |
|  | 17 | -0.282095000 | -4.093509000 | 0.823174000  |
|  | 6  | -1.432317000 | 4.062363000  | -0.627550000 |
|  | 8  | -0.270077000 | 4.337658000  | -0.302251000 |
|  | 6  | -2.433235000 | 5.172510000  | -0.974593000 |
|  | 1  | -1.895899000 | 6.094989000  | -1.205821000 |
|  | 1  | -3.071032000 | 4.883223000  | -1.813514000 |
|  | 1  | -3.078414000 | 5.343709000  | -0.106144000 |
|  | 8  | -1.967504000 | 2.878659000  | -0.706474000 |
|  | 6  | -4.099032000 | 0.944266000  | 3.181546000  |
|  | 6  | -2.973583000 | 1.650152000  | 2.416805000  |
|  | 7  | -2.257500000 | 0.716899000  | 1.652834000  |
|  | 6  | -2.723634000 | -0.510122000 | 1.892981000  |
|  | 6  | -3.913388000 | -0.538280000 | 2.835518000  |
|  | 1  | -4.004321000 | 1.160756000  | 4.249178000  |
|  | 1  | -4.769483000 | -0.986700000 | 2.322227000  |
|  | 8  | -2.239961000 | -1.581769000 | 1.416175000  |
|  | 8  | -2.713704000 | 2.842242000  | 2.481478000  |
|  | 1  | -3.683396000 | -1.171329000 | 3.697882000  |
|  | 1  | -5.058972000 | 1.349733000  | 2.848074000  |
|  | 6  | -3.857892000 | -1.373136000 | -2.630395000 |
|  | 6  | -2.713690000 | -0.931194000 | -1.735866000 |

|                   |   |              |              |              |
|-------------------|---|--------------|--------------|--------------|
|                   | 7 | -1.779259000 | -1.865527000 | -1.552874000 |
|                   | 6 | -2.067241000 | -2.973614000 | -2.366054000 |
|                   | 6 | -3.435207000 | -2.790807000 | -3.032873000 |
|                   | 1 | -4.794345000 | -1.329006000 | -2.065965000 |
|                   | 1 | -3.337742000 | -2.932243000 | -4.112466000 |
|                   | 8 | -1.315656000 | -3.919121000 | -2.546030000 |
|                   | 8 | -2.678235000 | 0.240942000  | -1.251281000 |
|                   | 1 | -4.112335000 | -3.564918000 | -2.658887000 |
|                   | 1 | -3.953004000 | -0.682123000 | -3.473428000 |
|                   | 6 | 4.794065000  | -1.459158000 | 0.670144000  |
|                   | 1 | 5.830193000  | -1.499418000 | 0.339950000  |
|                   | 6 | 4.494156000  | -1.264014000 | 1.991676000  |
|                   | 1 | 5.296032000  | -1.147820000 | 2.718743000  |
|                   | 6 | 3.929365000  | 2.746742000  | -0.772518000 |
|                   | 1 | 4.890727000  | 3.162385000  | -0.477014000 |
|                   | 6 | 3.671396000  | 2.463413000  | -2.086865000 |
|                   | 1 | 4.431330000  | 2.653294000  | -2.842866000 |
| Succinimide...OAc | 6 | -2.946949000 | -0.730860000 | 0.233602000  |
|                   | 6 | -1.513190000 | -1.149389000 | -0.090754000 |
|                   | 7 | -0.746639000 | -0.012938000 | -0.265398000 |
|                   | 6 | -1.463722000 | 1.157306000  | -0.104167000 |
|                   | 6 | -2.915595000 | 0.804300000  | 0.218069000  |
|                   | 1 | -3.620517000 | -1.163360000 | -0.512040000 |
|                   | 1 | -3.183693000 | 1.256719000  | 1.177369000  |
|                   | 8 | -1.003745000 | 2.289715000  | -0.209249000 |
|                   | 8 | -1.103012000 | -2.301744000 | -0.185625000 |
|                   | 1 | -3.564858000 | 1.247156000  | -0.543018000 |
|                   | 1 | -3.224171000 | -1.151358000 | 1.204874000  |
|                   | 1 | 0.315810000  | -0.036562000 | -0.456746000 |
|                   | 8 | 1.865194000  | -0.064963000 | -0.850199000 |
|                   | 8 | 2.349856000  | 0.003583000  | 1.359262000  |
|                   | 6 | 2.677251000  | -0.019618000 | 0.145220000  |
|                   | 6 | 4.168512000  | 0.013631000  | -0.223516000 |
|                   | 1 | 4.382036000  | 0.911427000  | -0.815003000 |
|                   | 1 | 4.799627000  | 0.011176000  | 0.668736000  |
|                   | 1 | 4.418056000  | -0.849582000 | -0.850617000 |
| succinimide       | 6 | 0.769611000  | -1.260304000 | -0.000317000 |
|                   | 6 | 1.169766000  | 0.210683000  | -0.000217000 |
|                   | 7 | 0.000000000  | 0.962507000  | -0.000049000 |
|                   | 6 | -1.169765000 | 0.210683000  | 0.000092000  |
|                   | 6 | -0.769610000 | -1.260305000 | 0.000297000  |
|                   | 1 | 1.203666000  | -1.741587000 | -0.881429000 |
|                   | 1 | -1.203649000 | -1.741507000 | 0.881463000  |
|                   | 8 | -2.297782000 | 0.677522000  | 0.000031000  |

|  |   |              |              |              |
|--|---|--------------|--------------|--------------|
|  | 8 | 2.297782000  | 0.677523000  | 0.000095000  |
|  | 1 | -1.204522000 | -1.742226000 | -0.880028000 |
|  | 1 | 1.204508000  | -1.742146000 | 0.880062000  |
|  | 1 | -0.000001000 | 1.985015000  | 0.000129000  |

**Table S1-6.** Some optimized Cartesian Coordinates of stationary points for the oxidative process (Pd<sup>II</sup> to Pd<sup>IV</sup>), involved in the discussion on PhI(OAc)<sub>2</sub> (**OX-a**), PhICl<sub>2</sub> (**OX-b**) and NCS (**OX-c**) as oxidant, computed at B3LYP-IDSCRF/DGDZVP level in dichloromethane with bond lengths in Å.

| Species   | Cartesian coordinates |              |              |              |
|-----------|-----------------------|--------------|--------------|--------------|
| <b>1m</b> | 6                     | -4.119534000 | -2.664667000 | -0.936169000 |
|           | 6                     | -2.897281000 | -3.341460000 | -0.997173000 |
|           | 6                     | -1.745827000 | -2.642590000 | -0.643214000 |
|           | 7                     | -1.753591000 | -1.361419000 | -0.237234000 |
|           | 6                     | -2.934803000 | -0.684564000 | -0.192606000 |
|           | 6                     | -4.134977000 | -1.330581000 | -0.537926000 |
|           | 1                     | -5.046161000 | -3.166160000 | -1.208017000 |
|           | 1                     | -2.829973000 | -4.378588000 | -1.314333000 |
|           | 1                     | -0.774916000 | -3.127436000 | -0.696322000 |
|           | 1                     | -5.074259000 | -0.787291000 | -0.512665000 |
|           | 6                     | -2.833887000 | 0.728995000  | 0.218582000  |
|           | 6                     | -3.978883000 | 1.483130000  | 0.544722000  |
|           | 6                     | -1.532130000 | 1.298527000  | 0.316680000  |
|           | 6                     | -3.859881000 | 2.797636000  | 0.996304000  |
|           | 6                     | -1.445703000 | 2.613223000  | 0.804747000  |
|           | 6                     | -2.585151000 | 3.358494000  | 1.138652000  |
|           | 1                     | -4.971495000 | 1.044339000  | 0.470058000  |
|           | 1                     | -4.749086000 | 3.370180000  | 1.252198000  |
|           | 1                     | -0.473128000 | 3.075122000  | 0.946630000  |
|           | 1                     | -2.475648000 | 4.374268000  | 1.516669000  |
|           | 46                    | -0.000004000 | -0.024589000 | -0.000138000 |
|           | 6                     | 4.119296000  | -2.664848000 | 0.936463000  |
|           | 6                     | 2.897022000  | -3.341624000 | 0.997192000  |
|           | 6                     | 1.745649000  | -2.642722000 | 0.643026000  |
|           | 7                     | 1.753509000  | -1.361534000 | 0.237104000  |
|           | 6                     | 2.934746000  | -0.684699000 | 0.192730000  |
|           | 6                     | 4.134839000  | -1.330748000 | 0.538266000  |
|           | 1                     | 5.045861000  | -3.166363000 | 1.208483000  |
|           | 1                     | 2.829631000  | -4.378764000 | 1.314293000  |
|           | 1                     | 0.774725000  | -3.127565000 | 0.695903000  |
|           | 1                     | 5.074135000  | -0.787473000 | 0.513208000  |
|           | 6                     | 2.833944000  | 0.728866000  | -0.218460000 |
|           | 6                     | 1.532222000  | 1.298428000  | -0.316790000 |
|           | 6                     | 3.979015000  | 1.482974000  | -0.544404000 |
|           | 6                     | 1.445902000  | 2.613111000  | -0.804917000 |

|               |    |              |              |              |
|---------------|----|--------------|--------------|--------------|
|               | 6  | 3.860118000  | 2.797472000  | -0.996035000 |
|               | 6  | 2.585424000  | 3.358349000  | -1.138640000 |
|               | 1  | 4.971606000  | 1.044167000  | -0.469549000 |
|               | 1  | 0.473357000  | 3.075016000  | -0.946988000 |
|               | 1  | 4.749380000  | 3.369996000  | -1.251773000 |
|               | 1  | 2.476012000  | 4.374111000  | -1.516715000 |
| <b>TS1m-a</b> | 6  | 0.143592000  | -2.827730000 | 0.964576000  |
|               | 6  | -0.511138000 | -4.067477000 | 0.864398000  |
|               | 6  | -0.219593000 | -4.921050000 | -0.197057000 |
|               | 6  | 0.714786000  | -4.522815000 | -1.158818000 |
|               | 6  | 1.324582000  | -3.280163000 | -1.002565000 |
|               | 7  | 1.062711000  | -2.465941000 | 0.031736000  |
|               | 1  | -1.253749000 | -4.357836000 | 1.600750000  |
|               | 1  | 0.961712000  | -5.148992000 | -2.011853000 |
|               | 1  | 2.035706000  | -2.909126000 | -1.736625000 |
|               | 6  | 0.325545000  | 0.382553000  | 2.918917000  |
|               | 6  | -0.478147000 | 0.090263000  | 4.031054000  |
|               | 6  | -1.103008000 | -1.157166000 | 4.140011000  |
|               | 6  | -0.907296000 | -2.109977000 | 3.140048000  |
|               | 6  | -0.097816000 | -1.826793000 | 2.022123000  |
|               | 6  | 0.523953000  | -0.554060000 | 1.896256000  |
|               | 1  | 0.808216000  | 1.353575000  | 2.872422000  |
|               | 1  | -0.608032000 | 0.836798000  | 4.813541000  |
|               | 1  | -1.384391000 | -3.082031000 | 3.242912000  |
|               | 46 | 1.808543000  | -0.416051000 | 0.284713000  |
|               | 6  | 2.388989000  | 1.524595000  | 0.494015000  |
|               | 6  | 1.530025000  | 2.601216000  | 0.746597000  |
|               | 6  | 3.748298000  | 1.802070000  | 0.191696000  |
|               | 6  | 1.999064000  | 3.921650000  | 0.758937000  |
|               | 1  | 0.473358000  | 2.420913000  | 0.923204000  |
|               | 6  | 4.215477000  | 3.131726000  | 0.217131000  |
|               | 6  | 3.350515000  | 4.187414000  | 0.507192000  |
|               | 1  | 1.308488000  | 4.740151000  | 0.957166000  |
|               | 1  | 5.254652000  | 3.355447000  | -0.013433000 |
|               | 1  | 3.723147000  | 5.209613000  | 0.515851000  |
|               | 6  | 4.701262000  | -1.577924000 | -0.787829000 |
|               | 6  | 6.085881000  | -1.558350000 | -0.946038000 |
|               | 6  | 6.755459000  | -0.353471000 | -0.709738000 |
|               | 6  | 6.020764000  | 0.768089000  | -0.331532000 |
|               | 6  | 4.624206000  | 0.677555000  | -0.197431000 |
|               | 7  | 3.985835000  | -0.499464000 | -0.432596000 |
|               | 1  | 4.141971000  | -2.495863000 | -0.952420000 |
|               | 1  | 6.615472000  | -2.460443000 | -1.240596000 |
|               | 1  | 7.836943000  | -0.290520000 | -0.811896000 |

|         |    |              |              |              |
|---------|----|--------------|--------------|--------------|
|         | 1  | 6.532073000  | 1.704181000  | -0.129670000 |
|         | 1  | -0.725630000 | -5.880628000 | -0.280735000 |
|         | 1  | -1.727865000 | -1.389595000 | 4.999747000  |
|         | 8  | -0.129630000 | 0.150387000  | -1.245757000 |
|         | 6  | 0.369364000  | 0.244947000  | -2.464480000 |
|         | 8  | 1.550905000  | -0.042272000 | -2.701026000 |
|         | 6  | -0.550436000 | 0.729645000  | -3.575889000 |
|         | 1  | -1.336808000 | -0.006853000 | -3.769529000 |
|         | 1  | 0.028982000  | 0.878286000  | -4.489040000 |
|         | 1  | -1.036545000 | 1.668308000  | -3.294048000 |
|         | 6  | -2.797267000 | 2.030616000  | -0.312276000 |
|         | 6  | -2.496520000 | 2.465803000  | 0.983881000  |
|         | 6  | -3.218313000 | 2.917338000  | -1.310971000 |
|         | 6  | -2.620217000 | 3.827877000  | 1.279089000  |
|         | 6  | -3.333735000 | 4.275661000  | -0.997069000 |
|         | 6  | -3.035883000 | 4.730937000  | 0.293191000  |
|         | 1  | -2.175936000 | 1.764820000  | 1.749128000  |
|         | 1  | -3.461789000 | 2.565067000  | -2.309784000 |
|         | 1  | -2.391402000 | 4.178732000  | 2.283093000  |
|         | 1  | -3.660527000 | 4.974646000  | -1.763852000 |
|         | 1  | -3.129692000 | 5.788434000  | 0.530321000  |
|         | 1  | -7.064650000 | -1.285494000 | 1.005974000  |
|         | 1  | -7.044701000 | -2.695443000 | -0.097756000 |
|         | 1  | -7.464947000 | -1.066879000 | -0.699533000 |
|         | 8  | -5.003685000 | -0.120240000 | -0.144314000 |
|         | 6  | -5.363104000 | -1.358505000 | -0.326359000 |
|         | 8  | -4.609126000 | -2.262045000 | -0.730140000 |
|         | 6  | -6.831962000 | -1.629121000 | -0.005875000 |
|         | 53 | -2.637708000 | -0.031544000 | -0.761610000 |
| INT1m-a | 6  | 2.860402000  | -0.537642000 | -0.199458000 |
|         | 6  | 4.238593000  | -0.688224000 | 0.031061000  |
|         | 6  | 4.900958000  | 0.205379000  | 0.870333000  |
|         | 6  | 4.183744000  | 1.243814000  | 1.474177000  |
|         | 6  | 2.820541000  | 1.340277000  | 1.204101000  |
|         | 7  | 2.183538000  | 0.478406000  | 0.396527000  |
|         | 1  | 4.791463000  | -1.494483000 | -0.440444000 |
|         | 1  | 4.662741000  | 1.961817000  | 2.134279000  |
|         | 1  | 2.205556000  | 2.125482000  | 1.638327000  |
|         | 6  | -0.125946000 | -1.960835000 | -2.012296000 |
|         | 6  | 0.441426000  | -3.048881000 | -2.691513000 |
|         | 6  | 1.807253000  | -3.324448000 | -2.561694000 |
|         | 6  | 2.600159000  | -2.510740000 | -1.752251000 |
|         | 6  | 2.042334000  | -1.414683000 | -1.063881000 |
|         | 6  | 0.656297000  | -1.133149000 | -1.200195000 |

