# Electronic Supplenentary Information

## Regular Patterns of the Effects of Hydrogen-Containing Additives on the Formation of CdSe Monomer

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*Physical Chemistry Chemical Physics*

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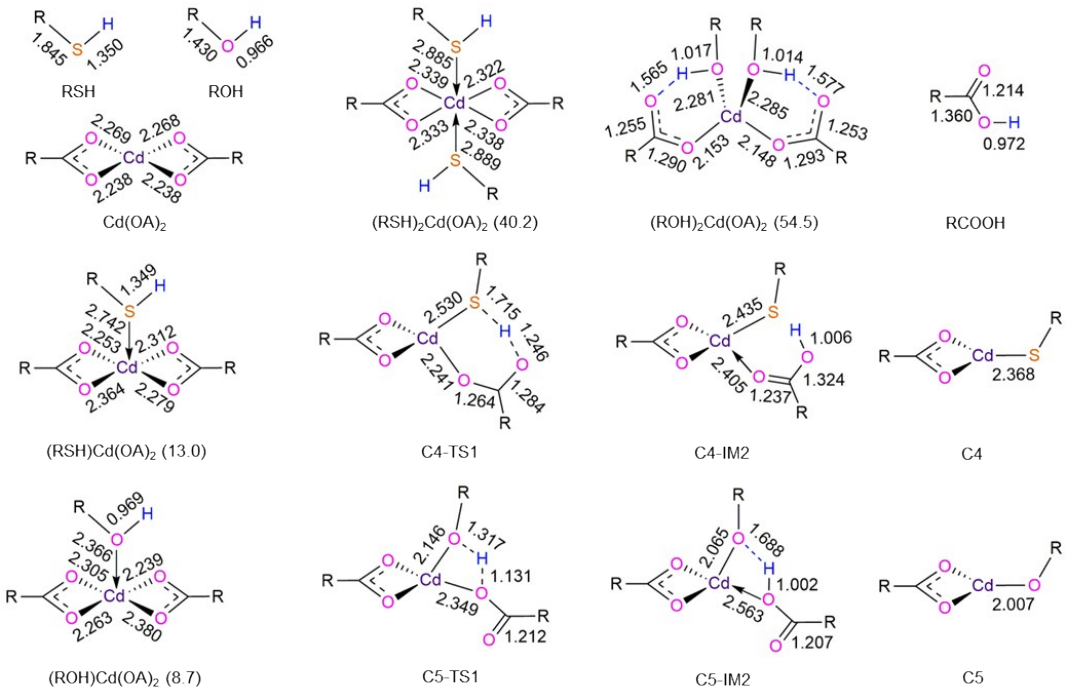
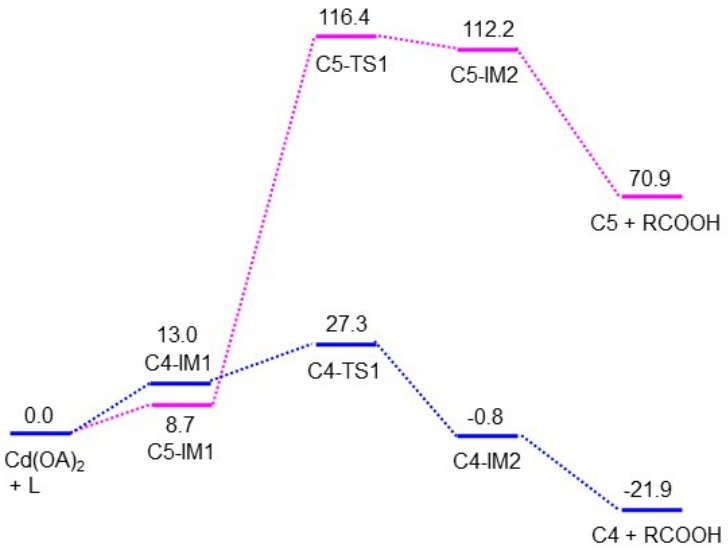
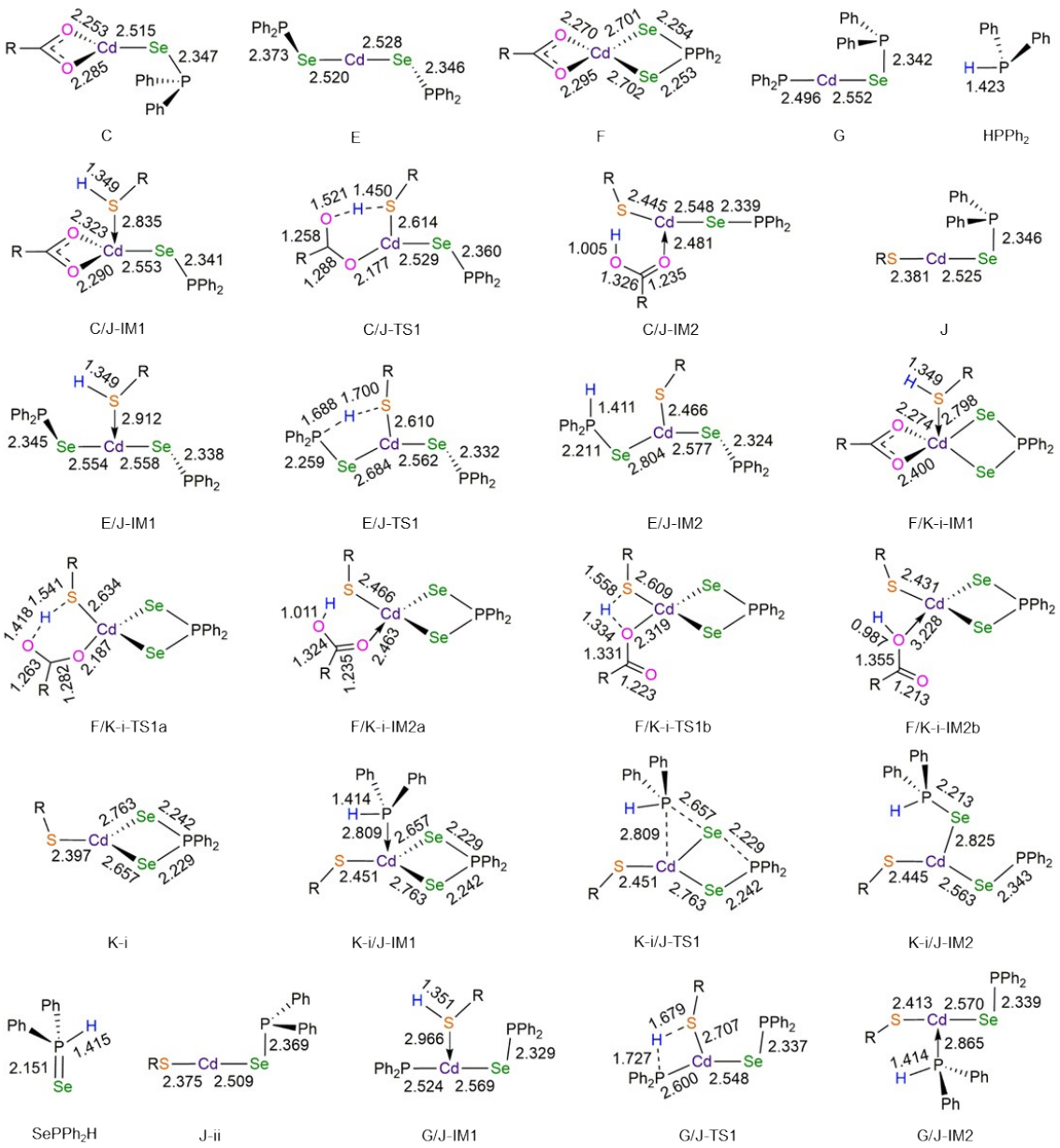



(**a**)

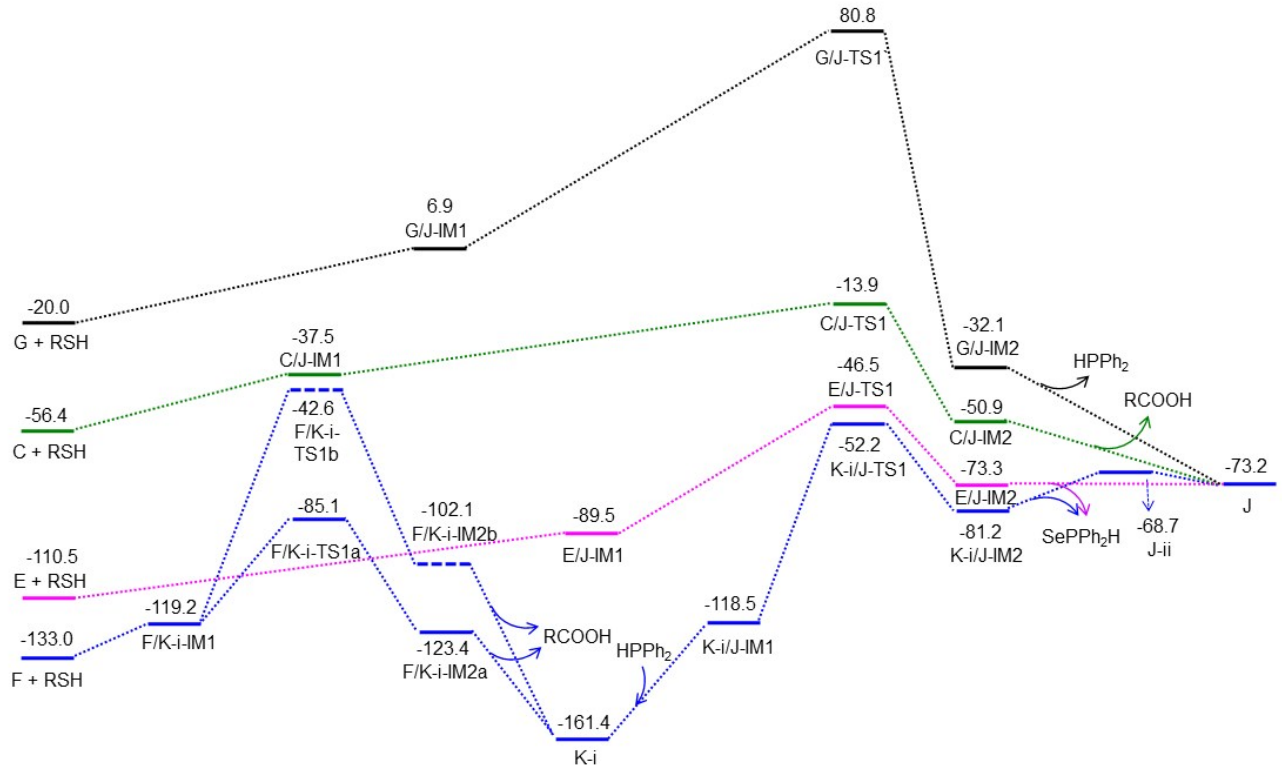



(**b**)

**Figure S1**. The geometric structures of various species (**a**), and the schematic energy diagrams (**b**) for the reaction (3) $Cd(OA)_2$ + H*Y* → RCOOCd–*Y* + RCOOH, *Y* = –SR (**C4**) and –OR (**C5**), respectively. Bond lengths are reported in Å. Relative Gibbs free energies ($G_r$, kJ mol$^{-1}$) for the corresponding species relative to $Cd(OA)_2$ + H*Y* (H*Y* = RSH and ROH) at the M06//B3LYP/6-31++G(d, p), SDD level are shown.


C
E
F
G
HPPh2
C/J-IM1
C/J-TS1
C/J-IM2
J
E/J-IM1
E/J-TS1
E/J-IM2
F/K-i-IM1
F/K-i-TS1a
F/K-i-IM2a
F/K-i-TS1b
F/K-i-IM2b
K-i
K-i/J-IM1
K-i/J-TS1
K-i/J-IM2
SePPh2H
J-ii
G/J-IM1
G/J-TS1
G/J-IM2

**(a)**




(**b**)

**Figure S2**. The geometric structures of various species (**a**), and the schematic energy diagrams (**b**) for the reaction (S1) $Cd(OA)_2$ + $SePPh_2H$ + RSH → RS–CdSe–$PPh_2$ (**J**) + 2RCOOH calculated at the M06//B3LYP/6-31++G(d, p), SDD level are shown. Bond lengths are reported in Å. Relative Gibbs free energies ($G_r$, kJ $mol^{-1}$) for the corresponding species plus RCOOH form **C** + RSH to **J**, for the corresponding species plus $HPPh_2$ + RCOOH − $SePPh_2H$ from **F** + RSH to **K-i**, for the corresponding species plus 2RCOOH − $SePPh_2H$ from **K-i** and **E** to **J**, and for the corresponding species plus 2RCOOH − $HPPh_2$ from **G** + RSH to **J** are shown relative to $Cd(OA)_2$ + $SePPh_2H$ + RSH. Green, red, blue, and black lines represent the reaction (S1-1) **C** + RSH → **J** + RCOOH, (S1-2) **E** + RSH → **J** + $SePPh_2H$, (S1-3) **F** + RSH + $HPPh_2$ → **J** + RCOOH + $SePPh_2H$, and (S1-4) **G** + RSH → **J** + $HPPh_2$, respectively.

In the reaction system of $HPPh_2$/RSH additives (**System 2**), the formation of RS–CdSe–$PPh_2$ (**J**) can be expressed to the overall reaction formula:

$Cd(OA)_2$ + $SePPh_2H$ + RSH → RS–CdSe–$PPh_2$ + RCOOH (S1)

For the **J** monomer formation, the reactions of **C**, **E**, **F**, and **G** with RSH and/or $HPPh_2$ can be dealt with the following four reaction formulas:

RCOOCdSe–$PPh_2$ + RSH → RS–CdSe–$PPh_2$ + RCOOH (S1-1)

$Ph_2P$–SeCdSe–$PPh_2$ + RSH → RS–CdSe–$PPh_2$ + $SePPh_2H$ (S1-2)

$RCOOCdSe_2PPh_2$ + RSH + $HPPh_2$ → RS–CdSe–$PPh_2$ + $SePPh_2H$ + RCOOH (S1-3)

$Ph_2P$–CdSe–$PPh_2$ + RSH → RS–CdSe–$PPh_2$ + $HPPh_2$ (S1-4)

The geometric structures and the schematic energy diagrams for reactions S1-1,2,3,4 are depicted in Figure S2a,b.

As depicted in Figure S2a,b, for the reaction S1-1 of **C** with RSH, in the beginning, when RSH interacts with the central Cd atom of **C**, a four-coordination complex **C/J-IM1** is formed. From **C/J-IM1**, H-shift from RSH to carboxylate occurs via a six-membered ring **C/J-TS1**, leading to a RCOOH molecular complex **C/J-IM2**. Then, **C/J-IM2** releases RCOOH free, leaving RS–CdSe–$PPh_2$ (**J**) monomer behind. This reaction pathway involves the HEB of 23.6 kJ $mol^{-11}$ at the reaction step of **C/J-IM1** → **C/J-TS1**, the EHHP of -13.9 kJ $mol^{-1}$ at **C/J-TS1**, and the exoergicity of 16.8 kJ $mol^{-1}$.

As pictured in Figure S2a,b, for the reaction S1-2 of **E** with RSH, to begin, when RSH interacts with the central Cd atom of **E**, a three-coordination complex **E/J-IM1** is formed. Then, from **E/J-IM1**, H-shift from RSH to $–PPh_2$ group occurs via a five-membered ring **E/J-TS1**, leading to a $SePPh_2H$ molecular complex **E/J-IM2**. Next, **E/J-IM2** releases the free $SePPh_2H$, leaving **J** monomer behind. This reaction pathway comprises the HEB of 43.0 kJ $mol^{-1}$ at the reaction step of **E/J-IM1** → **E/J-TS1**, the EHHP of -46.5 kJ $mol^{-1}$ at **E/J-TS1**, and the endoergicity of 37.3 kJ $mol^{-1}$.

As shown in Figure S2a,b, there are two reaction formulas for the formation **J** from **F**.

$RCOOCdSe_2PPh_2 + RSH \rightarrow RS–CdSe_2PPh_2 + RCOOH$ (S1-3a)

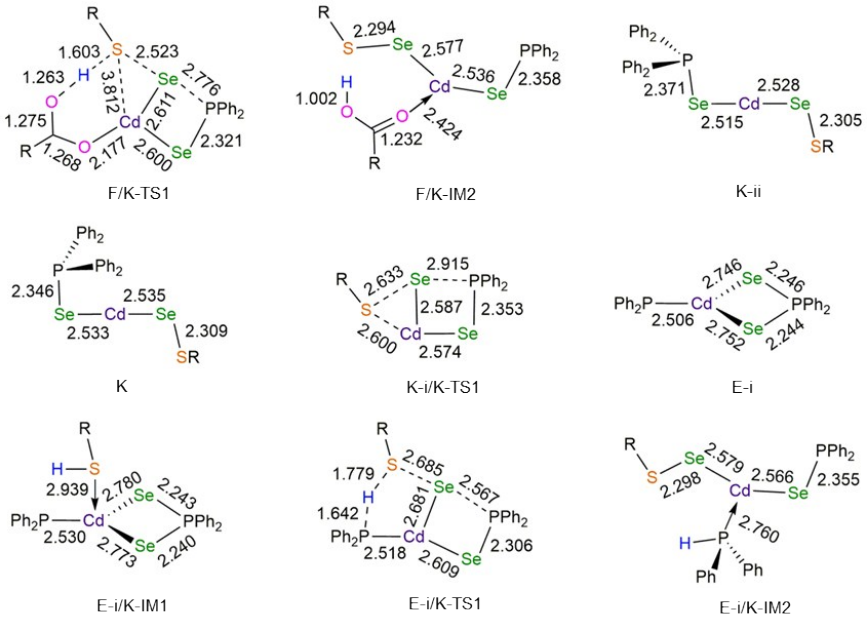
$RS–CdSe_2PPh_2 + HPPh_2 \rightarrow RS–CdSe–PPh_2 + SePPh_2H$ (S1-3b)

In the beginning, when RSH molecule coordinates to **F**, the five-coordination complex **F/K-i-IM1** is generated. From **F/K-i-IM1**, there are two reaction pathways for the formation of $RS–CdSe_2PPh_2$ (**K-i**). For one thing, H-shift from RSH to carboxylate proceeds via a six-membered ring **F/K-i-TS1a**, producing a complex **F/K-i-IM2a**, containing RCOOH molecular. For another, a [1,3]-H shift takes place via a four-membered ring **F/K-i-TS1b**, leading a RCOOH-containing molecular complex **F/K-i-IM2b**. After that, **F/K-i-IM2a,b** liberate the RCOOH free, leaving **K-i** with the four-membered ring Cd*–Se–P–Se–(Cd*) skeleton behind. Because the energy of **F/K-i-TS1a** locates 42.5 kJ $mol^{-1}$ below **F/K-i-TS1b**, the reaction pathway via **F/K-i-TS1a** is kinetically more favoured than that **F/K-i-TS1b**. This may be attributed to be the fact that the strain of six-membered ring is less than that of four-membered ring. That is to say, the formation of **K-i** should prefer via the six-membered **F/E-i-TS1a** to the four-membered **F/E-i-TS1b**. NBO results show that the occupancies of Cd–S are 1.982 *e* in the complex **K-i**, indicating a complete single-bond formed. Furthermore, there is a hyperconjugation interaction in Cd*–Se–P–Se–(Cd*) four-membered cycle. It is indicated that the stable complex **K-i** includes three-coordinated Cd center. That is to say, when RSH coordinates to four-coordinated **F**, a more stable three-coordinated complex **K-i** can be formed by releasing RCOOH free. This decrease of coordination number originates from the formation of Cd–S single bond.

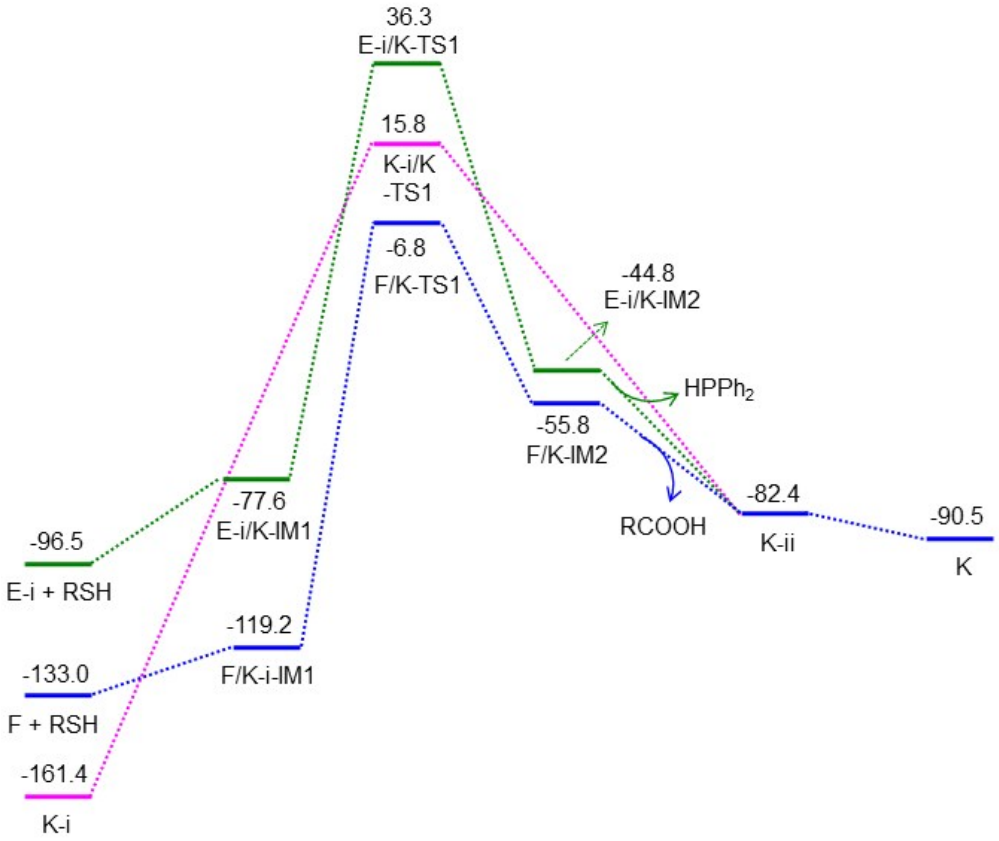
Next, in the reaction S1-3b, **K-i** interacts with $HPPh_2$ molecule though the P-end, producing a four-coordination complex **K-i/J-IM1**. From **K-i/J-IM1**, the Se–P bond cleavage of $–Se_2PR_2$ group occurs via a five-membered ring **K-i/J-TS1**, through the electrophilic attack of $HPPh_2$ toward Se atom, generating a $SePPh_2H$-containing molecular complex **K-i/J-IM2**.Then, **K-i/J-IM2** sets the $SePPh_2H$ molecule free, leaving *trans*-RS–CdSe–$PPh_2$ (**J-ii**). Lastly, **J-ii** can readily isomerize to **J**.

As for the reaction S1-3, the minimal energy reaction pathway (MERP) should include the EHHP of –52.2 kJ $mol^{-1}$ at **K-i/J-TS1**, the HEB of 66.3 kJ $mol^{-1}$ at the reaction step **K-i/J-IM1** → **K-i/J-TS1**, and the endoergicity of 59.8 kJ $mol^{-1}$.

As depicted in Figure S2a,b, for the reaction S1-4 of **G** with RSH, initially, when the S-end of RSH interacts with the central Cd atom of **G**, a three-coordination complex **G/J-IM1** is generated. Next, from **G/J-IM1**, H-shift from RSH to $–PPh_2$ group takes place via a four-membered ring **G/J-TS1**, resulting in a $HPPh_2$ molecular complex **G/J-IM2**. Lastly, **G/J-IM2** releases the free $HPPh_2$, leaving **J** behind. This reaction pathway comprises the HEB of 73.9 kJ $mol^{-1}$ at the reaction step of **G/J-IM1** → **G/J-TS1**, the EHHP of 80.8 kJ $mol^{-1}$ at **G/J-TS1**, and the exoergicity of 53.2 kJ $mol^{-1}$.




(**a**)




(**b**)

**Figure S3**. The geometric structures of various species (**a**), and the schematic energy diagrams (**b**) for the reaction (S2) $Cd(OA)_2$ + $2SePPh_2H$ + RSH → $Ph_2P$–SeCdSe–SR (**K**) + $HPPh_2$ + 2RCOOH calculated at the M06//B3LYP/6-31++G(d, p), SDD level are shown. Bond lengths are reported in Å. Relative Gibbs free energies ($G_r$, kJ $mol^{-1}$) for the corresponding species plus $HPPh_2$ + RCOOH from **F** + RSH to **K**, for the corresponding species plus $HPPh_2$ + 2RCOOH from **K-i** to **K**, and for the corresponding species plus 2RCOOH from **E-i** + RSH to **K** are shown relative to $Cd(OA)_2$ + $2SePPh_2H$ + RSH. Blue, red, and green lines represent the reaction (S2-1) **F** + RSH → **K** + RCOOH, (S2-2) **K-i** → **K**, and (S2-3) **E-i** + RSH → **K** + $HPPh_2$, respectively.

In the reaction system of $HPPh_2$/RSH additives (**System 2**), the formation of $Ph_2PSe–CdSe–SR$ (**K**) can be showed to the overall reaction formula:

$Cd(OA)_2 + 2SePPh_2H + RSH \rightarrow Ph_2P–SeCdSe–SR + HPPh_2 + 2RCOOH$ (S2)

For the K monomer formation, the reactions of $RCOOCdSe_2PPh_2$ (**F**), $RS–CdSe_2PPh_2$ (**K-i**), and $Ph_2P–CdSe_2PPh_2$ (**E-i**) with RSH can be referred to the following there reactions:

$RCOOCdSe_2PPh_2 + RSH \rightarrow Ph_2PSe–CdSe–SR + RCOOH$ (S2-1)

$RS–CdSe_2PPh_2 \rightarrow Ph_2P–SeCdSe–SR$ (S2-2)

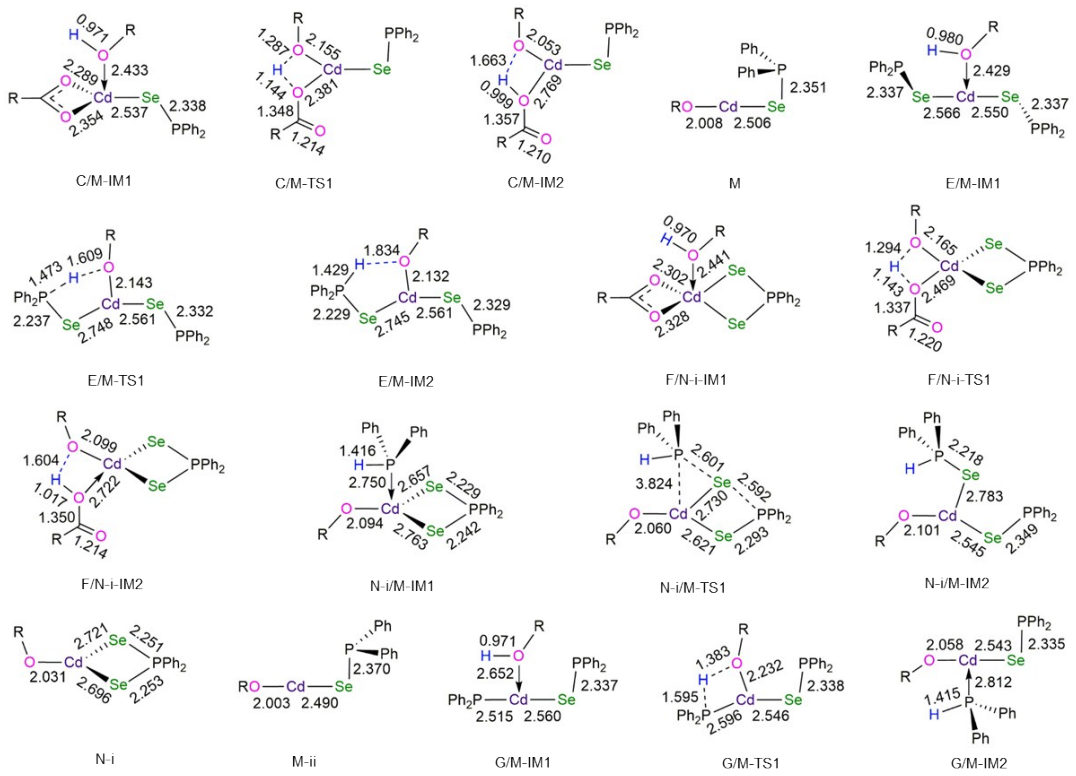
$Ph_2P–CdSe_2PPh_2 + RSH \rightarrow Ph_2P–SeCdSe–SR + HPPh_2$ (S2-3)

The geometric structures and the schematic energy diagrams for reactions S2-1,2,3 are depicted in Figure S3a,b.

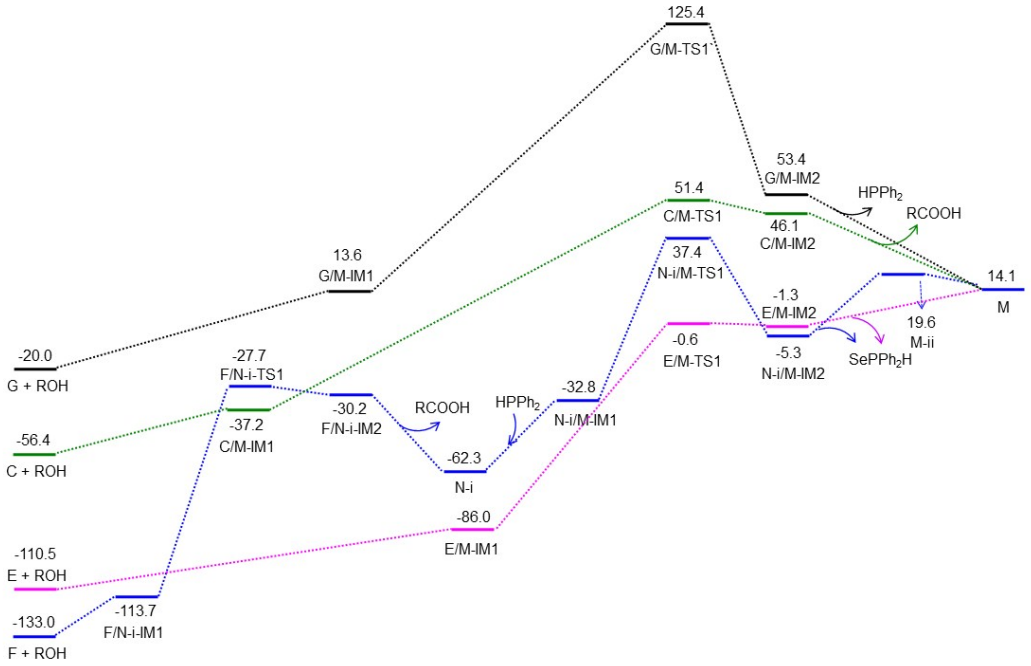
As shown in Figure S3a,b, for the reaction S2-1 of $RCOOCdSe_2PPh_2$ (**F**) with RSH, first of all, from five-coordination complex **F/K-i-IM1**, [1,5]-H shift in a six-membered cycle and Se exchange through the Se–P bond cleavage of $Se_2PPh_2$ moiety and Se–S bond formation take place simultaneously via a nine-membered **F/K-TS1**, resulting to a RCOOH-containing complex **F/K-IM2**. Next, **F/K-IM2** decomposes into the discrete *trans*-$Ph_2PSe–CdSe–SR$ (**K-ii**) and RCOOH. Last, **K-ii** can readily isomerize to **K**, with the Se–P single bond rotation. Combined with the formation of **C** and **F** in reaction **System 1**,[1] the reaction pathway of **K** from **C** is signified as **RP-CFK** (see Scheme 2b), which includes the HEB of 112.4 kJ $mol^{-1}$ at the reaction step of **F/K-i-IM1** → **F/K-TS1**, the EHHP of –6.8 kJ $mol^{-1}$ at **F/K-TS1**.

As pictured in Figure S3a,b, the reaction S2-2 is the isomerization of $RS–Cd–Se_2PPh_2$ (**K-i**). From **K-i**, Se exchange occurs through the synchronous Se–P bond cleavage of $Se_2PPh_2H$ moiety, Cd–S bond cleavage, and Se–S bond formation via a five-membered envelope-like **K-i/K-TS1**, producing an isomer **K-ii**. Last, **K-ii** can isomerize to **K**. Integrated with the formation of **C** and **F** in reaction **System 1**,[1] the reaction pathway of **K** from **C** via **K-i** is expressed as **RP-CFK-iK** (see Scheme 2b), which contains the HEB of 177.2 kJ $mol^{-1}$ at the reaction step of **K-i** → **K-i/K-TS1**, the EHHP of 15.8 kJ $mol^{-1}$ at **K-i/K-TS1**.

As depicted in Figure S3a,b, for the reaction S2-3 of $Ph_2P$-$CdSe_2PPh_2$ (**E-i**) with RSH, in the beginning, a four-coordination complex **E-i/K-IM1** is formed by coordinating RSH and the central Cd atom of **E-i**. Then, from **E-i/K-IM1**, [1,4]-H shift and Se exchange through the Se–P bond cleavage of $Se_2PPh_2$ moiety and Se–S bond formation occur simultaneously via a seven-membered twist-chair-like **E-i/K-TS1**, leading to a complex **E-i/K-IM2**, containing a $HPPh_2$ molecular. After that, **E-i/K-IM2** liberates the free $HPPh_2$, leaving the **K-ii** monomer behind. Finally, **K-ii** can readily isomerize to **K**. Together with the formation of **C**, **F**, and **E-i** in reaction **System 1**,[1] the reaction pathway of **K** formation from **C** via **E-i** is denoted as **RP-CFE-iK** (see Scheme 2b), which comprises the HEB of 113.9 kJ $mol^{-1}$ at the reaction step of **E-i/K-IM1** → **E-i/K-TS1**, the EHHP of 36.3 kJ $mol^{-1}$ at **E-i/K-TS1**.




(**a**)




(**b**)

**Figure S4**. The geometric structures of various species (**a**), and the schematic energy diagrams (**b**) for the reaction (S3) $Cd(OA)_2$ + $SePPh_2H$ + ROH→ RO–CdSe–$PPh_2$ (**M**) + 2RCOOH calculated at the M06//B3LYP/6-31++G(d, p), SDD level are shown. Bond lengths are reported in Å. Relative Gibbs free energies ($G_r$, kJ $mol^{-1}$) for the corresponding species plus RCOOH form **C** + ROH to **M**, for the corresponding species plus $HPPh_2$ + RCOOH − $SePPh_2H$ from **F** + ROH to **N-i**, for the corresponding species plus 2RCOOH − $SePPh_2H$ from **N-i** + $HPPh_2$ and **E** + ROH to **M**, and for the corresponding species plus 2RCOOH − $HPPh_2$ from **G** + ROH to **M** are shown relative to $Cd(OA)_2$ + $SePPh_2H$ + ROH. Green, red, blue, and black lines represent the reaction (S3-1) **C** + ROH → **M** + RCOOH, (S3-2) **E** + ROH → **M** + $SePPh_2H$, (S3-3) **F** + ROH + $HPPh_2$ → **M** + RCOOH + $SePPh_2H$, and (S3-4) **G** + ROH → **M** + $HPPh_2$, respectively.

In the reaction system of $HPPh_2$/ROH additives (**System 3**), the formation of RO–CdSe–$PPh_2$ (**M**) can be represented to the overall reaction formula:

$Cd(OA)_2 + SePPh_2H + ROH \rightarrow RO–CdSe–PPh_2 + RCOOH$ (S3)

For the M monomer formation, the reactions of **C**, **E**, **F**, and **G** with ROH and/or $HPPh_2$ can be referred to by the following four reaction formulas:

$RCOOCdSe–PPh_2 + ROH \rightarrow RO–CdSe–PPh_2 + RCOOH$ (S3-1)

$Ph_2P–SeCdSe–PPh_2 + ROH \rightarrow RO–CdSe–PPh_2 + SePPh_2H$ (S3-2)

$RCOOCdSe_2PPh_2 + ROH + HPPh_2 \rightarrow RO–CdSe–PPh_2 + SePPh_2H + RCOOH$ (S3-3)

$Ph_2P–CdSe–PPh_2 + ROH \rightarrow RO–CdSe–PPh_2 + HPPh_2$ (S3-4)

Supplementary Figure 4a,b presents the geometric structures and schematic energy diagrams of reactions S3-1,2,3,4 in the reaction **System 3**. As pictured in Figure S4a,b, for the reaction S3-1 of C with ROH, initially, ROH interacts with the central Cd atom of **C**, producing a four-coordination complex **C/M-IM1**. Then, a [1,3]-H shift occurs via a four-membered ring **C/M-TS1**, generating a RCOOH-containing molecular complex **C/M-IM2**. Lastly, **C/M-IM2** sets the RCOOH free, leaving RO–CdSe–$PPh_2$ (**M**) behind. For M, NBO results show that the occupancies of Cd–Se are 1.983 *e*, indicating a complete single-bond in Cd–Se. In addition, there is a very strong hyperconjugation interaction in P–Se–Cd–O skeleton. This reaction pathway denoted as **RP-CM** (see Scheme 2c) includes the EHHP of 51.4 kJ $mol^{-1}$ at **C/M-TS1**, the HEB of 88.6 kJ $mol^{-1}$ at the reaction step of **C/M-IM1** → **C/M-TS1**, and the endoergicity of 70.5 kJ $mol^{-1}$.

As depicted in Figure S4a,b, for the reaction S3-2 of **E** with ROH, in the beginning, when the O-end of ROH interacts with the central Cd atom of **E**, a three-coordination complex **E/M-IM1** is formed. Then, from **E/M-IM1**, a [1,4]-H shift from ROH to –$PPh_2$ group takes place via a five-membered ring **E/M-TS1**, forming to a $SePPh_2H$ molecular complex **E/M-IM2**. Next, **E/M-IM2** decomposes into the discrete M monomer and $SePPh_2H$. Combined with the formation of **C** and **E** in reaction **System 1**,[1] the reaction pathway of **M** formation from **C** via **E** is remarked as **RP-CEM** (see Scheme 2c), which comprises the EHHP of –0.6 kJ $mol^{-1}$ at **E/M-TS1** and the HEB of 85.4 kJ $mol^{-1}$ at the reaction step of **E/M-IM1** → **E/M-TS1**.

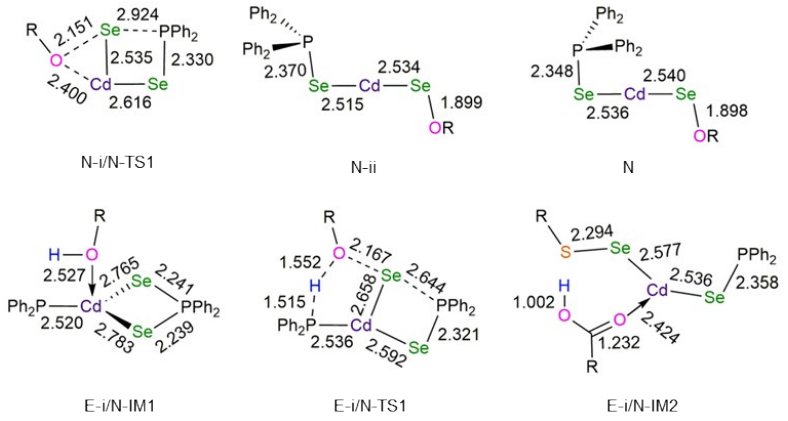
As shown in Figure S4a,b, there are two reaction formulas for the formation **M** from **F**,

$RCOOCdSe_2PPh_2 + ROH \rightarrow RO–CdSe_2PPh_2 + RCOOH$ (S3-3a)

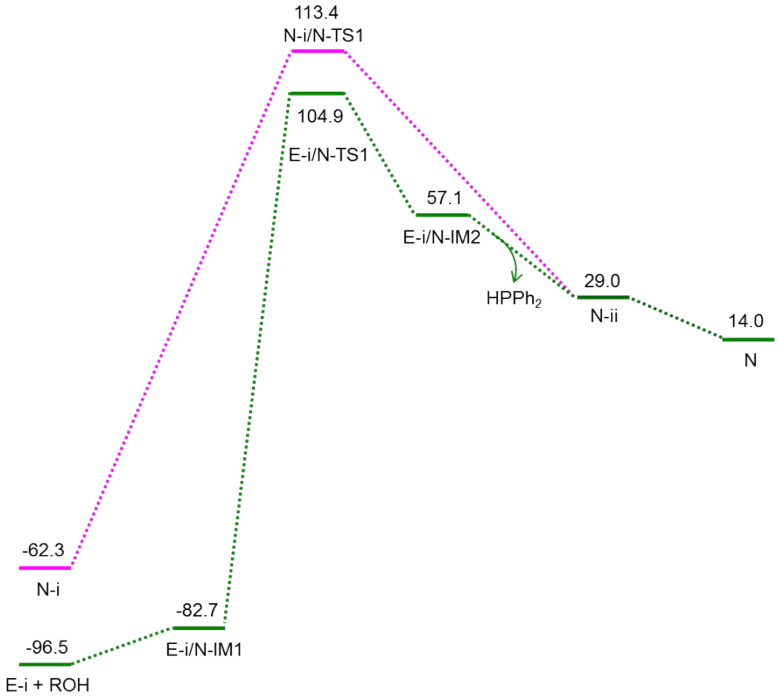
$RO–CdSe_2PPh_2 + HPPh_2 \rightarrow RO–CdSe–PPh_2 + SePPh_2H$ (S3-3b)

To begin, a five-coordination complex **F/N-i-IM1** is generated by coordinating ROH to F. A [1,3]-H shift from ROH to carboxylate occurs via a four-membered ring **F/N-i-TS1**, producing a RCOOH molecular complex **F/N-i-IM2**. After that, **F/N-i-IM2** liberates the RCOOH, leaving **N-i** behind. For the complex **N-i**, NBO results show that there is a very strong hyperconjugation interaction in four-membered O–Cd*–Se–P–Se–(Cd)* skeleton. Next, in the reaction S3-2b, when the P-end of $HPPh_2$ molecule interacts with **N-i**, a four-coordination complex **N-i/M-IM1** is formed. From **N-i/M-IM1**, Se–P bond cleavage takes place via a five-membered ring **N-i/M-TS1**, yielding a $SePPh_2H$-containing **N-i/M-IM2** molecular complex. Next, **N-i/M-IM2** separates into the discrete *trans*-RO–CdSe–$PPh_2$ (**M-ii**) and $SePPh_2H$ molecule. Finally, **M-ii** can readily isomerize to **M**. Together with the formation of **C** and **F** in reaction **System 1**,[1] the reaction pathway of **M** formation from **C** via **N-i** is signified as **RP-CFN-iM** (see Scheme 2c), which comprises the EHHP of 37.4 kJ $mol^{-1}$ at **N-i/M-TS1** and the HEB of 70.2 kJ $mol^{-1}$ at the reaction step of **N-i/M-IM1** → **N-i/M-TS1**.

As depicted in Figure S4a,b, for the reaction S3-4 of G with ROH, ROH interacts initially with **G** through coordination, forming a three-coordination complex **G/M-IM1**. Next, a [1,3]-H shift from ROH to –$PPh_2$ group takes place via a four-membered cyclic **G/M-TS1**, resulting in complex **G/M-IM2** with a $HPPh_2$ molecular. Finally, **G/M-IM2** releases the free $HPPh_2$, leaving M behind. Integrated with the formation of **C** and **F** in reaction **System 1**,[1] the reaction pathway of **M** formation from **C** via **E-i** and **G** is expressed as **RP-CFE-iGM** (see Scheme 2c), which contains the EHHP of 111.8 kJ $mol^{-1}$ at **G/M-TS1** and the HEB of 125.4 kJ $mol^{-1}$ at the reaction step of G/M-IM1 → G/M-TS1.




(**a**)




(**b**)

**Figure S5**. The geometric structures of various species (**a**), and the schematic energy diagrams (**b**) for the reaction (S4) $Cd(OA)_2$ + $2SePPh_2H$ + ROH → $Ph_2P$–SeCdSe–OR (**N**) + $HPPh_2$ + 2RCOOH are shown. Bond lengths are reported in Å. Relative Gibbs free energies ($G_r$, kJ $mol^{-1}$) for the corresponding species plus $HPPh_2$ + 2RCOOH from **N-i** to **N**, and for the corresponding species plus 2RCOOH from **E-i** + ROH to **N** are shown relative to $Cd(OA)_2$ + $2SePPh_2H$ + ROH at the M06//B3LYP/6-31++G(d, p), SDD level. Red and green lines represent the reaction (S4-1) **N-i** → **N** and (S4-2) **E-i** + ROH → **N** + $HPPh_2$, respectively.

In the reaction system of $HPPh_2$/ROH additives (**System 3**), the formation of $Ph_2PSe$–CdSe–OR (**N**) can be showed to the overall reaction formula:

$Cd(OA)_2$ + $2SePPh_2H$ + ROH → $Ph_2PSe$–CdSe–OR + $HPPh_2$ + 2RCOOH (S4)

For the N monomer formation, the reactions of RO–$CdSe_2PPh_2$ (**N-i**) and $Ph_2P$–$CdSe_2PPh_2$ (**E-i**) with ROH can be formulated upon the following two reactions:

RO–$CdSe_2PPh_2$ → $Ph_2P$–SeCdSe–OR (S4-1)

$Ph_2P$–$CdSe_2PPh_2$ + ROH → $Ph_2P$–SeCdSe–OR + $HPPh_2$ (S4-2)

Supplementary Figure 5a,b shows the geometric structures and schematic energy diagrams of reactions S4-1,2. As depicted in Figure S5a,b, the reaction S4-1 is the isomerization of RO–Cd–$Se_2PPh_2$ (**N-i**) through the synchronous Se–P and Cd–O bond cleavage, as well as Se–S bond formation via a five-membered envelope-like **N-i/N-TS1**. An isomer *trans*-$Ph_2PSe$–CdSe–OR (**N-ii**) is formed. Last, **N-ii** can isomerize to **N** by the rotation of –$PPh_2$ group. The reaction pathway of **K** from **C** via **N-i** is expressed as **RP-CFN-iN** (see Scheme 2d). This pathway involves the HEB of 175.7 kJ $mol^{-1}$ at the reaction step of **N-i** → **N-i/N-TS1**, the EHHP of 113.4 kJ $mol^{-1}$ at **N-i/N-TS1**, connecting with the formation of **C** and **F** in reaction **System 1**,[1] and the reaction (5-3a) of **F** + ROH → **N-i** + RCOOH.

As pictured in Figure S5a,b, for the reaction S4-2 of $Ph_2P$–$CdSe_2PPh_2$ (**E-i**) with ROH, in the beginning, when ROH coordinates to the central Cd atom of **E-i**, a four-coordination complex **E-i/N-IM1** is formed. Then, from **E-i/N-IM1**, Se exchange happens through the simultaneous Se–P bond cleavage of $Se_2PPh_2$ moiety, Se–N bond formation, and [1,4]-H shift occurs via a seven-membered twist-chair-like **E-i/N-TS1**, leading to a $HPPh_2$ molecular complex **E-i/N-IM2**. Next, **E-i/N-IM2** sets $HPPh_2$ free, leaving the *trans*-$Ph_2PSe$–CdSe–OR **(N-ii**) monomer behind. Finally, **N-ii** can readily isomerize to **N**. For the **N** formation from **C** via **E-i**, this reaction pathway **RP-CFE-iN** comprises the HEB of 187.6 kJ $mol^{-1}$ at the reaction step of **E-i/N-IM1** → **E-i/N-TS1** and the EHHP of 104.9 kJ $mol^{-1}$ at **E-i/N-TS1**, together with the formation of **C**, **F** and **E-i** in reaction **System 1**.[1]

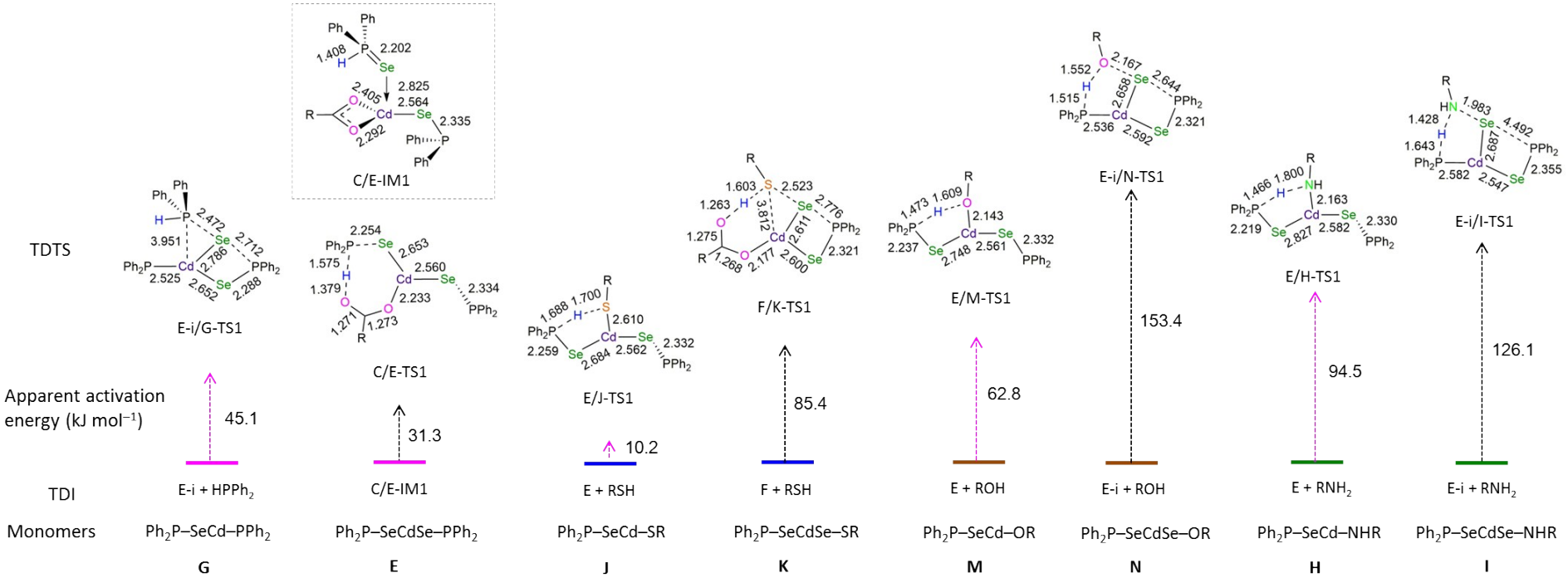
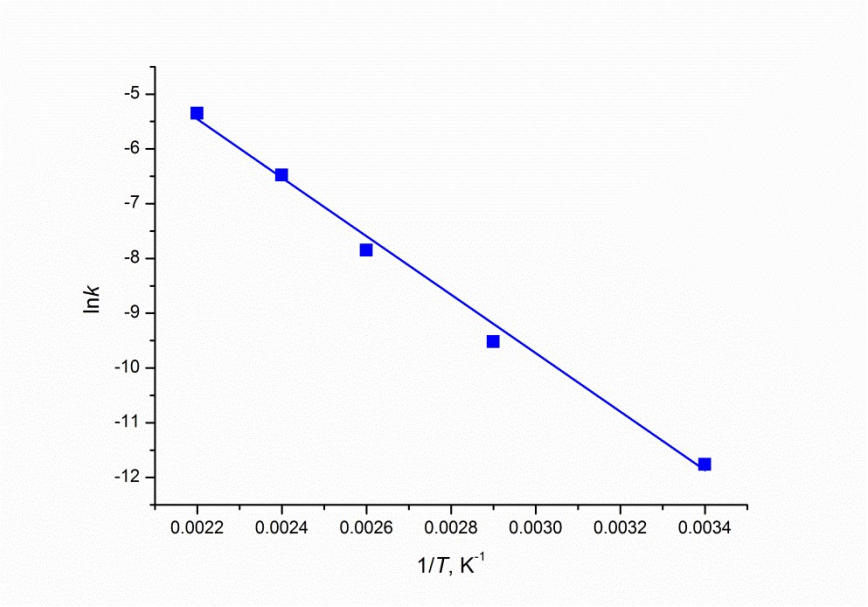
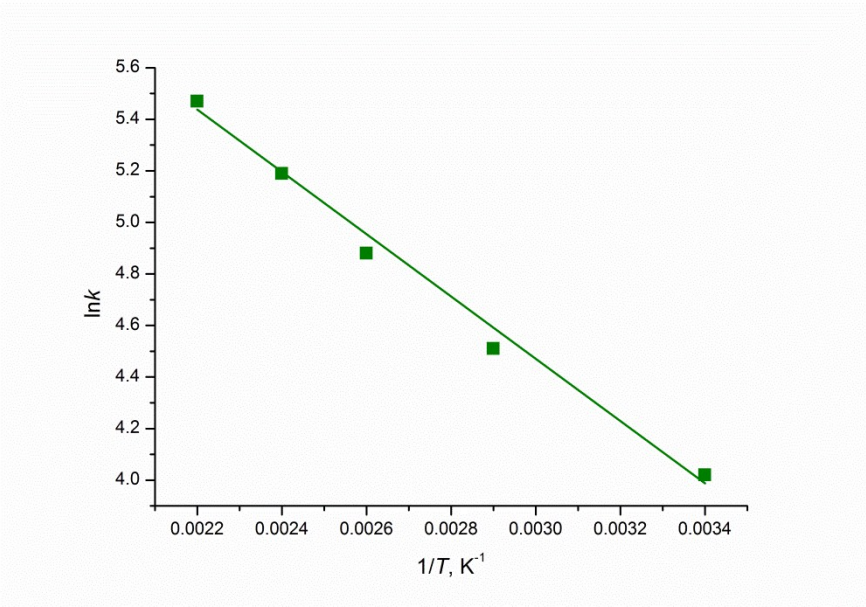



**Figure S6.** Rate-determining step for the formation of CdSe monomers. TDI and TDTS denote TOF-determining intermediate and transition state in optimal reaction pathway, respectively.



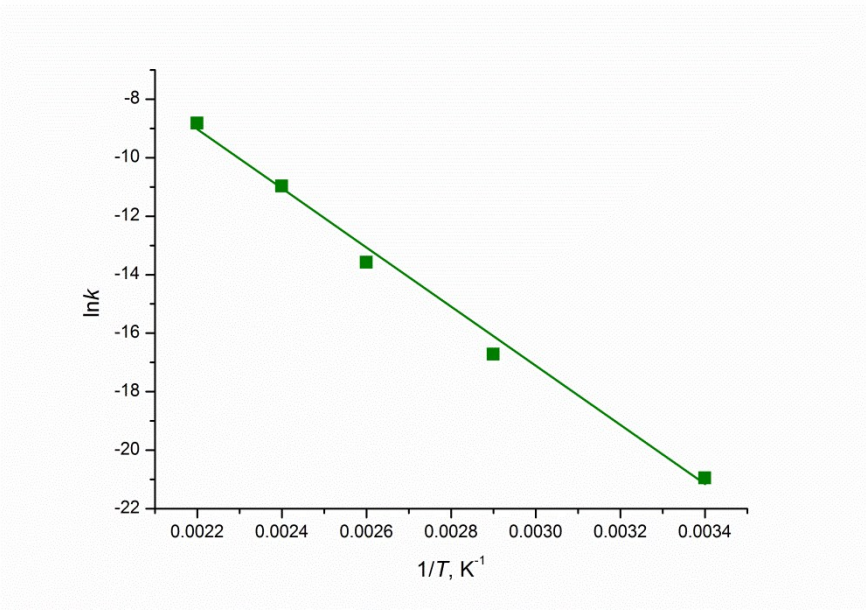

$$k_{\mathrm{G}}(T) = 6.219\times10^{2}\,\exp(-45,098\,/\,RT) \quad (\mathrm{s^{-1}\ mol^{-1}\ dm^{3}})$$

**Figure S7.** Arrhenius plots of rate constants for the crucial reaction step **E-i** + $HPPh_2$ → **E-i/G-TS1** for the formation of $Ph_2P$–CdSe–$PPh_2$ (**G**) in the reaction **System 1** (H*Y* = $HPPh_2$).



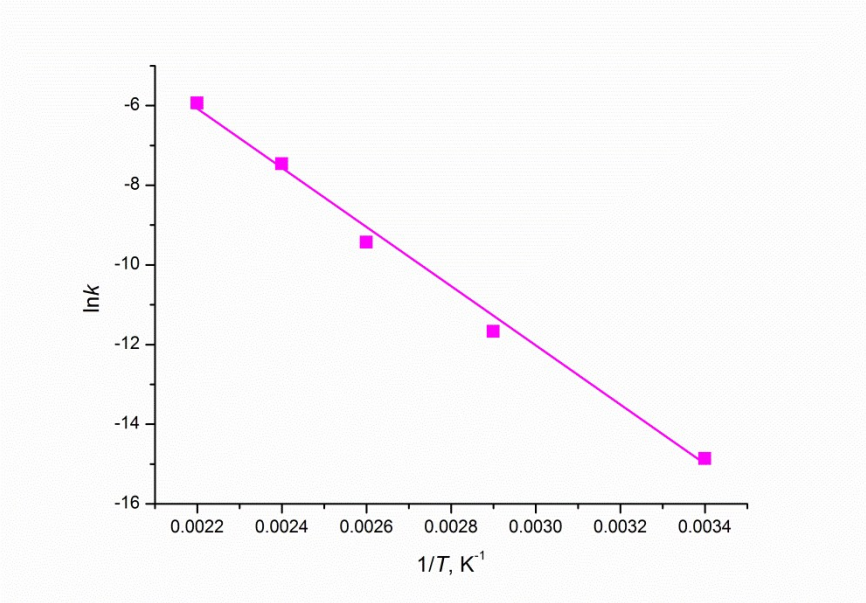

$$k_{\mathrm{J}} = 3.335 \times 10^{3} \exp(-10{,}170 / RT) \quad (\mathrm{s^{-1}\ mol^{-1}\ dm^{3}})$$

**Figure S8.** Arrhenius plots of rate constants for the crucial reaction step **E** + RSH → **E/J-TS1** for the formation of RS–CdSe–$PPh_2$ (**J**) in the reaction **System 2** (H*Y* = RSH + $HPPh_2$).



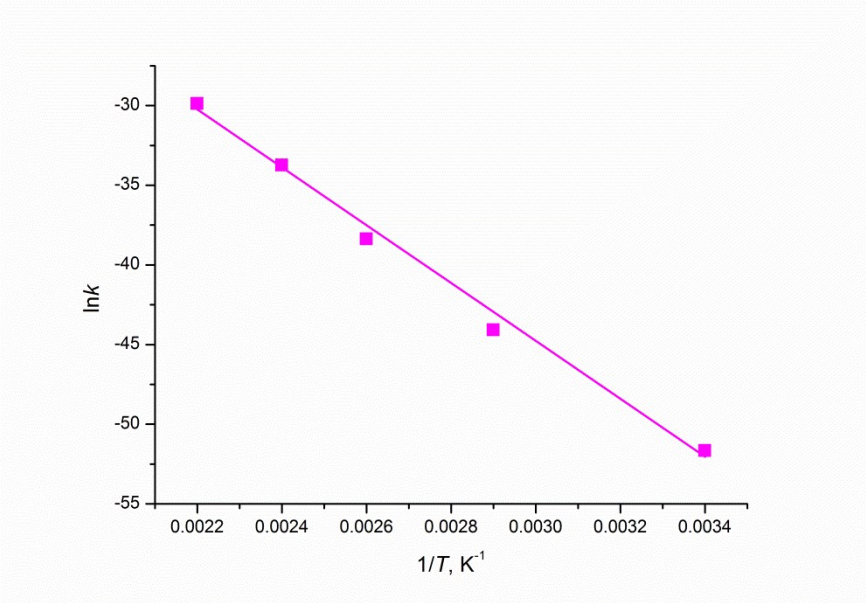

$$k_{\mathrm{K}} = 7.079\times10^{5}\exp(-85{,}352/RT)\ \ (\mathrm{s^{-1}\ mol^{-1}\ dm^{3}})$$

**Figure S9.** Arrhenius plots of rate constants for the crucial reaction step **F** + RSH → **F/K-TS1** for the formation of $Ph_2P$–SeCdSe–SR (**K**) in the reaction **System 2** (H*Y* = RSH + $HPPh_2$).



