# Supporting Information

Some optimized geometrical parameters of the complexes $[Pb(S_2COEt)_n]^{2-n}$ (n=1,2,3,4) are given at CL1 level. Here bond lengths are given in Å and angles are given in degrees.

**Table 1.** Geometry of complex $[Pb(S_2COEt)]^+$

| **Parameter** | **CL1** |
|---|---|
| **Bond lengths** | |
| PbS1 | 2.632 |
| PbS2 | 2.665 |
| S1C1 | 1.730 |
| S2C1 | 1.726 |
| C1O | 1.281 |
| **Angles** | |
| S1PbS2 | 69.6 |
| PbS1C1 | 84.6 |
| PbS2C1 | 83.6 |
| S1C1S2 | 122.1 |
| S2C1O | 122.5 |
| OC1S1 | 115.3 |

**Table 2.** Geometry of complex $Pb(S_2COEt)_2$

| **Parameter** | **CL1** | **Expt.**[a] |
|---|---|---|
| **Bond lengths** | | |
| PbS1 | 2.943 | 2.95 |
| PbS2 | 2.711 | 2.79 |
| PbS3 | 2.943 | 2.84 |
| PbS4 | 2.711 | 2.74 |
| S1S3 | 5.514 | 4.16 |
| S2S4 | 3.971 | 3.77 |
| S1C1 | 1.692 | 1.66 |
| S2C1 | 1.716 | 1.78 |
| **Angles** | | |
| S1C1S2 | 124.3 | 124 |
| C1S1Pb | 82.1 | 87 |
| PbS2C1 | 89.1 | 91 |

| | | |
|---|---|---|
| C1PbC2 | 107.3 | - |

[a] Reference [44]

**Table 3.** Geometry of complex $[Pb(S_2COEt)_3]^-$

| **Parameter** | **CL1** | **Expt**[b] |
|---|---|---|
| **Bond lengths** | | |
| PbS1 | 3.210 | 3.086 |
| PbS2 | 2.895 | 2.754 |
| C1S1 | 1.685 | - |
| C1S2 | 1.706 | - |
| PbS3 | 3.210 | 3.126 |
| PbS4 | 2.895 | 2.942 |
| C2S3 | 1.685 | - |
| C2S4 | 1.706 | - |
| PbS5 | 3.302 | 3.029 |
| PbS6 | 2.733 | 2.946 |
| C3S5 | 1.675 | - |
| C3S6 | 1.716 | - |
| **Angles** | | |
| C1PbC2 | 140.3 | - |
| C1PbC3 | 100.1 | - |
| C2PbC3 | 100.1 | - |

[b] Reference [45]

**Table 4.** Geometry of complex $[Pb(S_2COEt)_4]^{2-}$

| Parameter | CL1 |
|---|---|
| **Bond lengths** | |
| C1S1 | 1.692 |
| C1S2 | 1.687 |
| C2S3 | 1.693 |
| C2S4 | 1.687 |
| C3S5 | 1.692 |
| C3S6 | 1.687 |
| C4S7 | 1.693 |
| C4S8 | 1.687 |
| **Angles** | |
| S1PbS2 | 55.2 |
| S3PbS4 | 57.5 |
| S5PbS6 | 55.2 |
| S7PbS8 | 57.5 |
| S1C1S2 | 126.8 |
| S3C2S4 | 126.2 |
| S5C3S6 | 126.8 |
| S7C4S8 | 126.2 |
| C1PbC3 | 134.0 |
| C2PbC4 | 136.6 |
| C1PbC2 | 98.3 |
| C1PbC4 | 98.3 |
| C2PbC3 | 98.3 |
| C3PbC4 | 98.3 |

**Table 5.** NBO analysis of $[Pb^{II}(S_2COEt)]^+$ at CL1.

| | | Composition of NBO | | | | |
|---|---|---|---|---|---|---|
| **Interaction** | **Atom** | **%$\|c_A\|^2$** | **%s** | **%p** | **%d** | $\Delta E_{CT}$ |
| $LP_{S1} \rightarrow LP^*_{Pb}$ | S1(Pb) | - | 0.0(0.0) | 99.8(97.3) | 0.2(2.7) | 12.1 |
| $BD_{S2\text{-}C1} \rightarrow LP^*_{Pb}$ | S2(Pb) | 79.1 | 0.0(0.0) | 99.8(97.3) | 0.2(2.7) | 6.4 |
| | C1 | 20.9 | 0.0 | 99.8 | 0.2 | |

$\Delta E_{CT}$ is given in kcal/mol. The data inside parenthesis correspond to acceptor NBO.