|             |    |              |              |              |
|-------------|----|--------------|--------------|--------------|
|             | 1  | -1.187809000 | -1.766156000 | -2.129713000 |
|             | 1  | -0.185701000 | -3.678315000 | -3.321110000 |
|             | 1  | 3.660089000  | -2.737002000 | -1.662289000 |
|             | 46 | 0.048715000  | 0.521916000  | -0.127811000 |
|             | 6  | -1.894884000 | 0.353769000  | -0.701944000 |
|             | 6  | -2.404811000 | 0.947346000  | -1.858095000 |
|             | 6  | -2.751620000 | -0.363404000 | 0.164016000  |
|             | 6  | -3.765736000 | 0.826743000  | -2.173551000 |
|             | 1  | -1.745034000 | 1.508273000  | -2.515798000 |
|             | 6  | -4.118408000 | -0.475061000 | -0.163555000 |
|             | 6  | -4.622113000 | 0.113212000  | -1.324475000 |
|             | 1  | -4.155370000 | 1.289541000  | -3.078969000 |
|             | 1  | -4.800381000 | -1.018981000 | 0.486183000  |
|             | 1  | -5.678865000 | 0.018228000  | -1.564861000 |
|             | 6  | -0.219514000 | -1.243921000 | 2.644942000  |
|             | 6  | -0.873517000 | -2.011195000 | 3.607803000  |
|             | 6  | -2.239318000 | -2.258069000 | 3.431272000  |
|             | 6  | -2.891705000 | -1.736500000 | 2.316072000  |
|             | 6  | -2.173032000 | -0.968738000 | 1.382465000  |
|             | 7  | -0.850507000 | -0.742040000 | 1.576311000  |
|             | 1  | 0.842536000  | -1.020865000 | 2.726825000  |
|             | 1  | -0.326813000 | -2.399254000 | 4.463076000  |
|             | 1  | -2.790972000 | -2.853279000 | 4.156066000  |
|             | 1  | -3.950893000 | -1.926713000 | 2.173051000  |
|             | 1  | 5.967999000  | 0.093054000  | 1.051336000  |
|             | 1  | 2.252249000  | -4.166777000 | -3.087084000 |
|             | 8  | 0.359117000  | 2.760484000  | -1.294564000 |
|             | 6  | -0.035099000 | 3.255596000  | -0.200206000 |
|             | 8  | -0.331407000 | 2.525495000  | 0.813308000  |
|             | 6  | -0.198658000 | 4.759928000  | -0.061075000 |
|             | 1  | 0.410506000  | 5.288500000  | -0.797679000 |
|             | 1  | 0.060935000  | 5.085712000  | 0.949623000  |
|             | 1  | -1.250105000 | 5.017257000  | -0.233666000 |
| <b>2m-a</b> | 6  | -2.646024000 | 0.180794000  | -0.849084000 |
|             | 6  | -3.938627000 | 0.606334000  | -1.186759000 |
|             | 6  | -4.486105000 | 1.716051000  | -0.544873000 |
|             | 6  | -3.734112000 | 2.390049000  | 0.421271000  |
|             | 6  | -2.448674000 | 1.927022000  | 0.698054000  |
|             | 7  | -1.925339000 | 0.860504000  | 0.077276000  |
|             | 1  | -4.519345000 | 0.071713000  | -1.931679000 |
|             | 1  | -4.124346000 | 3.257022000  | 0.947306000  |
|             | 1  | -1.805710000 | 2.423691000  | 1.416322000  |
|             | 6  | -0.041049000 | -2.492161000 | -1.416698000 |
|             | 6  | -0.658206000 | -3.293995000 | -2.389979000 |

|  |    |              |              |              |
|--|----|--------------|--------------|--------------|
|  | 6  | -1.919263000 | -2.950686000 | -2.885858000 |
|  | 6  | -2.570513000 | -1.814952000 | -2.402331000 |
|  | 6  | -1.973311000 | -1.001492000 | -1.421131000 |
|  | 6  | -0.692997000 | -1.357129000 | -0.945440000 |
|  | 1  | 0.938327000  | -2.772058000 | -1.043188000 |
|  | 1  | -0.146476000 | -4.182361000 | -2.755635000 |
|  | 1  | -3.555936000 | -1.569299000 | -2.790394000 |
|  | 46 | 0.072809000  | -0.034459000 | 0.429018000  |
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|  | 6  | 2.286590000  | -1.865298000 | 1.445796000  |
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|  | 6  | 3.592896000  | -2.377316000 | 1.403218000  |
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|  | 6  | 4.501977000  | -1.925855000 | 0.437255000  |
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|  | 1  | 5.512680000  | -2.326638000 | 0.409550000  |
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|  | 6  | 1.119907000  | 2.544244000  | -2.950722000 |
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|  | 7  | 1.015311000  | 0.963848000  | -1.163463000 |
|  | 1  | -0.584036000 | 2.173595000  | -1.668621000 |
|  | 1  | 0.616728000  | 3.306031000  | -3.539372000 |
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|  | 1  | 4.078241000  | 0.916912000  | -2.571058000 |
|  | 8  | 0.472271000  | 3.298909000  | 0.843621000  |
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|  | 8  | 0.824958000  | 1.351878000  | 1.949802000  |
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|  | 8  | -0.486543000 | -1.196487000 | 2.042443000  |
|  | 6  | -1.661769000 | -2.440582000 | 3.649757000  |
|  | 1  | -2.680006000 | -2.715388000 | 3.931791000  |
|  | 1  | -1.202676000 | -1.840361000 | 4.440341000  |
|  | 1  | 1.560767000  | 4.423709000  | 2.858592000  |
|  | 1  | 2.666364000  | 3.030187000  | 2.997257000  |
|  | 1  | -1.060406000 | -3.348492000 | 3.534326000  |
|  | 1  | 1.166477000  | 3.039356000  | 3.922117000  |
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| COM1m-b | 6  | -0.143674000 | 3.932261000  | -3.034682000 |
|         | 6  | -0.394736000 | 2.680934000  | -3.605850000 |
|         | 6  | -0.902749000 | 1.677856000  | -2.784142000 |
|         | 7  | -1.174554000 | 1.859894000  | -1.480813000 |
|         | 6  | -0.914393000 | 3.066651000  | -0.906167000 |
|         | 6  | -0.397894000 | 4.121439000  | -1.678683000 |
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|         | 1  | -0.181244000 | 5.080008000  | -1.219041000 |
|         | 6  | -1.201268000 | 3.148505000  | 0.538593000  |
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|         | 6  | -1.535886000 | 4.450346000  | 2.570786000  |
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|         | 6  | -1.899175000 | 3.278526000  | 3.244080000  |
|         | 1  | -0.949795000 | 5.302577000  | 0.696222000  |
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|         | 1  | -2.202205000 | 1.165579000  | 3.122223000  |
|         | 1  | -2.192142000 | 3.320148000  | 4.291983000  |
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|         | 1  | -0.685824000 | -2.271927000 | 4.481808000  |
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|         | 6  | 4.394217000  | -1.944032000 | 0.282652000  |

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|               | 6  | 6.583376000  | -1.244144000 | -0.502040000 |
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|               | 17 | 2.370194000  | 0.735711000  | 2.396193000  |
| <b>TS1m-b</b> | 6  | -0.302982000 | 4.388450000  | -2.441111000 |
|               | 6  | -0.188597000 | 3.217201000  | -3.197952000 |
|               | 6  | -0.372862000 | 1.998652000  | -2.549518000 |
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|               | 1  | -0.164079000 | 5.362381000  | -2.905071000 |
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|               | 1  | -0.281276000 | 1.054408000  | -3.080106000 |
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|               | 7  | -2.937938000 | -0.786263000 | -1.243013000 |
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|         | 53 | 1.923679000  | -0.024480000 | 0.402843000  |
|         | 6  | 3.647543000  | -0.957540000 | -0.503942000 |
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|         | 1  | 3.411528000  | -0.529965000 | 4.885138000  |
|         | 1  | 1.120181000  | 1.962257000  | 2.226996000  |
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|             | 1  | 5.381093000  | 0.139307000  | -2.456026000 |
|             | 1  | 3.374708000  | -0.912565000 | -1.422605000 |
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|             | 53 | -1.575707000 | -0.938810000 | 1.023130000  |
|             | 6  | -3.183396000 | -1.116026000 | -0.381393000 |
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|             | 1  | -2.390716000 | -2.936083000 | -1.262518000 |
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|             | 17 | -0.370998000 | -0.080807000 | -2.601428000 |
|             | 17 | -4.236491000 | 2.553720000  | 2.041331000  |
| <b>2m-b</b> | 6  | -4.852265000 | -0.893375000 | -0.202856000 |
|             | 6  | -4.136405000 | -1.719169000 | -1.075364000 |
|             | 6  | -2.762522000 | -1.517473000 | -1.195745000 |
|             | 7  | -2.120071000 | -0.568317000 | -0.499419000 |
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|             | 1  | -4.624614000 | -2.498396000 | -1.653631000 |
|             | 1  | -2.141539000 | -2.116594000 | -1.857431000 |
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|        | 6  | 0.218146000  | 2.323787000  | 1.295139000  |
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|        | 1  | -2.100386000 | 3.790506000  | 3.330118000  |
|        | 1  | 1.267070000  | 2.407049000  | 1.031567000  |
|        | 1  | 0.313090000  | 3.946889000  | 2.713541000  |
|        | 46 | 0.028779000  | -0.035744000 | -0.678721000 |
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|        | 6  | 0.449452000  | -2.907447000 | 2.608156000  |
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|        | 7  | 0.704829000  | -1.243722000 | 0.913020000  |
|        | 6  | 2.035410000  | -1.135858000 | 1.174082000  |
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|        | 1  | 2.254559000  | -3.430392000 | 3.681167000  |
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|        | 1  | 3.670631000  | -1.849671000 | 2.391472000  |
|        | 6  | 2.748757000  | -0.173060000 | 0.331738000  |
|        | 6  | 2.001571000  | 0.505554000  | -0.654132000 |
|        | 6  | 4.125195000  | 0.099644000  | 0.449521000  |
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|        | 6  | 3.976036000  | 1.682166000  | -1.374169000 |
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|        | 1  | 2.021703000  | 1.935158000  | -2.265920000 |
|        | 1  | 5.797509000  | 1.229643000  | -0.300710000 |
|        | 1  | 4.449097000  | 2.401935000  | -2.039204000 |
|        | 17 | -0.593536000 | 1.504604000  | -2.384190000 |
|        | 17 | 0.577647000  | -1.923677000 | -2.260652000 |
| TS1m-c | 6  | 0.420043000  | 4.871865000  | -0.738644000 |
|        | 6  | 0.154222000  | 4.125999000  | -1.891481000 |
|        | 6  | -0.183618000 | 2.783541000  | -1.739526000 |
|        | 7  | -0.267602000 | 2.193352000  | -0.536963000 |
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|        | 6  | 0.344725000  | 4.255572000  | 0.508832000  |
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|        | 1  | 0.212960000  | 4.564648000  | -2.883718000 |
|        | 1  | -0.388732000 | 2.152721000  | -2.602577000 |
|        | 1  | 0.566131000  | 4.824026000  | 1.406634000  |
|        | 6  | -0.095167000 | 2.124486000  | 1.845067000  |
|        | 6  | 0.018140000  | 2.724414000  | 3.114657000  |

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|      | 6  | -0.070615000 | 1.960935000  | 4.278630000  |
|      | 6  | -0.391838000 | -0.039589000 | 2.936876000  |
|      | 6  | -0.274395000 | 0.580294000  | 4.190607000  |
|      | 1  | 0.171854000  | 3.797590000  | 3.198912000  |
|      | 1  | 0.020464000  | 2.441903000  | 5.249880000  |
|      | 1  | -0.545645000 | -1.111303000 | 2.887899000  |
|      | 1  | -0.341591000 | -0.024110000 | 5.093414000  |
|      | 46 | -0.714821000 | 0.083454000  | -0.139713000 |
|      | 6  | -5.387387000 | -0.488983000 | -1.881915000 |
|      | 6  | -4.784339000 | 0.755404000  | -2.090898000 |
|      | 6  | -3.471526000 | 0.925719000  | -1.657939000 |
|      | 7  | -2.771319000 | -0.052842000 | -1.061704000 |
|      | 6  | -3.342495000 | -1.268007000 | -0.847375000 |
|      | 6  | -4.665137000 | -1.503444000 | -1.256421000 |
|      | 1  | -6.412885000 | -0.666441000 | -2.199161000 |
|      | 1  | -5.311707000 | 1.574478000  | -2.572139000 |
|      | 1  | -2.959816000 | 1.876084000  | -1.788653000 |
|      | 1  | -5.131912000 | -2.467775000 | -1.082837000 |
|      | 6  | -2.479227000 | -2.260465000 | -0.175359000 |
|      | 6  | -1.198850000 | -1.855381000 | 0.283217000  |
|      | 6  | -2.883891000 | -3.597658000 | 0.008772000  |
|      | 6  | -0.358350000 | -2.791230000 | 0.891864000  |
|      | 6  | -2.040177000 | -4.521170000 | 0.626227000  |
|      | 6  | -0.773841000 | -4.118678000 | 1.064965000  |
|      | 1  | -3.859435000 | -3.930133000 | -0.337664000 |
|      | 1  | 0.632768000  | -2.499737000 | 1.226987000  |
|      | 1  | -2.366858000 | -5.550407000 | 0.757783000  |
|      | 1  | -0.103978000 | -4.834646000 | 1.537989000  |
|      | 6  | 5.828670000  | -2.039686000 | -0.742852000 |
|      | 6  | 4.404961000  | -1.970908000 | -0.168086000 |
|      | 7  | 3.773838000  | -0.851859000 | -0.656532000 |
|      | 6  | 4.561121000  | -0.121710000 | -1.514023000 |
|      | 6  | 5.932990000  | -0.802429000 | -1.643848000 |
|      | 1  | 6.543966000  | -2.042145000 | 0.085283000  |
|      | 1  | 6.110816000  | -1.039197000 | -2.697342000 |
|      | 8  | 4.239075000  | 0.915261000  | -2.095638000 |
|      | 8  | 3.924757000  | -2.798604000 | 0.607859000  |
|      | 17 | 1.679621000  | -0.343080000 | -0.139681000 |
|      | 1  | 6.708272000  | -0.095705000 | -1.332475000 |
|      | 1  | 5.946989000  | -2.985960000 | -1.279585000 |
| 2m-c | 6  | 4.518054000  | 2.223463000  | 0.107941000  |
|      | 6  | 3.401953000  | 3.064999000  | 0.107690000  |
|      | 6  | 2.139061000  | 2.485255000  | 0.007826000  |