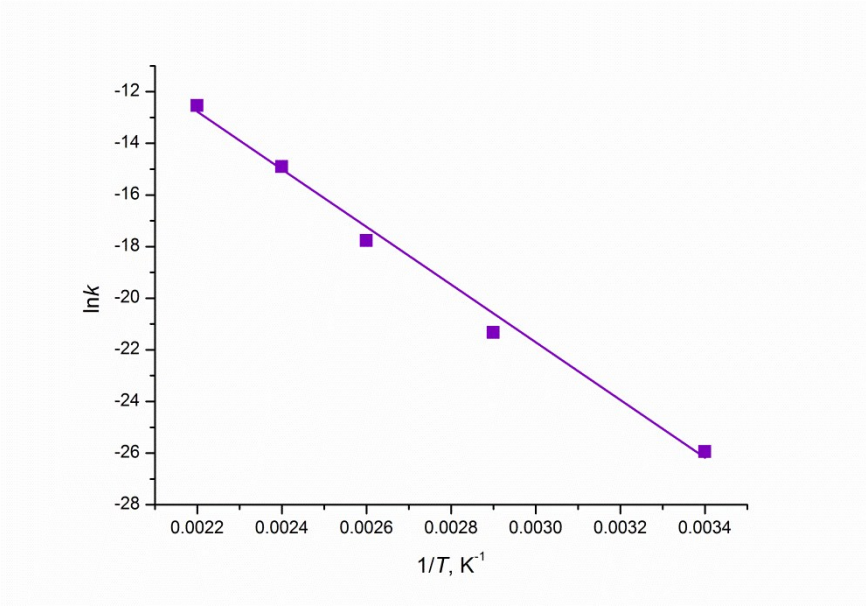

$$k_{\mathrm{M}} = 3.632\times10^{4}\,\exp(-62,809\,/\,RT) \quad (\mathrm{s^{-1}\ mol^{-1}\ dm^{3}})$$

**Figure S10.** Arrhenius plots of rate constants for the crucial reaction step **E** + ROH → **E/M-TS1** for the formation of RO–CdSe–$PPh_2$ (**M**) in the reaction **System 3** (H*Y* = ROH + $HPPh_2$).



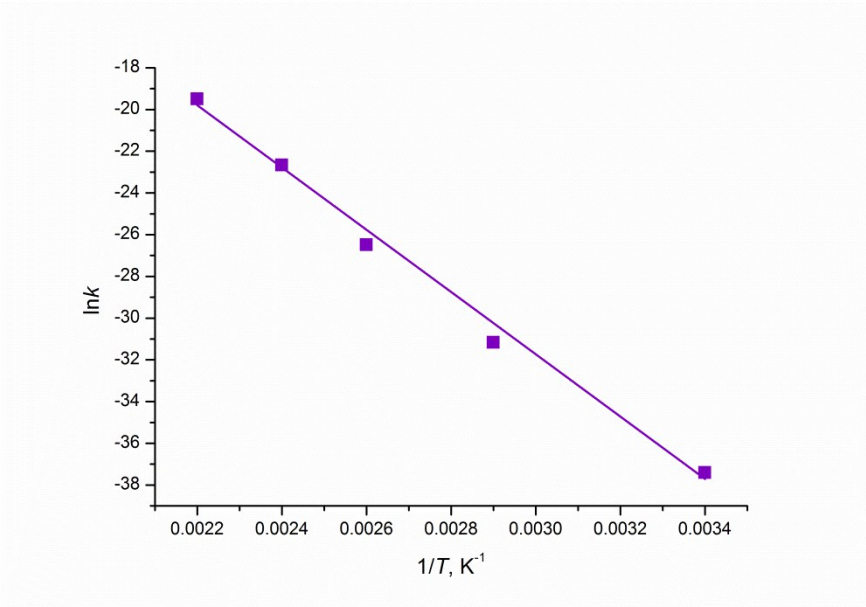

$$k_{\mathrm{N}} = 2.742\times10^{4}\exp(-153,443/RT) \quad (\mathrm{s^{-1}\ mol^{-1}\ dm^{3}})$$

**Figure S11.** Arrhenius plots of rate constants for the crucial reaction step **E-i** + ROH → **E-i/N-TS1** for the formation of $Ph_2P$–SeCdSe–OR (**N**) in the reaction **System 3** (H*Y* = ROH + $HPPh_2$).




$$k_{\mathrm{H}}(T) = 1.899 \times 10^{5} \exp(-94,514 / RT) \quad (\mathrm{s^{-1}\ mol^{-1}\ dm^{3}})$$

**Figure S12.** Arrhenius plots of rate constants for the crucial reaction step **E** + $RNH_2$ → **E/H-TS1** for the formation of RHN–CdSe–$PPh_2$ (**H**) in the reaction **System 4** (H*Y* = $RNH_2$ + $HPPh_2$).




$$k_1(T) = 6.945\times10^5 \exp(-126,090 / RT) \quad (\text{s}^{-1}\ \text{mol}^{-1}\ \text{dm}^3)$$

**Figure S13.** Arrhenius plots of rate constants for the crucial reaction step **E-i** + $RNH_2$ → **E-i/I-TS1** for the formation of $Ph_2P$–SeCdSe–NHR (**I**) in the reaction **System 4** (H*Y* = $RNH_2$ + $HPPh_2$).

**Table S1.** The Natural Bond Orbital (NBO, *e*) charges of the coordinated atom (*X* = Se, P, N, S, and O) in ligands (H*Y* = $SePPh_2H$, $HPPh_2$, $RNH_2$, RSH, and ROH) and stabilization energies (kJ $mol^{-1}$) of coordination complex (H*Y*)$Cd(OA)_2$ and $(HY)_2Cd(OA)_2$.

| item | $SePPh_2H$ | $HPPh_2$ | $RNH_2$ | RSH | ROH |
|---|---|---|---|---|---|
| NBO charges of *X* | –0.460 | 0.617 | –0.916 | –0.052 | –0.771 |
| Stabilization energies of (H*Y*)$Cd(OA)_2$ | 17.9 | –33.4 | 22.6 | –13.0 | –8.7 |
| Stabilization energies of $(HY)_2Cd(OA)_2$ | -8.9 | -79.0 | 6.0 | -40.2 | -54.5 |
| [a]The data of H*Y* = *S*$ePPh_2H$, $HPPh_2$, and $RNH_2$ from Ref. 1 | | | | | |

As depicted in Figure S1 and Table S1, when one ligand (H*Y*) coordinates to $Cd(OA)_2$, the five-coordination complexes (H*Y*)$Cd(OA)_2$ should be generated, with the stabilization energies of –13.0 and –8.7 kJ $mol^{-1}$ for RSH and ROH, respectively. Alternatively, when two RSH ligands coordinate to $Cd(OA)_2$, the six-coordination complexes $(RSH)_2Cd(OA)_2$ should be formed, with the stabilization energies of –40.2 kJ $mol^{-1}$. When two ROH ligands coordinate to $Cd(OA)_2$, the four-coordination complexes $(ROH)_2Cd(OA)_2$ is generated through two Cd–O bonds cleavage of four-coordination complex $Cd(OA)_2$, with the stabilization energies of –54.5 kJ $mol^{-1}$. It is indicated that the $G_r$ values of the five-coordination complex are lower than that of the six-coordination complex. Nevertheless, the five- and six-coordination complexes of H*Y* toward $Cd(OA)_2$ are unstable because of their positive $G_r$ values.

Based on previous works[1] and this study, Table S1 lists the natural bond orbital (NBO) charges of the coordinated atom in ligands (H*Y* = $SePPh_2H$, $HPPh_2$, $RNH_2$, RSH, and ROH) and stabilization energies in five-coordination complex (H*Y*)$Cd(OA)_2$. As shown in Table S1, the NBO charges of coordinated atoms are the following from negative to positive: –0.916 ($RNH_2$) > –0.771 (ROH) > –0.460 ($SePPh_2H$) > –0.052 (RSH) > 0.617 ($HPPh_2$). According to the stabilization energies values, the coordination stability of ligands to metal centres of $Cd(OA)_2$ decreases as $RNH_2$ > $SePPh_2H$ > ROH > RSH > $HPPh_2$. It is apparent that the coordination stability is related to NBO charges. The larger of negative charges of coordinated atoms is, the more stable of coordination complex is. Exceptionally, for $SePPh_2H$ and ROH, five-coordination complex of $SePPh_2H$ toward $Cd(OA)_2$ is more stable than that of ROH. This can be ascribed to the steric hindrance of ligands, in which the Se atom in the linear Se–P of $SePPh_2H$ coordinates more readily than the O atom in the triangle of ROH, toward $Cd(OA)_2$. Thereupon, coordination stability mainly stems from the electrostatic interaction and steric hindrance between the ligand and $Cd(OA)_2$.

As depicted in Figure S1, for the reaction of $Cd(OA)_2$ with RSH, initially, the five-coordination complex (RSH)$Cd(OA)_2$ (**C3-IM1**) is formed. From **C3-IM1**, a H-shift from RSH to carboxylate occurs via a six-membered ring **C3-TS1**, resulting in the carboxylic acid molecular complex **C3-IM2**, with the energy barrier of 14.3 kJ $mol^{-1}$ and the energy height of the highest point (EHHP) of 27.3 kJ $mol^{-1}$ at **C3-TS1**. Then, **C3-IM2** releases the RCOOH molecules free, leaving RCOOCd–SR (**C3**) behind, with the exoergicity of 21.1 kJ $mol^{-1}$.

In addition, as shown in Figure S1, for the reaction of $Cd(OA)_2$ with ROH, firstly, the five-coordination complex (ROH)$Cd(OA)_2$ (**C4-IM1**) is formed. From **C4-IM1**, a H-shift takes place via a four-membered cyclic **C4-TS1**, leading to the RCOOH-containing molecular complex **C4-IM2**, with the energy barrier of 107.7 kJ $mol^{-1}$ and the EHHP of 116.4 kJ $mol^{-1}$ at **C4-TS1**. Last, **C4-IM2** releases the carboxylic acid, leaving RCOOCd–OR (**C4**), with the exoergicity of 41.3 kJ $mol^{-1}$.

**Table S2.** Relative Gibbs Free Energies and Typical Data for the Reaction of $Cd(OA)_2$ + H*Y* → RCOOCd–*Y* + RCOOH[a,b]

| item | $SePPh_2H$ | $HPPh_2$ | $RNH_2$ | RSH | ROH |
|---|---|---|---|---|---|
| $G_r$ | –56.4 | 34.0 | 86.3 | –21.9 | 70.9 |
| EHHP | 4.2 | 103.6 | 125.0 | 27.3 | 116.4 |
| Radius of *X* | 1.17 | 1.10 | 0.70 | 1.04 | 0.66 |
| Bond length of H–*Y* | 1.415 | 1.423 | 1.017 | 1.350 | 0.971 |
| Cd–*X* distance | 2.765 | 2.668 | 2.365 | 2.742 | 2.366 |
| No. of TS cyclic members | 7 | 6 | 4 | 6 | 4 |

[a]Relative Gibbs free energies ($G_r$, kJ mol$^{-1}$), energy height of the highest point (EHHP, kJ mol$^{-1}$), radius (Å) of the coordinated atom (*X* = Se, P, N, S, and O), bond length (Å) of H*Y*, Cd–*X* Distance (Å) in complex (H*Y*)$Cd(OA)_2$, and the number of the TS cyclic members for the reaction $Cd(OA)_2$ + H*Y* → RCOOCd–*Y* + RCOOH (See Figure S1). H*Y* = $SePPh_2H$, $HPPh_2$, $RNH_2$, RSH, and ROH.

[b]The data of H*Y* = *S*$ePPh_2H$, $HPPh_2$, and $RNH_2$ from Ref. 1

Table S2 summarizes the radii of the coordinated atom (*X*), bond length in ligand, Cd–*X* distance in (H*Y*)$Cd(OA)_2$, and the relative activation Gibbs free energy ($G_r$) of TS, considering the reports in previous publications[1] and this study.

As shown in Table S2, for the release of RCOOH from $Cd(OA)_2$ and ligands in the reaction (3), $G_r$ increases as -56.4 kJ mol$^{-1}$ ($SePPh_2H$) < -21.9 kJ mol$^{-1}$ (RSH) < 34.0 kJ mol$^{-1}$ ($HPPh_2$) < 70.9kJ mol$^{-1}$ (ROH) < 86.3 kJ mol$^{-1}$ ($RNH_2$). The energy height of the highest point (EHHP) increase as 4.2 kJ mol$^{-1}$ ($SePPh_2H$) < 27.3 kJ mol$^{-1}$ (RSH) < 103.6 kJ mol$^{-1}$ ($HPPh_2$) < 116.4 kJ mol$^{-1}$ (ROH) < 125.0 kJ mol$^{-1}$ ($RNH_2$). It is indicated that the thermodynamics and kinetics of RCOOH release should decrease as $SePPh_2H$ > RSH > $HPPh_2$ > ROH > $RNH_2$.

Furthermore, the radiuses of the coordinated atom in ligands decrease as 1.17 Å ($SePPh_2H$) > 1.10 Å ($HPPh_2$) > 1.04 Å (RSH) > 0.70 Å ($RNH_2$) > 0.66 Å (ROH). The bond length of H–*Y* in ligands decreases as 1.423 Å ($HPPh_2$) > 1.415 Å ($SePPh_2H$) > 1.350 Å (RSH) > 1.017 Å ($RNH_2$) > 0.971 Å (ROH) ≈ 0.972 Å (RCOOH). Typical strengths of the H–*Y* bonds are the following order: 300.4 kJ mol$^{-1}$ (P–H in $SePPh_2H$) ≈ 300.2 kJ mol$^{-1}$ (P–H in $HPPh_2$) < 346.2 kJ mol$^{-1}$ (S–H in RSH) < 400.4 kJ mol$^{-1}$ (N–H in $RNH_2$) < 423.3 kJ mol$^{-1}$（O–H in ROH） < 456.0 kJ mol$^{-1}$ (O–H in RCOOH). The above data clearly indicate that $SePPh_2H$, RSH, and $HPPh_2$ are more easily providing hydrogen/proton toward $Cd(OA)_2$ to the release of RCOOH than $RNH_2$ and ROH. Cd–*X* distance in (H*Y*)$Cd(OA)_2$ shortens in the reverse order as as 2.765 Å ($SePPh_2H$) > 2.742 Å (RSH) > 2.668 Å ($HPPh_2$) > 2.366 Å (ROH) ≈ 2.365 Å ($RNH_2$), and the number of TS cyclic member lessens follows in the reverse order as 7 ($SePPh_2H$) > 6 (RSH and $HPPh_2$) > 4 (ROH and $RNH_2$). It is indicated that the longer the Cd–*X* distance is, and the more the number of TS cyclic members is, which lowers the activation Gibbs free energy is.The lower the activation strain is, the less the activation energy is, and the lower the activation Gibbs free energy is. In short, the longer the Cd–*X* distance and *Z*–H bond length make the size of TS cyclic member larger, which makes the activation strain less, and thereby makes the activation Gibbs free energy lower (Table S3).

**Table S3.** Activation strain analysis of transition state (kJ mol$^{-1}$) and typical lengths (Å) for the *Z*–H (*Z* = P, N, S and O) bond cleavage in reaction of $Cd(OA)_2$ with ligand (H*Y* = $SePPh_2H$, $HPPh_2$, $RNH_2$, RSH, and ROH).

| H*Y* | Bond | TS | Length in H*Y* | Length in TS | Stretching in TS | Stretching in TS (%) | $\Delta E^{\neq}_{strain}$ [H*Y*] | $\Delta E^{\neq}_{strain}$ [$Cd(OA)_2$] | $\Delta E^{\neq}_{strain}$ | $\Delta E^{\neq}_{int}$ | $\Delta E^{\neq}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| $SePPh_2H$ | P–H | C-TS1 | 1.415 | 1.549 | 0.134 | 9.5 | 30.9 | 100.8 | 131.7 | –176.4 | –44.7 |
| $HPPh_2$ | P–H | C′-TS1 | 1.423 | 1.596 | 0.173 | 12.2 | 72.0 | 96.7 | 168.7 | –116.3 | 52.4 |
| $RNH_2$ | N–H | C′′-TS1 | 1.017 | 1.424 | 0.407 | 40.0 | 113.4 | 165.9 | 279.3 | –199.9 | 79.4 |
| RSH | S–H | C4-TS1 | 1.350 | 1.715 | 0.365 | 27.0 | 77.6 | 92.8 | 170.4 | –192.3 | –21.9 |
| ROH | O–H | C5-TS1 | 0.966 | 1.317 | 0.351 | 36.3 | 96.5 | 118.5 | 215.0 | –142.5 | 72.5 |

To gain insight into how ligands ($SePPh_2H$, $HPPh_2$, $RNH_2$, RSH, and ROH) affect the generation of RCOOH or Se–P bond cleavage in the formation of CdSe monomers, the trends in reactivity are analysed using the Activation Strain Model of chemical reactivity.[6, 7] In this model, the activation energies $\Delta E^{\neq}$ of TS are decomposed into the activation strain energies $\Delta E^{\neq}_{strain}$ and the stabilizing interaction energies $\Delta E^{\neq}_{int}$, *i.e.*, $\Delta E^{\neq} = \Delta E^{\neq}_{strain} + \Delta E^{\neq}_{int}$. $\Delta E^{\neq}_{strain}$ is the strain energy associated with deforming the reactants from their equilibrium geometry to the geometry they acquire in the TS. $\Delta E^{\neq}_{int}$ is the actual interaction energy between the deformed reactants in the TS.[6, 7] The results of the activation strain analysis were summarized in Table S3, according to current data and previous literature.[1]

As illustrated in Table S3, for the *Z*–H (*Z* = P, N, S, and O) bond cleavage, $\Delta E^{\neq}$ increases as –44.7 kJ mol$^{-1}$ ($SePPh_2H$) < –21.9 kJ mol$^{-1}$ (RSH) < 52.4 kJ mol$^{-1}$ ($HPPh_2$) < 72.5 kJ mol$^{-1}$ (ROH) < 79.4 kJ mol$^{-1}$ ($RNH_2$). $\Delta E^{\neq}_{strain}$ increases obviously as 131.7 kJ mol$^{-1}$ ($SePPh_2H$) < 170.4 kJ mol$^{-1}$ (RSH) ≈ 168.7 kJ mol$^{-1}$ ($HPPh_2$) < 215.0 kJ mol$^{-1}$ (ROH) < 279.3 kJ mol$^{-1}$ ($RNH_2$). The ligand activation-strain term $\Delta E^{\neq}_{strain}$[H*Y*] increases as 30.9 kJ mol$^{-1}$ ($SePPh_2H$) < 77.6 kJ mol$^{-1}$ (RSH) ≈ 72.0 kJ mol$^{-1}$ ($HPPh_2$) < 96.5 kJ mol$^{-1}$ (ROH) < 113.4 kJ mol$^{-1}$ ($RNH_2$), whereas $\Delta E^{\neq}_{strain}$[$Cd(OA)_2$] increases as 92.8 kJ mol$^{-1}$ (RSH) ≈ 96.7 kJ mol$^{-1}$ ($HPPh_2$) ≈ 100.8 kJ mol$^{-1}$ ($SePPh_2H$) < 118.5 kJ mol$^{-1}$ (ROH) < 165.9 kJ mol$^{-1}$ ($RNH_2$). That is to say, the $\Delta E^{\neq}_{strain}$ of TS, $Cd(OA)_2$, and ligands change in the same order as $\Delta E^{\neq}$. Moreover, it is apparent that the activation strain is correlated nearly with the percentage-wise extent of bond stretching in the TS (see Table S3). The percentage-wise bond elongation in the TS increases as $SePPh_2H$ < $HPPh_2$ < RSH < ROH < $RNH_2$. This nearly relates to $\Delta E^{\neq}_{strain}$. It is indicated that the activation strain favors the P–H and S–H cleavage over the O–H and N–H cleavage.

On the other hand, $\Delta E^{\neq}_{int}$ of the TS decreases as –199.9 kJ mol$^{-1}$ ($RNH_2$) > –192.3 kJ mol$^{-1}$ (RSH) > –176.4 kJ mol$^{-1}$ ($SePPh_2H$) > –142.5 kJ mol$^{-1}$ (ROH) > –116.3 kJ mol$^{-1}$ ($HPPh_2$). It is indicated that the stabilizing interaction with $HPPh_2$ is the least. This may derived from the repulsion of the positive P in $HPPh_2$ and the positive Cd in $Cd(OA)_2$, whereas the electrostatic interaction exists between the negative N, S, Se, and O in ligands and the positive Cd. For $RNH_2$, the value of $\Delta E^{\neq}_{int}$ is the minimum, $\Delta E^{\neq}_{strain}$ is the strongest, and $\Delta E^{\neq}$ is the largest. The phenomenon shows that the activation strain plays an important role for the release of RCOOH from $Cd(OA)_2$ and ligands. Consequently, for the release of RCOOH from $Cd(OA)_2$, ligands meet the following demands, the lowering of the activation strain and the strengthening of the stabilizing TS interaction, which lower the activation energies. Thereby, interacting with $Cd(OA)_2$ for the release of RCOOH, $RNH_2$ and ROH are the most difficult owing to the strong activation strain of activated N–H and O–H bond. $SePPh_2H$ and RSH are the easiest both because of the weak activation strain of P–H and S–H bond activation and the strong stabilizing TS interaction. Whereas, thanks to the weak activation strain of P–H bond activation and the weak stabilizing TS interaction, $HPPh_2$ is in the middle among five ligands. In other words, the capacity of releasing RCOOH decreases as $SePPh_2H$ > RSH > $HPPh_2$ > ROH > $RNH_2$ in the reaction of $Cd(OA)_2$ and ligands.

**Table S4.** Relative Gibbs free energies ($G_r$, kJ mol$^{-1}$), energy height of the highest point (EHHP, kJ mol$^{-1}$), and highest energy barrier (HEB, kJ mol$^{-1}$) in the reaction (4) of $Ph_2P$–SeCd–*Y* + $SePPh_2H$ ⇌ $Ph_2P$–SeCdSe–*Y* + $HPPh_2$ calculated at the M06//B3LYP/6-31++G(d, p), SDD level in 1-octadecene under room temperature (298.15 K) and atmospheric pressure (1 atm). *Y* = –$PPh_2$, –SR, –OR, –NHR.

| *Y* | Reaction | $G_r$ | EHHP | HEB |
|---|---|---|---|---|
| –$PPh_2$ | $Ph_2P$–CdSe–$PPh_2$ (**G**) + $SePPh_2H$ ⇌ $Ph_2P$–SeCdSe–$PPh_2$ (**E**) + $HPPh_2$ | –90.5 | 25.1 | 45.1 |
| –SR | RS–CdSe–$PPh_2$ (**J**) + $SePPh_2H$ ⇌ $Ph_2P$–SeCdSe–SR (**K**) + $HPPh_2$ | –17.3 | 143.0 | 216.2 |
| –OR | RO–CdSe–$PPh_2$ (**M**) + $SePPh_2H$ ⇌ $Ph_2P$–SeCdSe–OR (**N**) + $HPPh_2$ | –0.1 | 199.0 | 184.9 |
| –NHR | RHN–CdSe–$PPh_2$ (**H**) + $SePPh_2H$ ⇌ $Ph_2P$–SeCdSe–NHR (**I**) + $HPPh_2$ | –48.0 | 221.2 | 190.2 |

As shown in Figure 5a,b, for *Y* = –$PPh_2$, $Ph_2P$–CdSe–$PPh_2$ (**G**) + $SePPh_2H$ ⇌ $Ph_2P$–SeCdSe–$PPh_2$ (**E**) + $HPPh_2$ have been discussed in previous works.[1] The reaction **G** + $SePPh_2H$ ⇌ **E** + $HPPh_2$ can take place Se exchange reaction, with the HEB of 45.1 kJ mol$^{-1}$, the EHHP of 25.1 kJ mol$^{-1}$, and the exoergicity of 90.5 kJ mol$^{-1}$.[1]

As indicated in Figure 5a,b and Table S4, for *Y* = –SR, RS–CdSe–$PPh_2$ (**J**) + $SePPh_2H$ ⇌ $Ph_2P$–SeCdSe–SR (**K**) + $HPPh_2$, in the beginning, **J** isomerizes to $Ph_2P$–CdSe–SR (**J-i**) via a four-membered ring **J/J-i-TS1**. Next, a three-coordination complex **K/J-i-IM2** is formed by the Se atom of $SePPh_2H$ interacting with the central Cd atom of **J-i**. After that, [1,4]-H shift takes place from –$PPh_2$ group to $HPPh_2$ via a five-membered cyclic **K/J-i-TS1**, resulting in a $HPPh_2$-containing molecular complex **K/J-i-IM1**. Last, **K/J-i-IM1** releases the $HPPh_2$molecular free, leaving isomer $Ph_2P$–SeCdSe–SR (**K**) monomer behind. For $Ph_2P$–CdSe–SR (**J-i**), the occupancies of P–Cd, Cd–Se, and Se–S are 1.766, 1.883, and 1.987 *e*, respectively, from NBO analysis. It is indicated that complete single-bond exist in the P–Cd–Se–S skeleton. This reaction includes the HEB of 216.2 kJ mol$^{-1}$ at the reaction step of **J** → **J/J-i-TS1**, the EHHP of 143.0 kJ mol$^{-1}$ at **J/J-i-TS1**, and the exoergicity of 17.3 kJ mol$^{-1}$.

As shown in Figure 5a,b, for *Y* = –NHR, RNH–CdSe–$PPh_2$ (**H**) + $SePPh_2H$ ⇌ $Ph_2P$–SeCdSe–NHR (**I**) + $HPPh_2$ have an analogous reaction process as mentioned above. NBO results show that the occupancies of P–Cd, Cd–Se, and Se–N in **H-i** monomer are 1.775, 1.884, and 1.983 *e*, respectively, indicating complete single-bond in the P–Cd–Se–N skeleton. This reaction includes the HEB of 190.2 kJ mol$^{-1}$ at the reaction step of **H** → **H/H-i-TS1**, the EHHP of 221.2 kJ mol$^{-1}$ at **H/H-i-TS1**, and the exoergicity of 48.0 kJ mol$^{-1}$.

As indicated in Figure 5a,b, for *Y* = –OR, RO–CdSe–$PPh_2$ (**M**) + $SePPh_2H$ ⇌ $Ph_2P$–SeCdSe–OR (**N**) + $HPPh_2$ have a similar reaction process as mentioned before. For $Ph_2P$–CdSe–OR (**M-i**), the occupancies of P–Cd, Cd–Se, and Se–O are 1.771, 1.875, and 1.985 *e*, respectively, indicating complete single-bond in the P–Cd–Se–O skeleton. This reaction includes the HEB of 184.9 kJ mol$^{-1}$ at the reaction step of **M** → **M/M-i-TS1**, the EHHP of 199.0 kJ mol$^{-1}$ at **M/M-i-TS1**, and the exoergicity of 0.1 kJ mol$^{-1}$.

**Table S5.** Relative Gibbs free energies (Δ*G*, kJ mol$^{-1}$) to **1** ($Ph_2P$–*Y*) + $Se=PPh_2H$ for all the species in the reaction of $Ph_2P$–*Y* (**1**) + $SePPh_2H$ ⇌ $Ph_2P(Se)$–*Y* (**2**) + $HPPh_2$ calculated at the M06//B3LYP/6-31++G(d, p), SDD level in 1-octadecene under room temperature (298.15 K) and atmospheric pressure (1 atm). *Y* = –OOCR (**a**), –$PPh_2$ (**b**), –NHR (**c**), –SR (**d**), and –OR (**e**).

| *Y* | Reaction | Δ*G* | EHHP or HEB | P-containing compounds detected[a] |
|---|---|---|---|---|
| –OOCR | $Ph_2P$–OOCR (**1a**) + $SePPh_2H$ ⇌ $Ph_2P(Se)$–OOCR (**2a**) + $HPPh_2$ | 8.3 | 133.8 | $Ph_2P$–OOCR (**1a**) |
| –$PPh_2$ | $Ph_2P$–$PPh_2$ (**1b**) + $SePPh_2H$ ⇌ $Ph_2P(Se)$–$PPh_2$ (**2b**) + $HPPh_2$ | 34.9 | 151.7 | $Ph_2P$–$PPh_2$ (**1b**) |
| –NHR | $Ph_2P$–NHR (**1c**) + $SePPh_2H$ ⇌ $Ph_2P(Se)$–NHR (**2c**) + $HPPh_2$ | –17.8 | 120.4 | $Ph_2P$–NHR (**1c**), $Ph_2P(Se)$–NHR (**2c**) |
| –SR | $Ph_2P$–SR (**1d**) + $SePPh_2H$ ⇌ $Ph_2P(Se)$–SR (**2d**) + $HPPh_2$ | 8.6 | 126.8 | $Ph_2P$–SR (**1d**) |
| –OR | $Ph_2P$–OR (**1e**) + $SePPh_2H$ ⇌ $Ph_2P(Se)$–OR (**2e**) + $HPPh_2$ | –24.5 | 114.1 | $Ph_2P$–OR (**1e**), $Ph_2P(Se)$–OR (**2e**) |

[a]From ref.[2-5]

**Table S6.** Apparent activation energy (AAE, kJ $mol^{-1}$), rate-determining step involved bond cleavage, and comparision of correlation parameters for the formation of P-containing compounds $Ph_2P$–*Y* (**1**) and $Ph_2P(Se)$–*Y* (**2**). *Y* = –OOCR (**a**), $–PPh_2$ (**b**),–NHR (**c**), –SR (**d**), and –OR (**e**).

| *Y* | $Ph_2P$–*Y* (**1**) | | | | | | $Ph_2P(Se)$–*Y* (**2**) | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Monomers | Optimal paths | EHHP | $G_r$ | AAE | Bond cleavage | Monomers | Optimal paths | EHHP | $G_r$ | AAE | Bond cleavage |
| –OOCR | RCOOCdSe–$PPh_2$ (**C**) | **RP-C** | 4.2 | –56.4 | | | RCOOCd$Se_2PPh_2$ (**F**) | **RP-CF** | 4.2 | –133.0 | | |
| $–PPh_2$ | $Ph_2P$–CdSe–$PPh_2$ (**G**) | **RP-CFE-iG** | 5.9 | –20.0 | 45.1 | Se–P | $Ph_2PSe$–Cd–$SePPh_2$ (**E**) | **RP-CE** | –42.8 | –110.5 | 31.3 | P–H |
| –NHR | RHN–CdSe–$PPh_2$ (**H**) | **RP-CEH, RP-CFEH** | 37.6 | 31.0 | 94.5 | N–H | $Ph_2PSe$–CdSe–NHR (**I**) | **RP-CFE-iI** | 71.0 | –17.0 | 126.1 | P–N, Se–P |
| –SR | RS–CdSe–$PPh_2$ (**J**) | **RP-CEJ** | –42.8 | –73.2 | 10.2 | S–H | $Ph_2PSe$–CdSe–SR (**K**) | **RP-CFK** | –6.8 | –90.5 | 85.4 | S–H, Se–P |
| –OR | RO–CdSe–$PPh_2$ (**M**) | **RP-CEM, RP-CFEM** | –0.6 | 14.1 | 62.8 | O–H | $Ph_2PSe$–CdSe–OR **(N)** | **RP-CFE-iN** | 104.9 | 14.0 | 153.4 | O–H, Se–P |

**Table S7**. Activation strain analysis of transition state (kJ mol$^{-1}$) and typical lengths (Å) for the Se–P Bond cleavage in reaction of $Ph_2P$–$CdSe_2PPh_2$ (**E-i**) or $RCOOCdSe_2PPh_2$ (**F**) with ligands (H*Y* = $HPPh_2$, $RNH_2$, RSH, and ROH).

| H*Y* | Bond | TS | Length in **E-i** or **F** | Length in TS | Stretching in TS | Stretching in TS (%) | $\Delta E^{\neq}_{strain}$ [H*Y*] | $\Delta E^{\neq}_{strain}$ [**E-i** or **F**] | $\Delta E^{\neq}_{strain}$ | $\Delta E^{\neq}_{int}$ | $\Delta E^{\neq}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| $HPPh_2$ | Se–P | E-i/G-TS1 | 2.246 | 2.712 | 0.466 | 20.7 | 7.6 | 99.8 | 107.4 | –64.4 | 43.0 |
| $RNH_2$ | Se–P | E-i/I-TS1 | 2.246 | 4.492 | 2.246 | 100 | 102.4 | 283.4 | 385.8 | –260.6 | 125.2 |
| RSH | Se–P | F/K-TS1 | 2.254 | 2.776 | 0.522 | 23.2 | 44.3 | 162.7 | 207.0 | –124.4 | 82.6 |
| ROH | Se–P | E-i/N-TS1 | 2.246 | 2.644 | 0.398 | 17.7 | 286.1 | 137.9 | 424.0 | –272.9 | 151.1 |

As shown in Table S7, for the Se–P bond cleavage in the CdSe monomers formation, $\Delta E^{\neq}$ increases as 43.0 kJ mol$^{-1}$ ($HPPh_2$) < 82.6 kJ mol$^{-1}$ (RSH) < 125.2 kJ mol$^{-1}$ ($RNH_2$) < 151.1 kJ mol$^{-1}$ (ROH). $\Delta E^{\neq}_{strain}$ increases significantly as 107.4 kJ mol$^{-1}$ ($HPPh_2$) < 207.0 kJ mol$^{-1}$ (RSH) < 385.8 kJ mol$^{-1}$ ($RNH_2$) < 424.0 kJ mol$^{-1}$ (ROH). The substrate ligand $\Delta E^{\neq}_{strain}[L]$ increases as 7.6 kJ mol$^{-1}$ ($HPPh_2$) < 44.3 kJ mol$^{-1}$ (RSH) < 102.4 kJ mol$^{-1}$ ($RNH_2$) < 286.1 kJ mol$^{-1}$ (ROH). The substrate **E-i** or **F** activation-strain term $\Delta E^{\neq}_{strain}$[**E-i** or **F**] increases as 99.8 kJ mol$^{-1}$ ($HPPh_2$) < 162.7 kJ mol$^{-1}$ (RSH) < 283.4 kJ mol$^{-1}$ ($RNH_2$) < 137.9 kJ mol$^{-1}$ (ROH). That is to say, for the Se–P cleavage, $\Delta E^{\neq}_{strain}$ varies in the same order as $\Delta E^{\neq}$. In addition, $\Delta E^{\neq}_{strain}$ is related to the percentage-wise extent of Se–P bond stretching in the TS, as inferred in the Table S7. It is indicated that the activation strain favors the Se–P bond cleavage in the presence of $HPPh_2$ and RSH over that in the presence of $RNH_2$ and ROH. For another, $\Delta E^{\neq}_{int}$ increases as –64.4 kJ mol$^{-1}$ ($HPPh_2$) < –124.4 kJ mol$^{-1}$ (RSH) < –260.6 kJ mol$^{-1}$ ($RNH_2$) < –272.9 kJ mol$^{-1}$ (ROH), which takes in the same order as the activation energy $\Delta E^{\neq}$. It is indicated that the stabilizing TS interaction prefers $RNH_2$ and ROH to $HPPh_2$ and RSH. Overall, for the Se–P bond cleavage, the activation strain $\Delta E^{\neq}_{strain}$ play a central role. The capacity of Se–P bond cleavage decreases as $HPPh_2$ > RSH > $RNH_2$ > ROH in the formation of CdSe monomers, which originates from the size of coordinated atom radius (*X* = P, S, N, and O). As indicated in Table S2, the radius of the coordinated atom of H*Y* decrease as 1.10 Å ($HPPh_2$) > 1.04 Å (RSH) > 0.70 Å ($RNH_2$) > 0.66 Å (ROH), which takes in the same order as above.

**Table S8.** The zero-point energies (*ZPE*, hartree), thermal correction to Gibbs free energy ($G_0$, hartree) of various species calculated at the B3LYP/6-31++G(d, p), SDD level in the gas phase under atmospheric pressure and room temperature (298.15 K and 1 atm). Polarizable continuum model correction energies (*PCM-E*, hartree), total energies ($E_c$, hartree) corrected by *ZPE*, sum of electronic and thermal free energies ($G_c$, hartree) corrected by $G_0$, relative energies ($E_r$, kJ mol$^{-1}$) and relative Gibbs free energies ($G_r$, kJ mol$^{-1}$) to $Cd(OA)_2$ + *n*H*Y* (H*Y* = RSH and ROH; *n* = 1 ~ 2) for all the species in the reaction of $Cd(OA)_2$ + *n*H*Y* → $(HY)_nCd(OA)_2$, $Cd(OA)_2$ + RSH → **C4** + RCOOH, and $Cd(OA)_2$ + ROH → **C5** + RCOOH calculated at the M06//B3LYP/6-31++G(d, p), SDD level in 1-octadecene solution under room temperature and atmospheric pressure (298.15 K and 1 atm).

| Species | M06//B3LYP/6-31++G(d, p), SDD (298.15 K and 1 atm) | | | | | | |
|---|---|---|---|---|---|---|---|
| | *ZPE* | $G_0$ | *PCM-E* | $E_c$ (*PCM-E + ZPE*) | $E_r$ | $G_c$(*PCM-E + $G_0$*) | $G_r$ |
| RSH | 0.07493 | 0.04829 | -477.92093 | -477.84600 | | -477.87264 | |
| ROH | 0.07988 | 0.05449 | -154.95830 | -154.87842 | | -154.90381 | |
| $Cd(OA)_2$ | 0.15896 | 0.11333 | -703.16954 | -703.01058 | | -703.05621 | |
| RCOOH | 0.09058 | 0.06013 | -268.27275 | -268.18218 | | -268.21262 | |
| RSH +$Cd(OA)_2$ | 0.23389 | 0.16161 | -1181.09047 | -1180.85658 | 0.0 | -1180.92886 | 0.0 |
| (RSH)$Cd(OA)_2$, C4-IM1 | 0.23515 | 0.17881 | -1181.10274 | -1180.86759 | -28.9 | -1180.92393 | 13.0 |
| C4-TS1 | 0.23302 | 0.17946 | -1181.09793 | -1180.86491 | -21.9 | -1180.91848 | 27.3 |
| C4-IM2 | 0.23853 | 0.18274 | -1181.11192 | -1180.87339 | -44.1 | -1180.92918 | -0.8 |
| C4 | 0.14684 | 0.10316 | -912.82773 | -912.68089 | | -912.72457 | |
| C4 + RCOOH | 0.23741 | 0.16329 | -1181.10048 | -1180.86307 | -17.0 | -1180.93719 | -21.9 |
| | | | | | | | |
| ROH +$Cd(OA)_2$ | 0.23884 | 0.16782 | -858.12784 | -857.88900 | 0.0 | -857.96002 | 0.0 |
| (ROH)$Cd(OA)_2$, C5-IM1 | 0.24034 | 0.18443 | -858.14112 | -857.90078 | -30.9 | -857.95669 | 8.7 |
| C5-TS1 | 0.23619 | 0.18188 | -858.09756 | -857.86137 | 72.5 | -857.91568 | 116.4 |
| C5-IM2 | 0.23973 | 0.18387 | -858.10116 | -857.86143 | 72.4 | -857.91729 | 112.2 |
| C5 | 0.14851 | 0.10556 | -589.82596 | -589.67745 | | -589.72040 | |
| C5 + RCOOH | 0.23909 | 0.16570 | -858.09871 | -857.85962 | 77.1 | -857.93302 | 70.9 |
| | | | | | | | |
| 2RSH +$Cd(OA)_2$ | 0.30882 | 0.20990 | -1659.01140 | -1658.70258 | 0.0 | -1658.80150 | 0.0 |
| $(RSH)_2Cd(OA)_2$ | 0.31117 | 0.24420 | -1659.03040 | -1658.71923 | -43.7 | -1658.78620 | 40.2 |
| 2ROH +$Cd(OA)_2$ | 0.31871 | 0.22231 | -1013.08614 | -1012.76742 | 0.0 | -1012.86383 | 0.0 |
| $(ROH)_2Cd(OA)_2$ | 0.32241 | 0.26055 | -1013.10363 | -1012.78122 | -36.2 | -1012.84307 | 54.5 |

**Table S9.** The zero-point energies (*ZPE*, hartree), thermal correction to Gibbs free energy ($G_0$, hartree) of various species calculated at the B3LYP/6-31++G(d, p), SDD level in the gas phase under atmospheric pressure and room temperature (298.15 K and 1 atm). Polarizable continuum model correction energies (*PCM-E*, hartree), total energies ($E_c$, hartree) corrected by *ZPE*, sum of electronic and thermal free energies ($G_c$, hartree) corrected by $G_0$, relative energies ($E_r$, kJ mol$^{-1}$) and relative Gibbs free energies ($G_r$, kJ mol$^{-1}$) to $Cd(OA)_2$ + $SePPh_2H$ + RSH for all the species in the reaction of $Cd(OA)_2$ + $SePPh_2H$ + RSH → **J** + 2RCOOH (**C** + RSH → **J** + RCOOH, **E** + RSH → **J** + $SePPh_2H$, **F** + RSH + $HPPh_2$ → **J** + RCOOH + $SePPh_2H$, and **G** + RSH → **J** + $HPPh_2$) calculated at the M06//B3LYP/6-31++G(d, p), SDD level in 1-octadecene solution under room temperature and atmospheric pressure (298.15 K and 1 atm).

| Species | M06//B3LYP/6-31++G(d, p), SDD (298.15 K and 1 atm) | | | | | | |
|---|---|---|---|---|---|---|---|
| | *ZPE* | $G_0$ | *PCM-E* | $E_c$ (*PCM-E* + *ZPE*) | $E_r$ | $G_c$(*PCM-E* + $G_0$) | $G_r$ |
| $Cd(OA)_2$ | 0.15896 | 0.11333 | -703.16954 | -703.01058 | | -703.05621 | |
| $SePPh_2H$ | 0.19343 | 0.15007 | -814.22030 | -814.02687 | | -814.07023 | |
| $HPPh_2$ | 0.19113 | 0.15188 | -804.87857 | -804.68745 | | -804.72669 | |
| RSH | 0.07493 | 0.04829 | -477.92093 | -477.84600 | | -477.87264 | |
| RCOOH | 0.09058 | 0.06013 | -268.27275 | -268.18218 | | -268.21262 | |
| $Cd(OA)_2$ + $SePPh_2H$ + RSH | 0.42732 | 0.31168 | -1995.31076 | -1994.88344 | 0.0 | -1994.99908 | 0.0 |
| C | 0.26354 | 0.20472 | -1249.14001 | -1248.87647 | | -1248.93529 | |
| C + RSH + RCOOH | 0.42904 | 0.31314 | -1995.33369 | -1994.90465 | -55.7 | -1995.02055 | -56.4 |
| C/J-IM1 | 0.33996 | 0.27260 | -1727.07332 | -1726.73337 | | -1726.80073 | |
| C/J-IM1 + RCOOH | 0.43053 | 0.33273 | -1995.34608 | -1994.91554 | -84.3 | -1995.01335 | -37.5 |
| C/J-TS1 | 0.33842 | 0.27066 | -1727.06242 | -1726.72401 | | -1726.79177 | |
| C/J-TS1 + RCOOH | 0.42899 | 0.33079 | -1995.33518 | -1994.90618 | -59.7 | -1995.00439 | -13.9 |
| C/J-IM2 | 0.34319 | 0.27543 | -1727.08110 | -1726.73792 | | -1726.80567 | |
| C/J-IM2 + RCOOH | 0.43376 | 0.33556 | -1995.35386 | -1994.92009 | -96.2 | -1995.01829 | -50.4 |
| J | 0.25157 | 0.19517 | -1458.79688 | -1458.54530 | | -1458.60171 | |
| J + 2RCOOH | 0.43273 | 0.31544 | -1995.34238 | -1994.90966 | -68.8 | -1995.02694 | -73.2 |
| | | | | | | | |
| E | 0.36828 | 0.29778 | -1795.11131 | -1794.74302 | | -1794.81353 | |
| E + RSH + 2RCOOH - $SePPh_2H$ | 0.43093 | 0.31626 | -1995.35744 | -1994.92651 | -113.1 | -1995.04118 | -110.5 |
| E/J-IM1 | 0.44429 | 0.36189 | -2273.04005 | -2272.59576 | | -2272.67816 | |
| E/J-IM1 + 2RCOOH- $SePPh_2H$ | 0.43201 | 0.33208 | -1995.36526 | -1994.93325 | -130.8 | -1995.03317 | -89.5 |
| E/J-TS1 | 0.44146 | 0.36449 | -2273.02628 | -2272.58481 | | -2272.66178 | |
| E/J-TS1 + 2RCOOH- $SePPh_2H$ | 0.42919 | 0.33469 | -1995.35148 | -1994.92230 | -102.0 | -1995.01679 | -46.5 |
| E/J-IM2 | 0.44575 | 0.36556 | -2273.03756 | -2272.59182 | | -2272.67200 | |
| E/J-IM2 + 2RCOOH - $SePPh_2H$ | 0.43347 | 0.33576 | -1995.36277 | -1994.92930 | -120.4 | -1995.02701 | -73.3 |
| | | | | | | | |
| F | 0.26560 | 0.20565 | -1258.51366 | -1258.24806 | | -1258.30802 | |
| F + RSH + $HPPh_2$ + RCOOH - $SePPh_2H$ | 0.42880 | 0.31588 | -1995.36562 | -1994.93682 | -140.1 | -1995.04974 | -133.0 |
| F/K-i-IM1 | 0.34150 | 0.26888 | -1736.44428 | -1736.10278 | | -1736.17540 | |
| F/K-i-IM1+ $HPPh_2$ + RCOOH - $SePPh_2H$ | 0.42977 | 0.33083 | -1995.37531 | -1994.94554 | -163.0 | -1995.04448 | -119.2 |

Continued

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| F/K-i-TS1a | 0.33933 | 0.27243 | -1736.43484 | -1736.09551 | | -1736.16241 | |
| F/K-i-TS1a + $HPPh_2$ + RCOOH - $SePPh_2H$ | 0.42760 | 0.33438 | -1995.36587 | -1994.93827 | -143.9 | -1995.03149 | -85.1 |
| F/K-i-IM2a | 0.34474 | 0.27569 | -1736.45269 | -1736.10794 | | -1736.17699 | |
| F/K-i-IM2a + $HPPh_2$ + RCOOH - $SePPh_2H$ | 0.43302 | 0.33764 | -1995.38371 | -1994.95070 | -176.6 | -1995.04607 | -123.4 |
| F/K-i-TS1b | 0.33880 | 0.27032 | -1736.41654 | -1736.07774 | | -1736.14622 | |
| F/K-i-TS1b + $HPPh_2$ + RCOOH - $SePPh_2H$ | 0.42707 | 0.33227 | -1995.34757 | -1994.92049 | -97.3 | -1995.01530 | -42.6 |
| F/K-i-IM2b | 0.34467 | 0.27413 | -1736.44300 | -1736.09833 | | -1736.16887 | |
| F/K-i-IM2b + $HPPh_2$ + RCOOH - $SePPh_2H$ | 0.43295 | 0.33608 | -1995.37403 | -1994.94108 | -151.3 | -1995.03795 | -102.1 |
| K-i | 0.24896 | 0.19022 | -1468.16906 | -1467.92010 | | -1467.97884 | |
| K-i + $HPPh_2$ + 2RCOOH - $SePPh_2H$ | 0.42781 | 0.31230 | -1995.37284 | -1994.94503 | -161.7 | -1995.06054 | -161.4 |
| K-i/J-IM1 | 0.440961 | 0.359823 | -2273.049041 | -2272.60808 | | -2272.689218 | |
| K-i/J-IM1 + 2RCOOH - $SePPh_2H$ | 0.428684 | 0.330021 | -1995.374247 | -1994.945563 | -163.1 | -1995.044226 | -118.5 |
| K-i/J-TS1 | 0.445045 | 0.366152 | -2273.030107 | -2272.585062 | | -2272.663955 | |
| K-i/J-TS1 + 2RCOOH - $SePPh_2H$ | 0.432768 | 0.33635 | -1995.355313 | -1994.922545 | -102.7 | -1995.018963 | -52.2 |
| K-i/J-IM2 | 0.44579 | 0.365049 | -2273.040053 | -2272.594263 | | -2272.675004 | |
| K-i/J-IM2 + 2RCOOH - $SePPh_2H$ | 0.433513 | 0.335247 | -1995.36526 | -1994.931747 | -126.8 | -1995.030013 | -81.2 |
| J-ii | 0.251478 | 0.19299 | -1458.792994 | -1458.541516 | | -1458.600004 | |
| J-ii + 2RCOOH | 0.43263 | 0.313256 | -1995.338498 | -1994.905868 | -58.9 | -1995.025242 | -68.7 |
| | | | | | | | |
| G | 0.36683 | 0.29875 | -1785.73426 | -1785.36743 | | -1785.43551 | |
| G + RSH + 2RCOOH - $HPPh_2$ | 0.43178 | 0.31542 | -1995.32212 | -1994.89034 | -18.1 | -1995.00670 | -20.0 |
| G/J-IM1 | 0.44302 | 0.36546 | -2263.66336 | -2263.22034 | | -2263.29789 | |
| G/J-IM1 + 2RCOOH - $HPPh_2$ | 0.43304 | 0.33385 | -1995.33029 | -1994.89725 | -36.3 | -1994.99644 | 6.9 |
| G/J-TS1 | 0.43982 | 0.36361 | -2263.63339 | -2263.19357 | | -2263.26977 | |
| G/J-TS1 + 2RCOOH - $HPPh_2$ | 0.42985 | 0.33200 | -1995.30032 | -1994.87047 | 34.0 | -1994.96832 | 80.8 |
| G/J-IM2 | 0.44367 | 0.36461 | -2263.67738 | -2263.23371 | | -2263.31276 | |
| G/J-IM2 + 2RCOOH - $HPPh_2$ | 0.43369 | 0.33300 | -1995.34431 | -1994.91062 | -71.4 | -1995.01131 | -32.1 |

**Table S10.** The zero-point energies (*ZPE*, hartree), thermal correction to Gibbs free energy ($G_0$, hartree) of various species calculated at the B3LYP/6-31++G(d, p), SDD level in the gas phase under atmospheric pressure and room temperature (298.15 K and 1 atm). Polarizable continuum model correction energies (*PCM-E*, hartree), total energies ($E_c$, hartree) corrected by *ZPE*, sum of electronic and thermal free energies ($G_c$, hartree) corrected by $G_0$, relative energies ($E_r$, kJ mol$^{-1}$) and relative Gibbs free energies ($G_r$, kJ mol$^{-1}$) to $Cd(OA)_2$ + $2SePPh_2H$ + RSH for all the species in the reaction of $Cd(OA)_2$ + $2SePPh_2H$ + RSH → **K** + $HPPh_2$ + 2RCOOH (**F** + RSH + $SePPh_2H$ → **K** + RCOOH, **K-i** → **K**, and **E-i** + RSH → **K** + $HPPh_2$) calculated at the M06//B3LYP/6-31++G(d, p), SDD level in 1-octadecene solution under room temperature and atmospheric pressure (298.15 K and 1 atm).

| Species | M06//B3LYP/6-31++G(d, p), SDD (298.15 K and 1 atm) | | | | | | |
|---|---|---|---|---|---|---|---|
| | *ZPE* | $G_0$ | *PCM-E* | $E_c$ (*PCM-E* + *ZPE*) | $E_r$ | $G_c$(*PCM-E* + $G_0$) | $G_r$ |
| $Cd(OA)_2$ | 0.15896 | 0.11333 | -703.16954 | -703.01058 | | -703.05621 | |
| $SePPh_2H$ | 0.19343 | 0.15007 | -814.22030 | -814.02687 | | -814.07023 | |
| $HPPh_2$ | 0.19113 | 0.15188 | -804.87857 | -804.68745 | | -804.72669 | |
| RSH | 0.07493 | 0.04829 | -477.92093 | -477.84600 | | -477.87264 | |
| RCOOH | 0.09058 | 0.06013 | -268.27275 | -268.18218 | | -268.21262 | |
| $Cd(OA)_2$ + $2SePPh_2H$ + RSH | 0.62075 | 0.46175 | -2809.53106 | -2808.91031 | 0.0 | -2809.06931 | 0.0 |
| F | 0.26560 | 0.20565 | -1258.51366 | -1258.24806 | | -1258.30802 | |
| F + RSH + DPP + RCOOH | 0.62223 | 0.46595 | -2809.58592 | -2808.96368 | -140.1 | -2809.11997 | -133.0 |
| F/K-i-IM1 | 0.34150 | 0.26888 | -1736.44428 | -1736.10278 | | -1736.17540 | |
| F/K-i-IM1 + DPP + RCOOH | 0.62320 | 0.48090 | -2809.59560 | -2808.97240 | -163.0 | -2809.11471 | -119.2 |
| F/K-TS1 | 0.33822 | 0.26821 | -1736.40082 | -1736.06260 | | -1736.13261 | |
| F/K-TS1 + DPP + RCOOH | 0.61992 | 0.48023 | -2809.55214 | -2808.93222 | -57.5 | -2809.07192 | -6.8 |
| F/K-IM2 | 0.34374 | 0.27029 | -1736.42153 | -1736.07779 | | -1736.15124 | |
| F/K-IM2 + DPP + RCOOH | 0.62544 | 0.48231 | -2809.57286 | -2808.94741 | -97.4 | -2809.09054 | -55.8 |
| K-ii | 0.25233 | 0.18874 | -1468.13749 | -1467.88516 | | -1467.94875 | |
| K-ii + DPP + 2RCOOH | 0.62461 | 0.46089 | -2809.56156 | -2808.93696 | -70.0 | -2809.10068 | -82.4 |
| K | 0.25230 | 0.19078 | -1468.14263 | -1467.89033 | | -1467.95185 | |
| K + DPP + 2RCOOH | 0.62458 | 0.46293 | -2809.56671 | -2808.94212 | -83.5 | -2809.10378 | -90.5 |
| K-i | 0.24896 | 0.19022 | -1468.16906 | -1467.92010 | | -1467.97884 | |
| K-i + DPP + 2RCOOH | 0.62124 | 0.46237 | -2809.59314 | -2808.97190 | -161.7 | -2809.13077 | -161.4 |
| K-i/K-TS1 | 0.25238 | 0.19501 | -1468.10638 | -1467.85400 | | -1467.91137 | |
| K-i/K-TS1 + DPP + 2RCOOH | 0.62466 | 0.46716 | -2809.53046 | -2808.90580 | 11.8 | -2809.06330 | 15.8 |
| E-i | 0.36870 | 0.29776 | -1795.10594 | -1794.73724 | | -1794.80818 | |
| E-i + RSH + 2RCOOH | 0.62478 | 0.46632 | -2809.57237 | -2808.94759 | -97.9 | -2809.10606 | -96.5 |
| E-i/K-IM1 | 0.44480 | 0.36408 | -2273.03773 | -2272.59293 | | -2272.67364 | |
| E-i/K-IM1 + 2RCOOH | 0.62595 | 0.48435 | -2809.58323 | -2808.95728 | -123.3 | -2809.09888 | -77.6 |
| E-i/K-TS1 | 0.44115 | 0.36243 | -2272.99268 | -2272.55153 | | -2272.63026 | |
| E-i/K-TS1 + 2RCOOH | 0.62230 | 0.48269 | -2809.53819 | -2808.91588 | -14.6 | -2809.05550 | 36.3 |
| E-i/K-IM2 | 0.44477 | 0.36142 | -2273.02254 | -2272.57777 | | -2272.66112 | |
| E-i/K-IM2 + 2RCOOH | 0.62592 | 0.48169 | -2809.56804 | -2808.94212 | -83.5 | -2809.08635 | -44.8 |

**Table S11.** The zero-point energies (*ZPE*, hartree), thermal correction to Gibbs free energy ($G_0$, hartree) of various species calculated at the B3LYP/6-31++G(d, p), SDD level in the gas phase under atmospheric pressure and room temperature (298.15 K and 1 atm). Polarizable continuum model correction energies (*PCM-E*, hartree), total energies ($E_c$, hartree) corrected by *ZPE*, sum of electronic and thermal free energies ($G_c$, hartree) corrected by $G_0$, relative energies ($E_r$, kJ mol$^{-1}$) and relative Gibbs free energies ($G_r$, kJ mol$^{-1}$) to $Cd(OA)_2$ + $SePPh_2H$ + ROH for all the species in the reaction of $Cd(OA)_2$ + $SePPh_2H$ + ROH → **M** + 2RCOOH (**C** + ROH → **M** + RCOOH, **E** + ROH → **M** + $SePPh_2H$, **F** + ROH + $HPPh_2$ → **M** + RCOOH + $SePPh_2H$, and **G** + ROH → **M** + $HPPh_2$) calculated at the M06//B3LYP/6-31++G(d, p), SDD level in 1-octadecene solution under room temperature and atmospheric pressure (298.15 K and 1 atm).

| Species | M06//B3LYP/6-31++G(d, p), SDD (298.15 K and 1 atm) | | | | | | |
|---|---|---|---|---|---|---|---|
| | *ZPE* | $G_0$ | *PCM-E* | $E_c$ (*PCM-E* + *ZPE*) | $E_r$ | $G_c$(*PCM-E* + $G_0$) | $G_r$ |
| $Cd(OA)_2$ | 0.15896 | 0.11333 | -703.16954 | -703.01058 | | -703.05621 | |
| $SePPh_2H$ | 0.19343 | 0.15007 | -814.22030 | -814.02687 | | -814.07023 | |
| $HPPh_2$ | 0.19113 | 0.15188 | -804.87857 | -804.68745 | | -804.72669 | |
| ROH | 0.07988 | 0.05449 | -154.95830 | -154.87842 | | -154.90381 | |
| RCOOH | 0.09058 | 0.06013 | -268.27275 | -268.18218 | | -268.21262 | |
| $Cd(OA)_2$ + $SePPh_2H$ + ROH | 0.43227 | 0.31789 | -1672.34814 | -1671.91587 | 0.0 | -1672.03025 | 0.0 |
| C | 0.26354 | 0.20472 | -1249.14001 | -1248.87647 | | -1248.93529 | |
| C + ROH + RCOOH | 0.43399 | 0.31935 | -1672.37106 | -1671.93707 | -55.7 | -1672.05171 | -56.4 |
| C/M-IM1 | 0.34533 | 0.27872 | -1404.11054 | -1403.76521 | | -1403.83182 | |
| C/M-IM1 + RCOOH | 0.43591 | 0.33886 | -1672.38329 | -1671.94738 | -82.7 | -1672.04444 | -37.2 |
| C/M-TS1 | 0.34064 | 0.27374 | -1404.07179 | -1403.73115 | | -1403.79805 | |
| C/M-TS1 + RCOOH | 0.43121 | 0.33387 | -1672.34454 | -1671.91333 | 6.7 | -1672.01067 | 51.4 |
| C/M-IM2 | 0.34469 | 0.27641 | -1404.07649 | -1403.73180 | | -1403.80008 | |
| C/M-IM2 + RCOOH | 0.43527 | 0.33654 | -1672.34924 | -1671.91398 | 5.0 | -1672.01270 | 46.1 |
| M | 0.25335 | 0.19864 | -1135.79829 | -1135.54493 | | -1135.59965 | |
| M + 2RCOOH | 0.43451 | 0.31890 | -1672.34379 | -1671.90928 | 17.3 | -1672.02489 | 14.1 |
| | | | | | | | |
| E | 0.36828 | 0.29778 | -1795.11131 | -1794.74302 | | -1794.81353 | |
| E + ROH + 2RCOOH - $SePPh_2H$ | 0.43588 | 0.32247 | -1672.39481 | -1671.95893 | -113.1 | -1672.07235 | -110.5 |
| E/M-IM1 | 0.44980 | 0.36855 | -1950.07654 | -1949.62674 | | -1949.70798 | |
| E/M-IM1 + 2RCOOH- $SePPh_2H$ | 0.43752 | 0.33875 | -1672.40174 | -1671.96422 | -126.9 | -1672.06299 | -86.0 |
| E/M-TS1 | 0.44589 | 0.36842 | -1950.04389 | -1949.59800 | | -1949.67547 | |
| E/M-TS1 + 2RCOOH- $SePPh_2H$ | 0.43362 | 0.33862 | -1672.36910 | -1671.93548 | -51.5 | -1672.03048 | -0.6 |
| E/M-IM2 | 0.44693 | 0.36802 | -1950.04375 | -1949.59682 | | -1949.67572 | |
| E/M-IM2 + 2RCOOH - $SePPh_2H$ | 0.43465 | 0.33822 | -1672.36895 | -1671.93430 | -48.4 | -1672.03073 | -1.3 |
| | | | | | | | |
| F | 0.26560 | 0.20565 | -1258.51366 | -1258.24806 | | -1258.30802 | |
| F + ROH + $HPPh_2$ + RCOOH - $SePPh_2H$ | 0.43375 | 0.32209 | -1672.40299 | -1671.96924 | -140.1 | -1672.08091 | -133.0 |
| F/N-i-IM1 | 0.34682 | 0.27612 | -1413.48058 | -1413.13376 | | -1413.20447 | |

