

Т а б л и ц а S1

**Критические точки электронной плотности (ат.ед.) между реакционными центрами в структуре комплексов реагентов, переходных состояний и продуктов (интермедиатов) на последней стадии замещения хлора на фенильную группу**

| Tt | Критические точки |                      | Ph...Tt(Ph) <sub>3</sub> Cl                                                                 | TS                                                                           | Tt(Ph) <sub>4</sub> ...Cl (Tt = C),<br>Ph...Tt(Ph) <sub>3</sub> ...Cl<br>(Tt = Si, Ge) |
|----|-------------------|----------------------|---------------------------------------------------------------------------------------------|------------------------------------------------------------------------------|----------------------------------------------------------------------------------------|
| C  | (3,-1)<br>связи   | C(Ph)-Tt             | —                                                                                           | —                                                                            | 0.092                                                                                  |
|    |                   | C(Ph)...другие атомы | C(Ph)...C (0.005);<br>C(Ph)...C (0.004);<br>C(Ph)...H (0.005)                               | C(Ph)...C (0.008);<br>C(Ph)...H (0.009);<br>C(Ph)...H (0.010)                | -                                                                                      |
|    |                   | Tt-Cl                | 0.128                                                                                       | 0.081                                                                        | -                                                                                      |
|    |                   | Cl...другие атомы    | —                                                                                           | --                                                                           | Cl...C (0.009);<br>Cl...C (0.005);<br>Cl...C (0.005);                                  |
|    | (3,+1)<br>цикла   | между Tt и Ph        | Tt-C-C-C(Ph)-H-C-C<br>(0.003);<br>Tt-C-C-H-C(Ph)-C-C<br>(0.003)<br>Tt-C-C-C(Ph)-C-C (0.003) | Tt-C-C(Ph)-H-C-C (0.007);<br>Tt-C-C(Ph)-H-C-C (0.007)                        | —                                                                                      |
|    |                   | между Tt и Cl        | —                                                                                           | —                                                                            | Tt-C-C-H-C-C(Ph) (0.012);<br>Cl-C-H-C-C (0.004);<br>Tt-C-C-C-Cl-C-C (0.003)            |
|    | (3,+3) клетки     |                      | 0.002                                                                                       | —                                                                            | —                                                                                      |
| Si | (3,-1)<br>связи   | C(Ph)-Tt             | —                                                                                           | —                                                                            | 0.111                                                                                  |
|    |                   | C(Ph)...другие атомы | C(Ph)...C (0.003);<br>C(Ph)...H (0.011);<br>C(Ph)...H (0.007)                               | C(Ph)...C (0.007);<br>C(Ph)...H (0.022);<br>C(Ph)...H (0.018)                | C(Ph)...C (0.301);<br>C(Ph)...C (0.298);<br>C(Ph)...H (0.014);                         |
|    |                   | Tt-Cl                | 0.084                                                                                       | 0.077                                                                        | —                                                                                      |
|    |                   | Cl...другие атомы    | Cl...H (0.010)                                                                              | Cl...H (0.011);<br>Cl...H (0.013)                                            | Cl...H (0.017);<br>Cl...H (0.008);<br>Cl...C (0.006)                                   |
|    | (3,+1)<br>цикла   | между Tt и Ph        | Tt-C-C(Ph)-H-C-C<br>(0.003);<br>Tt-C-C-H-C(Ph)-C (0.003)                                    | Tt-C-C(Ph)-H-C-C (0.006);<br>Tt-C-C-H-C(Ph)-C (0.006)                        | —                                                                                      |
|    |                   | между Tt и Cl        | —                                                                                           | —                                                                            | Tt-C-Cl-H-C-C (0.005);<br>Tt-C-C-H-Cl-C (0.005)                                        |
|    | (3,+3) клетки     |                      | —                                                                                           | —                                                                            | —                                                                                      |
| Ge | (3,-1)<br>связи   | C(Ph)-Tt             | —                                                                                           | 0.007                                                                        | 0.036                                                                                  |
|    |                   | C(Ph)...другие атомы | C(Ph)...H (0.006);<br>C(Ph)...H (0.015);<br>C(Ph)...H (0.015)                               | C(Ph)...H (0.002);<br>C(Ph)...H (0.017);<br>C(Ph)...H (0.013)                | C(Ph)...H (0.010);<br>C(Ph)...H (0.015);                                               |
|    |                   | Tt-Cl                | 0.083                                                                                       | 0.078                                                                        | —                                                                                      |
|    |                   | Cl...другие атомы    | Cl...H (0.012);<br>Cl...H (0.013)                                                           | Cl...H (0.012);<br>Cl...H (0.010);<br>Cl...H (0.012);                        | Cl...H (0.015)                                                                         |
|    | (3,+1)<br>цикла   | между Tt и Ph        | Tt-C-C-H-C(Ph) (0.004);<br>Tt-C-C-H-C(Ph) (0.004);<br>Tt-C-C-H-C(Ph) (0.004)                | Tt-C-C-H-C(Ph) (0.006);<br>Tt-C-C-H-C(Ph) (0.006);<br>Tt-C-C-H-C(Ph) (0.006) | —                                                                                      |
|    |                   | между Tt и Cl        | —                                                                                           | —                                                                            | -                                                                                      |
|    | (3,+3) клетки     |                      | 0.004                                                                                       | —                                                                            | —                                                                                      |