|  |    |              |              |              |
|--|----|--------------|--------------|--------------|
|  | 7  | 1.962962000  | 1.158584000  | -0.084773000 |
|  | 6  | 3.034719000  | 0.326704000  | -0.105079000 |
|  | 6  | 4.334345000  | 0.846685000  | -0.000910000 |
|  | 1  | 5.522309000  | 2.635106000  | 0.184185000  |
|  | 1  | 3.499507000  | 4.144625000  | 0.182147000  |
|  | 1  | 1.238810000  | 3.088461000  | 0.012109000  |
|  | 1  | 5.195731000  | 0.186759000  | -0.018395000 |
|  | 6  | 2.717883000  | -1.105900000 | -0.268676000 |
|  | 6  | 3.708349000  | -2.108065000 | -0.238296000 |
|  | 6  | 1.378742000  | -1.491665000 | -0.488131000 |
|  | 6  | 3.376204000  | -3.448891000 | -0.429571000 |
|  | 6  | 1.042847000  | -2.827377000 | -0.689017000 |
|  | 6  | 2.044533000  | -3.809036000 | -0.659689000 |
|  | 1  | 4.748552000  | -1.844230000 | -0.064474000 |
|  | 1  | 4.154151000  | -4.208614000 | -0.403010000 |
|  | 1  | 0.016327000  | -3.124754000 | -0.874764000 |
|  | 1  | 1.776774000  | -4.852128000 | -0.818084000 |
|  | 46 | 0.036698000  | 0.076084000  | -0.428513000 |
|  | 6  | -0.995689000 | -1.250558000 | 4.145514000  |
|  | 6  | 0.115304000  | -0.430207000 | 3.925673000  |
|  | 6  | 0.408808000  | -0.045362000 | 2.621437000  |
|  | 7  | -0.335860000 | -0.453336000 | 1.582405000  |
|  | 6  | -1.417718000 | -1.256497000 | 1.766146000  |
|  | 6  | -1.767139000 | -1.662763000 | 3.062140000  |
|  | 1  | -1.258502000 | -1.565897000 | 5.153004000  |
|  | 1  | 0.742459000  | -0.083494000 | 4.742091000  |
|  | 1  | 1.243049000  | 0.606984000  | 2.394336000  |
|  | 1  | -2.633573000 | -2.298393000 | 3.216695000  |
|  | 6  | -2.118178000 | -1.625368000 | 0.534235000  |
|  | 6  | -1.608315000 | -1.117626000 | -0.678018000 |
|  | 6  | -3.251100000 | -2.462081000 | 0.496804000  |
|  | 6  | -2.201859000 | -1.422803000 | -1.895881000 |
|  | 6  | -3.848126000 | -2.781125000 | -0.721842000 |
|  | 6  | -3.324108000 | -2.263876000 | -1.913770000 |
|  | 1  | -3.665338000 | -2.867257000 | 1.417284000  |
|  | 1  | -1.809253000 | -1.009702000 | -2.817326000 |
|  | 1  | -4.720577000 | -3.430273000 | -0.743737000 |
|  | 1  | -3.790781000 | -2.508457000 | -2.866311000 |
|  | 6  | -3.103080000 | 3.439052000  | -0.577871000 |
|  | 6  | -2.353838000 | 2.211771000  | -1.113693000 |
|  | 7  | -1.336472000 | 1.844155000  | -0.245970000 |
|  | 6  | -1.310749000 | 2.686452000  | 0.841966000  |
|  | 6  | -2.418772000 | 3.739572000  | 0.754910000  |
|  | 1  | -3.018637000 | 4.250689000  | -1.307266000 |

|  |    |              |             |              |
|--|----|--------------|-------------|--------------|
|  | 1  | -3.077785000 | 3.631115000 | 1.622344000  |
|  | 8  | -0.499259000 | 2.629167000 | 1.774542000  |
|  | 8  | -2.641508000 | 1.654173000 | -2.170716000 |
|  | 17 | 0.491969000  | 0.365801000 | -2.751029000 |
|  | 1  | -1.970369000 | 4.736210000 | 0.811735000  |
|  | 1  | -4.165501000 | 3.193699000 | -0.486741000 |

**Table S2-1.** Frequencies of some stationary points for the C-H activation, involved in the discussion on Pd(OAc)<sub>2</sub> as catalyst, computed at B3LYP-IDSCRF/DGDZVP level in dichloromethane.

| Species                                                   | Frequencies (cm <sup>-1</sup> ) |      |      |      |      |      |      |      |      |      |      |      |
|-----------------------------------------------------------|---------------------------------|------|------|------|------|------|------|------|------|------|------|------|
| <b>R</b>                                                  | 42                              | 95   | 148  | 243  | 323  | 395  | 412  | 414  | 476  | 560  | 620  | 631  |
|                                                           | 646                             | 702  | 752  | 754  | 765  | 813  | 852  | 898  | 936  | 977  | 986  | 1001 |
|                                                           | 1002                            | 1006 | 1011 | 1034 | 1059 | 1081 | 1100 | 1114 | 1169 | 1173 | 1197 | 1287 |
|                                                           | 1318                            | 1340 | 1357 | 1448 | 1476 | 1499 | 1528 | 1607 | 1626 | 1633 | 1647 | 1300 |
|                                                           | 3184                            | 3188 | 3194 | 3202 | 3207 | 3213 | 3214 |      |      |      |      | 3177 |
| <b>Pd<sub>2</sub>(μ-OAc)<sub>4</sub></b>                  | 27                              | 28   | 28   | 29   | 63   | 63   | 64   | 73   | 79   | 108  | 109  | 119  |
|                                                           | 163                             | 211  | 215  | 217  | 218  | 220  | 224  | 230  | 246  | 265  | 267  | 268  |
|                                                           | 284                             | 304  | 351  | 354  | 553  | 569  | 569  | 570  | 611  | 623  | 623  | 624  |
|                                                           | 682                             | 683  | 693  | 704  | 939  | 939  | 942  | 949  | 1041 | 1041 | 1042 | 1061 |
|                                                           | 1063                            | 1063 | 1064 | 1376 | 1380 | 1380 | 1385 | 1419 | 1423 | 1423 | 1428 | 1454 |
|                                                           | 1459                            | 1470 | 1489 | 1489 | 1489 | 1489 | 1504 | 1506 | 1516 | 1619 | 3064 | 1456 |
|                                                           | 3064                            | 3153 | 3153 | 3153 | 3154 | 3188 | 3188 | 3188 | 3188 |      | 3064 | 3064 |
| <b>Pd<sub>2</sub>(OAc)<sub>2</sub>(μ-OAc)<sub>2</sub></b> | 19                              | 24   | 24   | 29   | 34   | 35   | 43   | 60   | 64   | 84   | 92   | 112  |
|                                                           | 123                             | 156  | 165  | 178  | 186  | 200  | 214  | 235  | 249  | 278  | 292  | 338  |
|                                                           | 341                             | 358  | 372  | 494  | 498  | 579  | 579  | 604  | 604  | 614  | 620  | 686  |
|                                                           | 689                             | 690  | 694  | 950  | 951  | 951  | 957  | 1011 | 1012 | 1046 | 1046 | 1062 |
|                                                           | 1064                            | 1065 | 1385 | 1385 | 1385 | 1388 | 1428 | 1433 | 1434 | 1436 | 1466 | 1062 |
|                                                           | 1490                            | 1490 | 1505 | 1506 | 1507 | 1510 | 1536 | 1596 | 3061 | 3061 | 3065 | 1472 |
|                                                           | 3155                            | 3155 | 3180 | 3180 | 3189 | 3189 |      |      |      |      | 3148 | 1472 |
| <b>COM1<sup>bi</sup></b>                                  | 10                              | 13   | 23   | 24   | 27   | 29   | 30   | 35   | 37   | 50   | 61   | 63   |
|                                                           | 65                              | 65   | 76   | 82   | 97   | 110  | 113  | 123  | 147  | 161  | 208  | 214  |
|                                                           | 217                             | 219  | 221  | 224  | 225  | 236  | 251  | 263  | 265  | 268  | 283  | 300  |
|                                                           | 322                             | 348  | 350  | 389  | 414  | 415  | 486  | 550  | 560  | 566  | 567  | 568  |
|                                                           | 612                             | 621  | 623  | 623  | 624  | 631  | 646  | 682  | 683  | 694  | 703  | 704  |
|                                                           | 753                             | 755  | 766  | 811  | 853  | 898  | 936  | 939  | 940  | 942  | 949  | 984  |
|                                                           | 986                             | 1000 | 1003 | 1007 | 1012 | 1034 | 1040 | 1041 | 1042 | 1042 | 1059 | 1062 |
|                                                           | 1064                            | 1083 | 1100 | 1116 | 1169 | 1172 | 1197 | 1288 | 1301 | 1319 | 1342 | 1063 |
|                                                           | 1379                            | 1380 | 1385 | 1418 | 1423 | 1423 | 1428 | 1448 | 1457 | 1458 | 1460 | 1376 |
|                                                           | 1489                            | 1489 | 1489 | 1490 | 1501 | 1508 | 1509 | 1516 | 1528 | 1607 | 1622 | 1476 |
|                                                           | 3064                            | 3064 | 3064 | 3064 | 3153 | 3153 | 3153 | 3153 | 3176 | 3183 | 3184 | 1648 |
|                                                           | 3186                            | 3187 | 3189 | 3193 | 3201 | 3206 | 3211 | 3220 |      |      |      | 3186 |
| <b>TS1<sup>bi</sup></b>                                   | -49                             | 15   | 28   | 31   | 32   | 34   | 40   | 41   | 47   | 56   | 59   | 63   |
|                                                           | 69                              | 70   | 84   | 99   | 101  | 109  | 112  | 117  | 133  | 146  | 160  | 174  |
|                                                           | 186                             | 187  | 208  | 211  | 225  | 236  | 254  | 256  | 266  | 270  | 291  | 299  |

|                          |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |
|--------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|                          | 319 327 351 374 415 424 508 521 538 558 573 577<br>611 619 621 622 625 634 647 683 687 687 707 709<br>753 760 766 804 852 897 934 938 938 945 949 979<br>983 999 1009 1011 1013 1034 1034 1039 1040 1041 1060 1061 1062<br>1062 1063 1089 1099 1121 1171 1172 1196 1285 1304 1320 1339 1356<br>1362 1376 1378 1383 1403 1418 1419 1422 1449 1458 1469 1473 1474 1477<br>1488 1489 1489 1491 1502 1504 1529 1540 1569 1606 1618 1625 1638 1648<br>3061 3063 3063 3064 3148 3151 3152 3152 3177 3180 3183 3184 3185 3186<br>3190 3192 3200 3206 3208 3212 3225                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
| <b>INT1<sup>bi</sup></b> | 3 15 28 33 34 40 43 58 60 63 64 72 75<br>84 89 91 105 107 124 134 142 167 174 183 186<br>198 210 218 222 230 244 258 263 269 289 291 332<br>336 346 376 411 454 523 526 548 556 561 568 606<br>608 618 622 626 640 667 675 679 689 694 709 754<br>764 768 794 852 897 927 934 936 940 958 983 983<br>1004 1011 1015 1025 1030 1041 1043 1043 1047 1057 1058 1061 1063<br>1064 1093 1100 1131 1174 1176 1197 1287 1304 1308 1318 1336 1356<br>1372 1375 1387 1390 1414 1417 1445 1454 1462 1468 1473 1475 1482<br>1488 1490 1490 1492 1505 1510 1531 1535 1603 1608 1622 1645 1648 1690<br>3056 3062 3064 3064 3140 3150 3153 3153 3171 3179 3182 3183 3184<br>3186 3190 3198 3198 3206 3214 3218 3240                                                                                                                                                                                                                                                                                                        |
| <b>TS2<sup>bi</sup></b>  | -45 8 18 20 26 31 33 36 42 45 47 51<br>57 58 60 67 69 72 72 79 83 90 96 104<br>105 113 123 134 141 145 156 167 173 185 191 204<br>206 215 228 235 254 257 265 268 284 290 319 324<br>330 345 378 382 415 417 420 456 496 521 525 529<br>549 558 562 573 608 612 619 622 623 626 632 640<br>646 664 679 680 686 695 708 709 754 754 758 765<br>766 768 796 810 852 855 898 899 926 934 935 937<br>942 957 983 987 989 995 1001 1002 1004 1011 1011 1012 1013<br>1024 1030 1034 1036 1041 1043 1046 1056 1059 1060 1061 1063 1063<br>1086 1094 1101 1101 1117 1130 1170 1173 1173 1176 1198 1200 1285 1286<br>1302 1305 1309 1320 1322 1337 1344 1356 1359 1369 1373 1386 1389<br>1406 1412 1443 1448 1453 1471 1475 1475 1476 1479 1482 1488 1491<br>1491 1491 1504 1506 1530 1532 1533 1554 1605 1607 1610 1623 1625<br>1635 1646 1648 1648 1696 3056 3060 3063 3063 3140 3146 3151 3151<br>3171 3176 3178 3179 3180 3183 3184 3185 3186 3191 3192 3196 3198<br>3199 3201 3206 3208 3212 3213 3217 3219 3237 |
| <b>INT2<sup>bi</sup></b> | 18 19 22 23 25 27 29 33 38 40 46 46<br>50 61 63 64 67 75 80 84 86 86 99 101<br>112 120 125 126 149 156 161 170 181 186 190 192<br>207 209 217 235 246 252 268 286 293 295 322 324<br>339 339 375 376 416 416 456 456 515 516 522 522<br>557 557 568 569 611 612 613 616 627 627 640 640                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |