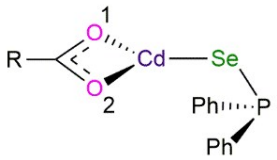
Continued

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| F/N-i-IM1+ $HPPh_2$ + RCOOH - $SePPh_2H$ | 0.43509 | 0.33806 | -1672.41161 | -1671.97651 | -159.2 | -1672.07354 | -113.7 |
| F/N-i-TS1 | 0.34285 | 0.27530 | -1413.44702 | -1413.10417 | | -1413.17172 | |
| F/N-i-TS1 + $HPPh_2$ + RCOOH - $SePPh_2H$ | 0.43113 | 0.33725 | -1672.37805 | -1671.94692 | -81.5 | -1672.04080 | -27.7 |
| F/N-i-IM2 | 0.34619 | 0.27677 | -1413.44944 | -1413.10324 | | -1413.17266 | |
| F/N-i-IM2 + $HPPh_2$ + RCOOH - $SePPh_2H$ | 0.43447 | 0.33872 | -1672.38046 | -1671.94599 | -79.1 | -1672.04174 | -30.2 |
| N-i | 0.25513 | 0.19667 | -1145.16894 | -1144.91382 | | -1144.97228 | |
| N-i + $HPPh_2$ + 2RCOOH - $SePPh_2H$ | 0.43398 | 0.31875 | -1672.37272 | -1671.93875 | -60.1 | -1672.05397 | -62.3 |
| N-i/J-IM1 | 0.44291 | 0.36542 | -1950.05315 | -1949.61024 | | -1949.68773 | |
| N-i/J-IM1 + 2RCOOH - $SePPh_2H$ | 0.43064 | 0.33562 | -1672.37836 | -1671.94772 | -83.6 | -1672.04274 | -32.8 |
| N-i/J-TS1 | 0.44695 | 0.37067 | -1950.03166 | -1949.58472 | | -1949.66099 | |
| N-i/J-TS1 + 2RCOOH - $SePPh_2H$ | 0.43467 | 0.34087 | -1672.35687 | -1671.92220 | -16.6 | -1672.01600 | 37.4 |
| N-i/J-IM2 | 0.44728 | 0.36701 | -1950.04426 | -1949.59698 | | -1949.67725 | |
| N-i/J-IM2 + 2RCOOH - $SePPh_2H$ | 0.43500 | 0.33721 | -1672.36947 | -1671.93447 | -48.8 | -1672.03226 | -5.3 |
| M-ii | 0.25340 | 0.19727 | -1135.79483 | -1135.54143 | | -1135.59756 | |
| M-ii + 2RCOOH | 0.43455 | 0.31753 | -1672.34033 | -1671.90578 | 26.5 | -1672.02280 | 19.6 |
| | | | | | | | |
| G | 0.36683 | 0.29875 | -1785.73426 | -1785.36743 | | -1785.43551 | |
| G + ROH + 2RCOOH - $HPPh_2$ | 0.43673 | 0.32162 | -1672.35949 | -1671.92276 | -18.1 | -1672.03787 | -20.0 |
| G/M-IM1 | 0.44845 | 0.37289 | -1940.69941 | -1940.25096 | | -1940.32652 | |
| G/M-IM1 + 2RCOOH - $HPPh_2$ | 0.43848 | 0.34127 | -1672.36634 | -1671.92786 | -31.5 | -1672.02507 | 13.6 |
| G/M-TS1 | 0.44247 | 0.36821 | -1940.65214 | -1940.20967 | | -1940.28393 | |
| G/M-TS1 + 2RCOOH - $HPPh_2$ | 0.43250 | 0.33659 | -1672.31907 | -1671.88657 | 76.9 | -1671.98248 | 125.4 |
| G/M-IM2 | 0.44559 | 0.36928 | -1940.68063 | -1940.23505 | | -1940.31135 | |
| G/M-IM2 + 2RCOOH - $HPPh_2$ | 0.43561 | 0.33766 | -1672.34757 | -1671.91195 | 10.3 | -1672.00990 | 53.4 |

**Table S12.** The zero-point energies (*ZPE*, hartree), thermal correction to Gibbs free energy ($G_0$, hartree) of various species calculated at the B3LYP/6-31++G(d, p), SDD level in the gas phase under atmospheric pressure and room temperature (298.15 K and 1 atm). Polarizable continuum model correction energies (*PCM-E*, hartree), total energies ($E_c$, hartree) corrected by *ZPE*, sum of electronic and thermal free energies ($G_c$, hartree) corrected by $G_0$, relative energies ($E_r$, kJ mol$^{-1}$) and relative Gibbs free energies ($G_r$, kJ mol$^{-1}$) to $Cd(OA)_2$ + $2SePPh_2H$ + ROH for all the species in the reaction of $Cd(OA)_2$ + $2SePPh_2H$ + ROH → **N** + $HPPh_2$ + 2RCOOH (**N-i** → **N** and **E-i** + ROH → **N** + $HPPh_2$) calculated at the M06//B3LYP/6-31++G(d, p), SDD level in 1-octadecene solution under room temperature and atmospheric pressure (298.15 K and 1 atm).

| Species | M06//B3LYP/6-31++G(d, p), SDD (298.15 K and 1 atm) | | | | | | |
|---|---|---|---|---|---|---|---|
| | *ZPE* | $G_0$ | *PCM-E* | $E_c$ (*PCM-E + ZPE*) | $E_r$ | $G_c$(*PCM-E + $G_0$*) | $G_r$ |
| $Cd(OA)_2$ | 0.15896 | 0.11333 | -703.16954 | -703.01058 | | -703.05621 | |
| $SePPh_2H$ | 0.19343 | 0.15007 | -814.22030 | -814.02687 | | -814.07023 | |
| $HPPh_2$ | 0.19113 | 0.15188 | -804.87857 | -804.68745 | | -804.72669 | |
| ROH | 0.07988 | 0.05449 | -154.95830 | -154.87842 | | -154.90381 | |
| RCOOH | 0.09058 | 0.06013 | -268.27275 | -268.18218 | | -268.21262 | |
| $Cd(OA)_2$ + $2SePPh_2H$ + ROH | 0.62570 | 0.46795 | -2486.56843 | -2485.94274 | 0.0 | -2486.10048 | 0.0 |
| N-i | 0.25513 | 0.19667 | -1145.16894 | -1144.91382 | | -1144.97228 | |
| N-i + DPP + 2RCOOH | 0.62741 | 0.46882 | -2486.59302 | -2485.96562 | -60.1 | -2486.12420 | -62.3 |
| N-i/N-TS1 | 0.25400 | 0.19708 | -1145.10245 | -1144.84844 | | -1144.90537 | |
| N-i/N-TS1 + DPP + 2RCOOH | 0.62628 | 0.46923 | -2486.52652 | -2485.90024 | 111.6 | -2486.05730 | 113.4 |
| N-ii | 0.25436 | 0.19573 | -1145.13322 | -1144.87887 | | -1144.93749 | |
| N-ii + DPP + 2RCOOH | 0.62664 | 0.46788 | -2486.55730 | -2485.93067 | 31.7 | -2486.08942 | 29.0 |
| N | 0.25447 | 0.19431 | -1145.13755 | -1144.88308 | | -1144.94323 | |
| N + DPP + 2RCOOH | 0.62675 | 0.46646 | -2486.56162 | -2485.93488 | 20.6 | -2486.09516 | 14.0 |
| | | | | | | | |
| E-i | 0.36870 | 0.29776 | -1795.10594 | -1794.73724 | | -1794.80818 | |
| E-i + ROH + 2RCOOH | 0.62972 | 0.47252 | -2486.60974 | -2485.98002 | -97.9 | -2486.13722 | -96.5 |
| E-i/N-IM1 | 0.44962 | 0.36739 | -1950.07413 | -1949.62451 | | -1949.70674 | |
| E-i/N-IM1 + 2RCOOH | 0.63077 | 0.48766 | -2486.61964 | -2485.98887 | -121.1 | -2486.13198 | -82.7 |
| E-i/N-TS1 | 0.44481 | 0.36765 | -1950.00295 | -1949.55813 | | -1949.63530 | |
| E-i/N-TS1 + 2RCOOH | 0.62596 | 0.48791 | -2486.54845 | -2485.92249 | 53.2 | -2486.06054 | 104.9 |
| E-i/N-IM2 | 0.44707 | 0.36567 | -1950.01915 | -1949.57208 | | -1949.65348 | |
| E-i/N-IM2 + 2RCOOH | 0.62822 | 0.48594 | -2486.56465 | -2485.93643 | 16.6 | -2486.07872 | 57.1 |

**Table S13.** Selected bond lengths (in Å), bond angles (in degree), the number of basis functions, and the number of primitive Gaussians of RCOOCdSe–$PPh_2$ species optimized using B3LYP or BPW91 functionals with SDD, cc-pVDZ-pp, or cc-pVTZ-pp basis sets.




| Levels | O1–Cd | O2–Cd | Cd–Se | Se–P | ∠O1–Cd–Se | ∠O2–Cd–Se | ∠Cd–Se–P | basis functions | primitive Gaussians |
|---|---|---|---|---|---|---|---|---|---|
| B3LYP/6-31++G(d,p), SDD | 2.253 | 2.285 | 2.515 | 2.347 | 149.6 | 152.0 | 102.4 | 465 | 804 |
| B3LYP/6-31++G(d,p), cc-pVDZ-pp | 2.250 | 2.291 | 2.498 | 2.310 | 150.7 | 150.8 | 102.2 | 479 | 940 |
| B3LYP/6-31++G(d,p), cc-pVTZ-pp | 2.240 | 2.285 | 2.490 | 2.302 | 151.0 | 150.4 | 102.6 | 520 | 1079 |
| BPW91/6-31++G(d,p), cc-pVDZ-pp | 2.272 | 2.293 | 2.498 | 2.305 | 149.0 | 152.2 | 101.8 | 479 | 940 |
| BPW91/6-31++G(d,p), cc-pVTZ-pp | 2.261 | 2.288 | 2.488 | 2.297 | 149.2 | 151.8 | 102.4 | 520 | 1079 |

From Table S13, there are only less than 0.045 Å differences in bond length and about 0.4 degree in bond angle between B3LYP/6-31++G(d,p), SDD and BPW91/6-31++G(d,p), cc-pVTZ-pp. It is indicated that the present B3LYP/6-31++G(d,p), SDD level is appropriate for the present reaction system.

Furthermore, the numbers of basis functions and primitive Gaussian functions are 465 and 864 for [6-31++G(d,p), SDD] basis set, and are 520 and 1079 for [6-31++G(d,p), cc-pVTZ-pp] basis set, respectively. To save computational time, the comparatively small basis set [6-31++G(d,p), SDD] is preferred in the present study.

## Descriptions for the turnover frequency (TOF) of the catalytic cycle and rate constants *k*(*T*)

The turnover frequency (TOF) of the catalytic cycle determines the efficiency of the catalyst. Based on the transition state theory (TST),[8, 9] TOF can be calculated by eqs i and ii,[10-12] in which δ*E* (the energetic span[13]) is defined as the energy difference between the summit and trough of the catalytic cycle.

$$\mathrm{TOF} = \frac{k_B T}{h} e^{-\frac{\delta E}{RT}} \quad \text{(i)}$$

$$\delta E = \begin{pmatrix} G_{\mathrm{TDTS}} - G_{\mathrm{TDI}} & \text{if TDTS appears after TDI} \\ G_{\mathrm{TDTS}} - G_{\mathrm{TDI}} + \Delta G_r & \text{if TDTS appears before TDI} \end{pmatrix} \quad \text{(ii)}$$

where $k_B$ is the Boltzmann constant, $T$ is the absolute temperature, and $h$ is the Planck constant. $G_{\mathrm{TDTS}}$ and $G_{\mathrm{TDI}}$ are the Gibbs free energies of the TOF-determining transition state (TDTS) and the TOF-determining intermediate (TDI), and $\Delta G_r$ is the global free energy of the entire cycle.

The rate constants $k(T)$ have been evaluated according to conventional transition state theory (TST) $k'(T)$, including tunneling correction $\kappa(T)$ based on Wigner's formulation as follows:[8, 9]

$$k'(T) = \frac{k_B T}{hc^0} e^{\frac{-\Delta G^{\neq}}{k_B T}} \quad \text{(iii)}$$

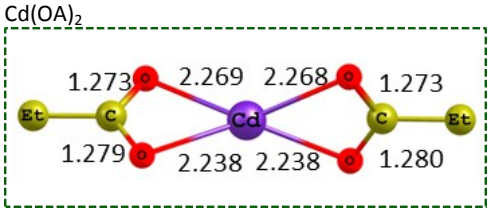
$$\kappa(T) = 1 + \frac{1}{24}\left|\frac{h\omega^{\neq}}{k_B T}\right|^2 \quad \text{(iv)}$$

$$k(T) = \kappa(T) k'(T) \quad \text{(v)}$$

where $k_B$ is the Boltzmann constant, $T$ is the absolute temperature, $h$ is the Planck constant, $c^0$ is the standard concentration (1 mol dm$^{-3}$), $\Delta G^{\neq}$ is the activation Gibbs free energy barrier, and $\omega^{\neq}$ is the imaginary frequency of TS.

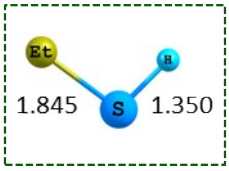
**Snapshot and standard orientation of all the species in the gas phase calculated at the B3LYP/6-31++G(d, p), SDD level. Distance lengths are reported in Å.**

$Cd(OA)_2$



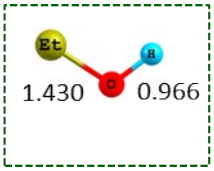

| | | | |
|---|---|---|---|
| Cd | 0.00019200 | -0.19527000 | 0.00561900 |
| O | -2.01693100 | 0.54343300 | -0.72606600 |
| O | -1.89855100 | -0.82833100 | 1.00721500 |
| C | -2.59113400 | -0.12964300 | 0.18946900 |
| C | -4.10111300 | -0.14244500 | 0.31582400 |
| H | -4.42769900 | -1.11683800 | -0.07236200 |
| H | -4.33800400 | -0.15651700 | 1.38467200 |
| C | -4.81776500 | 0.99626700 | -0.41224400 |
| H | -5.90143900 | 0.89458800 | -0.29523300 |
| H | -4.52262200 | 1.97044800 | -0.01058100 |
| H | -4.58147200 | 0.99294200 | -1.47936300 |
| O | 2.00009900 | 0.74006300 | 0.52602100 |
| O | 1.91279800 | -1.01990800 | -0.81391200 |
| C | 2.58917400 | -0.12440100 | -0.19911900 |
| C | 4.09618100 | -0.11452200 | -0.35804600 |
| H | 4.29421700 | -0.01905700 | -1.43292300 |
| H | 4.44727400 | -1.11759900 | -0.08737300 |
| C | 4.82515100 | 0.96746200 | 0.43942200 |
| H | 4.64867800 | 0.85535700 | 1.51287300 |
| H | 5.90332200 | 0.90456900 | 0.26008100 |
| H | 4.48622100 | 1.96669100 | 0.15259500 |

RSH



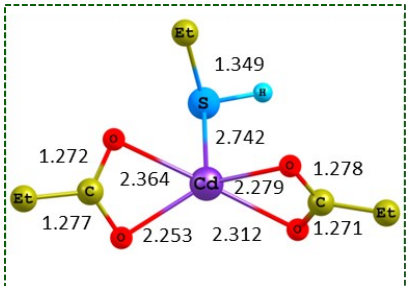

| | | | |
|---|---|---|---|
| C | -1.65187300 | -0.35211900 | -0.05355800 |
| H | -1.62605200 | -1.10588400 | 0.74074800 |
| H | -1.60259600 | -0.87316100 | -1.01422600 |
| H | -2.61586600 | 0.16750500 | 0.00995200 |
| C | -0.50485000 | 0.64488200 | 0.09148000 |
| H | -0.54210400 | 1.39746100 | -0.70193400 |
| H | -0.55876700 | 1.17787400 | 1.04503000 |
| S | 1.17483500 | -0.09909600 | -0.08018700 |
| H | 1.08836000 | -0.93484300 | 0.97589700 |

ROH



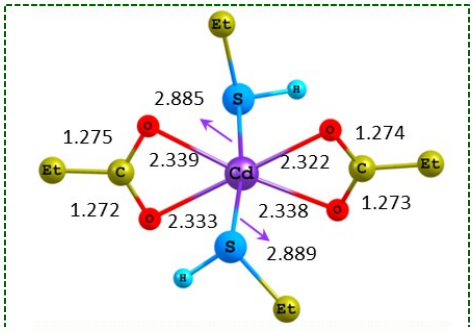

| | | | |
|---|---|---|---|
| C | -1.21816400 | -0.24157300 | -0.02147900 |
| H | -1.28417100 | -0.96277100 | 0.80271400 |
| H | -1.28245900 | -0.79362600 | -0.96448100 |
| H | -2.08576300 | 0.42470400 | 0.05147700 |
| C | 0.07984400 | 0.55710700 | 0.04725400 |
| H | 0.12794900 | 1.27982100 | -0.77264900 |
| H | 0.13135300 | 1.12419300 | 0.98908100 |
| H | 1.26905000 | -0.90511600 | 0.60810400 |
| O | 1.24424600 | -0.25755100 | -0.10861200 |

$(RSH)Cd(OA)_2$




| | | | |
|---|---|---|---|
| Cd | -0.00733200 | -0.27107700 | -0.07410600 |
| O | 2.04708500 | -1.05611500 | -0.78776600 |
| O | 1.79932100 | -0.38348700 | 1.31104200 |
| C | 2.52281100 | -0.86888100 | 0.37601500 |
| C | 3.96469800 | -1.22839000 | 0.69099000 |
| H | 4.41337800 | -0.35547500 | 1.17998800 |
| H | 3.92658700 | -2.00545900 | 1.46507700 |
| C | 4.79588800 | -1.68872900 | -0.50713500 |
| H | 5.81312000 | -1.94065000 | -0.18894700 |
| H | 4.35314300 | -2.56997500 | -0.97919700 |
| H | 4.85966800 | -0.90684100 | -1.26981600 |
| O | -1.89540400 | -1.46241300 | -0.37698700 |
| O | -2.09954600 | 0.41600600 | 0.78458800 |
| C | -2.61150900 | -0.63170900 | 0.27679700 |
| C | -4.09648100 | -0.89184200 | 0.46536000 |
| H | -4.62085000 | 0.01712400 | 0.14653700 |
| H | -4.26352300 | -0.95808300 | 1.54796900 |
| C | -4.63946900 | -2.12852400 | -0.25168100 |
| H | -4.12906600 | -3.03534800 | 0.08401300 |
| H | -5.71074500 | -2.24144100 | -0.05374500 |
| H | -4.49651300 | -2.05398500 | -1.33360500 |
| C | 0.54219500 | 3.31430700 | 1.19780000 |
| H | 1.49864600 | 3.72591400 | 0.85722600 |
| H | 0.72853100 | 2.32559300 | 1.62661200 |
| H | 0.16500000 | 3.96394500 | 1.99569000 |
| C | -0.48128200 | 3.26501200 | 0.06805100 |
| H | -1.43194500 | 2.84784400 | 0.40968200 |
| H | -0.66260600 | 4.25536100 | -0.35662500 |
| S | -0.01182000 | 2.15857200 | -1.34554500 |
| H | 1.30549700 | 2.44660500 | -1.38921700 |

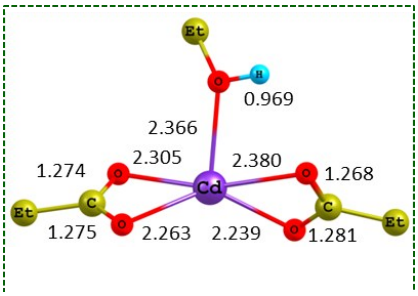
$(RSH)_2Cd(OA)_2$




| | | | |
|---|---|---|---|
| Cd | -0.08654500 | 0.01944500 | 0.04676000 |
| O | 2.03720900 | -0.07926900 | -0.92701000 |
| O | 1.83872800 | 0.73953400 | 1.12660300 |
| C | 2.55266300 | 0.43606100 | 0.11620200 |
| C | 4.04938100 | 0.70378700 | 0.18394300 |
| H | 4.16972800 | 1.75938300 | 0.45685600 |
| H | 4.43188600 | 0.14064900 | 1.04467200 |
| C | 4.83240300 | 0.36859400 | -1.08609100 |
| H | 5.89558100 | 0.59344200 | -0.94846700 |
| H | 4.73562900 | -0.68986200 | -1.34428000 |
| H | 4.46735800 | 0.94584300 | -1.94057400 |
| O | -2.04894800 | -0.87194300 | -0.84561100 |
| O | -2.20915400 | 0.45611700 | 0.92565000 |

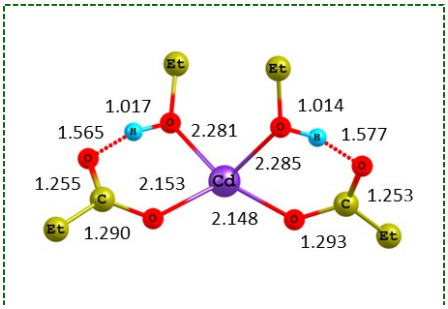
| | | | |
|---|---|---|---|
| C | -2.74998000 | -0.27505500 | 0.03158200 |
| C | -4.26562400 | -0.40756900 | 0.02411000 |
| H | -4.66053200 | 0.58331400 | -0.23699600 |
| H | -4.58025600 | -0.58294800 | 1.05919200 |
| C | -4.82078500 | -1.47447300 | -0.92086400 |
| H | -4.46602900 | -2.47242500 | -0.64461300 |
| H | -5.91554100 | -1.48181800 | -0.88620800 |
| H | -4.50694200 | -1.28938100 | -1.95161600 |
| C | 0.09961200 | 3.86192300 | 1.30866600 |
| H | 0.87088100 | 4.48075200 | 0.83584900 |
| H | 0.56953600 | 2.93580000 | 1.65051400 |
| H | -0.27278300 | 4.40694500 | 2.18397400 |
| C | -1.05808200 | 3.59307000 | 0.35143300 |
| H | -1.83618000 | 2.99069300 | 0.82776600 |
| H | -1.50681000 | 4.52356500 | -0.00596200 |
| S | -0.59871000 | 2.59769700 | -1.14315800 |
| H | 0.62290000 | 3.12865000 | -1.35297600 |
| S | 0.11024800 | -2.58923000 | 1.27229700 |
| H | -0.90466500 | -3.09254600 | 0.54063500 |
| C | 1.47581500 | -3.55648000 | 0.48248700 |
| H | 1.40289000 | -4.57848600 | 0.86429800 |
| H | 2.38630200 | -3.11399400 | 0.89664900 |
| C | 1.48823000 | -3.52299800 | -1.04298200 |
| H | 2.31895600 | -4.13588400 | -1.41320000 |
| H | 0.56130500 | -3.93268200 | -1.45822900 |
| H | 1.62186800 | -2.50450100 | -1.41598700 |

$(ROH)Cd(OA)_2$



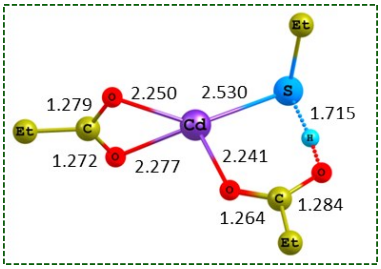

| | | | |
|---|---|---|---|
| Cd | 0.07545300 | -0.29234300 | 0.09702300 |
| O | -2.09683800 | -0.45829800 | -0.86136000 |
| O | -1.68641100 | -1.09165000 | 1.22384000 |
| C | -2.49475900 | -0.94038100 | 0.24212000 |
| C | -3.93831000 | -1.37033700 | 0.43688100 |
| H | -3.91529000 | -2.45392300 | 0.61030700 |
| H | -4.28041800 | -0.93353200 | 1.38230000 |
| C | -4.87975300 | -1.02239200 | -0.71675300 |
| H | -5.88974500 | -1.38947000 | -0.50613500 |
| H | -4.93680800 | 0.05966300 | -0.87069200 |
| H | -4.53765200 | -1.46955800 | -1.65398300 |
| O | 2.05856100 | -1.15946300 | -0.56501000 |
| O | 2.08170700 | 0.47569500 | 0.93215200 |
| C | 2.69842300 | -0.36929800 | 0.20462600 |
| C | 4.21417800 | -0.42644600 | 0.27406600 |
| H | 4.46844900 | -0.64483800 | 1.31888500 |
| H | 4.57798600 | 0.59256500 | 0.09470500 |
| C | 4.87338800 | -1.42793200 | -0.67500000 |
| H | 4.63946100 | -1.19806700 | -1.71847200 |
| H | 5.96157600 | -1.40479100 | -0.55337600 |
| H | 4.52632300 | -2.44606900 | -0.47833600 |
| C | -0.78956500 | 3.77034800 | 0.57553700 |
| H | -0.79938400 | 3.15452200 | 1.48025500 |
| H | -1.82157800 | 3.89170200 | 0.22530900 |
| H | -0.41022100 | 4.76315600 | 0.84218700 |
| C | 0.09302800 | 3.15070000 | -0.49859500 |
| H | 0.12211000 | 3.77537700 | -1.39982400 |
| H | 1.11543800 | 3.01454100 | -0.13963200 |
| H | -1.25662600 | 1.81121400 | -1.18298400 |
| O | -0.33765800 | 1.82427000 | -0.87523900 |

$(ROH)_2Cd(OA)_2$




| | | | |
|---|---|---|---|
| Cd | -0.09180100 | -0.27295000 | -0.24670800 |
| O | -1.97033800 | -1.30675700 | -0.05156800 |
| O | -3.26502900 | 0.50198600 | -0.44901400 |
| C | -3.10861300 | -0.71195600 | -0.16991200 |
| C | -4.35575700 | -1.56693200 | 0.03279000 |
| H | -5.01672600 | -1.00255400 | 0.70075000 |
| H | -4.87074100 | -1.58528300 | -0.93669200 |
| C | -4.11970000 | -2.98664200 | 0.54885100 |
| H | -5.07365300 | -3.51493300 | 0.65255900 |
| H | -3.48332700 | -3.55641700 | -0.13366300 |
| H | -3.62759800 | -2.97813000 | 1.52621700 |
| O | 1.71837600 | -0.83650600 | -1.25634300 |
| O | 3.12091400 | -0.28959400 | 0.43022200 |
| C | 2.89118200 | -0.71515000 | -0.72530800 |
| C | 4.04189500 | -1.13981300 | -1.63060200 |
| H | 3.97037900 | -0.53198200 | -2.54133400 |
| H | 3.83015500 | -2.16695700 | -1.95215900 |
| C | 5.43001900 | -1.03114000 | -1.00026200 |
| H | 5.50791700 | -1.65499100 | -0.10514200 |
| H | 6.19640900 | -1.35455300 | -1.71276300 |
| H | 5.65032000 | -0.00225000 | -0.70146600 |
| O | -1.05245400 | 1.65600200 | -0.99431200 |
| O | 0.96018800 | 0.14429100 | 1.73857800 |
| C | -0.82168100 | 3.02978200 | -0.63991800 |
| C | 0.85420900 | 1.22941400 | 2.67560300 |
| H | 0.25828500 | 3.19036600 | -0.71554000 |
| H | -1.11698300 | 3.19564900 | 0.40533200 |
| H | 1.23050800 | 2.15315700 | 2.21479000 |
| H | -0.21390700 | 1.36130800 | 2.87382700 |
| C | -1.57388800 | 3.97269200 | -1.56979600 |
| C | 1.60815200 | 0.92277800 | 3.96293600 |
| H | -1.36326600 | 5.01449100 | -1.30154100 |
| H | -1.27005300 | 3.81249800 | -2.60876700 |
| H | -2.65488300 | 3.81412500 | -1.49724200 |
| H | 2.67706600 | 0.78708900 | 3.76788300 |
| H | 1.49370400 | 1.75020700 | 4.67280300 |
| H | 1.22284800 | 0.00992400 | 4.42727200 |
| H | 1.90010100 | 0.02874000 | 1.37650100 |
| H | -2.00828300 | 1.35852800 | -0.81645900 |

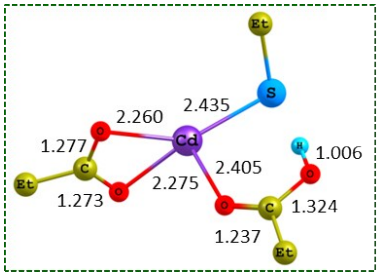
C4-TS1




| | | | |
|---|---|---|---|
| Cd | 0.57798300 | -0.50432500 | 0.48138000 |

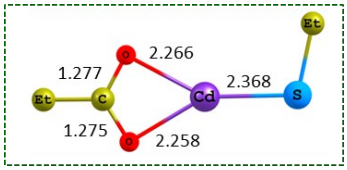
| | | | |
|---|---|---|---|
| O | -2.59899900 | 0.24448900 | -0.72428500 |
| O | -0.53254700 | 1.14381300 | -0.55420500 |
| C | -1.75495500 | 1.20170700 | -0.86976900 |
| C | -2.26687300 | 2.51424300 | -1.44116500 |
| H | -2.39502100 | 3.18635300 | -0.58092600 |
| H | -1.45612900 | 2.94544400 | -2.03617900 |
| C | -3.57054500 | 2.41707000 | -2.23763700 |
| H | -3.86924000 | 3.40707900 | -2.59672900 |
| H | -3.45491400 | 1.76169000 | -3.10666600 |
| H | -4.37977800 | 2.01112000 | -1.62526000 |
| O | 2.76366700 | -0.41965600 | -0.14974700 |
| O | 2.15174400 | 0.37596400 | 1.82682200 |
| C | 3.05170700 | 0.16221100 | 0.94381000 |
| C | 4.46803300 | 0.62330700 | 1.23239700 |
| H | 4.78897100 | 0.09606300 | 2.13984800 |
| H | 4.40312500 | 1.67982000 | 1.51848800 |
| C | 5.46330600 | 0.41482200 | 0.09049500 |
| H | 5.15299700 | 0.95569800 | -0.80805500 |
| H | 6.45501200 | 0.77542000 | 0.38339800 |
| H | 5.54571000 | -0.64279300 | -0.17490000 |
| C | -2.39168000 | -0.84895900 | 2.69252900 |
| H | -3.10313700 | -0.30453200 | 2.06536300 |
| H | -1.49914000 | -0.22538100 | 2.81924300 |
| H | -2.84289500 | -0.98350100 | 3.68283800 |
| C | -2.04649300 | -2.21141700 | 2.09879600 |
| H | -1.32425500 | -2.74293900 | 2.72372700 |
| H | -2.93685800 | -2.84021500 | 2.01169900 |
| S | -1.31717400 | -2.17774600 | 0.38806500 |
| H | -2.11398000 | -0.81246500 | -0.27717500 |

C4-IM2



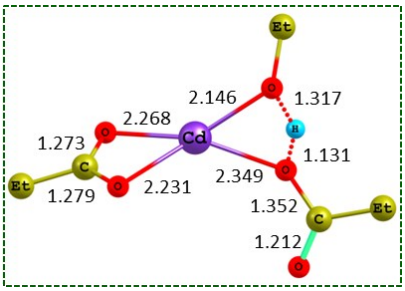

| | | | |
|---|---|---|---|
| Cd | 0.36311900 | -0.50176900 | -0.29298000 |
| O | -3.04967600 | 0.69196500 | 0.03693400 |
| O | -0.92988900 | 1.43157900 | 0.31817600 |
| C | -2.15285300 | 1.60494800 | 0.37614300 |
| C | -2.75642900 | 2.91855100 | 0.81011100 |
| H | -3.71825300 | 2.72433400 | 1.29300600 |
| H | -2.07614900 | 3.37159600 | 1.53595200 |
| C | -2.94967700 | 3.86242700 | -0.39506800 |
| H | -3.37140100 | 4.81326500 | -0.05656600 |
| H | -1.99476100 | 4.06921500 | -0.88733100 |
| H | -3.63446600 | 3.42896000 | -1.13013200 |
| O | 2.32209500 | 0.52847100 | -0.81689000 |
| O | 2.09944500 | -0.43491400 | 1.16589100 |
| C | 2.79574200 | 0.22993900 | 0.32633900 |
| C | 4.19815000 | 0.65455400 | 0.72030600 |
| H | 4.74045600 | -0.26174400 | 0.98470800 |
| H | 4.10368100 | 1.21584400 | 1.65798400 |
| C | 4.95440400 | 1.46120100 | -0.33594400 |
| H | 4.42455400 | 2.38588000 | -0.58167500 |
| H | 5.95230200 | 1.72336800 | 0.03126700 |
| H | 5.06740000 | 0.89208800 | -1.26298400 |
| C | -1.69572800 | -2.88094800 | 1.57353000 |
| H | -2.56424600 | -2.24409400 | 1.76934500 |
| H | -0.79884900 | -2.34812600 | 1.91088700 |
| H | -1.79234200 | -3.78474200 | 2.18808400 |
| C | -1.60221600 | -3.25705600 | 0.09700400 |
| H | -0.73986400 | -3.90340000 | -0.08726400 |
| H | -2.49446900 | -3.81004800 | -0.21255000 |
| S | -1.51236400 | -1.83315100 | -1.09158400 |
| H | -2.61965100 | -0.15557000 | -0.29178900 |

C4




| | | | |
|---|---|---|---|
| Cd | 0.27359000 | -0.32721900 | -0.01398500 |
| O | -1.92445100 | -0.79657900 | 0.20698600 |
| O | -1.31341900 | 1.25816500 | -0.33720700 |
| C | -2.23003600 | 0.40804400 | -0.07856600 |
| C | -3.67738600 | 0.85633400 | -0.11489000 |
| H | -3.84466500 | 1.29368400 | -1.10683900 |
| H | -3.76108100 | 1.69453600 | 0.58796500 |
| C | -4.70395400 | -0.23363400 | 0.19462100 |
| H | -4.54834200 | -0.65238700 | 1.19275800 |
| H | -5.71706900 | 0.17896100 | 0.14867300 |
| H | -4.63582200 | -1.05720200 | -0.52164600 |
| C | 3.31899300 | 1.70239800 | 0.53228100 |
| H | 3.59273300 | 1.40637100 | 1.54937200 |
| H | 2.28891400 | 2.07790100 | 0.55419700 |
| H | 3.96748700 | 2.53372800 | 0.22827900 |
| C | 3.46789500 | 0.53472500 | -0.43972600 |
| H | 3.19190400 | 0.82845700 | -1.45590400 |
| H | 4.51003100 | 0.20050800 | -0.47294000 |
| S | 2.54209200 | -1.00612000 | 0.02792500 |

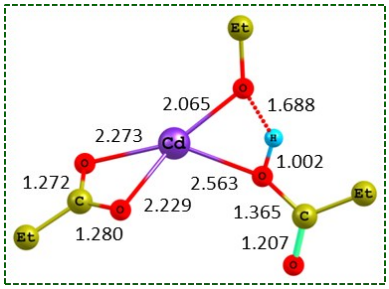
C5-TS1




| | | | |
|---|---|---|---|
| Cd | -0.49944200 | 0.32539400 | 0.10584000 |
| C | 1.38002900 | 2.92277900 | -0.28253000 |
| H | 1.27881300 | 2.91027900 | -1.37931800 |
| H | 0.58390600 | 3.56863400 | 0.11185900 |
| C | 2.74277100 | 3.48340500 | 0.10950300 |
| H | 2.84528200 | 3.51673300 | 1.19885400 |
| H | 3.55071000 | 2.86260600 | -0.29315200 |
| H | 2.86666000 | 4.49945000 | -0.28372300 |
| O | 1.95189100 | -2.69804000 | -0.30611800 |
| C | 2.37526800 | -1.56235700 | -0.33929400 |
| C | 3.82712300 | -1.17492100 | -0.09628800 |
| H | 4.19081200 | -0.68518300 | -1.00946900 |
| H | 3.84340800 | -0.40050100 | 0.68225700 |
| C | 4.71904500 | -2.35666000 | 0.28382600 |
| H | 5.75004300 | -2.02125500 | 0.43508300 |
| H | 4.37095100 | -2.83101600 | 1.20568100 |
| H | 4.71294700 | -3.11951100 | -0.49921500 |
| O | 1.56451800 | -0.52041500 | -0.63222600 |
| H | 1.76247600 | 0.53907200 | -0.28919400 |
| O | -2.16409900 | -0.60649500 | 1.26225000 |
| O | -2.57778700 | 0.13494500 | -0.78194100 |
| C | -2.97474000 | -0.42813200 | 0.28876800 |

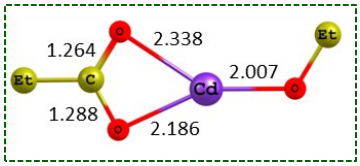
| | | | |
|---|---|---|---|
| C | -4.40546400 | -0.90394600 | 0.43772600 |
| H | -4.79236900 | -0.45332300 | 1.35964300 |
| H | -4.35271000 | -1.98059600 | 0.64160400 |
| C | -5.31525600 | -0.60867300 | -0.75513200 |
| H | -4.93835900 | -1.08034500 | -1.66673100 |
| H | -6.32332900 | -0.98940200 | -0.56186500 |
| H | -5.38508400 | 0.46623000 | -0.94466000 |
| O | 1.21502600 | 1.60878700 | 0.24960800 |

C5-IM2



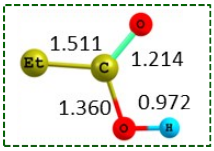

| | | | |
|---|---|---|---|
| Cd | -0.54480000 | 0.54922600 | 0.12027300 |
| C | 1.32413100 | 3.02975100 | -0.16174200 |
| H | 0.95260600 | 3.29033300 | -1.16628700 |
| H | 0.71466400 | 3.59002100 | 0.56468500 |
| C | 2.78296200 | 3.45700800 | -0.03121500 |
| H | 3.16242500 | 3.22597800 | 0.96967100 |
| H | 3.40625300 | 2.93505700 | -0.76581200 |
| H | 2.88529700 | 4.53562500 | -0.20115000 |
| O | 1.99824500 | -2.89191400 | -0.40088500 |
| C | 2.37885500 | -1.74670600 | -0.36733200 |
| C | 3.78553100 | -1.29687100 | -0.00540400 |
| H | 4.19449100 | -0.76228300 | -0.87368600 |
| H | 3.70696200 | -0.54872600 | 0.79471500 |
| C | 4.70114100 | -2.44970900 | 0.40552000 |
| H | 5.69911000 | -2.07149100 | 0.64763100 |
| H | 4.30639500 | -2.97086800 | 1.28198800 |
| H | 4.79334300 | -3.18353700 | -0.39949800 |
| O | 1.52108500 | -0.73378700 | -0.68784000 |
| H | 1.86452000 | 0.19253800 | -0.52177400 |
| O | -2.08716000 | -0.58033600 | 1.26735800 |
| O | -2.59363700 | 0.12284700 | -0.76769400 |
| C | -2.91675300 | -0.49475100 | 0.29671300 |
| C | -4.27526200 | -1.14932200 | 0.44134700 |
| H | -4.69871800 | -0.79492300 | 1.38857400 |
| H | -4.08545200 | -2.21971000 | 0.59098500 |
| C | -5.23466600 | -0.91611300 | -0.72614400 |
| H | -4.81434000 | -1.28969000 | -1.66373700 |
| H | -6.18237200 | -1.43260600 | -0.54273600 |
| H | -5.44531500 | 0.14884100 | -0.86032900 |
| O | 1.21333100 | 1.63229500 | 0.07321200 |

C5



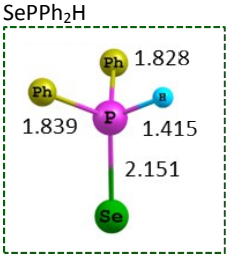

| | | | |
|---|---|---|---|
| Cd | 0.42429300 | -0.34479900 | 0.00219000 |
| C | 3.16471700 | 0.89839800 | 0.01412700 |
| H | 2.91841300 | 1.52739600 | -0.85742900 |
| H | 2.93713100 | 1.49256100 | 0.91478700 |
| C | 4.65378900 | 0.56665100 | -0.00789600 |
| H | 4.92312100 | -0.03875800 | 0.86364700 |
| H | 4.90585600 | -0.00069600 | -0.90970000 |
| H | 5.25287100 | 1.48577000 | 0.00603800 |
| O | -1.55653400 | -1.27040200 | 0.02147600 |
| O | -1.52840100 | 0.94086400 | -0.03883800 |
| C | -2.17851000 | -0.14324600 | -0.01209700 |
| C | -3.69328200 | -0.16866300 | -0.02622500 |
| H | -4.00802700 | -0.80581300 | 0.80874200 |
| H | -3.98610400 | -0.71414200 | -0.93239300 |
| C | -4.36051300 | 1.20562200 | 0.03292700 |
| H | -4.05816700 | 1.82920800 | -0.81274100 |
| H | -5.44951700 | 1.09626800 | 0.00953200 |
| H | -4.08904600 | 1.73855400 | 0.94864200 |
| O | 2.43121300 | -0.32203000 | -0.00129700 |

RCOOH



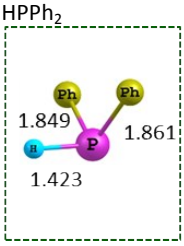

| | | | |
|---|---|---|---|
| C | 0.61869200 | -0.13356000 | 0.07306000 |
| O | 1.43908300 | -0.94444900 | -0.30394900 |
| O | 0.88489100 | 1.20023800 | 0.10120200 |
| H | 1.79301100 | 1.31592600 | -0.22618900 |
| C | -0.78170100 | -0.44345500 | 0.54906900 |
| C | -1.86819400 | 0.13721400 | -0.37412700 |
| H | -0.86333300 | -1.53055700 | 0.61357800 |
| H | -0.89620300 | -0.02920300 | 1.55770500 |
| H | -1.77704700 | -0.26234400 | -1.38919700 |
| H | -2.85996100 | -0.12840200 | 0.00384100 |
| H | 1.80103400 | 1.22707200 | -0.42577500 |

$SePPh_2H$



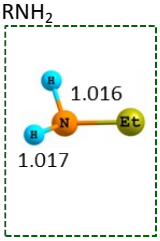

| | | | |
|---|---|---|---|
| P | -0.02183300 | 0.60467600 | -0.65425600 |
| C | 1.50151600 | -0.28608800 | -0.17583800 |
| C | 1.78581200 | -0.51600500 | 1.17918800 |
| C | 2.40666100 | -0.71455800 | -1.15698700 |
| C | 2.95472000 | -1.18383200 | 1.54369100 |
| H | 1.09923400 | -0.16563800 | 1.94479600 |
| C | 3.58040200 | -1.37905400 | -0.78760800 |
| H | 2.20401200 | -0.52738500 | -2.20847200 |
| C | 3.85355700 | -1.61606500 | 0.56142000 |
| H | 3.16853200 | -1.36141600 | 2.59362900 |
| H | 4.27867500 | -1.70601000 | -1.55263500 |
| H | 4.76565600 | -2.13112500 | 0.84884600 |
| C | -1.41616200 | -0.52925700 | -0.26345200 |
| C | -2.55877000 | -0.04286600 | 0.38126500 |
| C | -1.34820500 | -1.88125200 | -0.63823900 |
| C | -3.62767000 | -0.90271100 | 0.65198600 |
| H | -2.60174100 | 1.00428800 | 0.66793900 |
| C | -2.41923200 | -2.73525800 | -0.37007400 |
| H | -0.46060000 | -2.27230000 | -1.12865300 |
| C | -3.56040800 | -2.24616100 | 0.27548700 |
| H | -4.51126200 | -0.51976300 | 1.15434900 |
| H | -2.36217900 | -3.78007800 | -0.66164100 |
| H | -4.39242500 | -2.91253900 | 0.48485900 |
| Se | -0.23070000 | 2.61737700 | 0.07436500 |
| H | 0.07007000 | 0.50963600 | -2.06261100 |

$HPPh_2$



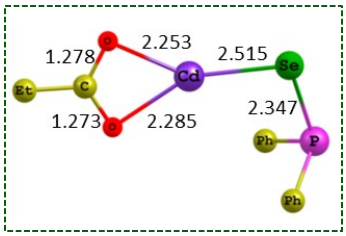

| | | | |
|---|---|---|---|
| P | 0.04767600 | 1.66775400 | -0.26849400 |
| H | -0.01274300 | 1.74307100 | -1.68842000 |
| C | -1.43536900 | 0.58308500 | -0.06540600 |
| C | -2.23731700 | 0.18364300 | -1.14730200 |
| C | -1.81986300 | 0.19686100 | 1.23097400 |
| C | -3.38751500 | -0.58460300 | -0.94044400 |
| H | -1.96439400 | 0.47250000 | -2.15872400 |
| C | -2.95870800 | -0.58307700 | 1.43720700 |
| H | -1.22472100 | 0.50911900 | 2.08569500 |
| C | -3.74844500 | -0.97429400 | 0.35115500 |
| H | -3.99583400 | -0.88230400 | -1.79007800 |
| H | -3.23539400 | -0.87715500 | 2.44577300 |
| H | -4.63938800 | -1.57439300 | 0.51184100 |
| C | 1.46097700 | 0.46359900 | -0.13878500 |
| C | 2.65267400 | 0.92736900 | 0.43944900 |
| C | 1.40353300 | -0.86508500 | -0.59079900 |
| C | 3.76770500 | 0.08996200 | 0.55143600 |
| H | 2.70804700 | 1.94913500 | 0.80634900 |
| C | 2.51347000 | -1.70383900 | -0.47436800 |
| H | 0.48614100 | -1.24857500 | -1.02801900 |
| C | 3.69966000 | -1.22737700 | 0.09460400 |
| H | 4.68278400 | 0.46606500 | 1.00029600 |
| H | 2.45348100 | -2.72946700 | -0.82813900 |
| H | 4.56206600 | -1.88176700 | 0.18451700 |

$RNH_2$



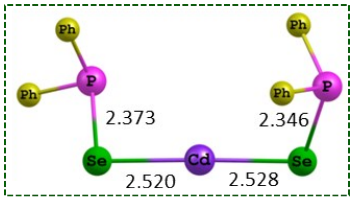

| | | | |
|---|---|---|---|
| C | 1.24988900 | -0.23947700 | -0.02923900 |
| H | 1.31064000 | -0.77205600 | -0.98348300 |
| H | 1.30747100 | -0.98229000 | 0.77615700 |
| H | 2.12135600 | 0.41771200 | 0.06350100 |
| C | -0.04775300 | 0.56173000 | 0.05608700 |
| H | -0.06279100 | 1.12854900 | 1.00344400 |
| H | -0.07431000 | 1.30043100 | -0.75376000 |
| N | -1.21041600 | -0.31956000 | -0.11451800 |
| H | -1.26382800 | -0.99793800 | 0.64179300 |
| H | -2.07843800 | 0.20899100 | -0.10711300 |

C




| | | | |
|---|---|---|---|
| Cd | 1.28084400 | 0.00127200 | -1.00375300 |
| Se | -0.85256400 | 0.29999000 | -2.30076100 |
| P | -2.46655800 | 0.40479600 | -0.59992400 |
| C | -1.71339700 | 1.58599700 | 0.61250800 |
| C | -2.13959400 | 2.92271900 | 0.53884900 |
| C | -0.74074800 | 1.23883800 | 1.56726600 |
| C | -1.59818500 | 3.89301500 | 1.38722900 |
| H | -2.89498000 | 3.20478500 | -0.19018500 |
| C | -0.20045600 | 2.20804800 | 2.41571400 |
| H | -0.41088300 | 0.20830900 | 1.66528400 |
| C | -0.62646600 | 3.53789700 | 2.32647800 |
| H | -1.93779700 | 4.92245100 | 1.31547300 |
| H | 0.55142000 | 1.92161300 | 3.14564000 |
| H | -0.20572900 | 4.29022800 | 2.98759600 |
| C | -2.35015800 | -1.20693300 | 0.30868300 |
| C | -2.92458800 | -1.28117200 | 1.59314500 |
| C | -1.88194000 | -2.39081600 | -0.28222700 |
| C | -2.99948000 | -2.49751500 | 2.27332500 |
| H | -3.30877600 | -0.38403300 | 2.07130400 |
| C | -1.96157800 | -3.60983500 | 0.39939000 |
| H | -1.45422300 | -2.36155700 | -1.27966600 |
| C | -2.51569200 | -3.66801000 | 1.67960700 |
| H | -3.43600500 | -2.52968300 | 3.26781400 |
| H | -1.58785900 | -4.51326300 | -0.07482000 |
| H | -2.57464200 | -4.61451200 | 2.20918200 |
| O | 3.53333700 | 0.01822700 | -0.93858500 |
| O | 2.43002200 | -0.58516000 | 0.88220400 |
| C | 3.53011400 | -0.37654200 | 0.27722100 |
| C | 4.85924300 | -0.59479300 | 0.97354600 |
| H | 5.40236000 | -1.33962600 | 0.37844300 |
| H | 5.42950300 | 0.33528000 | 0.86182500 |
| C | 4.76341400 | -1.01982400 | 2.43908400 |
| H | 5.76543100 | -1.16452400 | 2.85603400 |
| H | 4.24921400 | -0.26313500 | 3.03857200 |
| H | 4.20816800 | -1.95594800 | 2.54452000 |

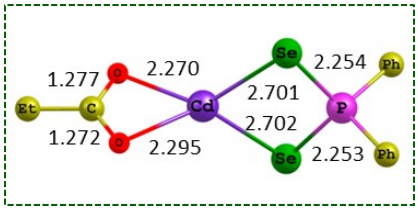
E




| | | | |
|---|---|---|---|
| Cd | 0.03011800 | 1.98446500 | -0.25455400 |
| P | 2.52043900 | -0.20994100 | 0.08240300 |
| Se | 2.63283400 | 2.08179200 | 0.06472500 |
| C | 3.61385300 | -0.85601100 | -1.25058300 |
| C | 3.89449900 | -2.23543000 | -1.26808100 |
| C | 4.08569300 | -0.05217400 | -2.29809900 |
| C | 4.64525800 | -2.79147600 | -2.30419100 |
| H | 3.53256300 | -2.87602000 | -0.46830100 |
| C | 4.83643200 | -0.61395600 | -3.33576200 |
| H | 3.87198700 | 1.01219000 | -2.29618200 |
| C | 5.11931600 | -1.98153700 | -3.34228500 |
| H | 4.85962300 | -3.85663000 | -2.30074300 |
| H | 5.20167200 | 0.02265000 | -4.13687900 |
| H | 5.70363800 | -2.41522700 | -4.14889500 |
| C | 3.33263100 | -0.77875400 | 1.63239600 |
| C | 4.72985900 | -0.79702800 | 1.78154100 |
| C | 2.52190400 | -1.16679800 | 2.71051700 |
| C | 5.30307000 | -1.20153700 | 2.98792200 |
| H | 5.36856800 | -0.49711800 | 0.95627300 |
| C | 3.09953400 | -1.56839700 | 3.91848300 |
| H | 1.44110500 | -1.15393000 | 2.60226500 |
| C | 4.48935200 | -1.58718200 | 4.05907700 |
| H | 6.38439700 | -1.21170000 | 3.09326700 |
| H | 2.46255300 | -1.86809600 | 4.74594800 |
| H | 4.93812900 | -1.90057500 | 4.99754900 |
| Se | -0.08960000 | -0.72803100 | -0.09589800 |

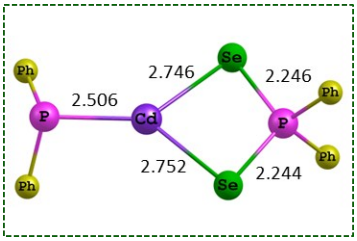
| | | | |
|---|---|---|---|
| O | -1.91519600 | 2.97167900 | 0.55969800 |
| O | -1.38414000 | 3.24310300 | -1.57576800 |
| C | -2.15375900 | 3.47068700 | -0.59144400 |
| C | -3.37756000 | 4.35771000 | -0.75923600 |
| H | -4.23061500 | 3.81664900 | -0.33210000 |
| H | -3.22460000 | 5.22229500 | -0.10052500 |
| C | -3.66214700 | 4.80630400 | -2.19323500 |
| H | -4.54760700 | 5.45043200 | -2.22189400 |
| H | -2.81624500 | 5.36208100 | -2.60654300 |
| H | -3.84036400 | 3.94882400 | -2.84902200 |
| P | -2.61353900 | -0.80819200 | -0.20082200 |
| H | -3.19207400 | 0.32946100 | -0.80612700 |
| C | -3.46877400 | -0.81919600 | 1.41719600 |
| C | -3.93284200 | -2.01194700 | 1.99291700 |
| C | -3.56759500 | 0.38600500 | 2.13554300 |
| C | -4.50704200 | -1.99747800 | 3.26686100 |
| H | -3.85655500 | -2.94912300 | 1.44942300 |
| C | -4.14559600 | 0.39073700 | 3.40666600 |
| H | -3.18682000 | 1.31329300 | 1.71228500 |
| C | -4.61694800 | -0.79745500 | 3.97466900 |
| H | -4.86862400 | -2.92434400 | 3.70313800 |
| H | -4.22356600 | 1.32609300 | 3.95346900 |
| H | -5.06452100 | -0.78815200 | 4.96440300 |
| C | -3.31930000 | -2.17770500 | -1.19420400 |
| C | -2.47102200 | -3.18340500 | -1.67877800 |
| C | -4.69143300 | -2.22326700 | -1.49876100 |
| C | -2.98924200 | -4.22747400 | -2.45201800 |
| H | -1.40766200 | -3.14134500 | -1.46157400 |
| C | -5.20357000 | -3.26365200 | -2.27472500 |
| H | -5.35864700 | -1.45015800 | -1.12763500 |
| C | -4.35266900 | -4.26816000 | -2.75062400 |
| H | -2.32496100 | -5.00199100 | -2.82409000 |
| H | -6.26385400 | -3.28991600 | -2.50934400 |
| H | -4.75333900 | -5.07667000 | -3.35544700 |

F




| | | | |
|---|---|---|---|
| Cd | 1.94348900 | -0.20149700 | -0.00299400 |
| P | -1.33674000 | 0.01406500 | 0.00098200 |
| Se | -0.03648500 | -0.16190800 | 1.83337000 |
| Se | -0.03590500 | -0.05525100 | -1.83706900 |
| C | -2.30983100 | 1.56615800 | 0.06119300 |
| C | -3.32398600 | 1.69020100 | 1.02668000 |
| C | -2.03084500 | 2.63769600 | -0.79625300 |
| C | -4.05520600 | 2.87358800 | 1.12198700 |
| H | -3.54410200 | 0.86784900 | 1.70119300 |
| C | -2.76675700 | 3.82221400 | -0.69435400 |
| H | -1.24476000 | 2.54452600 | -1.53898400 |
| C | -3.77772300 | 3.94177600 | 0.26131300 |
| H | -4.83844900 | 2.96256500 | 1.86904100 |
| H | -2.54731100 | 4.64821200 | -1.36443500 |
| H | -4.34787600 | 4.86306000 | 0.33839200 |
| C | -2.58424500 | -1.32720300 | -0.05208900 |
| C | -3.65169100 | -1.22537900 | -0.96082000 |
| C | -2.45969900 | -2.46908300 | 0.74958400 |
| C | -4.58614000 | -2.25608600 | -1.05730800 |
| H | -3.75665900 | -0.34602700 | -1.58940900 |
| C | -3.39952300 | -3.49877100 | 0.64749500 |
| H | -1.63531700 | -2.54908900 | 1.45113900 |
| C | -4.46125000 | -3.39480200 | -0.25381800 |
| H | -5.40930800 | -2.17086200 | -1.76061500 |
| H | -3.29911400 | -4.37952900 | 1.27487600 |
| H | -5.18989100 | -4.19656400 | -0.33150500 |
| O | 3.89891300 | -1.35428100 | -0.04343600 |
| O | 3.97806700 | 0.86053100 | 0.00621900 |
| C | 4.56768700 | -0.26621700 | -0.02342100 |
| C | 6.08380100 | -0.34790800 | -0.04269000 |
| H | 6.37415000 | -1.03295400 | 0.76276500 |
| H | 6.35573200 | -0.86242200 | -0.97309800 |
| C | 6.80756500 | 0.99372100 | 0.07721500 |
| H | 7.89198800 | 0.84291000 | 0.04819700 |
| H | 6.53088400 | 1.66679700 | -0.73899500 |
| H | 6.55611200 | 1.49640800 | 1.01563500 |

E-i

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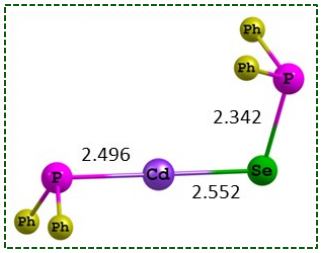
| Cd | -0.91607100 | -0.20243600 | -0.59249400 |
| P | -3.33449200 | -0.32566200 | -1.23642400 |
| C | -4.03379500 | -1.46471300 | 0.05437200 |
| C | -3.68009300 | -1.46280700 | 1.41732900 |
| C | -4.96784800 | -2.42105800 | -0.38298300 |
| C | -4.24292300 | -2.37800200 | 2.30953700 |
| H | -2.96055100 | -0.73714900 | 1.78759100 |
| C | -5.53171200 | -3.34129000 | 0.50744900 |
| H | -5.25447800 | -2.44307500 | -1.43100600 |
| C | -5.17027300 | -3.32253800 | 1.85609300 |
| H | -3.95220400 | -2.35776300 | 3.35645500 |
| H | -6.25064200 | -4.07096300 | 0.14484600 |
| H | -5.60369500 | -4.03814900 | 2.54915600 |
| C | -3.91790500 | 1.35706400 | -0.71142700 |
| C | -4.84153500 | 1.59078100 | 0.32179700 |
| C | -3.48219700 | 2.46144900 | -1.47160700 |
| C | -5.30078300 | 2.88433800 | 0.59284400 |
| H | -5.20852900 | 0.76304300 | 0.91967900 |
| C | -3.93389100 | 3.75146000 | -1.19496900 |
| H | -2.78332600 | 2.30925200 | -2.29183900 |
| C | -4.84751600 | 3.97130300 | -0.15749200 |
| H | -6.01560000 | 3.03822700 | 1.39722700 |
| H | -3.57557600 | 4.58552200 | -1.79252800 |
| H | -5.20259700 | 4.97494600 | 0.05805100 |
| P | 2.35945500 | -0.01134600 | 0.04820900 |
| Se | 0.99204300 | -1.64794900 | 0.75237800 |
| Se | 1.19322700 | 1.46712400 | -1.17277000 |
| C | 3.74928700 | -0.71721500 | -0.91889100 |
| C | 4.70473200 | -1.50441900 | -0.25351000 |
| C | 3.85249200 | -0.52031500 | -2.30143000 |
| C | 5.75515000 | -2.07962000 | -0.96779600 |
| H | 4.63182200 | -1.66732200 | 0.81788200 |
| C | 4.90701400 | -1.10128100 | -3.01263600 |
| H | 3.11414600 | 0.08661700 | -2.81607800 |
| C | 5.85778500 | -1.87946700 | -2.34918500 |
| H | 6.49095600 | -2.68558400 | -0.44723900 |
| H | 4.98237800 | -0.94170100 | -4.08431400 |
| H | 6.67613700 | -2.32955200 | -2.90382900 |
| C | 3.16469900 | 0.83029200 | 1.46577900 |
| C | 4.19387200 | 1.75178100 | 1.20696100 |
| C | 2.74995100 | 0.60423600 | 2.78384600 |
| C | 4.80311000 | 2.43207900 | 2.26074000 |
| H | 4.51943100 | 1.93872000 | 0.18774400 |

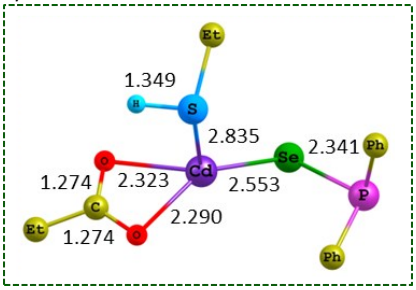
| | | | |
|---|---|---|---|
| C | 3.36342000 | 1.29077000 | 3.83640000 |
| H | 1.95396300 | -0.10626900 | 2.98359100 |
| C | 4.38820400 | 2.20315700 | 3.57768000 |
| H | 5.59862000 | 3.14201700 | 2.05400300 |
| H | 3.03868900 | 1.10819300 | 4.85662600 |
| H | 4.86341200 | 2.73518600 | 4.39684000 |