**Table 6.** NBO analysis of $Pb^{II}(S_2COEt)_2$ at CL1.

| Interaction | Composition of NBO | | | | | |
|---|---|---|---|---|---|---|
| | **Atom** | **%$\|c_A\|^2$** | **%s** | **%p** | **%d** | $\Delta E_{CT}$ |
| $BD_{Pb\text{-}S1} \rightarrow BD^*_{Pb\text{-}S3}$ | Pb(Pb) | 6.0(94.0) | 3.6(3.6) | 60.1(60.1) | 36.3(36.3) | 39.0 |
| | S1(S3) | 94.0(6.0) | 8.3(8.3) | 91.6(91.6) | 0.1(0.1) | |
| $BD_{Pb\text{-}S1} \rightarrow BD^*_{Pb\text{-}S1}$ | Pb(Pb) | 6.0(94.0) | 3.6(3.6) | 60.1(60.1) | 36.3(36.3) | 12.7 |
| | S1(S1) | 94.0(6.0) | 8.3(8.3) | 91.6(91.6) | 0.1(0.1) | |
| $BD_{Pb\text{-}S1} \rightarrow BD^*_{Pb\text{-}S2}$ | Pb(Pb) | 6.0(85.0) | 3.6(2.1) | 60.1(90.4) | 36.3(7.5) | 12.2 |
| | S1(S2) | 94.0(15.0) | 8.3(11.0) | 91.6(89.0) | 0.1(0.0) | |
| $BD_{Pb\text{-}S1} \rightarrow BD^*_{Pb\text{-}S4}$ | Pb(Pb) | 6.0(85.0) | 3.6(2.1) | 60.1(90.4) | 36.3(7.5) | 9.3 |
| | S1(S4) | 94.0(15.0) | 8.3(11.0) | 91.6(89.0) | 0.1(0.0) | |
| $BD_{Pb\text{-}S1} \rightarrow RY^*_{Pb}$ | Pb(Pb) | 6.0 | 3.6(88.0) | 60.1(0.9) | 36.3(11.1) | 8.1 |
| | S1 | 94.0 | 8.3 | 91.6 | 0.1 | |
| $BD_{Pb\text{-}S3} \rightarrow BD^*_{Pb\text{-}S1}$ | Pb(Pb) | 6.0(94.0) | 3.6(3.6) | 60.1(60.1) | 36.3(36.3) | 39.0 |
| | S3(S1) | 94.0(6.0) | 8.3(8.3) | 91.6(91.6) | 0.1(0.1) | |
| $BD_{Pb\text{-}S3} \rightarrow BD^*_{Pb\text{-}S3}$ | Pb(Pb) | 6.0(94.0) | 3.6(3.6) | 60.1(60.1) | 36.3(36.3) | 12.7 |
| | S3(S3) | 94.0(6.0) | 8.3(8.3) | 91.6(91.6) | 0.1(0.1) | |
| $BD_{Pb\text{-}S3} \rightarrow BD^*_{Pb\text{-}S4}$ | Pb(Pb) | 6.0(85.0) | 3.6(2.1) | 60.1(90.4) | 36.3(7.5) | 12.2 |
| | S3(S4) | 94.0(15.0) | 8.3(11.0) | 91.6(89.0) | 0.1(0.0) | |
| $BD_{Pb\text{-}S3} \rightarrow BD^*_{Pb\text{-}S2}$ | Pb(Pb) | 6.0(85.0) | 3.6(2.1) | 60.1(90.4) | 36.3(7.5) | 9.3 |
| | S3(S2) | 94.0(15.0) | 8.3(11.0) | 91.6(89.0) | 0.1(0.0) | |
| $BD_{Pb\text{-}S3} \rightarrow RY^*_{Pb}$ | Pb(Pb) | 6.0 | 3.6(88.0) | 60.1(0.9) | 36.3(11.1) | 8.1 |
| | S3 | 94.0 | 8.3 | 91.6 | 0.1 | |
| BDPb-S2→BD*Pb-S3 | Pb(Pb) | 15.0(94.0) | 2.1(3.6) | 90.4(60.1) | 7.5(36.3) | 19.1 |
| | S2(S3) | 85.0(6.0) | 11.0(8.3) | 89.0(91.6) | 0.0(0.1) | |
| BDPb-S2→BD*Pb-S1 | Pb(Pb) | 15.0(94.0) | 2.1(3.6) | 90.4(60.1) | 7.5(36.3) | 18.8 |
| | S2(S1) | 85.0(6.0) | 11.0(8.3) | 89.0(91.6) | 0.0(0.1) | |
| BDPb-S2→RY*Pb | Pb(Pb) | 15.0 | 2.1(88.0) | 90.4(0.9) | 7.5(11.1) | 7.0 |
| | S2 | 85.0 | 11.0 | 89.0 | 0.0 | |
| BDPb-S4→BD*Pb-S1 | Pb(Pb) | 15.0(94.0) | 2.1(3.6) | 90.4(60.1) | 7.5(36.3) | 19.1 |
| | S4(S1) | 85.0(6.0) | 11.0(8.3) | 89.0(91.6) | 0.0(0.1) | |
| BDPb-S4→BD*Pb-S3 | Pb(Pb) | 15.0(94.0) | 2.1(3.6) | 90.4(60.1) | 7.5(36.3) | 18.8 |
| | S4(S3) | 85.0(6.0) | 11.0(8.3) | 89.0(91.6) | 0.0(0.1) | |
| BDPb-S4→RY*Pb | Pb(Pb) | 15.0 | 2.1(88.0) | 90.4(0.9) | 7.5(11.1) | 7.0 |
| | S4 | 85.0 | 11.0 | 89.0 | 0.0 | |