|                          |      |      |      |      |      |      |      |      |      |      |      |      |
|--------------------------|------|------|------|------|------|------|------|------|------|------|------|------|
|                          | 663  | 664  | 674  | 675  | 678  | 681  | 711  | 711  | 755  | 755  | 764  | 764  |
|                          | 770  | 770  | 797  | 797  | 858  | 858  | 900  | 900  | 929  | 930  | 942  | 942  |
|                          | 951  | 955  | 990  | 990  | 996  | 997  | 1004 | 1004 | 1011 | 1011 | 1014 | 1026 |
|                          | 1027 | 1029 | 1030 | 1044 | 1045 | 1047 | 1047 | 1060 | 1060 | 1061 | 1062 | 1063 |
|                          | 1094 | 1095 | 1102 | 1102 | 1129 | 1129 | 1173 | 1173 | 1175 | 1175 | 1202 | 1280 |
|                          | 1280 | 1308 | 1308 | 1319 | 1320 | 1331 | 1335 | 1340 | 1342 | 1360 | 1360 | 1383 |
|                          | 1396 | 1397 | 1433 | 1437 | 1452 | 1453 | 1474 | 1475 | 1475 | 1476 | 1481 | 1488 |
|                          | 1489 | 1492 | 1492 | 1508 | 1509 | 1532 | 1532 | 1559 | 1603 | 1607 | 1607 | 1623 |
|                          | 1644 | 1644 | 1648 | 1648 | 1674 | 1675 | 3057 | 3057 | 3063 | 3063 | 3140 | 3150 |
|                          | 3150 | 3172 | 3172 | 3179 | 3179 | 3183 | 3184 | 3185 | 3185 | 3194 | 3194 | 3195 |
|                          | 3203 | 3203 | 3214 | 3214 | 3215 | 3215 | 3218 | 3218 | 3247 | 3248 |      |      |
| <b>TS3<sup>bi</sup></b>  | -35  | 17   | 20   | 23   | 28   | 28   | 29   | 31   | 33   | 34   | 38   | 40   |
|                          | 44   | 47   | 55   | 61   | 61   | 67   | 72   | 77   | 88   | 90   | 92   | 98   |
|                          | 107  | 111  | 118  | 127  | 130  | 143  | 152  | 155  | 165  | 185  | 188  | 195  |
|                          | 197  | 204  | 213  | 225  | 238  | 254  | 272  | 282  | 286  | 294  | 314  | 332  |
|                          | 338  | 351  | 378  | 408  | 416  | 438  | 440  | 453  | 462  | 505  | 513  | 521  |
|                          | 556  | 557  | 558  | 572  | 611  | 612  | 614  | 615  | 618  | 626  | 631  | 637  |
|                          | 640  | 662  | 670  | 676  | 680  | 682  | 711  | 731  | 752  | 754  | 763  | 765  |
|                          | 768  | 769  | 798  | 802  | 856  | 887  | 896  | 900  | 901  | 928  | 929  | 941  |
|                          | 950  | 954  | 979  | 987  | 988  | 989  | 1004 | 1011 | 1012 | 1014 | 1014 | 1025 |
|                          | 1029 | 1029 | 1044 | 1046 | 1046 | 1050 | 1056 | 1058 | 1060 | 1061 | 1062 | 1080 |
|                          | 1093 | 1097 | 1102 | 1126 | 1129 | 1135 | 1173 | 1174 | 1176 | 1179 | 1201 | 1283 |
|                          | 1292 | 1307 | 1308 | 1319 | 1329 | 1330 | 1338 | 1339 | 1346 | 1359 | 1380 | 1385 |
|                          | 1396 | 1399 | 1432 | 1436 | 1450 | 1452 | 1471 | 1473 | 1474 | 1476 | 1479 | 1488 |
|                          | 1491 | 1491 | 1492 | 1494 | 1505 | 1527 | 1531 | 1553 | 1578 | 1597 | 1605 | 1614 |
|                          | 1623 | 1627 | 1645 | 1647 | 1649 | 1670 | 1926 | 3046 | 3058 | 3062 | 3064 | 3126 |
|                          | 3151 | 3151 | 3154 | 3173 | 3179 | 3184 | 3185 | 3185 | 3186 | 3192 | 3194 | 3199 |
|                          | 3200 | 3203 | 3207 | 3210 | 3214 | 3215 | 3218 | 3219 | 3231 | 3243 |      |      |
| <b>INT3<sup>bi</sup></b> | 18   | 23   | 23   | 25   | 30   | 31   | 35   | 39   | 41   | 55   | 57   | 61   |
|                          | 63   | 72   | 78   | 91   | 95   | 100  | 107  | 114  | 122  | 129  | 140  | 153  |
|                          | 162  | 172  | 181  | 189  | 193  | 196  | 205  | 219  | 229  | 234  | 253  | 264  |
|                          | 284  | 285  | 298  | 312  | 332  | 337  | 371  | 378  | 415  | 422  | 436  | 453  |
|                          | 478  | 485  | 515  | 519  | 541  | 557  | 558  | 570  | 612  | 614  | 618  | 626  |
|                          | 637  | 640  | 659  | 661  | 672  | 677  | 678  | 680  | 710  | 723  | 746  | 754  |
|                          | 760  | 765  | 768  | 773  | 797  | 805  | 856  | 877  | 893  | 896  | 928  | 940  |
|                          | 945  | 950  | 958  | 980  | 985  | 988  | 994  | 1004 | 1010 | 1011 | 1013 | 1026 |
|                          | 1029 | 1036 | 1041 | 1044 | 1045 | 1048 | 1059 | 1061 | 1062 | 1063 | 1071 | 1093 |
|                          | 1102 | 1125 | 1128 | 1140 | 1171 | 1173 | 1175 | 1178 | 1201 | 1259 | 1282 | 1301 |
|                          | 1320 | 1331 | 1336 | 1339 | 1340 | 1360 | 1379 | 1383 | 1396 | 1428 | 1436 | 1449 |
|                          | 1466 | 1476 | 1476 | 1478 | 1482 | 1484 | 1489 | 1492 | 1493 | 1506 | 1516 | 1531 |
|                          | 1597 | 1606 | 1607 | 1613 | 1623 | 1625 | 1644 | 1648 | 1649 | 1674 | 3056 | 3059 |
|                          | 3138 | 3145 | 3147 | 3170 | 3173 | 3179 | 3179 | 3180 | 3181 | 3185 | 3194 | 3195 |
|                          | 3198 | 3203 | 3207 | 3211 | 3212 | 3214 | 3216 | 3217 | 3228 | 3248 |      |      |
| <b>TS4<sup>bi</sup></b>  | -116 | 16   | 21   | 29   | 31   | 33   | 35   | 36   | 38   | 41   | 50   | 55   |

|                            |      |      |      |      |      |      |      |      |      |      |      |      |
|----------------------------|------|------|------|------|------|------|------|------|------|------|------|------|
|                            | 65   | 68   | 76   | 90   | 98   | 101  | 105  | 110  | 117  | 122  | 131  | 135  |
|                            | 148  | 154  | 174  | 186  | 190  | 195  | 203  | 207  | 217  | 229  | 245  | 262  |
|                            | 278  | 287  | 293  | 316  | 328  | 350  | 371  | 408  | 422  | 435  | 440  | 441  |
|                            | 467  | 476  | 485  | 505  | 542  | 547  | 554  | 568  | 597  | 613  | 615  | 620  |
|                            | 632  | 637  | 637  | 659  | 669  | 676  | 679  | 683  | 722  | 731  | 745  | 752  |
|                            | 761  | 763  | 767  | 772  | 803  | 805  | 869  | 877  | 891  | 895  | 901  | 912  |
|                            | 945  | 948  | 959  | 979  | 986  | 987  | 994  | 1011 | 1011 | 1015 | 1020 | 1024 |
|                            | 1036 | 1041 | 1043 | 1048 | 1049 | 1056 | 1057 | 1062 | 1063 | 1071 | 1078 | 1084 |
|                            | 1122 | 1125 | 1135 | 1140 | 1171 | 1173 | 1178 | 1179 | 1217 | 1259 | 1290 | 1301 |
|                            | 1310 | 1324 | 1332 | 1337 | 1339 | 1340 | 1379 | 1380 | 1383 | 1395 | 1424 | 1433 |
|                            | 1449 | 1466 | 1469 | 1474 | 1479 | 1479 | 1484 | 1490 | 1491 | 1492 | 1492 | 1515 |
|                            | 1540 | 1569 | 1597 | 1598 | 1606 | 1612 | 1613 | 1625 | 1626 | 1648 | 1649 | 1748 |
|                            | 3061 | 3062 | 3128 | 3146 | 3148 | 3156 | 3175 | 3180 | 3181 | 3182 | 3183 | 3190 |
|                            | 3198 | 3199 | 3199 | 3207 | 3208 | 3212 | 3213 | 3216 | 3217 | 3226 | 3227 |      |
| <b>1a</b>                  | 12   | 17   | 23   | 28   | 29   | 33   | 34   | 57   | 63   | 67   | 80   | 93   |
|                            | 95   | 108  | 120  | 121  | 131  | 139  | 174  | 180  | 186  | 188  | 193  | 194  |
|                            | 201  | 219  | 226  | 245  | 261  | 263  | 282  | 300  | 316  | 330  | 371  | 371  |
|                            | 422  | 423  | 435  | 436  | 477  | 477  | 484  | 485  | 530  | 533  | 569  | 569  |
|                            | 616  | 619  | 637  | 638  | 657  | 659  | 673  | 674  | 679  | 680  | 724  | 724  |
|                            | 745  | 746  | 760  | 761  | 772  | 772  | 805  | 806  | 877  | 878  | 893  | 894  |
|                            | 942  | 943  | 958  | 958  | 986  | 986  | 993  | 993  | 1010 | 1010 | 1024 | 1024 |
|                            | 1036 | 1040 | 1040 | 1047 | 1048 | 1062 | 1062 | 1069 | 1070 | 1083 | 1083 | 1124 |
|                            | 1139 | 1140 | 1171 | 1171 | 1178 | 1178 | 1258 | 1259 | 1301 | 1301 | 1309 | 1309 |
|                            | 1336 | 1336 | 1339 | 1339 | 1379 | 1380 | 1434 | 1436 | 1448 | 1449 | 1466 | 1466 |
|                            | 1478 | 1480 | 1483 | 1483 | 1493 | 1493 | 1514 | 1515 | 1578 | 1596 | 1597 | 1605 |
|                            | 1610 | 1612 | 1624 | 1627 | 1647 | 1647 | 3058 | 3058 | 3142 | 3142 | 3173 | 3173 |
|                            | 3175 | 3175 | 3180 | 3180 | 3195 | 3195 | 3198 | 3198 | 3205 | 3205 | 3212 | 3212 |
|                            | 3216 | 3216 | 3226 | 3226 |      |      |      |      |      |      |      |      |
| <b>AcOH</b>                | 57   | 427  | 543  | 581  | 651  | 870  | 1006 | 1066 | 1211 | 1346 | 1419 | 1481 |
|                            | 1783 | 3066 | 3147 | 3194 | 3501 |      |      |      |      |      |      |      |
| <b>Pd(OAc)<sub>2</sub></b> | 33   | 35   | 54   | 76   | 120  | 175  | 201  | 237  | 279  | 369  | 384  | 472  |
|                            | 539  | 600  | 606  | 683  | 699  | 952  | 953  | 1011 | 1012 | 1065 | 1065 | 1386 |
|                            | 1435 | 1438 | 1471 | 1473 | 1505 | 1507 | 1510 | 1514 | 3061 | 3061 | 3149 | 3149 |
|                            | 3181 |      |      |      |      |      |      |      |      |      |      |      |
| <b>COM1<sup>mo</sup></b>   | 8    | 10   | 22   | 27   | 30   | 37   | 37   | 44   | 54   | 57   | 76   | 95   |
|                            | 151  | 178  | 201  | 228  | 246  | 277  | 324  | 369  | 381  | 396  | 414  | 415  |
|                            | 467  | 478  | 537  | 560  | 601  | 606  | 621  | 631  | 646  | 681  | 697  | 703  |
|                            | 753  | 755  | 765  | 813  | 853  | 898  | 937  | 951  | 952  | 981  | 987  | 1001 |
|                            | 1003 | 1006 | 1011 | 1012 | 1013 | 1034 | 1059 | 1065 | 1065 | 1082 | 1101 | 1115 |
|                            | 1169 | 1173 | 1199 | 1288 | 1300 | 1318 | 1341 | 1358 | 1385 | 1387 | 1438 | 1439 |
|                            | 1448 | 1472 | 1473 | 1476 | 1500 | 1507 | 1508 | 1511 | 1514 | 1528 | 1607 | 1626 |
|                            | 1633 | 1647 | 3061 | 3061 | 3148 | 3148 | 3172 | 3177 | 3180 | 3181 | 3184 | 3187 |
|                            | 3194 | 3202 | 3206 | 3212 | 3222 |      |      |      |      |      |      |      |
| <b>TS1<sup>mo</sup></b>    | -102 | 19   | 30   | 32   | 38   | 47   | 50   | 54   | 60   | 72   | 75   | 99   |
|                            | 113  | 133  | 148  | 158  | 230  | 259  | 289  | 318  | 325  | 350  | 382  | 415  |

|                          |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
|--------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|                          | 419 477 498 511 560 604 608 624 632 646 681 696<br>708 754 758 766 808 855 900 939 941 947 984 988<br>1002 1005 1009 1012 1013 1015 1033 1060 1064 1065 1086 1101 1118<br>1171 1173 1199 1286 1302 1319 1340 1359 1373 1384 1422 1436 1448<br>1475 1476 1477 1488 1498 1502 1528 1530 1578 1605 1625 1635 1648<br>3059 3060 3146 3147 3176 3177 3178 3183 3184 3191 3193 3202 3208<br>3213 3220                                                                                                 |
| <b>INT1<sup>mo</sup></b> | 17 26 28 32 42 53 62 72 73 96 108 127<br>150 174 177 194 205 260 283 321 334 348 385 417<br>446 491 519 523 559 606 614 626 640 662 677 687<br>712 753 765 767 797 862 896 927 948 950 980 994<br>1010 1011 1014 1015 1024 1029 1044 1060 1063 1066 1093 1105 1130<br>1174 1176 1206 1286 1304 1317 1323 1339 1365 1384 1395 1448 1451<br>1473 1477 1481 1488 1502 1505 1520 1532 1605 1623 1644 1647 1671<br>3059 3060 3142 3147 3174 3178 3179 3184 3190 3197 3198 3204 3214<br>3218 3230     |
| <b>TS2<sup>mo</sup></b>  | -56 33 36 39 41 51 60 64 70 85 97 107<br>119 150 175 196 199 221 272 290 310 342 386 417<br>444 495 508 517 556 611 614 625 639 666 669 692<br>719 750 766 767 800 859 902 925 932 935 985 994<br>1008 1012 1016 1020 1022 1029 1047 1057 1060 1063 1086 1101 1129<br>1174 1175 1193 1293 1303 1317 1325 1337 1356 1358 1390 1412 1453<br>1476 1478 1481 1486 1489 1501 1531 1607 1618 1627 1639 1647 1656<br>3058 3059 3131 3143 3145 3174 3175 3185 3194 3199 3204 3212 3213<br>3217 3231     |
| <b>INT2<sup>mo</sup></b> | 21 29 34 39 49 51 63 68 75 80 109 120<br>131 148 179 189 208 230 277 287 302 343 384 420<br>435 498 513 517 550 612 615 624 637 667 671 687<br>723 748 764 766 796 851 897 918 924 930 975 987<br>1008 1016 1016 1022 1024 1030 1047 1056 1059 1060 1082 1099 1129<br>1173 1176 1190 1289 1305 1314 1328 1333 1337 1362 1390 1397 1452<br>1476 1481 1481 1488 1489 1497 1529 1605 1616 1633 1648 1653 1670<br>3058 3058 3096 3141 3144 3172 3173 3188 3197 3200 3207 3212 3218<br>3221 3245     |
| <b>TS3<sup>mo</sup></b>  | -1369 19 26 36 42 57 66 81 84 106 121 127<br>163 177 188 204 226 245 258 288 309 324 360 419<br>439 453 498 503 533 565 612 632 637 656 671 673<br>691 740 748 765 774 803 886 901 926 938 971 994<br>1005 1015 1022 1024 1027 1039 1047 1060 1068 1073 1085 1120 1134<br>1174 1184 1194 1257 1298 1309 1328 1330 1340 1366 1387 1398 1445<br>1453 1471 1481 1481 1488 1489 1489 1519 1589 1597 1611 1625 1645<br>1658 3056 3066 3138 3149 3170 3183 3189 3190 3197 3199 3207 3213<br>3218 3225 |
| <b>INT3<sup>mo</sup></b> | 19 24 29 43 56 78 81 85 106 113 117 137                                                                                                                                                                                                                                                                                                                                                                                                                                                         |