G



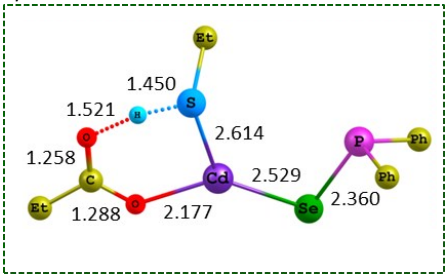

| | | | |
|---|---|---|---|
| Se | 1.57528500 | -0.27864800 | 2.27999400 |
| P | 3.39607400 | 0.51419500 | 1.03814300 |
| C | 2.60956000 | 1.74566100 | -0.10870800 |
| C | 2.06822000 | 1.43338200 | -1.36882000 |
| C | 2.55918900 | 3.07989200 | 0.33209100 |
| C | 1.48075300 | 2.42629700 | -2.15856200 |
| H | 2.12000100 | 0.41565200 | -1.74536800 |
| C | 1.96807500 | 4.07180900 | -0.45491300 |
| H | 2.98200400 | 3.34012400 | 1.29918800 |
| C | 1.42697400 | 3.74760200 | -1.70292200 |
| H | 1.06598500 | 2.16591900 | -3.12841100 |
| H | 1.93767800 | 5.09722700 | -0.09695700 |
| H | 0.97224500 | 4.51834800 | -2.31874000 |
| C | 3.84636700 | -0.84916600 | -0.13897700 |
| C | 4.81327200 | -0.55001300 | -1.11934400 |
| C | 3.40262800 | -2.17395700 | -0.02123600 |
| C | 5.29453300 | -1.54142800 | -1.97514700 |
| H | 5.18994700 | 0.46517600 | -1.22037500 |
| C | 3.89158300 | -3.16962100 | -0.87502800 |
| H | 2.67555300 | -2.42940500 | 0.74341200 |
| C | 4.83393600 | -2.85767600 | -1.85648600 |
| H | 6.03229000 | -1.28714700 | -2.73129400 |
| H | 3.53267100 | -4.18975500 | -0.76798600 |
| H | 5.21208700 | -3.63082400 | -2.51925500 |
| P | -2.12803800 | -0.19185800 | -1.14926400 |
| C | -3.09686400 | -1.69288100 | -0.63613000 |
| C | -3.31488800 | -2.67796600 | -1.61509200 |
| C | -3.59806600 | -1.92218400 | 0.66004400 |
| C | -4.00449000 | -3.85718700 | -1.31037600 |
| H | -2.94459800 | -2.51750800 | -2.62426800 |
| C | -4.29271300 | -3.09378800 | 0.96420400 |
| H | -3.45111200 | -1.17486000 | 1.43556800 |
| C | -4.49533000 | -4.06807000 | -0.02069200 |
| H | -4.16021000 | -4.60497600 | -2.08313000 |
| H | -4.67014700 | -3.24997500 | 1.97116800 |
| H | -5.03190400 | -4.98183800 | 0.21830900 |
| C | -3.15064700 | 1.23284600 | -0.54139600 |
| C | -4.54333000 | 1.14815800 | -0.36793200 |
| C | -2.54099900 | 2.49435000 | -0.39245000 |
| C | -5.29519300 | 2.28166400 | -0.04201800 |
| H | -5.04919100 | 0.19552300 | -0.48826300 |
| C | -3.29197400 | 3.62371500 | -0.06491000 |
| H | -1.46753600 | 2.60069200 | -0.53616200 |
| C | -4.67587400 | 3.52355800 | 0.11499200 |
| H | -6.37013900 | 2.18846900 | 0.08866700 |
| H | -2.79398100 | 4.58241500 | 0.05282600 |
| H | -5.26118300 | 4.40140000 | 0.37272300 |
| Cd | -0.30143800 | -0.23740900 | 0.55050500 |

C/J-IM1




| | | | |
|---|---|---|---|
| Cd | -1.19962300 | -0.37236600 | 0.55853200 |
| P | 2.31056200 | 1.19815700 | 1.13528100 |
| Se | 0.66227200 | -0.01821800 | 2.26895300 |
| C | 3.06421100 | 0.01262600 | -0.07843100 |
| C | 3.22686400 | -1.34772300 | 0.23535900 |
| C | 3.68792100 | 0.50635900 | -1.24042600 |
| C | 3.97408400 | -2.19045200 | -0.59300300 |
| H | 2.76456900 | -1.74588500 | 1.13405500 |
| C | 4.42716700 | -0.33847600 | -2.07209900 |
| H | 3.59524700 | 1.55622700 | -1.50325100 |
| C | 4.57421700 | -1.69157500 | -1.75278900 |
| H | 4.09346500 | -3.23762300 | -0.32588000 |
| H | 4.89085100 | 0.06405800 | -2.96865400 |
| H | 5.15494500 | -2.34675400 | -2.39585200 |
| C | 1.35008400 | 2.33940700 | 0.03837800 |
| C | 1.23718600 | 3.67309800 | 0.46443300 |
| C | 0.71269100 | 1.95897900 | -1.15628000 |
| C | 0.49735300 | 4.60034100 | -0.27612500 |
| H | 1.72732300 | 3.98416000 | 1.38338500 |
| C | -0.02556300 | 2.88368000 | -1.89693400 |
| H | 0.80463200 | 0.93951400 | -1.52142200 |
| C | -0.13695300 | 4.20706300 | -1.45674500 |
| H | 0.41772200 | 5.62689700 | 0.07053800 |
| H | -0.51962000 | 2.56955600 | -2.81183700 |
| H | -0.71543400 | 4.92465000 | -2.03147400 |
| C | 0.13079100 | -3.58041600 | -1.06408600 |
| H | 0.04425300 | -4.32081700 | -1.86370500 |
| H | 1.18353200 | -3.29678900 | -0.98465300 |
| C | -0.40669500 | -4.11202100 | 0.26066700 |
| H | -0.25971200 | -3.39011800 | 1.06945400 |
| H | -1.47365600 | -4.34862100 | 0.19984200 |
| H | 0.12742800 | -5.03122800 | 0.52842200 |
| O | -3.37777700 | -1.17479000 | 0.64974300 |
| O | -2.92379200 | 0.61211400 | -0.58197200 |
| C | -3.75982300 | -0.22665800 | -0.11126000 |
| C | -5.23819000 | -0.10473200 | -0.44161500 |
| H | -5.57566700 | -1.09219700 | -0.77860700 |
| H | -5.75285900 | 0.06595900 | 0.51261500 |
| C | -5.59137800 | 0.98395100 | -1.45599700 |
| H | -6.67382700 | 1.01316700 | -1.62023500 |
| H | -5.26807700 | 1.96797400 | -1.10595000 |
| H | -5.10427600 | 0.80282300 | -2.41887400 |
| S | -0.68926700 | -2.03907800 | -1.67691400 |
| H | -1.95758600 | -2.49839100 | -1.68091000 |

C/J-TS1



| | | | |
|---|---|---|---|
| Cd | 1.59350000 | -0.00799300 | -0.44424300 |
| P | -1.87358200 | -0.13677700 | 0.53682500 |
| Se | -0.65080100 | -0.65102500 | -1.41532800 |
| C | -2.59070100 | 1.54572000 | 0.21064700 |
| C | -3.21782100 | 2.16186900 | 1.30953900 |
| C | -2.51932300 | 2.24658600 | -1.00142200 |
| C | -3.78073900 | 3.43428500 | 1.19166000 |
| H | -3.26670700 | 1.64329900 | 2.26473500 |
| C | -3.07413200 | 3.52573500 | -1.11700500 |
| H | -2.02509200 | 1.79280300 | -1.85508300 |
| C | -3.70858400 | 4.12168700 | -0.02431900 |
| H | -4.26478400 | 3.89135400 | 2.05038100 |
| H | -3.00974800 | 4.05440500 | -2.06434000 |
| H | -4.13746500 | 5.11562000 | -0.11594800 |
| C | -3.34130500 | -1.22814900 | 0.24308200 |
| C | -4.42901500 | -0.88740000 | -0.57753200 |
| C | -3.35252800 | -2.47152900 | 0.89897100 |
| C | -5.49901600 | -1.77073100 | -0.73906800 |
| H | -4.44305500 | 0.07060200 | -1.08781600 |
| C | -4.42037000 | -3.35673000 | 0.73412000 |
| H | -2.52064900 | -2.74615500 | 1.54298600 |
| C | -5.49706100 | -3.00740400 | -0.08616600 |
| H | -6.33392600 | -1.49314700 | -1.37675100 |
| H | -4.41325300 | -4.31403000 | 1.24799300 |
| H | -6.33082700 | -3.69225200 | -0.21307300 |
| C | 1.96526400 | -0.32141700 | 3.10084900 |
| H | 2.52814900 | -0.02891500 | 3.99148300 |
| H | 0.90093800 | -0.26029100 | 3.34072100 |
| C | 2.35334300 | -1.72507800 | 2.64521600 |
| H | 1.74767800 | -2.05195800 | 1.79193700 |
| H | 3.40910000 | -1.77911500 | 2.36430100 |
| H | 2.18130000 | -2.43765600 | 3.46047400 |
| O | 4.84267900 | 0.24145700 | 0.64314300 |
| O | 3.62144600 | -0.17422800 | -1.21707000 |
| C | 4.73160100 | -0.05506000 | -0.57467400 |
| C | 5.98436100 | -0.30395000 | -1.40678700 |
| H | 5.88236500 | -1.30674600 | -1.84022500 |
| H | 5.93663900 | 0.38466600 | -2.25969100 |
| C | 7.30457000 | -0.15767700 | -0.65039100 |
| H | 8.14852700 | -0.34841700 | -1.32180600 |
| H | 7.41471600 | 0.84887400 | -0.23693600 |
| H | 7.36370900 | -0.86218000 | 0.18422900 |
| S | 2.26406500 | 1.02453100 | 1.86131600 |
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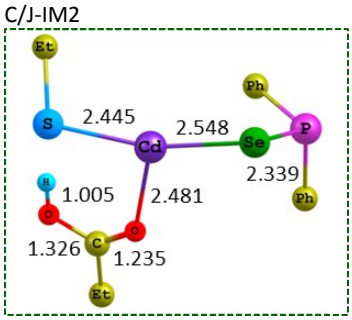
C/J-IM2




| | | | |
|---|---|---|---|
| Cd | -1.24454700 | 0.21702500 | -0.97549400 |
| P | 1.67410500 | -2.22785000 | -0.43121200 |
| Se | 0.24137100 | -1.50010800 | -2.13034400 |
| C | 2.88298600 | -0.85103800 | -0.13282700 |
| C | 3.73529000 | -0.98182100 | 0.98161000 |
| C | 3.10158500 | 0.21041100 | -1.02127300 |
| C | 4.75715800 | -0.06015700 | 1.21279500 |
| H | 3.59922000 | -1.80672300 | 1.67723000 |
| C | 4.13192600 | 1.12948300 | -0.79355400 |
| H | 2.46084600 | 0.32311700 | -1.88997300 |
| C | 4.96026200 | 1.00114500 | 0.32314200 |
| H | 5.39886200 | -0.17503600 | 2.08224000 |
| H | 4.28375100 | 1.94612200 | -1.49443400 |
| H | 5.76148000 | 1.71411200 | 0.49691000 |
| C | 0.60958900 | -2.11342200 | 1.08587700 |
| C | 0.40471900 | -0.93224200 | 1.82229000 |
| C | -0.03300400 | -3.28920500 | 1.50879100 |
| C | -0.42954800 | -0.92781700 | 2.94390500 |
| H | 0.91303300 | -0.01888200 | 1.52662600 |
| C | -0.87143300 | -3.28424000 | 2.62773200 |
| H | 0.12282700 | -4.21234100 | 0.95632200 |
| C | -1.07240800 | -2.10341900 | 3.34799800 |
| H | -0.57232400 | -0.00868300 | 3.50617300 |
| H | -1.36041900 | -4.20309200 | 2.93929500 |
| H | -1.71722200 | -2.09950300 | 4.22230800 |
| C | -4.19037800 | 0.05636100 | 0.78435800 |
| H | -3.53778400 | -0.27943700 | 1.59441200 |
| H | -5.01939000 | 0.60953600 | 1.23661600 |
| C | -4.71823400 | -1.12724100 | -0.02278200 |
| H | -5.37055000 | -0.79114200 | -0.83438600 |
| H | -3.90074000 | -1.70758800 | -0.46445800 |
| H | -5.29324600 | -1.79954300 | 0.62618000 |
| O | -1.28138900 | 3.24439500 | 1.21331000 |
| O | 0.10842200 | 2.14196600 | -0.18703600 |
| C | -0.10379600 | 3.03223100 | 0.64216700 |
| C | 0.96519600 | 4.00393500 | 1.08201500 |
| H | 0.89224200 | 4.13186300 | 2.16711900 |
| H | 1.93348800 | 3.55916700 | 0.84147300 |
| C | 0.80833600 | 5.37155000 | 0.38693200 |
| H | 1.60089800 | 6.04889700 | 0.71833400 |
| H | 0.88265100 | 5.27081500 | -0.70041000 |
| H | -0.15569800 | 5.82811700 | 0.62827800 |
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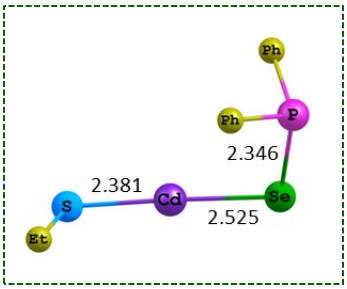
J




| | | | |
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| Se | -0.61915700 | -1.01727600 | -2.05369200 |
| P | -2.03225900 | 0.63579100 | -1.17334900 |
| C | -0.83849600 | 1.88723800 | -0.50210500 |
| C | -0.24144400 | 1.81913700 | 0.76980900 |
| C | -0.50905300 | 2.96353800 | -1.34355300 |
| C | 0.66876900 | 2.79625000 | 1.18222400 |
| H | -0.50238000 | 1.01423600 | 1.45147000 |
| C | 0.40496600 | 3.93833000 | -0.93348900 |
| H | -0.96846500 | 3.03480800 | -2.32616100 |
| C | 0.99655900 | 3.85665300 | 0.33020000 |
| H | 1.11600600 | 2.73078500 | 2.17034200 |
| H | 0.64865600 | 4.76270100 | -1.59777400 |
| H | 1.70238100 | 4.61684100 | 0.65273900 |
| C | -2.74054200 | -0.07755900 | 0.38593800 |
| C | -3.42011900 | 0.80632300 | 1.24772900 |
| C | -2.77878100 | -1.45020400 | 0.67189300 |
| C | -4.08843600 | 0.33117200 | 2.37672700 |
| H | -3.42299200 | 1.87396700 | 1.04219800 |
| C | -3.45445700 | -1.92599900 | 1.80133900 |
| H | -2.28074000 | -2.15138500 | 0.00946500 |

| | | | |
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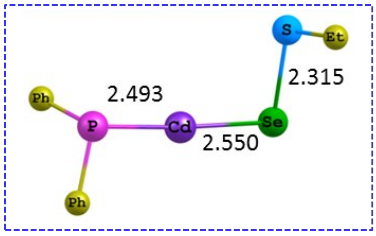
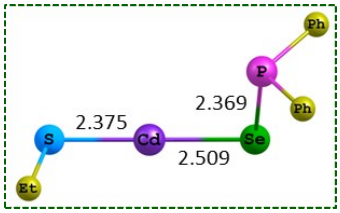
| C | -4.10682700 | -1.03908700 | 2.65946000 |
| H | -4.59669200 | 1.03131600 | 3.03404200 |
| H | -3.46756800 | -2.99296600 | 2.00662600 |
| H | -4.62908600 | -1.40918900 | 3.53701600 |
| Cd | 1.23889100 | -1.12024800 | -0.34772600 |
| C | 4.09777000 | 0.15298200 | 0.82738200 |
| H | 4.49706500 | 0.05947200 | -0.18606000 |
| H | 3.48874800 | 1.05948900 | 0.87546000 |
| C | 5.23919900 | 0.22537100 | 1.84146000 |
| H | 5.85989900 | -0.67546300 | 1.80339400 |
| H | 5.87870600 | 1.08975700 | 1.62460700 |
| H | 4.85557600 | 0.33046100 | 2.86127000 |
| S | 3.03216700 | -1.32857900 | 1.20424100 |

J-i




| | | | |
|---|---|---|---|
| Cd | 0.58076800 | -0.15031200 | -0.07250400 |
| Se | 2.85373200 | -0.25413500 | -1.22430900 |
| C | 4.61518500 | 0.02367700 | 1.51677700 |
| H | 3.86932700 | -0.66882800 | 1.91968100 |
| H | 4.92153000 | 0.68935000 | 2.33372400 |
| C | 5.81442200 | -0.72347400 | 0.94099400 |
| H | 6.57285600 | -0.02600100 | 0.57254800 |
| H | 6.27038400 | -1.35538500 | 1.71301100 |
| H | 5.51036500 | -1.36974600 | 0.11183300 |
| S | 3.78409400 | 1.17379500 | 0.34283900 |
| P | -1.54024400 | -0.01042600 | 1.22982900 |
| C | -2.31655500 | 1.49051200 | 0.45868900 |
| C | -2.83886800 | 2.45555100 | 1.33784100 |
| C | -2.38877900 | 1.74468300 | -0.92468800 |
| C | -3.41447900 | 3.63544100 | 0.85351200 |
| H | -2.79397000 | 2.27996700 | 2.40932500 |
| C | -2.96508700 | 2.91956400 | -1.41054100 |
| H | -1.99680500 | 1.01600800 | -1.62983100 |
| C | -3.47846400 | 3.87043400 | -0.52113100 |
| H | -3.81060900 | 4.36746400 | 1.55179000 |
| H | -3.00730800 | 3.09590500 | -2.48185100 |
| H | -3.92169500 | 4.78715600 | -0.89943600 |
| C | -2.47393600 | -1.43888600 | 0.49731200 |
| C | -3.69464100 | -1.31063300 | -0.18647200 |
| C | -1.99070100 | -2.73784600 | 0.75360900 |
| C | -4.39859500 | -2.44274600 | -0.61149200 |
| H | -4.10445400 | -0.32646300 | -0.38816900 |
| C | -2.68923800 | -3.86534700 | 0.32266700 |
| H | -1.05938200 | -2.87078400 | 1.30140800 |
| C | -3.89989400 | -3.72341400 | -0.36530800 |
| H | -5.34096100 | -2.31722700 | -1.13817300 |
| H | -2.29060000 | -4.85524800 | 0.52771600 |
| H | -4.44650500 | -4.60003900 | -0.70037800 |

J-ii

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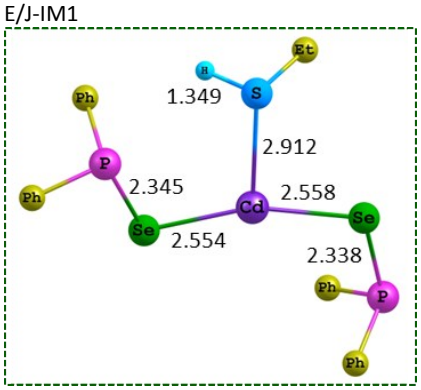
| Se | -0.04148900 | -0.44762300 | -1.41078100 |
| P | -1.13638300 | 0.01250300 | 0.63956300 |
| C | -2.56563100 | -1.15456000 | 0.51368700 |
| C | -3.64509800 | -0.98151100 | -0.36961600 |
| C | -2.54664400 | -2.28377800 | 1.34884500 |
| C | -4.67938200 | -1.91734400 | -0.41413800 |
| H | -3.67789300 | -0.11269800 | -1.02042200 |
| C | -3.58202200 | -3.22236400 | 1.30302600 |
| H | -1.71929200 | -2.42735900 | 2.03947100 |
| C | -4.64983500 | -3.04024800 | 0.42102100 |
| H | -5.50809300 | -1.77226600 | -1.10175300 |
| H | -3.55470400 | -4.08977300 | 1.95659800 |
| H | -5.45667300 | -3.76683900 | 0.38445800 |
| C | -1.97310900 | 1.63931900 | 0.32325600 |
| C | -2.94313000 | 2.04008800 | 1.26315400 |
| C | -1.61843900 | 2.53437700 | -0.69562500 |
| C | -3.55241300 | 3.29183200 | 1.17149900 |
| H | -3.23067700 | 1.36834600 | 2.06843000 |
| C | -2.22749900 | 3.79155200 | -0.78394200 |
| H | -0.87358000 | 2.24591800 | -1.43048500 |
| C | -3.19568500 | 4.17443800 | 0.14580300 |
| H | -4.30374800 | 3.57837800 | 1.90226500 |
| H | -1.94400900 | 4.46778100 | -1.58598600 |
| H | -3.66818300 | 5.15004100 | 0.07531000 |
| Cd | 2.23472800 | -0.54579800 | -0.35908100 |
| C | 4.97914900 | 1.04070000 | 0.71516600 |
| H | 4.97997100 | 1.49650400 | -0.27847000 |
| H | 4.28707200 | 1.59853100 | 1.35137500 |
| C | 6.38627600 | 1.07035000 | 1.31139300 |
| H | 7.09404900 | 0.52222400 | 0.68152400 |
| H | 6.73487700 | 2.10679400 | 1.39588300 |
| H | 6.40145100 | 0.62250000 | 2.31003100 |
| S | 4.40685000 | -0.72845300 | 0.58372400 |

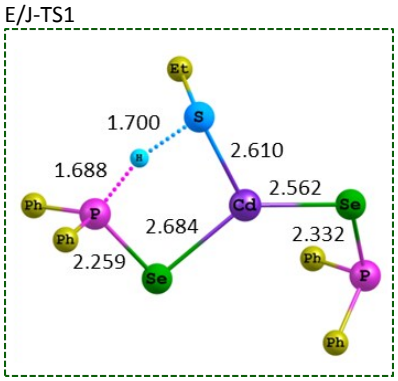
E/J-IM1




| | | | |
|---|---|---|---|
| Se | 2.77016400 | -1.57932100 | -1.21303300 |
| P | 4.41311900 | -0.53963200 | 0.08532700 |
| C | 3.59102200 | -0.33278200 | 1.73400100 |
| C | 2.76349700 | 0.74891500 | 2.08298200 |
| C | 3.81822900 | -1.34155700 | 2.68638500 |
| C | 2.17117400 | 0.81287800 | 3.34677500 |
| H | 2.58879800 | 1.55112900 | 1.37184400 |
| C | 3.22201000 | -1.28063400 | 3.94879300 |
| H | 4.46355400 | -2.17952600 | 2.43457400 |
| C | 2.39651600 | -0.20268800 | 4.28183700 |
| H | 1.53157400 | 1.65435800 | 3.59794100 |
| H | 3.40837800 | -2.06951100 | 4.67243900 |
| H | 1.93512200 | -0.15091000 | 5.26402000 |
| C | 4.50092000 | 1.21627300 | -0.50931700 |
| C | 5.26874600 | 2.11454700 | 0.25833300 |
| C | 3.98643300 | 1.65864400 | -1.73629300 |
| C | 5.48681700 | 3.42236700 | -0.17625100 |
| H | 5.69392200 | 1.79443300 | 1.20654900 |
| C | 4.21077900 | 2.96871600 | -2.17441100 |

| | | | |
|---|---|---|---|
| H | 3.40866000 | 0.97705100 | -2.35258000 |
| C | 4.95647400 | 3.85600100 | -1.39644200 |
| H | 6.07310700 | 4.10144700 | 0.43685700 |
| H | 3.79810500 | 3.29227300 | -3.12624000 |
| H | 5.12787300 | 4.87330000 | -1.73665700 |
| Cd | 0.54841000 | -0.49514800 | -0.55485100 |
| Se | -1.09276600 | 1.10835200 | 0.56775300 |
| C | -0.42930300 | -4.08415700 | -1.23910600 |
| H | -0.38701500 | -3.98958100 | -0.15142800 |
| H | 0.59969600 | -4.15119800 | -1.60190500 |
| C | -1.25642100 | -5.29277000 | -1.66871400 |
| H | -1.28815300 | -5.38575300 | -2.75824400 |
| H | -0.81154000 | -6.20705400 | -1.25860000 |
| H | -2.28536800 | -5.22585000 | -1.30073800 |
| P | -2.98117800 | 0.56169200 | -0.70987000 |
| C | -3.98506400 | 2.09401400 | -0.44917200 |
| C | -4.71139100 | 2.37087700 | 0.72101600 |
| C | -4.00698500 | 3.02915300 | -1.49782200 |
| C | -5.44194900 | 3.55526100 | 0.83714600 |
| H | -4.70886700 | 1.65971000 | 1.54149600 |
| C | -4.73376900 | 4.21671300 | -1.37929100 |
| H | -3.45302200 | 2.82496400 | -2.41070400 |
| C | -5.45362700 | 4.48161600 | -0.21104400 |
| H | -6.00016400 | 3.75623400 | 1.74754300 |
| H | -4.74039200 | 4.92993000 | -2.19887200 |
| H | -6.02252600 | 5.40247700 | -0.11787000 |
| C | -3.91408500 | -0.66889100 | 0.33150800 |
| C | -5.08125800 | -1.20478800 | -0.24811400 |
| C | -3.51017900 | -1.14850300 | 1.58612000 |
| C | -5.83388000 | -2.17292200 | 0.41925000 |
| H | -5.40652400 | -0.85919900 | -1.22724400 |
| C | -4.25935400 | -2.12667900 | 2.25087700 |
| H | -2.60908600 | -0.75130700 | 2.04446100 |
| C | -5.42341900 | -2.63884500 | 1.67343200 |
| H | -6.73566900 | -2.56668400 | -0.04169000 |
| H | -3.93222900 | -2.48230500 | 3.22444600 |
| H | -6.00449800 | -3.39652200 | 2.19160300 |
| S | -1.05430000 | -2.49035000 | -1.94427400 |
| H | -2.20082300 | -2.41169000 | -1.23697500 |

E/J-TS1

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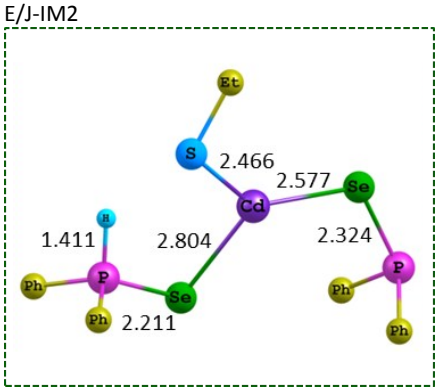
| C | -3.94416500 | -1.21335300 | -0.76092000 |
| C | -2.86334300 | -1.23124300 | -1.65905900 |
| C | -4.72408100 | -2.37471500 | -0.62611000 |
| C | -2.57192100 | -2.37916400 | -2.39919400 |
| H | -2.25046600 | -0.34490500 | -1.79090700 |
| C | -4.42835500 | -3.52719600 | -1.35981100 |
| H | -5.56699000 | -2.37501200 | 0.06049100 |
| C | -3.35132600 | -3.53166900 | -2.25006900 |
| H | -1.73612700 | -2.37206000 | -3.09392600 |
| H | -5.04237600 | -4.41568900 | -1.24064700 |
| H | -3.12322900 | -4.42341800 | -2.82746300 |
| C | -3.84074400 | 1.66846100 | -0.72413200 |
| C | -4.27311200 | 1.75896500 | -2.06229900 |
| C | -3.13875700 | 2.75415600 | -0.17778200 |
| C | -3.98605900 | 2.88660700 | -2.83305300 |
| H | -4.83295400 | 0.94183300 | -2.50937500 |
| C | -2.85463000 | 3.88550900 | -0.94996900 |
| H | -2.81339900 | 2.71553700 | 0.85735500 |
| C | -3.27260200 | 3.95554000 | -2.28032000 |
| H | -4.32074800 | 2.92963100 | -3.86610400 |
| H | -2.30222700 | 4.71009200 | -0.50750000 |
| H | -3.04864400 | 4.83291700 | -2.88044100 |
| Cd | -0.59025500 | 0.04432000 | 1.29118000 |
| Se | 0.78316700 | 0.80183000 | -0.88725700 |
| C | 1.30219500 | -2.63691500 | 2.60391800 |
| H | 1.46362000 | -2.86318400 | 1.54460900 |
| H | 0.29728000 | -2.97621700 | 2.86796500 |
| C | 2.35386100 | -3.32956500 | 3.46919800 |
| H | 2.19432500 | -3.11493200 | 4.53028300 |
| H | 2.30010900 | -4.41588100 | 3.32707700 |
| H | 3.36435300 | -3.00143900 | 3.20518700 |
| P | 2.74955600 | 0.02037500 | -0.09575700 |
| C | 3.96339200 | 1.38209300 | 0.03313100 |
| C | 4.46299900 | 2.04740700 | -1.09902100 |
| C | 4.37982200 | 1.78574500 | 1.31197900 |
| C | 5.37173200 | 3.09509400 | -0.95126500 |
| H | 4.14015200 | 1.74784200 | -2.09184100 |
| C | 5.28996800 | 2.83771100 | 1.45561600 |
| H | 3.99602600 | 1.28257300 | 2.19525900 |
| C | 5.78638600 | 3.49163700 | 0.32591100 |
| H | 5.75367300 | 3.60528000 | -1.83087200 |
| H | 5.60826400 | 3.14274000 | 2.44823800 |
| H | 6.49239400 | 4.30955600 | 0.43754000 |
| C | 3.47835200 | -1.18381700 | -1.27334200 |
| C | 4.84871100 | -1.49085100 | -1.18003300 |
| C | 2.68170500 | -1.88195600 | -2.19375600 |
| C | 5.40676600 | -2.47535700 | -1.99708500 |
| H | 5.48263800 | -0.95895300 | -0.47649600 |
| C | 3.24635900 | -2.86596200 | -3.00958700 |
| H | 1.62612100 | -1.64346900 | -2.27970500 |
| C | 4.60762200 | -3.16600200 | -2.91399000 |
| H | 6.46675300 | -2.69968600 | -1.91872300 |
| H | 2.62043300 | -3.39317700 | -3.72396400 |
| H | 5.04452600 | -3.92974400 | -3.55077900 |
| S | 1.34473000 | -0.79446400 | 2.82888800 |
| H | 2.28674600 | -0.47694000 | 1.44960100 |

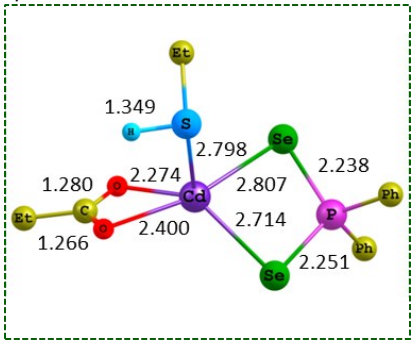
E/J-IM2




| | | | |
|---|---|---|---|
| Se | 3.11071100 | 1.32323200 | -1.33140800 |
| P | 4.28514900 | -0.32927700 | -0.19510300 |
| C | 3.40912300 | -1.91388100 | -0.59544300 |
| C | 2.47801100 | -2.55791600 | 0.23620400 |
| C | 3.75731600 | -2.52750300 | -1.81305300 |
| C | 1.91063100 | -3.77913700 | -0.14167800 |

| | | | |
|---|---|---|---|
| H | 2.19909500 | -2.11378400 | 1.18639000 |
| C | 3.18132000 | -3.73979700 | -2.19637100 |
| H | 4.48348400 | -2.04787400 | -2.46469400 |
| C | 2.25702100 | -4.37248500 | -1.35838400 |
| H | 1.19291400 | -4.26162100 | 0.51636300 |
| H | 3.46191900 | -4.19506000 | -3.14233100 |
| H | 1.81501400 | -5.32142800 | -1.64948000 |
| C | 3.91966500 | -0.12643000 | 1.61288700 |
| C | 4.49026500 | -1.07360200 | 2.48684700 |
| C | 3.24924400 | 0.97144800 | 2.16956800 |
| C | 4.36261700 | -0.94155700 | 3.87001900 |
| H | 5.03688100 | -1.92313900 | 2.08411300 |
| C | 3.12721900 | 1.10840500 | 3.55708200 |
| H | 2.83009400 | 1.72935200 | 1.51507600 |
| C | 3.67782800 | 0.15215200 | 4.41205800 |
| H | 4.80331400 | -1.68892400 | 4.52447200 |
| H | 2.60093400 | 1.96713600 | 3.96556100 |
| H | 3.58316700 | 0.25911200 | 5.48907000 |
| Cd | 0.56576900 | 1.19404800 | -0.94757000 |
| Se | -0.74059200 | -1.07929100 | 0.04645300 |
| C | -0.47040900 | 4.11892400 | -2.42576800 |
| H | -0.16054200 | 3.66475900 | -3.37082200 |
| H | 0.42347700 | 4.49628700 | -1.92180400 |
| C | -1.45794100 | 5.25653200 | -2.68213300 |
| H | -1.76852600 | 5.72710500 | -1.74347700 |
| H | -0.99413600 | 6.02505700 | -3.31323600 |
| H | -2.35565300 | 4.89209400 | -3.19241200 |
| P | -2.78589000 | -0.24052700 | 0.00425400 |
| C | -3.37158100 | 0.48900400 | 1.56175700 |
| C | -3.77280600 | -0.33375800 | 2.62705000 |
| C | -3.35614500 | 1.88446200 | 1.71501600 |
| C | -4.17270500 | 0.23979600 | 3.83351700 |
| H | -3.77546900 | -1.41436200 | 2.51564400 |
| C | -3.75748700 | 2.44957000 | 2.92884200 |
| H | -3.02027000 | 2.52463800 | 0.90301200 |
| C | -4.16599100 | 1.63139900 | 3.98480100 |
| H | -4.48511700 | -0.39737900 | 4.65550700 |
| H | -3.74595500 | 3.52905200 | 3.04597900 |
| H | -4.47574300 | 2.07493200 | 4.92665700 |
| C | -4.03362000 | -1.45553300 | -0.55040800 |
| C | -5.39873400 | -1.13673500 | -0.44462900 |
| C | -3.64272800 | -2.67210200 | -1.12485100 |
| C | -6.36036700 | -2.03245700 | -0.91349100 |
| H | -5.71199400 | -0.19853500 | 0.00411900 |
| C | -4.61195800 | -3.56675300 | -1.58704500 |
| H | -2.58780000 | -2.91486000 | -1.20783400 |
| C | -5.96801100 | -3.24857200 | -1.48321600 |
| H | -7.41380300 | -1.78192600 | -0.83122100 |
| H | -4.30395400 | -4.50967300 | -2.02883700 |
| H | -6.71900900 | -3.94495900 | -1.84481700 |
| S | -1.24890600 | 2.81146700 | -1.35987200 |
| H | -2.83833300 | 0.83841400 | -0.90355900 |

F/K-i-IM1




| | | | |
|---|---|---|---|
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| Se | -0.38920200 | 0.27661200 | 1.73526300 |
| Se | -0.44900400 | -0.58465700 | -1.83759500 |
| C | -2.82927300 | 1.28337800 | -0.34268100 |
| C | -3.80129400 | 1.60106900 | 0.62174100 |
| C | -2.71216500 | 2.07067500 | -1.49466500 |
| C | -4.64895900 | 2.69099300 | 0.42724500 |
| H | -3.89586700 | 1.00108600 | 1.52222500 |
| C | -3.56399600 | 3.16398800 | -1.68364000 |
| H | -1.95988600 | 1.82800900 | -2.23891700 |
| C | -4.53168300 | 3.47500400 | -0.72643700 |
| H | -5.39852600 | 2.92955600 | 1.17624900 |
| H | -3.46881400 | 3.76804400 | -2.58133300 |
| H | -5.19243000 | 4.32422500 | -0.87565600 |
| C | -2.83137000 | -1.54515500 | 0.31482300 |
| C | -3.94110400 | -1.75526800 | -0.52124600 |
| C | -2.56436500 | -2.44636500 | 1.35339500 |
| C | -4.77609600 | -2.85283900 | -0.31114400 |
| H | -4.15591700 | -1.06554600 | -1.33212200 |
| C | -3.40356500 | -3.54528400 | 1.55775000 |
| H | -1.70702800 | -2.28467400 | 1.99935600 |
| C | -4.50863400 | -3.75015400 | 0.72852500 |
| H | -5.63333800 | -3.00776400 | -0.95989800 |
| H | -3.19141900 | -4.23800100 | 2.36694700 |
| H | -5.15986100 | -4.60451700 | 0.88960700 |
| C | 2.72231800 | 3.03703500 | 1.47916000 |
| H | 3.04343000 | 4.08184000 | 1.46586200 |
| H | 1.71972900 | 2.99821600 | 1.91458900 |
| C | 3.70124200 | 2.15905200 | 2.25330000 |
| H | 3.39074300 | 1.11032600 | 2.26616900 |
| H | 4.70716100 | 2.20911000 | 1.82254200 |
| H | 3.76480600 | 2.51076100 | 3.28957400 |
| O | 3.28095500 | -1.35797900 | 0.83951600 |
| O | 3.74030900 | -0.63714100 | -1.20872600 |
| C | 4.06546100 | -1.28234800 | -0.16929700 |
| C | 5.40318800 | -2.00206900 | -0.08132800 |
| H | 5.88236600 | -1.67790800 | 0.85054700 |
| H | 5.17447500 | -3.06511800 | 0.06664200 |
| C | 6.32793100 | -1.80340000 | -1.28279400 |
| H | 7.25737900 | -2.36691300 | -1.14601400 |
| H | 5.85114200 | -2.14181000 | -2.20687200 |
| H | 6.58437500 | -0.74801500 | -1.41645800 |
| S | 2.45574400 | 2.53034900 | -0.28115400 |
| H | 3.74272400 | 2.28930600 | -0.60560300 |

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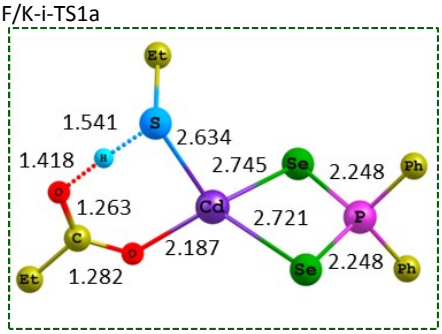


| | | | |
|---|---|---|---|
| Cd | -1.60470600 | 0.02963800 | 0.26240400 |
| O | -3.30833900 | -1.33719600 | 0.15207600 |
| C | -4.55100800 | -1.02471900 | 0.11225000 |
| C | -5.55136500 | -2.18010600 | 0.05315600 |
| H | -6.08042100 | -2.17219400 | 1.01959600 |
| H | -6.30975000 | -1.90897800 | -0.69518100 |
| C | -4.95804200 | -3.56073000 | -0.22640300 |
| H | -5.75531200 | -4.31608100 | -0.25039400 |

| | | | |
|---|---|---|---|
| H | -4.43659100 | -3.58179000 | -1.19333900 |
| H | -4.23399100 | -3.84434600 | 0.54484500 |
| O | -5.02029500 | 0.14782800 | 0.12558700 |
| H | -4.07770400 | 1.19035900 | 0.31020500 |
| P | 1.68270300 | -0.20113000 | 0.03224800 |
| Se | 0.29420500 | 0.03459700 | -1.72016000 |
| Se | 0.49403300 | -0.46988900 | 1.92135300 |
| C | 2.80011900 | 1.25061900 | 0.15115600 |
| C | 3.69512300 | 1.49829200 | -0.90272300 |
| C | 2.75252100 | 2.12442100 | 1.24559300 |
| C | 4.53774300 | 2.60512300 | -0.85198600 |
| H | 3.73323200 | 0.82910500 | -1.75828600 |
| C | 3.59841500 | 3.23485200 | 1.28548900 |
| H | 2.05450300 | 1.93515800 | 2.05698100 |
| C | 4.49039200 | 3.48011600 | 0.24055200 |
| H | 5.23082600 | 2.79180400 | -1.66887000 |
| H | 3.55726400 | 3.90952100 | 2.13641200 |
| H | 5.14938300 | 4.34308200 | 0.27439400 |
| C | 2.80270900 | -1.63448500 | -0.21921800 |
| C | 2.45930600 | -2.66852800 | -1.09788400 |
| C | 3.98491900 | -1.72450800 | 0.53480500 |
| C | 3.29505100 | -3.78038600 | -1.22980800 |
| H | 1.54619200 | -2.60365900 | -1.68084000 |
| C | 4.81527700 | -2.83330600 | 0.39814700 |
| H | 4.25950900 | -0.92717800 | 1.22117600 |
| C | 4.47198200 | -3.86679900 | -0.48213000 |
| H | 3.02533600 | -4.57928000 | -1.91670100 |
| H | 5.72890000 | -2.89565400 | 0.98213000 |
| H | 5.12132700 | -4.73091400 | -0.58497300 |
| C | -2.97453100 | 2.97223000 | -1.22096300 |
| H | -2.80274800 | 2.16680200 | -1.94411500 |
| H | -3.97626900 | 3.37679800 | -1.38853100 |
| C | -1.90794200 | 4.06275900 | -1.35049000 |
| H | -2.07646600 | 4.87114100 | -0.63120000 |
| H | -0.90027500 | 3.66048200 | -1.19011300 |
| H | -1.94119700 | 4.49097100 | -2.36285300 |
| S | -2.98534100 | 2.26093400 | 0.49633900 |

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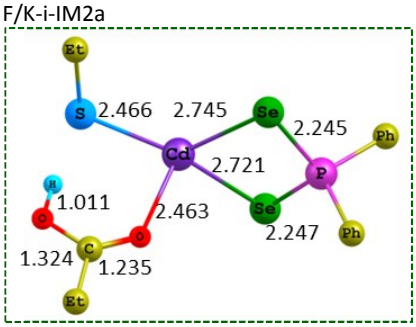


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| Cd | 1.44961400 | -0.69349000 | -0.31930100 |
| O | 2.46213500 | 1.52803700 | 0.00781000 |
| C | 3.64272700 | 1.87316100 | 0.11501000 |
| C | 4.04804300 | 3.30775300 | 0.36828200 |
| H | 3.13816600 | 3.87124600 | 0.58631600 |
| H | 4.68798700 | 3.32370000 | 1.25827100 |
| C | 4.80644700 | 3.92221400 | -0.82295400 |
| H | 5.07576800 | 4.95881400 | -0.59894400 |
| H | 5.72367300 | 3.36603700 | -1.03389600 |
| H | 4.18767300 | 3.92252600 | -1.72619800 |
| O | 4.67142600 | 1.04556100 | 0.01242400 |
| H | 4.37368600 | 0.09781300 | -0.17587200 |
| P | -1.76933900 | -0.01919600 | -0.00526000 |
| Se | -0.63914600 | -0.06613100 | -1.94716300 |
| Se | -0.46190300 | -0.79163700 | 1.64834700 |
| C | -3.30646100 | -1.01048900 | -0.14564800 |
| C | -3.39743400 | -2.28795700 | 0.42173600 |
| C | -4.38508600 | -0.49849200 | -0.88657300 |
| C | -4.56067500 | -3.04473200 | 0.25499500 |
| H | -2.56390000 | -2.68389500 | 0.99356000 |
| C | -5.54322300 | -1.25887500 | -1.04993000 |
| H | -4.32481800 | 0.48992500 | -1.33240900 |
| C | -5.63304900 | -2.53315500 | -0.47933400 |
| H | -4.62587300 | -4.03277900 | 0.70127400 |
| H | -6.37386900 | -0.85659400 | -1.62253000 |
| H | -6.53605200 | -3.12317600 | -0.60748200 |
| C | -2.34656000 | 1.67912600 | 0.38344800 |
| C | -3.20652000 | 1.86535600 | 1.47945000 |
| C | -1.91889100 | 2.78598900 | -0.35941000 |
| C | -3.63863800 | 3.14684300 | 1.81865400 |
| H | -3.53768100 | 1.01422500 | 2.06745400 |
| C | -2.35358400 | 4.06935900 | -0.01290700 |
| H | -1.24991800 | 2.64272500 | -1.20214100 |
| C | -3.21242400 | 4.25195300 | 1.07256900 |
| H | -4.30456100 | 3.28311300 | 2.66581100 |
| H | -2.01951500 | 4.92315800 | -0.59534700 |
| H | -3.54911000 | 5.24971600 | 1.33928700 |
| C | 3.82587900 | -2.67829600 | 1.10590300 |
| H | 3.73698200 | -1.93492900 | 1.90372800 |
| H | 3.01535500 | -3.40195800 | 1.22817400 |
| C | 5.18140900 | -3.38015400 | 1.18111200 |
| H | 5.27961500 | -4.13134700 | 0.39098800 |
| H | 6.00384600 | -2.66571200 | 1.07229800 |
| H | 5.29258800 | -3.88412400 | 2.14924900 |
| S | 3.61774900 | -1.84595800 | -0.54529800 |

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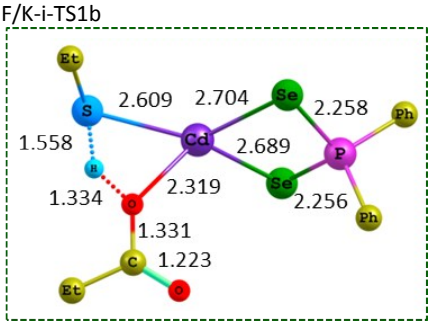


| | | | |
|---|---|---|---|
| Cd | -1.36195500 | -0.82540000 | 0.22912900 |
| C | -4.13240900 | -2.61269500 | -1.08204300 |
| H | -3.76837200 | -1.91955500 | -1.84506000 |
| H | -3.58499200 | -3.55271600 | -1.18916800 |
| C | -5.63661800 | -2.83943200 | -1.22103100 |
| H | -6.00557700 | -3.53051300 | -0.45683700 |
| H | -6.19055600 | -1.90029000 | -1.12591500 |
| H | -5.85977800 | -3.26739000 | -2.20579900 |
| O | -2.30550600 | 2.73793700 | 0.20304200 |
| C | -3.25464700 | 1.96851600 | 0.14633800 |
| C | -4.70168400 | 2.41039200 | 0.33911200 |
| H | -5.25347100 | 2.12634900 | -0.56644900 |
| H | -5.12906000 | 1.80122200 | 1.14699400 |
| C | -4.86229500 | 3.90138400 | 0.63425500 |
| H | -5.92024400 | 4.15405900 | 0.76190400 |
| H | -4.32727600 | 4.18134100 | 1.54614400 |
| H | -4.45757200 | 4.50810200 | -0.18067100 |
| O | -3.10349300 | 0.66983400 | -0.10349100 |
| H | -3.79203300 | -0.41393600 | 0.25989400 |
| P | 1.77843300 | -0.03823200 | -0.02016900 |
| Se | 0.63179700 | -0.18804000 | 1.91636600 |
| Se | 0.55598000 | -0.97353600 | -1.67158500 |
| C | 3.39619500 | -0.87869400 | 0.15836300 |
| C | 3.81409200 | -1.85947700 | -0.75006200 |
| C | 4.22124300 | -0.53731800 | 1.24414900 |

| | | | |
|---|---|---|---|
| C | 5.05460500 | -2.48306800 | -0.58288400 |
| H | 3.17062800 | -2.14146300 | -1.57742600 |
| C | 5.45671300 | -1.16364400 | 1.40599300 |
| H | 3.89941500 | 0.20931500 | 1.96438100 |
| C | 5.87596600 | -2.13694600 | 0.49183900 |
| H | 5.37224800 | -3.24212000 | -1.29174300 |
| H | 6.08823100 | -0.89595000 | 2.24800000 |
| H | 6.83712800 | -2.62587500 | 0.62204300 |
| C | 2.14189700 | 1.71124400 | -0.41748000 |
| C | 3.40419900 | 2.09305600 | -0.89941200 |
| C | 1.12136700 | 2.66892000 | -0.29078800 |
| C | 3.64520700 | 3.42574600 | -1.24355600 |
| H | 4.19835400 | 1.36194300 | -1.00734400 |
| C | 1.37230200 | 3.99628900 | -0.63914900 |
| H | 0.13243200 | 2.39957100 | 0.06951200 |
| C | 2.63173600 | 4.37823100 | -1.11279100 |
| H | 4.62517200 | 3.71488400 | -1.61231200 |
| H | 0.57581800 | 4.72717900 | -0.53816000 |
| H | 2.82173100 | 5.41391500 | -1.38021500 |
| S | -3.69590700 | -1.93369000 | 0.59115700 |

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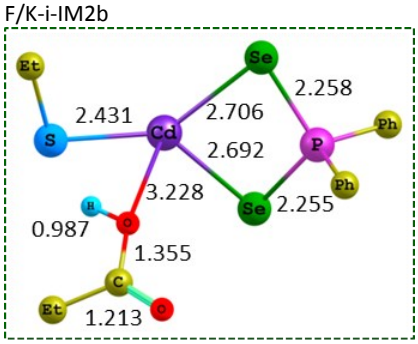


| | | | |
|---|---|---|---|
| Cd | -1.12065100 | -1.39799500 | 0.28100100 |
| C | -3.84897300 | -2.65621300 | -1.29996900 |
| H | -3.50456600 | -1.97962400 | -2.08670600 |
| H | -3.28291500 | -3.58803400 | -1.38019400 |
| C | -5.34500500 | -2.93120600 | -1.44588300 |
| H | -5.69973100 | -3.61038800 | -0.66418100 |
| H | -5.92711900 | -2.00613000 | -1.38109700 |
| H | -5.54859900 | -3.39357600 | -2.41938400 |
| O | -2.93782200 | 3.40607600 | 0.05163500 |
| C | -3.51621000 | 2.34904300 | 0.18695300 |
| C | -4.88167900 | 2.18724600 | 0.83890900 |
| H | -5.55367600 | 1.73998300 | 0.09388200 |
| H | -4.78955400 | 1.44020700 | 1.63858600 |
| C | -5.45755200 | 3.49748300 | 1.37505000 |
| H | -6.44077000 | 3.32300700 | 1.82305300 |
| H | -4.80272900 | 3.93172400 | 2.13550600 |
| H | -5.56611700 | 4.23452600 | 0.57488000 |
| O | -2.94331000 | 1.20886400 | -0.26771800 |
| H | -3.45508200 | 0.39149500 | -0.05596500 |
| P | 1.79643800 | 0.01269900 | -0.01695400 |
| Se | 0.63781400 | -0.17111000 | 1.90938600 |
| Se | 0.89702100 | -1.40881100 | -1.52277300 |
| C | 3.56182900 | -0.36164900 | 0.28336900 |
| C | 4.19269900 | -1.45318100 | -0.32638700 |
| C | 4.27856400 | 0.44555000 | 1.18426300 |
| C | 5.53560600 | -1.72694800 | -0.04881300 |
| H | 3.63675300 | -2.08794900 | -1.00926400 |
| C | 5.61668700 | 0.16546000 | 1.45852800 |
| H | 3.79542800 | 1.28762200 | 1.67146100 |
| C | 6.24771600 | -0.92089000 | 0.84150100 |
| H | 6.01979000 | -2.57282400 | -0.52788900 |
| H | 6.16465000 | 0.79253300 | 2.15561500 |
| H | 7.28972400 | -1.13784700 | 1.05815400 |
| C | 1.72910100 | 1.72650800 | -0.65405500 |
| C | 2.81943100 | 2.26993600 | -1.35377000 |
| C | 0.54931600 | 2.47301900 | -0.51283100 |
| C | 2.72670700 | 3.55379600 | -1.89549900 |
| H | 3.73576400 | 1.70163600 | -1.47680300 |
| C | 0.46073500 | 3.75211000 | -1.06320600 |
| H | -0.30545700 | 2.06855000 | 0.01774200 |
| C | 1.54997300 | 4.29521200 | -1.75118500 |
| H | 3.57465100 | 3.97123200 | -2.43091900 |
| H | -0.46514900 | 4.30673300 | -0.94705600 |
| H | 1.48218000 | 5.29283500 | -2.17587700 |
| S | -3.49761500 | -1.89914200 | 0.36466900 |

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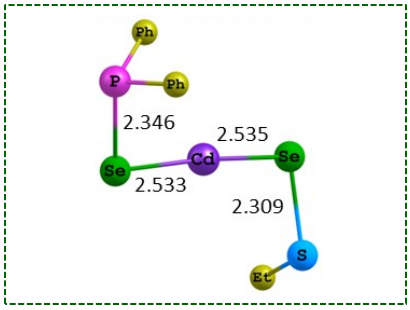
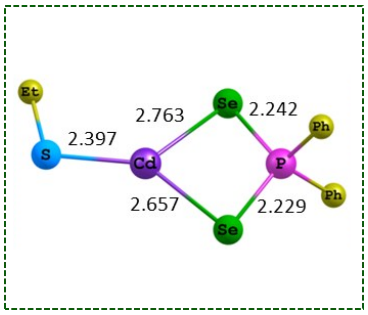


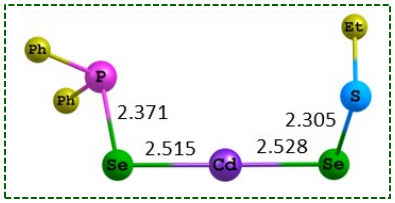

| | | | |
|---|---|---|---|
| Se | 0.88907200 | -0.57647900 | 2.21124100 |
| P | 2.81571400 | 0.29961900 | 1.19871700 |
| C | 2.12497300 | 1.70568900 | 0.20220400 |
| C | 1.59615500 | 1.57475500 | -1.09568300 |
| C | 2.11561000 | 2.97389000 | 0.80735500 |
| C | 1.05805500 | 2.68088100 | -1.76083500 |
| H | 1.62874400 | 0.61346600 | -1.60156700 |
| C | 1.57316000 | 4.07840800 | 0.14420300 |
| H | 2.52919400 | 3.09431900 | 1.80541600 |
| C | 1.04073300 | 3.93439300 | -1.14018800 |
| H | 0.65758900 | 2.56275700 | -2.76396500 |
| H | 1.57136100 | 5.05048500 | 0.62925000 |
| H | 0.62159800 | 4.79265400 | -1.65726300 |
| C | 3.27891300 | -0.90218000 | -0.13719400 |
| C | 4.30177700 | -0.50357500 | -1.02056600 |
| C | 2.78626800 | -2.21143700 | -0.23074100 |
| C | 4.79187400 | -1.38092400 | -1.98842100 |
| H | 4.71565900 | 0.50018700 | -0.95791600 |
| C | 3.28371900 | -3.09289800 | -1.19760300 |
| H | 2.01340000 | -2.54553500 | 0.45453200 |
| C | 4.28268000 | -2.68112400 | -2.08134000 |
| H | 5.57350800 | -1.05041100 | -2.66691200 |
| H | 2.88563100 | -4.10222600 | -1.25631900 |
| H | 4.66659500 | -3.36581800 | -2.83211600 |
| Cd | -0.83146600 | -0.13157400 | 0.40583000 |
| Se | -2.70351800 | 0.22069300 | -1.26694500 |
| C | -5.14221500 | -0.75751900 | 0.67169600 |
| H | -4.55850000 | -0.26864700 | 1.45824500 |
| H | -5.64788000 | -1.61917200 | 1.12578900 |
| C | -6.15014800 | 0.20238200 | 0.04728300 |
| H | -6.75862400 | -0.30248300 | -0.70923200 |
| H | -6.81851800 | 0.60074100 | 0.82034100 |
| H | -5.64214800 | 1.04727300 | -0.42773700 |
| S | -3.98256800 | -1.55087600 | -0.51926800 |

K-i




| | | | |
|---|---|---|---|
| Cd | -2.05482800 | -0.10086100 | 0.43609000 |
| C | -5.02504600 | -0.05234800 | -1.13282500 |
| H | -4.58435700 | 0.77192600 | -1.70045200 |
| H | -4.69163900 | -0.99262900 | -1.58080500 |
| C | -6.55079600 | 0.03757800 | -1.17029400 |
| H | -7.00785300 | -0.78582300 | -0.61200500 |
| H | -6.90080900 | 0.97846000 | -0.73356900 |
| H | -6.90679500 | -0.01234400 | -2.20683000 |
| P | 1.16954900 | -0.04221900 | -0.01193000 |
| Se | -0.29785600 | -0.30744900 | -1.68653200 |
| Se | 0.12603300 | -0.18393400 | 1.95220200 |
| C | 2.03164700 | 1.57018800 | -0.17781000 |
| C | 1.98114800 | 2.54306800 | 0.82774300 |
| C | 2.74681600 | 1.82669900 | -1.36065600 |
| C | 2.64809100 | 3.76078600 | 0.65587300 |
| H | 1.42212000 | 2.35104500 | 1.73808200 |
| C | 3.41193700 | 3.04070700 | -1.52489400 |
| H | 2.78012000 | 1.08474600 | -2.15325800 |
| C | 3.36361400 | 4.01041800 | -0.51630100 |
| H | 2.60460200 | 4.51046100 | 1.44049200 |
| H | 3.96245800 | 3.23233100 | -2.44125500 |
| H | 3.87964200 | 4.95705500 | -0.64826800 |
| C | 2.50362800 | -1.29686500 | -0.10276100 |
| C | 3.72081300 | -1.05975200 | 0.55749200 |
| C | 2.29959600 | -2.51292500 | -0.76883200 |
| C | 4.72242000 | -2.03126900 | 0.54473900 |
| H | 3.89144500 | -0.12073200 | 1.07526600 |
| C | 3.30643000 | -3.48143900 | -0.77789900 |
| H | 1.36104800 | -2.69650900 | -1.28249900 |
| C | 4.51690000 | -3.24339700 | -0.12208200 |
| H | 5.66204500 | -1.84044700 | 1.05487300 |
| H | 3.14305500 | -4.41939900 | -1.30040400 |
| H | 5.29856200 | -3.99752500 | -0.13134000 |
| S | -4.44039400 | 0.03077100 | 0.63167600 |

K-ii




| | | | |
|---|---|---|---|
| Cd | -1.54599300 | -0.55597400 | -0.86450500 |
| Se | -3.90391800 | -1.04459800 | -0.09429700 |
| Se | 0.77792600 | -0.01104600 | -1.65534200 |
| P | 1.62693000 | 0.27184700 | 0.54006900 |
| C | 2.94879100 | 1.51336900 | 0.17380300 |
| C | 2.61435600 | 2.86745400 | 0.35322800 |
| C | 4.24761100 | 1.18757200 | -0.25013500 |
| C | 3.55137100 | 3.87254100 | 0.10539700 |
| H | 1.61538600 | 3.13470700 | 0.68897200 |
| C | 5.18625800 | 2.19353600 | -0.49263000 |
| H | 4.52935600 | 0.14840500 | -0.38714200 |
| C | 4.84085000 | 3.53706200 | -0.31844700 |
| H | 3.27672100 | 4.91401600 | 0.24753300 |
| H | 6.18751200 | 1.92668400 | -0.81966200 |
| H | 5.57286500 | 4.31707300 | -0.50789900 |
| C | 2.61929700 | -1.26632400 | 0.84598100 |
| C | 2.92613900 | -2.25076700 | -0.10425200 |
| C | 3.05371300 | -1.45002800 | 2.17207500 |
| C | 3.66375100 | -3.38284700 | 0.25795200 |
| H | 2.58189300 | -2.13676300 | -1.12757400 |
| C | 3.79868600 | -2.57523700 | 2.53122900 |
| H | 2.80814600 | -0.70890100 | 2.92966600 |
| C | 4.10484400 | -3.54710100 | 1.57333800 |
| H | 3.89238700 | -4.13592000 | -0.49138200 |
| H | 4.12895500 | -2.69726300 | 3.55906000 |
| H | 4.67573400 | -4.42815000 | 1.85252000 |
| C | -4.08133400 | 1.34046200 | 2.10241300 |
| H | -3.00865900 | 1.18005800 | 2.24637700 |
| H | -4.62441300 | 0.57466800 | 2.66245100 |
| C | -4.48938700 | 2.74497400 | 2.55307100 |
| H | -4.26005100 | 2.86980400 | 3.61728400 |
| H | -3.94767800 | 3.51786600 | 1.99828400 |
| H | -5.56242600 | 2.91269400 | 2.41663900 |
| S | -4.48049800 | 1.15024600 | 0.31122900 |

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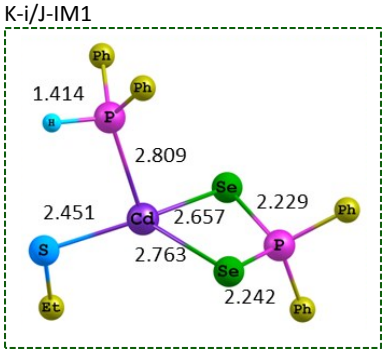