$\Delta E_{CT}$ is given in kcal/mol. The data inside parenthesis correspond to acceptor NBO.

**Table 7.** NBO analysis of $[Pb^{II}(S_2COEt)_3]^-$ at CL1.

| Interaction | Composition of NBO | | | | | $\Delta E_{CT}$ |
|---|---|---|---|---|---|---|
| | Atom | $\%\lvert c_A\rvert^2$ | %s | %p | %d | |
| $BD_{Pb\text{-}S1} \rightarrow BD^*_{Pb\text{-}S3}$ | Pb(Pb) | 2.68 (97.32) | 11.03(11.03) | 54.21(54.21) | 34.76(34.76) | 32.8 |
| | S1(S3) | 97.32(2.68) | 6.78(6.78) | 93.18(93.18) | 0.04(0.04) | |
| $BD_{Pb\text{-}S1} \rightarrow BD^*_{Pb\text{-}S4}$ | Pb(Pb) | 2.68(93.13) | 11.03(2.61) | 54.21(71.66) | 34.76(25.73) | 27.5 |
| | S1(S4) | 97.32(6.87) | 6.78(12.07) | 93.18(87.86) | 0.04(0.07) | |
| $BD_{Pb\text{-}S1} \rightarrow BD^*_{Pb\text{-}S1}$ | Pb(Pb) | 2.68(97.32) | 11.03(11.03) | 54.21(54.21) | 34.76(34.76) | 21.2 |
| | S1(S1) | 97.32(2.68) | 6.78(6.78) | 93.18(93.18) | 0.04(0.04) | |
| $BD_{Pb\text{-}S1} \rightarrow RY^*_{Pb}$ | Pb(Pb) | 2.7 | 11.03(53.71) | 54.21( 1.39) | 34.76(44.90) | 16.6 |
| | S1 | 97.3 | 6.8 | 93.2 | 0.0 | |
| $BD_{Pb\text{-}S1} \rightarrow RY^*_{Pb}$ | Pb(Pb) | 2.7 | 11.03(12.6) | 54.21( 0.8) | 34.76(86.6) | 10.8 |
| | S1 | 97.3 | 6.8 | 93.2 | 0.0 | |
| $BD_{Pb\text{-}S1} \rightarrow RY^*_{Pb}$ | Pb(Pb) | 2.7 | 11.03(3.5) | 54.21(1.0) | 34.76(95.5) | 6.1 |
| | S1 | 97.3 | 6.8 | 93.2 | 0.0 | |
| $BD_{Pb\text{-}S3} \rightarrow BD^*_{Pb\text{-}S1}$ | Pb(Pb) | 2.68(97.32) | 11.03(11.03) | 54.21(54.21) | 34.76(34.76) | 32.8 |
| | S3(S1) | 97.32( 2.68) | 6.78(6.78) | 93.18(93.18) | 0.04( 0.04) | |
| $BD_{Pb\text{-}S3} \rightarrow BD^*_{Pb\text{-}S2}$ | Pb(Pb) | 2.68(93.13) | 11.03(2.61) | 54.21(71.66) | 34.76(25.73) | 27.5 |
| | S3(S2) | 97.32(6.87) | 6.78(12.07) | 93.18(87.86) | 0.04(0.07) | |
| $BD_{Pb\text{-}S3} \rightarrow BD^*_{Pb\text{-}S3}$ | Pb(Pb) | 2.68(97.32) | 11.03(11.03) | 54.21(54.21) | 34.76(34.76) | 21.2 |
| | S3(S3) | 97.32(2.68) | 6.78( 6.78) | 93.18(93.18) | 0.04(0.04) | |
| $BD_{Pb\text{-}S3} \rightarrow RY^*_{Pb}$ | Pb(Pb) | 2.7 | 11.03(53.71) | 54.21(1.39) | 34.76(44.90) | 16.6 |
| | S3 | 97.3 | 6.8 | 93.2 | 0.0 | |
| $BD_{Pb\text{-}S3} \rightarrow RY^*_{Pb}$ | Pb(Pb) | 2.7 | 11.03(12.6) | 54.21( 0.8) | 34.76(86.6) | 10.9 |
| | S3 | 97.3 | 6.8 | 93.2 | 0.0 | |
| $BD_{Pb\text{-}S3} \rightarrow RY^*_{Pb}$ | Pb(Pb) | 2.7 | 11.03(3.5) | 54.21(1.0) | 34.76(95.5) | 6.1 |
| | S3 | 97.3 | 6.8 | 93.2 | 0.0 | |
| $BD_{Pb\text{-}S2} \rightarrow BD^*_{Pb\text{-}S3}$ | Pb(Pb) | 6.87(97.32) | 2.61(11.03) | 71.66(54.21) | 25.73(34.76) | 34.0 |
| | S2(S3) | 93.13(2.68) | 12.07( 6.78) | 87.86(93.18) | 0.07(0.04) | |
| $BD_{Pb\text{-}S2} \rightarrow BD^*_{Pb\text{-}S2}$ | Pb(Pb) | 6.87(93.13) | 2.61(2.61) | 71.66(71.66) | 25.73(25.73) | 13.0 |
| | S2(S2) | 93.13(6.87) | 12.07( 12.07) | 87.86(87.86) | 0.07(0.07) | |
| $BD_{Pb\text{-}S2} \rightarrow RY^*_{Pb}$ | Pb(Pb) | 6.9 | 2.61(53.71) | 71.66(1.39) | 25.73(44.90) | 5.0 |
| | S2 | 93.1 | 12.1 | 87.9 | 0.1 | |
| $BD_{Pb\text{-}S4} \rightarrow BD^*_{Pb\text{-}S1}$ | Pb(Pb) | 6.87(97.32) | 2.61(11.03) | 71.66(54.21) | 25.73(34.76) | 34.0 |
| | S4(S1) | 93.13(2.68) | 12.07(6.78) | 87.86(93.18) | 0.07(0.04) | |
| $BD_{Pb\text{-}S4} \rightarrow BD^*_{Pb\text{-}S4}$ | Pb(Pb) | 6.9 | 2.6 | 71.7 | 25.7 | 13.0 |
| | S4(S4) | 93.1 | 12.1 | 87.9 | 0.1 | |
| $BD_{Pb\text{-}S4} \rightarrow RY^*_{Pb}$ | Pb(Pb) | 6.9 | 2.61(53.71) | 71.66(1.39) | 25.73(44.90) | 5.0 |
| | S4 | 93.1 | 12.1 | 87.9 | 0.1 | |
| $BD_{Pb\text{-}S6} \rightarrow BD^*_{Pb\text{-}S1}$ | Pb(Pb) | 14.65(97.32) | 2.35(11.03) | 95.07(54.21) | 2.57(34.76) | 12.7 |