|              |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
|--------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|              | 1047 1048 1057 1057 1062 1063 1069 1069 1071 1084 1084 1096 1125<br>1125 1140 1140 1171 1171 1174 1178 1179 1196 1259 1260 1269 1301 1303<br>1306 1310 1312 1323 1336 1337 1339 1341 1346 1379 1381 1382 1388<br>1432 1435 1448 1449 1464 1467 1467 1478 1478 1481 1482 1484 1485<br>1489 1492 1492 1494 1494 1515 1517 1573 1594 1597 1601 1608 1611<br>1613 1614 1619 1623 1625 1647 1648 1658 3058 3060 3060 3061 3143<br>3144 3144 3151 3168 3174 3176 3176 3178 3180 3181 3183 3187 3195<br>3196 3197 3199 3200 3205 3207 3211 3212 3213 3213 3216 3217 3227<br>3229 3231                                                                                                                                                                                                                                                                                                                                                                                                      |
| <b>INT1a</b> | 13 25 25 31 32 33 36 37 44 51 55 73<br>78 85 94 98 102 119 120 121 137 140 142 154<br>179 181 186 190 198 202 214 217 225 246 248 264<br>271 282 301 315 331 368 371 423 425 436 439 472<br>477 481 484 485 535 537 566 568 606 617 620 635<br>637 639 659 660 678 679 680 685 720 723 746 746<br>761 762 772 772 801 805 876 879 893 894 905 945<br>947 961 962 986 987 995 996 1012 1012 1013 1020 1024 1034<br>1036 1040 1041 1047 1048 1052 1062 1063 1069 1071 1084 1086 1126<br>1126 1140 1141 1172 1172 1179 1179 1260 1261 1301 1303 1305 1311 1313<br>1336 1338 1340 1341 1377 1380 1382 1433 1437 1448 1450 1467 1468<br>1475 1479 1480 1484 1486 1488 1492 1493 1516 1517 1571 1592 1599<br>1602 1611 1613 1623 1626 1648 1648 1656 3053 3060 3060 3139 3145<br>3146 3165 3175 3178 3178 3179 3182 3185 3196 3196 3199 3202 3208<br>3213 3213 3217 3217 3217 3228 3230                                                                                                   |
| <b>2a</b>    | 20 34 35 38 41 42 44 45 45 47 54 59<br>62 67 72 72 74 89 100 109 115 116 126 128<br>139 143 145 149 164 167 180 190 195 198 205 213<br>218 229 242 257 267 271 274 278 295 313 324 340<br>370 370 425 428 438 441 480 482 483 485 486 488<br>538 543 563 564 610 610 620 625 633 633 650 650<br>662 663 678 680 688 692 714 715 741 743 759 761<br>772 773 794 796 869 870 887 888 913 916 948 950<br>958 958 984 984 994 994 1011 1011 1014 1017 1019 1019 1037<br>1038 1039 1039 1050 1051 1055 1055 1063 1064 1070 1072 1087 1087<br>1129 1129 1142 1142 1172 1173 1179 1180 1260 1261 1305 1306 1307 1315<br>1315 1317 1340 1340 1344 1344 1379 1379 1380 1382 1424 1425 1448<br>1450 1470 1470 1479 1479 1481 1481 1487 1488 1488 1488 1491 1491<br>1519 1520 1575 1588 1601 1601 1611 1612 1627 1627 1641 1648 1648<br>1663 3055 3055 3062 3062 3141 3141 3148 3148 3166 3166 3181 3181<br>3182 3182 3188 3188 3197 3197 3204 3204 3216 3216 3219 3219 3226<br>3226 3250 3250 |
| <b>PhI</b>   | 151 219 262 408 459 620 659 696 740 840 919 980<br>999 1003 1029 1074 1092 1171 1195 1317 1342 1462 1495 1615 1621<br>3187 3194 3205 3212 3215                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |

|                          |      |      |      |      |      |      |      |      |      |      |      |      |
|--------------------------|------|------|------|------|------|------|------|------|------|------|------|------|
| <b>1b</b>                | 14   | 16   | 26   | 27   | 29   | 31   | 34   | 57   | 62   | 65   | 79   | 99   |
|                          | 107  | 115  | 123  | 140  | 164  | 164  | 176  | 182  | 189  | 193  | 201  | 209  |
|                          | 213  | 221  | 234  | 235  | 258  | 274  | 275  | 279  | 284  | 297  | 325  | 330  |
|                          | 430  | 431  | 439  | 439  | 477  | 477  | 499  | 499  | 509  | 509  | 510  | 511  |
|                          | 533  | 536  | 565  | 565  | 574  | 575  | 615  | 618  | 618  | 619  | 659  | 660  |
|                          | 674  | 677  | 729  | 729  | 729  | 730  | 762  | 763  | 770  | 771  | 794  | 795  |
|                          | 844  | 844  | 850  | 850  | 879  | 880  | 916  | 917  | 931  | 931  | 942  | 944  |
|                          | 968  | 968  | 981  | 981  | 990  | 990  | 997  | 997  | 1028 | 1029 | 1040 | 1061 |
|                          | 1062 | 1064 | 1065 | 1093 | 1093 | 1125 | 1125 | 1158 | 1158 | 1166 | 1166 | 1209 |
|                          | 1233 | 1237 | 1238 | 1264 | 1265 | 1340 | 1340 | 1348 | 1350 | 1372 | 1372 | 1379 |
|                          | 1427 | 1428 | 1434 | 1436 | 1440 | 1440 | 1449 | 1449 | 1478 | 1479 | 1480 | 1493 |
|                          | 1493 | 1522 | 1522 | 1532 | 1534 | 1577 | 1603 | 1608 | 1614 | 1619 | 1619 | 1635 |
|                          | 1658 | 1659 | 3059 | 3059 | 3143 | 3143 | 3171 | 3171 | 3174 | 3174 | 3175 | 3185 |
|                          | 3185 | 3187 | 3187 | 3191 | 3191 | 3200 | 3200 | 3208 | 3208 | 3221 | 3221 |      |
| <b>PhICl<sub>2</sub></b> | 25   | 59   | 96   | 101  | 200  | 217  | 240  | 256  | 258  | 406  | 463  | 614  |
|                          | 657  | 684  | 743  | 831  | 929  | 983  | 991  | 1010 | 1025 | 1066 | 1097 | 1195 |
|                          | 1327 | 1343 | 1467 | 1490 | 1604 | 1624 | 3191 | 3200 | 3208 | 3216 | 3217 |      |
| <b>TS1b</b>              | -62  | 13   | 15   | 17   | 21   | 24   | 29   | 29   | 34   | 35   | 37   | 44   |
|                          | 46   | 53   | 58   | 62   | 63   | 66   | 74   | 79   | 83   | 102  | 108  | 121  |
|                          | 127  | 147  | 149  | 163  | 169  | 171  | 176  | 182  | 188  | 196  | 200  | 202  |
|                          | 212  | 217  | 224  | 226  | 234  | 237  | 243  | 262  | 273  | 276  | 280  | 287  |
|                          | 298  | 324  | 331  | 403  | 429  | 430  | 439  | 440  | 448  | 474  | 475  | 499  |
|                          | 499  | 507  | 508  | 509  | 509  | 535  | 539  | 565  | 565  | 570  | 571  | 613  |
|                          | 615  | 615  | 616  | 620  | 656  | 660  | 661  | 675  | 678  | 681  | 722  | 724  |
|                          | 729  | 729  | 746  | 763  | 764  | 767  | 769  | 789  | 792  | 835  | 835  | 837  |
|                          | 845  | 847  | 878  | 879  | 916  | 916  | 932  | 932  | 937  | 944  | 947  | 967  |
|                          | 969  | 978  | 980  | 984  | 987  | 990  | 995  | 996  | 996  | 1009 | 1021 | 1029 |
|                          | 1041 | 1042 | 1061 | 1062 | 1063 | 1065 | 1067 | 1094 | 1095 | 1100 | 1125 | 1160 |
|                          | 1167 | 1167 | 1176 | 1200 | 1209 | 1210 | 1235 | 1235 | 1239 | 1240 | 1265 | 1266 |
|                          | 1345 | 1350 | 1352 | 1356 | 1375 | 1379 | 1382 | 1383 | 1429 | 1431 | 1433 | 1441 |
|                          | 1443 | 1452 | 1453 | 1466 | 1477 | 1479 | 1483 | 1486 | 1491 | 1495 | 1496 | 1524 |
|                          | 1535 | 1536 | 1576 | 1603 | 1607 | 1611 | 1613 | 1615 | 1622 | 1625 | 1638 | 1661 |
|                          | 1663 | 3056 | 3057 | 3141 | 3142 | 3173 | 3173 | 3176 | 3176 | 3176 | 3182 | 3186 |
|                          | 3187 | 3189 | 3189 | 3193 | 3193 | 3195 | 3204 | 3204 | 3204 | 3210 | 3211 | 3223 |
|                          | 3225 | 3234 |      |      |      |      |      |      |      |      |      |      |
| <b>INT1b</b>             | 11   | 15   | 16   | 24   | 31   | 34   | 39   | 42   | 43   | 44   | 48   | 49   |
|                          | 53   | 56   | 62   | 65   | 71   | 77   | 82   | 86   | 108  | 109  | 121  | 126  |
|                          | 129  | 145  | 151  | 165  | 174  | 177  | 185  | 187  | 197  | 202  | 205  | 214  |
|                          | 218  | 220  | 227  | 228  | 235  | 239  | 241  | 264  | 274  | 279  | 281  | 291  |
|                          | 302  | 326  | 334  | 404  | 429  | 430  | 439  | 440  | 458  | 474  | 474  | 499  |
|                          | 500  | 507  | 507  | 509  | 509  | 538  | 544  | 565  | 566  | 568  | 571  | 612  |
|                          | 614  | 617  | 618  | 620  | 658  | 660  | 661  | 678  | 681  | 688  | 719  | 724  |
|                          | 729  | 730  | 744  | 763  | 764  | 769  | 769  | 788  | 792  | 833  | 835  | 840  |
|                          | 846  | 847  | 878  | 880  | 916  | 920  | 928  | 932  | 932  | 947  | 949  | 968  |

|              |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
|--------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|              | 969 980 981 982 990 990 997 998 1001 1005 1025 1029 1029<br>1041 1043 1063 1064 1066 1067 1068 1095 1096 1097 1125 1126 1160 1161<br>1168 1168 1174 1196 1209 1211 1235 1235 1239 1241 1266 1266 1327 1344<br>1346 1350 1351 1352 1376 1379 1382 1383 1429 1430 1432 1438 1442<br>1444 1452 1454 1465 1478 1480 1484 1486 1494 1495 1496 1524 1525<br>1536 1537 1574 1602 1611 1613 1615 1621 1623 1626 1638 1640 1662<br>1664 3058 3059 3144 3145 3174 3177 3177 3177 3178 3182 3183 3187<br>3188 3190 3191 3192 3193 3195 3201 3204 3208 3208 3211 3212 3218<br>3224 3226                                                                                                                                                                                                                                                                                                                                                                                                                                                        |
| <b>INT2b</b> | 13 24 32 34 35 38 41 44 45 52 54 59<br>61 62 65 67 72 87 92 92 97 114 120 128<br>137 139 147 168 171 179 185 191 193 210 216 227<br>230 232 233 235 244 248 270 277 283 284 285 296<br>308 325 337 407 429 432 439 440 459 474 476 498<br>499 504 507 509 509 540 545 565 566 567 568 607<br>610 620 620 624 658 659 660 688 691 695 711 714<br>728 730 744 763 764 766 767 785 787 826 828 843<br>846 846 872 876 912 913 925 929 931 950 952 968<br>970 979 981 983 988 990 998 1000 1001 1006 1028 1028 1030<br>1039 1041 1063 1065 1068 1069 1072 1093 1097 1098 1124 1126 1161 1162<br>1169 1169 1172 1195 1208 1210 1237 1237 1242 1242 1266 1266 1321 1344<br>1346 1349 1352 1353 1381 1381 1382 1384 1419 1425 1432 1433 1444<br>1444 1453 1455 1462 1478 1481 1486 1488 1491 1494 1496 1524 1525<br>1533 1536 1571 1588 1605 1611 1616 1618 1626 1627 1641 1642 1663<br>1666 3059 3062 3147 3149 3178 3179 3180 3181 3182 3183 3185 3186<br>3189 3191 3194 3195 3196 3197 3198 3205 3210 3214 3216 3216 3222<br>3228 3232 |
| <b>2b</b>    | 15 31 38 39 42 46 57 67 68 80 85 87<br>91 94 98 113 124 134 137 147 171 179 182 190<br>195 209 211 218 230 233 235 240 261 271 279 283<br>287 287 295 308 325 335 432 435 440 441 478 480<br>499 499 508 508 511 514 541 546 566 567 570 571<br>612 614 620 624 660 660 691 694 719 720 728 728<br>763 764 769 770 789 791 837 837 849 850 874 877<br>914 914 930 930 949 951 970 970 982 982 990 990<br>1000 1000 1029 1030 1039 1040 1062 1063 1067 1068 1096 1096 1123<br>1126 1160 1160 1168 1168 1208 1209 1236 1236 1240 1240 1265 1266 1342<br>1343 1350 1352 1378 1379 1380 1382 1420 1421 1431 1431 1443 1443<br>1451 1452 1479 1479 1484 1484 1490 1490 1522 1523 1531 1533 1573<br>1589 1606 1606 1624 1624 1639 1639 1660 1661 3063 3063 3149 3149<br>3179 3179 3180 3180 3184 3184 3189 3189 3194 3194 3196 3196 3214<br>3214 3219 3219 3230 3230                                                                                                                                                                     |
| <b>1c</b>    | 8 15 23 24 28 46 51 59 63 64 78 94<br>95 97 102 104 134 135 147 159 167 168 188 192                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |