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| Cd | -0.45617600 | 1.35299900 | -0.54177900 |
| C | 0.10009200 | 4.72027900 | -0.74971500 |
| H | 0.38867800 | 4.60588700 | 0.29964100 |
| H | 0.95965100 | 4.44506700 | -1.36838900 |
| C | -0.30361000 | 6.16865000 | -1.02786200 |
| H | -0.58802100 | 6.30225100 | -2.07679500 |
| H | -1.15572600 | 6.46491600 | -0.40710700 |
| H | 0.53144900 | 6.84707700 | -0.81017500 |
| P | 2.13589700 | -0.49635300 | 0.13777900 |
| Se | 1.28505500 | -0.28613800 | -1.92614900 |
| Se | 0.76571400 | 0.43144900 | 1.63063200 |
| C | 3.80385200 | 0.27491800 | 0.21759900 |
| C | 4.04984900 | 1.41091000 | 0.99764700 |
| C | 4.84120700 | -0.27787600 | -0.55259700 |
| C | 5.32410600 | 1.98741300 | 1.01161100 |
| H | 3.24866600 | 1.84036800 | 1.59091300 |
| C | 6.11028600 | 0.29922700 | -0.53324600 |
| H | 4.65941500 | -1.15418600 | -1.16807300 |
| C | 6.35404000 | 1.43462900 | 0.24842400 |
| H | 5.50655900 | 2.86858200 | 1.61994800 |
| H | 6.90717000 | -0.13397900 | -1.13080700 |
| H | 7.34280600 | 1.88427400 | 0.25997300 |
| C | 2.44218700 | -2.25894100 | 0.55835400 |
| C | 2.95046800 | -2.57257200 | 1.83026800 |
| C | 2.18121100 | -3.28644900 | -0.35593100 |
| C | 3.19782100 | -3.90051800 | 2.17660000 |
| H | 3.14989400 | -1.78369600 | 2.54990700 |
| C | 2.43216000 | -4.61698800 | -0.00406200 |
| H | 1.78521200 | -3.04493000 | -1.33770900 |
| C | 2.93837000 | -4.92591500 | 1.25978400 |
| H | 3.58941800 | -4.13512300 | 3.16215000 |

| | | | |
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| H | 2.23013600 | -5.40840000 | -0.72021800 |
| H | 3.13027000 | -5.95981100 | 1.53218000 |
| S | -1.31058900 | 3.57424400 | -1.12705500 |
| P | -2.99568900 | 0.15183200 | -0.52526500 |
| H | -3.89696700 | 0.97413400 | -1.24022900 |
| C | -3.79844900 | 0.20881600 | 1.13022200 |
| C | -4.35442700 | 1.41517000 | 1.58742400 |
| C | -3.77208000 | -0.90242500 | 1.98679100 |
| C | -4.88936900 | 1.50029400 | 2.87500500 |
| H | -4.36556900 | 2.29095200 | 0.94376400 |
| C | -4.31018600 | -0.81292600 | 3.27314800 |
| H | -3.33961300 | -1.84089000 | 1.65183200 |
| C | -4.87061900 | 0.38680600 | 3.72026400 |
| H | -5.32087600 | 2.43740000 | 3.21515300 |
| H | -4.28832500 | -1.68170100 | 3.92498700 |
| H | -5.28825300 | 0.45444400 | 4.72066800 |
| C | -3.40692600 | -1.50083500 | -1.21766100 |
| C | -2.36203400 | -2.37694500 | -1.54776400 |
| C | -4.73689300 | -1.90130200 | -1.43832000 |
| C | -2.64336600 | -3.63775700 | -2.08552900 |
| H | -1.32996800 | -2.07132500 | -1.39953200 |
| C | -5.01339900 | -3.15748700 | -1.97851400 |
| H | -5.55530700 | -1.23334300 | -1.18399200 |
| C | -3.96593300 | -4.02853900 | -2.30161800 |
| H | -1.82720300 | -4.30790200 | -2.33965000 |
| H | -6.04374800 | -3.45666000 | -2.14890500 |
| H | -4.18326500 | -5.00583900 | -2.72333700 |

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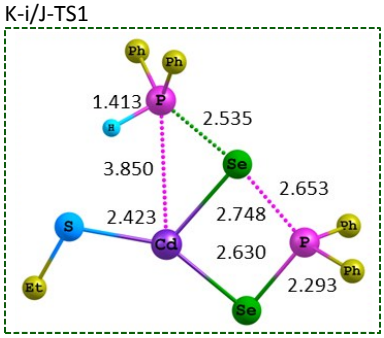


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| Se | 2.69023000 | 1.77048000 | -0.53415900 |
| P | -2.77645000 | -0.64131200 | -0.25623400 |
| Se | -0.26034200 | -0.70205000 | 0.04530500 |
| H | -3.19852100 | 0.28512200 | -1.23583000 |
| Cd | 0.07998300 | 1.87076600 | -0.85445100 |
| C | -1.26744400 | 4.79269800 | -2.04545500 |
| H | -0.54077100 | 4.68139600 | -2.85521200 |
| H | -2.14693300 | 5.28960300 | -2.46813200 |
| C | -0.68819000 | 5.62688700 | -0.90466800 |
| H | -1.41554000 | 5.74415700 | -0.09527200 |
| H | 0.20904000 | 5.15858000 | -0.48448200 |
| H | -0.40816300 | 6.62553300 | -1.26500100 |
| S | -1.88117500 | 3.11612700 | -1.54624700 |
| C | 3.42392900 | -1.49543400 | -0.80872700 |
| C | 3.90330100 | -1.13041000 | -2.07521800 |
| C | 3.65798800 | -2.80239500 | -0.34118800 |
| C | 4.61468400 | -2.04885100 | -2.85318300 |
| H | 3.72852100 | -0.12480600 | -2.44489200 |
| C | 4.36924700 | -3.71565800 | -1.12046000 |
| H | 3.29134300 | -3.10693800 | 0.63523700 |
| C | 4.85064200 | -3.34166500 | -2.37985800 |
| H | 4.98721300 | -1.74845100 | -3.82862100 |
| H | 4.54803500 | -4.71870100 | -0.74298100 |
| H | 5.40540000 | -4.05304000 | -2.98509500 |
| C | 3.09469700 | -0.49073700 | 1.88816100 |
| C | 2.22777800 | -0.57088000 | 2.98857300 |
| C | 4.48291300 | -0.46180400 | 2.10611600 |
| C | 2.74127700 | -0.62392100 | 4.28828900 |
| H | 1.15386600 | -0.59165400 | 2.82565100 |
| C | 4.99178400 | -0.51670200 | 3.40398500 |
| H | 5.16399700 | -0.39638700 | 1.26280700 |
| C | 4.12187300 | -0.59731400 | 4.49777600 |
| H | 2.06152000 | -0.68763400 | 5.13336300 |
| H | 6.06637200 | -0.49291500 | 3.56259500 |
| H | 4.52081800 | -0.63868400 | 5.50747800 |
| C | -3.77307400 | -0.09632600 | 1.17585400 |
| C | -4.11680300 | -0.99940400 | 2.19537500 |
| C | -4.10981200 | 1.26139600 | 1.31114900 |
| C | -4.80542800 | -0.55322400 | 3.32490500 |
| H | -3.85627200 | -2.05038900 | 2.10581100 |
| C | -4.79561100 | 1.70122800 | 2.44613500 |
| H | -3.83203400 | 1.97592000 | 0.54002600 |
| C | -5.14643200 | 0.79718700 | 3.45295100 |
| H | -5.07382900 | -1.26026500 | 4.10479500 |
| H | -5.05585600 | 2.75166100 | 2.53988500 |
| H | -5.68158100 | 1.14218000 | 4.33300500 |
| C | -3.50856400 | -2.22175000 | -0.83766200 |
| C | -2.66696700 | -3.31289800 | -1.09583000 |
| C | -4.89299900 | -2.35001600 | -1.04782600 |
| C | -3.20296500 | -4.51939300 | -1.55847000 |
| H | -1.59639900 | -3.21439000 | -0.94111900 |
| C | -5.42294100 | -3.55438000 | -1.51189500 |
| H | -5.55524800 | -1.51288400 | -0.84568100 |
| C | -4.57813100 | -4.64114200 | -1.76681100 |
| H | -2.54363200 | -5.35955500 | -1.75634700 |
| H | -6.49309700 | -3.64490600 | -1.67498600 |
| H | -4.99320700 | -5.57790400 | -2.12780300 |

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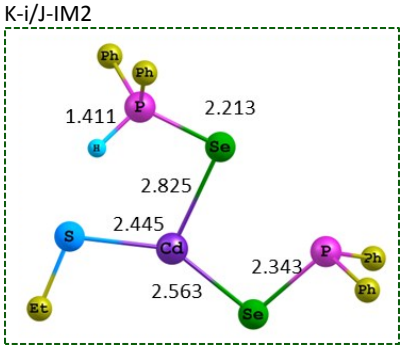


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| Se | -2.57103000 | -1.41702600 | -0.83294000 |
| P | 3.06332500 | 0.52524600 | 0.07397400 |
| Se | 0.91923700 | 0.77100200 | 0.56546000 |
| H | 3.21152900 | -0.31726300 | -1.04817100 |
| Cd | -0.01040100 | -1.43557700 | -0.93350000 |
| C | 1.38388800 | -3.68163800 | -3.13474900 |
| H | 0.86075600 | -3.08318200 | -3.88571500 |
| H | 2.29634600 | -4.06388500 | -3.60380900 |
| C | 0.51094800 | -4.83857600 | -2.65327500 |
| H | 1.03581000 | -5.44242700 | -1.90651400 |
| H | -0.41753300 | -4.47537600 | -2.19938000 |
| H | 0.24160500 | -5.48850800 | -3.49611700 |
| S | 1.98608700 | -2.56419500 | -1.78181900 |
| C | -3.71199900 | 1.69860300 | -0.55946900 |
| C | -3.85373500 | 1.58988700 | -1.95005100 |
| C | -4.22750300 | 2.84331200 | 0.07971500 |
| C | -4.50505700 | 2.58974100 | -2.68165800 |
| H | -3.46368100 | 0.71437100 | -2.45989200 |
| C | -4.88133100 | 3.83728000 | -0.64941700 |
| H | -4.12436600 | 2.95664200 | 1.15630700 |

| | | | |
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| C | -5.02298400 | 3.71427700 | -2.03641900 |
| H | -4.61072600 | 2.48197600 | -3.75805900 |
| H | -5.27986300 | 4.70751600 | -0.13461800 |
| H | -5.53110600 | 4.48805300 | -2.60523000 |
| C | -4.01736500 | -0.01072200 | 1.71665400 |
| C | -3.57917500 | -0.28016200 | 3.02352900 |
| C | -5.38054800 | -0.16968000 | 1.41445600 |
| C | -4.47986700 | -0.69971300 | 4.00739300 |
| H | -2.52727500 | -0.15981500 | 3.27075900 |
| C | -6.28060300 | -0.58665300 | 2.39640100 |
| H | -5.73805500 | 0.03398600 | 0.40942600 |
| C | -5.83280400 | -0.85376000 | 3.69536100 |
| H | -4.12470400 | -0.90276600 | 5.01410600 |
| H | -7.33171400 | -0.70667200 | 2.14769600 |
| H | -6.53550500 | -1.17835100 | 4.45790100 |
| C | 4.07392100 | -0.30359200 | 1.33757700 |
| C | 4.43377200 | 0.36998200 | 2.51612500 |
| C | 4.43665000 | -1.64749600 | 1.15632900 |
| C | 5.16797500 | -0.29386600 | 3.49847600 |
| H | 4.14402700 | 1.40629200 | 2.66559200 |
| C | 5.17073300 | -2.30556400 | 2.14726200 |
| H | 4.13924500 | -2.18249100 | 0.25806100 |
| C | 5.53722800 | -1.63149300 | 3.31458800 |
| H | 5.44811000 | 0.22972800 | 4.40771800 |
| H | 5.45034700 | -3.34513900 | 2.00494100 |
| H | 6.10659900 | -2.14658100 | 4.08287800 |
| C | 3.89131900 | 2.09914200 | -0.35295500 |
| C | 3.14058400 | 3.25731800 | -0.59338000 |
| C | 5.28995300 | 2.12960000 | -0.49098300 |
| C | 3.78529800 | 4.43986800 | -0.96722500 |
| H | 2.06030900 | 3.23148600 | -0.48661200 |
| C | 5.92626100 | 3.31225500 | -0.86951400 |
| H | 5.88130900 | 1.23865300 | -0.30021000 |
| C | 5.17473600 | 4.46838500 | -1.10677200 |
| H | 3.19881300 | 5.33547100 | -1.14918500 |
| H | 7.00687200 | 3.33127900 | -0.97591900 |
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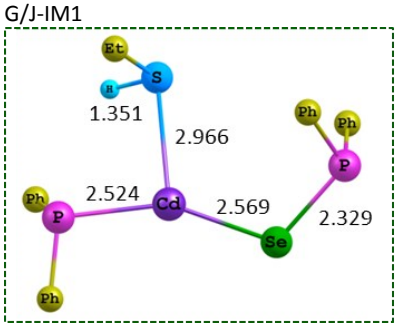


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| C | 3.26632500 | -1.22781000 | 0.97636100 |
| C | 3.70938700 | -0.00086800 | 1.49772100 |
| C | 2.94179500 | -2.25921100 | 1.87987000 |
| C | 3.82496900 | 0.18748900 | 2.88032100 |
| H | 3.97275500 | 0.81114100 | 0.82830300 |
| C | 3.04091100 | -2.06505900 | 3.25775100 |
| H | 2.60559700 | -3.21982200 | 1.49801200 |
| C | 3.48899700 | -0.83959000 | 3.76548100 |
| H | 4.18163100 | 1.14117400 | 3.26137300 |
| H | 2.78163700 | -2.87418600 | 3.93513600 |
| H | 3.58255200 | -0.69248800 | 4.83785000 |
| C | 3.68635600 | -0.02922100 | -1.62638900 |
| C | 5.06030800 | 0.27820300 | -1.65853600 |
| C | 2.79364000 | 0.83656500 | -2.27212700 |
| C | 5.52090200 | 1.43890200 | -2.28342800 |
| H | 5.77641800 | -0.39669400 | -1.19473800 |
| C | 3.25495600 | 1.99310100 | -2.90916100 |
| H | 1.73569600 | 0.59504100 | -2.29321000 |
| C | 4.61718500 | 2.30210400 | -2.91167300 |
| H | 6.58455000 | 1.66091000 | -2.29094300 |
| H | 2.54672800 | 2.65003200 | -3.40717800 |
| H | 4.97425500 | 3.19961500 | -3.40884700 |
| Cd | -0.57708000 | -0.50695600 | 0.00904100 |
| P | -2.80989200 | 0.09182100 | 1.02222300 |
| H | -0.40543000 | 2.73096700 | 0.61245700 |
| C | -3.95323700 | -1.14961000 | 0.25826100 |
| C | -3.66424600 | -2.52192700 | 0.38985200 |
| C | -5.18245600 | -0.78875600 | -0.32299200 |
| C | -4.56183700 | -3.49511800 | -0.05089700 |
| H | -2.72451700 | -2.83749100 | 0.83847300 |
| C | -6.07984600 | -1.76426400 | -0.76807100 |
| H | -5.44606400 | 0.25893600 | -0.42910000 |
| C | -5.77610500 | -3.12143900 | -0.63648200 |
| H | -4.30787200 | -4.54620900 | 0.05665100 |
| H | -7.02092500 | -1.45772000 | -1.21736900 |
| H | -6.47339900 | -3.87760600 | -0.98523300 |
| C | -3.14867200 | 1.65275900 | 0.06667800 |
| C | -3.34597300 | 2.83579300 | 0.80209200 |
| C | -3.17440200 | 1.73914400 | -1.33976200 |
| C | -3.54565600 | 4.06447500 | 0.15986400 |
| H | -3.35638600 | 2.78977500 | 1.88829100 |
| C | -3.38382400 | 2.96026400 | -1.98272800 |
| H | -3.03556000 | 0.84077100 | -1.93557600 |
| C | -3.56418700 | 4.13039400 | -1.23456400 |
| H | -3.69789700 | 4.96358800 | 0.75102000 |
| H | -3.39943900 | 3.00061700 | -3.06861500 |
| H | -3.72200300 | 5.08085400 | -1.73624200 |
| C | 0.34501900 | 1.90933900 | 2.75752700 |
| H | -0.63520600 | 1.44686200 | 2.89744100 |
| H | 1.10316700 | 1.21562200 | 3.13000700 |
| C | 0.43862700 | 3.26094300 | 3.46057200 |
| H | -0.31552600 | 3.96042000 | 3.08530300 |
| H | 0.26887900 | 3.12957000 | 4.53585700 |
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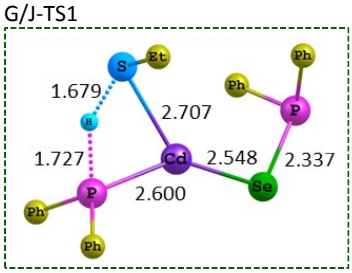


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| C | 3.85375800 | -1.18360200 | -0.29420100 |
| C | 3.51370700 | -1.07263800 | 1.06478800 |
| C | 4.45347700 | -2.37383700 | -0.74323700 |
| C | 3.76920900 | -2.12473500 | 1.94827800 |
| H | 3.05157500 | -0.16550500 | 1.44019900 |
| C | 4.69773100 | -3.43059700 | 0.13731200 |
| H | 4.73020600 | -2.47097900 | -1.79013400 |
| C | 4.35886000 | -3.30681800 | 1.48789400 |
| H | 3.50786200 | -2.01777200 | 2.99777500 |
| H | 5.16090900 | -4.34276800 | -0.22865900 |
| H | 4.55786900 | -4.12217200 | 2.17798700 |
| C | 3.53499000 | 1.67601900 | -0.54542900 |

| | | | |
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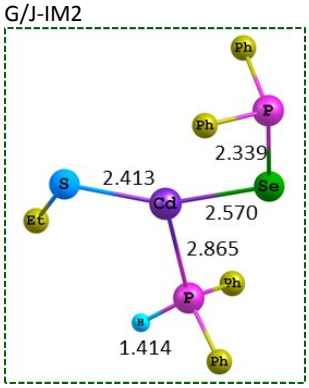
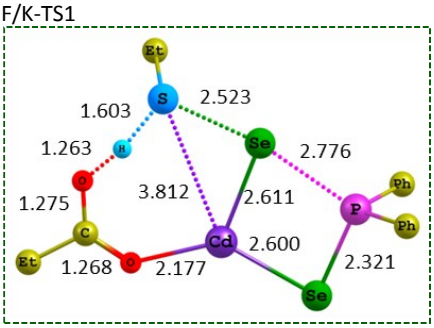
| C | 2.54659700 | 2.66206800 | -0.68843400 |
| C | 4.72264400 | 3.15900500 | 0.98549000 |
| H | 5.42585000 | 1.21552100 | 0.41006700 |
| C | 2.63738300 | 3.87419700 | 0.00448300 |
| H | 1.70443800 | 2.48567900 | -1.35048200 |
| C | 3.72129800 | 4.12626400 | 0.84732600 |
| H | 5.57449700 | 3.34383400 | 1.63436300 |
| H | 1.85676200 | 4.62025600 | -0.11845400 |
| H | 3.78999200 | 5.06632600 | 1.38727200 |
| Cd | -0.18046300 | -0.21740700 | -0.36755800 |
| P | -2.66377900 | -0.16445600 | 0.39923700 |
| H | -1.72158600 | -0.35825300 | 1.83299000 |
| C | -4.04646700 | -1.12161600 | -0.33645600 |
| C | -3.76428900 | -2.27094400 | -1.09636800 |
| C | -5.39123100 | -0.78413200 | -0.09572000 |
| C | -4.79749000 | -3.06618800 | -1.59662700 |
| H | -2.73271300 | -2.53992900 | -1.30959200 |
| C | -6.42186700 | -1.57758400 | -0.60333900 |
| H | -5.63254600 | 0.10071200 | 0.48575100 |
| C | -6.13033100 | -2.72211200 | -1.35262300 |
| H | -4.55998400 | -3.94731600 | -2.18619400 |
| H | -7.45499200 | -1.30092900 | -0.41136300 |
| H | -6.93432300 | -3.33661000 | -1.74711100 |
| C | -3.23747800 | 1.57998100 | 0.49414300 |
| C | -3.27463900 | 2.23432500 | 1.73767900 |
| C | -3.60822900 | 2.29699400 | -0.65905700 |
| C | -3.66876500 | 3.57358100 | 1.82613700 |
| H | -2.99768300 | 1.69548400 | 2.63932500 |
| C | -4.01410500 | 3.62894100 | -0.56727400 |
| H | -3.58034900 | 1.80947900 | -1.62974100 |
| C | -4.04138400 | 4.27229900 | 0.67572000 |
| H | -3.68985200 | 4.06499400 | 2.79481900 |
| H | -4.30128500 | 4.16744300 | -1.46615200 |
| H | -4.35166300 | 5.31105100 | 0.74450800 |
| C | -0.22139900 | -2.27369700 | 2.43613700 |
| H | -0.96256000 | -2.62300300 | 1.70510200 |
| H | 0.75231900 | -2.67194600 | 2.13973000 |
| C | -0.60305800 | -2.74507900 | 3.83911800 |
| H | -1.58352200 | -2.35772700 | 4.13344900 |
| H | -0.64582100 | -3.84091100 | 3.86931500 |
| H | 0.12928900 | -2.41035000 | 4.58034000 |
| S | -0.11951900 | -0.42755000 | 2.33009200 |

G/J-IM2




| | | | |
|---|---|---|---|
| Se | 0.53935200 | 0.11405400 | -1.72390100 |
| P | 2.86056100 | 0.01257000 | -1.99554500 |
| C | 3.36063000 | -1.39423800 | -0.89905200 |
| C | 3.51221300 | -1.30064400 | 0.49549900 |
| C | 3.58198200 | -2.63535200 | -1.51984900 |
| C | 3.86407300 | -2.42216000 | 1.24941300 |
| H | 3.36206400 | -0.34934800 | 0.99790400 |
| C | 3.93424600 | -3.75861800 | -0.76585400 |
| H | 3.47508100 | -2.72102800 | -2.59841400 |
| C | 4.07466800 | -3.65414100 | 0.62072000 |
| H | 3.96464800 | -2.33266400 | 2.32722500 |
| H | 4.10127900 | -4.71101300 | -1.26163400 |
| H | 4.34712100 | -4.52591200 | 1.20904100 |
| C | 3.54029000 | 1.46759600 | -1.06421000 |
| C | 4.92341600 | 1.48099100 | -0.79605100 |
| C | 2.79299500 | 2.61617000 | -0.76433500 |
| C | 5.53086100 | 2.59891300 | -0.22259900 |
| H | 5.53103500 | 0.60989600 | -1.02758700 |
| C | 3.40352100 | 3.73819000 | -0.19360800 |
| H | 1.72788900 | 2.63116900 | -0.97376000 |
| C | 4.77212100 | 3.73409700 | 0.08234100 |
| H | 6.59725200 | 2.58261300 | -0.01422500 |
| H | 2.80348800 | 4.61437800 | 0.03763900 |
| H | 5.24466900 | 4.60464200 | 0.52839400 |
| Cd | 0.04683200 | -0.21795900 | 0.77687600 |
| P | -2.80738400 | -0.07659600 | 0.57595900 |
| H | -3.52082900 | -0.24630800 | 1.78446700 |
| C | -3.62825300 | -1.37347100 | -0.43987800 |
| C | -2.99057600 | -1.84053100 | -1.60063100 |
| C | -4.87318700 | -1.91441000 | -0.07531600 |
| C | -3.59896300 | -2.81840100 | -2.39236100 |
| H | -2.01686100 | -1.45234300 | -1.88800700 |
| C | -5.47254500 | -2.89895600 | -0.86354000 |
| H | -5.37739300 | -1.56914000 | 0.82307000 |
| C | -4.83815900 | -3.34917300 | -2.02578900 |
| H | -3.09684100 | -3.16958300 | -3.28905700 |
| H | -6.43310200 | -3.31291100 | -0.57019400 |
| H | -5.30564500 | -4.11465400 | -2.63842600 |
| C | -3.52461700 | 1.53122400 | 0.04023100 |
| C | -4.66253000 | 2.07256300 | 0.66177600 |
| C | -2.90794200 | 2.24409700 | -1.00154500 |
| C | -5.18036800 | 3.29989100 | 0.24134600 |
| H | -5.14756200 | 1.53921300 | 1.47479500 |
| C | -3.43570400 | 3.46587800 | -1.42658900 |
| H | -2.01246200 | 1.85424200 | -1.47905900 |
| C | -4.57059800 | 3.99599200 | -0.80660500 |
| H | -6.05909900 | 3.70985600 | 0.73109700 |
| H | -2.95249900 | 4.00553800 | -2.23586800 |
| H | -4.97479300 | 4.94946900 | -1.13413500 |
| C | -0.82266900 | -0.12343300 | 4.07606100 |
| H | -1.11302900 | 0.90790400 | 3.85411200 |
| H | -1.65422800 | -0.77973900 | 3.80144700 |
| C | -0.51488200 | -0.26904200 | 5.56708400 |
| H | 0.30898900 | 0.38793000 | 5.86347900 |
| H | -1.39611300 | -0.00531300 | 6.16542900 |
| H | -0.23110200 | -1.29788500 | 5.81105200 |
| S | 0.67652000 | -0.57641400 | 3.07860200 |

F/K-TS1

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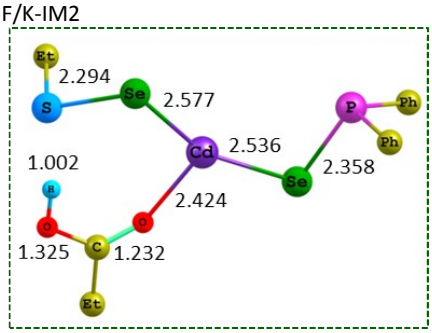
| Cd | -1.25530700 | -0.92552700 | -0.30135700 |
| Se | -0.44958800 | 1.20186100 | 0.98092600 |
| O | -4.55556100 | 0.16362200 | 0.41332800 |
| O | -3.34128800 | -1.51194600 | -0.51630500 |

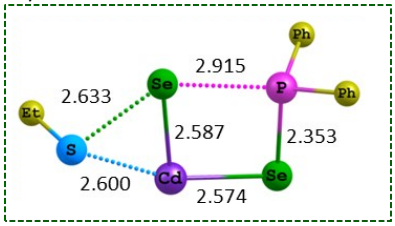
| | | | |
|---|---|---|---|
| C | -4.43152800 | -0.94663500 | -0.20054000 |
| C | -5.73490300 | -1.63965300 | -0.57081300 |
| H | -6.24509100 | -1.85659000 | 0.37651900 |
| H | -6.35955200 | -0.88921900 | -1.06954600 |
| C | -5.59084500 | -2.90244000 | -1.41970000 |
| H | -6.57768500 | -3.32800000 | -1.62836100 |
| H | -5.10381300 | -2.68661800 | -2.37515100 |
| H | -4.99183800 | -3.66027900 | -0.90752500 |
| Se | 1.02439300 | -1.89511200 | -1.08939100 |
| P | 1.84351600 | -0.01742200 | 0.00094600 |
| H | -3.65518000 | 0.86397400 | 0.95462300 |
| C | 2.81797600 | 0.91925700 | -1.24805900 |
| C | 2.31764600 | 2.15055200 | -1.69813600 |
| C | 4.02515700 | 0.43202000 | -1.77809400 |
| C | 3.01505200 | 2.88593700 | -2.66210900 |
| H | 1.38467500 | 2.53175100 | -1.29212600 |
| C | 4.71862700 | 1.16797000 | -2.73897500 |
| H | 4.42136500 | -0.52065300 | -1.43931800 |
| C | 4.21469500 | 2.39638500 | -3.18310400 |
| H | 2.62118300 | 3.83997700 | -3.00114000 |
| H | 5.65033200 | 0.78269700 | -3.14377600 |
| H | 4.75696100 | 2.96749000 | -3.93147100 |
| C | 3.11865600 | -0.59596400 | 1.19738300 |
| C | 3.14612600 | -1.90715800 | 1.69518600 |
| C | 4.02013600 | 0.35056000 | 1.71968800 |
| C | 4.06546900 | -2.26833800 | 2.68454300 |
| H | 2.45680600 | -2.64725000 | 1.30095100 |
| C | 4.93670800 | -0.01451200 | 2.70644600 |
| H | 4.01196700 | 1.37312100 | 1.35264700 |
| C | 4.96270600 | -1.32601800 | 3.19245600 |
| H | 4.07996800 | -3.29002000 | 3.05389000 |
| H | 5.62972800 | 0.72628200 | 3.09538900 |
| H | 5.67667000 | -1.60907200 | 3.96065000 |
| C | -3.08540200 | 3.34280800 | 0.53224000 |
| H | -2.96080900 | 2.96841100 | -0.48791400 |
| H | -2.30892100 | 4.09116000 | 0.71146900 |
| C | -4.48057800 | 3.93201900 | 0.74337200 |
| H | -4.64043900 | 4.76378000 | 0.04667800 |
| H | -5.25984400 | 3.18478700 | 0.56474600 |
| H | -4.60007900 | 4.31413600 | 1.76190900 |
| S | -2.74794900 | 1.95394700 | 1.70179300 |

F/K-IM2




| | | | |
|---|---|---|---|
| Cd | -1.04990200 | -0.16384300 | -0.13179500 |
| Se | -2.50327000 | -2.18886500 | 0.52157300 |
| O | -4.78916700 | 1.21129200 | -1.20075700 |
| O | -2.55388300 | 1.48040300 | -1.08516500 |
| C | -3.65927500 | 1.83558100 | -1.49733800 |
| C | -3.86355800 | 3.03666000 | -2.39243300 |
| H | -4.38936300 | 2.68075500 | -3.28749800 |
| H | -4.57621400 | 3.69726600 | -1.88257600 |
| C | -2.57422900 | 3.77272400 | -2.75359300 |
| H | -2.80030800 | 4.62665600 | -3.39909100 |
| H | -2.06404900 | 4.14248400 | -1.86008300 |
| H | -1.87778900 | 3.11711400 | -3.28333300 |
| Se | 1.10381300 | 1.14693000 | -0.40062900 |
| P | 2.48493700 | -0.41369300 | 0.70301400 |
| H | -4.63209400 | 0.42353000 | -0.60231300 |
| C | 3.80148800 | 0.74500200 | 1.30163500 |
| C | 3.67244700 | 1.22743500 | 2.61610600 |
| C | 4.90758300 | 1.15429100 | 0.53895800 |
| C | 4.61799100 | 2.10436300 | 3.15221900 |
| H | 2.82661500 | 0.91236900 | 3.22235400 |
| C | 5.85688600 | 2.02687400 | 1.07727800 |
| H | 5.03154100 | 0.78883700 | -0.47556300 |
| C | 5.71410400 | 2.50630300 | 2.38288200 |
| H | 4.50197300 | 2.46780100 | 4.16962200 |
| H | 6.70771700 | 2.33346300 | 0.47470400 |
| H | 6.45413500 | 3.18419600 | 2.79907700 |
| C | 3.37112800 | -1.30040100 | -0.66886300 |
| C | 3.31646900 | -0.96892400 | -2.03010100 |
| C | 4.12117300 | -2.42598300 | -0.27967500 |
| C | 4.00602700 | -1.73368100 | -2.97725800 |
| H | 2.72852600 | -0.11383900 | -2.34978300 |
| C | 4.81798400 | -3.18345900 | -1.22340700 |
| H | 4.16009300 | -2.71315900 | 0.76893500 |
| C | 4.76096600 | -2.83928300 | -2.57789700 |
| H | 3.95189200 | -1.46205700 | -4.02822300 |
| H | 5.39469200 | -4.04666800 | -0.90252100 |
| H | 5.29437000 | -3.43277900 | -3.31518800 |
| C | -4.60155900 | -0.53222200 | 2.39192100 |
| H | -3.85482600 | 0.26711500 | 2.41938900 |
| H | -4.29807200 | -1.31094900 | 3.09586100 |
| C | -5.99796000 | -0.00010300 | 2.71852800 |
| H | -5.99682200 | 0.43746600 | 3.72306000 |
| H | -6.31074900 | 0.77823500 | 2.01474100 |
| H | -6.74436500 | -0.80021200 | 2.69900800 |
| S | -4.60410800 | -1.28541000 | 0.70511700 |

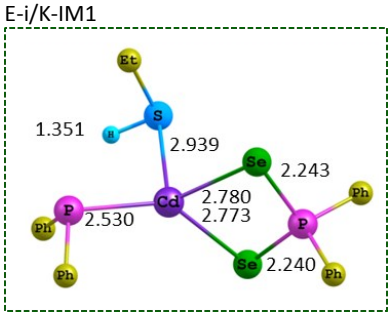
K-i/K-TS1




| | | | |
|---|---|---|---|
| Cd | 1.86277100 | -0.83459400 | 0.98128400 |
| C | 4.66713800 | 1.01020500 | -0.30932900 |
| H | 3.92425700 | 1.66190700 | 0.15878200 |
| H | 5.47552700 | 0.83699800 | 0.40910100 |
| C | 5.19911800 | 1.63214500 | -1.59875300 |
| H | 5.94736200 | 0.98810900 | -2.07107200 |
| H | 4.38778100 | 1.79942800 | -2.31367600 |
| H | 5.66774400 | 2.59923000 | -1.38003000 |
| P | -1.16435600 | 0.03269900 | -0.20604400 |
| Se | -0.52672000 | -0.71433600 | 1.93186100 |
| Se | 1.46788800 | -0.05946900 | -1.45529500 |
| C | -1.85893300 | 1.71342300 | 0.08927700 |
| C | -1.19041600 | 2.80756500 | -0.48132400 |
| C | -3.00458000 | 1.94099100 | 0.87229200 |
| C | -1.66328400 | 4.10867200 | -0.27978500 |
| H | -0.29915600 | 2.63948500 | -1.08014900 |
| C | -3.47264500 | 3.23936800 | 1.07318300 |
| H | -3.52927800 | 1.10358700 | 1.32250700 |
| C | -2.80320700 | 4.32592600 | 0.49679300 |
| H | -1.14063400 | 4.94763500 | -0.73047300 |
| H | -4.35827600 | 3.40483300 | 1.68039800 |
| H | -3.17095100 | 5.33596200 | 0.65446000 |
| C | -2.64956000 | -0.97514100 | -0.63274400 |

| | | | |
|---|---|---|---|
| C | -3.60654200 | -0.43796100 | -1.51453100 |
| C | -2.77329200 | -2.31680700 | -0.23604100 |
| C | -4.66802500 | -1.22125300 | -1.97168900 |
| H | -3.52898200 | 0.59443800 | -1.84219300 |
| C | -3.83740000 | -3.09645800 | -0.69564300 |
| H | -2.04545100 | -2.74699700 | 0.44448900 |
| C | -4.78852400 | -2.55285300 | -1.56331700 |
| H | -5.40126300 | -0.78802500 | -2.64629000 |
| H | -3.92293400 | -4.12958300 | -0.37047900 |
| H | -5.61564800 | -3.16064100 | -1.91872300 |
| S | 3.89771500 | -0.64211600 | -0.62632500 |

E-i/K-IM1




| | | | |
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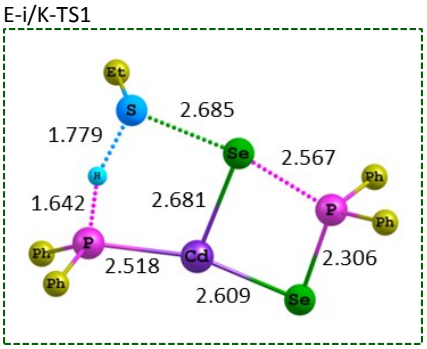
| Cd | -0.84790900 | -0.29704100 | -0.41588400 |
| P | -3.22263200 | 0.36646800 | -0.98210600 |
| C | -4.07496400 | -0.31514500 | 0.52567200 |
| C | -3.81005700 | 0.09045900 | 1.84880000 |
| C | -5.01579300 | -1.34294000 | 0.32931100 |
| C | -4.45688700 | -0.51097100 | 2.92954400 |
| H | -3.09179600 | 0.88484600 | 2.03229000 |
| C | -5.65651300 | -1.95759500 | 1.41244600 |
| H | -5.25855900 | -1.65239800 | -0.68454900 |
| C | -5.37931600 | -1.54321400 | 2.71672000 |
| H | -4.23392100 | -0.18073900 | 3.94075100 |
| H | -6.38075500 | -2.74802500 | 1.23306500 |
| H | -5.87787200 | -2.01382200 | 3.55940500 |
| C | -3.21889100 | 2.19722100 | -0.69392400 |
| C | -4.27978000 | 2.85278300 | -0.04128800 |
| C | -2.21116900 | 2.99406000 | -1.27147000 |
| C | -4.32136800 | 4.24738800 | 0.04305800 |
| H | -5.08171900 | 2.27251100 | 0.40525000 |
| C | -2.25691000 | 4.38714700 | -1.19455200 |
| H | -1.37553900 | 2.52236200 | -1.78399800 |
| C | -3.31164400 | 5.02369300 | -0.53227300 |
| H | -5.15029000 | 4.72641300 | 0.55801800 |
| H | -1.46161400 | 4.97445700 | -1.64614400 |
| H | -3.34533400 | 6.10742400 | -0.46603700 |
| P | 2.44842200 | 0.05750000 | 0.11638900 |
| Se | 0.89157400 | -0.01643000 | 1.72552000 |
| Se | 1.51027100 | -0.30204100 | -1.88872800 |
| C | 3.77588800 | -1.16511200 | 0.45491000 |
| C | 4.60066700 | -0.97454800 | 1.57669400 |
| C | 3.95461800 | -2.29391300 | -0.35364100 |
| C | 5.59687600 | -1.90292600 | 1.87719800 |
| H | 4.46652000 | -0.10528700 | 2.21398600 |
| C | 4.95464700 | -3.22223500 | -0.04724100 |
| H | 3.31614800 | -2.44149900 | -1.21913200 |
| C | 5.77557800 | -3.02912700 | 1.06557900 |
| H | 6.23131600 | -1.74885900 | 2.74523300 |
| H | 5.08947600 | -4.09391700 | -0.68116200 |
| H | 6.55169300 | -3.75142000 | 1.30214500 |
| C | 3.31407800 | 1.67825900 | 0.11853300 |
| C | 4.45468900 | 1.83889000 | -0.68680900 |
| C | 2.83810700 | 2.75937200 | 0.87010600 |
| C | 5.11214300 | 3.06790600 | -0.73052100 |
| H | 4.82934600 | 1.00879000 | -1.27876100 |
| C | 3.50002500 | 3.99033300 | 0.82061800 |
| H | 1.95608400 | 2.63645200 | 1.49087500 |
| C | 4.63543600 | 4.14668400 | 0.02324200 |
| H | 5.99396700 | 3.18398400 | -1.35395600 |
| H | 3.12523200 | 4.82360700 | 1.40797700 |
| H | 5.14823900 | 5.10362900 | -0.01330500 |
| C | -2.58251200 | -4.89604700 | -2.11735000 |
| H | -3.50975600 | -4.91285100 | -1.53533600 |
| H | -1.95265900 | -5.72386300 | -1.77832000 |
| H | -2.84319200 | -5.06877700 | -3.16831100 |
| C | -1.86317600 | -3.55679500 | -1.97755800 |
| H | -0.93702200 | -3.54301000 | -2.55927600 |
| H | -2.48439500 | -2.72636000 | -2.32274000 |
| S | -1.31095600 | -3.19502700 | -0.24937700 |
| H | -2.54089400 | -3.06851900 | 0.29447800 |

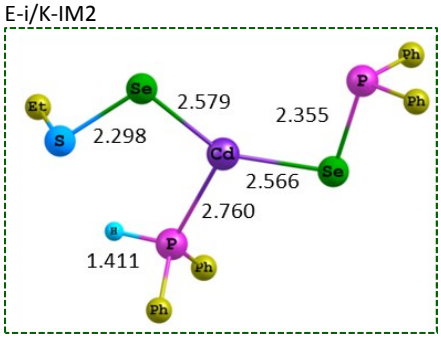
E-i/K-TS1




| | | | |
|---|---|---|---|
| Cd | 0.48662400 | 0.16453500 | -0.73225900 |
| Se | -0.81579100 | -0.15194600 | 1.58945600 |
| Se | -1.68196400 | 0.32269200 | -2.17354200 |
| P | -2.71247900 | 0.04591400 | -0.12890100 |
| C | -3.79660700 | -1.43263500 | -0.26631700 |
| C | -3.47833300 | -2.57855700 | 0.47704400 |
| C | -4.91687200 | -1.44922700 | -1.11541800 |
| C | -4.27296300 | -3.72538100 | 0.37682800 |
| H | -2.61205200 | -2.56873900 | 1.13246900 |
| C | -5.70634100 | -2.59488600 | -1.21293700 |
| H | -5.17152300 | -0.56856600 | -1.69778300 |
| C | -5.38564700 | -3.73545400 | -0.46674900 |
| H | -4.02132600 | -4.60659100 | 0.96021100 |
| H | -6.57013800 | -2.59934600 | -1.87185500 |
| H | -6.00261900 | -4.62631300 | -0.54452900 |
| C | -3.88799500 | 1.44023600 | 0.10311100 |
| C | -3.71913800 | 2.67294900 | -0.54479700 |
| C | -4.91627000 | 1.30176500 | 1.05356400 |
| C | -4.57020900 | 3.74339700 | -0.25686900 |
| H | -2.92952100 | 2.79047900 | -1.28025400 |
| C | -5.76372000 | 2.37356800 | 1.33731100 |
| H | -5.05935100 | 0.35737900 | 1.57067800 |
| C | -5.59389400 | 3.59788300 | 0.68267100 |
| H | -4.43267200 | 4.68998900 | -0.77204800 |
| H | -6.55626500 | 2.25104600 | 2.07018000 |
| H | -6.25486100 | 4.43094800 | 0.90429600 |
| H | 2.45122100 | -0.14704200 | 1.57032900 |
| C | 1.66561500 | -2.16700700 | 3.06192900 |
| H | 1.84060800 | -2.51811100 | 2.03742100 |
| H | 0.71619300 | -2.59706500 | 3.39320800 |
| C | 2.80881500 | -2.60009800 | 3.98156300 |
| H | 2.90093400 | -3.69383200 | 3.98377700 |
| H | 3.76518500 | -2.18031500 | 3.65253800 |
| H | 2.63265100 | -2.26882700 | 5.00976600 |
| P | 2.89305200 | 0.09309200 | 0.00705200 |
| C | 4.00011600 | -1.14378300 | -0.76232200 |
| C | 3.50953300 | -2.06328700 | -1.70498200 |
| C | 5.34485000 | -1.24288600 | -0.35597900 |

| | | | |
|---|---|---|---|
| C | 4.33802200 | -3.06186500 | -2.22418100 |
| H | 2.47914800 | -1.99660700 | -2.04437700 |
| C | 6.17289400 | -2.23319200 | -0.88566000 |
| H | 5.74339300 | -0.54442400 | 0.37425100 |
| C | 5.67192400 | -3.14832400 | -1.81828900 |
| H | 3.94145700 | -3.76350000 | -2.95251900 |
| H | 7.20887300 | -2.29424600 | -0.56426000 |
| H | 6.31778500 | -3.92028000 | -2.22635200 |
| C | 3.75568500 | 1.70798500 | -0.02246300 |
| C | 4.55602500 | 2.10929700 | -1.10644400 |
| C | 3.57779300 | 2.58934700 | 1.05922100 |
| C | 5.16980700 | 3.36304100 | -1.10420800 |
| H | 4.70253800 | 1.44099500 | -1.95009100 |
| C | 4.18489900 | 3.84804600 | 1.05055600 |
| H | 2.97383300 | 2.29183200 | 1.91171900 |
| C | 4.98299400 | 4.23773100 | -0.02829400 |
| H | 5.78906500 | 3.65898500 | -1.94647300 |
| H | 4.03894700 | 4.51863900 | 1.89257100 |
| H | 5.45771700 | 5.21465500 | -0.03115500 |
| S | 1.44512600 | -0.33695500 | 3.02537600 |

E-i/K-IM2

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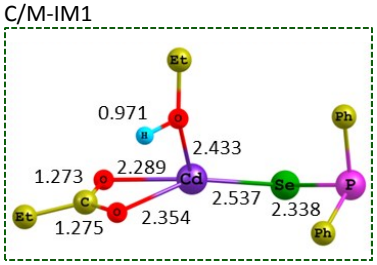
| Cd | 0.46443600 | -0.75568300 | -0.19786500 |
| Se | 1.16134600 | -3.13427800 | -0.91042100 |
| Se | -1.49328900 | 0.74889500 | 0.49909800 |
| P | -3.22648700 | -0.69909700 | -0.16973400 |
| C | -4.19210400 | 0.40413800 | -1.30393900 |
| C | -4.23614400 | 0.04651900 | -2.66093900 |
| C | -4.85653600 | 1.57210300 | -0.89098200 |
| C | -4.92874700 | 0.83463700 | -3.58679900 |
| H | -3.72733400 | -0.85480400 | -2.99401900 |
| C | -5.54857000 | 2.35826000 | -1.81264500 |
| H | -4.83266900 | 1.86507100 | 0.15465400 |
| C | -5.58628700 | 1.99159200 | -3.16373900 |
| H | -4.95570400 | 0.54189600 | -4.63286900 |
| H | -6.05878300 | 3.25787500 | -1.47871400 |
| H | -6.12695900 | 2.60483600 | -3.87942700 |
| C | -4.33157000 | -0.72372400 | 1.32270000 |
| C | -3.85332400 | -0.57568200 | 2.63377900 |
| C | -5.68418600 | -1.07130000 | 1.13894200 |
| C | -4.70411200 | -0.75610600 | 3.72928900 |
| H | -2.81513800 | -0.30508800 | 2.79893200 |
| C | -6.53255700 | -1.24886900 | 2.23310200 |
| H | -6.08206900 | -1.19764200 | 0.13555100 |
| C | -6.04572100 | -1.09167700 | 3.53503600 |
| H | -4.31391900 | -0.62951900 | 4.73572900 |
| H | -7.57458400 | -1.50904800 | 2.06730800 |
| H | -6.70576600 | -1.22996500 | 4.38679100 |
| H | 3.82209900 | 0.26951800 | -0.74616900 |
| C | 3.85610200 | -2.57665000 | -2.62489800 |
| H | 3.41907500 | -1.60673100 | -2.88483000 |
| H | 3.38942200 | -3.33796300 | -3.25546700 |
| C | 5.37452400 | -2.56439100 | -2.81274600 |
| H | 5.61727700 | -2.33813000 | -3.85725900 |
| H | 5.85358900 | -1.80552700 | -2.18457800 |
| H | 5.81381600 | -3.53616700 | -2.56609800 |
| P | 2.74295000 | 0.78976300 | -0.00131800 |
| C | 2.69693200 | 2.52156500 | -0.60464800 |
| C | 1.46251900 | 3.17098700 | -0.76160300 |
| C | 3.88264200 | 3.20730800 | -0.92559800 |
| C | 1.41616700 | 4.49028300 | -1.22454100 |
| H | 0.53471800 | 2.65358100 | -0.53217500 |
| C | 3.83128300 | 4.52123400 | -1.39176000 |
| H | 4.84487800 | 2.71666600 | -0.80666600 |
| C | 2.59700900 | 5.16480200 | -1.54037400 |
| H | 0.45528500 | 4.98247900 | -1.34184200 |
| H | 4.75181300 | 5.04173600 | -1.63995200 |
| H | 2.55874600 | 6.18743700 | -1.90466000 |
| C | 3.49638700 | 0.84185200 | 1.67703300 |
| C | 3.33046500 | 1.95100800 | 2.51912100 |
| C | 4.17439500 | -0.29373200 | 2.15167200 |
| C | 3.84866500 | 1.92860400 | 3.81718700 |
| H | 2.80705500 | 2.83452000 | 2.16577600 |
| C | 4.69389500 | -0.30694000 | 3.44776700 |
| H | 4.29495400 | -1.16449600 | 1.51177900 |
| C | 4.53158700 | 0.80250400 | 4.28368600 |
| H | 3.71744300 | 2.79346300 | 4.46120100 |
| H | 5.22243500 | -1.18661500 | 3.80374400 |
| H | 4.93342800 | 0.78796000 | 5.29261200 |
| S | 3.45292400 | -2.96309600 | -0.86660700 |

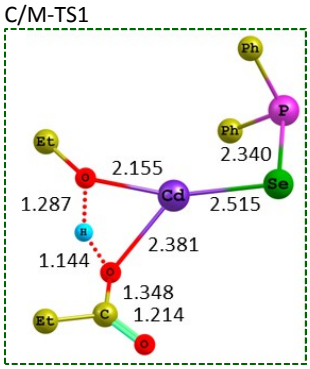
C/M-IM1




| | | | |
|---|---|---|---|
| Cd | -1.24653900 | -0.08600500 | 0.77845300 |
| P | 2.55248300 | 0.83394700 | 0.94848400 |
| Se | 0.71529500 | 0.37258600 | 2.31961900 |
| C | 2.87403800 | -0.72736500 | -0.00012800 |
| C | 2.72416100 | -1.98648100 | 0.60753900 |
| C | 3.48431700 | -0.66826400 | -1.26747700 |
| C | 3.15683300 | -3.14923000 | -0.03630100 |
| H | 2.26244300 | -2.05523100 | 1.58839300 |
| C | 3.91024100 | -1.83207100 | -1.91310600 |
| H | 3.62767300 | 0.28952500 | -1.75881900 |
| C | 3.74953700 | -3.07842800 | -1.30079300 |
| H | 3.03372900 | -4.11094500 | 0.45517100 |
| H | 4.37192700 | -1.76141100 | -2.89437500 |
| H | 4.08796200 | -3.98212000 | -1.79985600 |
| C | 1.89065000 | 1.97736200 | -0.34822700 |
| C | 2.24019800 | 3.33205100 | -0.22298100 |
| C | 1.05499900 | 1.59133400 | -1.41144400 |
| C | 1.76131300 | 4.28186700 | -1.13108500 |
| H | 2.88731600 | 3.64404100 | 0.59276000 |
| C | 0.57790600 | 2.53899800 | -2.31885400 |
| H | 0.77734000 | 0.54844700 | -1.53763200 |
| C | 0.92838100 | 3.88703200 | -2.18025500 |
| H | 2.03947900 | 5.32589100 | -1.01724100 |
| H | -0.07212200 | 2.22630300 | -3.13147600 |
| H | 0.55339700 | 4.62246200 | -2.88648500 |
| C | -0.57710600 | -2.74229300 | -1.59300000 |
| H | -0.39701500 | -2.79615500 | -2.67373100 |
| H | 0.37452400 | -2.91567600 | -1.08650100 |
| C | -1.63141000 | -3.75098900 | -1.15825100 |
| H | -1.80841000 | -3.69443400 | -0.07951700 |
| H | -2.58470500 | -3.58149400 | -1.67220900 |

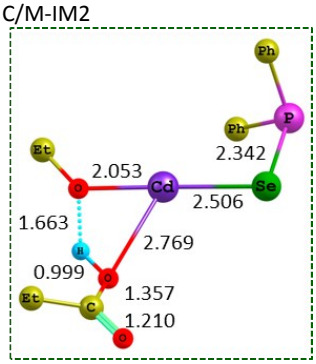
| | | | |
|---|---|---|---|
| H | -1.29852700 | -4.76691700 | -1.39929500 |
| O | -3.45869000 | -0.54629400 | 1.14285800 |
| O | -2.94418000 | 0.49298700 | -0.74584300 |
| C | -3.81249000 | 0.00616200 | 0.05152600 |
| C | -5.29448500 | 0.08402700 | -0.27413600 |
| H | -5.70805000 | -0.92161600 | -0.13345100 |
| H | -5.74908800 | 0.69565200 | 0.51572600 |
| C | -5.63175300 | 0.64199200 | -1.65739500 |
| H | -6.71739600 | 0.68643700 | -1.79381900 |
| H | -5.22559000 | 1.64876800 | -1.78672400 |
| H | -5.21597400 | 0.01567500 | -2.45289600 |
| H | -1.74335000 | -1.10037100 | -1.71309500 |
| O | -0.93474500 | -1.38418700 | -1.25561200 |

C/M-TS1




| | | | |
|---|---|---|---|
| Cd | -0.99597500 | -0.06758400 | -0.35423200 |
| P | 2.57354400 | 0.86433200 | -1.18734400 |
| Se | 0.48727500 | 0.70157100 | -2.23406600 |
| C | 2.16548200 | 1.73087700 | 0.40067100 |
| C | 1.72714900 | 1.08852300 | 1.57227700 |
| C | 2.29298300 | 3.13010500 | 0.40812900 |
| C | 1.41330500 | 1.82871100 | 2.71520800 |
| H | 1.65467300 | 0.00471200 | 1.60198200 |
| C | 1.97246200 | 3.87132800 | 1.54888200 |
| H | 2.63810000 | 3.64129100 | -0.48690400 |
| C | 1.53046100 | 3.22271400 | 2.70494500 |
| H | 1.08333700 | 1.31689600 | 3.61530200 |
| H | 2.07207900 | 4.95293700 | 1.53444300 |
| H | 1.28487300 | 3.79680200 | 3.59367400 |
| C | 2.99525500 | -0.84189200 | -0.59519100 |
| C | 4.06450600 | -0.96712300 | 0.31428800 |
| C | 2.42859400 | -2.01137300 | -1.12399500 |
| C | 4.52862300 | -2.22425100 | 0.70350500 |
| H | 4.53548700 | -0.07845700 | 0.72696100 |
| C | 2.89843800 | -3.27153800 | -0.73681300 |
| H | 1.62079500 | -1.93841400 | -1.84571500 |
| C | 3.94543500 | -3.38346300 | 0.17975900 |
| H | 5.34845200 | -2.29795200 | 1.41276600 |
| H | 2.44263300 | -4.16430100 | -1.15622400 |
| H | 4.30908300 | -4.36199700 | 0.47985600 |
| C | -1.27751900 | -1.48953600 | 2.60726500 |
| H | -0.80142600 | -0.60823100 | 3.06432100 |
| H | -2.12984400 | -1.76225200 | 3.24624700 |
| C | -0.29025600 | -2.64938900 | 2.54373000 |
| H | -0.77065800 | -3.53833600 | 2.12256500 |
| H | 0.57269300 | -2.40133300 | 1.91526800 |
| H | 0.07973500 | -2.89651500 | 3.54591600 |
| O | -3.24263800 | 0.32954600 | 0.32861100 |
| O | -4.71217500 | 0.67394200 | -1.32296800 |
| C | -4.46323700 | 0.20808700 | -0.22965200 |
| C | -5.47713400 | -0.52451800 | 0.64005800 |
| H | -5.04979200 | -1.50209000 | 0.90209000 |
| H | -5.55428100 | 0.02788700 | 1.58595100 |
| C | -6.84859200 | -0.68261600 | -0.01583600 |
| H | -7.53436500 | -1.20742200 | 0.65720300 |
| H | -7.27990600 | 0.29182400 | -0.26041600 |
| H | -6.77587500 | -1.25058700 | -0.94761100 |
| H | -2.81174100 | -0.44111200 | 1.05582600 |
| O | -1.78687200 | -1.17418500 | 1.31743800 |

C/M-IM2




| | | | |
|---|---|---|---|
| Cd | -0.89761100 | 0.04535300 | -0.10346400 |
| P | 2.62000900 | 0.08500300 | -1.48387800 |
| Se | 0.44016700 | -0.43311900 | -2.16729500 |
| C | 2.35930100 | 1.56145300 | -0.39223900 |
| C | 2.14644400 | 1.50067900 | 0.99664700 |
| C | 2.37596800 | 2.82151000 | -1.01618100 |
| C | 1.94347500 | 2.66925200 | 1.73721700 |
| H | 2.16100000 | 0.54160100 | 1.50641200 |
| C | 2.16392400 | 3.98779000 | -0.27720600 |
| H | 2.54886000 | 2.88694100 | -2.08736000 |
| C | 1.94670100 | 3.91500200 | 1.10206800 |
| H | 1.78852200 | 2.60528600 | 2.81084900 |
| H | 2.17510800 | 4.95203000 | -0.77739800 |
| H | 1.78789500 | 4.82165600 | 1.67869000 |
| C | 3.10465100 | -1.21819900 | -0.25596300 |
| C | 4.33292000 | -1.03370200 | 0.40986900 |
| C | 2.41474200 | -2.42358900 | -0.06255900 |
| C | 4.83514300 | -2.01224700 | 1.26837500 |
| H | 4.90082900 | -0.11822900 | 0.26115500 |
| C | 2.92324400 | -3.40791700 | 0.79307500 |
| H | 1.48240600 | -2.60072900 | -0.58960900 |
| C | 4.12983400 | -3.20497800 | 1.46475200 |
| H | 5.77956400 | -1.84551700 | 1.77902900 |
| H | 2.37250800 | -4.33474700 | 0.92891900 |
| H | 4.52324300 | -3.96969300 | 2.12827200 |
| C | -1.57776600 | 0.64418200 | 2.88447200 |
| H | -0.91155700 | 1.52093500 | 2.91370000 |
| H | -2.45922900 | 0.89625400 | 3.49303200 |
| C | -0.87064300 | -0.56473800 | 3.49427700 |
| H | -1.53260600 | -1.43712100 | 3.50022200 |
| H | 0.02903700 | -0.82488400 | 2.92147500 |
| H | -0.56146100 | -0.35799800 | 4.52631400 |
| O | -3.63202700 | 0.38888200 | -0.37407800 |
| O | -5.21244400 | -0.44822000 | -1.70374600 |
| C | -4.84884300 | -0.17504600 | -0.58296500 |
| C | -5.67493700 | -0.40165800 | 0.67695100 |
| H | -5.06793000 | -0.98949200 | 1.37870700 |
| H | -5.82169600 | 0.57571900 | 1.15679300 |
| C | -7.01667200 | -1.08161100 | 0.40656500 |
| H | -7.57220100 | -1.21098200 | 1.34083800 |
| H | -7.62462500 | -0.48701400 | -0.28034300 |
| H | -6.87319600 | -2.06467800 | -0.05035000 |
| H | -3.37929400 | 0.48547500 | 0.58778300 |
| O | -2.03685700 | 0.40585600 | 1.56562700 |

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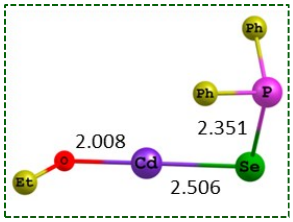


| | | | |
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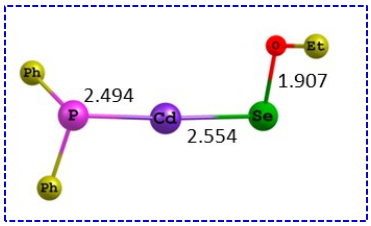
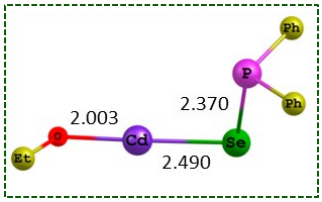
| Se | -0.37794100 | -1.18787400 | -1.94308200 |
| P | -1.81292700 | 0.54461900 | -1.26100200 |
| C | -0.63063400 | 1.79984800 | -0.57713800 |
| C | -0.10932500 | 1.76949400 | 0.72972300 |
| C | -0.22344800 | 2.83015800 | -1.44139400 |
| C | 0.80698900 | 2.73624800 | 1.15292300 |
| H | -0.43530800 | 1.00297000 | 1.42791300 |
| C | 0.69496500 | 3.79573400 | -1.01876200 |
| H | -0.62399200 | 2.87216600 | -2.45102700 |
| C | 1.21366000 | 3.74976000 | 0.27819500 |
| H | 1.19866500 | 2.69843500 | 2.16553000 |
| H | 1.00059300 | 4.58426400 | -1.70066800 |
| H | 1.92553100 | 4.50074700 | 0.60849000 |
| C | -2.63852900 | -0.06461500 | 0.28469900 |
| C | -3.37166000 | 0.87878900 | 1.03169100 |
| C | -2.70377200 | -1.41352800 | 0.66239700 |
| C | -4.12153200 | 0.48487300 | 2.14049900 |
| H | -3.35316700 | 1.92945000 | 0.75209700 |
| C | -3.46163400 | -1.80799700 | 1.77087500 |
| H | -2.16222200 | -2.15955000 | 0.08911500 |
| C | -4.16849600 | -0.86236200 | 2.51563100 |
| H | -4.67104700 | 1.22985100 | 2.70933900 |
| H | -3.49558100 | -2.85780400 | 2.04912200 |
| H | -4.75479900 | -1.16972000 | 3.37679200 |
| Cd | 1.43043100 | -1.04714600 | -0.21380800 |
| C | 3.96036600 | -0.16843000 | 1.20881700 |
| H | 4.57454800 | -0.25098200 | 0.29574200 |
| H | 3.61040400 | 0.87653900 | 1.26582800 |
| C | 4.82986600 | -0.47583100 | 2.42563300 |
| H | 5.20909800 | -1.50166800 | 2.37392400 |
| H | 5.68451400 | 0.21087400 | 2.47431100 |
| H | 4.24714800 | -0.37429500 | 3.34723500 |
| O | 2.87099500 | -1.07783600 | 1.18451600 |