| | | | | | | |
|---|---|---|---|---|---|---|
| | S6(S1) | 85.35(2.68) | 14.17(6.78) | 85.74(93.18) | 0.09(0.04) | |
| $BD_{Pb\text{-}S6} \rightarrow BD^{*}_{Pb\text{-}S3}$ | Pb(Pb) | 14.65(97.32) | 2.35(11.03) | 95.07(54.21) | 2.57(34.76) | 12.7 |
| | S6(S3) | 85.35(2.68) | 14.17(6.78) | 85.74(93.18) | 0.09(0.04) | |
| $BD_{Pb\text{-}S6} \rightarrow RY^{*}_{Pb}$ | Pb(Pb) | 14.7 | 2.35(53.71) | 95.07(1.39) | 2.57(44.90) | 8.2 |
| | S6 | 85.4 | 14.2 | 85.7 | 0.1 | |
| $BD_{Pb\text{-}S6} \rightarrow RY^{*}_{Pb}$ | Pb(Pb) | 14.7 | 2.35(12.60) | 95.07(0.75) | 2.57(86.64) | 5.3 |
| | S6 | 85.4 | 14.2 | 85.7 | 0.1 | |
| $LPS5 \rightarrow BD^{*}_{Pb\text{-}S2}$ | (Pb) | (93.13 | (2.61 | (71.66 | (25.73 | 3.1 |
| | S5(S2) | (6.87 | 77.04(12.07) | 22.93(87.86) | 0.02(0.07) | |

$\Delta E_{CT}$ is given in kcal/mol. The data inside parenthesis correspond to acceptor NBO.