|              |      |      |      |      |      |      |      |      |      |      |      |      |
|--------------|------|------|------|------|------|------|------|------|------|------|------|------|
|              | 207  | 210  | 226  | 233  | 233  | 245  | 262  | 267  | 275  | 276  | 289  | 294  |
|              | 322  | 323  | 431  | 431  | 438  | 438  | 457  | 458  | 477  | 477  | 498  | 499  |
|              | 509  | 509  | 511  | 511  | 564  | 564  | 572  | 573  | 575  | 576  | 578  | 579  |
|              | 587  | 591  | 619  | 619  | 659  | 660  | 664  | 665  | 684  | 684  | 729  | 729  |
|              | 729  | 730  | 761  | 762  | 768  | 769  | 793  | 794  | 835  | 836  | 844  | 844  |
|              | 850  | 851  | 879  | 879  | 895  | 895  | 912  | 913  | 931  | 931  | 968  | 968  |
|              | 981  | 981  | 988  | 989  | 996  | 997  | 997  | 997  | 1021 | 1021 | 1028 | 1030 |
|              | 1030 | 1067 | 1068 | 1095 | 1095 | 1125 | 1125 | 1159 | 1159 | 1163 | 1163 | 1167 |
|              | 1212 | 1233 | 1233 | 1239 | 1239 | 1245 | 1245 | 1252 | 1254 | 1266 | 1266 | 1279 |
|              | 1314 | 1315 | 1341 | 1341 | 1349 | 1350 | 1369 | 1369 | 1394 | 1394 | 1429 | 1440 |
|              | 1440 | 1448 | 1448 | 1465 | 1465 | 1480 | 1480 | 1484 | 1484 | 1523 | 1523 | 1534 |
|              | 1607 | 1608 | 1613 | 1620 | 1620 | 1630 | 1636 | 1636 | 1659 | 1659 | 1761 | 1764 |
|              | 3075 | 3084 | 3084 | 3126 | 3126 | 3141 | 3141 | 3171 | 3171 | 3174 | 3174 | 3185 |
|              | 3188 | 3188 | 3191 | 3191 | 3203 | 3203 | 3207 | 3207 | 3220 | 3220 |      |      |
| <b>NCS</b>   | 79   | 106  | 189  | 211  | 330  | 517  | 562  | 562  | 564  | 640  | 649  | 825  |
|              | 955  | 1018 | 1019 | 1032 | 1172 | 1176 | 1251 | 1271 | 1324 | 1326 | 1459 | 1478 |
|              | 3086 | 3091 | 3140 | 3153 |      |      |      |      |      |      |      |      |
| <b>TS1c</b>  | -922 | 10   | 14   | 19   | 20   | 25   | 27   | 33   | 33   | 35   | 38   | 41   |
|              | 46   | 48   | 53   | 54   | 58   | 61   | 69   | 75   | 84   | 87   | 88   | 92   |
|              | 102  | 105  | 106  | 111  | 113  | 119  | 122  | 136  | 143  | 153  | 159  | 172  |
|              | 176  | 181  | 199  | 202  | 205  | 212  | 223  | 232  | 235  | 239  | 241  | 262  |
|              | 263  | 278  | 282  | 287  | 288  | 301  | 314  | 318  | 326  | 418  | 429  | 431  |
|              | 438  | 439  | 462  | 463  | 475  | 477  | 498  | 499  | 504  | 507  | 508  | 509  |
|              | 511  | 549  | 563  | 564  | 565  | 566  | 567  | 569  | 570  | 573  | 580  | 582  |
|              | 586  | 590  | 606  | 610  | 615  | 645  | 652  | 658  | 661  | 664  | 669  | 671  |
|              | 680  | 682  | 710  | 722  | 727  | 729  | 761  | 763  | 765  | 773  | 787  | 793  |
|              | 831  | 832  | 833  | 833  | 842  | 849  | 852  | 868  | 877  | 895  | 900  | 904  |
|              | 916  | 916  | 925  | 927  | 931  | 957  | 964  | 970  | 983  | 985  | 992  | 996  |
|              | 1002 | 1002 | 1003 | 1007 | 1017 | 1019 | 1025 | 1025 | 1027 | 1027 | 1028 | 1030 |
|              | 1061 | 1069 | 1070 | 1098 | 1099 | 1121 | 1125 | 1160 | 1161 | 1162 | 1167 | 1168 |
|              | 1192 | 1210 | 1213 | 1233 | 1235 | 1236 | 1241 | 1241 | 1243 | 1247 | 1247 | 1248 |
|              | 1267 | 1269 | 1281 | 1286 | 1311 | 1315 | 1316 | 1339 | 1344 | 1346 | 1349 | 1352 |
|              | 1374 | 1377 | 1385 | 1406 | 1414 | 1430 | 1430 | 1442 | 1442 | 1451 | 1452 | 1459 |
|              | 1463 | 1463 | 1479 | 1480 | 1481 | 1483 | 1484 | 1484 | 1490 | 1515 | 1522 | 1524 |
|              | 1534 | 1599 | 1606 | 1617 | 1623 | 1625 | 1627 | 1637 | 1639 | 1659 | 1660 | 1693 |
|              | 1769 | 1781 | 1800 | 3052 | 3075 | 3080 | 3080 | 3084 | 3086 | 3087 | 3125 | 3131 |
|              | 3133 | 3140 | 3146 | 3150 | 3165 | 3179 | 3181 | 3183 | 3185 | 3189 | 3192 | 3194 |
|              | 3196 |      |      |      |      |      |      |      |      |      |      |      |
|              | 3198 | 3199 | 3211 | 3212 | 3216 | 3225 | 3233 | 3244 |      |      |      |      |
| <b>INT1c</b> | 22   | 32   | 37   | 42   | 52   | 54   | 60   | 65   | 73   | 83   | 86   | 91   |
|              | 95   | 100  | 103  | 113  | 119  | 134  | 138  | 153  | 159  | 172  | 176  | 182  |
|              | 201  | 204  | 213  | 223  | 233  | 236  | 240  | 241  | 264  | 278  | 283  | 287  |
|              | 288  | 302  | 316  | 319  | 326  | 429  | 431  | 438  | 439  | 461  | 463  | 475  |
|              | 477  | 498  | 499  | 503  | 507  | 509  | 510  | 563  | 564  | 565  | 567  | 568  |
|              | 572  | 579  | 582  | 586  | 589  | 604  | 613  | 651  | 657  | 660  | 663  | 677  |

|                          |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
|--------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|                          | 681 707 720 726 729 761 763 765 774 787 793 829<br>831 833 841 849 853 866 876 895 906 917 924 929<br>930 964 968 985 986 994 997 1003 1003 1004 1009 1016 1025<br>1026 1027 1030 1031 1069 1071 1098 1099 1120 1124 1162 1162 1168 1169<br>1170 1170 1188 1209 1212 1235 1237 1239 1241 1243 1246 1248 1265 1266<br>1281 1287 1316 1316 1343 1346 1349 1351 1374 1377 1383 1410 1430<br>1430 1442 1442 1451 1452 1461 1462 1478 1479 1483 1484 1520 1523<br>1528 1532 1596 1603 1615 1622 1625 1628 1636 1639 1658 1659 1772<br>1800 3080 3080 3087 3088 3132 3134 3147 3150 3181 3182 3184 3186<br>3190 3192 3195 3197 3199 3200 3212 3212 3215 3225 3235 3242                                                                                                                                                                                                                                                                                                                                                                                                   |
| <b>2c</b>                | 21 29 34 39 42 50 52 53 57 60 65 67<br>75 82 87 91 95 99 110 111 115 122 136 150<br>153 154 161 177 178 181 188 200 209 211 230 232<br>238 240 253 263 267 281 286 288 290 300 318 324<br>433 435 439 439 463 465 477 479 489 499 499 509<br>509 511 515 565 566 568 568 569 570 579 582 585<br>588 605 612 614 649 653 656 659 662 679 682 717<br>719 729 729 761 763 768 768 787 789 832 833 836<br>836 848 848 872 876 893 895 914 915 916 929 930<br>958 960 981 982 989 990 997 998 1000 1002 1019 1023 1025<br>1027 1027 1031 1032 1052 1070 1072 1099 1099 1123 1125 1160 1160 1166<br>1166 1168 1169 1211 1212 1213 1220 1237 1237 1242 1242 1247 1248 1267<br>1267 1282 1283 1304 1312 1313 1343 1344 1352 1353 1375 1377 1379<br>1392 1393 1432 1432 1443 1443 1452 1453 1463 1464 1480 1481 1482<br>1486 1487 1488 1524 1525 1533 1534 1605 1607 1625 1625 1627 1629<br>1640 1640 1655 1662 1663 1784 1789 3056 3078 3078 3086 3086 3130<br>3130 3144 3146 3146 3167 3178 3178 3179 3179 3188 3189 3193 3194<br>3195 3195 3212 3213 3230 3235 3237 3241 |
| <b>Succinimide...OAc</b> | 21 28 54 67 89 104 108 155 183 399 458 545<br>562 573 614 629 636 661 833 841 902 950 1017 1021<br>1028 1056 1131 1178 1234 1249 1272 1320 1353 1368 1412 1463 1479<br>1484 1492 1506 1616 1731 1798 2502 3043 3079 3087 3121 3130 3144<br>3151                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
| <b>succinimide</b>       | 86 140 388 535 538 566 632 642 655 831 855 913<br>1014 1026 1174 1185 1250 1277 1325 1357 1364 1461 1480 1756 1824<br>3084 3091 3136 3150 3486                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |

**Table S2-3.** Frequencies of some stationary points for the oxidative process ( $\text{Pd}^{\text{II}}$  to  $\text{Pd}^{\text{IV}}$ ), involved in the discussion on  $\text{PhI}(\text{OAc})_2$  (**OX-a**),  $\text{PhICl}_2$  (**OX-b**) and  $\text{NCS}$  (**OX-c**) as oxidant, computed at B3LYP-IDSCRF/DGDZVP level in dichloromethane.

| Species   | Frequencies ( $\text{cm}^{-1}$ ) |     |     |     |     |     |     |     |     |     |     |     |
|-----------|----------------------------------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| <b>1m</b> | 29                               | 36  | 47  | 83  | 86  | 108 | 121 | 136 | 151 | 175 | 194 | 203 |
|           | 235                              | 244 | 268 | 278 | 303 | 355 | 368 | 422 | 426 | 427 | 442 | 467 |

|                |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |
|----------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|                | 469 485 497 567 572 638 640 645 648 668 671 722<br>728 746 751 758 758 769 770 808 813 871 885 889<br>892 953 960 965 972 989 997 1007 1007 1018 1019 1027 1033<br>1037 1043 1072 1081 1081 1087 1120 1124 1137 1143 1171 1172 1182 1184<br>1262 1273 1293 1300 1305 1306 1325 1329 1333 1336 1446 1450 1458 1462<br>1481 1484 1509 1510 1592 1593 1609 1611 1619 1622 1643 1644 3167 3168<br>3178 3178 3192 3192 3194 3195 3201 3203 3206 3207 3217 3218 3220 3221                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
| <b>TS1m-a</b>  | -238 7 12 16 17 22 27 29 32 39 40 44<br>45 48 64 67 75 80 88 103 108 116 119 129 133<br>148 151 153 170 173 183 197 209 226 233 245 260<br>263 274 295 355 365 409 418 423 431 439 447 456<br>462 465 469 479 494 567 570 602 616 618 624 636<br>639 643 644 648 662 666 672 692 719 725 744 745<br>749 757 760 769 770 807 810 844 870 881 890 891<br>893 929 933 954 960 970 977 987 989 995 1000 1007 1007<br>1009 1009 1015 1017 1019 1024 1026 1028 1039 1042 1060 1061 1070 1071<br>1077 1082 1085 1097 1120 1122 1137 1141 1171 1172 1175 1182 1183 1197<br>1263 1271 1285 1295 1300 1306 1310 1315 1324 1326 1329 1333 1336 1347<br>1386 1396 1446 1447 1459 1462 1464 1479 1481 1482 1483 1487 1495 1496<br>1509 1512 1592 1593 1609 1610 1611 1617 1619 1619 1624 1641 1645 1657<br>3058 3062 3141 3148 3169 3169 3170 3179 3180 3181 3187 3191 3192 3195<br>3196 3197 3198 3201 3203 3205 3210 3212 3214 3216 3218 3218 3220 |
| <b>INT1m-a</b> | 24 26 35 39 42 53 79 82 95 102 107 133<br>138 142 160 172 189 199 221 246 256 260 287 293<br>359 366 419 424 431 432 456 471 473 478 488 567<br>569 617 635 638 644 650 662 670 674 722 727 745<br>746 758 761 769 770 807 810 874 876 890 896 933<br>957 958 975 991 992 994 1009 1011 1017 1021 1022 1024 1029<br>1041 1043 1063 1070 1072 1083 1086 1121 1122 1138 1140 1171 1173 1182<br>1185 1264 1270 1297 1300 1310 1311 1325 1326 1333 1337 1375 1442 1446<br>1447 1462 1463 1475 1482 1484 1493 1507 1511 1573 1594 1596 1611 1612<br>1620 1622 1639 1644 3054 3137 3166 3173 3173 3182 3183 3188 3192 3193<br>3195 3198 3199 3200 3207 3214 3216 3219 3221                                                                                                                                                                                                                                                                    |
| <b>2m-a</b>    | 33 36 38 42 44 48 54 60 62 70 78 87<br>95 112 122 128 138 156 168 178 187 202 208 212<br>229 245 273 277 297 313 323 364 372 425 427 435<br>444 475 484 488 488 491 523 564 566 608 614 635<br>637 650 657 660 672 675 679 718 720 745 747 760<br>762 771 772 798 803 873 878 888 890 922 927 958<br>965 973 975 993 999 1010 1012 1012 1018 1026 1027 1032 1037<br>1045 1049 1056 1058 1070 1075 1087 1090 1125 1131 1142 1143 1172 1173<br>1180 1185 1258 1272 1304 1304 1308 1313 1315 1332 1338 1341 1343 1350<br>1388 1399 1449 1450 1466 1470 1481 1483 1488 1489 1490 1490 1516 1519<br>1598 1600 1611 1615 1625 1628 1641 1647 1649 1694 3052 3057 3133 3141                                                                                                                                                                                                                                                                    |