M-i




| | | | |
|---|---|---|---|
| Cd | 0.73625700 | -0.18192100 | 0.03923500 |
| Se | 3.06748500 | -0.33910600 | -0.99187100 |
| C | 4.61552200 | 0.41168100 | 1.24799200 |
| H | 4.17773300 | -0.46313400 | 1.75251000 |
| H | 4.69514900 | 1.22163300 | 1.98568300 |
| C | 5.99072700 | 0.07345300 | 0.68414900 |
| H | 6.43022900 | 0.94808000 | 0.19410400 |
| H | 6.66168000 | -0.24837000 | 1.48974000 |
| H | 5.92744900 | -0.73992200 | -0.04643900 |
| P | -1.44250800 | 0.02933100 | 1.23376500 |
| C | -2.15308800 | 1.53715200 | 0.41453000 |
| C | -2.74889400 | 2.49247300 | 1.25718200 |
| C | -2.11125900 | 1.80630700 | -0.96720900 |
| C | -3.28620100 | 3.67589300 | 0.73899900 |
| H | -2.79130400 | 2.30657000 | 2.32700100 |
| C | -2.64843800 | 2.98532700 | -1.48719000 |
| H | -1.66029000 | 1.08650000 | -1.64572200 |
| C | -3.23683400 | 3.92536700 | -0.63380400 |
| H | -3.74046200 | 4.39985800 | 1.40974800 |
| H | -2.60199500 | 3.17278100 | -2.55641600 |
| H | -3.64973400 | 4.84520600 | -1.03797100 |
| C | -2.36771700 | -1.38932500 | 0.47030000 |
| C | -3.51162900 | -1.24539600 | -0.33247800 |
| C | -1.95887900 | -2.69314900 | 0.81623300 |
| C | -4.21321300 | -2.36847700 | -0.78457200 |
| H | -3.86316300 | -0.25608100 | -0.60585400 |
| C | -2.65343100 | -3.81200300 | 0.35698500 |
| H | -1.09095000 | -2.83545900 | 1.45770100 |
| C | -3.78712900 | -3.65509800 | -0.44883800 |
| H | -5.09641000 | -2.23154000 | -1.40299800 |
| H | -2.31346400 | -4.80640100 | 0.63347900 |
| H | -4.33172800 | -4.52469800 | -0.80488500 |
| O | 3.70910600 | 0.93519600 | 0.27381500 |

M-ii

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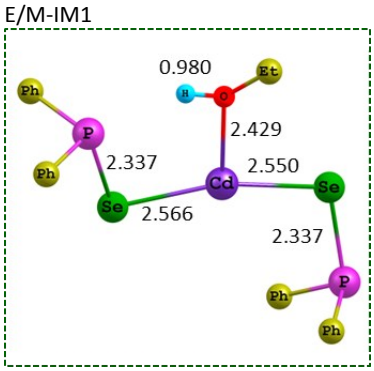
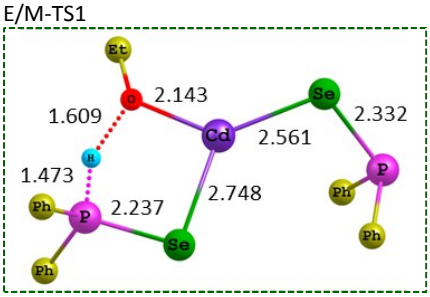
| P | -0.95546900 | 0.00948800 | 0.65150900 |
| C | -2.15114200 | -1.38032500 | 0.41472300 |
| C | -3.18543100 | -1.37475100 | -0.53747000 |
| C | -1.98742000 | -2.51057800 | 1.23193500 |
| C | -4.03410600 | -2.47443400 | -0.66581000 |
| H | -3.32774500 | -0.50856400 | -1.17715600 |
| C | -2.83823200 | -3.61326300 | 1.10345300 |
| H | -1.19259100 | -2.52677900 | 1.97357100 |
| C | -3.86218600 | -3.59646400 | 0.15401600 |
| H | -4.82880800 | -2.45846100 | -1.40658900 |
| H | -2.70114000 | -4.47943800 | 1.74466500 |
| H | -4.52479600 | -4.45126500 | 0.05172700 |
| C | -2.05802400 | 1.48403300 | 0.42979800 |
| C | -3.21335200 | 1.55966400 | 1.23223900 |
| C | -1.72245100 | 2.59057700 | -0.36521700 |
| C | -4.01385000 | 2.70295000 | 1.22584800 |
| H | -3.49611000 | 0.71991900 | 1.86140800 |
| C | -2.52576200 | 3.73570500 | -0.36951200 |
| H | -0.83956600 | 2.55438700 | -0.99545600 |
| C | -3.67316100 | 3.79713300 | 0.42380000 |
| H | -4.90503400 | 2.73680400 | 1.84651000 |
| H | -2.25261000 | 4.57768200 | -0.99978700 |
| H | -4.29684400 | 4.68646100 | 0.41784800 |
| Cd | 2.45977900 | -0.16038200 | -0.33862600 |
| C | 5.05364500 | 0.65161500 | 1.01356900 |
| H | 5.24437100 | 1.45378500 | 0.28048500 |
| H | 4.52914100 | 1.11383900 | 1.86682700 |
| C | 6.38630800 | 0.08202700 | 1.49234200 |
| H | 6.93541000 | -0.36013500 | 0.65459700 |
| H | 7.00524800 | 0.87018100 | 1.93941100 |
| H | 6.22010500 | -0.69863200 | 2.24184800 |
| O | 4.28826100 | -0.40081000 | 0.44341800 |

E/M-IM1




| | | | |
|---|---|---|---|
| Se | -2.80693800 | -0.97844400 | 1.86959000 |
| P | -4.45439300 | -0.45504400 | 0.29679000 |
| C | -3.80988400 | -1.20271700 | -1.27173600 |
| C | -2.88597300 | -0.58414300 | -2.13229800 |
| C | -4.28253800 | -2.48458500 | -1.60092900 |
| C | -2.44015600 | -1.23545100 | -3.28489900 |
| H | -2.52184700 | 0.41522900 | -1.91170700 |
| C | -3.83304800 | -3.13916200 | -2.75110800 |
| H | -5.00317800 | -2.97269200 | -0.94955800 |
| C | -2.91010100 | -2.51596500 | -3.59555400 |
| H | -1.72393900 | -0.74339800 | -3.93712100 |
| H | -4.20713700 | -4.13125700 | -2.98844700 |
| H | -2.56095200 | -3.02180300 | -4.49133700 |
| C | -4.27654200 | 1.35975700 | -0.04968700 |
| C | -4.95218300 | 1.87888600 | -1.17209400 |
| C | -3.65565600 | 2.26061200 | 0.82843900 |
| C | -4.97833400 | 3.25184100 | -1.42059000 |
| H | -5.45581900 | 1.20734100 | -1.86286300 |
| C | -3.68649400 | 3.63751400 | 0.58112800 |
| H | -3.14678300 | 1.88322700 | 1.71015400 |
| C | -4.34313100 | 4.13865200 | -0.54436000 |
| H | -5.49608000 | 3.62861200 | -2.29854100 |
| H | -3.19418600 | 4.31662800 | 1.27222900 |
| H | -4.36468800 | 5.20754900 | -0.73674800 |
| Cd | -0.58797000 | -0.52961400 | 0.69576100 |
| Se | 1.18618000 | -0.13906500 | -1.11579400 |
| H | 1.74167500 | -0.13411300 | 2.31949300 |
| C | 0.62780800 | -0.01466500 | 4.00073300 |
| H | -0.42701200 | -0.23035300 | 4.18941500 |
| H | 0.76804000 | 1.07136600 | 4.08116600 |
| C | 1.52457300 | -0.75883200 | 4.98085900 |
| H | 2.58271700 | -0.54449800 | 4.79329400 |
| H | 1.29511800 | -0.45153900 | 6.00767500 |
| H | 1.37184800 | -1.83926400 | 4.90000600 |
| P | 3.00648900 | 0.22410200 | 0.30421500 |
| C | 3.74217200 | 1.77089100 | -0.38492200 |
| C | 4.38306000 | 1.83046300 | -1.63422900 |
| C | 3.63066900 | 2.94485000 | 0.37683200 |
| C | 4.90155500 | 3.03691900 | -2.10587900 |
| H | 4.47681300 | 0.93200100 | -2.23691500 |
| C | 4.14867200 | 4.15455800 | -0.09627600 |
| H | 3.13797300 | 2.91319800 | 1.34547100 |
| C | 4.78541900 | 4.20186100 | -1.33844400 |
| H | 5.39417500 | 3.06976700 | -3.07374700 |
| H | 4.05656000 | 5.05443000 | 0.50546200 |
| H | 5.19015400 | 5.13974900 | -1.70824000 |
| C | 4.24989800 | -1.05342900 | -0.20059400 |
| C | 5.58528400 | -0.86203100 | 0.20416800 |
| C | 3.90701500 | -2.25376800 | -0.83916300 |
| C | 6.55059500 | -1.84041600 | -0.03740100 |
| H | 5.87714700 | 0.05854500 | 0.70327900 |
| C | 4.87578200 | -3.23482600 | -1.07715600 |
| H | 2.88352100 | -2.41677200 | -1.16183400 |
| C | 6.19869800 | -3.03288300 | -0.67931100 |
| H | 7.57716300 | -1.67092000 | 0.27586000 |
| H | 4.59162100 | -4.15577900 | -1.57901400 |
| H | 6.94981000 | -3.79504800 | -0.86632000 |
| O | 0.86390600 | -0.42910900 | 2.64063300 |

E/M-TS1




| | | | |
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| C | -3.80626900 | 1.02691900 | -0.88064300 |
| C | -2.66474700 | 1.84304400 | -0.79689500 |
| C | -4.68257000 | 1.20715500 | -1.96401200 |
| C | -2.40483800 | 2.80554300 | -1.77506600 |
| H | -1.97811300 | 1.73429100 | 0.03761200 |
| C | -4.42123000 | 2.16723700 | -2.94617100 |
| H | -5.57299800 | 0.58802000 | -2.03911900 |
| C | -3.28067700 | 2.96890200 | -2.85422500 |
| H | -1.51716300 | 3.42756100 | -1.69498000 |
| H | -5.10939800 | 2.29002600 | -3.77802100 |
| H | -3.07620300 | 3.71780900 | -3.61438400 |
| C | -3.49198200 | 0.32946100 | 1.89831000 |
| C | -3.85567600 | 1.61869300 | 2.33514800 |
| C | -2.71975000 | -0.47020600 | 2.75497800 |
| C | -3.43673200 | 2.09859900 | 3.57711600 |
| H | -4.46446600 | 2.25666800 | 1.69972300 |
| C | -2.30279600 | 0.01053900 | 4.00084900 |
| H | -2.44233700 | -1.47319800 | 2.44523000 |
| C | -2.65605200 | 1.29607900 | 4.41598700 |
| H | -3.72156600 | 3.09981100 | 3.88948200 |
| H | -1.69796100 | -0.62349500 | 4.64350300 |
| H | -2.32990600 | 1.66939200 | 5.38264900 |
| Cd | -0.54561400 | -1.24047100 | -0.51217000 |
| Se | 0.86711500 | 0.36318500 | 1.21538600 |
| C | 0.98145700 | -2.04999000 | -3.18187500 |
| H | 1.96365300 | -1.93085900 | -3.67032700 |
| H | 0.27051300 | -1.43169300 | -3.75486300 |
| C | 0.55726000 | -3.51647200 | -3.26434500 |
| H | -0.43785000 | -3.66085500 | -2.82709100 |
| H | 0.51846300 | -3.85336700 | -4.30809100 |
| H | 1.26466800 | -4.15311600 | -2.72135200 |
| P | 2.66210300 | 0.21970900 | -0.11198800 |
| C | 4.01619600 | -0.75292200 | 0.61764000 |
| C | 4.88972400 | -0.20833900 | 1.57221800 |
| C | 4.14432200 | -2.09940400 | 0.23895800 |
| C | 5.88925600 | -1.00296300 | 2.13462400 |
| H | 4.79199600 | 0.83065600 | 1.87373800 |
| C | 5.14686700 | -2.88944300 | 0.80749600 |
| H | 3.46006600 | -2.52414300 | -0.49086200 |
| C | 6.01884400 | -2.34310600 | 1.75302700 |
| H | 6.56426600 | -0.57809200 | 2.87181300 |
| H | 5.24505100 | -3.92962300 | 0.51092600 |
| H | 6.79720000 | -2.95932700 | 2.19378000 |
| C | 3.34738500 | 1.85782700 | -0.55047500 |
| C | 4.53888300 | 1.91890400 | -1.29536900 |
| C | 2.68443100 | 3.04257400 | -0.20517200 |
| C | 5.05514200 | 3.15411300 | -1.68797400 |

| | | | |
|---|---|---|---|
| H | 5.06518400 | 1.00753400 | -1.56559500 |
| C | 3.20862600 | 4.27767600 | -0.59838900 |
| H | 1.76542400 | 2.99501000 | 0.37098800 |
| C | 4.39091500 | 4.33550200 | -1.33961700 |
| H | 5.97476600 | 3.19396300 | -2.26441700 |
| H | 2.69118900 | 5.19201300 | -0.32299100 |
| H | 4.79557200 | 5.29600000 | -1.64534600 |
| H | 2.17225700 | -0.54570700 | -1.27110000 |
| O | 1.09373600 | -1.59221200 | -1.84690400 |

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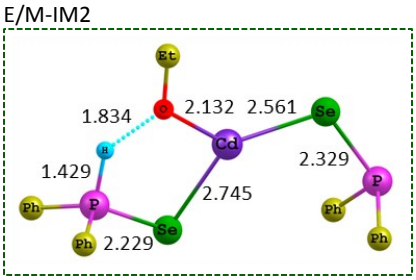


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| C | 3.49709000 | 1.81331600 | -0.36813500 |
| C | 2.64037500 | 1.78029600 | -1.48134200 |
| C | 3.79102800 | 3.05849400 | 0.21659100 |
| C | 2.08895900 | 2.96005100 | -1.99014600 |
| H | 2.40678500 | 0.83411500 | -1.95921700 |
| C | 3.23135900 | 4.23568800 | -0.28441400 |
| H | 4.46081600 | 3.10285600 | 1.07183500 |
| C | 2.37944300 | 4.18986400 | -1.39243600 |
| H | 1.42884500 | 2.91448600 | -2.85211200 |
| H | 3.46816300 | 5.18736700 | 0.18354900 |
| H | 1.94904600 | 5.10515200 | -1.78929500 |
| C | 4.13680100 | -0.93060400 | -0.96830800 |
| C | 4.84063300 | -0.69176500 | -2.16570300 |
| C | 3.46861400 | -2.15423300 | -0.82295800 |
| C | 4.84607500 | -1.63426800 | -3.19454500 |
| H | 5.38619600 | 0.23963600 | -2.29825000 |
| C | 3.47979200 | -3.10290900 | -1.85202400 |
| H | 2.94569300 | -2.37069300 | 0.10348600 |
| C | 4.16287800 | -2.84620000 | -3.04198800 |
| H | 5.38837600 | -1.42475500 | -4.11270700 |
| H | 2.95309000 | -4.04409700 | -1.71776900 |
| H | 4.17124500 | -3.58310300 | -3.84022300 |
| Cd | 0.48279500 | -0.28407900 | 1.35160800 |
| Se | -0.79942800 | 0.89293000 | -0.77101700 |
| C | -1.22634700 | -1.63340500 | 3.58394200 |
| H | -0.89274400 | -0.86027700 | 4.29791700 |
| H | -0.51378700 | -2.47177700 | 3.67486900 |
| C | -2.61644500 | -2.11695500 | 4.00000400 |
| H | -2.96598600 | -2.91287100 | 3.33207100 |
| H | -2.60347400 | -2.51116300 | 5.02394900 |
| H | -3.33963100 | -1.29387900 | 3.96019500 |
| P | -2.75995500 | 0.07006100 | -0.10314600 |
| C | -3.28774800 | -1.42515600 | -0.99147900 |
| C | -3.90689000 | -1.35774300 | -2.24941400 |
| C | -3.00865200 | -2.67231000 | -0.40857400 |
| C | -4.25537600 | -2.53363400 | -2.91459900 |
| H | -4.11894700 | -0.39523800 | -2.70616500 |
| C | -3.36115300 | -3.84450700 | -1.08244000 |
| H | -2.51243500 | -2.71589200 | 0.55799400 |
| C | -3.98348900 | -3.77666800 | -2.33193400 |
| H | -4.73622500 | -2.48043300 | -3.88694500 |
| H | -3.14793000 | -4.80875000 | -0.63040900 |
| H | -4.25531400 | -4.68994500 | -2.85336600 |
| C | -4.11086100 | 1.29528400 | -0.20788500 |
| C | -5.42749000 | 0.88508500 | 0.06773400 |
| C | -3.84819800 | 2.63966000 | -0.50163800 |
| C | -6.46644200 | 1.81605900 | 0.04784400 |
| H | -5.64398200 | -0.15511000 | 0.29436800 |
| C | -4.89470600 | 3.56624800 | -0.52481000 |
| H | -2.83063400 | 2.95690700 | -0.70828300 |
| C | -6.20150300 | 3.15735200 | -0.24998300 |
| H | -7.48094100 | 1.49394700 | 0.26341600 |
| H | -4.68476800 | 4.60627600 | -0.75632300 |
| H | -7.01249900 | 3.87967000 | -0.26648700 |
| H | -2.56668100 | -0.36583200 | 1.24413400 |
| O | -1.24759300 | -1.13488900 | 2.26054200 |

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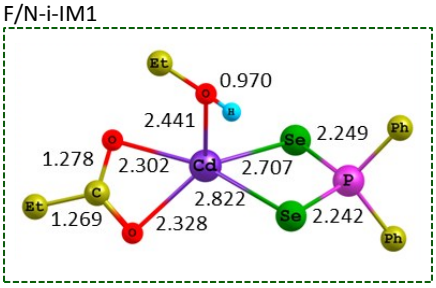


| | | | |
|---|---|---|---|
| Cd | 1.75009900 | 0.01897700 | 0.10087300 |
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| Se | -0.30008400 | -0.22150900 | 1.85222600 |
| Se | -0.30911000 | -0.07920500 | -1.82657000 |
| C | -2.73342100 | 1.28234300 | 0.09631900 |
| C | -3.44159300 | 1.51758800 | 1.28672000 |
| C | -2.92206200 | 2.13153900 | -1.00172600 |
| C | -4.33690100 | 2.58390100 | 1.36829700 |
| H | -3.28907300 | 0.87642100 | 2.14982500 |
| C | -3.81968900 | 3.20065400 | -0.91370900 |
| H | -2.36628800 | 1.95944700 | -1.91844900 |
| C | -4.52721500 | 3.42799100 | 0.26839500 |
| H | -4.87904500 | 2.76045100 | 2.29269800 |
| H | -3.96056700 | 3.85428800 | -1.76975600 |
| H | -5.22074300 | 4.26124800 | 0.33651600 |
| C | -2.68933000 | -1.62443800 | -0.04937800 |
| C | -3.91047500 | -1.55821600 | -0.73988300 |
| C | -2.28669200 | -2.83409100 | 0.53392800 |
| C | -4.71820000 | -2.69228500 | -0.84169500 |
| H | -4.23550200 | -0.62737200 | -1.19390400 |
| C | -3.09857300 | -3.96530200 | 0.42721900 |
| H | -1.34759600 | -2.88632100 | 1.07562100 |
| C | -4.31375600 | -3.89735100 | -0.25964300 |
| H | -5.66256200 | -2.63230800 | -1.37492800 |
| H | -2.78078600 | -4.89771900 | 0.88457200 |
| H | -4.94425400 | -4.77827400 | -0.33937200 |
| C | 2.88882400 | 3.27586700 | -0.82888100 |
| H | 3.57583100 | 2.82774600 | -1.55799700 |
| H | 2.47891300 | 4.19836400 | -1.25798800 |
| C | 3.59679600 | 3.55483300 | 0.48438000 |
| H | 2.90838500 | 4.00957400 | 1.20371600 |
| H | 3.99756300 | 2.63009300 | 0.90822800 |
| H | 4.42753600 | 4.24867800 | 0.31390300 |
| O | 3.93964500 | 0.18142900 | 0.79335400 |
| O | 3.37459900 | -1.54538600 | -0.47503900 |
| C | 4.24333500 | -0.90268200 | 0.18934500 |
| C | 5.67259400 | -1.41088800 | 0.29273500 |
| H | 6.32967200 | -0.57744800 | 0.01627400 |
| H | 5.86318100 | -1.58891100 | 1.35881300 |
| C | 5.97824200 | -2.65938600 | -0.53561200 |
| H | 7.02187700 | -2.96207100 | -0.39679200 |
| H | 5.33461700 | -3.49375600 | -0.24356100 |
| H | 5.81236000 | -2.47753000 | -1.60155100 |

| | | | |
|---|---|---|---|
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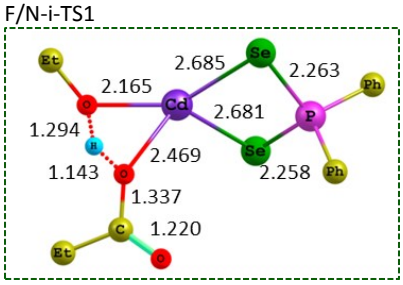
| O | 1.79164200 | 2.36274700 | -0.58120200 |

F/N-i-TS1




| | | | |
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| Cd | -1.36702500 | -1.08248300 | -0.03078500 |
| C | -4.10525600 | -2.64674300 | -0.71915900 |
| H | -3.98636200 | -2.44310800 | -1.79575700 |
| H | -3.62802600 | -3.61542200 | -0.51600200 |
| C | -5.58747500 | -2.71994500 | -0.36500200 |
| H | -5.71648500 | -2.93671500 | 0.70032500 |
| H | -6.08889600 | -1.77121400 | -0.58578600 |
| H | -6.08229900 | -3.50889300 | -0.94418700 |
| O | -2.70891600 | 2.71094700 | 0.16628500 |
| C | -3.46924800 | 1.75975100 | 0.09341500 |
| C | -4.89847900 | 1.78239700 | 0.62361500 |
| H | -5.56483400 | 1.59025000 | -0.22798600 |
| H | -5.02072900 | 0.92098300 | 1.29369300 |
| C | -5.27618900 | 3.08482600 | 1.32862400 |
| H | -6.31226000 | 3.04161800 | 1.68045500 |
| H | -4.62633200 | 3.26831400 | 2.18902300 |
| H | -5.17408400 | 3.93942600 | 0.65417600 |
| O | -3.10142900 | 0.61348200 | -0.48803600 |
| H | -3.59378700 | -0.39189500 | -0.25575400 |
| P | 1.67642800 | -0.02868200 | -0.00639800 |
| Se | 0.39233800 | -0.29374200 | 1.83157000 |
| Se | 0.72196300 | -1.16359100 | -1.71560300 |
| C | 3.36803800 | -0.64135800 | 0.32954400 |
| C | 3.93933600 | -1.66786200 | -0.43299600 |
| C | 4.08813000 | -0.08274500 | 1.40027500 |
| C | 5.22773300 | -2.12308400 | -0.13608400 |
| H | 3.37903200 | -2.11352000 | -1.24879400 |
| C | 5.37166600 | -0.54288500 | 1.69221700 |
| H | 3.64942200 | 0.70539200 | 2.00539000 |
| C | 5.94386600 | -1.56308800 | 0.92358800 |
| H | 5.66586800 | -2.91766400 | -0.73280200 |
| H | 5.92235800 | -0.10805400 | 2.52108700 |
| H | 6.94305900 | -1.92095300 | 1.15453500 |
| C | 1.83563300 | 1.74245000 | -0.43803700 |
| C | 3.04826200 | 2.24679100 | -0.93675600 |
| C | 0.71741300 | 2.58564400 | -0.33296800 |
| C | 3.14085200 | 3.58764900 | -1.31675800 |
| H | 3.91787100 | 1.60435000 | -1.02852600 |
| C | 0.81875800 | 3.92212400 | -0.72100600 |
| H | -0.23592100 | 2.22463200 | 0.04062500 |
| C | 2.02799000 | 4.42632100 | -1.20925800 |
| H | 4.08280600 | 3.97267700 | -1.69664300 |
| H | -0.05555600 | 4.56005600 | -0.63696300 |
| H | 2.10289800 | 5.46853000 | -1.50650900 |
| O | -3.45707600 | -1.64087100 | 0.05520800 |

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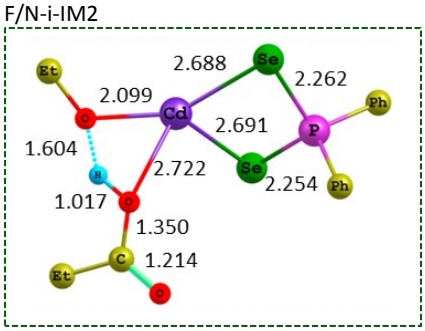


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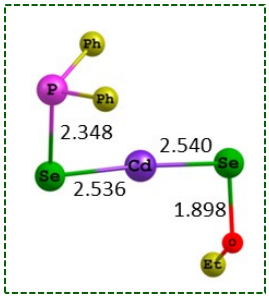
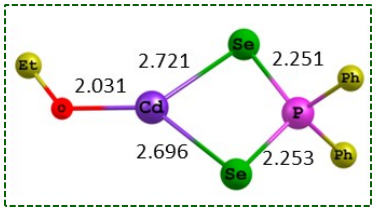
| Cd | -1.34817700 | -1.18272600 | -0.09593700 |
| C | -4.03095700 | -2.62127300 | -0.82368100 |
| H | -3.86497800 | -2.52493400 | -1.91029500 |
| H | -3.59423900 | -3.58495500 | -0.51672800 |
| C | -5.53073800 | -2.63822500 | -0.53868500 |
| H | -5.71569100 | -2.75879500 | 0.53394300 |
| H | -5.99815300 | -1.70218300 | -0.86453600 |
| H | -6.01630700 | -3.46536400 | -1.07107400 |
| O | -2.82808900 | 2.95140400 | 0.25945300 |
| C | -3.48019700 | 1.92890100 | 0.19815100 |
| C | -4.80703800 | 1.71065300 | 0.91139200 |
| H | -5.56649100 | 1.52561000 | 0.13952000 |
| H | -4.73455400 | 0.77552400 | 1.48189200 |
| C | -5.21691500 | 2.87790700 | 1.80884000 |
| H | -6.18101400 | 2.67046800 | 2.28405700 |
| H | -4.47483300 | 3.04958800 | 2.59368500 |
| H | -5.30526400 | 3.80318800 | 1.23312800 |
| O | -3.05022800 | 0.89143400 | -0.55188900 |
| H | -3.54824400 | 0.01445900 | -0.42225600 |
| P | 1.66769800 | -0.03526300 | 0.00081800 |
| Se | 0.30759700 | -0.21054500 | 1.78938000 |
| Se | 0.83804900 | -1.33932400 | -1.65127000 |
| C | 3.36620300 | -0.54102200 | 0.45503100 |
| C | 3.90724000 | -1.75568600 | 0.01468500 |
| C | 4.10927700 | 0.28368000 | 1.31773500 |
| C | 5.18743400 | -2.13806100 | 0.42558000 |
| H | 3.33035400 | -2.39780300 | -0.64346400 |
| C | 5.38503900 | -0.10521600 | 1.72544600 |
| H | 3.69649200 | 1.22488300 | 1.66866200 |
| C | 5.92625200 | -1.31611700 | 1.27945900 |
| H | 5.60339200 | -3.07882100 | 0.07725100 |
| H | 5.95481300 | 0.53615400 | 2.39134200 |
| H | 6.92014500 | -1.61638400 | 1.59852600 |
| C | 1.78158000 | 1.69647100 | -0.57837500 |
| C | 2.89762600 | 2.10186400 | -1.33107600 |
| C | 0.72639100 | 2.59297700 | -0.35462300 |
| C | 2.95843800 | 3.39896300 | -1.84125600 |
| H | 3.71574800 | 1.41333800 | -1.51897000 |
| C | 0.79170400 | 3.88683600 | -0.87680600 |
| H | -0.14942100 | 2.29674000 | 0.21298900 |
| C | 1.90598900 | 4.29271200 | -1.61508900 |
| H | 3.82544200 | 3.70856700 | -2.41763500 |
| H | -0.03698600 | 4.56609600 | -0.70307300 |
| H | 1.95481500 | 5.30070400 | -2.01714600 |
| O | -3.41342200 | -1.55445600 | -0.11921500 |

N



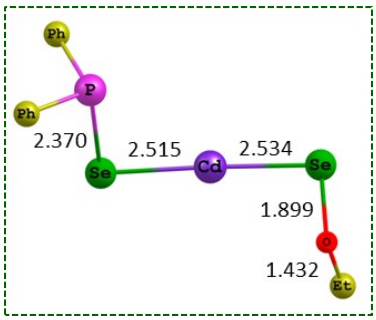

| | | | |
|---|---|---|---|
| Se | 0.85621800 | -0.87133400 | 2.12534300 |
| P | 2.64134400 | 0.34062100 | 1.20008800 |
| C | 1.75067700 | 1.71923600 | 0.32726800 |
| C | 1.25349400 | 1.63474300 | -0.98737400 |
| C | 1.55189500 | 2.91092700 | 1.04590700 |
| C | 0.56023000 | 2.70820800 | -1.55730600 |
| H | 1.43069800 | 0.74028100 | -1.57852900 |
| C | 0.85532200 | 3.98100100 | 0.47748900 |
| H | 1.93929700 | 2.99707900 | 2.05792000 |
| C | 0.35479900 | 3.88161000 | -0.82416400 |
| H | 0.18791100 | 2.62787500 | -2.57500500 |
| H | 0.70819000 | 4.89265600 | 1.04968300 |
| H | -0.18407800 | 4.71391800 | -1.26738000 |
| C | 3.24375000 | -0.66445600 | -0.23924600 |
| C | 4.26912100 | -0.08829800 | -1.01490700 |
| C | 2.84439700 | -1.97714700 | -0.52511300 |
| C | 4.85293800 | -0.79573900 | -2.06625000 |
| H | 4.61283600 | 0.92116000 | -0.79989800 |
| C | 3.43644400 | -2.68912000 | -1.57494400 |
| H | 2.07277200 | -2.44746600 | 0.07643200 |
| C | 4.43705500 | -2.10142700 | -2.35073400 |
| H | 5.63604200 | -0.33032400 | -2.65839600 |
| H | 3.11139800 | -3.70498600 | -1.78239800 |
| H | 4.89517300 | -2.65532200 | -3.16512000 |
| Cd | -0.94777700 | -0.30036000 | 0.43681700 |
| Se | -2.88418400 | 0.16527600 | -1.13926400 |
| C | -4.92794000 | -1.20032700 | 0.24689700 |
| H | -4.60524100 | -0.63701500 | 1.13579400 |
| H | -5.18845300 | -2.21737500 | 0.56895600 |
| C | -6.12884300 | -0.52889000 | -0.40862900 |
| H | -6.45468600 | -1.09771100 | -1.28530300 |
| H | -6.96402300 | -0.47295700 | 0.29979100 |
| H | -5.88607100 | 0.49106200 | -0.72464800 |
| O | -3.82598000 | -1.40610800 | -0.64256000 |

N-i




| | | | |
|---|---|---|---|
| Cd | 2.26703000 | -0.05180200 | 0.18705200 |
| C | 5.16327200 | 0.00671100 | -0.73027700 |
| H | 5.03241900 | -0.89220900 | -1.35908500 |
| H | 4.98328800 | 0.87893500 | -1.38408100 |
| C | 6.60520700 | 0.05336400 | -0.22714100 |
| H | 6.76997500 | 0.95399800 | 0.37377200 |
| H | 6.81722400 | -0.81824200 | 0.40113800 |
| H | 7.31091000 | 0.05910700 | -1.06797100 |
| P | -1.03429600 | -0.01127500 | -0.00019200 |
| Se | 0.36724400 | -0.01133000 | -1.76119400 |
| Se | 0.18082000 | -0.15028300 | 1.89243500 |
| C | -2.22071600 | -1.40224000 | -0.12216200 |
| C | -2.06480800 | -2.55897500 | 0.65278100 |
| C | -3.27034500 | -1.32243900 | -1.05348400 |
| C | -2.95454600 | -3.62594200 | 0.50005800 |
| H | -1.25603100 | -2.62152900 | 1.37395800 |
| C | -4.15534900 | -2.39049600 | -1.20013400 |
| H | -3.40053400 | -0.43119100 | -1.66013100 |
| C | -3.99840000 | -3.54421700 | -0.42433700 |
| H | -2.83047800 | -4.51785900 | 1.10710700 |
| H | -4.96534700 | -2.32194900 | -1.92031500 |
| H | -4.68897300 | -4.37452400 | -0.54032800 |
| C | -2.07058200 | 1.50039300 | 0.02167100 |
| C | -3.10429400 | 1.59587800 | 0.96956900 |
| C | -1.82720400 | 2.56707100 | -0.85228600 |
| C | -3.88983600 | 2.74614700 | 1.03077300 |
| H | -3.29660000 | 0.77739900 | 1.65727400 |
| C | -2.61775700 | 3.71848600 | -0.78471800 |
| H | -1.02544100 | 2.49582300 | -1.58052400 |
| C | -3.64761500 | 3.80963300 | 0.15359100 |
| H | -4.68759900 | 2.81367600 | 1.76456100 |
| H | -2.42571100 | 4.54093200 | -1.46747600 |
| H | -4.25988200 | 4.70533500 | 0.20473100 |
| O | 4.28792900 | -0.00218400 | 0.38202200 |

N-ii




| | | | |
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| Se | 0.52053100 | -0.40565600 | 1.31186500 |
| P | 1.79362100 | -0.07772400 | -0.65989300 |
| C | 3.06812700 | -1.39592600 | -0.42095100 |
| C | 4.15170800 | -1.29084500 | 0.46755300 |
| C | 2.92453800 | -2.56910300 | -1.18098400 |
| C | 5.06816700 | -2.33664600 | 0.59152900 |
| H | 4.28201000 | -0.38953400 | 1.05894400 |
| C | 3.84064400 | -3.61683400 | -1.05442800 |
| H | 2.09339100 | -2.66093100 | -1.87574200 |
| C | 4.91423100 | -3.50207500 | -0.16734300 |
| H | 5.90191300 | -2.24280900 | 1.28194500 |
| H | 3.71749300 | -4.51713900 | -1.64986100 |
| H | 5.62953400 | -4.31383800 | -0.06934700 |
| C | 2.78192400 | 1.45339400 | -0.30202700 |
| C | 3.72107300 | 1.82005100 | -1.28581000 |
| C | 2.59956200 | 2.30055900 | 0.79927100 |
| C | 4.47121200 | 2.98939100 | -1.15715200 |
| H | 3.87150500 | 1.18614900 | -2.15685400 |
| C | 3.34691300 | 3.47772200 | 0.92346900 |
| H | 1.87649900 | 2.03938300 | 1.56550700 |
| C | 4.28513700 | 3.82494700 | -0.05004400 |
| H | 5.19577300 | 3.25048100 | -1.92354100 |
| H | 3.19384600 | 4.11975200 | 1.78678500 |
| H | 4.86451400 | 4.73854400 | 0.04841200 |
| Cd | -1.66112700 | 0.14177300 | 0.18661200 |
| Se | -3.90188100 | 0.62138600 | -0.89621600 |
| C | -5.54009100 | -1.05945000 | 0.67077800 |
| H | -5.10046700 | -0.56103400 | 1.54812700 |
| H | -5.66275400 | -2.12328500 | 0.91363500 |
| C | -6.88579500 | -0.43774000 | 0.31765300 |
| H | -7.32520800 | -0.94068900 | -0.54961200 |

| | | | |
|---|---|---|---|
| H | -7.57859600 | -0.53231800 | 1.16236900 |
| H | -6.78011700 | 0.62756400 | 0.08724700 |
| O | -4.60846700 | -1.07488000 | -0.41602000 |

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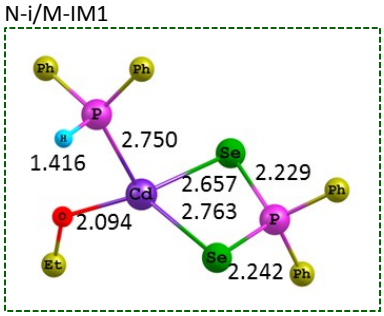
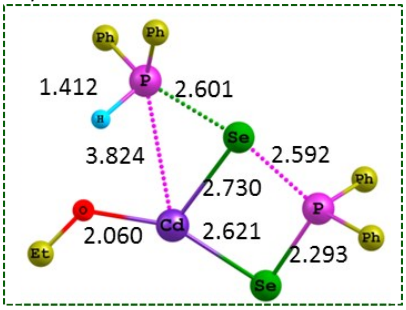



| | | | |
|---|---|---|---|
| Cd | -0.65830100 | -1.20465000 | 0.37490600 |
| C | -1.18619600 | -4.22120500 | 0.76885800 |
| H | -0.57689000 | -4.50030800 | -0.11200500 |
| H | -0.50219600 | -4.24186500 | 1.63792300 |
| C | -2.26447100 | -5.28776100 | 0.97335600 |
| H | -2.86633600 | -5.05580200 | 1.85921100 |
| H | -2.93457000 | -5.32558800 | 0.10678800 |
| H | -1.81575900 | -6.28094500 | 1.10742100 |
| P | 2.30000000 | 0.08137300 | -0.06705900 |
| Se | 1.37867300 | -0.21181000 | 1.95608900 |
| Se | 0.78806900 | -0.29533500 | -1.66047900 |
| C | 3.75259100 | -1.02456200 | -0.27051000 |
| C | 3.79253700 | -2.01524000 | -1.25879800 |
| C | 4.83437400 | -0.88017500 | 0.61529100 |
| C | 4.90889600 | -2.85161300 | -1.36524100 |
| H | 2.95430600 | -2.13263300 | -1.93854200 |
| C | 5.94582000 | -1.71412900 | 0.50230400 |
| H | 4.80745600 | -0.12345400 | 1.39407100 |
| C | 5.98481400 | -2.70244200 | -0.48850000 |
| H | 4.93185900 | -3.61862400 | -2.13392300 |
| H | 6.77806700 | -1.59696700 | 1.19029500 |
| H | 6.84992100 | -3.35407800 | -0.57181200 |
| C | 2.98467400 | 1.77674600 | -0.24175100 |
| C | 3.90565800 | 2.04622300 | -1.26794000 |
| C | 2.55876000 | 2.81385800 | 0.59829100 |
| C | 4.39592800 | 3.34048100 | -1.44508200 |
| H | 4.24298500 | 1.24996100 | -1.92476000 |
| C | 3.05373200 | 4.10830500 | 0.41655800 |
| H | 1.84864100 | 2.60556100 | 1.39270300 |
| C | 3.97080500 | 4.37392200 | -0.60323700 |
| H | 5.10990600 | 3.54076100 | -2.23873800 |
| H | 2.72309800 | 4.90570000 | 1.07588100 |
| H | 4.35567900 | 5.38034000 | -0.74141400 |
| P | -2.87760500 | 0.38091900 | 0.72345300 |
| H | -3.40124900 | 0.28495600 | 2.03512800 |
| C | -4.32104800 | -0.15599000 | -0.29035800 |
| C | -4.44280000 | -1.53149500 | -0.55559400 |
| C | -5.27427200 | 0.74147600 | -0.79560100 |
| C | -5.52809500 | -1.99586900 | -1.30486200 |
| H | -3.69190000 | -2.23095100 | -0.18360600 |
| C | -6.34849800 | 0.26707800 | -1.55305600 |
| H | -5.18030000 | 1.80630000 | -0.60567500 |
| C | -6.47903500 | -1.10197500 | -1.80531000 |
| H | -5.62111400 | -3.05972300 | -1.50446300 |
| H | -7.08134400 | 0.96731400 | -1.94443900 |
| H | -7.31530000 | -1.46852900 | -2.39428700 |
| C | -2.76745400 | 2.20364000 | 0.57334000 |
| C | -1.94855800 | 2.75655700 | -0.42609500 |
| C | -3.45604400 | 3.06283400 | 1.44653500 |
| C | -1.83722700 | 4.14254700 | -0.55972200 |
| H | -1.38537300 | 2.10677900 | -1.09070000 |
| C | -3.33538200 | 4.44891400 | 1.31622900 |
| H | -4.08777000 | 2.65075300 | 2.22885600 |
| C | -2.52961400 | 4.99028100 | 0.31007400 |
| H | -1.19998800 | 4.55714200 | -1.33544200 |
| H | -3.87105500 | 5.10302900 | 1.99837500 |
| H | -2.43724200 | 6.06791600 | 0.20856700 |
| O | -1.78245100 | -2.95596500 | 0.60717000 |

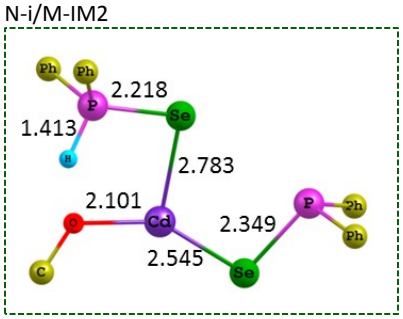
N-i/M-TS1




| | | | |
|---|---|---|---|
| P | -2.35762600 | 0.27346600 | 0.16371000 |
| Se | -2.65631800 | -1.83461400 | -0.68823600 |
| P | 2.77658800 | 0.62328300 | -0.34071300 |
| Se | 0.20100900 | 0.66099000 | 0.01990800 |
| H | 3.13144900 | -0.07997900 | -1.51199100 |
| Cd | -0.04752000 | -1.88581900 | -0.93209700 |
| C | 1.87026700 | -3.96249400 | -2.14263200 |
| H | 1.57188000 | -3.80441200 | -3.19472500 |
| H | 2.93918200 | -4.23542800 | -2.16309300 |
| C | 1.07489900 | -5.13830400 | -1.57048500 |
| H | 1.37299000 | -5.33866200 | -0.53522700 |
| H | -0.00248000 | -4.92270800 | -1.57815400 |
| H | 1.23557700 | -6.05003200 | -2.16029800 |
| C | -3.43423900 | 1.43232500 | -0.77453900 |
| C | -3.84308300 | 1.16244200 | -2.08922500 |
| C | -3.75911300 | 2.67502600 | -0.19974200 |
| C | -4.57164300 | 2.11200700 | -2.81091300 |
| H | -3.60197700 | 0.20550900 | -2.54145100 |
| C | -4.48725000 | 3.61992400 | -0.92430700 |
| H | -3.45109300 | 2.90473100 | 0.81624900 |
| C | -4.89620700 | 3.34161000 | -2.23257500 |
| H | -4.88844400 | 1.88536600 | -3.82511600 |
| H | -4.73608300 | 4.57251800 | -0.46490100 |
| H | -5.46414900 | 4.07736400 | -2.79482100 |
| C | -3.05871200 | 0.28716000 | 1.86373700 |
| C | -2.18477000 | 0.38531900 | 2.95667600 |
| C | -4.44012700 | 0.16536600 | 2.09416200 |
| C | -2.68582100 | 0.36704300 | 4.26241700 |
| H | -1.11599400 | 0.47394800 | 2.78381800 |
| C | -4.93605600 | 0.14918300 | 3.39774000 |
| H | -5.12588100 | 0.08314600 | 1.25608600 |
| C | -4.05948600 | 0.24992500 | 4.48470800 |
| H | -2.00106800 | 0.44504500 | 5.10217200 |
| H | -6.00513100 | 0.05407500 | 3.56611800 |
| H | -4.44805700 | 0.23532400 | 5.49914000 |
| C | 3.80952300 | -0.23858000 | 0.90362700 |
| C | 4.47130700 | 0.46362200 | 1.92294800 |
| C | 3.85286300 | -1.64444800 | 0.88133400 |
| C | 5.18633600 | -0.23156300 | 2.90180000 |
| H | 4.44115300 | 1.54914600 | 1.94973200 |
| C | 4.57217600 | -2.32896500 | 1.86401600 |
| H | 3.31822200 | -2.19411900 | 0.10623300 |
| C | 5.23982400 | -1.62804700 | 2.87376100 |
| H | 5.70178700 | 0.31940900 | 3.68360000 |
| H | 4.60889200 | -3.41461000 | 1.83927200 |
| H | 5.79760500 | -2.16670500 | 3.63470900 |

| | | | |
|---|---|---|---|
| C | 3.54973200 | 2.26432700 | -0.61492900 |
| C | 2.83953900 | 3.42348400 | -0.26960000 |
| C | 4.83328500 | 2.38510400 | -1.17620000 |
| C | 3.40773300 | 4.68552000 | -0.47196200 |
| H | 1.83867300 | 3.33836700 | 0.14396200 |
| C | 5.39497000 | 3.64588500 | -1.38310200 |
| H | 5.39461300 | 1.49528500 | -1.44786600 |
| C | 4.68355600 | 4.79794400 | -1.02857200 |
| H | 2.84934200 | 5.57695400 | -0.20102400 |
| H | 6.38591900 | 3.72946300 | -1.82033900 |
| H | 5.12248600 | 5.77835700 | -1.19064600 |
| O | 1.75383100 | -2.77387000 | -1.39268200 |

N-i/M-IM2

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| Se | -2.50236100 | -1.16777500 | -1.21119200 |
| P | 3.13743300 | 0.39365400 | 0.10861900 |
| Se | 1.06526500 | 0.65588300 | 0.85371100 |
| H | 3.06762100 | -0.05238600 | -1.22981100 |
| Cd | 0.03419300 | -0.96517500 | -1.16011200 |
| C | 1.94619700 | -2.16008900 | -3.29149200 |
| H | 1.55198200 | -1.51395000 | -4.09561000 |
| H | 3.01524200 | -2.31655600 | -3.51882400 |
| C | 1.23095200 | -3.51231700 | -3.34228800 |
| H | 1.62545800 | -4.18724400 | -2.57432200 |
| H | 0.15364700 | -3.39371600 | -3.16799900 |
| H | 1.36040900 | -3.98980800 | -4.32209100 |
| C | -3.79645200 | 1.73065700 | -0.19114000 |
| C | -3.85745600 | 1.99008100 | -1.56723800 |
| C | -4.36092100 | 2.66981400 | 0.69422800 |
| C | -4.47816900 | 3.14900900 | -2.04828900 |
| H | -3.42735800 | 1.27834200 | -2.26512600 |
| C | -4.98613400 | 3.82108600 | 0.21420000 |
| H | -4.31796500 | 2.49785500 | 1.76730700 |
| C | -5.04639600 | 4.06627100 | -1.16250900 |
| H | -4.51954000 | 3.32827300 | -3.11952900 |
| H | -5.42332200 | 4.52771800 | 0.91464600 |
| H | -5.52988300 | 4.96407800 | -1.53751300 |
| C | -4.26986800 | -0.57401900 | 1.43603000 |
| C | -3.96202000 | -1.23969300 | 2.63415500 |
| C | -5.58953300 | -0.62282800 | 0.95563900 |
| C | -4.94739300 | -1.93971400 | 3.33672100 |
| H | -2.94539600 | -1.20739700 | 3.01839700 |
| C | -6.57445600 | -1.31996400 | 1.65759500 |
| H | -5.84766100 | -0.11297900 | 0.03222500 |
| C | -6.25622700 | -1.98088100 | 2.84938900 |
| H | -4.69296500 | -2.44763400 | 4.26303700 |
| H | -7.59059700 | -1.34981000 | 1.27334700 |
| H | -7.02481700 | -2.52207400 | 3.39434000 |
| C | 4.09448600 | -0.91270800 | 0.93597500 |
| C | 4.80730500 | -0.66430400 | 2.11906100 |
| C | 4.05634000 | -2.20640800 | 0.38980100 |
| C | 5.49229900 | -1.70610900 | 2.74605100 |
| H | 4.83304200 | 0.33374200 | 2.54694100 |
| C | 4.74588100 | -3.24190200 | 1.02569300 |
| H | 3.47642400 | -2.38802800 | -0.51323300 |
| C | 5.46326300 | -2.99383100 | 2.19954100 |
| H | 6.04624500 | -1.51334700 | 3.66012200 |
| H | 4.72007600 | -4.24238800 | 0.60372800 |
| H | 5.99749300 | -3.80225700 | 2.69051300 |
| C | 4.12243300 | 1.93162600 | 0.16474800 |
| C | 3.55191800 | 3.14141100 | 0.58004200 |
| C | 5.46241900 | 1.90039700 | -0.26035200 |
| C | 4.31743700 | 4.31139500 | 0.57601100 |
| H | 2.51431600 | 3.16638600 | 0.89908200 |
| C | 6.21904000 | 3.07248500 | -0.26788500 |
| H | 5.91640100 | 0.96696800 | -0.58177900 |
| C | 5.64767200 | 4.27891800 | 0.15221800 |
| H | 3.86993400 | 5.24579500 | 0.90144100 |
| H | 7.25270700 | 3.04336000 | -0.59976200 |
| H | 6.23932200 | 5.18979900 | 0.14694900 |
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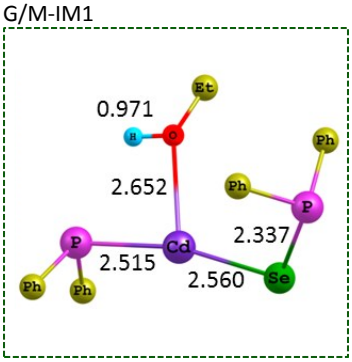


| | | | |
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| C | 2.63010600 | 2.05032400 | 0.26177800 |
| C | 2.10027200 | 1.77596100 | -1.01237100 |
| C | 2.71561700 | 3.38820200 | 0.68097400 |
| C | 1.66469400 | 2.81452500 | -1.83878000 |
| H | 2.02827100 | 0.75189400 | -1.36730900 |
| C | 2.27633800 | 4.42834100 | -0.14498100 |
| H | 3.12598000 | 3.61554600 | 1.66149800 |
| C | 1.75043400 | 4.14380600 | -1.40715900 |
| H | 1.26035800 | 2.58591000 | -2.82141500 |
| H | 2.34928900 | 5.45689600 | 0.19733200 |
| H | 1.41254900 | 4.94938000 | -2.05313400 |
| C | 3.95463000 | -0.52239100 | 0.35920800 |
| C | 4.81451600 | -0.13563700 | -0.68671500 |
| C | 3.86188400 | -1.88948700 | 0.67270500 |
| C | 5.53987100 | -1.08781300 | -1.40762300 |
| H | 4.91967800 | 0.91410800 | -0.94527800 |
| C | 4.59457800 | -2.84042500 | -0.04347000 |
| H | 3.20603500 | -2.20955000 | 1.47706400 |
| C | 5.43507500 | -2.44515800 | -1.08837900 |
| H | 6.19081600 | -0.76599500 | -2.21617600 |
| H | 4.50718200 | -3.89177000 | 0.21807600 |
| H | 6.00518800 | -3.18433100 | -1.64412500 |
| Cd | -0.43075500 | -0.26582200 | 0.38776000 |
| P | -2.47766800 | -0.22874500 | -1.07361300 |
| H | -0.27021300 | -1.23951200 | -2.36012200 |
| C | -3.27944700 | 1.39584000 | -0.69320700 |
| C | -4.66772200 | 1.51603600 | -0.50147400 |
| C | -2.51273100 | 2.57626700 | -0.73048200 |
| C | -5.26318000 | 2.77048400 | -0.33951000 |
| H | -5.29051100 | 0.62718100 | -0.47649600 |
| C | -3.10845400 | 3.82836000 | -0.57194400 |
| H | -1.43641000 | 2.52206900 | -0.87968000 |
| C | -4.48893500 | 3.93300700 | -0.37254600 |
| H | -6.33742100 | 2.83539200 | -0.18744700 |

| | | | |
|---|---|---|---|
| H | -2.49042800 | 4.72189100 | -0.59507000 |
| H | -4.95284100 | 4.90646100 | -0.24250400 |
| C | -3.55090600 | -1.47454700 | -0.20986500 |
| C | -3.94925200 | -1.37533300 | 1.13753800 |
| C | -3.96600000 | -2.60027100 | -0.94232600 |
| C | -4.73322100 | -2.36691000 | 1.72869400 |
| H | -3.64735600 | -0.51305300 | 1.72602500 |
| C | -4.74372400 | -3.60120900 | -0.34870400 |
| H | -3.68367200 | -2.68901000 | -1.98825900 |
| C | -5.13000500 | -3.48692300 | 0.98793400 |
| H | -5.02851200 | -2.26995800 | 2.76997400 |
| H | -5.05185100 | -4.46300400 | -0.93454100 |
| H | -5.73578700 | -4.26079900 | 1.45079900 |
| C | 1.43225800 | -2.28819900 | -2.40325200 |
| H | 1.64832400 | -2.04224300 | -3.45150900 |
| H | 2.36173600 | -2.19689800 | -1.83791600 |
| C | 0.85673700 | -3.69344300 | -2.28161200 |
| H | -0.07803900 | -3.79336800 | -2.84583700 |
| H | 1.56755700 | -4.42703100 | -2.67903100 |
| H | 0.65576100 | -3.94165800 | -1.23468700 |
| O | 0.55694600 | -1.28313100 | -1.85364000 |

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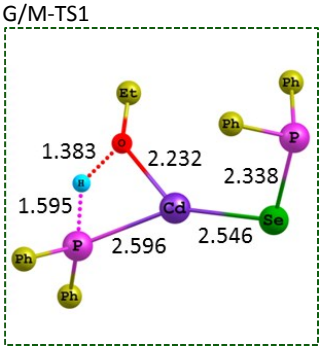


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| Se | -1.64613300 | -0.61557500 | -2.32515900 |
| P | -3.58485900 | 0.30736600 | -1.40118300 |
| C | -2.97023300 | 1.83406900 | -0.54750600 |
| C | -2.35368500 | 1.84917500 | 0.71593000 |
| C | -3.12203100 | 3.04878500 | -1.23686500 |
| C | -1.89432500 | 3.04656000 | 1.26892400 |
| H | -2.23702600 | 0.92654800 | 1.27693400 |
| C | -2.65827400 | 4.24725800 | -0.68606200 |
| H | -3.60224000 | 3.05376500 | -2.21209600 |
| C | -2.04286900 | 4.24867800 | 0.56831300 |
| H | -1.42120900 | 3.03890400 | 2.24714900 |
| H | -2.78133800 | 5.17682900 | -1.23483100 |
| H | -1.68407600 | 5.17907600 | 0.99948100 |
| C | -4.04622400 | -0.77487000 | 0.03291300 |
| C | -4.93701600 | -0.26079900 | 0.99589900 |
| C | -3.70382400 | -2.13437000 | 0.10083000 |
| C | -5.44791500 | -1.07681000 | 2.00668900 |
| H | -5.23109700 | 0.78494000 | 0.96186300 |
| C | -4.22035600 | -2.95228700 | 1.11118100 |
| H | -3.02982100 | -2.55473500 | -0.63949100 |
| C | -5.09111900 | -2.42802900 | 2.06905100 |
| H | -6.12646600 | -0.65652900 | 2.74416400 |
| H | -3.93879900 | -4.00133700 | 1.14681700 |
| H | -5.49076700 | -3.06413800 | 2.85374100 |
| Cd | 0.10308600 | -0.43765500 | -0.48369000 |
| P | 2.54095000 | -0.09994600 | 0.34338100 |
| H | 1.62423000 | -0.49640000 | 1.58738800 |
| C | 3.33384100 | 1.54090300 | 0.49116100 |
| C | 4.41955700 | 1.92120900 | -0.31657800 |
| C | 2.81227600 | 2.46953000 | 1.40979100 |
| C | 4.97385400 | 3.19799200 | -0.20097000 |
| H | 4.83492300 | 1.21930000 | -1.03378400 |
| C | 3.36205300 | 3.74905300 | 1.51357600 |
| H | 1.97866500 | 2.18813800 | 2.04781100 |
| C | 4.44600600 | 4.11735300 | 0.71082500 |
| H | 5.81562700 | 3.47569200 | -0.82935900 |
| H | 2.94882100 | 4.45451100 | 2.22918600 |
| H | 4.87679600 | 5.11073900 | 0.79639500 |
| C | 3.83391200 | -1.32073300 | -0.09227600 |
| C | 3.68715200 | -2.14753600 | -1.21822300 |
| C | 4.96857800 | -1.48497200 | 0.72501300 |
| C | 4.64469800 | -3.12234800 | -1.51706100 |
| H | 2.82671100 | -2.02353300 | -1.86981700 |
| C | 5.92984800 | -2.44857600 | 0.41781000 |
| H | 5.09750000 | -0.85761700 | 1.60245700 |
| C | 5.76841200 | -3.27292300 | -0.70190000 |
| H | 4.51446100 | -3.75423200 | -2.39101900 |
| H | 6.80102200 | -2.56204200 | 1.05702400 |
| H | 6.51567900 | -4.02563300 | -0.93621800 |
| C | -0.44862400 | -1.35920500 | 2.76454300 |
| H | -0.15938600 | -0.90766500 | 3.72711100 |
| H | -1.52566800 | -1.17446400 | 2.63672000 |
| C | -0.18931400 | -2.86554400 | 2.80331100 |
| H | 0.87531800 | -3.07331000 | 2.95806600 |
| H | -0.75365800 | -3.33764600 | 3.61718600 |
| H | -0.49544700 | -3.33274700 | 1.86033900 |
| O | 0.26500300 | -0.71126300 | 1.72580500 |

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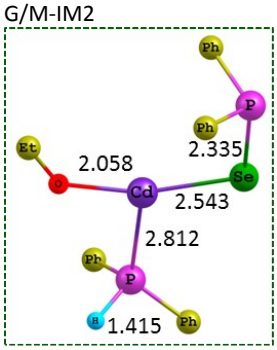


| | | | |
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| Se | 0.81833700 | -1.69646700 | -1.03556400 |
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| C | 3.68994100 | -1.33342400 | 0.55537100 |
| C | 3.62323600 | -0.18544800 | 1.36337300 |
| C | 4.19977000 | -2.51862500 | 1.11179400 |
| C | 4.04765100 | -0.22510500 | 2.69313800 |
| H | 3.25057200 | 0.74819400 | 0.95189900 |
| C | 4.62047500 | -2.56124800 | 2.44430100 |
| H | 4.26370600 | -3.41330100 | 0.49751300 |
| C | 4.54494100 | -1.41406200 | 3.23833800 |
| H | 3.98956700 | 0.67236400 | 3.30302800 |
| H | 5.01035800 | -3.48716300 | 2.85808700 |
| H | 4.87440300 | -1.44304300 | 4.27319300 |
| C | 3.40260200 | 0.32651700 | -1.77825600 |
| C | 4.69205600 | 0.87526700 | -1.63022000 |
| C | 2.44641000 | 1.06040300 | -2.49694700 |
| C | 5.00288000 | 2.12760900 | -2.16202000 |
| H | 5.45843200 | 0.32587800 | -1.08971800 |
| C | 2.76000700 | 2.31405300 | -3.03340900 |
| H | 1.45215900 | 0.64845200 | -2.64057200 |
| C | 4.03629500 | 2.85456200 | -2.86541000 |
| H | 6.00124400 | 2.53493900 | -2.02694100 |
| H | 2.00152800 | 2.86628100 | -3.58186000 |
| H | 4.27848300 | 3.82899500 | -3.27994100 |
| Cd | -0.02994200 | 0.16001000 | 0.48203900 |
| P | -2.80971600 | -0.13371600 | 0.79132700 |
| H | -3.17524300 | -0.18557600 | 2.15774600 |

| | | | |
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| C | -3.71035100 | -1.60450200 | 0.17491500 |
| C | -3.32877500 | -2.17588700 | -1.05081900 |
| C | -4.75353700 | -2.19501000 | 0.90886700 |
| C | -3.99001700 | -3.30456800 | -1.54068000 |
| H | -2.50721200 | -1.74881700 | -1.62005900 |
| C | -5.40647700 | -3.32999000 | 0.42170800 |
| H | -5.05739300 | -1.76901800 | 1.86120000 |
| C | -5.02813600 | -3.88357600 | -0.80513400 |
| H | -3.68377300 | -3.73750700 | -2.48836000 |
| H | -6.20867000 | -3.77976900 | 0.99980500 |
| H | -5.53533000 | -4.76685000 | -1.18246900 |
| C | -3.75246400 | 1.34767200 | 0.22462700 |
| C | -3.16536500 | 2.60527600 | 0.44943300 |
| C | -4.99476100 | 1.26378900 | -0.42170200 |
| C | -3.83446000 | 3.76457800 | 0.04812500 |
| H | -2.18958300 | 2.67024300 | 0.93064600 |
| C | -5.65006600 | 2.42902800 | -0.83070200 |
| H | -5.45214100 | 0.29723400 | -0.60927600 |
| C | -5.07414800 | 3.68015000 | -0.59296800 |
| H | -3.37934700 | 4.73427300 | 0.22949900 |
| H | -6.61053700 | 2.35647000 | -1.33335800 |
| H | -5.58657400 | 4.58384900 | -0.91088400 |
| C | 0.94674800 | 2.62840000 | 2.05999500 |
| H | 1.55813700 | 2.05365000 | 2.77851200 |
| H | 1.61545300 | 2.90360300 | 1.22465000 |
| C | 0.46069800 | 3.90706600 | 2.74314800 |
| H | -0.18964800 | 3.66344500 | 3.59035500 |
| H | 1.30775100 | 4.49879200 | 3.11341900 |
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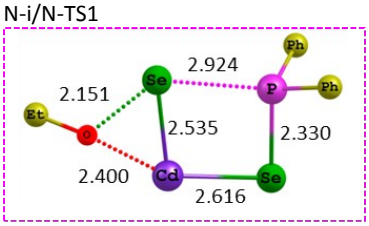
| O | -0.16107700 | 1.87334600 | 1.61533100 |