**Table 8.** NBO analysis of $[Pb^{II}(S_2COEt)_4]^{2-}$ at CL1.

| **Interaction** | **Composition of NBO** | | | | | $\Delta E_{CT}$ |
|---|---|---|---|---|---|---|
| | **Atom** | **%$\lvert c_A \rvert^2$** | **%s** | **%p** | **%d** | |
| $LP_{S1} \rightarrow LP^{*}_{Pb}$ | S1(Pb) | - | 0.0(0.0) | 99.8(97.3) | 0.2(2.7) | 12.1 |
| $BD_{S2\text{-}C1} \rightarrow LP^{*}_{Pb}$ | S2(Pb) | 79.1 | 0.0(0.0) | 99.8(97.3) | 0.2(2.7) | 6.4 |
| | C1 | 20.9 | 0.0 | 99.8 | 0.2 | |
| $BD_{Pb\text{-}S1} \rightarrow BD^{*}_{Pb\text{-}S3}$ | Pb(Pb) | 6.0(94.0) | 3.6(3.6) | 60.1(60.1) | 36.3(36.3) | 39.0 |
| | S1(S3) | 94.0(6.0) | 8.3(8.3) | 91.6(91.6) | 0.1(0.1) | |
| $BD_{Pb\text{-}S1} \rightarrow BD^{*}_{Pb\text{-}S1}$ | Pb(Pb) | 6.0(94.0) | 3.6(3.6) | 60.1(60.1) | 36.3(36.3) | 12.7 |
| | S1(S1) | 94.0(6.0) | 8.3(8.3) | 91.6(91.6) | 0.1(0.1) | |
| $BD_{Pb\text{-}S1} \rightarrow BD^{*}_{Pb\text{-}S2}$ | Pb(Pb) | 6.0(85.0) | 3.6(2.1) | 60.1(90.4) | 36.3(7.5) | 12.2 |
| | S1(S2) | 94.0(15.0) | 8.3(11.0) | 91.6(89.0) | 0.1(0.0) | |
| $BD_{Pb\text{-}S1} \rightarrow BD^{*}_{Pb\text{-}S4}$ | Pb(Pb) | 6.0(85.0) | 3.6(2.1) | 60.1(90.4) | 36.3(7.5) | 9.3 |
| | S1(S4) | 94.0(15.0) | 8.3(11.0) | 91.6(89.0) | 0.1(0.0) | |
| $BD_{Pb\text{-}S1} \rightarrow RY^{*}_{Pb}$ | Pb(Pb) | 6.0 | 3.6(88.0) | 60.1(0.9) | 36.3(11.1) | 8.1 |
| | S1 | 94.0 | 8.3 | 91.6 | 0.1 | |
| $BD_{Pb\text{-}S3} \rightarrow BD^{*}_{Pb\text{-}S1}$ | Pb(Pb) | 6.0(94.0) | 3.6(3.6) | 60.1(60.1) | 36.3(36.3) | 39.0 |
| | S3(S1) | 94.0(6.0) | 8.3(8.3) | 91.6(91.6) | 0.1(0.1) | |
| $BD_{Pb\text{-}S3} \rightarrow BD^{*}_{Pb\text{-}S3}$ | Pb(Pb) | 6.0(94.0) | 3.6(3.6) | 60.1(60.1) | 36.3(36.3) | 12.7 |
| | S3(S3) | 94.0(6.0) | 8.3(8.3) | 91.6(91.6) | 0.1(0.1) | |
| $BD_{Pb\text{-}S3} \rightarrow BD^{*}_{Pb\text{-}S4}$ | Pb(Pb) | 6.0(85.0) | 3.6(2.1) | 60.1(90.4) | 36.3(7.5) | 12.2 |
| | S3(S4) | 94.0(15.0) | 8.3(11.0) | 91.6(89.0) | 0.1(0.0) | |
| $BD_{Pb\text{-}S3} \rightarrow BD^{*}_{Pb\text{-}S2}$ | Pb(Pb) | 6.0(85.0) | 3.6(2.1) | 60.1(90.4) | 36.3(7.5) | 9.3 |
| | S3(S2) | 94.0(15.0) | 8.3(11.0) | 91.6(89.0) | 0.1(0.0) | |
| $BD_{Pb\text{-}S3} \rightarrow RY^{*}_{Pb}$ | Pb(Pb) | 6.0 | 3.6(88.0) | 60.1(0.9) | 36.3(11.1) | 8.1 |
| | S3 | 94.0 | 8.3 | 91.6 | 0.1 | |