|                |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
|----------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|                | 3162 3171 3180 3180 3187 3189 3194 3198 3203 3203 3213 3216 3219 3219<br>3220 3221 3244 3259                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
| <b>COM1m-b</b> | 11 13 18 23 24 27 31 35 40 54 67 86<br>89 103 107 109 124 139 152 177 195 200 203 219<br>235 236 244 250 252 268 278 303 356 368 405 422<br>426 428 442 462 467 469 484 495 565 571 616 638<br>640 646 649 656 669 671 687 720 726 741 745 750<br>757 758 769 770 805 810 834 870 885 888 891 927<br>954 962 967 974 982 990 994 1000 1007 1007 1008 1020 1021<br>1026 1026 1032 1038 1044 1068 1073 1083 1083 1088 1097 1122 1126 1138<br>1145 1173 1174 1176 1184 1186 1195 1264 1275 1296 1303 1309 1310 1326<br>1327 1330 1336 1339 1347 1449 1453 1460 1464 1468 1484 1487 1493 1512<br>1513 1595 1597 1610 1612 1615 1622 1625 1627 1647 1648 3169 3169 3180<br>3180 3189 3192 3193 3196 3197 3197 3206 3208 3208 3210 3213 3215 3215<br>3220 3221 3223 3226 |
| <b>TS1m-b</b>  | -103 14 18 20 25 32 36 43 49 57 71 72<br>82 88 95 102 119 132 152 159 169 171 195 202<br>207 218 233 236 242 257 277 284 356 366 404 414<br>423 429 432 459 466 471 472 490 565 567 616 636<br>638 642 649 653 667 670 686 713 723 740 743 745<br>755 760 768 769 805 807 834 869 876 890 893 925<br>955 959 974 981 985 990 994 994 1006 1007 1010 1015 1017<br>1023 1025 1028 1040 1041 1066 1074 1076 1083 1087 1096 1120 1124 1140<br>1143 1173 1174 1175 1186 1187 1194 1269 1274 1294 1299 1313 1313 1323<br>1326 1328 1335 1336 1346 1447 1448 1461 1464 1467 1482 1485 1492 1510<br>1514 1596 1597 1609 1613 1614 1622 1624 1626 1640 1647 3170 3174 3181<br>3182 3185 3186 3189 3193 3194 3194 3200 3201 3203 3204 3210 3213 3213<br>3218 3219 3222 3223  |
| <b>INT1m-b</b> | 14 31 35 37 42 45 48 56 68 76 82 87<br>92 94 104 113 115 123 155 175 178 188 203 218 222<br>232 257 262 269 277 296 304 360 368 412 423 426<br>431 437 457 472 477 482 486 560 564 616 630 633<br>646 656 657 667 675 689 704 710 742 745 745 763<br>764 768 769 794 803 850 871 874 887 901 946 964<br>969 977 991 997 999 1000 1002 1006 1012 1014 1017 1024 1026<br>1029 1035 1042 1046 1068 1072 1074 1086 1088 1104 1125 1129 1143 1146<br>1173 1175 1176 1183 1187 1206 1262 1271 1303 1305 1314 1318 1330 1331<br>1338 1340 1348 1360 1443 1447 1466 1467 1467 1485 1486 1500 1514 1521<br>1597 1600 1609 1609 1612 1625 1625 1626 1645 1647 3119 3185 3186 3186<br>3194 3195 3196 3196 3201 3202 3206 3207 3207 3218 3218 3219 3219 3219<br>3223 3223 3248 |
| <b>2m-b</b>    | 35 38 45 65 81 88 99 109 114 121 127 163<br>174 193 203 209 228 250 266 272 289 298 331 362<br>371 425 426 434 441 473 482 486 487 564 567 634                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |

|               |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
|---------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|               | 635 649 659 670 676 717 718 745 746 762 764 769<br>771 798 805 871 876 890 899 959 964 978 995 999<br>999 1008 1013 1015 1015 1031 1036 1042 1048 1071 1072 1086 1088 1124<br>1130 1142 1144 1173 1174 1182 1184 1264 1270 1302 1304 1313 1315 1330<br>1336 1338 1343 1446 1448 1466 1469 1486 1487 1513 1519 1596 1599 1610<br>1612 1625 1626 1643 1648 3181 3181 3188 3190 3194 3199 3200 3204 3204<br>3216 3216 3218 3220 3221 3225 3237                                                                                                                                                                                                                                                                                              |
| <b>TS1m-c</b> | -65 20 27 30 33 39 49 52 78 86 88 91<br>103 107 120 142 149 162 172 180 193 202 214 238<br>251 269 276 294 357 367 412 418 422 430 435 462<br>474 475 489 548 558 565 567 574 634 637 640 647<br>649 657 668 672 710 724 744 746 759 760 768 769<br>802 808 829 851 868 881 894 895 957 966 975 980<br>982 993 999 1004 1013 1013 1017 1019 1020 1023 1031 1042 1044 1073<br>1075 1084 1086 1122 1123 1140 1143 1153 1173 1174 1184 1186 1244 1253<br>1265 1267 1272 1298 1299 1302 1312 1313 1315 1327 1331 1335 1336 1445<br>1448 1463 1464 1465 1483 1484 1485 1512 1515 1595 1596 1610 1611 1621<br>1623 1642 1646 1667 1741 3074 3082 3126 3141 3178 3181 3187 3187 3189<br>3195 3198 3201 3202 3204 3210 3218 3218 3222 3222 3233  |
| <b>2m-c</b>   | 30 35 41 43 51 67 81 88 96 99 112 119<br>127 131 135 151 165 175 194 205 225 233 249 268<br>273 285 301 334 362 370 425 426 429 435 443 474<br>483 487 489 557 564 565 576 582 634 635 645 649<br>658 670 674 676 717 721 743 746 760 760 770 771<br>796 802 835 866 869 872 885 889 960 961 972 974<br>982 995 996 1009 1011 1012 1016 1027 1027 1030 1036 1044 1048 1071<br>1076 1087 1088 1126 1130 1143 1144 1157 1173 1174 1181 1185 1246 1247<br>1265 1269 1272 1303 1305 1307 1313 1314 1330 1337 1340 1342 1343 1448<br>1450 1465 1466 1469 1486 1488 1489 1514 1520 1597 1599 1611 1614 1626<br>1627 1645 1647 1666 1764 3070 3080 3120 3136 3180 3180 3187 3190 3195<br>3198 3203 3203 3214 3216 3220 3221 3222 3241 3251 3257 |

**Table S3-1.** The total energies ( $E_{\text{tot}}/\text{a.u.} = E_{\text{elec}}/\text{a.u.} + \text{ZPE}/\text{a.u.}$ ), electronic energies ( $E_{\text{elec}}/\text{a.u.}$ ) and Gibbs free energies ( $G/\text{a.u.}$ ) for the C-H activation, involved in the discussion on  $\text{Pd}(\text{OAc})_2$  as catalyst, computed at B3LYP-IDSCRF/DGDZVP level in dichloromethane at 313K.

| Species                                                         | $E_{\text{tot}}/\text{a.u.}$ | $E_{\text{elec}}/\text{a.u.}$ | $G/\text{a.u.}$ |
|-----------------------------------------------------------------|------------------------------|-------------------------------|-----------------|
| <b>R</b>                                                        | -479.228025                  | -479.3970521                  | -479.25176      |
| <b><math>\text{Pd}_2(\mu\text{-OAc})_4</math></b>               | -10793.4088                  | -10793.61677                  | -10793.45149    |
| <b><math>\text{Pd}_2(\text{OAc})_2(\mu\text{-OAc})_2</math></b> | -10793.40151                 | -10793.60844                  | -10793.44654    |
| <b>COM1<sup>bi</sup></b>                                        | -11272.63885                 | -11273.01639                  | -11272.69504    |
| <b>TS1<sup>bi</sup></b>                                         | -11272.63512                 | -11273.0124                   | -11272.68952    |
| <b>INT1<sup>bi</sup></b>                                        | -11272.64784                 | -11273.02585                  | -11272.70375    |
| <b>TS2<sup>bi</sup></b>                                         | -11751.87417                 | -11752.422                    | -11751.9403     |

|                            |              |              |              |
|----------------------------|--------------|--------------|--------------|
| <b>INT2<sup>bi</sup></b>   | -11751.8998  | -11752.44869 | -11751.96696 |
| <b>TS3<sup>bi</sup></b>    | -11751.85666 | -11752.4017  | -11751.92321 |
| <b>INT3<sup>bi</sup></b>   | -11522.82758 | -11523.31346 | -11522.8874  |
| <b>TS4<sup>bi</sup></b>    | -11522.86333 | -11523.26883 | -11522.84622 |
| <b>1a</b>                  | -11293.75503 | -11294.17784 | -11293.80817 |
| <b>AcOH</b>                | -229.076626  | -229.1377595 | -229.09339   |
| <b>Pd(OAc)<sub>2</sub></b> | -5396.686051 | -5396.788635 | -5396.71407  |
| <b>COM1<sup>mo</sup></b>   | -5875.914717 | -5876.186785 | -5875.95823  |
| <b>TS1<sup>mo</sup></b>    | -5875.909569 | -5876.181587 | -5875.95063  |
| <b>INT1<sup>mo</sup></b>   | -5875.936545 | -5876.209826 | -5875.97807  |
| <b>TS2<sup>mo</sup></b>    | -5875.923101 | -5876.195655 | -5875.96356  |
| <b>INT2<sup>mo</sup></b>   | -5875.924443 | -5876.196986 | -5875.96603  |
| <b>TS3<sup>mo</sup></b>    | -5875.906639 | -5876.174696 | -5875.94676  |
| <b>INT3<sup>mo</sup></b>   | -5875.949938 | -5876.222518 | -5875.99078  |
| <b>B</b>                   | -6355.181493 | -6355.625597 | -6355.23405  |

**Table S3-2.** The total energies ( $E_{\text{tot}}/\text{a.u.} = E_{\text{elec}}/\text{a.u.} + \text{ZPE}/\text{a.u.}$ ), electronic energies ( $E_{\text{elec}}/\text{a.u.}$ ) and Gibbs free energies ( $G/\text{a.u.}$ ) for the oxidative process ( $\text{Pd}^{\text{II}}$  to  $\text{Pd}^{\text{III}}$ ), involved in the discussion on  $\text{PhI}(\text{OAc})_2$  (**OX-a**),  $\text{PhICl}_2$  (**OX-b**) and NCS (**OX-c**) as oxidant, computed at B3LYP-IDSCRF/DGDZVP level in dichloromethane at 238K(**OX-a**), 243K(**OX-b**), 195K(**OX-c**).

| Species                     | $E_{\text{tot}}/\text{a.u.}$ | $E_{\text{elec}}/\text{a.u.}$ | $G/\text{a.u.}$ |
|-----------------------------|------------------------------|-------------------------------|-----------------|
| <b>PhI(OAc)<sub>2</sub></b> | -7608.331455                 | -7608.522826                  | -7608.35679     |
| <b>TS1a</b>                 | -18902.04864                 | -18902.66232                  | -18902.09854    |
| <b>INT1a</b>                | -11522.18901                 | -11522.66282                  | -11522.22877    |
| <b>2a</b>                   | -11750.62716                 | -11751.15272                  | -11750.66923    |
| <b>PhI</b>                  | -7151.450199                 | -7151.539913                  | -7151.46482     |
| <b>OAc-radical</b>          | -228.411795                  | -228.4594773                  | -228.42423      |
| <b>1b</b>                   | -11446.16008                 | -11446.60878                  | -11446.19677    |
| <b>PhICl<sub>2</sub></b>    | -8071.742501                 | -8071.834146                  | -8071.75997     |
| <b>TS1b</b>                 | -19517.86657                 | -19518.4071                   | -19517.91239    |
| <b>INT1b</b>                | -19517.88244                 | -19518.42382                  | -19517.9283     |
| <b>INT2b</b>                | -19517.88238                 | -19518.42444                  | -19517.92705    |
| <b>2b</b>                   | -12366.46661                 | -12366.91869                  | -12366.5048     |
| <b>1c</b>                   | -11709.34261                 | -11709.8514                   | -11709.37026    |
| <b>NCS</b>                  | -820.171193                  | -820.2527436                  | -820.18298      |
| <b>TS1c</b>                 | -12758.5482                  | -12759.1967                   | -12758.584      |
| <b>INT1c</b>                | -12169.27195                 | -12169.78316                  | -12169.29911    |
| <b>2c</b>                   | -12397.91746                 | -12398.47901                  | -12397.9479     |
| <b>Succinimide...OAc</b>    | -589.272392                  | -589.4133622                  | -589.28805      |
| <b>succinimide</b>          | -360.648443                  | -360.7400759                  | -360.65881      |

**Table S3-3.** The total energies ( $E_{\text{tot}}/\text{a.u.} = E_{\text{elec}}/\text{a.u.} + \text{ZPE}/\text{a.u.}$ ), electronic energies ( $E_{\text{elec}}/\text{a.u.}$ ) and Gibbs free energies ( $G/\text{a.u.}$ ) for the oxidative process ( $\text{Pd}^{\text{II}}$  to  $\text{Pd}^{\text{IV}}$ ), involved in the discussion on  $\text{PhI}(\text{OAc})_2$  (**OX-a**),  $\text{PhICl}_2$  (**OX-b**) and NCS (**OX-c**) as oxidant, computed at B3LYP-IDSCRF/DGDZVP level in dichloromethane at 298K.

| Species | $E_{\text{tot}}/\text{a.u.}$ | $E_{\text{elec}}/\text{a.u.}$ | $G/\text{a.u.}$ |
|---------|------------------------------|-------------------------------|-----------------|
|---------|------------------------------|-------------------------------|-----------------|

|                |               |                |              |
|----------------|---------------|----------------|--------------|
| <b>1m</b>      | -5896.998745  | -5897.317236   | -5897.03317  |
| <b>TS1m-a</b>  | -13505.29958  | -13505.80807   | -13505.3574  |
| <b>INT1m-a</b> | -6125.458569  | -6125.827527   | -6125.50047  |
| <b>2m-a</b>    | -6353.929224  | -6354.350844   | -6353.97523  |
| <b>COM1m-b</b> | -13968.760494 | -13969.1711579 | -13968.81040 |
| <b>TS1m-b</b>  | -13968.743517 | -13969.1531934 | -13968.79232 |
| <b>INT1m-b</b> | -13968.776827 | -13969.1884588 | -13968.82477 |
| <b>2m-b</b>    | -6817.365714  | -6817.68748987 | -6817.40408  |
| <b>TS1m-c</b>  | -6717.157715  | -6717.55702    | -6717.20227  |
| <b>2m-c</b>    | -6717.210782  | -6717.612576   | -6717.25352  |

**Table S3-4.** The electronic energies ( $E_{\text{elec/a.u.}}$ ) for the C-H activation, involved in the discussion on  $\text{Pd}(\text{OAc})_2$  as catalyst, computed at B2PLYP-IDSCRF/DGDZVP level in dichloromethane at 313K.