N-i/N-TS1




| | | | |
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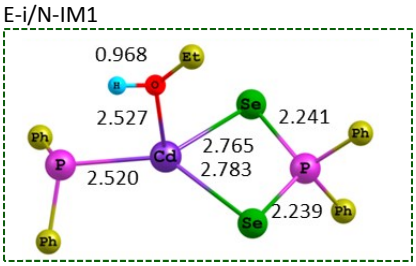
| H | 4.35209800 | 1.66115400 | -0.68469200 |
| H | 5.55287900 | 0.41685300 | -0.26983900 |
| C | 5.07038500 | 0.51188900 | -2.37687300 |
| H | 5.43778100 | -0.49543600 | -2.59713700 |
| H | 4.20737900 | 0.71265500 | -3.02144000 |
| H | 5.85616700 | 1.23544600 | -2.62618400 |
| P | -0.98165800 | 0.01785400 | -0.12193600 |
| Se | -0.43636700 | -0.36549600 | 2.11067800 |
| Se | 1.69115400 | 0.01637500 | -1.30798900 |
| C | -1.93922200 | 1.59040900 | -0.10661000 |
| C | -1.34046200 | 2.72654200 | -0.67285900 |
| C | -3.22053700 | 1.69903400 | 0.46180700 |
| C | -2.01289800 | 3.95286900 | -0.67348000 |
| H | -0.34891900 | 2.64947000 | -1.11116900 |
| C | -3.88892500 | 2.92341400 | 0.45823400 |
| H | -3.69465500 | 0.82750900 | 0.90309100 |
| C | -3.28624500 | 4.05283200 | -0.10865100 |
| H | -1.54163700 | 4.82517300 | -1.11736300 |
| H | -4.87851100 | 2.99781900 | 0.90045900 |
| H | -3.80941100 | 5.00492500 | -0.10921500 |
| C | -2.23357100 | -1.25972200 | -0.57244300 |
| C | -3.06651100 | -1.01068000 | -1.67950900 |
| C | -2.28295100 | -2.51950800 | 0.04345400 |
| C | -3.93736200 | -1.99653500 | -2.14647400 |
| H | -3.04012300 | -0.04595700 | -2.17815400 |
| C | -3.15533900 | -3.50401400 | -0.42868900 |
| H | -1.64810900 | -2.72633000 | 0.89897400 |
| C | -3.98521400 | -3.24716800 | -1.52279000 |
| H | -4.57709100 | -1.78579800 | -2.99891300 |
| H | -3.18660600 | -4.47161100 | 0.06442400 |
| H | -4.66276000 | -4.01375800 | -1.88762000 |
| O | 3.67734500 | -0.30567200 | -0.54796800 |

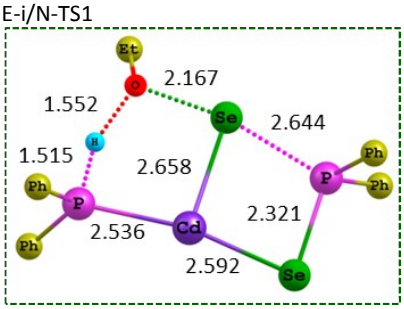
E-i/N-IM1




| | | | |
|---|---|---|---|
| Cd | 0.89181900 | -0.63166000 | 0.01499300 |
| Se | -1.14748000 | 0.04784200 | 1.78242700 |
| Se | -1.03198000 | -0.05251700 | -1.88451800 |
| P | -2.30879900 | 0.39864000 | -0.09946400 |
| C | -3.83389400 | -0.62800100 | -0.13727900 |
| C | -4.15843900 | -1.50002400 | 0.90885600 |
| C | -4.68419800 | -0.53308500 | -1.25219600 |
| C | -5.32665400 | -2.26727200 | 0.84387300 |
| H | -3.49963900 | -1.57642700 | 1.76856700 |
| C | -5.84770600 | -1.29926800 | -1.31181600 |
| H | -4.43693200 | 0.13338600 | -2.07356600 |
| C | -6.17117900 | -2.16888100 | -0.26347300 |
| H | -5.57317200 | -2.93873100 | 1.66148000 |
| H | -6.49937700 | -1.22074000 | -2.17719800 |
| H | -7.07745000 | -2.76577900 | -0.31268100 |
| C | -2.93246700 | 2.12581000 | -0.15405000 |
| C | -2.40446400 | 3.06449100 | -1.04890400 |
| C | -3.93227700 | 2.51505000 | 0.75330300 |
| C | -2.87603300 | 4.38083100 | -1.04013300 |
| H | -1.63182200 | 2.76466300 | -1.74999000 |
| C | -4.39958700 | 3.82900300 | 0.75710000 |
| H | -4.34499300 | 1.79650500 | 1.45544900 |
| C | -3.87168700 | 4.76486400 | -0.13959800 |
| H | -2.46346600 | 5.10237800 | -1.73939000 |
| H | -5.17332100 | 4.12262400 | 1.46058100 |
| H | -4.23662700 | 5.78799700 | -0.13436300 |
| H | 1.54527800 | -3.54260500 | 0.19333900 |
| C | -0.36421400 | -4.12119100 | 0.02274900 |
| H | -0.17190200 | -4.92037600 | -0.70523600 |
| H | -1.25809700 | -3.58237400 | -0.30038200 |
| C | -0.54213200 | -4.68740300 | 1.42582200 |
| H | -1.37618900 | -5.39858400 | 1.44189100 |
| H | 0.35650100 | -5.22182900 | 1.75701800 |
| H | -0.75385900 | -3.88814900 | 2.14249500 |
| P | 3.38050100 | -0.95190200 | 0.24498700 |
| C | 4.05003400 | -0.22767200 | -1.32863900 |
| C | 3.65824800 | 1.01458100 | -1.86374900 |
| C | 4.98989000 | -0.98806500 | -2.04644000 |
| C | 4.18943000 | 1.47948100 | -3.06825700 |
| H | 2.93282100 | 1.62399000 | -1.33156300 |
| C | 5.51941700 | -0.52851600 | -3.25777700 |
| H | 5.31064300 | -1.94749500 | -1.64911800 |
| C | 5.12081300 | 0.70698200 | -3.77173400 |
| H | 3.87046300 | 2.44089600 | -3.46206900 |
| H | 6.24362400 | -1.13545900 | -3.79463000 |
| H | 5.52932200 | 1.06650000 | -4.71211600 |
| C | 3.85657300 | 0.28139600 | 1.54247300 |
| C | 4.83340900 | 1.27503600 | 1.35343900 |
| C | 3.29642500 | 0.14634400 | 2.82900800 |

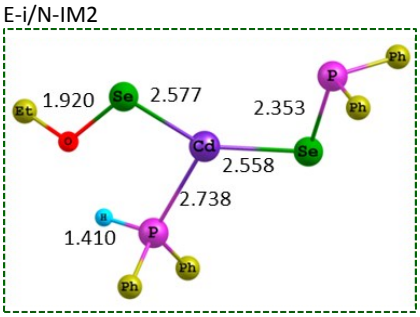
| | | | |
|---|---|---|---|
| C | 5.22376900 | 2.10810600 | 2.40733000 |
| H | 5.29496900 | 1.40342500 | 0.37970300 |
| C | 3.68347600 | 0.97913700 | 3.87851400 |
| H | 2.54512800 | -0.61932400 | 3.01268700 |
| C | 4.65123100 | 1.96933300 | 3.67353700 |
| H | 5.97988000 | 2.86938900 | 2.23232300 |
| H | 3.22687300 | 0.85641400 | 4.85719300 |
| H | 4.95334600 | 2.62006100 | 4.48913100 |
| O | 0.69501200 | -3.14989900 | -0.05159500 |

E-i/N-TS1




| | | | |
|---|---|---|---|
| Cd | 0.47921400 | -0.13088400 | -0.86438500 |
| Se | -0.57447500 | 0.11135200 | 1.56415300 |
| Se | -1.75003300 | -0.26300100 | -2.18057700 |
| P | -2.65783000 | -0.01910300 | -0.05795800 |
| C | -3.78792100 | -1.45324900 | 0.17392600 |
| C | -3.40612900 | -2.46424700 | 1.06886800 |
| C | -4.99874700 | -1.57719000 | -0.52908100 |
| C | -4.22353000 | -3.58303900 | 1.25888400 |
| H | -2.47214000 | -2.36968600 | 1.61605600 |
| C | -5.81199600 | -2.69419100 | -0.33668500 |
| H | -5.30602200 | -0.80081200 | -1.22352400 |
| C | -5.42555200 | -3.69987200 | 0.55733800 |
| H | -3.92076000 | -4.35841000 | 1.95706800 |
| H | -6.74569500 | -2.78178600 | -0.88536200 |
| H | -6.06100100 | -4.56862700 | 0.70539700 |
| C | -3.80233600 | 1.42376700 | -0.12192000 |
| C | -3.72707900 | 2.41206200 | -1.11362600 |
| C | -4.70785500 | 1.59264300 | 0.94214000 |
| C | -4.55099200 | 3.54019300 | -1.05109500 |
| H | -3.03044000 | 2.29475200 | -1.93770200 |
| C | -5.52951500 | 2.71882700 | 0.99999700 |
| H | -4.77500000 | 0.84340700 | 1.72621700 |
| C | -5.45413300 | 3.69703400 | 0.00264800 |
| H | -4.48618000 | 4.29376800 | -1.83117300 |
| H | -6.22654700 | 2.83263100 | 1.82557200 |
| H | -6.09395200 | 4.57373100 | 0.04889500 |
| H | 2.39606300 | -0.10819700 | 1.38080800 |
| C | 1.46271800 | -0.59247000 | 3.67597200 |
| H | 1.38034900 | -1.66618800 | 3.42992500 |
| H | 0.62239200 | -0.35621900 | 4.34684600 |
| C | 2.78144600 | -0.32745700 | 4.40426900 |
| H | 2.84123700 | -0.92754100 | 5.32101700 |
| H | 3.64006200 | -0.58641800 | 3.77403700 |
| H | 2.86417800 | 0.73003200 | 4.67683000 |
| P | 2.88107000 | -0.05400100 | -0.05349400 |
| C | 4.10504900 | -1.35234100 | -0.45981200 |
| C | 3.79467000 | -2.35899500 | -1.38739500 |
| C | 5.35183900 | -1.38410500 | 0.19159100 |
| C | 4.70795100 | -3.38332500 | -1.65497300 |
| H | 2.84046300 | -2.34273500 | -1.90704900 |
| C | 6.26437900 | -2.40330600 | -0.08320300 |
| H | 5.60889500 | -0.61130600 | 0.91033700 |
| C | 5.94362400 | -3.40653000 | -1.00470200 |
| H | 4.45386400 | -4.15630400 | -2.37445700 |
| H | 7.22386900 | -2.41695100 | 0.42592200 |
| H | 6.65505500 | -4.19991800 | -1.21472000 |
| C | 3.70551800 | 1.57531300 | -0.16429500 |
| C | 4.62163500 | 1.88355100 | -1.18345000 |
| C | 3.36115000 | 2.55880200 | 0.78038600 |
| C | 5.19369100 | 3.15549200 | -1.25071500 |
| H | 4.89432600 | 1.13179600 | -1.91896800 |
| C | 3.92987300 | 3.83269900 | 0.69892500 |
| H | 2.65791300 | 2.32165600 | 1.57506200 |
| C | 4.84693300 | 4.13336500 | -0.31225600 |
| H | 5.90652000 | 3.38341500 | -2.03827700 |
| H | 3.65974400 | 4.58679400 | 1.43269800 |
| H | 5.29097600 | 5.12310200 | -0.36872300 |
| O | 1.37451200 | 0.20131200 | 2.50719200 |

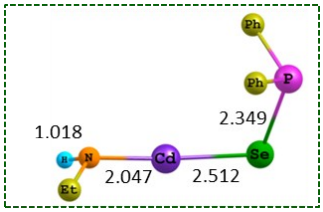
E-i/N-IM2




| | | | |
|---|---|---|---|
| Se | -1.47207200 | 1.01026500 | -0.03953700 |
| P | -3.20487700 | -0.53619300 | -0.41840400 |
| C | -4.56858700 | 0.65086000 | -0.82805300 |
| C | -5.36450600 | 1.30647400 | 0.12559000 |
| C | -4.81141100 | 0.89291800 | -2.19150500 |
| C | -6.37487700 | 2.18390600 | -0.27579800 |
| H | -5.19797200 | 1.12845700 | 1.18345600 |
| C | -5.81747700 | 1.77474200 | -2.59309600 |
| H | -4.20844200 | 0.38663700 | -2.94140300 |
| C | -6.60279500 | 2.42244200 | -1.63477900 |
| H | -6.98334500 | 2.68254300 | 0.47402900 |
| H | -5.99086300 | 1.95085400 | -3.65122400 |
| H | -7.38972900 | 3.10466600 | -1.94433900 |
| C | -3.71326100 | -1.09588600 | 1.28030500 |
| C | -4.66693300 | -2.13058700 | 1.31919100 |
| C | -3.19268500 | -0.61885400 | 2.49120800 |
| C | -5.10631800 | -2.65441600 | 2.53636600 |
| H | -5.06896300 | -2.53019800 | 0.39058800 |
| C | -3.62476000 | -1.15105600 | 3.71112100 |
| H | -2.44496100 | 0.16842000 | 2.47903800 |
| C | -4.58407500 | -2.16596000 | 3.73876100 |
| H | -5.84666300 | -3.44978500 | 2.54504800 |
| H | -3.20916500 | -0.76900100 | 4.63991400 |
| H | -4.91708600 | -2.57905100 | 4.68684000 |
| Cd | 0.48526800 | -0.53014000 | -0.62415800 |
| Se | 1.24445500 | -2.87368700 | -1.38019800 |
| C | 3.76809500 | -2.81048400 | -2.64725500 |
| H | 3.53779900 | -3.85777300 | -2.89010000 |
| H | 4.83679500 | -2.75942200 | -2.39677300 |
| C | 3.45909000 | -1.90609800 | -3.83663100 |
| H | 3.73260000 | -0.86760300 | -3.61920800 |
| H | 4.02800500 | -2.23160300 | -4.71584600 |
| H | 2.39467100 | -1.94003900 | -4.08774100 |
| P | 2.87429000 | 0.71877700 | -0.14777300 |
| H | 3.83887400 | 0.43769000 | -1.13734800 |
| C | 2.94227900 | 2.54868700 | -0.11652300 |
| C | 4.09102100 | 3.24104600 | -0.53880300 |
| C | 1.82357600 | 3.27816600 | 0.31802200 |
| C | 4.12021600 | 4.63677100 | -0.51949500 |
| H | 4.96387300 | 2.69102300 | -0.87987800 |
| C | 1.85891500 | 4.67516900 | 0.34350500 |

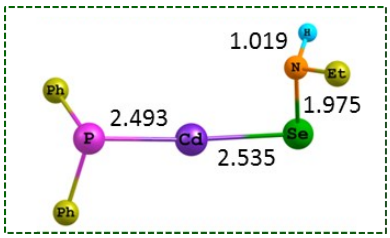
| | | | |
|---|---|---|---|
| H | 0.91912600 | 2.76213800 | 0.62860700 |
| C | 3.00509300 | 5.35522400 | -0.07562000 |
| H | 5.01136700 | 5.16175900 | -0.85134700 |
| H | 0.98649900 | 5.22743200 | 0.67976900 |
| H | 3.02847800 | 6.44109700 | -0.06299700 |
| C | 3.72772500 | 0.12821400 | 1.37497800 |
| C | 4.02763700 | -1.24197200 | 1.47622200 |
| C | 4.02591200 | 0.98748300 | 2.44228600 |
| C | 4.63870400 | -1.73383900 | 2.63154900 |
| H | 3.78952600 | -1.91391200 | 0.65442600 |
| C | 4.62942400 | 0.48298000 | 3.59843400 |
| H | 3.79607200 | 2.04632700 | 2.37606800 |
| C | 4.93897600 | -0.87575800 | 3.69453600 |
| H | 4.87333200 | -2.79219300 | 2.70126700 |
| H | 4.85797400 | 1.15532700 | 4.42056900 |
| H | 5.40859200 | -1.26504200 | 4.59338000 |
| O | 3.11057800 | -2.42568600 | -1.43733300 |

H




| | | | |
|---|---|---|---|
| Se | -0.36898000 | -0.88725600 | -2.10840000 |
| P | -1.85308300 | 0.66356800 | -1.15466500 |
| C | -0.71570700 | 1.91796800 | -0.39865400 |
| C | -0.09060300 | 1.77815700 | 0.85357200 |
| C | -0.45678600 | 3.07376700 | -1.15475800 |
| C | 0.78035200 | 2.76187300 | 1.32834600 |
| H | -0.29285900 | 0.90697600 | 1.47077000 |
| C | 0.41610300 | 4.05769000 | -0.68115500 |
| H | -0.93837600 | 3.20024900 | -2.12108300 |
| C | 1.03783900 | 3.90315400 | 0.56083100 |
| H | 1.25478600 | 2.63591800 | 2.29751900 |
| H | 0.60583700 | 4.94412600 | -1.27994600 |
| H | 1.71441900 | 4.66782200 | 0.93182000 |
| C | -2.55310800 | -0.16689500 | 0.34916700 |
| C | -3.21392400 | 0.64076700 | 1.29593400 |
| C | -2.61352500 | -1.56032100 | 0.50343100 |
| C | -3.88772000 | 0.07025300 | 2.37676300 |
| H | -3.19823000 | 1.72295400 | 1.19507100 |
| C | -3.29454400 | -2.13112700 | 1.58418100 |
| H | -2.12796600 | -2.20260100 | -0.22487000 |
| C | -3.92987300 | -1.32013200 | 2.52646200 |
| H | -4.38110200 | 0.71267800 | 3.10101800 |
| H | -3.32561800 | -3.21262400 | 1.68581100 |
| H | -4.45632200 | -1.76409000 | 3.36649000 |
| Cd | 1.41773900 | -1.09104300 | -0.35384600 |
| N | 2.79481200 | -1.20200600 | 1.15699900 |
| H | 2.96806000 | -2.15858000 | 1.46029500 |
| C | 4.05828600 | -0.45592900 | 1.10287300 |
| H | 4.78033800 | -0.86843400 | 0.37688100 |
| H | 3.83961800 | 0.56756700 | 0.77194400 |
| C | 4.72799000 | -0.39988000 | 2.48096700 |
| H | 4.97660900 | -1.40807500 | 2.83515500 |
| H | 5.65944800 | 0.17834800 | 2.44023600 |
| H | 4.05906400 | 0.05897800 | 3.21633600 |

H-i




| | | | |
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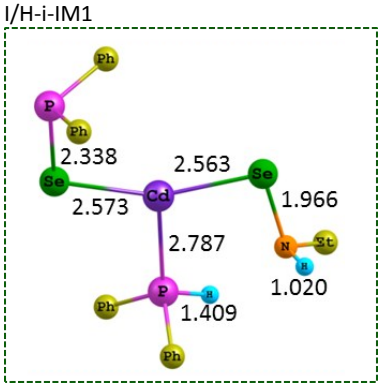
| P | -1.30036300 | 0.10495800 | 1.21302500 |
| C | -1.97853600 | 1.61797200 | 0.37330300 |
| C | -2.37156200 | 2.68221600 | 1.20397900 |
| C | -2.09731100 | 1.78600500 | -1.02000000 |
| C | -2.86603800 | 3.87467700 | 0.66357800 |
| H | -2.29055900 | 2.57371200 | 2.28225000 |
| C | -2.59512700 | 2.97238200 | -1.56158400 |
| H | -1.80458800 | 0.98024700 | -1.68838500 |
| C | -2.97927300 | 4.02266800 | -0.71995200 |
| H | -3.16271400 | 4.68358000 | 1.32553600 |
| H | -2.67683200 | 3.07972700 | -2.63979900 |
| H | -3.36160200 | 4.94777200 | -1.14194200 |
| C | -2.36792800 | -1.28101500 | 0.58903800 |
| C | -3.60746400 | -1.09034200 | -0.04482000 |
| C | -1.97065100 | -2.60105600 | 0.88249300 |
| C | -4.41203400 | -2.18282300 | -0.38693500 |
| H | -3.95322300 | -0.08753200 | -0.27278900 |
| C | -2.77050600 | -3.68974600 | 0.53577500 |
| H | -1.02570900 | -2.78109700 | 1.39206800 |
| C | -3.99835300 | -3.48613400 | -0.10462000 |
| H | -5.36630700 | -2.00856900 | -0.87716700 |
| H | -2.43627400 | -4.69731800 | 0.76817000 |
| H | -4.62323900 | -4.33222800 | -0.37525900 |
| Cd | 0.76696900 | -0.27838000 | -0.12618000 |
| Se | 3.02209800 | -0.59094300 | -1.24192000 |
| N | 3.64115600 | 0.58601400 | 0.21766200 |
| H | 4.00106600 | 1.41498900 | -0.25395800 |
| C | 4.71646700 | -0.01504800 | 1.02124900 |
| H | 4.30819500 | -0.91120800 | 1.50123500 |
| H | 5.57187200 | -0.34270700 | 0.40818000 |
| C | 5.18764900 | 0.98265600 | 2.08188600 |
| H | 5.96658500 | 0.53223800 | 2.70708500 |
| H | 5.61143200 | 1.88327800 | 1.62114900 |
| H | 4.35738700 | 1.28844800 | 2.72622100 |

I/H-i-IM1




| | | | |
|---|---|---|---|
| Se | -0.95130400 | -2.11959400 | -0.48816100 |
| P | -3.27882200 | -1.97437000 | -0.32820100 |
| C | -3.67817600 | -0.42044200 | -1.25656500 |
| C | -3.68890100 | 0.86686300 | -0.69115300 |
| C | -3.98911600 | -0.55931500 | -2.62054000 |
| C | -3.99141000 | 1.98462000 | -1.47362000 |
| H | -3.46788300 | 0.99915400 | 0.36370600 |
| C | -4.28543700 | 0.55874900 | -3.40445300 |
| H | -3.99533700 | -1.54951100 | -3.06955800 |
| C | -4.28679000 | 1.83425400 | -2.83237200 |

| | | | |
|---|---|---|---|
| H | -3.99277000 | 2.97238700 | -1.02087100 |
| H | -4.52074900 | 0.43256500 | -4.45774100 |
| H | -4.51930800 | 2.70493600 | -3.43902500 |
| C | -3.64026500 | -1.45968000 | 1.41978800 |
| C | -4.98659600 | -1.18547500 | 1.73217200 |
| C | -2.70183200 | -1.46057400 | 2.46085500 |
| C | -5.37323600 | -0.89184000 | 3.04026800 |
| H | -5.73909600 | -1.19514800 | 0.94697400 |
| C | -3.09088700 | -1.17329500 | 3.77432800 |
| H | -1.66305100 | -1.68896900 | 2.24353500 |
| C | -4.42438800 | -0.88443600 | 4.06903500 |
| H | -6.41552500 | -0.67356500 | 3.25674800 |
| H | -2.34591200 | -1.17500000 | 4.56571200 |
| H | -4.72499800 | -0.66051600 | 5.08870200 |
| Cd | -0.05987700 | 0.29162500 | -0.38059600 |
| Se | -0.28807500 | 2.83688300 | -0.18850200 |
| N | 1.59947900 | 3.09855100 | 0.29568800 |
| H | 1.57792600 | 3.42187700 | 1.26259900 |
| C | 2.28490000 | 4.09958300 | -0.53395300 |
| H | 2.25136800 | 3.74391800 | -1.57056300 |
| H | 3.34197300 | 4.08200300 | -0.22412900 |
| C | 1.76361400 | 5.53960700 | -0.46035400 |
| H | 1.81077600 | 5.92203800 | 0.56667100 |
| H | 2.36620900 | 6.20112300 | -1.09425700 |
| H | 0.72452000 | 5.59758800 | -0.79936700 |
| P | 2.71672300 | 0.05992200 | -0.33721800 |
| H | 3.40865700 | 1.18570400 | -0.82523700 |
| C | 3.42315900 | -0.04000800 | 1.35538700 |
| C | 4.23786800 | 0.97809700 | 1.87406100 |
| C | 3.10193500 | -1.14075600 | 2.16745700 |
| C | 4.73055400 | 0.89198000 | 3.17935300 |
| H | 4.48424600 | 1.84061300 | 1.26191900 |
| C | 3.60110400 | -1.22715500 | 3.46848600 |
| H | 2.46556100 | -1.93490200 | 1.78477300 |
| C | 4.41525600 | -0.21056200 | 3.97803100 |
| H | 5.36204100 | 1.68540000 | 3.56928400 |
| H | 3.34920400 | -2.08542500 | 4.08471000 |
| H | 4.79979000 | -0.27713300 | 4.99163100 |
| C | 3.54000200 | -1.29984100 | -1.27355700 |
| C | 4.94045100 | -1.42522600 | -1.30437700 |
| C | 2.75598400 | -2.21898100 | -1.98624500 |
| C | 5.54142400 | -2.44791100 | -2.03834800 |
| H | 5.56162000 | -0.72787500 | -0.74871400 |
| C | 3.36098400 | -3.24598300 | -2.71959100 |
| H | 1.67205300 | -2.14515000 | -1.97073400 |
| C | 4.75152200 | -3.36066600 | -2.74791700 |
| H | 6.62422900 | -2.53439700 | -2.05640700 |
| H | 2.74106100 | -3.95276300 | -3.26330300 |
| H | 5.22114700 | -4.15755000 | -3.31751800 |

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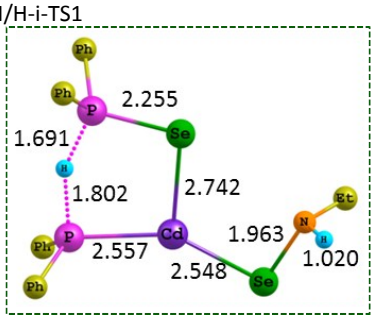


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| Cd | -0.28480900 | -1.52065600 | 0.08551900 |
| Se | -0.59248000 | 1.18228600 | -0.25664800 |
| P | 2.24474700 | -1.54984200 | 0.46026000 |
| H | 2.26960100 | 0.25129400 | 0.43240000 |
| C | 2.83082400 | -2.28565400 | 2.03653100 |
| C | 2.20814600 | -3.41266900 | 2.60232900 |
| C | 3.90750700 | -1.69502300 | 2.72330800 |
| C | 2.65558200 | -3.93923700 | 3.81696300 |
| H | 1.37258600 | -3.88040300 | 2.08946500 |
| C | 4.35651100 | -2.22351100 | 3.93648700 |
| H | 4.39516300 | -0.81835300 | 2.30621400 |
| C | 3.73061800 | -3.34625900 | 4.48578400 |
| H | 2.16265200 | -4.80998600 | 4.24004900 |
| H | 5.18957500 | -1.75514900 | 4.45319900 |
| H | 4.07588700 | -3.75465400 | 5.43135500 |
| C | 3.20626900 | -2.31254600 | -0.89906700 |
| C | 4.29137500 | -3.17856300 | -0.67463300 |
| C | 2.87527400 | -1.98159100 | -2.22855300 |
| C | 5.02112300 | -3.69584400 | -1.74853100 |
| H | 4.56485400 | -3.45425400 | 0.33896500 |
| C | 3.60828300 | -2.49915900 | -3.29702100 |
| H | 2.03381200 | -1.32341300 | -2.43410600 |
| C | 4.68668400 | -3.35933500 | -3.06303700 |
| H | 5.85287600 | -4.36751600 | -1.55327300 |
| H | 3.33107100 | -2.23465100 | -4.31384900 |
| H | 5.25395600 | -3.76589000 | -3.89511700 |
| P | 1.52837300 | 1.76031300 | 0.24832700 |
| C | 1.57031400 | 2.87011200 | 1.70921400 |
| C | 0.51668000 | 2.89313700 | 2.63562100 |
| C | 2.72736300 | 3.62907100 | 1.96787200 |
| C | 0.61656400 | 3.66348800 | 3.79748800 |
| H | -0.38364600 | 2.31981000 | 2.43670900 |
| C | 2.82097800 | 4.39789000 | 3.12887300 |
| H | 3.55139500 | 3.62819100 | 1.25996400 |
| C | 1.76645700 | 4.41636600 | 4.04815400 |
| H | -0.20953800 | 3.67773800 | 4.50286800 |
| H | 3.71659900 | 4.98456800 | 3.31335800 |
| H | 1.84083800 | 5.01637200 | 4.95057700 |
| C | 2.28163800 | 2.72108400 | -1.11633300 |
| C | 3.31770700 | 2.13741800 | -1.86285500 |
| C | 1.83121300 | 4.00878700 | -1.45299300 |
| C | 3.90040500 | 2.83492300 | -2.92574000 |
| H | 3.67182700 | 1.13931300 | -1.62021900 |
| C | 2.41597400 | 4.70235200 | -2.51278300 |
| H | 1.02311500 | 4.46499400 | -0.88867600 |
| C | 3.45125500 | 4.11667400 | -3.25096500 |
| H | 4.70261300 | 2.37502200 | -3.49568100 |
| H | 2.06114100 | 5.69725400 | -2.76649100 |
| H | 3.90333000 | 4.65839600 | -4.07692500 |
| N | -3.51331100 | -1.24093400 | -0.49784500 |
| H | -3.92149000 | -1.41860400 | -1.41508600 |
| C | -4.59216200 | -1.02614100 | 0.47581700 |
| H | -5.25658200 | -1.89996500 | 0.58570600 |
| H | -4.12460000 | -0.85807900 | 1.45236700 |
| C | -5.41288300 | 0.20114600 | 0.07048600 |
| H | -5.90136100 | 0.05020900 | -0.90016000 |
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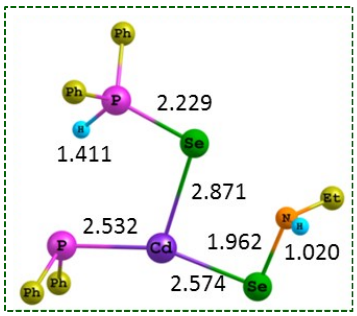


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| Se | -1.52659700 | 3.39032600 | -1.19460900 |
| Cd | -1.16055200 | 1.02357200 | -0.25051800 |
| Se | 1.68607900 | 1.20664600 | -0.57314400 |
| P | -1.73361100 | -1.23624700 | 0.73785800 |
| H | 1.17951800 | -1.28438000 | 1.09682500 |
| C | -3.01077500 | -0.80705500 | 2.01418700 |
| C | -4.22921100 | -0.16123900 | 1.72839900 |
| C | -2.72553500 | -1.11752200 | 3.35528900 |
| C | -5.12776000 | 0.15927000 | 2.74677700 |
| H | -4.47564900 | 0.09164500 | 0.70071700 |
| C | -3.61900900 | -0.78522900 | 4.38004700 |
| H | -1.79688100 | -1.62837900 | 3.59695200 |
| C | -4.82394800 | -0.14783800 | 4.07875100 |
| H | -6.06185500 | 0.65819500 | 2.50246800 |
| H | -3.37452800 | -1.03263700 | 5.40968700 |
| H | -5.52140800 | 0.10870500 | 4.87121600 |
| C | -2.70526300 | -2.05123400 | -0.61315200 |
| C | -3.85461300 | -2.81934800 | -0.34695700 |
| C | -2.21728300 | -2.03954300 | -1.93495800 |
| C | -4.49451800 | -3.53390200 | -1.36361300 |
| H | -4.25614700 | -2.85955100 | 0.66100700 |
| C | -2.85238200 | -2.75863700 | -2.94906800 |
| H | -1.33307900 | -1.45543100 | -2.18206500 |
| C | -3.99881500 | -3.50971900 | -2.67021300 |
| H | -5.38452300 | -4.11257600 | -1.12962400 |
| H | -2.45589200 | -2.72153900 | -3.96039500 |
| H | -4.49968100 | -4.06266400 | -3.45964900 |
| P | 2.24231200 | -0.75008900 | 0.33794000 |
| C | 3.66872400 | -0.66077400 | 1.48543700 |
| C | 4.14157100 | 0.58182700 | 1.92700800 |
| C | 4.26501600 | -1.84233200 | 1.95817000 |
| C | 5.20172200 | 0.64272000 | 2.83609200 |
| H | 3.68191600 | 1.49300800 | 1.55606700 |
| C | 5.32056700 | -1.77524600 | 2.86866600 |
| H | 3.91374700 | -2.81088800 | 1.61386100 |
| C | 5.78991900 | -0.53275200 | 3.30857900 |
| H | 5.56519400 | 1.60925400 | 3.17252200 |
| H | 5.77752900 | -2.69145000 | 3.23112300 |
| H | 6.61347100 | -0.48314100 | 4.01512700 |
| C | 2.56907000 | -2.11618000 | -0.82167100 |
| C | 1.70151800 | -3.21887500 | -0.85545100 |
| C | 3.64935300 | -2.04805100 | -1.71613500 |
| C | 1.92339900 | -4.25203800 | -1.77106300 |
| H | 0.85102300 | -3.26926000 | -0.18065000 |
| C | 3.86880800 | -3.08522300 | -2.62225400 |
| H | 4.31369900 | -1.18838900 | -1.70592300 |
| C | 3.00577400 | -4.18722800 | -2.65145200 |
| H | 1.24623900 | -5.10057700 | -1.79641400 |
| H | 4.70744900 | -3.03106800 | -3.31018500 |
| H | 3.17594000 | -4.99018000 | -3.36285500 |
| N | 0.39060400 | 3.67874700 | -1.49311900 |
| H | 0.47998400 | 3.80884300 | -2.50040000 |
| C | 0.90217700 | 4.87209100 | -0.80279000 |
| H | 0.30147200 | 5.77191200 | -1.01244000 |
| H | 0.82731000 | 4.68210600 | 0.27371900 |
| C | 2.36045500 | 5.11953300 | -1.19656400 |
| H | 2.45206900 | 5.33403500 | -2.26857600 |
| H | 2.76011100 | 5.98176200 | -0.65081900 |
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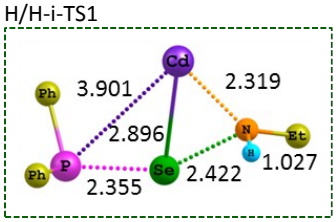
H/H-i-TS1

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| Cd | -1.29079600 | 0.63769400 | -1.44356500 |
| C | -4.28750900 | -0.40688500 | 0.03762100 |
| H | -4.25602300 | 0.57532100 | 0.52709200 |
| H | -5.00004300 | -0.31526400 | -0.79938600 |
| C | -4.80355400 | -1.47071100 | 1.01634900 |
| H | -4.89526400 | -2.44582000 | 0.52278400 |
| H | -4.12501900 | -1.58265400 | 1.86732900 |
| H | -5.79185000 | -1.19330100 | 1.40069100 |
| N | -2.95439400 | -0.67390600 | -0.50140100 |
| H | -2.92218600 | -1.64788200 | -0.82441000 |
| P | 1.09275800 | -0.23615700 | 1.51786700 |
| Se | -1.21050600 | -0.59086700 | 1.17724900 |
| C | 2.04401000 | -1.40012100 | 0.44867400 |
| C | 1.46633400 | -2.54179000 | -0.13024000 |
| C | 3.43848200 | -1.22468700 | 0.33760500 |
| C | 2.25485800 | -3.47108600 | -0.81587400 |
| H | 0.39655400 | -2.70195800 | -0.04149700 |
| C | 4.22301500 | -2.15100700 | -0.35073100 |
| H | 3.91486600 | -0.36005400 | 0.79214000 |
| C | 3.63340400 | -3.27920300 | -0.93149100 |
| H | 1.78726200 | -4.34587500 | -1.25978300 |
| H | 5.29533300 | -1.99380600 | -0.42885500 |
| H | 4.24461900 | -4.00215200 | -1.46424100 |
| C | 1.47463300 | 1.40216900 | 0.79980400 |
| C | 1.92180400 | 1.60754200 | -0.52122700 |
| C | 1.26037800 | 2.52918700 | 1.62022100 |
| C | 2.17992800 | 2.90103900 | -0.99161700 |
| H | 2.10462000 | 0.75755300 | -1.17013200 |
| C | 1.50292300 | 3.81580200 | 1.14323400 |
| H | 0.90660800 | 2.38861800 | 2.63837700 |
| C | 1.97352500 | 4.00453200 | -0.16352500 |
| H | 2.53827600 | 3.03952100 | -2.00806400 |
| H | 1.33771600 | 4.67186000 | 1.79143400 |
| H | 2.17594100 | 5.00703700 | -0.52987400 |

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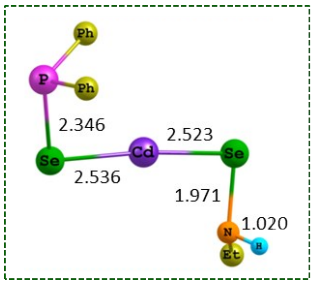


| | | | |
|---|---|---|---|
| Se | 0.80674000 | -0.68312400 | 2.17191800 |
| P | 2.68519800 | 0.28740000 | 1.15654200 |
| C | 1.94104300 | 1.70357100 | 0.21412700 |
| C | 1.39541800 | 1.59967800 | -1.07921500 |
| C | 1.91177300 | 2.95244000 | 0.85801900 |
| C | 0.82336600 | 2.71306300 | -1.70238200 |
| H | 1.43745000 | 0.65349900 | -1.61207600 |
| C | 1.33552500 | 4.06403500 | 0.23680500 |

| | | | |
|---|---|---|---|
| H | 2.33809200 | 3.05179300 | 1.85301200 |
| C | 0.78811000 | 3.94683600 | -1.04402300 |
| H | 0.40972100 | 2.61609600 | -2.70245200 |
| H | 1.31914800 | 5.02084200 | 0.75107500 |
| H | 0.34270500 | 4.81057800 | -1.52908300 |
| C | 3.16748200 | -0.85771000 | -0.22193800 |
| C | 4.16528600 | -0.40054000 | -1.10557000 |
| C | 2.71911300 | -2.18035100 | -0.34629300 |
| C | 4.67461300 | -1.23413400 | -2.10177200 |
| H | 4.54506800 | 0.61494900 | -1.01976100 |
| C | 3.23597200 | -3.01802700 | -1.34144400 |
| H | 1.96647500 | -2.55907900 | 0.33825600 |
| C | 4.21028100 | -2.54867500 | -2.22408100 |
| H | 5.43688400 | -0.85882900 | -2.77904800 |
| H | 2.87285100 | -4.03902700 | -1.42248900 |
| H | 4.60993100 | -3.19987000 | -2.99620500 |
| Cd | -0.98224300 | -0.18286800 | 0.44568600 |
| Se | -2.93324100 | 0.18611000 | -1.11024900 |
| N | -3.79962600 | -1.35880100 | -0.24641400 |
| H | -3.92305400 | -2.04121200 | -0.99373600 |
| C | -5.10310200 | -1.05127200 | 0.35948200 |
| H | -4.93535200 | -0.29119000 | 1.13070400 |
| H | -5.40967900 | -1.97052000 | 0.88023800 |
| C | -6.21876500 | -0.60086500 | -0.58928000 |
| H | -6.42123600 | -1.36432900 | -1.35043000 |
| H | -7.14827300 | -0.42468400 | -0.03510600 |
| H | -5.94930100 | 0.32942900 | -1.10040300 |

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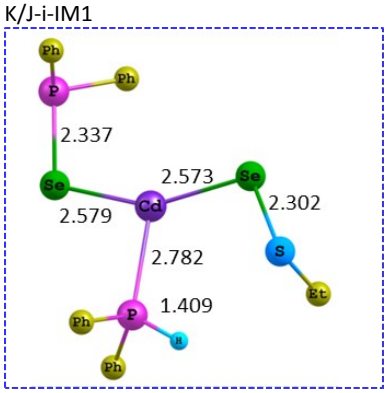


| | | | |
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| Se | 0.80014900 | -1.51251900 | 1.46409000 |
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| C | 3.50531400 | 0.37720400 | 1.50655400 |
| C | 3.65070900 | 1.12402000 | 0.32422900 |
| C | 3.65140900 | 1.03421900 | 2.74078400 |
| C | 3.92485300 | 2.49327400 | 0.37715300 |
| H | 3.55979900 | 0.63598700 | -0.64160100 |
| C | 3.92035600 | 2.40440400 | 2.79389600 |
| H | 3.55176400 | 0.46804300 | 3.66361600 |
| C | 4.05742200 | 3.13741900 | 1.61152800 |
| H | 4.03057100 | 3.05561500 | -0.54635800 |
| H | 4.02895400 | 2.89620800 | 3.75673000 |
| H | 4.26891600 | 4.20224800 | 1.65025500 |
| C | 3.73361800 | -1.98189100 | -0.10980800 |
| C | 5.12463600 | -1.92425700 | -0.32646000 |
| C | 2.92757800 | -2.55731400 | -1.10130400 |
| C | 5.68478400 | -2.40079400 | -1.51214300 |
| H | 5.77545700 | -1.49831700 | 0.43377700 |
| C | 3.49014900 | -3.04145000 | -2.28799900 |
| H | 1.85593900 | -2.62890400 | -0.94396400 |
| C | 4.86761500 | -2.96246600 | -2.49981900 |
| H | 6.75903800 | -2.33744900 | -1.66301300 |
| H | 2.84617300 | -3.47872300 | -3.04644400 |
| H | 5.30316000 | -3.33730100 | -3.42174800 |
| Cd | 0.00342500 | 0.40195600 | -0.06865000 |
| Se | 0.49496300 | 2.48555200 | -1.49647200 |
| C | -2.30583700 | 4.13764600 | -1.34771600 |
| H | -2.34599800 | 3.73304300 | -0.33074800 |
| H | -3.33738600 | 4.21841100 | -1.71406700 |
| C | -1.61443600 | 5.49830200 | -1.37072400 |
| H | -1.60944800 | 5.91941600 | -2.38083300 |
| H | -2.13496300 | 6.19835000 | -0.70534800 |
| H | -0.57854100 | 5.41297600 | -1.02901100 |
| P | -2.71638900 | -0.17227400 | -0.16715400 |
| H | -3.48527000 | 0.75312700 | -0.90092500 |
| C | -3.15273400 | -1.71756000 | -1.05990500 |
| C | -4.13131900 | -1.72513700 | -2.06737300 |
| C | -2.47597000 | -2.90909500 | -0.74942800 |
| C | -4.43862100 | -2.90931000 | -2.74225900 |
| H | -4.65304200 | -0.80917700 | -2.33032800 |
| C | -2.79439500 | -4.09255600 | -1.41909700 |
| H | -1.69503600 | -2.91668100 | 0.00684400 |
| C | -3.77483900 | -4.09512100 | -2.41583100 |
| H | -5.19530100 | -2.90341500 | -3.52158600 |
| H | -2.26823000 | -5.00880600 | -1.16756800 |
| H | -4.01568400 | -5.01540900 | -2.94002900 |
| C | -3.64717500 | -0.19903600 | 1.41893200 |
| C | -4.99816800 | 0.18476200 | 1.47673400 |
| C | -2.99594500 | -0.59798300 | 2.59716900 |
| C | -5.68578500 | 0.16326100 | 2.69154700 |
| H | -5.51563700 | 0.49992600 | 0.57474900 |
| C | -3.69039400 | -0.62650900 | 3.80997700 |
| H | -1.94678700 | -0.88128500 | 2.57786600 |
| C | -5.03340100 | -0.24553500 | 3.85943800 |
| H | -6.72868700 | 0.46524800 | 2.72581000 |
| H | -3.17634000 | -0.93890100 | 4.71421000 |
| H | -5.56939400 | -0.26142600 | 4.80404200 |
| S | -1.56139700 | 2.86969600 | -2.45805600 |

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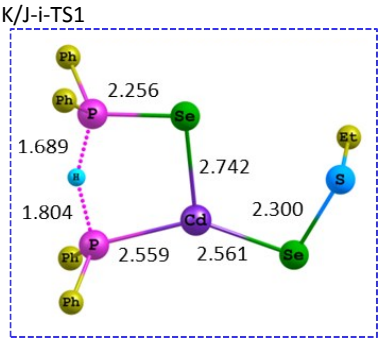


| | | | |
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| Se | 4.15238600 | -0.08769200 | -0.49869300 |
| Cd | 1.62302200 | 0.20716100 | -0.22442700 |
| Se | 0.08132700 | -2.03809900 | -0.53945000 |
| P | -0.23834100 | 1.89762600 | 0.25353700 |
| H | -1.44747800 | 0.56257900 | 0.15868700 |
| C | -0.14999900 | 2.68684700 | 1.90718100 |
| C | 0.74433300 | 3.73796300 | 2.18424600 |
| C | -0.96142600 | 2.20034000 | 2.94746000 |
| C | 0.81359400 | 4.29278200 | 3.46278100 |
| H | 1.38725200 | 4.12144600 | 1.39706000 |
| C | -0.87841100 | 2.74674700 | 4.23196100 |
| H | -1.66608900 | 1.39610500 | 2.75471700 |
| C | 0.00573000 | 3.79607000 | 4.49229400 |
| H | 1.50726300 | 5.10581200 | 3.65849200 |
| H | -1.51143400 | 2.35610300 | 5.02382100 |
| H | 0.06730500 | 4.22423500 | 5.48864800 |
| C | -0.43046600 | 3.22848400 | -0.98896800 |
| C | -1.13295500 | 4.41327600 | -0.69484700 |
| C | 0.04601600 | 3.04083300 | -2.29996100 |

| | | | |
|---|---|---|---|
| C | -1.34073300 | 5.37988100 | -1.68049000 |
| H | -1.51397300 | 4.58211500 | 0.30791100 |
| C | -0.17737300 | 4.00308000 | -3.28750500 |
| H | 0.60673700 | 2.14425700 | -2.55285900 |
| C | -0.86795200 | 5.17916000 | -2.98165200 |
| H | -1.87746400 | 6.29110600 | -1.43047600 |
| H | 0.20388400 | 3.83812500 | -4.29138800 |
| H | -1.03114000 | 5.93301500 | -3.74623300 |
| P | -1.89191400 | -1.05032200 | -0.07169600 |
| C | -2.69472700 | -1.84835000 | 1.37208600 |
| C | -1.96949300 | -2.64495500 | 2.27079900 |
| C | -4.04721800 | -1.56537900 | 1.64332400 |
| C | -2.58726100 | -3.15599600 | 3.41616300 |
| H | -0.92843100 | -2.87321800 | 2.06372100 |
| C | -4.65894700 | -2.07855700 | 2.78768700 |
| H | -4.62621100 | -0.95346000 | 0.95710900 |
| C | -3.93039200 | -2.87535900 | 3.67802700 |
| H | -2.01651300 | -3.77832700 | 4.09962700 |
| H | -5.70482800 | -1.85827000 | 2.98215500 |
| H | -4.40866800 | -3.27543700 | 4.56742500 |
| C | -3.06389200 | -1.25784300 | -1.46155800 |
| C | -3.36742800 | -0.14288500 | -2.25935200 |
| C | -3.63644300 | -2.50327500 | -1.76998200 |
| C | -4.23655900 | -0.27086700 | -3.34694700 |
| H | -2.92774500 | 0.82544400 | -2.03667400 |
| C | -4.50476000 | -2.62641100 | -2.85487200 |
| H | -3.40201300 | -3.37354500 | -1.16397400 |
| C | -4.80580500 | -1.51100100 | -3.64511300 |
| H | -4.46609400 | 0.59758700 | -3.95751600 |
| H | -4.94252700 | -3.59303400 | -3.08723400 |
| H | -5.48014100 | -1.61076300 | -4.49083100 |
| C | 4.33184000 | -3.11682800 | 0.63632500 |
| H | 5.22634100 | -2.71939700 | 1.12399600 |
| H | 3.45954500 | -2.84811500 | 1.23996200 |
| C | 4.42774100 | -4.63444400 | 0.46397700 |
| H | 5.29820500 | -4.91366000 | -0.13865200 |
| H | 4.52768100 | -5.11360600 | 1.44484100 |
| H | 3.53231200 | -5.03850800 | -0.01958100 |
| S | 4.16716600 | -2.32780300 | -1.02183900 |

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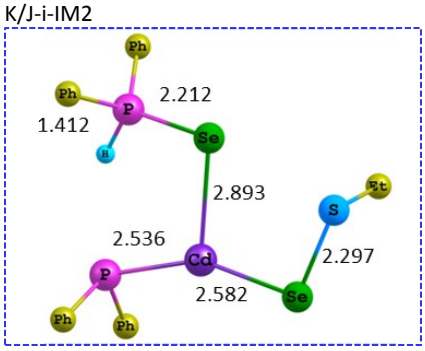


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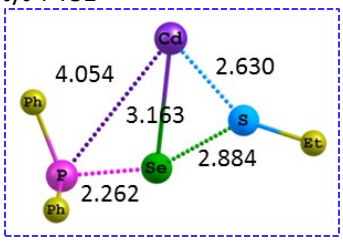
| Se | 1.62431800 | 1.20615700 | -0.65262100 |
| P | -1.51363700 | -1.48619100 | 0.77746800 |
| H | 1.26454000 | -1.31555900 | 0.97025100 |
| C | -2.83350100 | -1.17272400 | 2.04215400 |
| C | -4.11606900 | -0.67634600 | 1.73909100 |
| C | -2.51937900 | -1.41681300 | 3.39048100 |
| C | -5.04835000 | -0.43422300 | 2.74872600 |
| H | -4.38620900 | -0.47847900 | 0.70542300 |
| C | -3.44816800 | -1.16232600 | 4.40600100 |
| H | -1.54016200 | -1.81430900 | 3.64512100 |
| C | -4.71628700 | -0.67250000 | 4.08795900 |
| H | -6.03176100 | -0.04988300 | 2.49146100 |
| H | -3.18113800 | -1.35554400 | 5.44157700 |
| H | -5.44096700 | -0.47686100 | 4.87330100 |
| C | -2.37716300 | -2.44172100 | -0.55414900 |
| C | -3.43727700 | -3.32367100 | -0.27129300 |
| C | -1.88149600 | -2.41492600 | -1.87297700 |
| C | -3.98582500 | -4.13357200 | -1.26962900 |
| H | -3.84088100 | -3.37883200 | 0.73508100 |
| C | -2.42522300 | -3.22869000 | -2.86861000 |
| H | -1.06499600 | -1.74452400 | -2.13387300 |
| C | -3.48434200 | -4.09304200 | -2.57355400 |
| H | -4.80906100 | -4.79935200 | -1.02336400 |
| H | -2.02722100 | -3.17674400 | -3.87863900 |
| H | -3.91469200 | -4.72016500 | -3.34895900 |
| P | 2.31851500 | -0.67385800 | 0.28334200 |
| C | 3.66204400 | -0.44288900 | 1.50548700 |
| C | 3.99511700 | 0.83853400 | 1.96264400 |
| C | 4.33428700 | -1.56540600 | 2.01874500 |
| C | 4.99355200 | 0.99681900 | 2.92809700 |
| H | 3.47765600 | 1.70370400 | 1.55929100 |
| C | 5.32702200 | -1.40091500 | 2.98553900 |
| H | 4.09098800 | -2.56253900 | 1.66308200 |
| C | 5.65750800 | -0.11986500 | 3.44097700 |
| H | 5.25015900 | 1.99294100 | 3.27629700 |
| H | 5.84341800 | -2.27117800 | 3.37979700 |
| H | 6.43274400 | 0.00548000 | 4.19138600 |
| C | 2.85276900 | -1.97376300 | -0.87257500 |
| C | 2.09774600 | -3.15163200 | -0.98357800 |
| C | 3.98265800 | -1.78577100 | -1.68460700 |
| C | 2.48116300 | -4.14009600 | -1.89490600 |
| H | 1.21185000 | -3.29742500 | -0.37124500 |
| C | 4.36206100 | -2.77822900 | -2.58764700 |
| H | 4.56025800 | -0.86825600 | -1.61426400 |
| C | 3.61149900 | -3.95528400 | -2.69425200 |
| H | 1.89190200 | -5.04818700 | -1.98005300 |
| H | 5.23783800 | -2.63137600 | -3.21276000 |
| H | 3.90667000 | -4.72379600 | -3.40273200 |
| C | 0.24053900 | 5.01871700 | -0.18538100 |
| H | -0.61530500 | 5.66556200 | 0.02597600 |
| H | 0.36157100 | 4.32117100 | 0.64891800 |
| C | 1.51237000 | 5.84172600 | -0.40102400 |
| H | 1.39667400 | 6.54447800 | -1.23258100 |
| H | 1.73713600 | 6.42075600 | 0.50232000 |
| H | 2.37319500 | 5.19918500 | -0.61376100 |
| S | -0.12717700 | 4.04992900 | -1.71098300 |

J/J-i-TS1

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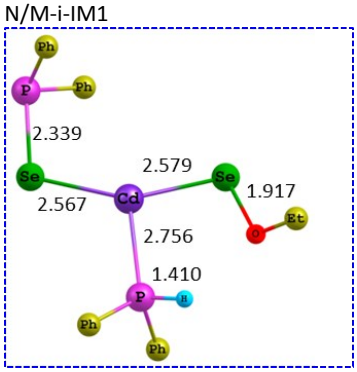
| Cd | 1.59924600 | -1.59525300 | -0.52884200 |
| C | 4.03639300 | 1.99535000 | -0.41805300 |
| H | 4.24036400 | 2.46642500 | 0.55053700 |
| H | 4.93026000 | 1.41773300 | -0.68053000 |
| C | 3.70551100 | 3.03621100 | -1.48574600 |
| H | 3.50661600 | 2.56012000 | -2.45119300 |
| H | 2.82053800 | 3.61674000 | -1.20689200 |
| H | 4.54344600 | 3.73356500 | -1.61517100 |
| P | -1.54125000 | 0.12417700 | 1.37309000 |
| Se | 0.66137700 | 0.23584500 | 1.87430300 |
| C | -2.01068000 | 1.58895400 | 0.35357600 |
| C | -1.14535900 | 2.20847200 | -0.56267000 |

| | | | |
|---|---|---|---|
| C | -3.30334400 | 2.10954200 | 0.53399000 |
| C | -1.57652900 | 3.31651600 | -1.29604400 |
| H | -0.13304800 | 1.83700900 | -0.69316300 |
| C | -3.73367700 | 3.21536800 | -0.20557300 |
| H | -3.97400700 | 1.65177400 | 1.25695000 |
| C | -2.87001400 | 3.82036100 | -1.12225700 |
| H | -0.89869200 | 3.78852000 | -2.00205600 |
| H | -4.73612200 | 3.60694300 | -0.05715000 |
| H | -3.19932500 | 4.68430000 | -1.69278100 |
| C | -1.79226400 | -1.29818400 | 0.24176700 |
| C | -2.49471400 | -1.19708700 | -0.97462700 |
| C | -1.35081000 | -2.57286400 | 0.65863400 |
| C | -2.75635100 | -2.33612800 | -1.73949000 |
| H | -2.83667500 | -0.22864200 | -1.32391600 |
| C | -1.62460500 | -3.71095200 | -0.10712000 |
| H | -0.82445700 | -2.67539700 | 1.60420900 |
| C | -2.33183000 | -3.59667200 | -1.30594000 |
| H | -3.29480800 | -2.23685100 | -2.67800800 |
| H | -1.28754400 | -4.68380300 | 0.23971500 |
| H | -2.54653800 | -4.47980100 | -1.90057800 |
| S | 2.69048500 | 0.75992500 | -0.10692900 |

N/M-i-IM1




| | | | |
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| P | 3.28791200 | 1.19277500 | -1.60089000 |
| C | 3.34378100 | -0.65994600 | -1.57663700 |
| C | 3.40492300 | -1.44115400 | -0.40863700 |
| C | 3.31900100 | -1.31170800 | -2.82159100 |
| C | 3.43030200 | -2.83679600 | -0.48702500 |
| H | 3.44327600 | -0.96101100 | 0.56428700 |
| C | 3.33626100 | -2.70698000 | -2.89976100 |
| H | 3.28109700 | -0.72155100 | -3.73393600 |
| C | 3.39105700 | -3.47312600 | -1.73235900 |
| H | 3.48083700 | -3.42511500 | 0.42513900 |
| H | 3.31175400 | -3.19325200 | -3.87107300 |
| H | 3.40617800 | -4.55769000 | -1.79035200 |
| C | 4.01089700 | 1.60764100 | 0.05891400 |
| C | 5.35980300 | 1.25995200 | 0.27097200 |
| C | 3.35561800 | 2.36441600 | 1.04049200 |
| C | 6.02012800 | 1.63291500 | 1.44228300 |
| H | 5.89822900 | 0.68823900 | -0.48130400 |
| C | 4.02060000 | 2.74494400 | 2.21181200 |
| H | 2.32196100 | 2.65890600 | 0.88711900 |
| C | 5.35150400 | 2.37864300 | 2.41971900 |
| H | 7.05745000 | 1.34460900 | 1.58962400 |
| H | 3.49281100 | 3.32925700 | 2.96103600 |
| H | 5.86623300 | 2.67387600 | 3.32970800 |
| Cd | -0.00014600 | -0.18488300 | 0.03568800 |
| Se | 0.22116100 | -2.49007700 | 1.17038300 |
| C | -1.45989900 | -2.70375500 | 3.43283300 |
| H | -0.85678800 | -3.59820100 | 3.64552000 |
| H | -2.50182000 | -2.94323500 | 3.68690800 |
| C | -0.97195400 | -1.52157600 | 4.26531300 |
| H | -1.59588000 | -0.63769600 | 4.09172500 |
| H | -1.01919900 | -1.76733800 | 5.33307300 |
| H | 0.06424100 | -1.26963100 | 4.01996700 |
| P | -2.67440600 | 0.33198900 | 0.45788500 |
| H | -3.07034400 | -0.02267400 | 1.76383100 |
| C | -3.32886600 | 2.04104000 | 0.35316700 |
| C | -4.46920600 | 2.42604500 | 1.08107600 |
| C | -2.67865900 | 2.98884600 | -0.45311100 |
| C | -4.95163400 | 3.73306900 | 0.99703500 |
| H | -4.98297100 | 1.70376600 | 1.70968100 |
| C | -3.16860300 | 4.29555000 | -0.54056800 |
| H | -1.78407000 | 2.71789000 | -1.00689600 |
| C | -4.30277900 | 4.66892200 | 0.18396900 |
| H | -5.83123600 | 4.02064100 | 1.56585400 |
| H | -2.65595900 | 5.01914600 | -1.16734200 |
| H | -4.67840300 | 5.68616800 | 0.12056200 |
| C | -3.79744600 | -0.72484600 | -0.54960500 |
| C | -3.75094100 | -2.11697500 | -0.35665500 |
| C | -4.63125800 | -0.18619300 | -1.54006000 |
| C | -4.55013700 | -2.95196400 | -1.14036000 |
| H | -3.09459100 | -2.54014900 | 0.40065600 |
| C | -5.42174700 | -1.03170700 | -2.32456400 |
| H | -4.67310500 | 0.88705100 | -1.69867700 |
| C | -5.38481700 | -2.41388700 | -2.12539200 |
| H | -4.51408000 | -4.02618800 | -0.98277600 |
| H | -6.06622000 | -0.60647300 | -3.08875800 |
| H | -6.00030800 | -3.06870100 | -2.73563700 |
| O | -1.49405300 | -2.45101600 | 2.02624100 |