| | | | | | | |
|---|---|---|---|---|---|---|
| $BD_{Pb\text{-}S2} \rightarrow BD^*_{Pb\text{-}S3}$ | Pb(Pb) | 15.0(94.0) | 2.1(3.6) | 90.4(60.1) | 7.5(36.3) | 19.1 |
| | S2(S3) | 85.0(6.0) | 11.0(8.3) | 89.0(91.6) | 0.0(0.1) | |
| $BD_{Pb\text{-}S2} \rightarrow BD^*_{Pb\text{-}S1}$ | Pb(Pb) | 15.0(94.0) | 2.1(3.6) | 90.4(60.1) | 7.5(36.3) | 18.8 |
| | S2(S1) | 85.0(6.0) | 11.0(8.3) | 89.0(91.6) | 0.0(0.1) | |
| $BD_{Pb\text{-}S2} \rightarrow RY^*_{Pb}$ | Pb(Pb) | 15.0 | 2.1(88.0) | 90.4(0.9) | 7.5(11.1) | 7.0 |
| | S2 | 85.0 | 11.0 | 89.0 | 0.0 | |
| $BD_{Pb\text{-}S4} \rightarrow BD^*_{Pb\text{-}S1}$ | Pb(Pb) | 15.0(94.0) | 2.1(3.6) | 90.4(60.1) | 7.5(36.3) | 19.1 |
| | S4(S1) | 85.0(6.0) | 11.0(8.3) | 89.0(91.6) | 0.0(0.1) | |
| $BD_{Pb\text{-}S4} \rightarrow BD^*_{Pb\text{-}S3}$ | Pb(Pb) | 15.0(94.0) | 2.1(3.6) | 90.4(60.1) | 7.5(36.3) | 18.8 |
| | S4(S3) | 85.0(6.0) | 11.0(8.3) | 89.0(91.6) | 0.0(0.1) | |
| $BD_{Pb\text{-}S4} \rightarrow RY^*_{Pb}$ | Pb(Pb) | 15.0 | 2.1(88.0) | 90.4(0.9) | 7.5(11.1) | 7.0 |
| | S4 | 85.0 | 11.0 | 89.0 | 0.0 | |
| $BD_{Pb\text{-}S1} \rightarrow BD^*_{Pb\text{-}S3}$ | Pb(Pb) | 2.68 (97.32) | 11.03(11.03) | 54.21(54.21) | 34.76(34.76) | 32.8 |
| | S1(S3) | 97.32(2.68) | 6.78(6.78) | 93.18(93.18) | 0.04(0.04) | |
| $BD_{Pb\text{-}S1} \rightarrow BD^*_{Pb\text{-}S4}$ | Pb(Pb) | 2.68(93.13) | 11.03(2.61) | 54.21(71.66) | 34.76(25.73) | 27.5 |
| | S1(S4) | 97.32(6.87) | 6.78(12.07) | 93.18(87.86) | 0.04(0.07) | |
| $BD_{Pb\text{-}S1} \rightarrow BD^*_{Pb\text{-}S1}$ | Pb(Pb) | 2.68(97.32) | 11.03(11.03) | 54.21(54.21) | 34.76(34.76) | 21.2 |
| | S1(S1) | 97.32(2.68) | 6.78(6.78) | 93.18(93.18) | 0.04(0.04) | |
| $BD_{Pb\text{-}S1} \rightarrow RY^*_{Pb}$ | Pb(Pb) | 2.7 | 11.03(53.71) | 54.21( 1.39) | 34.76(44.90) | 16.6 |
| | S1 | 97.3 | 6.8 | 93.2 | 0.0 | |