| <b>Species</b>                                    | <b><math>E_{\text{elec/a.u.}}</math></b> | <b>Species</b>                                                  | <b><math>E_{\text{elec/a.u.}}</math></b> |
|---------------------------------------------------|------------------------------------------|-----------------------------------------------------------------|------------------------------------------|
| <b>R</b>                                          | -478.8311177                             | <b><math>\text{Pd}_2(\text{OAc})_2(\mu\text{-OAc})_2</math></b> | -10791.36655                             |
| <b><math>\text{Pd}_2(\mu\text{-OAc})_4</math></b> | -10791.37777                             | <b>AcOH</b>                                                     | -228.8907035                             |
| <b>COM1<sup>bi</sup></b>                          | -11270.21921                             | <b><math>\text{Pd}(\text{OAc})_2</math></b>                     | -5395.664309                             |
| <b>TS1<sup>bi</sup></b>                           | -11270.21669                             | <b>COM1mo</b>                                                   | -5874.502277                             |
| <b>INT1<sup>bi</sup></b>                          | -11270.23126                             | <b>TS1mo</b>                                                    | -5874.494225                             |
| <b>TS2<sup>bi</sup></b>                           | -11749.06804                             | <b>INT1mo</b>                                                   | -5874.528225                             |
| <b>INT2<sup>bi</sup></b>                          | -11749.09428                             | <b>TS2mo</b>                                                    | -5874.507141                             |
| <b>TS3<sup>bi</sup></b>                           | -11749.05077                             | <b>INT2mo</b>                                                   | -5874.516092                             |
| <b>INT3<sup>bi</sup></b>                          | -11520.19887                             | <b>TS3mo</b>                                                    | -5874.485751                             |
| <b>TS4<sup>bi</sup></b>                           | -11520.16399                             | <b>INT3mo</b>                                                   | -5874.540749                             |
| <b>1a</b>                                         | -11291.31271                             | <b>B</b>                                                        | -6353.390011                             |

**Table S3-5.** The electronic energies ( $E_{\text{elec/a.u.}}$ ) for the oxidative process ( $\text{Pd}^{\text{II}}$  to  $\text{Pd}^{\text{III}}$ ), involved in the discussion on  $\text{PhI}(\text{OAc})_2$  (**OX-a**),  $\text{PhICl}_2$  (**OX-b**) and  $\text{NCS}$  (**OX-c**) as oxidant, computed at B2PLYP-IDSCRF/DGDZVP level in dichloromethane at 238K(**OX-a**), 243K(**OX-b**), 195K(**OX-c**).

| <b>Species</b>                               | <b><math>E_{\text{elec/a.u.}}</math></b> | <b>Species</b>           | <b><math>E_{\text{elec/a.u.}}</math></b> |
|----------------------------------------------|------------------------------------------|--------------------------|------------------------------------------|
| <b><math>\text{PhI}(\text{OAc})_2</math></b> | -7607.054784                             | <b>INT2b</b>             | -19514.16012                             |
| <b>TS1a</b>                                  | -18898.343                               | <b>2b</b>                | -12363.63777                             |
| <b>INT1a</b>                                 | -11519.56736                             | <b>1c</b>                | -11706.5622                              |
| <b>2a</b>                                    | -11747.85475                             | <b>NCS</b>               | -819.7084437                             |
| <b>PhI</b>                                   | -7150.537903                             | <b>TS1c</b>              | -12755.14264                             |
| <b>OAc-radical</b>                           | -228.2220439                             | <b>INT1c</b>             | -12166.34698                             |
| <b>1b</b>                                    | -11443.6333                              | <b>2c</b>                | -12394.81448                             |
| <b><math>\text{PhICl}_2</math></b>           | -8070.498449                             | <b>Succinimide...OAc</b> | -588.7916266                             |
| <b>TS1b</b>                                  | -19514.11186                             | <b>succinimide</b>       | -360.3557501                             |
| <b>INT1b</b>                                 | -19514.13514                             |                          |                                          |

**Table S3-6.** The electronic energies ( $E_{\text{elec/a.u.}}$ ) for the oxidative process ( $\text{Pd}^{\text{II}}$  to  $\text{Pd}^{\text{IV}}$ ), involved in the discussion on  $\text{PhI}(\text{OAc})_2$  (**OX-a**),  $\text{PhICl}_2$  (**OX-b**) and  $\text{NCS}$  (**OX-c**) as oxidant, computed at B2PLYP-IDSCRF/DGDZVP level in dichloromethane at 298K.

| <b>Species</b> | <b><math>E_{\text{elec/a.u.}}</math></b> | <b>Species</b> | <b><math>E_{\text{elec/a.u.}}</math></b> |
|----------------|------------------------------------------|----------------|------------------------------------------|
| <b>1m</b>      | -5895.560545                             | <b>TS1m-b</b>  | -13966.05858                             |

|                |              |                |              |
|----------------|--------------|----------------|--------------|
| <b>TS1m-a</b>  | -13502.58649 | <b>INT1m-b</b> | -13966.10805 |
| <b>INT1m-a</b> | -6123.843366 | <b>2m-b</b>    | -6815.603856 |
| <b>2m-a</b>    | -6352.145006 | <b>TS1m-c</b>  | -6715.264904 |
| <b>COM1m-b</b> | -13966.07195 | <b>2m-c</b>    | -6715.335496 |

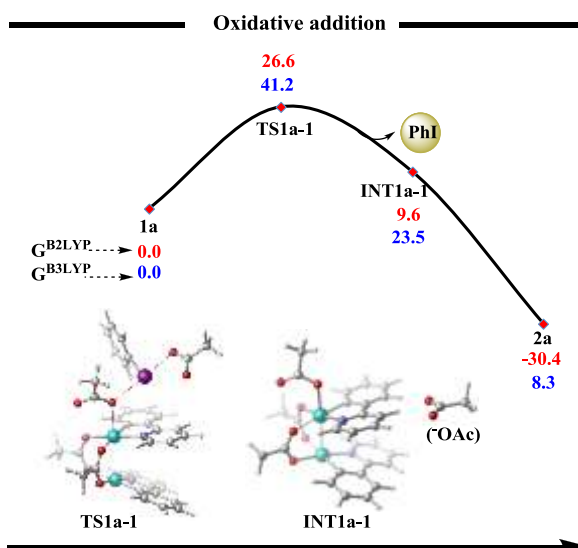
**Table S4.** Calculated free energy barriers (kcal mol<sup>-1</sup>) with the oxidation of 1a→2a for different calculation methods.

| method         | d <sub>2a</sub><br>(Pd <sup>III</sup> -Pd <sup>III</sup> ) | ΔE<br>(1a→2a) | ΔG<br>(1a→2a) | ΔE<br>(TS) | ΔG<br>(TS) |
|----------------|------------------------------------------------------------|---------------|---------------|------------|------------|
| B3LYP-IDSCRF   | 2.68                                                       | 5.0           | 8.3           | 24.1       | 30.6       |
| B2LYP-IDSCRF   | 2.67                                                       | -15.8         | -12.5         | 15.4       | 21.9       |
| Tpsstps-IDSCRF | 2.65                                                       | -11.0         | -8.0          | 14.0       | 20.5       |
| Wb97xd-IDSCRF  | 2.60                                                       | 6.0           | 7.7           | -          | -          |
| Wb97-IDSCRF    | 2.59                                                       | 17.1          | 20.2          | -          | -          |
| Pbepbe-IDSCRF  | 2.68                                                       | -9.9          | -6.2          | 11.4       | 18.1       |
| Pbe1pbe-IDSCRF | 2.62                                                       | 4.5           | 7.5           | -          | -          |
| M06L-IDSCRF    | 2.63                                                       | -14.3         | -11.5         | -          | -          |
| M06-IDSCRF     | 2.63                                                       | 6.6           | 8.1           | -          | -          |
| Exp.           | 2.55                                                       | -             | -             | -          | -          |

**Table S5.** Calculated free energy barriers (ΔG, kcal mol<sup>-1</sup>) with the oxidation of B3LYP-IDSCRF+D3/DGDZVP.

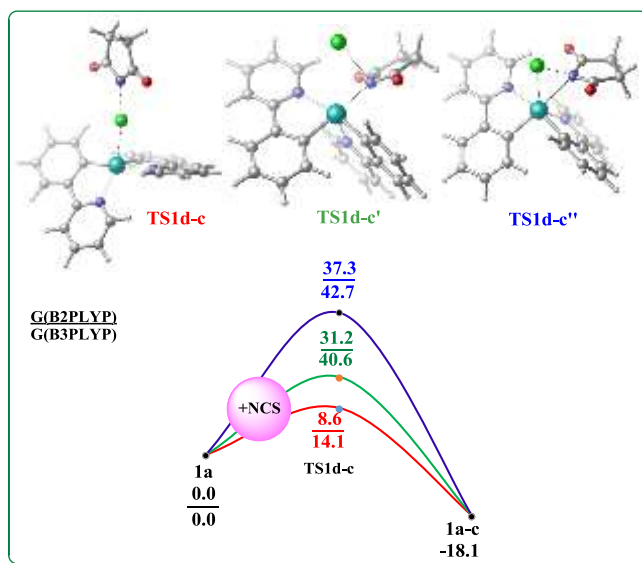
| method          | TS1m-a | TS1m-b | TS1m-c | TS1a | TS1b | TS1c |
|-----------------|--------|--------|--------|------|------|------|
| B3LYP-IDSCRF+D3 | 4.8    | 0.2    | 2.1    | 12.0 | 10.8 | 17.7 |

**Figure S1.** Gibbs free-energy profiles (ΔG, kcal mol<sup>-1</sup>) for the oxidative process (Pd<sup>II</sup> to Pd<sup>III</sup>), involved in the discussion on PhI(OAc)<sub>2</sub> (**OX-a**) as oxidant, with the schematic representation of stationary points along the reaction coordinates in dichloromethane at 238K(**OX-a**).

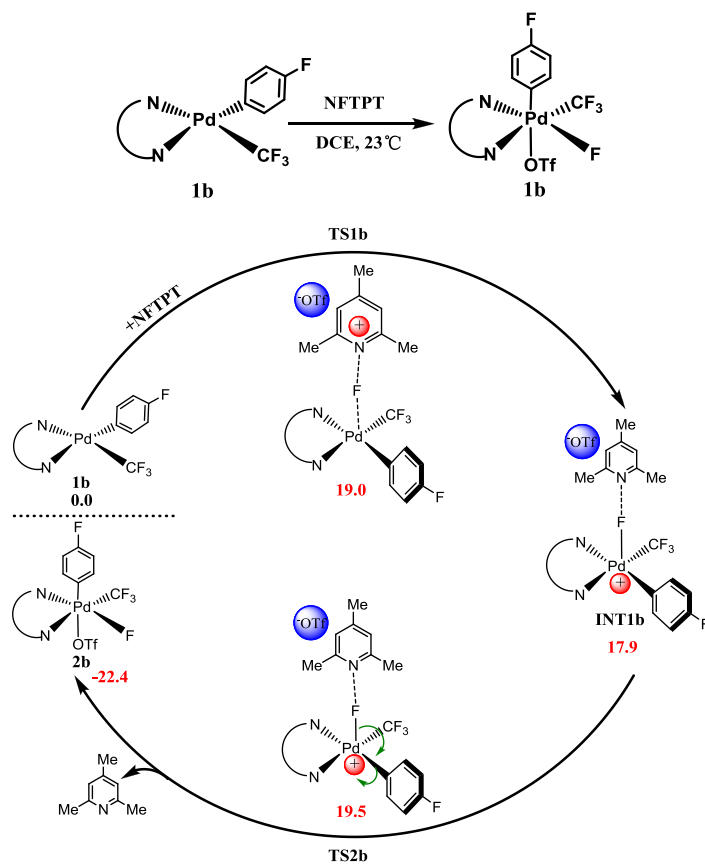


**Figure S2.** Gibbs free-energy profiles (ΔG, kcal mol<sup>-1</sup>) for the oxidative process (Pd<sup>II</sup> to Pd<sup>IV</sup>), involved in the

discussion on NCS (**OX-c**) as oxidant, with the schematic representation of stationary points along the reaction coordinates in dichloromethane at 298K.

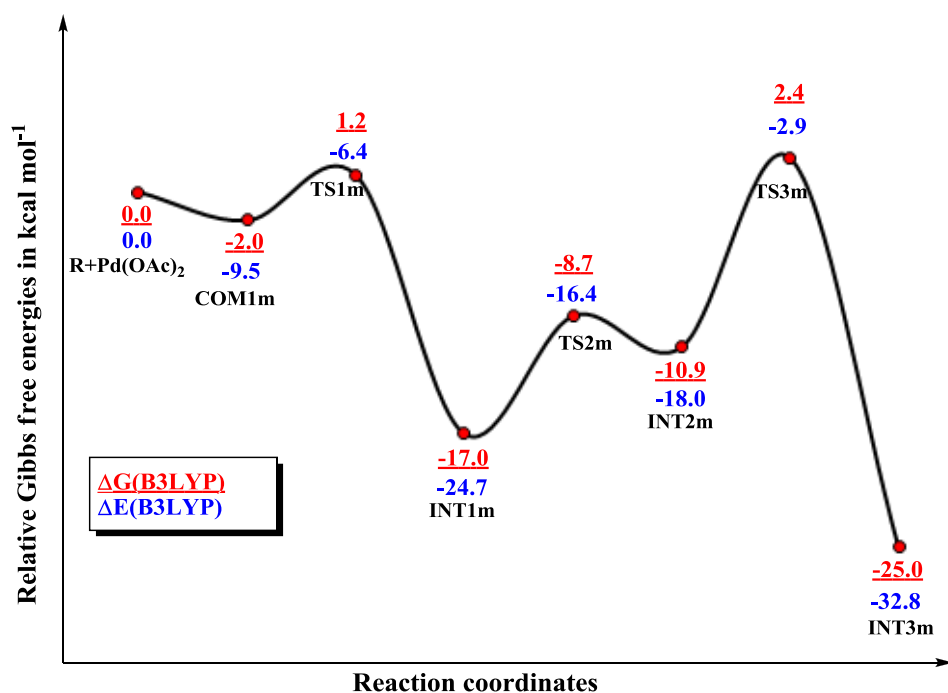


**Figure S3.** Gibbs free-energy profiles ( $\Delta G$ , kcal mol<sup>-1</sup>) for the oxidative process (Pd<sup>II</sup> to Pd<sup>IV</sup>), involved in the discussion on NFTPT (**OX-d**) as oxidant, computed at B3LYP-IDSCRF/DGDZVP level, with the schematic representation of stationary points along the reaction coordinates in DCE at 296K.



**Figure S4.** Gibbs free-energy profiles ( $\Delta G$ , kcal mol<sup>-1</sup>) for the C-H activation process, involved in the mononuclear

mechanism, computed at B3LYP-IDSCRF+D3/DGDZVP in dichloromethane at 298K.



**Figure S5.** The bond length change (Å) and the change of  $\langle S^2 \rangle$  expectation value along the distance of O1-Pd (Å) under IRC of TS1m-a.