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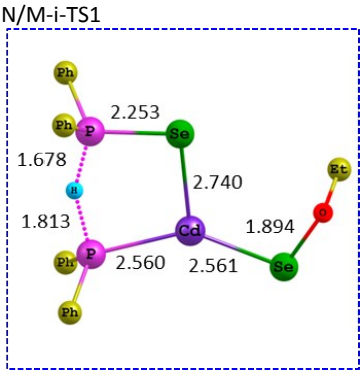


| | | | |
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| Cd | 1.69936500 | -0.36095100 | -0.09092300 |
| Se | -0.37043400 | -2.13242100 | -0.38689600 |
| P | 0.32740200 | 1.77856200 | 0.21297900 |
| H | -1.19146300 | 0.79215400 | 0.12065900 |
| C | 0.55266700 | 2.66045200 | 1.80350400 |
| C | 1.42828700 | 3.75198500 | 1.94882500 |
| C | -0.14890300 | 2.20403700 | 2.93494800 |
| C | 1.58792200 | 4.37279700 | 3.18914400 |
| H | 1.98583900 | 4.11684800 | 1.09141400 |
| C | 0.02536000 | 2.81764700 | 4.17773900 |
| H | -0.83975200 | 1.36948400 | 2.84613800 |
| C | 0.89140100 | 3.90664200 | 4.30921100 |
| H | 2.26645900 | 5.21644200 | 3.28199200 |
| H | -0.52418200 | 2.44954900 | 5.03971300 |
| H | 1.02238600 | 4.38816000 | 5.27390400 |
| C | 0.50371700 | 3.00512600 | -1.13663500 |
| C | -0.20087200 | 4.22523000 | -1.08962800 |
| C | 1.26310800 | 2.71588800 | -2.28455000 |
| C | -0.13409400 | 5.12809000 | -2.15127400 |
| H | -0.79985700 | 4.46948800 | -0.21678800 |
| C | 1.31354900 | 3.61377700 | -3.35513600 |
| H | 1.83269900 | 1.79207000 | -2.34159900 |
| C | 0.61978200 | 4.82434600 | -3.29098300 |
| H | -0.67802200 | 6.06690100 | -2.09164900 |

| | | | |
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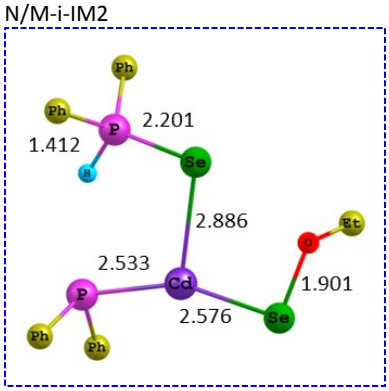
| H | 1.90836300 | 3.36989900 | -4.23087500 |
| H | 0.66743100 | 5.52680700 | -4.11801400 |
| P | -2.03380800 | -0.64640400 | -0.06858700 |
| C | -3.06923200 | -1.11910800 | 1.36850100 |
| C | -2.64790500 | -2.07956200 | 2.30009800 |
| C | -4.26979400 | -0.41968500 | 1.59767000 |
| C | -3.41870800 | -2.34353100 | 3.43648600 |
| H | -1.72493300 | -2.62464800 | 2.12703600 |
| C | -5.03503000 | -0.68737900 | 2.73310800 |
| H | -4.61172300 | 0.32766100 | 0.88682900 |
| C | -4.61138400 | -1.65048000 | 3.65606400 |
| H | -3.08566900 | -3.09544900 | 4.14628700 |
| H | -5.96186200 | -0.14480700 | 2.89647800 |
| H | -5.20884500 | -1.85802300 | 4.53912500 |
| C | -3.15722400 | -0.61185800 | -1.51068200 |
| C | -2.98044700 | 0.40018600 | -2.46877600 |
| C | -4.15630000 | -1.57987100 | -1.70651200 |
| C | -3.79458100 | 0.44562300 | -3.60331300 |
| H | -2.20846800 | 1.15278300 | -2.33407900 |
| C | -4.96914300 | -1.52892100 | -2.83977600 |
| H | -4.29786200 | -2.37092600 | -0.97617100 |
| C | -4.78971300 | -0.51726800 | -3.78961600 |
| H | -3.65107400 | 1.23307900 | -4.33744400 |
| H | -5.73849400 | -2.28207700 | -2.98416600 |
| H | -5.42255400 | -0.48191700 | -4.67173100 |
| C | 3.60814200 | -3.91922900 | 0.34071100 |
| H | 4.53825000 | -3.90212800 | 0.92781300 |
| H | 2.78404600 | -3.62963100 | 1.01223000 |
| C | 3.36385600 | -5.30724800 | -0.23847300 |
| H | 4.18713000 | -5.60064600 | -0.89721200 |
| H | 3.28577200 | -6.04240000 | 0.57129800 |
| H | 2.43484300 | -5.32757300 | -0.81671700 |
| O | 3.69270100 | -3.01376800 | -0.75904800 |

N/M-i-IM2

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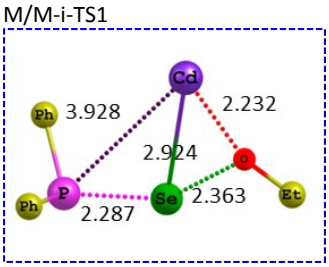
| Se | 1.62057300 | 1.28360500 | -0.68561500 |
| P | -1.55567000 | -1.32240900 | 0.78968000 |
| H | 1.23997200 | -1.17791400 | 0.99634600 |
| C | -2.89356200 | -0.96471200 | 2.02323400 |
| C | -4.18287100 | -0.51342200 | 1.68136100 |
| C | -2.58830400 | -1.12672000 | 3.38585100 |
| C | -5.13022900 | -0.23538700 | 2.66738200 |
| H | -4.44616500 | -0.37929300 | 0.63581200 |
| C | -3.53221400 | -0.83502100 | 4.37710100 |
| H | -1.60410300 | -1.48946000 | 3.67140300 |
| C | -4.80703400 | -0.39103900 | 4.02087700 |
| H | -6.11903900 | 0.11221100 | 2.38014800 |
| H | -3.27164200 | -0.96432200 | 5.42420700 |
| H | -5.54364700 | -0.16765000 | 4.78747000 |
| C | -2.40088600 | -2.32560200 | -0.51852400 |
| C | -3.43526200 | -3.22829400 | -0.20598500 |
| C | -1.91651600 | -2.31681500 | -1.84146400 |
| C | -3.97013600 | -4.07546600 | -1.18025000 |
| H | -3.82907800 | -3.27003600 | 0.80505500 |
| C | -2.44587000 | -3.16859000 | -2.81312400 |
| H | -1.12095800 | -1.63073000 | -2.12494800 |
| C | -3.47952100 | -4.05283800 | -2.48895600 |
| H | -4.77377200 | -4.75644000 | -0.91180100 |
| H | -2.05715900 | -3.13011200 | -3.82734700 |
| H | -3.89923500 | -4.70924500 | -3.24575400 |
| P | 2.30372600 | -0.56153100 | 0.30177000 |
| C | 3.63731600 | -0.29997600 | 1.52811200 |
| C | 3.97332900 | 0.99304900 | 1.94894800 |
| C | 4.29830400 | -1.41012400 | 2.08130500 |
| C | 4.96454500 | 1.17524100 | 2.91756400 |
| H | 3.46365500 | 1.84837800 | 1.51575700 |
| C | 5.28357400 | -1.22152500 | 3.05130700 |
| H | 4.05245400 | -2.41636600 | 1.75413000 |
| C | 5.61761200 | 0.07108600 | 3.47003800 |
| H | 5.22357000 | 2.18013500 | 3.23756200 |
| H | 5.79154700 | -2.08209200 | 3.47655500 |
| H | 6.38717500 | 0.21508400 | 4.22293100 |
| C | 2.84134700 | -1.89702700 | -0.81097000 |
| C | 2.07655600 | -3.07048400 | -0.89810000 |
| C | 3.98209400 | -1.74149300 | -1.61455700 |
| C | 2.46145800 | -4.08754600 | -1.77674200 |
| H | 1.18172800 | -3.19102200 | -0.29316600 |
| C | 4.36252600 | -2.76202200 | -2.48530100 |
| H | 4.56709700 | -0.82743300 | -1.56289900 |
| C | 3.60254400 | -3.93501400 | -2.56753000 |
| H | 1.86508800 | -4.99251200 | -1.84357800 |
| H | 5.24655500 | -2.64037900 | -3.10415700 |
| H | 3.89882400 | -4.72560400 | -3.25080700 |
| C | 0.17771100 | 4.86928200 | -0.69858700 |
| H | -0.55584700 | 5.68843800 | -0.72324600 |
| H | 0.19660700 | 4.46917500 | 0.32738400 |
| C | 1.55608900 | 5.37507400 | -1.10629900 |
| H | 1.53249400 | 5.78314700 | -2.12156300 |
| H | 1.88246200 | 6.16590700 | -0.42020100 |
| H | 2.29065400 | 4.56401900 | -1.07692700 |
| O | -0.18723500 | 3.84457900 | -1.62301800 |

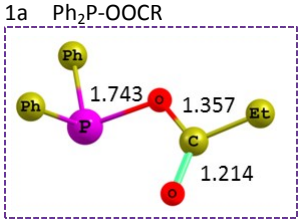
M/M-i-TS1




| | | | |
|---|---|---|---|
| Cd | 1.36561300 | -1.27549700 | -1.06056300 |
| C | 4.13300000 | 0.59740000 | 0.20648000 |
| H | 4.27686300 | 0.75247400 | 1.28961400 |
| H | 4.95401600 | -0.06742600 | -0.11153800 |
| C | 4.21933800 | 1.93520100 | -0.52895400 |
| H | 4.10551300 | 1.78950400 | -1.60906700 |
| H | 3.42778000 | 2.61182900 | -0.18958700 |
| H | 5.18681800 | 2.42021600 | -0.34705800 |
| P | -1.16378300 | 0.37362800 | 1.45134200 |
| Se | 1.10164500 | 0.06796300 | 1.52303500 |
| C | -1.57040900 | 1.81527700 | 0.37632200 |
| C | -0.60020800 | 2.61395800 | -0.24874300 |
| C | -2.92515800 | 2.18620200 | 0.26781500 |
| C | -0.97696700 | 3.74628100 | -0.97821600 |
| H | 0.44948900 | 2.35207500 | -0.16199700 |

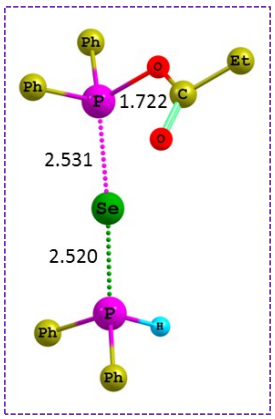
| | | | |
|---|---|---|---|
| C | -3.29858000 | 3.31218700 | -0.46701000 |
| H | -3.69231300 | 1.59316700 | 0.75964100 |
| C | -2.32395600 | 4.09740000 | -1.09264800 |
| H | -0.21295900 | 4.35149700 | -1.45845300 |
| H | -4.34864200 | 3.58027400 | -0.54409200 |
| H | -2.61365500 | 4.97745800 | -1.65973800 |
| C | -1.88152900 | -1.05318600 | 0.55468300 |
| C | -2.28987600 | -1.01368500 | -0.79284900 |
| C | -2.01210600 | -2.26368200 | 1.26493100 |
| C | -2.83758000 | -2.14850400 | -1.40153000 |
| H | -2.20428200 | -0.09213500 | -1.35939400 |
| C | -2.54519300 | -3.39583100 | 0.65022200 |
| H | -1.69550700 | -2.31214500 | 2.30349600 |
| C | -2.96877000 | -3.33831200 | -0.68359700 |
| H | -3.15842400 | -2.09784100 | -2.43841900 |
| H | -2.64146900 | -4.31987000 | 1.21325400 |
| H | -3.39558300 | -4.21744500 | -1.15788900 |
| O | 2.91021700 | -0.06964400 | 0.00793700 |

1a $Ph_2P$-OOCR




| | | | |
|---|---|---|---|
| O | -2.80301300 | -0.75467200 | -1.00780000 |
| C | -2.18411400 | -1.40192400 | -0.18833700 |
| C | -2.77720200 | -2.44388500 | 0.73940800 |
| H | -2.22471600 | -3.37825300 | 0.57986300 |
| H | -2.54465300 | -2.13612500 | 1.76668400 |
| C | -4.27975700 | -2.64313600 | 0.54546700 |
| H | -4.65289400 | -3.40083400 | 1.24141000 |
| H | -4.82664000 | -1.71283900 | 0.72149000 |
| H | -4.50566400 | -2.96916800 | -0.47349100 |
| O | -0.84978000 | -1.26284500 | 0.01322500 |
| P | 0.03646100 | -0.21535200 | -1.06235500 |
| C | -0.26482600 | 1.42315700 | -0.25465900 |
| C | -1.16443900 | 2.28835800 | -0.89966800 |
| C | 0.34982500 | 1.84444500 | 0.93630000 |
| C | -1.45061400 | 3.54555500 | -0.36137300 |
| H | -1.65012800 | 1.96839300 | -1.81715800 |
| C | 0.06392200 | 3.10086400 | 1.47340500 |
| H | 1.05813900 | 1.19429100 | 1.44060000 |
| C | -0.83620500 | 3.95313300 | 0.82527600 |
| H | -2.15111800 | 4.20341800 | -0.86765700 |
| H | 0.54654600 | 3.41680000 | 2.39410900 |
| H | -1.05482500 | 4.93179700 | 1.24325400 |
| C | 1.70031900 | -0.66103100 | -0.40026300 |
| C | 2.80756700 | -0.18487000 | -1.12324900 |
| C | 1.92377700 | -1.47191800 | 0.72299700 |
| C | 4.10854200 | -0.48592600 | -0.71679500 |
| H | 2.65411000 | 0.42462100 | -2.01133400 |
| C | 3.22742000 | -1.78340300 | 1.12148400 |
| H | 1.07934600 | -1.86333700 | 1.27919500 |
| C | 4.32182100 | -1.28887400 | 0.40781700 |
| H | 4.95274800 | -0.10443000 | -1.28398500 |
| H | 3.38589700 | -2.41407600 | 1.99201400 |
| H | 5.33306700 | -1.53310300 | 0.72008300 |

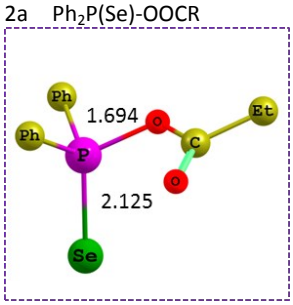
a-TS1




| | | | |
|---|---|---|---|
| Se | 0.38000900 | 0.01134900 | -0.63343000 |
| P | 2.87590100 | -0.06110800 | -0.97245500 |
| H | 3.32507000 | -0.17512700 | -2.31159800 |
| C | 3.78722200 | -1.47395900 | -0.24078500 |
| C | 4.64155600 | -2.28181900 | -1.00813700 |
| C | 3.58265100 | -1.79001100 | 1.11326800 |
| C | 5.29024000 | -3.37732300 | -0.42940100 |
| H | 4.80266300 | -2.05845400 | -2.05948900 |
| C | 4.23970900 | -2.87684800 | 1.69163000 |
| H | 2.90000600 | -1.19044200 | 1.70948400 |
| C | 5.09445100 | -3.67367000 | 0.92178100 |
| H | 5.94815200 | -3.99494900 | -1.03447500 |
| H | 4.07676900 | -3.10834600 | 2.74048400 |
| H | 5.59980900 | -4.52331900 | 1.37206900 |
| C | 3.78306700 | 1.44832600 | -0.41518500 |
| C | 3.04113900 | 2.61032200 | -0.15733000 |
| C | 5.17889400 | 1.47247200 | -0.25754800 |
| C | 3.68865700 | 3.78446500 | 0.24102900 |
| H | 1.95957600 | 2.58732800 | -0.25996600 |
| C | 5.82164100 | 2.64548100 | 0.14329100 |
| H | 5.76389300 | 0.57533000 | -0.43926900 |
| C | 5.07715700 | 3.80417100 | 0.39127600 |
| H | 3.10471500 | 4.67908200 | 0.43826500 |
| H | 6.90146800 | 2.65442500 | 0.26384000 |
| H | 5.57879300 | 4.71568600 | 0.70440100 |
| P | -2.11097100 | -0.07689700 | -0.19239200 |
| C | -2.87194800 | -1.66495200 | -0.71065000 |
| C | -2.14572000 | -2.83947900 | -0.45020700 |
| C | -4.10917400 | -1.75540300 | -1.36796600 |
| C | -2.66229600 | -4.08372100 | -0.81570800 |
| H | -1.17029900 | -2.77628300 | 0.02384800 |
| C | -4.61750900 | -3.00327800 | -1.74109500 |
| H | -4.66685700 | -0.85375500 | -1.59441700 |
| C | -3.89928200 | -4.16909700 | -1.46248700 |
| H | -2.09169200 | -4.98423800 | -0.60706400 |
| H | -5.57474900 | -3.06149700 | -2.25206500 |
| H | -4.29654400 | -5.13721200 | -1.75448200 |
| C | -2.64156200 | 0.12149100 | 1.55999300 |
| C | -1.80276500 | 0.84583900 | 2.42107200 |
| C | -3.83635000 | -0.42414800 | 2.05783300 |
| C | -2.15955500 | 1.03039700 | 3.75869900 |
| H | -0.87646400 | 1.26177500 | 2.03686700 |
| C | -4.19058300 | -0.23704900 | 3.39570200 |
| H | -4.48587000 | -1.00085800 | 1.40639900 |
| C | -3.35258400 | 0.49015200 | 4.24740100 |
| H | -1.50566300 | 1.59486300 | 4.41742000 |
| H | -5.11551100 | -0.66395500 | 3.77362700 |
| H | -3.62780300 | 0.63160200 | 5.28899800 |
| O | -3.21217500 | 0.94194200 | -1.03782100 |
| C | -3.06838900 | 2.29771800 | -0.99314800 |
| C | -4.01261600 | 2.97418600 | -1.96675700 |
| H | -3.78005600 | 2.58495500 | -2.96614900 |

| | | | |
|---|---|---|---|
| H | -5.02763800 | 2.62291100 | -1.74246200 |
| O | -2.28539900 | 2.85797700 | -0.25921600 |
| C | -3.92831500 | 4.49966100 | -1.92841700 |
| H | -2.91896600 | 4.84376300 | -2.17009500 |
| H | -4.62489300 | 4.93426400 | -2.65219000 |
| H | -4.17801600 | 4.88376700 | -0.93529100 |

2a $Ph_2P(Se)$-OOCR




| | | | |
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| P | -0.12272700 | -0.16468900 | 0.42084800 |
| C | -1.80178900 | -0.45983000 | -0.24211100 |
| C | -2.88963100 | 0.07670300 | 0.46539000 |
| C | -2.03462500 | -1.19391200 | -1.41516700 |
| C | -4.19080400 | -0.10556700 | -0.00405600 |
| H | -2.71766200 | 0.62092100 | 1.38915700 |
| C | -3.34121400 | -1.37890500 | -1.87695700 |
| H | -1.20233500 | -1.62638800 | -1.95767400 |
| C | -4.41954300 | -0.83445500 | -1.17565200 |
| H | -5.02528200 | 0.31301900 | 0.55084300 |
| H | -3.51322500 | -1.95371300 | -2.78256000 |
| H | -5.43367700 | -0.98207900 | -1.53581900 |
| C | 0.37799200 | 1.49719200 | -0.15863000 |
| C | 1.24725100 | 2.27462400 | 0.61864800 |
| C | -0.10118400 | 1.99779000 | -1.38027200 |
| C | 1.63836200 | 3.53838800 | 0.17427600 |
| H | 1.61224900 | 1.88320700 | 1.56276800 |
| C | 0.29529500 | 3.26231900 | -1.82115100 |
| H | -0.78734500 | 1.41159000 | -1.98377600 |
| C | 1.16441900 | 4.03384900 | -1.04432600 |
| H | 2.31405000 | 4.13470800 | 0.78038300 |
| H | -0.08077500 | 3.64551400 | -2.76542400 |
| H | 1.46859500 | 5.01912700 | -1.38628800 |
| Se | 0.09015600 | -0.53087800 | 2.50363000 |
| O | 0.69722600 | -1.23922300 | -0.60079400 |
| C | 2.07058500 | -1.35141100 | -0.63731900 |
| O | 2.81112300 | -0.58974600 | -0.06668900 |
| C | 2.47848400 | -2.54154700 | -1.47799900 |
| H | 2.02773000 | -3.42899700 | -1.01540700 |
| H | 1.99284500 | -2.44073600 | -2.45678100 |
| C | 3.99320000 | -2.69090400 | -1.61527300 |
| H | 4.23067500 | -3.57208500 | -2.21904500 |
| H | 4.43522000 | -1.81382700 | -2.09651400 |
| H | 4.46696600 | -2.80432500 | -0.63655000 |

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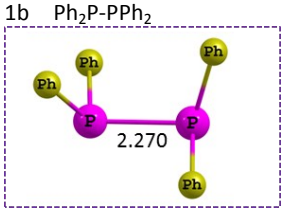
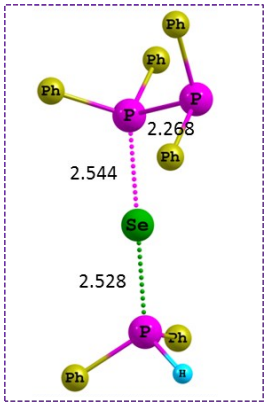



| | | | |
|---|---|---|---|
| P | 0.51739400 | 0.36280200 | -1.48919700 |
| C | 0.40082400 | 1.83719500 | -0.36967500 |
| C | 0.75535300 | 1.86324200 | 0.99157800 |
| C | -0.10667000 | 3.01298000 | -0.95175300 |
| C | 0.60477400 | 3.03030200 | 1.74352000 |
| H | 1.14918900 | 0.97197900 | 1.46695300 |
| C | -0.25615500 | 4.18190600 | -0.19956700 |
| H | -0.38519400 | 3.00923100 | -2.00232200 |
| C | 0.09886800 | 4.19211100 | 1.15125000 |
| H | 0.88222800 | 3.03042400 | 2.79396600 |
| H | -0.64627500 | 5.08030800 | -0.66960400 |
| H | -0.01559300 | 5.09837600 | 1.73928500 |
| C | 2.26257500 | -0.23103000 | -1.27408700 |
| C | 2.61173900 | -1.49332300 | -1.79393100 |
| C | 3.28805300 | 0.57945300 | -0.75935700 |
| C | 3.93378800 | -1.93836600 | -1.77133900 |
| H | 1.84373300 | -2.13571800 | -2.21526900 |
| C | 4.61411600 | 0.13453000 | -0.74466400 |
| H | 3.05945600 | 1.56494200 | -0.36861100 |
| C | 4.94350700 | -1.12637300 | -1.24433400 |
| H | 4.17535000 | -2.91949900 | -2.17092100 |
| H | 5.38858600 | 0.78028200 | -0.33968300 |
| H | 5.97335100 | -1.47117500 | -1.23015000 |
| P | -0.59387400 | -1.39080000 | -0.57130500 |
| C | -0.36799200 | -1.34652900 | 1.26622300 |
| C | -1.34964400 | -0.95051800 | 2.18909800 |
| C | 0.85968800 | -1.82965300 | 1.76211000 |
| C | -1.10600300 | -1.01998800 | 3.56428600 |
| H | -2.31138300 | -0.59149500 | 1.84030300 |
| C | 1.10730600 | -1.88218800 | 3.13423000 |
| H | 1.62585000 | -2.16632800 | 1.06937000 |
| C | 0.12353400 | -1.47755400 | 4.04281900 |
| H | -1.88158300 | -0.71252600 | 4.26055000 |
| H | 2.06407200 | -2.25115200 | 3.49333700 |
| H | 0.31103900 | -1.52828900 | 5.11152700 |
| C | -2.35363300 | -0.88061500 | -0.84465000 |
| C | -3.19494800 | -1.84073800 | -1.43296500 |
| C | -2.89314400 | 0.38088300 | -0.53570600 |
| C | -4.53754600 | -1.55527500 | -1.69795900 |
| H | -2.79281100 | -2.81777800 | -1.68696400 |
| C | -4.23306300 | 0.66913400 | -0.80513300 |
| H | -2.26857600 | 1.14345300 | -0.08302700 |
| C | -5.05904700 | -0.29821500 | -1.38548800 |
| H | -5.17066900 | -2.31240300 | -2.15183400 |
| H | -4.63050500 | 1.65070200 | -0.56201400 |
| H | -6.10074200 | -0.07159800 | -1.59438700 |

b-TS1




| | | | |
|---|---|---|---|
| P | 1.27179100 | 0.50915800 | 0.20891500 |
| C | 1.89761800 | -0.29017700 | 1.75251300 |
| C | 3.20985000 | -0.13732900 | 2.23809100 |
| C | 1.00488300 | -1.12091200 | 2.45135300 |
| C | 3.61412000 | -0.80054500 | 3.39902400 |
| H | 3.91747900 | 0.49446900 | 1.71265900 |
| C | 1.41381600 | -1.78208900 | 3.61330000 |
| H | -0.00792800 | -1.24330300 | 2.07699200 |
| C | 2.71797500 | -1.62403200 | 4.08909100 |
| H | 4.63059700 | -0.67491700 | 3.76171400 |

| | | | |
|---|---|---|---|
| H | 0.71124600 | -2.41836800 | 4.14437800 |
| H | 3.03633100 | -2.13833100 | 4.99180300 |
| C | 1.60491200 | 2.31060200 | 0.40822100 |
| C | 1.41204400 | 3.15252900 | -0.70399100 |
| C | 1.92131900 | 2.89258500 | 1.64633100 |
| C | 1.56147800 | 4.53439900 | -0.58384100 |
| H | 1.13776200 | 2.72564500 | -1.66398700 |
| C | 2.06320500 | 4.27911200 | 1.76432400 |
| H | 2.05566000 | 2.27002500 | 2.52406700 |
| C | 1.89037400 | 5.10428900 | 0.65127200 |
| H | 1.41412700 | 5.16676500 | -1.45507800 |
| H | 2.30903800 | 4.71025600 | 2.73099900 |
| H | 2.00324000 | 6.18073500 | 0.74453300 |
| P | 2.56836200 | 0.00255100 | -1.58226400 |
| C | 4.32772400 | 0.04045300 | -1.00063700 |
| C | 5.13937700 | -1.09237300 | -0.82292700 |
| C | 4.90858700 | 1.31294100 | -0.82554200 |
| C | 6.48432200 | -0.95720400 | -0.46324200 |
| H | 4.72879200 | -2.08508900 | -0.97009600 |
| C | 6.24606700 | 1.44542600 | -0.44996400 |
| H | 4.30957600 | 2.20562200 | -0.98302100 |
| C | 7.04140000 | 0.30863300 | -0.26750200 |
| H | 7.09496800 | -1.84707200 | -0.33535600 |
| H | 6.66957000 | 2.43664200 | -0.31264500 |
| H | 8.08577400 | 0.41030800 | 0.01377400 |
| C | 2.18545600 | -1.79105700 | -1.81423400 |
| C | 1.81802400 | -2.17809800 | -3.11419600 |
| C | 2.21990500 | -2.77082100 | -0.80595100 |
| C | 1.50511100 | -3.50918200 | -3.40499900 |
| H | 1.76961800 | -1.42986600 | -3.90063400 |
| C | 1.90078200 | -4.09927400 | -1.09444000 |
| H | 2.48956600 | -2.50046300 | 0.20937700 |
| C | 1.54557800 | -4.47248100 | -2.39463500 |
| H | 1.22370700 | -3.78855300 | -4.41646400 |
| H | 1.92563900 | -4.84158700 | -0.30132500 |
| H | 1.29769200 | -5.50692500 | -2.61597700 |
| Se | -1.17421800 | 0.04564400 | -0.31500700 |
| P | -3.63305300 | -0.32084900 | -0.77371200 |
| H | -3.95929800 | -0.96502600 | -1.99321700 |
| C | -4.66228700 | 1.20765800 | -0.89950600 |
| C | -6.04898800 | 1.15650200 | -1.12258500 |
| C | -4.03111500 | 2.45328400 | -0.77782600 |
| C | -6.78968700 | 2.33503400 | -1.22553300 |
| H | -6.55183300 | 0.19682300 | -1.20715100 |
| C | -4.77632600 | 3.63329000 | -0.87990700 |
| H | -2.95915800 | 2.49050800 | -0.60269500 |
| C | -6.15337100 | 3.57612900 | -1.10410000 |
| H | -7.86132300 | 2.28605200 | -1.39842100 |
| H | -4.27825400 | 4.59394600 | -0.78264500 |
| H | -6.73155800 | 4.49271500 | -1.18291500 |
| C | -4.56117500 | -1.41131900 | 0.37407800 |
| C | -5.06192600 | -2.65561400 | -0.04060500 |
| C | -4.70628700 | -1.03309200 | 1.71990200 |
| C | -5.70519600 | -3.50045400 | 0.86940100 |
| H | -4.95236900 | -2.96875900 | -1.07565700 |
| C | -5.35753700 | -1.87288800 | 2.62402600 |
| H | -4.30691400 | -0.08124000 | 2.05995700 |
| C | -5.85763000 | -3.11002100 | 2.20206200 |
| H | -6.08948500 | -4.45983800 | 0.53400600 |
| H | -5.46925800 | -1.56484700 | 3.65991100 |
| H | -6.36050900 | -3.76452600 | 2.90830400 |

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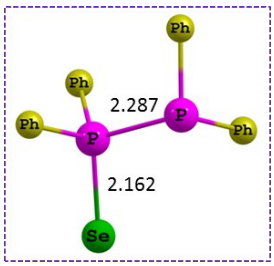
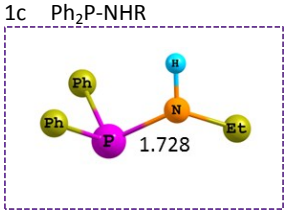



| | | | |
|---|---|---|---|
| P | 0.50786900 | -0.97840100 | -0.01527200 |
| C | 0.31003500 | -0.41073200 | 1.72900400 |
| C | -0.26315800 | -1.28001900 | 2.66877400 |
| C | 0.68438400 | 0.88540600 | 2.12836200 |
| C | -0.45073100 | -0.86487600 | 3.98988800 |
| H | -0.55665400 | -2.27777500 | 2.35534500 |
| C | 0.49220600 | 1.29597100 | 3.44944800 |
| H | 1.12574000 | 1.57550200 | 1.41786000 |
| C | -0.07498500 | 0.42240900 | 4.38292600 |
| H | -0.89020000 | -1.54977900 | 4.70951700 |
| H | 0.78614700 | 2.29872200 | 3.74624900 |
| H | -0.22183900 | 0.74427200 | 5.41016600 |
| C | 2.27666500 | -0.70541300 | -0.44355200 |
| C | 2.66141900 | -0.81484700 | -1.79148100 |
| C | 3.26093000 | -0.49536700 | 0.53357400 |
| C | 4.00267300 | -0.69001900 | -2.15464200 |
| H | 1.91391500 | -1.01185300 | -2.55375300 |
| C | 4.60451000 | -0.37534000 | 0.16547100 |
| H | 2.98892800 | -0.43172200 | 1.58128400 |
| C | 4.97823900 | -0.46686100 | -1.17695700 |
| H | 4.28598000 | -0.77568000 | -3.19978200 |
| H | 5.35694700 | -0.21511900 | 0.93248600 |
| H | 6.02292600 | -0.37455400 | -1.46007800 |
| Se | -0.12900900 | -3.01612000 | -0.35821600 |
| P | -0.58053100 | 0.37452000 | -1.50370200 |
| C | -2.34152400 | 0.06034900 | -1.05200100 |
| C | -3.18275500 | -0.32682100 | -2.10893300 |
| C | -2.88656000 | 0.16371600 | 0.24046500 |
| C | -4.53705100 | -0.59149000 | -1.88552800 |
| H | -2.77246600 | -0.42918900 | -3.10963800 |
| C | -4.23718300 | -0.10791700 | 0.46462400 |
| H | -2.25743600 | 0.44889500 | 1.07693600 |
| C | -5.06609700 | -0.48298500 | -0.59798500 |
| H | -5.17214800 | -0.88968800 | -2.71476300 |
| H | -4.64089800 | -0.03087300 | 1.47037400 |
| H | -6.11676100 | -0.69465700 | -0.42023100 |
| C | -0.23890100 | 2.10809900 | -0.94483200 |
| C | 1.03916800 | 2.62808900 | -1.23445300 |
| C | -1.18799000 | 2.96264600 | -0.35852400 |
| C | 1.36871700 | 3.94462300 | -0.90879700 |
| H | 1.78190500 | 1.99957200 | -1.71762800 |
| C | -0.86167100 | 4.28686700 | -0.04967900 |
| H | -2.18870100 | 2.60306500 | -0.14850200 |
| C | 0.41815200 | 4.78063100 | -0.31322700 |
| H | 2.36322900 | 4.32033700 | -1.13304600 |
| H | -1.61289700 | 4.93117000 | 0.39903200 |
| H | 0.66958800 | 5.80894800 | -0.06956800 |

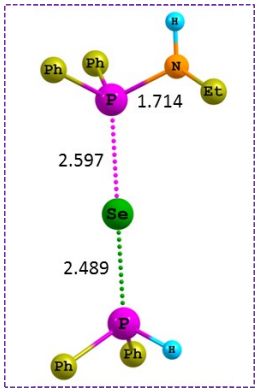
1c $Ph_2P-NHR$




| | | | |
|---|---|---|---|
| P | -0.01100000 | 0.65676200 | -0.92854400 |

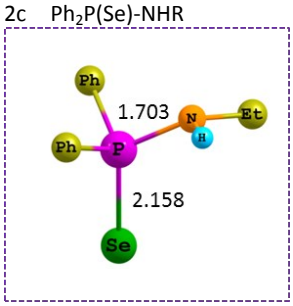
| | | | |
|---|---|---|---|
| C | 1.48408900 | -0.27502500 | -0.35967600 |
| C | 2.58946700 | 0.38822000 | 0.19724500 |
| C | 1.58567600 | -1.65617000 | -0.60565900 |
| C | 3.75614000 | -0.31358000 | 0.51691900 |
| H | 2.53059700 | 1.45656500 | 0.37930200 |
| C | 2.75190100 | -2.35504100 | -0.29001400 |
| H | 0.74582700 | -2.19386100 | -1.03777900 |
| C | 3.84254500 | -1.68635800 | 0.27519500 |
| H | 4.59824300 | 0.21648500 | 0.95384100 |
| H | 2.80753200 | -3.42286200 | -0.48312800 |
| H | 4.74960500 | -2.23052900 | 0.52230000 |
| C | -1.37157300 | -0.43390900 | -0.26333100 |
| C | -2.48617400 | -0.66414800 | -1.08431800 |
| C | -1.36836800 | -0.98241400 | 1.03150600 |
| C | -3.57208700 | -1.41981500 | -0.62754700 |
| H | -2.50238900 | -0.25017600 | -2.08970200 |
| C | -2.45111200 | -1.73219500 | 1.49279400 |
| H | -0.50795700 | -0.83563300 | 1.67992700 |
| C | -3.55658300 | -1.95278000 | 0.66258900 |
| H | -4.42519900 | -1.59051400 | -1.27833800 |
| H | -2.43223600 | -2.14986300 | 2.49584400 |
| H | -4.39768300 | -2.53949600 | 1.02104200 |
| N | 0.05281600 | 2.00703800 | 0.14833300 |
| H | 0.01157700 | 1.78082100 | 1.14035600 |
| C | -0.73340100 | 3.20543800 | -0.17196200 |
| H | -0.62513900 | 3.38974700 | -1.24640200 |
| H | -1.80907300 | 3.05819400 | 0.01853700 |
| C | -0.23784200 | 4.41673800 | 0.61814900 |
| H | 0.81540500 | 4.61852500 | 0.39886000 |
| H | -0.82532500 | 5.30635000 | 0.36570200 |
| H | -0.33456200 | 4.25179500 | 1.69811900 |

c-TS1




| | | | |
|---|---|---|---|
| Se | -0.24964300 | 0.03504100 | 0.66239500 |
| P | -2.73068900 | 0.08990200 | 0.85340500 |
| H | -3.25119500 | 0.23571400 | 2.16307600 |
| C | -3.60090500 | -1.44054300 | 0.29499600 |
| C | -5.00296900 | -1.53532300 | 0.27965800 |
| C | -2.83244700 | -2.54001400 | -0.11146400 |
| C | -5.62405600 | -2.71592600 | -0.13126400 |
| H | -5.61025500 | -0.68572000 | 0.58001300 |
| C | -3.45786900 | -3.72174800 | -0.52395300 |
| H | -1.74846800 | -2.46218700 | -0.10409000 |
| C | -4.85132700 | -3.81181900 | -0.53331000 |
| H | -6.70866600 | -2.78087900 | -0.13929200 |
| H | -2.85364400 | -4.56821200 | -0.83820100 |
| H | -5.33629500 | -4.72969400 | -0.85408900 |
| C | -3.62667900 | 1.46823400 | 0.03894000 |
| C | -3.50472100 | 1.64391600 | -1.35009400 |
| C | -4.37428200 | 2.39695800 | 0.78005000 |
| C | -4.13656500 | 2.71384800 | -1.98474000 |
| H | -2.90940000 | 0.94622800 | -1.93305300 |
| C | -4.99773900 | 3.47493400 | 0.14351200 |
| H | -4.47293500 | 2.28162400 | 1.85633500 |
| C | -4.88336700 | 3.63355000 | -1.23967400 |
| H | -4.03921500 | 2.83504200 | -3.05998000 |
| H | -5.57355400 | 4.18620200 | 0.72921300 |
| H | -5.36981300 | 4.46910300 | -1.73489100 |
| P | 2.33477000 | -0.08211900 | 0.43421100 |
| C | 2.99123500 | -1.39961000 | -0.66441900 |
| C | 3.05229300 | -1.19884200 | -2.05458500 |
| C | 3.32162300 | -2.66317700 | -0.14673900 |
| C | 3.45129900 | -2.23236000 | -2.90394100 |
| H | 2.79244300 | -0.23207400 | -2.47596000 |
| C | 3.72585400 | -3.69446200 | -0.99941100 |
| H | 3.25827900 | -2.83267000 | 0.92335200 |
| C | 3.79283900 | -3.48314200 | -2.37919000 |
| H | 3.49723900 | -2.05942600 | -3.97565400 |
| H | 3.98467500 | -4.66441700 | -0.58330300 |
| H | 4.10547800 | -4.28606200 | -3.04090700 |
| C | 3.11709000 | 1.45783300 | -0.24276300 |
| C | 2.31873100 | 2.59736700 | -0.42135300 |
| C | 4.49313800 | 1.53897500 | -0.52127600 |
| C | 2.88529700 | 3.79654000 | -0.86837700 |
| H | 1.25391500 | 2.53694700 | -0.21135900 |
| C | 5.05855800 | 2.73554500 | -0.96464900 |
| H | 5.12563900 | 0.66184800 | -0.40592500 |
| C | 4.25357200 | 3.86788000 | -1.13882600 |
| H | 2.25586000 | 4.67167600 | -1.00470600 |
| H | 6.12279100 | 2.78484300 | -1.17905200 |
| H | 4.69344700 | 4.79886600 | -1.48585800 |
| C | 2.67305900 | 0.15117300 | 3.16477000 |
| H | 2.98793200 | 1.20357000 | 3.24645000 |
| H | 1.57918000 | 0.14366800 | 3.14908400 |
| C | 3.19211800 | -0.63631500 | 4.36760600 |
| H | 2.84630600 | -0.17732400 | 5.30045500 |
| H | 2.83772000 | -1.67152100 | 4.33626200 |
| H | 4.28894300 | -0.65157400 | 4.39300200 |
| N | 3.13148100 | -0.45592400 | 1.90498800 |
| H | 4.14717900 | -0.49108100 | 1.84150200 |

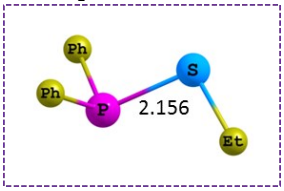
2c $Ph_2P(Se)$-NHR




| | | | |
|---|---|---|---|
| P | -0.00448900 | 0.44427200 | 0.08093100 |
| C | -1.28706000 | -0.86116300 | -0.10512900 |
| C | -1.81800100 | -1.13882600 | -1.37309500 |
| C | -1.71766100 | -1.61093000 | 1.00177200 |
| C | -2.75709600 | -2.15996900 | -1.53347900 |
| H | -1.50586300 | -0.54083500 | -2.22402800 |
| C | -2.66270000 | -2.62682100 | 0.83834800 |
| H | -1.32322200 | -1.39031500 | 1.98822800 |
| C | -3.18096800 | -2.90568400 | -0.42956000 |
| H | -3.16291200 | -2.36605600 | -2.51975600 |
| H | -2.99512900 | -3.19663700 | 1.70159100 |
| H | -3.91595400 | -3.69580100 | -0.55533500 |
| C | 1.62590600 | -0.40838400 | 0.13451700 |
| C | 2.57683000 | -0.16411400 | -0.86470400 |
| C | 1.92235100 | -1.31934100 | 1.16341700 |
| C | 3.81116600 | -0.81903400 | -0.83466800 |

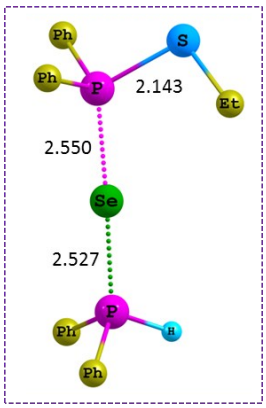
| | | | |
|---|---|---|---|
| H | 2.34574100 | 0.54553500 | -1.65378300 |
| C | 3.15717300 | -1.97034100 | 1.19047900 |
| H | 1.19279400 | -1.52116800 | 1.94069300 |
| C | 4.10331200 | -1.72185400 | 0.19070500 |
| H | 4.54296700 | -0.62043300 | -1.61245300 |
| H | 3.37864300 | -2.67204700 | 1.98968600 |
| H | 5.06316900 | -2.23028800 | 0.21211800 |
| Se | -0.14366700 | 1.96730900 | -1.44139900 |
| N | -0.16812200 | 0.89511300 | 1.71516500 |
| H | 0.71121200 | 1.22741700 | 2.10184200 |
| C | -1.32412800 | 1.69508100 | 2.17115900 |
| H | -1.63829900 | 1.30637900 | 3.14858900 |
| H | -2.15322900 | 1.51627600 | 1.47946800 |
| C | -1.03511200 | 3.19464000 | 2.26682800 |
| H | -0.76620600 | 3.60146400 | 1.28835100 |
| H | -1.91755900 | 3.72782700 | 2.63821100 |
| H | -0.21137300 | 3.39073700 | 2.96446600 |

1d $Ph_2P$-SR




| | | | |
|---|---|---|---|
| P | -0.05614700 | 0.47270600 | 0.88353400 |
| C | 1.61162500 | -0.04374100 | 0.25863100 |
| C | 1.81260700 | -0.96349000 | -0.78232100 |
| C | 2.73336900 | 0.51962900 | 0.89062200 |
| C | 3.10606300 | -1.30541300 | -1.18575900 |
| H | 0.95983700 | -1.41823200 | -1.27633700 |
| C | 4.02550600 | 0.18220000 | 0.48342200 |
| H | 2.59300500 | 1.22483600 | 1.70582500 |
| C | 4.21447800 | -0.73254800 | -0.55660600 |
| H | 3.24620900 | -2.01856300 | -1.99334300 |
| H | 4.88208200 | 0.62738900 | 0.98160100 |
| H | 5.21902500 | -1.00067300 | -0.87123600 |
| C | -1.12642300 | -0.94948200 | 0.34382500 |
| C | -1.20231000 | -2.03939400 | 1.22921700 |
| C | -1.88523500 | -0.98529000 | -0.83435600 |
| C | -1.99602400 | -3.14842300 | 0.93075600 |
| H | -0.63773800 | -2.02105900 | 2.15887700 |
| C | -2.68996700 | -2.09098300 | -1.12783700 |
| H | -1.84821400 | -0.14399000 | -1.52028800 |
| C | -2.74462800 | -3.17627400 | -0.25006300 |
| H | -2.03828500 | -3.98381900 | 1.62403100 |
| H | -3.27243400 | -2.10259900 | -2.04513400 |
| H | -3.37067800 | -4.03384300 | -0.47936600 |
| C | -1.72664700 | 3.00898200 | 0.39681900 |
| H | -2.63494600 | 2.40633800 | 0.48664800 |
| H | -1.33833700 | 3.19888900 | 1.40120600 |
| C | -2.01996900 | 4.31843000 | -0.33391500 |
| H | -2.77397100 | 4.89037800 | 0.21841100 |
| H | -1.11999900 | 4.93529500 | -0.42036300 |
| H | -2.40685600 | 4.13686500 | -1.34179700 |
| S | -0.45569800 | 2.04043600 | -0.54102200 |

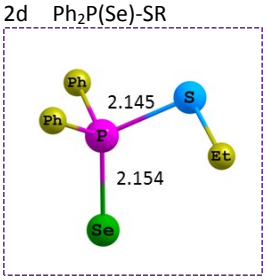
d-TS1




| | | | |
|---|---|---|---|
| Se | 0.26300000 | -0.01677400 | 0.61391500 |
| P | 2.78036100 | 0.02172200 | 0.83495300 |
| H | 3.26812300 | 0.07671300 | 2.16400700 |
| C | 3.68848000 | 1.45648700 | 0.14223600 |
| C | 4.48538400 | 2.28359900 | 0.94980400 |
| C | 3.53351300 | 1.77599700 | -1.21752400 |
| C | 5.12602000 | 3.40128500 | 0.40558500 |
| H | 4.60920800 | 2.05751000 | 2.00567800 |
| C | 4.18232100 | 2.88528600 | -1.76099000 |
| H | 2.89856800 | 1.15973700 | -1.84831700 |
| C | 4.97935500 | 3.70170200 | -0.95076700 |
| H | 5.73987800 | 4.03279600 | 1.04182400 |
| H | 4.05761000 | 3.11890400 | -2.81457300 |
| H | 5.47832700 | 4.56870400 | -1.37419100 |
| C | 3.66738500 | -1.46564100 | 0.19130700 |
| C | 2.90931100 | -2.58308300 | -0.18656500 |
| C | 5.06769700 | -1.51557000 | 0.08589100 |
| C | 3.54372400 | -3.73950300 | -0.65298600 |
| H | 1.82555100 | -2.53907100 | -0.11799100 |
| C | 5.69777300 | -2.67024200 | -0.38170400 |
| H | 5.66601500 | -0.65168200 | 0.36164200 |
| C | 4.93615600 | -3.78525500 | -0.75014200 |
| H | 2.94751800 | -4.60023800 | -0.94289000 |
| H | 6.78114500 | -2.69983600 | -0.45945400 |
| H | 5.42816000 | -4.68290100 | -1.11436300 |
| P | -2.26873400 | 0.00236100 | 0.31367500 |
| C | -2.94973500 | 1.64737300 | -0.16277900 |
| C | -4.11291300 | 1.79404100 | -0.93501300 |
| C | -2.26470400 | 2.79272100 | 0.27467000 |
| C | -4.58675600 | 3.06847800 | -1.25783900 |
| H | -4.64631200 | 0.91776000 | -1.28975600 |
| C | -2.74404500 | 4.06418800 | -0.04651700 |
| H | -1.35101100 | 2.68153400 | 0.85146200 |
| C | -3.90545000 | 4.20479400 | -0.81264100 |
| H | -5.48720300 | 3.17130600 | -1.85714700 |
| H | -2.20559500 | 4.94375600 | 0.29508700 |
| H | -4.27464100 | 5.19473000 | -1.06606800 |
| C | -2.89400400 | -1.13966800 | -0.99973700 |
| C | -2.12152700 | -1.25490100 | -2.16881500 |
| C | -4.06257100 | -1.90517200 | -0.87538000 |
| C | -2.52680300 | -2.10171000 | -3.20234700 |
| H | -1.19792700 | -0.69019700 | -2.26157400 |
| C | -4.46049200 | -2.75985500 | -1.90853200 |
| H | -4.65787500 | -1.83367700 | 0.03014700 |
| C | -3.69694100 | -2.85750400 | -3.07458500 |
| H | -1.92253700 | -2.17910200 | -4.10199400 |
| H | -5.36782100 | -3.34787200 | -1.79943300 |
| H | -4.00714300 | -3.52231700 | -3.87595800 |
| C | -2.42632400 | -1.70169700 | 2.88168600 |
| H | -2.60348200 | -2.64820900 | 2.36296700 |
| H | -1.37366500 | -1.43021100 | 2.76229100 |
| C | -2.81201100 | -1.80839500 | 4.35671700 |

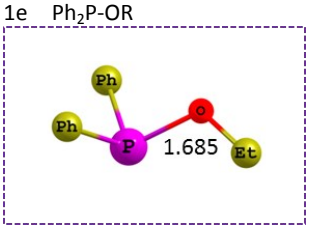
| | | | |
|---|---|---|---|
| H | -2.22301900 | -2.60090300 | 4.83242600 |
| H | -2.61389700 | -0.87127300 | 4.88601700 |
| H | -3.87127600 | -2.05625200 | 4.48349300 |
| S | -3.43938300 | -0.38044900 | 2.06787000 |

2d $Ph_2P(Se)$-SR



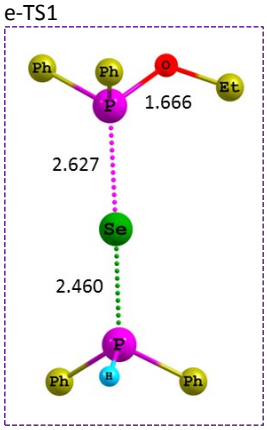

| | | | |
|---|---|---|---|
| P | -0.01402800 | -0.30836400 | 0.19104000 |
| C | -1.72912300 | 0.23527400 | -0.16892200 |
| C | -2.06960900 | 1.59174300 | -0.27265100 |
| C | -2.73402600 | -0.74124700 | -0.27253500 |
| C | -3.39938300 | 1.96474200 | -0.48974200 |
| H | -1.30731100 | 2.35804400 | -0.18362800 |
| C | -4.05783400 | -0.36311300 | -0.49573500 |
| H | -2.48042500 | -1.79183300 | -0.17008000 |
| C | -4.39338700 | 0.99069500 | -0.60468500 |
| H | -3.65442600 | 3.01772800 | -0.56736000 |
| H | -4.82740700 | -1.12500300 | -0.57870700 |
| H | -5.42564600 | 1.28358000 | -0.77390500 |
| C | 1.05299300 | 1.18331600 | 0.00417100 |
| C | 1.65831400 | 1.75145900 | 1.13373900 |
| C | 1.26128500 | 1.76343200 | -1.25857200 |
| C | 2.45405200 | 2.89339700 | 1.00317600 |
| H | 1.51035200 | 1.29122800 | 2.10589800 |
| C | 2.05754300 | 2.90334800 | -1.38394200 |
| H | 0.81163600 | 1.31939500 | -2.14126200 |
| C | 2.65452100 | 3.47076400 | -0.25305400 |
| H | 2.91996100 | 3.32567500 | 1.88402200 |
| H | 2.21500500 | 3.34394400 | -2.36430800 |
| H | 3.27701500 | 4.35548000 | -0.35309500 |
| Se | 0.23211100 | -1.31606900 | 2.07858700 |
| C | 1.96973300 | -2.28794700 | -1.10616800 |
| H | 2.74232300 | -1.51501100 | -1.14475300 |
| H | 1.89137000 | -2.65649000 | -0.07961100 |
| C | 2.27749000 | -3.42166600 | -2.08446300 |
| H | 3.24067400 | -3.87353000 | -1.82254000 |
| H | 1.51266800 | -4.20307700 | -2.04105400 |
| H | 2.34441400 | -3.06215600 | -3.11638700 |
| S | 0.34581400 | -1.51883400 | -1.54340600 |

1e $Ph_2P$-OR




| | | | |
|---|---|---|---|
| P | 0.01596900 | 0.62280400 | -1.02879200 |
| C | -1.47964700 | -0.24576000 | -0.38131800 |
| C | -1.68910300 | -1.59010700 | -0.73331200 |
| C | -2.46363700 | 0.42090500 | 0.36317200 |
| C | -2.84927800 | -2.25665600 | -0.33765700 |
| H | -0.93903000 | -2.12535000 | -1.31095000 |
| C | -3.62586000 | -0.24933000 | 0.75914000 |
| H | -2.31050600 | 1.45838900 | 0.63943800 |
| C | -3.82324900 | -1.58705500 | 0.41067400 |
| H | -2.99243000 | -3.29806200 | -0.61215300 |
| H | -4.37659500 | 0.27787100 | 1.34167300 |
| H | -4.72729800 | -2.10493200 | 0.71796800 |
| C | 1.36151300 | -0.40644400 | -0.26992400 |
| C | 2.34843500 | -0.93498200 | -1.11444700 |
| C | 1.44255100 | -0.65492100 | 1.11107000 |
| C | 3.39131400 | -1.71095400 | -0.59522900 |
| H | 2.30231000 | -0.73679600 | -2.18283300 |
| C | 2.48754800 | -1.41778000 | 1.63176000 |
| H | 0.68436000 | -0.24850100 | 1.77445000 |
| C | 3.46181800 | -1.95072300 | 0.77805800 |
| H | 4.14719400 | -2.11880300 | -1.26050600 |
| H | 2.54211600 | -1.60363600 | 2.70094400 |
| H | 4.27242600 | -2.54854800 | 1.18525600 |
| O | -0.04526000 | 1.94431400 | 0.01504200 |
| C | 0.76546400 | 3.08411200 | -0.31928100 |
| H | 1.82645500 | 2.82985300 | -0.18847900 |
| H | 0.60950500 | 3.35277200 | -1.37322300 |
| C | 0.37792400 | 4.23243600 | 0.59717800 |
| H | 0.98937600 | 5.11347900 | 0.37277900 |
| H | -0.67511400 | 4.49834600 | 0.46232900 |
| H | 0.53502300 | 3.96089500 | 1.64556000 |

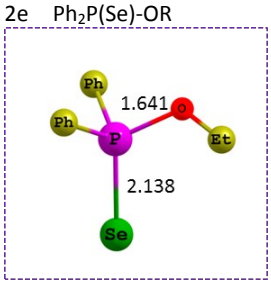
e-TS1




| | | | |
|---|---|---|---|
| Se | 0.30550200 | -0.21570500 | -0.29565100 |
| P | 2.69163600 | -0.14449400 | -0.88955800 |
| H | 2.99612600 | -0.45742200 | -2.23692800 |
| C | 3.80979600 | -1.33644100 | -0.05857000 |
| C | 4.41777500 | -2.38177100 | -0.77138000 |
| C | 3.99969400 | -1.25637600 | 1.33145000 |
| C | 5.21107700 | -3.32340400 | -0.10856600 |
| H | 4.27415800 | -2.46419300 | -1.84562100 |
| C | 4.79950900 | -2.19147100 | 1.98914900 |
| H | 3.51891100 | -0.46424300 | 1.89911200 |
| C | 5.40615300 | -3.22849200 | 1.27144300 |
| H | 5.67685200 | -4.12706900 | -0.67211200 |
| H | 4.94391500 | -2.11520800 | 3.06318700 |
| H | 6.02458200 | -3.95832400 | 1.78607100 |
| C | 3.51364900 | 1.49681700 | -0.70456500 |
| C | 2.74501400 | 2.59502100 | -0.29547500 |
| C | 4.88149800 | 1.67333700 | -0.97490300 |
| C | 3.33648300 | 3.85576100 | -0.15965000 |
| H | 1.68798100 | 2.45529900 | -0.08482400 |
| C | 5.46812400 | 2.93257100 | -0.84029100 |
| H | 5.49051900 | 0.82725900 | -1.28184000 |
| C | 4.69537100 | 4.02623500 | -0.43209700 |
| H | 2.73313200 | 4.70094000 | 0.15951200 |
| H | 6.52618900 | 3.06064900 | -1.05155300 |
| H | 5.15396200 | 5.00551700 | -0.32627700 |
| P | -2.24698800 | -0.24108900 | 0.32571600 |
| C | -3.04279600 | 1.37554200 | 0.67092800 |
| C | -2.99097100 | 2.36856000 | -0.32177800 |
| C | -3.63469600 | 1.67150300 | 1.90750500 |

| | | | |
|---|---|---|---|
| C | -3.54098600 | 3.62937500 | -0.08814000 |
| H | -2.51607800 | 2.15805200 | -1.27675600 |
| C | -4.18192300 | 2.93795900 | 2.13871900 |
| H | -3.66534300 | 0.91143600 | 2.68045600 |
| C | -4.13848400 | 3.91782600 | 1.14403100 |
| H | -3.49835700 | 4.38772900 | -0.86502000 |
| H | -4.64100300 | 3.15660900 | 3.09916300 |
| H | -4.56293300 | 4.90104400 | 1.32707200 |
| C | -3.35148300 | -0.98561900 | -0.95521000 |
| C | -2.79357300 | -1.42564300 | -2.16379800 |
| C | -4.73078400 | -1.14375000 | -0.73390700 |
| C | -3.60561700 | -2.00581300 | -3.14499300 |
| H | -1.72483500 | -1.31430100 | -2.32799200 |
| C | -5.53718600 | -1.72957400 | -1.71005500 |
| H | -5.17033600 | -0.80762600 | 0.20107400 |
| C | -4.97522500 | -2.15882900 | -2.91909400 |
| H | -3.16587700 | -2.34149800 | -4.08015200 |
| H | -6.60269000 | -1.84802700 | -1.53242100 |
| H | -5.60539100 | -2.61129700 | -3.67995100 |
| O | -2.69638700 | -1.03720400 | 1.71818800 |
| C | -2.06654900 | -2.30253700 | 2.01829500 |
| H | -2.42940000 | -3.05886000 | 1.30975500 |
| H | -0.98198500 | -2.20556400 | 1.89147200 |
| C | -2.42759800 | -2.68204200 | 3.44403800 |
| H | -1.97697900 | -3.64869700 | 3.69546700 |
| H | -2.05601300 | -1.93348800 | 4.15080400 |
| H | -3.51245700 | -2.76580700 | 3.56407900 |

2e $Ph_2P(Se)$-OR




| | | | |
|---|---|---|---|
| P | -0.01155700 | -0.49311000 | -0.08361900 |
| C | 1.61614200 | 0.32782000 | 0.02377300 |
| C | 2.08476200 | 1.03458100 | -1.09488000 |
| C | 2.40334100 | 0.26144800 | 1.18259700 |
| C | 3.32112600 | 1.67915600 | -1.04882900 |
| H | 1.48993500 | 1.06868500 | -2.00313200 |
| C | 3.64420200 | 0.90471100 | 1.22071000 |
| H | 2.04883500 | -0.29465600 | 2.04277100 |
| C | 4.10369100 | 1.61484000 | 0.10906800 |
| H | 3.67645700 | 2.22387800 | -1.91870500 |
| H | 4.25135900 | 0.84576300 | 2.11965900 |
| H | 5.06872500 | 2.11261000 | 0.14164400 |
| C | -1.26653800 | 0.84583100 | -0.01097100 |
| C | -2.27608400 | 0.94884200 | -0.97613700 |
| C | -1.21186800 | 1.78115500 | 1.03746400 |
| C | -3.22414200 | 1.97305900 | -0.89319400 |
| H | -2.31165500 | 0.22526700 | -1.78538800 |
| C | -2.16121800 | 2.80071700 | 1.11845500 |
| H | -0.42933500 | 1.71459900 | 1.78784400 |
| C | -3.16857100 | 2.89845800 | 0.15198100 |
| H | -4.00365700 | 2.04604000 | -1.64616800 |
| H | -2.11273600 | 3.51989300 | 1.93119200 |
| H | -3.90504900 | 3.69471300 | 0.21398700 |
| Se | -0.25920000 | -1.83143900 | -1.73261600 |
| O | -0.06428600 | -1.16382400 | 1.41292500 |
| C | -1.15489200 | -2.03699600 | 1.79589600 |
| H | -2.08097600 | -1.45006100 | 1.83220700 |
| H | -1.26513700 | -2.81574400 | 1.03396000 |
| C | -0.82416200 | -2.62832200 | 3.15423100 |
| H | -1.63531700 | -3.29235100 | 3.47237100 |
| H | 0.10081200 | -3.21097100 | 3.10871400 |
| H | -0.70658200 | -1.84330000 | 3.90787000 |

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