| $BD_{Pb\text{-}S1} \rightarrow RY^*_{Pb}$ | Pb(Pb) | 2.7 | 11.03(12.6) | 54.21( 0.8) | 34.76(86.6) | 10.8 |
| | S1 | 97.3 | 6.8 | 93.2 | 0.0 | |
| $BD_{Pb\text{-}S1} \rightarrow RY^*_{Pb}$ | Pb(Pb) | 2.7 | 11.03(3.5) | 54.21(1.0) | 34.76(95.5) | 6.1 |
| $LP_{S1} \rightarrow LP^*_{Pb}$ | S1(Pb) | - | 12.1(0.0) | 87.9(100.0) | 0(0.0) | 56.1 |
| $LP_{S1} \rightarrow LP^*_{Pb}$ | S1(Pb) | - | 70.1(0.0) | 29.9(100.0) | 0(0.0) | 14.0 |
| $LP_{S1} \rightarrow RY^*_{Pb}$ | S1(Pb) | - | 70.1(0.0) | 29.9(100.0) | 0.0(0.0) | 4.5 |
| $LP_{S5} \rightarrow LP^*_{Pb}$ | S5(Pb) | - | 12.1(0.0) | 87.9(100.0) | 0(0.0) | 56.2 |
| $LP_{S5} \rightarrow LP^*_{Pb}$ | S5(Pb) | - | 70.1(0.0) | 29.9(100.0) | 0(0.0) | 13.9 |
| $LP_{S5} \rightarrow RY^*_{Pb}$ | S5(Pb) | - | 70.1(0.0) | 29.9(100.0) | 0.0(0.0) | 4.5 |
| $LP_{S3} \rightarrow LP^*_{Pb}$ | S3(Pb) | - | 12.7(0.2) | 87.3(99.8) | 0.0(0.0) | 41.7 |
| $LP_{S3} \rightarrow LP^*_{Pb}$ | S3(Pb) | - | 12.7(0.0) | 87.3(98.6) | 0.0(1.4) | 18.3 |
| $LP_{S3} \rightarrow LP^*_{Pb}$ | S3(Pb) | - | 69.6(0.2) | 30.4(99.8) | 0.0(0.0) | 9.7 |
| $LP_{S3} \rightarrow RY^*_{Pb}$ | S3(Pb) | - | 69.6(0.5) | 30.4(99.1) | 0.0(0.4) | 3.2 |
| $LP_{S7} \rightarrow LP^*_{Pb}$ | S7(Pb) | - | 12.7(0.2) | 87.3(99.8) | 0.0(0.0) | 41.5 |
| $LP_{S7} \rightarrow LP^*_{Pb}$ | S7(Pb) | - | 12.7(0.0) | 87.3(98.6) | 0.0(1.4) | 18.5 |
| $LP_{S7} \rightarrow LP^*_{Pb}$ | S7(Pb) | - | 69.6(0.2) | 30.4(99.8) | 0.0(0.0) | 9.7 |
| $LP_{S7} \rightarrow RY^*_{Pb}$ | S7(Pb) | - | 69.6(0.5) | 30.4(99.1) | 0.0(0.4) | 3.2 |
| $LP_{S4} \rightarrow LP^*_{Pb}$ | S4(Pb) | - | 8.4(0.0) | 91.6(98.6) | 0.0(1.4) | 38.1 |
| $LP_{S4} \rightarrow LP^*_{Pb}$ | S4(Pb) | - | 73.3(0.0) | 26.7(98.6) | 0.0(1.4) | 12.2 |
| $LP_{S4} \rightarrow RY^*_{Pb}$ | S4(Pb) | | 73.3(0.0) | 26.7(85.5) | 0.0(14.5) | 3.4 |

| | | | | | | |
|---|---|---|---|---|---|---|
| $LP_{S8} \rightarrow LP^{*}_{Pb}$ | S8(Pb) | - | 8.4(0.0) | 91.6(98.6) | 0.0(1.4) | 38.0 |
| $LP_{S8} \rightarrow LP^{*}_{Pb}$ | S8(Pb) | - | 73.3(0.0) | 26.7(98.6) | 0.0(1.4) | 12.2 |
| $LP_{S8} \rightarrow RY^{*}_{Pb}$ | S8(Pb) | | 73.3(0.0) | 26.7(85.5) | 0.0(14.5) | 3.4 |
| $LP_{S2} \rightarrow LP^{*}_{Pb}$ | S2(Pb) | - | 5.4(0.2) | 94.6(99.8) | 0.0(0.0) | 20.0 |
| $LP_{S2} \rightarrow LP^{*}_{Pb}$ | S2(Pb) | - | 5.4(0.0) | 94.6(100.0) | 0.0(0.0) | 9.4 |
| $LP_{S2} \rightarrow LP^{*}_{Pb}$ | S2(Pb) | - | 76.1(0.2) | 23.9(99.8) | 0.0(0.0) | 5.4 |
| $LP_{S6} \rightarrow LP^{*}_{Pb}$ | S6(Pb) | - | 5.4(0.2) | 94.6(99.8) | 0.0(0.0) | 20.0 |
| $LP_{S6} \rightarrow LP^{*}_{Pb}$ | S6(Pb) | - | 5.4(0.0) | 94.6(100.0) | 0.0(0.0) | 9.4 |
| $LP_{S6} \rightarrow LP^{*}_{Pb}$ | S6(Pb) | - | 76.1(0.2) | 23.9(99.8) | 0.0(0.0) | 5.4 |

$\Delta E_{CT}$ is given in kcal/mol. The data inside parenthesis correspond to acceptor NBO.